Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:44 PM UTC

PDB ID	:	9HDF / pdb_00009hdf
Title	:	Glucocorticoid Receptor Ligand Binding Domain in complex with dexamethasone
Authors	:	Alegre-Marti, A.; Jimenez-Panizo, A.; Fuentes-Prior, P.; Estebanez-Perpina, E.
Deposited on	:	2024-11-12
Resolution	:	2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

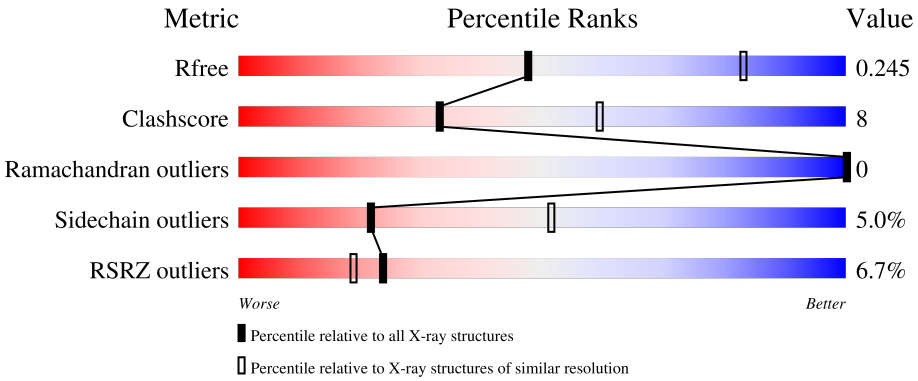
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	248	6% 82% 14%
1	C	248	2% 82% 14%
1	D	248	4% 83% 15%
1	F	248	11% 85% 13%

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Mol	Chain	Length	Quality of chain
1	G	248	2% 85% 13%
1	H	248	28% 73% 21%
1	I	248	3% 84% 14%
1	L	248	2% 84% 14%
1	M	248	7% 84% 14%
1	P	248	14% 80% 16%
2	B	248	2% 82% 15%
2	E	248	6% 80% 17%
2	J	248	2% 83% 16%
2	K	248	3% 82% 14%
2	N	248	3% 76% 19%
2	O	248	6% 77% 18%
3	a	15	13% 60% 27% 7% 7%
3	b	15	7% 73% 20% 7%
3	c	15	7% 73% 20% 7%
3	d	15	7% 60% 27% 7% 7%
3	e	15	20% 80% 13% 7%
3	f	15	27% 67% 20% 13%
3	g	15	7% 67% 20% 13%
3	h	15	7% 67% 13% 7% 13%
3	i	15	13% 67% 27% 7%
3	j	15	13% 73% 20% 7%
3	k	15	7% 73% 13% 7% 7%
3	l	15	13% 73% 13% 7% 7%
3	m	15	13% 80% 7% 7% 7%

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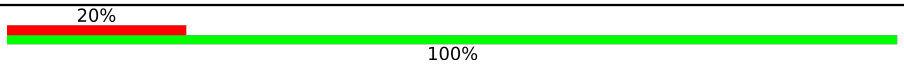
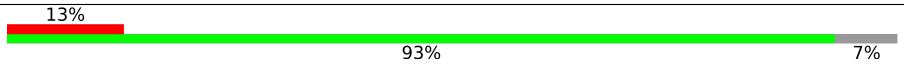
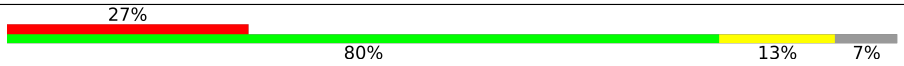
Mol	Chain	Length	Quality of chain
3	n	15	
3	o	15	
3	p	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	IMD	d	101	-	-	X	-
5	CAC	A	1002	-	X	-	-
5	CAC	D	801	-	X	-	-
5	CAC	E	1002	-	X	-	-
5	CAC	H	801	-	X	-	-
5	CAC	I	1002	-	X	-	-
5	CAC	K	803	-	X	-	-
5	CAC	M	803	-	X	-	-
5	CAC	O	1002	-	X	-	-
6	EPE	P	1002	-	-	X	-
7	GOL	C	1002	-	-	X	-
7	GOL	L	1004	-	-	X	-
7	GOL	P	1003	-	-	X	-
8	SO4	C	1006	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 34585 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ancestral Glucocorticoid Receptor2 ligand binding domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	C	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	D	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	F	248	Total	C	N	O	S	0	1	0
			2008	1297	328	365	18			
1	G	248	Total	C	N	O	S	0	1	0
			2011	1299	329	366	17			
1	H	245	Total	C	N	O	S	0	0	0
			1986	1286	323	360	17			
1	I	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	L	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	M	248	Total	C	N	O	S	0	0	0
			2007	1297	328	365	17			
1	P	243	Total	C	N	O	S	0	0	0
			1974	1280	321	356	17			

- Molecule 2 is a protein called Ancestral Glucocorticoid Receptor2 ligand binding domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	1	0
			2010	1297	328	367	18			
2	E	244	Total	C	N	O	S	0	2	0
			1988	1287	323	360	18			
2	J	248	Total	C	N	O	S	0	1	0
			2014	1300	331	366	17			
2	K	245	Total	C	N	O	S	0	1	0
			1992	1288	324	362	18			

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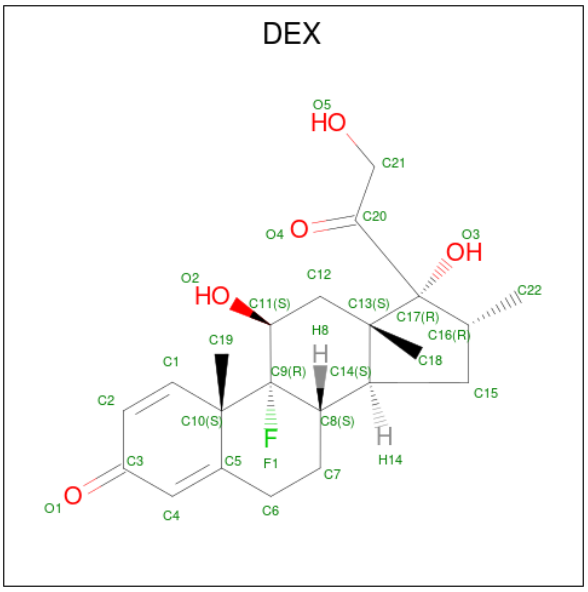
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	245	Total	C	N	O	S	0	2	0
			1997	1290	327	362	18			
2	O	244	Total	C	N	O	S	0	1	0
			1986	1285	323	360	18			

- Molecule 3 is a protein called Nuclear receptor subfamily 0 group B member 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	a	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	b	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	c	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	d	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	e	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	f	13	Total	C	N	O	0	0	0
			96	62	16	18			
3	g	13	Total	C	N	O	0	0	0
			96	62	16	18			
3	h	13	Total	C	N	O	0	0	0
			96	62	16	18			
3	i	15	Total	C	N	O	0	0	0
			109	71	18	20			
3	j	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	k	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	l	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	m	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	n	15	Total	C	N	O	0	0	0
			109	71	18	20			
3	o	14	Total	C	N	O	0	0	0
			104	68	17	19			
3	p	14	Total	C	N	O	0	0	0
			104	68	17	19			

- Molecule 4 is DEXAMETHASONE (CCD ID: DEX) (formula: $C_{22}H_{29}FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			28	22	1	5		
4	B	1	Total	C	F	O	0	0
			28	22	1	5		
4	C	1	Total	C	F	O	0	0
			28	22	1	5		
4	D	1	Total	C	F	O	0	0
			28	22	1	5		
4	E	1	Total	C	F	O	0	0
			28	22	1	5		
4	F	1	Total	C	F	O	0	0
			28	22	1	5		
4	G	1	Total	C	F	O	0	0
			28	22	1	5		
4	H	1	Total	C	F	O	0	0
			28	22	1	5		
4	I	1	Total	C	F	O	0	0
			28	22	1	5		
4	J	1	Total	C	F	O	0	0
			28	22	1	5		
4	K	1	Total	C	F	O	0	0
			28	22	1	5		
4	L	1	Total	C	F	O	0	0
			28	22	1	5		
4	M	1	Total	C	F	O	0	0
			28	22	1	5		
4	N	1	Total	C	F	O	0	0
			28	22	1	5		

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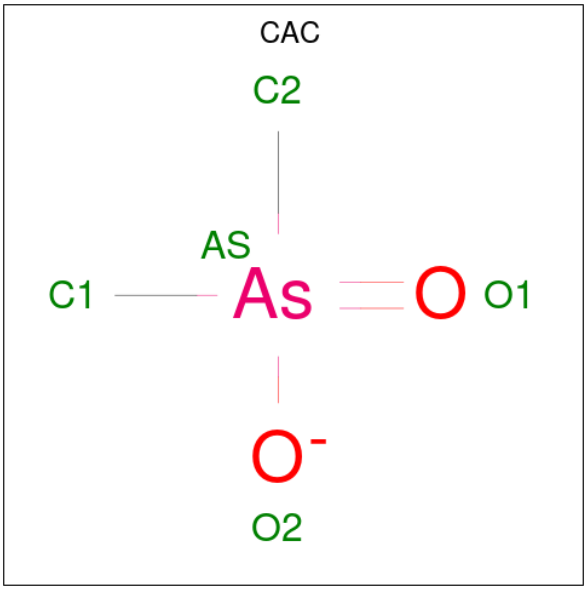
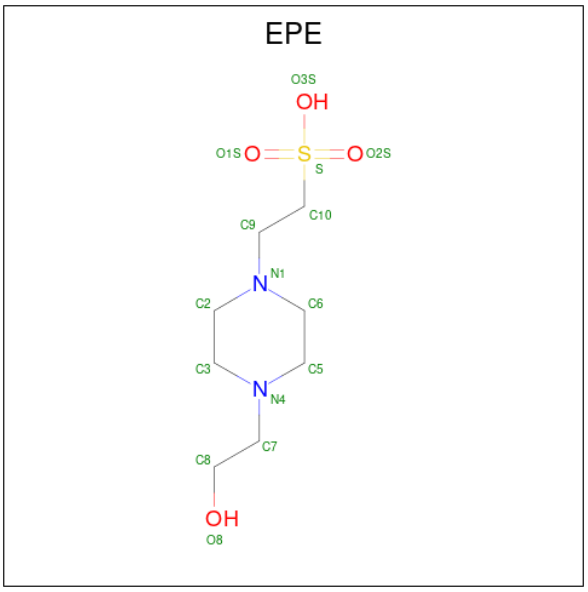
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	1	Total C F O 28 22 1 5	0	0
4	P	1	Total C F O 28 22 1 5	0	0

- Molecule 5 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



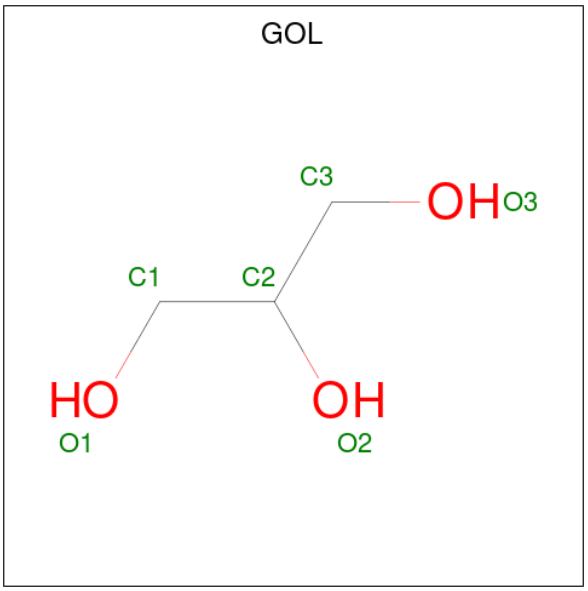
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total As C O 5 1 2 2	0	0
5	D	1	Total As C O 5 1 2 2	0	0
5	E	1	Total As C O 5 1 2 2	0	0
5	H	1	Total As C O 5 1 2 2	0	0
5	I	1	Total As C O 5 1 2 2	0	0
5	K	1	Total As C O 5 1 2 2	0	0
5	M	1	Total As C O 5 1 2 2	0	0
5	O	1	Total As C O 5 1 2 2	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	P	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	K	1	Total	C	O	0	0
			6	3	3		
7	K	1	Total	C	O	0	0
			6	3	3		

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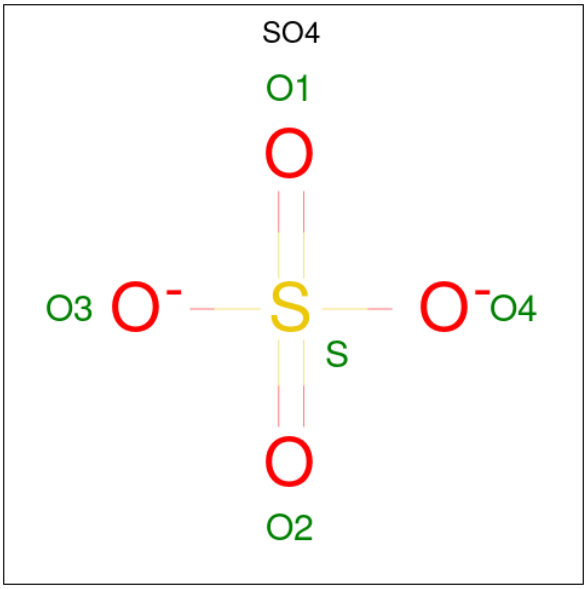
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 3 3	0	0
7	L	1	Total C O 6 3 3	0	0
7	M	1	Total C O 6 3 3	0	0
7	N	1	Total C O 6 3 3	0	0
7	O	1	Total C O 6 3 3	0	0
7	P	1	Total C O 6 3 3	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

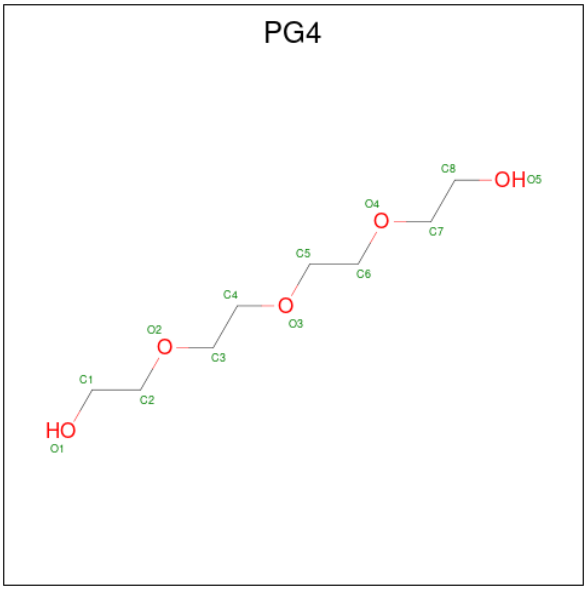


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	J	1	Total O S 5 4 1	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total Cl 3 3	0	0
9	C	1	Total Cl 1 1	0	0
9	D	1	Total Cl 1 1	0	0
9	E	1	Total Cl 1 1	0	0
9	F	1	Total Cl 1 1	0	0
9	J	1	Total Cl 1 1	0	0
9	L	1	Total Cl 1 1	0	0
9	M	1	Total Cl 1 1	0	0
9	N	1	Total Cl 1 1	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 13 8 5	0	0
10	D	1	Total C O 13 8 5	0	0

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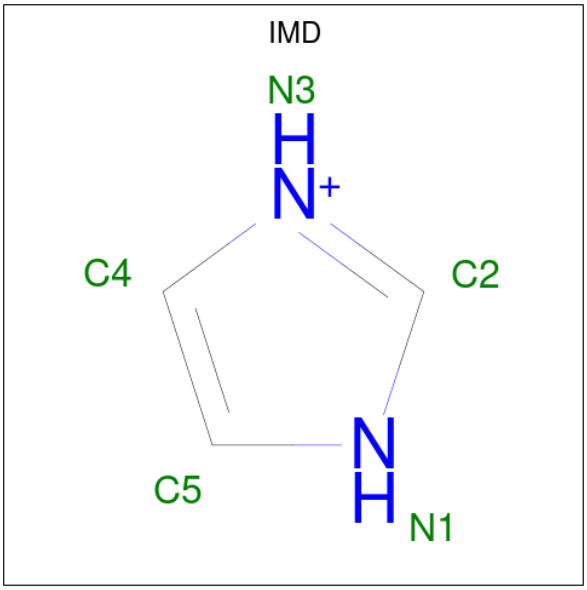
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total C O 13 8 5	0	0
10	L	1	Total C O 13 8 5	0	0

- Molecule 11 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N 5 3 2	0	0
11	B	1	Total C N 5 3 2	0	0
11	C	1	Total C N 5 3 2	0	0
11	E	1	Total C N 5 3 2	0	0
11	F	1	Total C N 5 3 2	0	0
11	I	1	Total C N 5 3 2	0	0
11	J	1	Total C N 5 3 2	0	0
11	J	1	Total C N 5 3 2	0	0
11	L	1	Total C N 5 3 2	0	0

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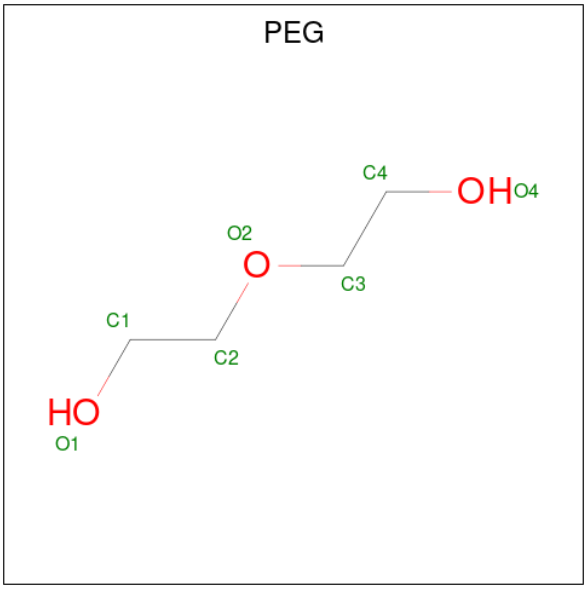
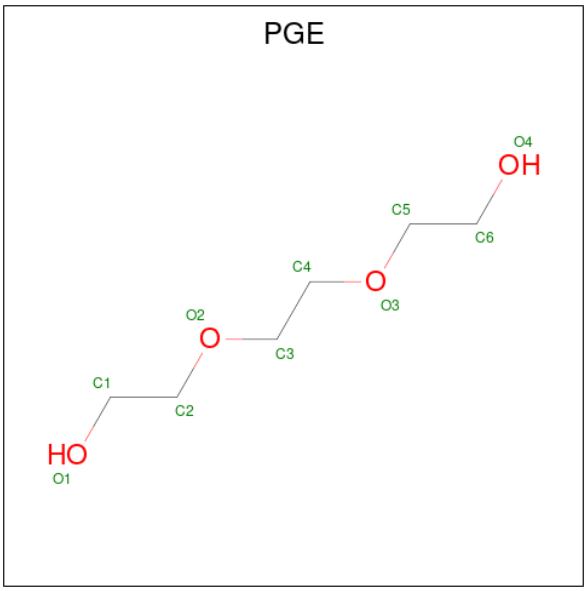
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C N 5 3 2	0	0
11	M	1	Total C N 5 3 2	0	0
11	N	1	Total C N 5 3 2	0	0
11	O	1	Total C N 5 3 2	0	0
11	b	1	Total C N 5 3 2	0	0
11	d	1	Total C N 5 3 2	0	0

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	F	1	Total C O 7 4 3	0	0
12	I	1	Total C O 7 4 3	0	0
12	K	1	Total C O 7 4 3	0	0
12	M	1	Total C O 7 4 3	0	0

- Molecule 13 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C O 10 6 4	0	0

- Molecule 14 is water.

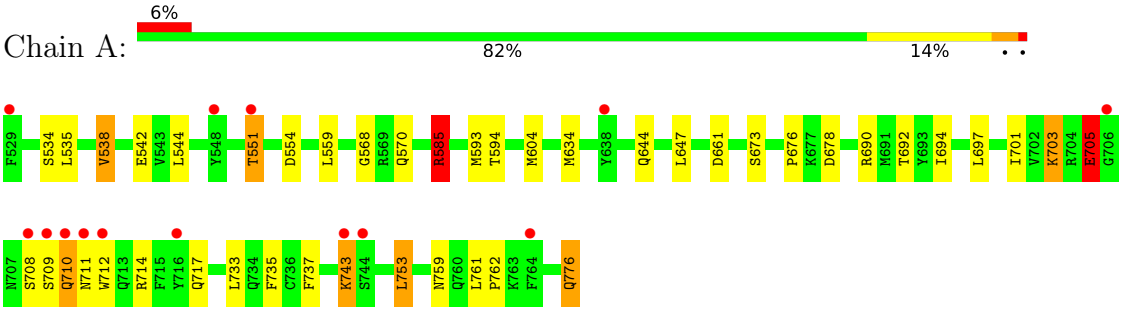
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	D	1	Total O 1 1	0	0
14	I	3	Total O 3 3	0	0
14	J	3	Total O 3 3	0	0
14	K	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0
14	O	2	Total O 2 2	0	0
14	P	1	Total O 1 1	0	0
14	i	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

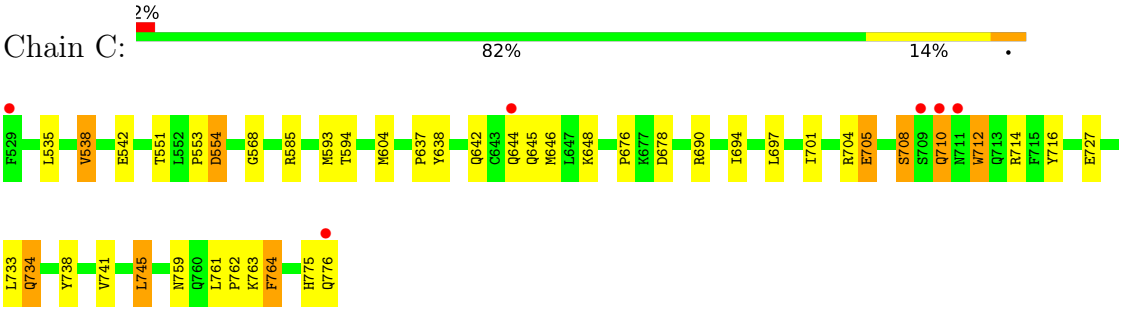
• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain A:



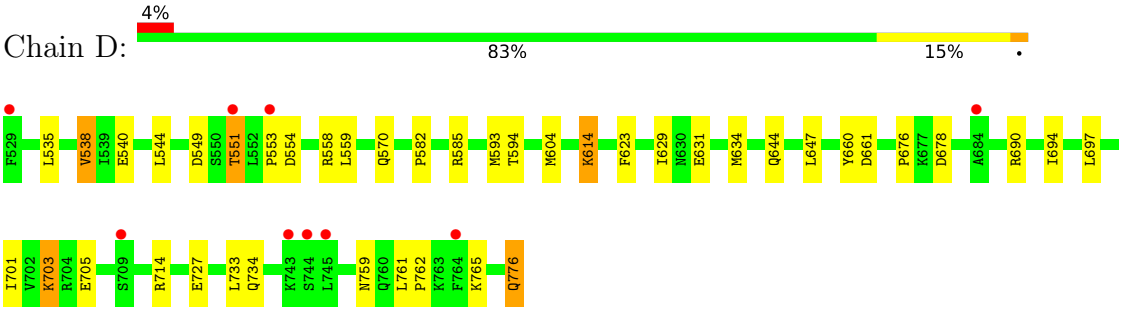
• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain C:



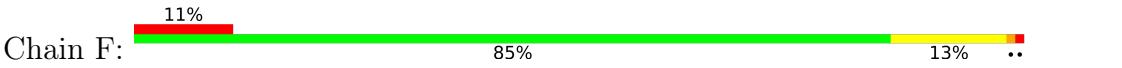
• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

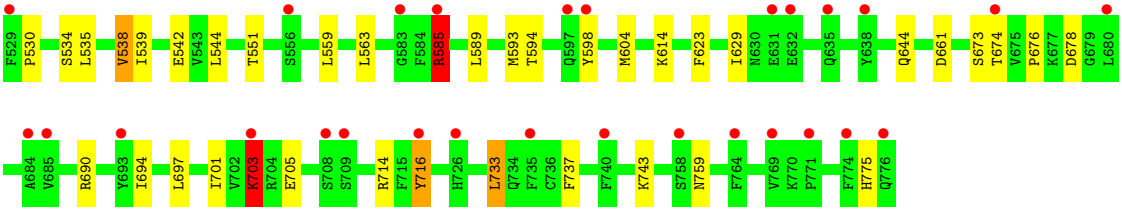
Chain D:



• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain F:

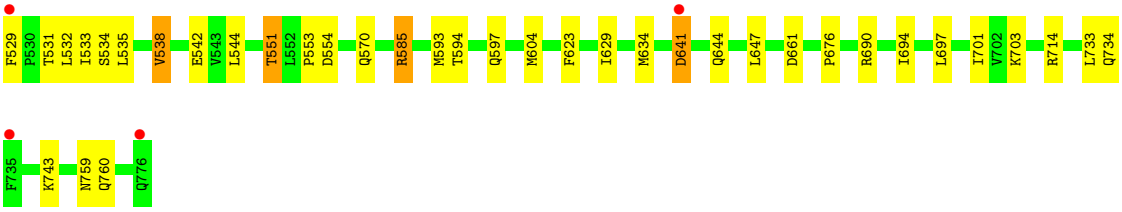




• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain G:

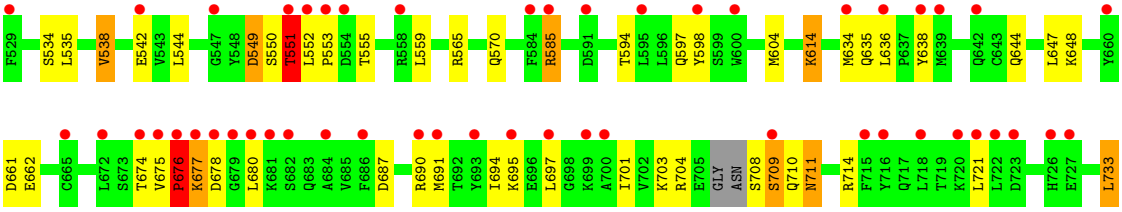




• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain H:

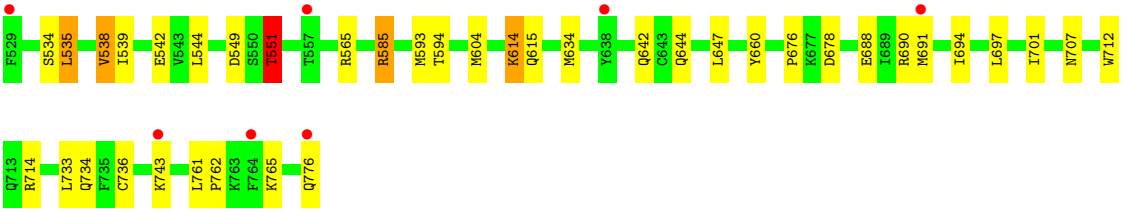




• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain I:

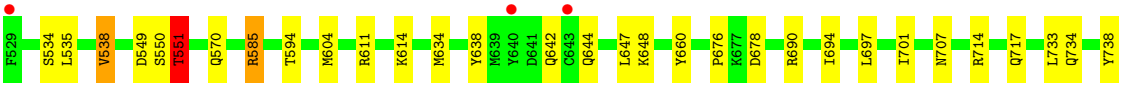


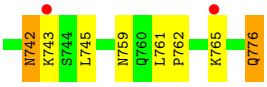


• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain L:



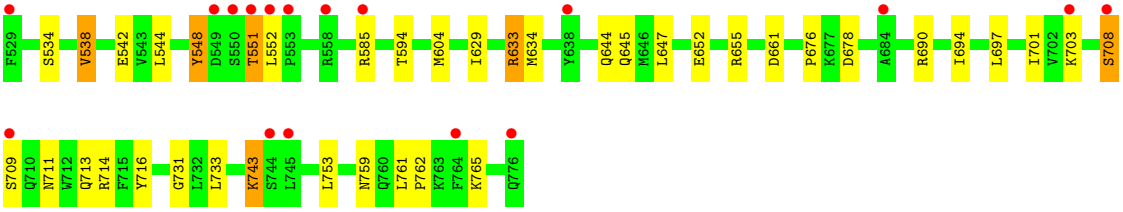




• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain M:

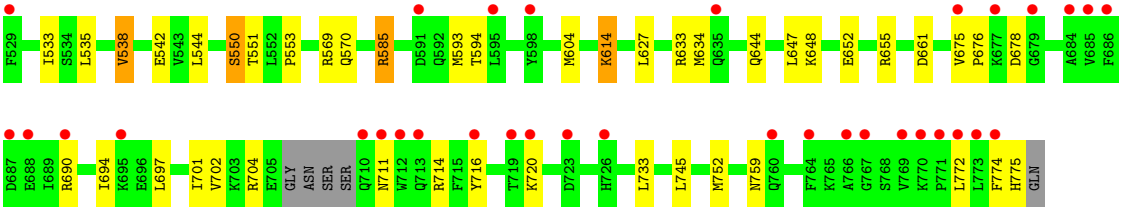




• Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain P:

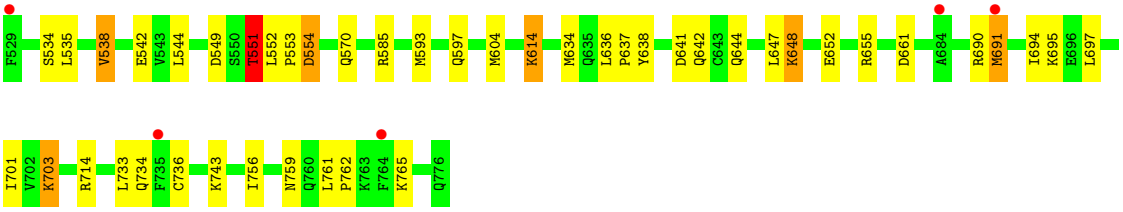




• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain B:

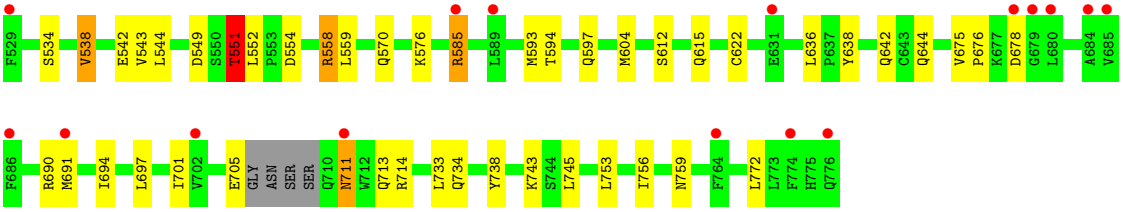




• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain E:

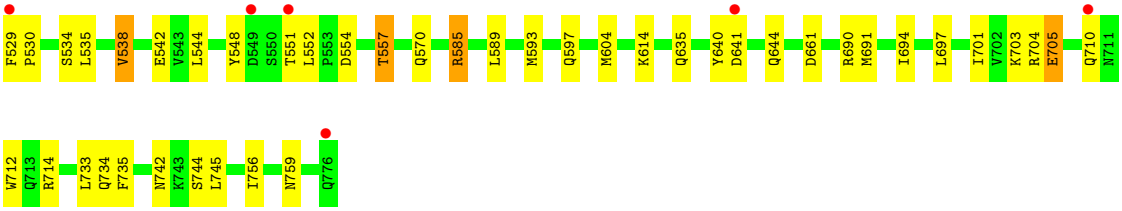




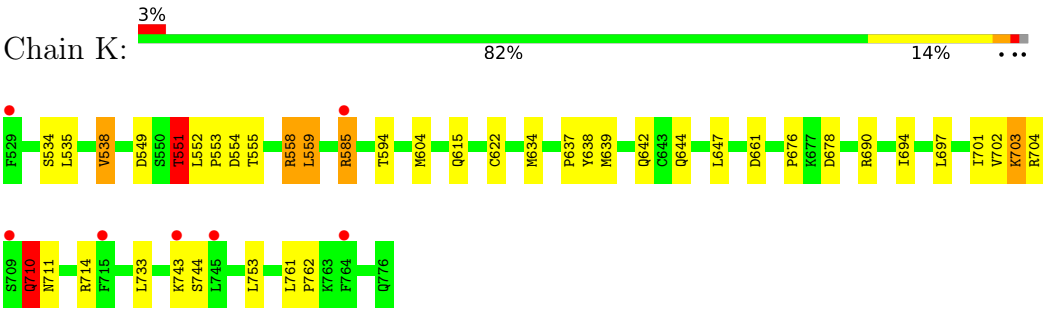
• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

Chain J:

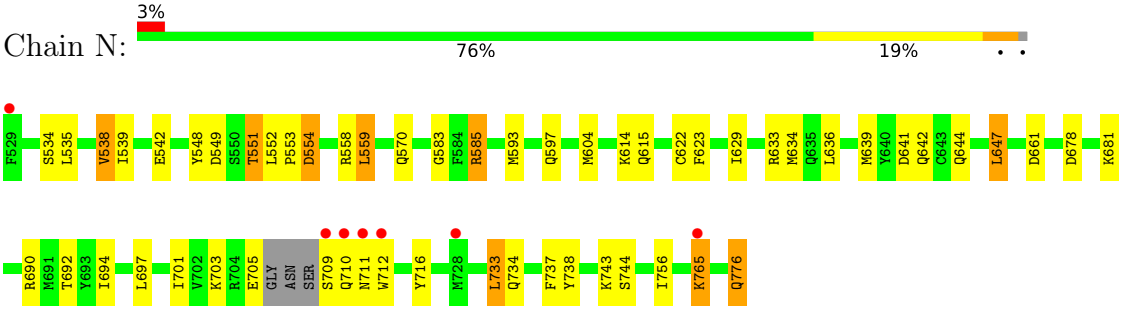




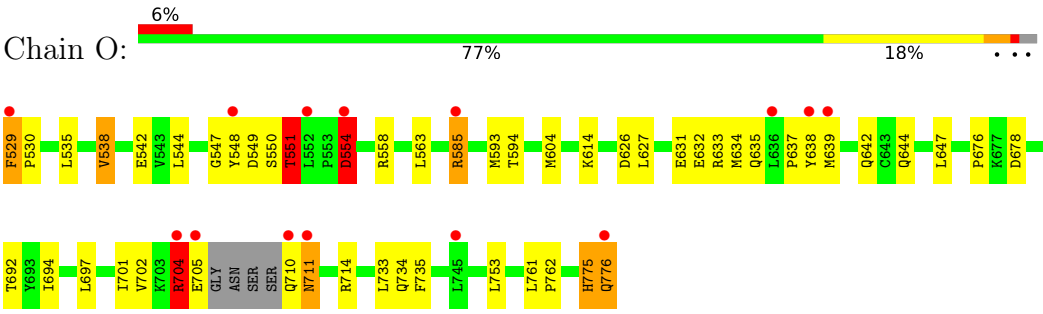
• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain



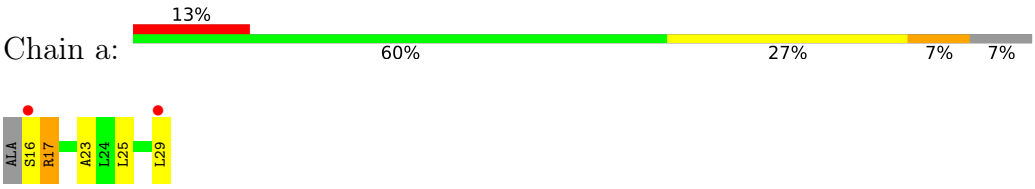
• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain



• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

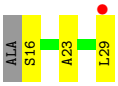


• Molecule 3: Nuclear receptor subfamily 0 group B member 2



• Molecule 3: Nuclear receptor subfamily 0 group B member 2

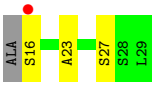




• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain c:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain d:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain e:

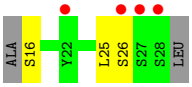




• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain f:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain g:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain h:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain i:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain j:

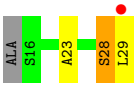




• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain k:

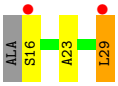




• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain l:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

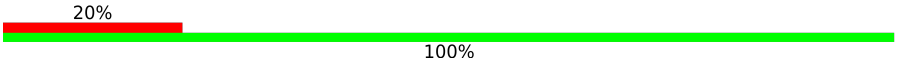
Chain m:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

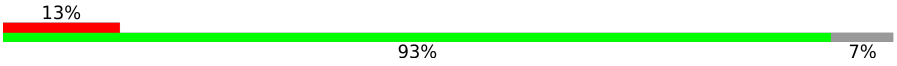
Chain n:





• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain o:

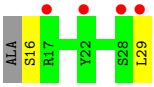




• Molecule 3: Nuclear receptor subfamily 0 group B member 2

Chain p:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	264.41Å 265.46Å 109.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.57 – 2.78 101.57 – 2.78	Depositor EDS
% Data completeness (in resolution range)	96.3 (101.57-2.78) 96.3 (101.57-2.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.244 0.211 , 0.245	Depositor DCC
R_{free} test set	1946 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	34585	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CAC, GOL, CL, PEG, PG4, DEX, IMD, EPE, PGE, CSO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	1/2051 (0.0%)	1.08	9/2769 (0.3%)
1	C	0.67	0/2051	1.14	5/2769 (0.2%)
1	D	0.57	0/2051	1.08	6/2769 (0.2%)
1	F	0.57	0/2057	1.12	4/2777 (0.1%)
1	G	0.53	0/2060	1.11	6/2781 (0.2%)
1	H	0.62	1/2029 (0.0%)	1.27	7/2738 (0.3%)
1	I	0.56	0/2051	1.08	4/2769 (0.1%)
1	L	0.58	0/2051	1.08	4/2769 (0.1%)
1	M	0.58	0/2051	1.16	10/2769 (0.4%)
1	P	0.58	0/2017	1.06	2/2722 (0.1%)
2	B	0.57	0/2044	1.06	3/2758 (0.1%)
2	E	0.61	0/2026	1.09	2/2733 (0.1%)
2	J	0.65	0/2055	1.09	6/2772 (0.2%)
2	K	0.61	0/2025	1.11	9/2731 (0.3%)
2	N	0.61	0/2036	1.12	6/2745 (0.2%)
2	O	0.62	0/2019	1.15	10/2723 (0.4%)
3	a	0.73	0/105	1.68	1/142 (0.7%)
3	b	0.58	0/105	0.98	0/142
3	c	0.68	0/105	0.99	0/142
3	d	0.67	0/105	1.03	0/142
3	e	0.58	0/105	0.99	0/142
3	f	0.64	0/97	0.94	0/131
3	g	0.73	0/97	1.06	0/131
3	h	0.63	0/97	1.79	1/131 (0.8%)
3	i	0.67	0/110	1.27	2/149 (1.3%)
3	j	0.75	0/105	0.99	0/142
3	k	0.73	0/105	1.07	1/142 (0.7%)
3	l	0.67	0/105	0.94	0/142
3	m	0.68	0/105	1.22	1/142 (0.7%)
3	n	0.67	0/110	0.96	0/149
3	o	0.57	0/105	0.96	0/142
3	p	0.56	0/105	0.95	0/142

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.60	2/34340 (0.0%)	1.12	99/46347 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	F	0	1
1	H	0	2
1	M	0	1
2	J	0	1
2	O	0	3
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	709	SER	CA-CB	-5.48	1.45	1.52
1	A	709	SER	CA-CB	-5.33	1.45	1.53

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	676	PRO	CA-C-O	-23.80	88.75	122.31
1	H	676	PRO	CB-CA-C	20.69	142.46	111.22
3	a	17	ARG	CG-CD-NE	15.72	146.58	112.00
1	F	585	ARG	CG-CD-NE	15.50	146.10	112.00
1	M	552	LEU	N-CA-C	-15.28	88.40	108.11
3	h	17	ARG	CG-CD-NE	14.86	144.70	112.00
2	N	711	ASN	CB-CA-C	14.71	129.32	111.22
1	G	641	ASP	CA-CB-CG	14.46	127.06	112.60
1	I	585	ARG	CG-CD-NE	11.87	138.12	112.00
2	O	688	GLU	CB-CG-CD	10.60	130.63	112.60
1	D	727	GLU	CB-CG-CD	10.19	129.92	112.60
1	H	585	ARG	CG-CD-NE	9.56	133.03	112.00
2	O	554	ASP	CA-CB-CG	-9.01	103.59	112.60
1	H	676	PRO	N-CA-CB	-8.74	91.89	103.42
2	K	710	GLN	N-CA-C	8.38	123.09	109.76
2	K	637	PRO	N-CA-CB	8.33	112.23	103.15
1	M	633	ARG	CB-CG-CD	8.28	130.34	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	642	GLN	CB-CG-CD	8.22	126.57	112.60
1	M	548	TYR	CB-CA-C	8.18	123.30	109.72
1	H	768	SER	CA-C-O	8.15	129.61	119.59
1	M	585	ARG	CB-CG-CD	7.99	129.69	111.30
1	F	551	THR	CB-CA-C	7.85	125.06	110.70
2	E	711	ASN	CA-CB-CG	7.76	120.36	112.60
1	C	705	GLU	CB-CA-C	7.74	125.82	110.42
2	O	633	ARG	CG-CD-NE	-7.68	95.11	112.00
1	C	551	THR	CB-CA-C	7.63	124.67	110.70
1	P	551	THR	CB-CA-C	7.60	124.61	110.70
2	O	554	ASP	CB-CA-C	7.59	126.12	110.40
2	O	704	ARG	O-C-N	-7.55	111.22	122.39
1	M	551	THR	O-C-N	-7.45	113.14	122.82
2	B	551	THR	CA-CB-OG1	-7.28	98.68	109.60
2	N	551	THR	CA-CB-OG1	-7.28	98.68	109.60
2	J	705	GLU	CB-CA-C	7.23	124.80	110.42
2	O	711	ASN	CB-CA-C	7.17	123.54	111.22
3	i	28	SER	CA-C-N	7.13	134.54	121.70
3	i	28	SER	C-N-CA	7.13	134.54	121.70
2	J	557	THR	CA-CB-OG1	7.09	120.24	109.60
3	m	29	LEU	CB-CA-C	7.01	123.41	110.10
2	K	551	THR	CA-CB-OG1	-6.99	99.12	109.60
1	H	551	THR	CA-CB-OG1	-6.94	99.20	109.60
1	L	551	THR	CA-CB-OG1	-6.93	99.20	109.60
1	D	551	THR	CA-CB-OG1	-6.88	99.28	109.60
2	E	551	THR	CA-CB-OG1	-6.86	99.31	109.60
1	M	552	LEU	N-CA-CB	6.82	120.25	110.77
2	O	551	THR	CA-CB-OG1	-6.76	99.46	109.60
1	A	551	THR	CA-CB-OG1	-6.72	99.52	109.60
2	O	642	GLN	CB-CG-CD	6.69	123.98	112.60
1	G	734	GLN	CB-CA-C	6.67	121.45	110.90
1	G	551	THR	CA-CB-OG1	-6.67	99.59	109.60
2	K	637	PRO	CA-C-O	-6.59	109.64	120.05
1	I	551	THR	CA-CB-OG1	-6.59	99.72	109.60
1	H	676	PRO	N-CA-C	-6.52	102.09	111.22
1	C	554	ASP	CA-CB-CG	6.46	119.06	112.60
3	k	28	SER	N-CA-C	6.27	121.01	113.23
1	A	705	GLU	CB-CA-C	6.25	122.87	110.42
1	D	538	VAL	CA-CB-CG2	6.16	120.87	110.40
1	G	585	ARG	CB-CG-CD	-6.01	97.47	111.30
2	O	538	VAL	CA-CB-CG2	5.99	120.57	110.40
1	A	710	GLN	CA-C-N	5.91	128.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	710	GLN	C-N-CA	5.91	128.47	120.38
1	F	703	LYS	CG-CD-CE	5.91	124.88	111.30
2	B	554	ASP	CA-CB-CG	5.83	118.43	112.60
2	N	712	TRP	CB-CA-C	5.81	122.14	109.99
2	N	710	GLN	CB-CA-C	5.80	121.33	111.35
2	B	765	LYS	CB-CG-CD	5.79	124.62	111.30
1	L	734	GLN	CA-CB-CG	5.79	125.67	114.10
1	C	712	TRP	CB-CA-C	5.75	121.22	109.55
1	F	716	TYR	CA-CB-CG	5.64	124.06	113.90
1	C	538	VAL	CA-CB-CG2	5.63	119.97	110.40
1	M	765	LYS	CB-CG-CD	5.62	124.22	111.30
2	K	710	GLN	CB-CG-CD	5.58	122.09	112.60
1	M	551	THR	N-CA-C	-5.58	97.11	107.71
1	A	712	TRP	CB-CA-C	5.55	121.60	109.99
1	M	551	THR	CA-CB-OG1	-5.45	101.42	109.60
2	J	712	TRP	CB-CA-C	5.41	121.30	109.99
1	D	554	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	554	ASP	CB-CA-C	-5.36	100.47	109.53
1	P	538	VAL	CA-CB-CG2	5.35	119.50	110.40
1	G	554	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	765	LYS	CB-CG-CD	5.28	123.44	111.30
2	J	551	THR	CA-CB-OG1	5.25	117.48	109.60
1	M	716	TYR	CA-CB-CG	5.24	123.34	113.90
2	K	585	ARG	CG-CD-NE	5.22	123.48	112.00
2	K	711	ASN	CA-C-O	5.18	126.31	120.92
2	J	551	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	585	ARG	CB-CG-CD	5.15	123.14	111.30
2	K	558	ARG	NE-CZ-NH1	-5.13	116.37	121.50
2	N	554	ASP	CB-CA-C	-5.11	100.91	109.65
1	A	717	GLN	CB-CG-CD	5.10	121.27	112.60
1	I	707	ASN	CA-C-N	5.10	127.36	120.38
1	I	707	ASN	C-N-CA	5.10	127.36	120.38
1	G	554	ASP	CB-CA-C	-5.09	100.92	109.53
2	K	554	ASP	CB-CA-C	-5.06	101.60	109.84
1	A	554	ASP	CB-CA-C	-5.04	101.01	109.53
2	J	548	TYR	CA-CB-CG	5.04	122.97	113.90
1	A	743	LYS	CB-CG-CD	5.03	122.87	111.30
1	L	707	ASN	CA-C-N	5.03	127.02	120.28
1	L	707	ASN	C-N-CA	5.03	127.02	120.28
2	O	639	MET	N-CA-CB	5.03	118.05	110.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	704	ARG	Peptide
1	C	708	SER	Peptide
1	C	738	TYR	Sidechain
1	F	775	HIS	Sidechain
1	H	549	ASP	Sidechain
1	H	676	PRO	Mainchain
2	J	704	ARG	Peptide
1	M	551	THR	Mainchain
2	O	554	ASP	Peptide
2	O	704	ARG	Peptide
2	O	775	HIS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2007	0	2030	31	0
1	C	2007	0	2029	43	0
1	D	2007	0	2030	30	0
1	F	2008	0	2031	29	0
1	G	2011	0	2034	28	0
1	H	1986	0	2012	66	1
1	I	2007	0	2030	27	0
1	L	2007	0	2030	31	0
1	M	2007	0	2030	29	0
1	P	1974	0	2002	51	0
2	B	2010	0	2031	40	0
2	E	1988	0	2016	31	0
2	J	2014	0	2039	32	0
2	K	1992	0	2016	32	0
2	N	1997	0	2021	50	1
2	O	1986	0	2010	42	0
3	a	104	0	113	4	0
3	b	104	0	113	3	0
3	c	104	0	113	3	0
3	d	104	0	113	9	0
3	e	104	0	113	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	f	96	0	102	2	0
3	g	96	0	102	3	0
3	h	96	0	102	2	0
3	i	109	0	118	4	0
3	j	104	0	113	3	0
3	k	104	0	113	4	0
3	l	104	0	113	3	0
3	m	104	0	113	3	0
3	n	109	0	118	0	0
3	o	104	0	113	0	0
3	p	104	0	113	3	0
4	A	28	0	29	1	0
4	B	28	0	29	4	0
4	C	28	0	29	3	0
4	D	28	0	29	0	0
4	E	28	0	29	3	0
4	F	28	0	29	2	0
4	G	28	0	29	0	0
4	H	28	0	29	1	0
4	I	28	0	29	2	0
4	J	28	0	29	2	0
4	K	28	0	29	2	0
4	L	28	0	29	1	0
4	M	28	0	29	1	0
4	N	28	0	29	2	0
4	O	28	0	29	2	0
4	P	28	0	29	0	0
5	A	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	H	5	0	0	1	0
5	I	5	0	0	0	0
5	K	5	0	0	0	0
5	M	5	0	0	0	0
5	O	5	0	0	0	0
6	A	15	0	18	0	0
6	B	15	0	18	1	0
6	D	15	0	18	1	0
6	I	15	0	18	2	0
6	J	15	0	18	0	0
6	L	15	0	18	1	0
6	P	15	0	18	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	16	1	0
7	B	6	0	8	0	0
7	C	12	0	16	8	0
7	E	18	0	24	0	0
7	I	6	0	8	1	0
7	J	18	0	24	0	0
7	K	12	0	16	0	0
7	L	12	0	16	5	0
7	M	6	0	8	0	0
7	N	6	0	8	1	0
7	O	6	0	8	0	0
7	P	6	0	8	4	0
8	A	5	0	0	1	0
8	B	5	0	0	0	0
8	C	10	0	0	3	0
8	J	5	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	J	1	0	0	0	0
9	L	1	0	0	1	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
10	B	13	0	18	0	0
10	D	13	0	18	1	0
10	H	13	0	18	1	0
10	L	13	0	18	0	0
11	B	10	0	10	0	0
11	C	5	0	5	0	0
11	E	5	0	5	0	0
11	F	5	0	5	0	0
11	I	5	0	5	0	0
11	J	10	0	10	0	0
11	L	10	0	10	2	0
11	M	5	0	5	0	0
11	N	5	0	5	2	0
11	O	5	0	5	1	0
11	b	5	0	5	0	0
11	d	5	0	5	4	0
12	F	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	7	0	10	0	0
12	K	7	0	10	1	0
12	M	7	0	10	0	0
13	M	10	0	14	2	0
14	D	1	0	0	0	0
14	I	3	0	0	1	0
14	J	3	0	0	0	0
14	K	1	0	0	0	0
14	M	1	0	0	0	0
14	O	2	0	0	0	0
14	P	1	0	0	0	0
14	i	1	0	0	1	0
All	All	34585	0	35127	544	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:711:ASN:HB2	6:P:1002:EPE:C6	1.19	1.65
1:P:711:ASN:CB	6:P:1002:EPE:H62	1.30	1.56
1:P:711:ASN:CB	6:P:1002:EPE:C6	1.84	1.50
1:P:711:ASN:CG	6:P:1002:EPE:H62	1.40	1.44
1:C:763:LYS:NZ	8:C:1006:SO4:O4	1.59	1.32
1:I:551:THR:O	1:P:553:PRO:HB3	1.16	1.25
2:J:742:ASN:OD1	2:N:552:LEU:HD21	1.40	1.18
2:J:640:TYR:CE2	2:K:744:SER:HB2	1.82	1.14
1:I:585:ARG:NH2	3:i:25:LEU:O	1.83	1.12
2:J:640:TYR:HE2	2:K:744:SER:HB2	0.98	1.08
1:P:716:TYR:HE1	1:P:775:HIS:CD2	1.71	1.08
1:P:711:ASN:HB3	6:P:1002:EPE:H92	1.29	1.08
2:J:742:ASN:OD1	2:N:552:LEU:CD2	2.02	1.07
1:H:598:TYR:HE2	1:H:676:PRO:HB3	1.17	1.03
1:H:676:PRO:HD3	1:H:680:LEU:HD21	1.37	1.03
1:I:551:THR:O	1:P:553:PRO:CB	2.08	1.00
1:H:759:ASN:ND2	3:h:16:SER:O	1.96	0.99
1:H:598:TYR:CE2	1:H:676:PRO:HB3	1.96	0.99
1:M:711:ASN:HB3	13:M:804:PGE:H4	1.42	0.97
1:P:711:ASN:CB	6:P:1002:EPE:H61	1.68	0.97
1:P:759:ASN:ND2	3:p:16:SER:O	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:677:LYS:N	1:H:768:SER:O	2.01	0.93
1:G:585:ARG:NH2	3:g:25:LEU:O	2.01	0.92
1:L:660:TYR:HB2	6:L:1003:EPE:H101	1.52	0.90
1:D:593:MET:SD	3:d:21:LEU:HD13	2.12	0.90
2:E:759:ASN:ND2	3:e:16:SER:O	2.04	0.90
1:H:676:PRO:CD	1:H:680:LEU:CD2	2.51	0.89
1:P:716:TYR:CE1	1:P:775:HIS:CD2	2.61	0.88
2:O:548:TYR:CD2	2:O:627:LEU:HD13	2.09	0.87
1:H:676:PRO:CD	1:H:680:LEU:HD21	2.04	0.87
1:I:565:ARG:NH1	14:I:1101:HOH:O	2.04	0.87
1:P:711:ASN:HB2	6:P:1002:EPE:H61	0.87	0.86
1:P:711:ASN:HB3	6:P:1002:EPE:C6	2.06	0.86
2:J:640:TYR:HE2	2:K:744:SER:CB	1.86	0.86
2:B:553:PRO:HD2	1:C:638:TYR:OH	1.76	0.85
1:P:716:TYR:CE1	1:P:775:HIS:NE2	2.45	0.85
1:H:675:VAL:O	1:H:676:PRO:O	1.96	0.83
3:j:28:SER:O	3:j:29:LEU:HB2	1.79	0.82
1:L:759:ASN:ND2	3:l:16:SER:O	2.12	0.82
1:P:716:TYR:HE1	1:P:775:HIS:NE2	1.78	0.82
1:P:711:ASN:HB3	6:P:1002:EPE:C9	2.10	0.81
1:H:676:PRO:C	1:H:768:SER:O	2.24	0.80
1:D:759:ASN:ND2	3:d:16:SER:O	2.14	0.80
1:H:676:PRO:HA	1:H:768:SER:O	1.80	0.80
2:O:775:HIS:O	2:O:776:GLN:HG3	1.81	0.80
3:i:16:SER:HB2	14:i:101:HOH:O	1.82	0.79
2:K:559:LEU:CD2	2:K:639:MET:HE2	2.13	0.78
1:H:676:PRO:HD3	1:H:680:LEU:CD2	2.13	0.78
1:H:676:PRO:CG	1:H:680:LEU:HD23	2.14	0.77
2:N:641:ASP:HB3	2:O:637:PRO:CD	2.14	0.76
1:H:675:VAL:C	1:H:676:PRO:O	2.18	0.76
2:N:692:THR:HG21	3:m:29:LEU:HD12	1.67	0.76
2:B:637:PRO:HB3	1:H:553:PRO:HG3	1.66	0.76
1:C:763:LYS:NZ	8:C:1006:SO4:S	2.52	0.76
1:H:676:PRO:CD	1:H:680:LEU:HD23	2.16	0.76
3:k:28:SER:O	3:k:29:LEU:HB2	1.85	0.76
2:N:641:ASP:HB3	2:O:637:PRO:HD2	1.68	0.76
1:P:704:ARG:NH2	1:P:714:ARG:NH1	2.33	0.75
1:C:712:TRP:CE2	1:M:713:GLN:HG3	2.22	0.75
2:N:738:TYR:CD2	2:O:635:GLN:HG3	2.22	0.74
1:H:677:LYS:HB2	1:H:768:SER:HA	1.70	0.73
2:O:690:ARG:O	2:O:694:ILE:HG13	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:648:LYS:NZ	1:H:638:TYR:OH	2.20	0.73
1:L:690:ARG:O	1:L:694:ILE:HG13	1.89	0.73
2:E:690:ARG:O	2:E:694:ILE:HG13	1.88	0.73
2:N:690:ARG:O	2:N:694:ILE:HG13	1.89	0.72
1:A:690:ARG:O	1:A:694:ILE:HG13	1.89	0.72
2:B:690:ARG:O	2:B:694:ILE:HG13	1.89	0.72
1:F:690:ARG:O	1:F:694:ILE:HG13	1.88	0.72
1:G:690:ARG:O	1:G:694:ILE:HG13	1.89	0.72
1:I:690:ARG:O	1:I:694:ILE:HG13	1.89	0.72
1:P:690:ARG:O	1:P:694:ILE:HG13	1.89	0.72
2:K:690:ARG:O	2:K:694:ILE:HG13	1.89	0.72
2:J:690:ARG:O	2:J:694:ILE:HG13	1.90	0.71
1:M:690:ARG:O	1:M:694:ILE:HG13	1.89	0.71
1:D:690:ARG:O	1:D:694:ILE:HG13	1.89	0.71
2:N:623:PHE:CE2	2:N:629:ILE:HD12	2.25	0.71
1:C:690:ARG:O	1:C:694:ILE:HG13	1.90	0.71
1:H:690:ARG:O	1:H:694:ILE:HG13	1.89	0.70
1:P:711:ASN:CG	6:P:1002:EPE:C6	2.36	0.70
2:N:765:LYS:HE3	11:N:1003:IMD:HN3	1.55	0.70
1:C:727:GLU:OE2	2:E:738:TYR:OH	2.10	0.69
1:H:604:MET:HE2	1:H:604:MET:HA	1.74	0.69
1:A:759:ASN:ND2	3:a:16:SER:O	2.21	0.69
1:F:623:PHE:CE2	1:F:629:ILE:HD12	2.27	0.69
1:C:568:GLY:HA3	7:C:1002:GOL:C3	2.23	0.69
1:D:623:PHE:CE2	1:D:629:ILE:HD12	2.28	0.69
1:G:623:PHE:CE2	1:G:629:ILE:HD12	2.28	0.69
2:N:559:LEU:HD23	2:N:639:MET:HE2	1.76	0.68
1:P:604:MET:HE2	1:P:604:MET:HA	1.75	0.68
1:L:604:MET:HA	1:L:604:MET:HE2	1.76	0.68
1:F:604:MET:HE2	1:F:604:MET:HA	1.76	0.68
1:P:711:ASN:OD1	6:P:1002:EPE:H62	1.92	0.68
2:K:604:MET:HE2	2:K:604:MET:HA	1.74	0.68
1:H:598:TYR:HE2	1:H:676:PRO:CB	1.99	0.67
2:E:604:MET:HA	2:E:604:MET:HE2	1.76	0.67
2:B:604:MET:HE2	2:B:604:MET:HA	1.77	0.67
2:J:742:ASN:OD1	2:N:552:LEU:HD22	1.95	0.67
1:G:604:MET:HE2	1:G:604:MET:HA	1.76	0.67
2:J:604:MET:HA	2:J:604:MET:HE2	1.77	0.66
1:I:604:MET:HE2	1:I:604:MET:HA	1.77	0.66
1:M:604:MET:HE2	1:M:604:MET:HA	1.76	0.66
1:C:554:ASP:OD1	1:H:551:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:589:LEU:HD23	2:J:589:LEU:O	1.95	0.66
2:N:738:TYR:CG	2:O:635:GLN:HG3	2.31	0.66
2:O:604:MET:HA	2:O:604:MET:HE2	1.78	0.66
2:N:641:ASP:HB3	2:O:637:PRO:HG2	1.79	0.65
2:O:585:ARG:NH1	1:P:585:ARG:HG3	2.10	0.65
2:J:589:LEU:HD23	2:J:589:LEU:C	2.22	0.65
2:N:604:MET:HE2	2:N:604:MET:HA	1.78	0.65
2:B:637:PRO:CB	1:H:553:PRO:HG3	2.27	0.65
2:K:559:LEU:HD23	2:K:639:MET:HE2	1.76	0.65
1:A:604:MET:HE2	1:A:604:MET:HA	1.77	0.65
1:C:568:GLY:C	7:C:1002:GOL:H31	2.21	0.65
1:C:604:MET:HA	1:C:604:MET:HE2	1.77	0.64
1:D:604:MET:HE2	1:D:604:MET:HA	1.79	0.64
2:O:638:TYR:HB3	2:O:735:PHE:HZ	1.62	0.64
1:D:553:PRO:HA	1:G:553:PRO:HB3	1.80	0.64
1:H:687:ASP:O	1:H:691:MET:HG2	1.97	0.64
1:H:674:THR:HG23	1:H:769:VAL:HG13	1.79	0.64
1:H:674:THR:CG2	1:H:769:VAL:HG13	2.28	0.63
1:M:759:ASN:ND2	3:m:16:SER:O	2.28	0.63
1:H:676:PRO:CG	1:H:680:LEU:CD2	2.77	0.63
2:N:776:GLN:OE1	2:N:776:GLN:HA	1.98	0.62
11:O:1004:IMD:HN1	1:P:569:ARG:HE	1.47	0.62
1:C:568:GLY:HA3	7:C:1002:GOL:H31	1.82	0.62
1:D:660:TYR:HB2	6:D:804:EPE:H101	1.81	0.62
1:F:589:LEU:HD23	1:F:589:LEU:O	2.00	0.61
1:L:776:GLN:HA	1:L:776:GLN:OE1	2.00	0.61
2:N:641:ASP:HB3	2:O:637:PRO:CG	2.30	0.61
2:N:623:PHE:HE2	2:N:629:ILE:HD12	1.63	0.61
1:D:553:PRO:HA	1:G:553:PRO:CB	2.30	0.61
1:L:638:TYR:HD1	7:L:1004:GOL:H2	1.66	0.61
1:G:531:THR:HG22	1:G:533:ILE:H	1.65	0.61
1:D:701:ILE:HG23	1:D:714:ARG:HG2	1.83	0.61
4:E:1001:DEX:O2	4:E:1001:DEX:H821	2.01	0.61
2:B:701:ILE:HG23	2:B:714:ARG:HG2	1.83	0.60
2:J:710:GLN:OE1	2:J:710:GLN:N	2.34	0.60
1:P:704:ARG:NH2	1:P:714:ARG:HH12	1.97	0.60
1:H:594:THR:HG21	1:H:676:PRO:HG3	1.84	0.60
1:F:589:LEU:HD23	1:F:589:LEU:C	2.26	0.60
1:D:623:PHE:HE2	1:D:629:ILE:HD12	1.67	0.60
1:M:701:ILE:HG23	1:M:714:ARG:HG2	1.84	0.60
1:F:701:ILE:HG23	1:F:714:ARG:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:585:ARG:HH11	1:L:585:ARG:HE	1.51	0.59
2:K:638:TYR:CD2	2:K:638:TYR:N	2.70	0.59
1:G:534:SER:O	1:G:538:VAL:HG13	2.02	0.59
1:M:534:SER:O	1:M:538:VAL:HG13	2.02	0.59
1:F:534:SER:O	1:F:538:VAL:HG13	2.02	0.59
1:H:534:SER:O	1:H:538:VAL:HG13	2.02	0.59
1:L:642:GLN:HB2	4:L:1001:DEX:C22	2.33	0.59
2:J:534:SER:O	2:J:538:VAL:HG13	2.03	0.59
2:K:534:SER:O	2:K:538:VAL:HG13	2.03	0.59
1:D:776:GLN:OE1	1:D:776:GLN:HA	2.01	0.59
1:C:775:HIS:O	1:C:776:GLN:C	2.46	0.59
2:E:534:SER:O	2:E:538:VAL:HG13	2.02	0.59
1:G:701:ILE:HG23	1:G:714:ARG:HG2	1.84	0.58
1:A:534:SER:O	1:A:538:VAL:HG13	2.02	0.58
2:B:549:ASP:OD1	2:B:551:THR:HB	2.04	0.58
2:N:554:ASP:HB3	2:N:636:LEU:HD11	1.85	0.58
1:L:638:TYR:CD1	7:L:1004:GOL:H2	2.38	0.58
1:I:534:SER:O	1:I:538:VAL:HG13	2.03	0.58
2:K:535:LEU:HD11	3:l:23:ALA:HB1	1.85	0.58
2:K:615:GLN:HB2	2:K:622[B]:CSO:OD	2.04	0.58
2:N:559:LEU:CD2	2:N:639:MET:HE2	2.34	0.58
1:L:534:SER:O	1:L:538:VAL:HG13	2.03	0.58
1:I:701:ILE:HG23	1:I:714:ARG:HG2	1.86	0.58
2:B:534:SER:O	2:B:538:VAL:HG13	2.03	0.57
2:B:642:GLN:OE1	4:B:802:DEX:O3	2.18	0.57
2:J:701:ILE:HG23	2:J:714:ARG:HG2	1.86	0.57
2:N:534:SER:O	2:N:538:VAL:HG13	2.03	0.57
1:L:701:ILE:HG23	1:L:714:ARG:HG2	1.85	0.57
2:O:632:GLU:OE1	2:O:632:GLU:N	2.38	0.57
3:j:28:SER:O	3:j:29:LEU:CB	2.50	0.57
1:A:776:GLN:OE1	1:A:776:GLN:HA	2.04	0.57
2:K:549:ASP:OD1	2:K:551:THR:HB	2.04	0.57
1:C:716:TYR:CE1	1:M:709:SER:HB3	2.40	0.56
1:C:701:ILE:HG23	1:C:714:ARG:HG2	1.87	0.56
1:D:593:MET:SD	3:d:21:LEU:CD1	2.91	0.56
2:E:642:GLN:OE1	4:E:1001:DEX:O3	2.12	0.56
1:G:585:ARG:HD2	1:H:585:ARG:NH1	2.20	0.56
1:L:745:LEU:HD21	7:L:1005:GOL:H12	1.87	0.56
1:C:764:PHE:HB2	7:C:1003:GOL:C3	2.35	0.56
1:P:711:ASN:HB2	6:P:1002:EPE:C5	2.22	0.56
2:B:553:PRO:HD2	1:C:638:TYR:CZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:GLY:CA	7:C:1002:GOL:H31	2.36	0.56
1:L:549:ASP:OD1	1:L:551:THR:HB	2.04	0.56
2:N:765:LYS:HE3	11:N:1003:IMD:N3	2.20	0.56
2:O:549:ASP:OD1	2:O:551:THR:HB	2.05	0.56
2:E:549:ASP:OD1	2:E:551:THR:HB	2.05	0.56
1:A:585:ARG:NH2	3:a:25:LEU:O	2.29	0.56
1:I:549:ASP:OD1	1:I:551:THR:HB	2.05	0.56
6:I:1004:EPE:O8	7:I:1005:GOL:H11	2.06	0.56
2:O:701:ILE:HG23	2:O:714:ARG:HG2	1.86	0.56
2:O:702:VAL:HG22	2:O:710:GLN:HA	1.87	0.55
1:P:652:GLU:OE2	1:P:655:ARG:NH1	2.39	0.55
2:E:691:MET:HG2	1:I:688:GLU:HB2	1.88	0.55
1:A:701:ILE:HG23	1:A:714:ARG:HG2	1.88	0.55
2:O:529:PHE:N	2:O:530:PRO:HD2	2.22	0.55
2:B:652:GLU:OE2	2:B:655:ARG:NH1	2.40	0.55
2:K:549:ASP:O	2:K:558:ARG:NH1	2.40	0.55
2:B:549:ASP:OD2	2:B:552:LEU:HD13	2.07	0.55
2:B:641:ASP:OD2	1:H:636:LEU:HD22	2.07	0.55
1:F:585:ARG:NH1	3:f:25:LEU:O	2.40	0.55
1:M:652:GLU:OE2	1:M:655:ARG:NH1	2.41	0.54
1:M:743:LYS:H	1:M:743:LYS:CD	2.20	0.54
1:L:742:ASN:HD22	1:L:742:ASN:C	2.14	0.54
2:O:710:GLN:HG3	2:O:711:ASN:N	2.22	0.54
1:H:676:PRO:CA	1:H:768:SER:O	2.54	0.54
1:H:708:SER:CB	1:H:710:GLN:HG3	2.38	0.54
1:H:662:GLU:CD	1:H:714:ARG:HH21	2.15	0.54
2:O:529:PHE:N	2:O:530:PRO:CD	2.71	0.54
1:C:710:GLN:N	1:C:710:GLN:OE1	2.41	0.53
2:B:691:MET:HE3	2:B:695:LYS:HE2	1.89	0.53
1:F:623:PHE:HE2	1:F:629:ILE:HD12	1.72	0.53
4:K:802:DEX:O2	4:K:802:DEX:H821	2.08	0.53
2:B:641:ASP:OD2	1:H:555:THR:HA	2.09	0.53
1:A:568:GLY:HA2	1:A:753:LEU:HD13	1.91	0.53
1:F:661:ASP:OD2	1:F:703:LYS:HE2	2.08	0.53
1:C:763:LYS:CE	8:C:1006:SO4:O4	2.53	0.53
1:D:540:GLU:OE2	10:D:803:PG4:H22	2.08	0.53
2:J:745:LEU:HD11	2:N:552:LEU:HB3	1.89	0.53
1:A:708:SER:CB	1:A:710:GLN:OE1	2.56	0.53
1:A:708:SER:OG	1:A:710:GLN:OE1	2.23	0.53
3:k:28:SER:O	3:k:29:LEU:CB	2.54	0.53
2:O:544:LEU:HD22	1:P:542:GLU:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:583:GLY:HA2	3:m:29:LEU:HD22	1.91	0.52
2:B:759:ASN:ND2	3:b:16:SER:O	2.30	0.52
2:J:529:PHE:N	2:J:530:PRO:CD	2.72	0.52
2:K:702:VAL:HG22	2:K:710:GLN:HB2	1.92	0.52
1:M:711:ASN:CB	13:M:804:PGE:H4	2.29	0.52
1:L:742:ASN:O	1:L:742:ASN:ND2	2.31	0.52
1:P:533:ILE:CG1	1:P:661:ASP:OD2	2.57	0.52
1:G:531:THR:HG21	1:G:533:ILE:HG22	1.91	0.52
2:K:559:LEU:HD22	2:K:639:MET:HE2	1.91	0.52
1:L:717:GLN:HG2	9:L:1008:CL:CL	2.46	0.52
2:O:548:TYR:CG	2:O:627:LEU:HD13	2.44	0.52
1:P:550:SER:OG	7:P:1003:GOL:O1	2.27	0.52
1:C:712:TRP:NE1	1:M:713:GLN:HG3	2.25	0.51
1:G:623:PHE:HE2	1:G:629:ILE:HD12	1.73	0.51
1:H:711:ASN:OD1	10:H:803:PG4:H52	2.10	0.51
1:P:633:ARG:NH1	7:P:1003:GOL:H12	2.25	0.51
1:G:544:LEU:HD22	1:H:542:GLU:HG3	1.92	0.51
2:B:641:ASP:OD2	1:H:636:LEU:CD2	2.58	0.51
1:G:531:THR:CG2	1:G:533:ILE:HG22	2.40	0.51
1:P:627:LEU:HA	7:P:1003:GOL:H11	1.93	0.51
4:F:1001:DEX:H821	4:F:1001:DEX:O2	2.11	0.51
1:M:544:LEU:CD2	2:N:542:GLU:HG3	2.40	0.51
1:G:542:GLU:HG3	1:H:544:LEU:CD2	2.41	0.51
1:M:544:LEU:HD22	2:N:542:GLU:HG3	1.93	0.51
2:E:542:GLU:HG3	1:F:544:LEU:HD22	1.93	0.50
2:J:597:GLN:HG2	2:J:756:ILE:HG23	1.93	0.50
1:C:775:HIS:HA	1:M:708:SER:OG	2.11	0.50
2:E:542:GLU:HG3	1:F:544:LEU:CD2	2.41	0.50
1:C:716:TYR:CD1	1:M:709:SER:CB	2.95	0.50
1:H:535:LEU:HD11	3:g:23:ALA:HB1	1.93	0.50
1:M:743:LYS:H	1:M:743:LYS:HD3	1.76	0.50
1:C:716:TYR:CE1	1:M:709:SER:CB	2.95	0.50
1:C:542:GLU:HG3	1:D:544:LEU:HD22	1.93	0.50
1:F:697:LEU:O	1:F:701:ILE:HG13	2.12	0.50
1:M:697:LEU:O	1:M:701:ILE:HG13	2.12	0.50
1:G:759:ASN:ND2	3:g:16:SER:O	2.34	0.49
2:J:744:SER:O	2:N:558:ARG:HD2	2.12	0.49
1:D:661:ASP:OD1	1:D:703:LYS:HE3	2.12	0.49
2:J:535:LEU:HD11	3:i:23:ALA:HB1	1.94	0.49
2:N:641:ASP:CB	2:O:637:PRO:HD2	2.41	0.49
2:E:576:LYS:NZ	1:F:539:ILE:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:633:ARG:HH12	7:P:1003:GOL:H12	1.77	0.49
2:B:638:TYR:OH	1:C:553:PRO:HG2	2.13	0.49
1:L:697:LEU:O	1:L:701:ILE:HG13	2.12	0.49
2:B:697:LEU:O	2:B:701:ILE:HG13	2.12	0.49
2:E:697:LEU:O	2:E:701:ILE:HG13	2.12	0.49
1:A:697:LEU:O	1:A:701:ILE:HG13	2.13	0.49
2:N:554:ASP:CB	2:N:636:LEU:HD11	2.42	0.49
2:O:542:GLU:HG3	1:P:544:LEU:CD2	2.43	0.49
1:P:697:LEU:O	1:P:701:ILE:HG13	2.13	0.49
1:A:542:GLU:HG3	2:B:544:LEU:CD2	2.42	0.49
4:B:802:DEX:H931	4:B:802:DEX:O2	2.12	0.49
2:O:547:GLY:N	2:O:626:ASP:OD2	2.42	0.49
3:d:21:LEU:HD22	3:d:21:LEU:O	2.13	0.49
1:A:585:ARG:NH1	8:A:1006:SO4:O1	2.46	0.49
1:C:759:ASN:ND2	3:c:16:SER:O	2.42	0.49
1:G:544:LEU:CD2	1:H:542:GLU:HG3	2.43	0.49
1:H:634:MET:HE1	1:H:647:LEU:HD11	1.95	0.49
2:O:544:LEU:CD2	1:P:542:GLU:HG3	2.42	0.49
2:B:634:MET:HE1	2:B:647:LEU:HD11	1.95	0.48
1:C:697:LEU:O	1:C:701:ILE:HG13	2.13	0.48
1:M:629:ILE:HG23	1:M:633:ARG:HB3	1.95	0.48
4:N:1001:DEX:O2	4:N:1001:DEX:H931	2.13	0.48
2:O:638:TYR:HB3	2:O:735:PHE:CZ	2.44	0.48
1:G:697:LEU:O	1:G:701:ILE:HG13	2.12	0.48
1:I:697:LEU:O	1:I:701:ILE:HG13	2.13	0.48
4:A:1001:DEX:H931	4:A:1001:DEX:O2	2.13	0.48
2:B:661:ASP:OD2	2:B:703:LYS:HE3	2.13	0.48
4:J:802:DEX:H821	4:J:802:DEX:O2	2.14	0.48
2:B:736:CYS:HA	4:B:802:DEX:O4	2.14	0.48
1:C:594:THR:HG21	1:C:676:PRO:HG3	1.94	0.48
1:D:697:LEU:O	1:D:701:ILE:HG13	2.13	0.48
2:O:697:LEU:O	2:O:701:ILE:HG13	2.12	0.48
1:H:721:LEU:C	1:H:721:LEU:HD23	2.38	0.48
2:K:701:ILE:HG23	2:K:714:ARG:HG2	1.94	0.48
1:M:661:ASP:OD2	1:M:703:LYS:HE2	2.14	0.48
1:A:542:GLU:HG3	2:B:544:LEU:HD22	1.96	0.48
2:J:697:LEU:O	2:J:701:ILE:HG13	2.13	0.48
1:C:716:TYR:CD1	1:M:709:SER:HB3	2.48	0.48
1:H:708:SER:HB3	1:H:710:GLN:HG3	1.95	0.48
2:N:661:ASP:OD1	2:N:703:LYS:HE3	2.14	0.48
2:J:759:ASN:ND2	3:j:16:SER:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:697:LEU:O	2:K:701:ILE:HG13	2.13	0.47
1:H:676:PRO:HG3	1:H:680:LEU:CD2	2.44	0.47
1:L:535:LEU:HD11	3:k:23:ALA:HB1	1.96	0.47
1:A:735:PHE:HE2	7:A:1005:GOL:H32	1.79	0.47
1:H:697:LEU:O	1:H:701:ILE:HG13	2.13	0.47
3:d:29:LEU:C	11:d:101:IMD:H2	2.39	0.47
1:C:568:GLY:HA3	7:C:1002:GOL:H32	1.96	0.47
2:B:551:THR:HG22	2:B:552:LEU:HD12	1.97	0.47
1:G:531:THR:HG22	1:G:532:LEU:N	2.29	0.47
2:K:661:ASP:OD2	2:K:703:LYS:HE3	2.15	0.47
2:N:697:LEU:O	2:N:701:ILE:HG13	2.14	0.47
2:B:637:PRO:CA	1:H:553:PRO:HG3	2.45	0.47
1:F:563:LEU:HB3	4:F:1001:DEX:H11	1.97	0.47
2:O:634:MET:HE1	2:O:647:LEU:HD11	1.96	0.47
2:E:675:VAL:HG21	2:E:772:LEU:HD21	1.97	0.47
1:A:733:LEU:HD22	1:A:737:PHE:CZ	2.50	0.47
1:D:594:THR:HG21	1:D:676:PRO:HG3	1.97	0.47
2:O:585:ARG:HH11	1:P:585:ARG:HG3	1.78	0.47
1:D:535:LEU:HD11	3:c:23:ALA:HB1	1.97	0.46
1:G:593:MET:HB3	1:G:593:MET:HE3	1.79	0.46
1:H:674:THR:HG23	1:H:769:VAL:CG1	2.42	0.46
3:d:28:SER:O	11:d:101:IMD:H2	2.15	0.46
1:L:742:ASN:C	1:L:742:ASN:ND2	2.73	0.46
3:h:17:ARG:NH2	3:h:22:TYR:CZ	2.83	0.46
1:A:661:ASP:OD2	1:A:703:LYS:HE3	2.15	0.46
2:E:713:GLN:HA	1:I:712:TRP:CH2	2.51	0.46
1:H:661:ASP:OD2	1:H:703:LYS:HE2	2.15	0.46
2:O:593:MET:HE3	2:O:593:MET:HB3	1.79	0.46
1:C:642:GLN:HB2	4:C:1001:DEX:C22	2.46	0.46
1:C:734:GLN:OE1	2:E:638:TYR:N	2.45	0.46
2:N:634:MET:HE1	2:N:647:LEU:HD21	1.97	0.46
2:E:593:MET:HE3	2:E:593:MET:HB3	1.81	0.46
1:G:661:ASP:OD2	1:G:703:LYS:HE2	2.15	0.46
2:K:704:ARG:CZ	2:K:714:ARG:NH2	2.79	0.46
1:P:593:MET:HE3	1:P:593:MET:HB3	1.80	0.46
2:O:563:LEU:HB3	4:O:1001:DEX:H11	1.98	0.46
1:A:604:MET:HE2	1:A:604:MET:CA	2.46	0.46
1:F:604:MET:HE2	1:F:604:MET:CA	2.46	0.46
2:J:554:ASP:OD2	2:O:551:THR:HG23	2.16	0.46
4:J:802:DEX:O2	4:J:802:DEX:H931	2.15	0.46
2:N:593:MET:HE3	2:N:593:MET:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:544:LEU:CD2	1:F:542:GLU:HG3	2.46	0.45
1:A:678:ASP:OD2	1:A:678:ASP:N	2.50	0.45
1:A:692:THR:HG21	3:b:29:LEU:HD22	1.98	0.45
2:B:637:PRO:HA	1:H:553:PRO:HG3	1.97	0.45
2:E:544:LEU:HD22	1:F:542:GLU:HG3	1.98	0.45
1:H:676:PRO:HD2	1:H:680:LEU:CD2	2.42	0.45
1:M:678:ASP:OD2	1:M:678:ASP:N	2.49	0.45
2:K:559:LEU:HD23	2:K:639:MET:CE	2.45	0.45
1:F:733:LEU:HD22	1:F:737:PHE:CZ	2.51	0.45
1:I:544:LEU:HD22	2:J:542:GLU:HG3	1.99	0.45
1:I:736:CYS:HA	4:I:1001:DEX:O4	2.16	0.45
2:K:552:LEU:CD2	2:N:633:ARG:HB2	2.45	0.45
2:N:549:ASP:H	7:N:1002:GOL:H12	1.81	0.45
1:P:716:TYR:CE1	1:P:775:HIS:CE1	3.04	0.45
1:D:678:ASP:OD2	1:D:678:ASP:N	2.49	0.45
2:K:555:THR:HG22	2:N:553:PRO:HB3	1.97	0.45
1:H:711:ASN:N	1:H:711:ASN:HD22	2.14	0.45
1:M:594:THR:HG21	1:M:676:PRO:HG3	1.98	0.45
2:N:634:MET:HE1	2:N:647:LEU:CD2	2.46	0.45
1:A:593:MET:HE3	1:A:593:MET:HB3	1.84	0.45
2:J:661:ASP:OD2	2:J:703:LYS:HE3	2.17	0.45
1:L:611:ARG:HD2	11:L:1007:IMD:N1	2.32	0.45
1:I:542:GLU:HG3	2:J:544:LEU:CD2	2.47	0.45
1:C:642:GLN:HB2	4:C:1001:DEX:H222	1.98	0.45
1:G:542:GLU:HG3	1:H:544:LEU:HD22	1.99	0.45
1:G:634:MET:HE1	1:G:647:LEU:HD11	1.98	0.45
1:H:678:ASP:OD2	1:H:678:ASP:N	2.50	0.45
2:N:548:TYR:CE2	2:N:633:ARG:NH1	2.85	0.45
2:O:585:ARG:NH1	1:P:585:ARG:HE	2.13	0.45
1:H:549:ASP:OD1	1:H:552:LEU:HG	2.16	0.45
1:L:604:MET:HE2	1:L:604:MET:CA	2.45	0.45
2:K:678:ASP:OD2	2:K:678:ASP:N	2.49	0.44
1:L:594:THR:HG21	1:L:676:PRO:HG3	1.98	0.44
1:P:678:ASP:OD2	1:P:678:ASP:N	2.50	0.44
1:A:535:LEU:HD11	3:b:23:ALA:HB1	1.99	0.44
1:C:542:GLU:HG3	1:D:544:LEU:CD2	2.46	0.44
2:E:678:ASP:OD2	2:E:678:ASP:N	2.50	0.44
1:G:594:THR:HG21	1:G:676:PRO:HG3	1.99	0.44
1:I:594:THR:HG21	1:I:676:PRO:HG3	1.99	0.44
1:H:733:LEU:HD22	1:H:737:PHE:CZ	2.52	0.44
2:N:597:GLN:HG2	2:N:756:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:594:THR:HG21	2:O:676:PRO:HG3	2.00	0.44
2:E:585:ARG:HH22	1:F:585:ARG:HG3	1.83	0.44
2:O:678:ASP:N	2:O:678:ASP:OD2	2.50	0.44
1:D:604:MET:HE2	1:D:604:MET:CA	2.47	0.44
2:K:553:PRO:HG3	2:N:554:ASP:CG	2.42	0.44
1:C:604:MET:HE2	1:C:604:MET:CA	2.46	0.44
1:F:678:ASP:OD2	1:F:678:ASP:N	2.50	0.44
2:B:554:ASP:CB	2:B:636:LEU:HD11	2.48	0.44
1:P:533:ILE:HG12	1:P:661:ASP:OD2	2.18	0.44
1:D:582:PRO:HA	3:c:27:SER:O	2.18	0.44
2:E:594:THR:HG21	2:E:676:PRO:HG3	2.00	0.44
1:F:585:ARG:HD2	1:F:585:ARG:HA	1.75	0.44
2:B:614:LYS:HE2	6:B:804:EPE:H22	2.00	0.43
2:J:552:LEU:HD21	2:N:744:SER:OG	2.18	0.43
1:C:637:PRO:O	1:C:638:TYR:HB2	2.18	0.43
2:N:733:LEU:HD22	2:N:737:PHE:CZ	2.53	0.43
1:A:594:THR:HG21	1:A:676:PRO:HG3	2.00	0.43
2:B:554:ASP:HB3	2:B:636:LEU:HD11	2.00	0.43
2:E:675:VAL:CG2	2:E:772:LEU:HD21	2.48	0.43
1:F:530:PRO:HG2	1:F:535:LEU:HD21	2.01	0.43
1:G:604:MET:HE2	1:G:604:MET:CA	2.46	0.43
4:N:1001:DEX:O2	4:N:1001:DEX:H821	2.18	0.43
1:I:660:TYR:HB2	6:I:1004:EPE:H92	1.99	0.43
1:F:598:TYR:HD2	1:F:674:THR:HG22	1.84	0.43
1:H:542:GLU:H	5:H:801:CAC:C2	2.31	0.43
1:I:604:MET:HE2	1:I:604:MET:CA	2.46	0.43
2:J:604:MET:HE2	2:J:604:MET:CA	2.46	0.43
1:C:535:LEU:HD11	3:d:23:ALA:HB1	2.00	0.43
1:I:642:GLN:HB2	4:I:1001:DEX:C22	2.47	0.43
1:P:594:THR:HG21	1:P:676:PRO:HG3	2.00	0.43
1:F:593:MET:HE3	1:F:593:MET:HB3	1.82	0.43
2:N:615:GLN:HB2	2:N:622[A]:CSO:OD	2.19	0.43
2:O:705:GLU:OE1	2:O:705:GLU:HA	2.18	0.43
2:B:597:GLN:HG2	2:B:756:ILE:HG23	2.00	0.43
2:E:559:LEU:HD12	2:E:559:LEU:HA	1.89	0.43
2:E:615:GLN:HB2	2:E:622[A]:CSO:OD	2.18	0.43
1:P:701:ILE:HG23	1:P:714:ARG:HG2	2.01	0.43
2:N:604:MET:HE2	2:N:604:MET:CA	2.46	0.43
1:P:634:MET:HE1	1:P:647:LEU:HD11	2.01	0.43
2:B:552:LEU:HD23	1:C:745:LEU:HD13	1.99	0.43
4:C:1001:DEX:O2	4:C:1001:DEX:H931	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:585:ARG:HH11	1:L:585:ARG:NE	2.14	0.43
2:N:559:LEU:HD23	2:N:639:MET:CE	2.46	0.43
2:O:548:TYR:CE2	2:O:627:LEU:HD13	2.52	0.43
2:B:535:LEU:HD11	3:a:23:ALA:HB1	2.01	0.42
2:J:735:PHE:CZ	12:K:801:PEG:H22	2.55	0.42
1:L:611:ARG:HD2	11:L:1007:IMD:HN1	1.83	0.42
2:O:542:GLU:HG3	1:P:544:LEU:HD22	2.00	0.42
1:D:553:PRO:CA	1:G:553:PRO:CB	2.97	0.42
2:J:635:GLN:OE1	2:J:635:GLN:HA	2.19	0.42
3:a:29:LEU:HD23	3:a:29:LEU:HA	1.90	0.42
3:i:29:LEU:HD13	3:i:29:LEU:HA	1.87	0.42
2:B:593:MET:HB3	2:B:593:MET:HE3	1.81	0.42
1:L:738:TYR:CD2	7:L:1004:GOL:H32	2.53	0.42
1:P:652:GLU:CD	1:P:655:ARG:HH12	2.28	0.42
1:P:675:VAL:HG21	1:P:772:LEU:HD21	2.01	0.42
3:d:29:LEU:HA	11:d:101:IMD:H2	2.01	0.42
1:A:559:LEU:HD12	1:A:559:LEU:HA	1.90	0.42
2:B:604:MET:HE2	2:B:604:MET:CA	2.46	0.42
3:k:29:LEU:HD23	3:k:29:LEU:HA	1.88	0.42
2:E:701:ILE:HG23	2:E:714:ARG:HG2	2.00	0.42
2:J:593:MET:HE3	2:J:593:MET:HB3	1.80	0.42
3:l:29:LEU:HD12	3:l:29:LEU:HA	1.85	0.42
1:C:764:PHE:HB2	7:C:1003:GOL:O3	2.19	0.42
2:E:612:SER:HA	2:E:622[A]:CSO:SG	2.60	0.42
1:F:594:THR:HG21	1:F:676:PRO:HG3	2.02	0.42
1:I:614:LYS:HA	1:I:614:LYS:HD2	1.86	0.42
1:C:764:PHE:HB2	7:C:1003:GOL:H31	2.01	0.42
1:D:559:LEU:HD12	1:D:559:LEU:HA	1.90	0.42
3:d:29:LEU:CA	11:d:101:IMD:H2	2.50	0.42
2:B:642:GLN:HB2	4:B:802:DEX:H222	2.01	0.42
2:K:604:MET:HE2	2:K:604:MET:CA	2.48	0.42
1:L:738:TYR:CE2	7:L:1004:GOL:H32	2.55	0.42
2:O:604:MET:HE2	2:O:604:MET:CA	2.46	0.42
1:P:774:PHE:C	1:P:775:HIS:CG	2.98	0.41
1:C:678:ASP:OD1	1:C:678:ASP:N	2.53	0.41
1:H:597:GLN:HG2	1:H:756:ILE:HG23	2.01	0.41
2:N:570:GLN:HB3	2:N:604:MET:SD	2.60	0.41
1:P:614:LYS:HD2	1:P:614:LYS:HA	1.86	0.41
2:B:570:GLN:HB3	2:B:604:MET:SD	2.60	0.41
2:E:597:GLN:HG2	2:E:756:ILE:HG23	2.01	0.41
1:L:678:ASP:OD1	1:L:678:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:692:THR:HG21	3:p:29:LEU:HD11	2.02	0.41
1:A:570:GLN:HB3	1:A:604:MET:SD	2.61	0.41
4:E:1001:DEX:O2	4:E:1001:DEX:C18	2.66	0.41
1:G:597:GLN:CD	1:G:760[B]:GLN:HE21	2.25	0.41
1:H:761:LEU:HB3	1:H:762:PRO:CD	2.51	0.41
4:O:1001:DEX:O2	4:O:1001:DEX:H931	2.21	0.41
1:P:702:VAL:HA	1:P:711:ASN:HD21	1.85	0.41
1:D:761:LEU:HB3	1:D:762:PRO:CD	2.51	0.41
2:K:634:MET:HE1	2:K:647:LEU:HD11	2.02	0.41
1:M:753:LEU:HD23	1:M:753:LEU:HA	1.94	0.41
1:D:634:MET:HE1	1:D:647:LEU:HD11	2.02	0.41
2:E:604:MET:HE2	2:E:604:MET:CA	2.47	0.41
1:F:759:ASN:ND2	3:f:16:SER:O	2.34	0.41
1:H:604:MET:HE2	1:H:604:MET:CA	2.45	0.41
1:A:634:MET:HE1	1:A:647:LEU:HD11	2.03	0.41
1:A:708:SER:O	1:A:711:ASN:HB2	2.20	0.41
2:E:552:LEU:HB2	2:E:558:ARG:NH2	2.35	0.41
1:F:559:LEU:HD12	1:F:559:LEU:HA	1.90	0.41
1:I:761:LEU:HB3	1:I:762:PRO:CD	2.51	0.41
1:I:765:LYS:HD2	1:I:765:LYS:HA	1.82	0.41
2:K:594:THR:HG21	2:K:676:PRO:HG3	2.02	0.41
2:N:678:ASP:OD1	2:N:678:ASP:N	2.54	0.41
1:D:549:ASP:O	1:D:558:ARG:NH1	2.52	0.41
1:I:542:GLU:HG3	2:J:544:LEU:HD22	2.01	0.41
2:K:552:LEU:HD23	2:N:633:ARG:HB2	2.01	0.41
1:C:761:LEU:HB3	1:C:762:PRO:CD	2.51	0.41
1:G:570:GLN:HB3	1:G:604:MET:SD	2.61	0.41
1:H:559:LEU:HD12	1:H:559:LEU:HA	1.90	0.41
1:H:614:LYS:HA	1:H:614:LYS:HD2	1.89	0.41
1:H:635:GLN:HA	1:H:635:GLN:OE1	2.20	0.41
1:H:770:LYS:HA	1:H:771:PRO:HD2	1.94	0.41
1:I:634:MET:HE1	1:I:647:LEU:HD11	2.03	0.41
2:J:570:GLN:HB3	2:J:604:MET:SD	2.61	0.41
1:L:634:MET:HE1	1:L:647:LEU:HD11	2.03	0.41
2:N:629:ILE:HG23	2:N:633:ARG:HB3	2.03	0.41
1:P:570:GLN:HB3	1:P:604:MET:SD	2.61	0.41
1:H:570:GLN:HB3	1:H:604:MET:SD	2.61	0.41
2:K:761:LEU:HB3	2:K:762:PRO:CD	2.51	0.41
1:L:585:ARG:HD2	1:L:585:ARG:HA	1.89	0.41
3:p:29:LEU:HD23	3:p:29:LEU:HA	1.90	0.41
1:A:544:LEU:CD2	2:B:542:GLU:HG3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:MET:HE3	1:C:593:MET:HB3	1.83	0.40
1:D:593:MET:HE3	1:D:593:MET:HB3	1.82	0.40
2:E:570:GLN:HB3	2:E:604:MET:SD	2.60	0.40
1:I:593:MET:HE3	1:I:593:MET:HB3	1.83	0.40
4:M:802:DEX:H931	4:M:802:DEX:O2	2.21	0.40
2:N:585:ARG:HD2	2:N:585:ARG:HA	1.88	0.40
1:A:761:LEU:HB3	1:A:762:PRO:CD	2.51	0.40
1:D:570:GLN:HB3	1:D:604:MET:SD	2.61	0.40
4:H:802:DEX:O2	4:H:802:DEX:H821	2.21	0.40
1:I:535:LEU:O	1:I:539:ILE:HG12	2.22	0.40
1:I:678:ASP:OD1	1:I:678:ASP:N	2.53	0.40
1:L:570:GLN:HB3	1:L:604:MET:SD	2.61	0.40
1:M:761:LEU:HB3	1:M:762:PRO:CD	2.51	0.40
2:N:535:LEU:O	2:N:539:ILE:HG12	2.21	0.40
3:e:29:LEU:HD23	3:e:29:LEU:HA	1.87	0.40
1:A:705:GLU:OE1	1:A:711:ASN:ND2	2.50	0.40
2:E:554:ASP:HB3	2:E:636:LEU:HD11	2.04	0.40
1:H:708:SER:HB2	1:H:710:GLN:HG3	2.03	0.40
1:L:761:LEU:HB3	1:L:762:PRO:CD	2.52	0.40
1:M:604:MET:HE2	1:M:604:MET:CA	2.46	0.40
1:M:645:GLN:NE2	1:M:731:GLY:HA3	2.37	0.40
2:O:761:LEU:HB3	2:O:762:PRO:CD	2.52	0.40
2:B:761:LEU:HB3	2:B:762:PRO:CD	2.52	0.40
1:F:589:LEU:C	1:F:589:LEU:CD2	2.95	0.40
2:K:642:GLN:HB2	4:K:802:DEX:H212	2.03	0.40
1:M:634:MET:HE1	1:M:647:LEU:HD11	2.03	0.40
1:A:705:GLU:HG2	1:A:711:ASN:HD21	1.85	0.40
1:D:614:LYS:HD2	1:D:614:LYS:HA	1.91	0.40
1:H:711:ASN:N	1:H:711:ASN:ND2	2.69	0.40
2:J:585:ARG:HA	2:J:585:ARG:HD2	1.88	0.40
2:O:530:PRO:HG2	2:O:535:LEU:HD21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:709:SER:OG	2:N:716:TYR:CD1[3_545]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
1	C	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
1	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
1	F	247/248 (100%)	240 (97%)	7 (3%)	0	100	100
1	G	247/248 (100%)	240 (97%)	7 (3%)	0	100	100
1	H	241/248 (97%)	234 (97%)	7 (3%)	0	100	100
1	I	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
1	L	246/248 (99%)	239 (97%)	7 (3%)	0	100	100
1	M	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
1	P	239/248 (96%)	233 (98%)	6 (2%)	0	100	100
2	B	245/248 (99%)	238 (97%)	7 (3%)	0	100	100
2	E	240/248 (97%)	233 (97%)	7 (3%)	0	100	100
2	J	246/248 (99%)	239 (97%)	7 (3%)	0	100	100
2	K	240/248 (97%)	235 (98%)	5 (2%)	0	100	100
2	N	241/248 (97%)	234 (97%)	7 (3%)	0	100	100
2	O	239/248 (96%)	232 (97%)	7 (3%)	0	100	100
3	a	12/15 (80%)	12 (100%)	0	0	100	100
3	b	12/15 (80%)	12 (100%)	0	0	100	100
3	c	12/15 (80%)	12 (100%)	0	0	100	100
3	d	12/15 (80%)	12 (100%)	0	0	100	100
3	e	12/15 (80%)	12 (100%)	0	0	100	100
3	f	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
3	g	11/15 (73%)	11 (100%)	0	0	100	100
3	h	11/15 (73%)	10 (91%)	1 (9%)	0	100	100
3	i	13/15 (87%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	j	12/15 (80%)	12 (100%)	0	0	100	100
3	k	12/15 (80%)	12 (100%)	0	0	100	100
3	l	12/15 (80%)	12 (100%)	0	0	100	100
3	m	12/15 (80%)	12 (100%)	0	0	100	100
3	n	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
3	o	12/15 (80%)	12 (100%)	0	0	100	100
3	p	12/15 (80%)	12 (100%)	0	0	100	100
All	All	4092/4208 (97%)	3972 (97%)	120 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/227 (100%)	217 (96%)	10 (4%)	25	56
1	C	227/227 (100%)	213 (94%)	14 (6%)	16	42
1	D	227/227 (100%)	216 (95%)	11 (5%)	23	53
1	F	228/227 (100%)	218 (96%)	10 (4%)	25	56
1	G	228/227 (100%)	220 (96%)	8 (4%)	32	64
1	H	225/227 (99%)	209 (93%)	16 (7%)	13	36
1	I	227/227 (100%)	216 (95%)	11 (5%)	23	53
1	L	227/227 (100%)	215 (95%)	12 (5%)	20	49
1	M	227/227 (100%)	220 (97%)	7 (3%)	35	68
1	P	223/227 (98%)	212 (95%)	11 (5%)	22	52
2	B	226/226 (100%)	215 (95%)	11 (5%)	22	52
2	E	224/226 (99%)	210 (94%)	14 (6%)	16	41
2	J	227/226 (100%)	217 (96%)	10 (4%)	25	56
2	K	224/226 (99%)	215 (96%)	9 (4%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	225/226 (100%)	210 (93%)	15 (7%)	15 39
2	O	223/226 (99%)	207 (93%)	16 (7%)	13 35
3	a	12/12 (100%)	11 (92%)	1 (8%)	10 29
3	b	12/12 (100%)	12 (100%)	0	100 100
3	c	12/12 (100%)	12 (100%)	0	100 100
3	d	12/12 (100%)	11 (92%)	1 (8%)	10 29
3	e	12/12 (100%)	12 (100%)	0	100 100
3	f	11/12 (92%)	10 (91%)	1 (9%)	9 25
3	g	11/12 (92%)	11 (100%)	0	100 100
3	h	11/12 (92%)	10 (91%)	1 (9%)	9 25
3	i	12/12 (100%)	11 (92%)	1 (8%)	10 29
3	j	12/12 (100%)	12 (100%)	0	100 100
3	k	12/12 (100%)	12 (100%)	0	100 100
3	l	12/12 (100%)	11 (92%)	1 (8%)	10 29
3	m	12/12 (100%)	11 (92%)	1 (8%)	10 29
3	n	12/12 (100%)	12 (100%)	0	100 100
3	o	12/12 (100%)	12 (100%)	0	100 100
3	p	12/12 (100%)	12 (100%)	0	100 100
All	All	3804/3818 (100%)	3612 (95%)	192 (5%)	22 51

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	VAL
1	A	551	THR
1	A	585	ARG
1	A	644	GLN
1	A	673	SER
1	A	703	LYS
1	A	705	GLU
1	A	743	LYS
1	A	753	LEU
1	A	776	GLN
2	B	538	VAL
2	B	551	THR
2	B	585	ARG

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Mol	Chain	Res	Type
2	B	614	LYS
2	B	644	GLN
2	B	648	LYS
2	B	691	MET
2	B	703	LYS
2	B	733	LEU
2	B	734	GLN
2	B	743	LYS
1	C	538	VAL
1	C	585	ARG
1	C	644	GLN
1	C	645	GLN
1	C	646	MET
1	C	648	LYS
1	C	705	GLU
1	C	708	SER
1	C	710	GLN
1	C	733	LEU
1	C	734	GLN
1	C	741	VAL
1	C	745	LEU
1	C	764	PHE
1	D	538	VAL
1	D	551	THR
1	D	585	ARG
1	D	614	LYS
1	D	631	GLU
1	D	644	GLN
1	D	703	LYS
1	D	705	GLU
1	D	733	LEU
1	D	734	GLN
1	D	776	GLN
2	E	538	VAL
2	E	543[A]	VAL
2	E	543[B]	VAL
2	E	551	THR
2	E	558	ARG
2	E	585	ARG
2	E	644	GLN
2	E	705	GLU
2	E	711	ASN

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Mol	Chain	Res	Type
2	E	733	LEU
2	E	734	GLN
2	E	743	LYS
2	E	745	LEU
2	E	753	LEU
1	F	538	VAL
1	F	585	ARG
1	F	614	LYS
1	F	644	GLN
1	F	673	SER
1	F	703	LYS
1	F	705	GLU
1	F	716	TYR
1	F	733	LEU
1	F	743	LYS
1	G	529	PHE
1	G	535	LEU
1	G	538	VAL
1	G	551	THR
1	G	641	ASP
1	G	644	GLN
1	G	733	LEU
1	G	743	LYS
1	H	538	VAL
1	H	550	SER
1	H	551	THR
1	H	565	ARG
1	H	614	LYS
1	H	644	GLN
1	H	648	LYS
1	H	676	PRO
1	H	677	LYS
1	H	695	LYS
1	H	704	ARG
1	H	711	ASN
1	H	733	LEU
1	H	734	GLN
1	H	753	LEU
1	H	772	LEU
1	I	535	LEU
1	I	538	VAL
1	I	551	THR

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Mol	Chain	Res	Type
1	I	614	LYS
1	I	615	GLN
1	I	644	GLN
1	I	691	MET
1	I	733	LEU
1	I	734	GLN
1	I	743	LYS
1	I	776	GLN
2	J	538	VAL
2	J	557	THR
2	J	585	ARG
2	J	614	LYS
2	J	641	ASP
2	J	644	GLN
2	J	691	MET
2	J	705	GLU
2	J	733	LEU
2	J	734	GLN
2	K	538	VAL
2	K	551	THR
2	K	559	LEU
2	K	644	GLN
2	K	703	LYS
2	K	710	GLN
2	K	733	LEU
2	K	743	LYS
2	K	753	LEU
1	L	538	VAL
1	L	550	SER
1	L	551	THR
1	L	585	ARG
1	L	614	LYS
1	L	644	GLN
1	L	648	LYS
1	L	733	LEU
1	L	742	ASN
1	L	743	LYS
1	L	765	LYS
1	L	776	GLN
1	M	538	VAL
1	M	542	GLU
1	M	548	TYR

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Mol	Chain	Res	Type
1	M	644	GLN
1	M	708	SER
1	M	733	LEU
1	M	743	LYS
2	N	538	VAL
2	N	551	THR
2	N	559	LEU
2	N	585	ARG
2	N	614	LYS
2	N	644	GLN
2	N	647	LEU
2	N	681	LYS
2	N	705	GLU
2	N	709	SER
2	N	733	LEU
2	N	734	GLN
2	N	743	LYS
2	N	765	LYS
2	N	776	GLN
2	O	529	PHE
2	O	538	VAL
2	O	550	SER
2	O	551	THR
2	O	554	ASP
2	O	558	ARG
2	O	585	ARG
2	O	614	LYS
2	O	631	GLU
2	O	644	GLN
2	O	688	GLU
2	O	704	ARG
2	O	733	LEU
2	O	734	GLN
2	O	753	LEU
2	O	776	GLN
1	P	535	LEU
1	P	538	VAL
1	P	550	SER
1	P	585	ARG
1	P	614	LYS
1	P	644	GLN
1	P	648	LYS

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Mol	Chain	Res	Type
1	P	720	LYS
1	P	733	LEU
1	P	745	LEU
1	P	752	MET
3	a	17	ARG
3	d	21	LEU
3	f	26	SER
3	h	17	ARG
3	i	29	LEU
3	l	29	LEU
3	m	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	GLN
1	A	615	GLN
1	A	619	ASN
1	A	711	ASN
2	B	615	GLN
2	B	726	HIS
1	C	615	GLN
1	C	644	GLN
1	C	711	ASN
1	C	726	HIS
1	D	615	GLN
1	D	645	GLN
1	D	742	ASN
2	E	615	GLN
2	E	635	GLN
2	E	726	HIS
1	F	597	GLN
1	F	615	GLN
1	F	644	GLN
1	F	775	HIS
1	G	615	GLN
1	G	619	ASN
1	H	615	GLN
1	I	597	GLN
1	I	619	ASN
1	I	645	GLN
2	J	597	GLN

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Mol	Chain	Res	Type
2	J	615	GLN
2	J	619	ASN
2	J	645	GLN
2	J	711	ASN
2	K	615	GLN
2	K	726	HIS
2	K	742	ASN
1	L	570	GLN
1	L	597	GLN
1	M	615	GLN
1	M	619	ASN
1	M	645	GLN
1	M	776	GLN
2	N	644	GLN
2	O	597	GLN
2	O	711	ASN
2	O	726	HIS
1	P	615	GLN
1	P	711	ASN
1	P	726	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CSO	O	622[B]	-	3,6,7	0.55	0	1,6,8	1.41	0
2	CSO	J	622	2	3,6,7	0.90	0	1,6,8	1.51	0
2	CSO	K	622[B]	-	3,6,7	0.59	0	1,6,8	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CSO	N	622[A]	-	3,6,7	0.55	0	1,6,8	1.58	0
2	CSO	N	622[B]	-	3,6,7	0.55	0	1,6,8	1.58	0
2	CSO	E	622[A]	-	3,6,7	0.47	0	1,6,8	1.39	0
2	CSO	B	622[A]	-	3,6,7	0.70	0	1,6,8	1.49	0
2	CSO	B	622[B]	-	3,6,7	0.70	0	1,6,8	1.49	0
2	CSO	E	622[B]	-	3,6,7	0.47	0	1,6,8	1.39	0
2	CSO	O	622[A]	-	3,6,7	0.55	0	1,6,8	1.41	0
2	CSO	K	622[A]	-	3,6,7	0.59	0	1,6,8	1.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	O	622[B]	-	-	1/1/5/7	-
2	CSO	J	622	2	-	1/1/5/7	-
2	CSO	K	622[B]	-	-	1/1/5/7	-
2	CSO	N	622[A]	-	-	1/1/5/7	-
2	CSO	N	622[B]	-	-	0/1/5/7	-
2	CSO	E	622[A]	-	-	1/1/5/7	-
2	CSO	B	622[A]	-	-	1/1/5/7	-
2	CSO	B	622[B]	-	-	1/1/5/7	-
2	CSO	E	622[B]	-	-	0/1/5/7	-
2	CSO	O	622[A]	-	-	0/1/5/7	-
2	CSO	K	622[A]	-	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	622[B]	CSO	N-CA-CB-SG
2	E	622[A]	CSO	N-CA-CB-SG
2	K	622[B]	CSO	N-CA-CB-SG
2	O	622[B]	CSO	N-CA-CB-SG
2	B	622[A]	CSO	N-CA-CB-SG
2	J	622	CSO	N-CA-CB-SG
2	K	622[A]	CSO	N-CA-CB-SG
2	N	622[A]	CSO	N-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	622[B]	CSO	1	0
2	N	622[A]	CSO	1	0
2	E	622[A]	CSO	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 91 ligands modelled in this entry, 11 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EPE	A	1003	-	15,15,15	0.66	1 (6%)	19,20,20	0.79	1 (5%)
6	EPE	D	804	-	15,15,15	0.66	1 (6%)	19,20,20	0.89	1 (5%)
11	IMD	M	806	-	5,5,5	0.28	0	5,5,5	0.63	0
4	DEX	N	1001	-	31,31,31	0.40	0	53,53,53	1.11	2 (3%)
11	IMD	J	808	-	5,5,5	0.28	0	5,5,5	0.53	0
11	IMD	B	806	-	5,5,5	0.22	0	5,5,5	0.53	0
7	GOL	E	1004	-	5,5,5	0.21	0	5,5,5	0.61	0
4	DEX	M	802	-	31,31,31	0.42	0	53,53,53	1.11	5 (9%)
4	DEX	K	802	-	31,31,31	0.45	0	53,53,53	1.28	8 (15%)
6	EPE	I	1004	-	15,15,15	0.84	1 (6%)	19,20,20	1.05	1 (5%)
7	GOL	N	1002	-	5,5,5	0.14	0	5,5,5	0.31	0
5	CAC	I	1002	-	2,4,4	3.17	2 (100%)	4,6,6	3.38	2 (50%)
4	DEX	P	1001	-	31,31,31	0.55	0	53,53,53	1.12	6 (11%)
4	DEX	A	1001	-	31,31,31	0.46	0	53,53,53	0.97	2 (3%)
4	DEX	J	802	-	31,31,31	0.44	0	53,53,53	1.10	4 (7%)
4	DEX	B	802	-	31,31,31	0.59	0	53,53,53	1.30	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	J	806	-	5,5,5	0.22	0	5,5,5	0.72	0
5	CAC	E	1002	-	2,4,4	3.87	2 (100%)	4,6,6	3.52	3 (75%)
5	CAC	D	801	-	2,4,4	3.48	2 (100%)	4,6,6	5.02	3 (75%)
11	IMD	B	807	-	5,5,5	0.25	0	5,5,5	0.57	0
7	GOL	L	1004	-	5,5,5	0.18	0	5,5,5	0.67	0
6	EPE	L	1003	-	15,15,15	0.88	1 (6%)	19,20,20	0.79	0
7	GOL	O	1003	-	5,5,5	0.08	0	5,5,5	0.42	0
12	PEG	K	801	-	6,6,6	0.57	0	5,5,5	0.60	0
11	IMD	d	101	-	5,5,5	0.22	0	5,5,5	0.47	0
8	SO4	B	808	-	4,4,4	0.33	0	6,6,6	0.09	0
11	IMD	C	1004	-	5,5,5	0.28	0	5,5,5	0.52	0
11	IMD	N	1003	-	5,5,5	0.23	0	5,5,5	0.56	0
7	GOL	C	1003	-	5,5,5	0.23	0	5,5,5	0.75	0
7	GOL	E	1003	-	5,5,5	0.14	0	5,5,5	0.42	0
10	PG4	L	1002	-	12,12,12	0.29	0	11,11,11	0.23	0
10	PG4	B	803	-	12,12,12	0.46	0	11,11,11	0.32	0
5	CAC	A	1002	-	2,4,4	3.47	2 (100%)	4,6,6	5.97	2 (50%)
8	SO4	J	801	-	4,4,4	0.30	0	6,6,6	0.10	0
5	CAC	K	803	-	2,4,4	3.79	2 (100%)	4,6,6	5.50	3 (75%)
7	GOL	J	804	-	5,5,5	0.21	0	5,5,5	0.55	0
4	DEX	I	1001	-	31,31,31	0.45	0	53,53,53	1.27	5 (9%)
7	GOL	K	804	-	5,5,5	0.13	0	5,5,5	0.40	0
11	IMD	L	1007	-	5,5,5	0.32	0	5,5,5	0.59	0
12	PEG	I	1003	-	6,6,6	0.39	0	5,5,5	0.30	0
11	IMD	L	1006	-	5,5,5	0.27	0	5,5,5	0.51	0
10	PG4	D	803	-	12,12,12	0.41	0	11,11,11	0.27	0
4	DEX	F	1001	-	31,31,31	0.45	0	53,53,53	0.79	0
7	GOL	A	1005	-	5,5,5	0.20	0	5,5,5	0.56	0
7	GOL	P	1003	-	5,5,5	0.10	0	5,5,5	0.37	0
12	PEG	M	805	-	6,6,6	0.29	0	5,5,5	0.23	0
12	PEG	F	1002	-	6,6,6	0.35	0	5,5,5	0.26	0
7	GOL	A	1004	-	5,5,5	0.11	0	5,5,5	0.43	0
5	CAC	M	803	-	2,4,4	2.92	2 (100%)	4,6,6	7.86	2 (50%)
6	EPE	B	804	-	15,15,15	0.73	1 (6%)	19,20,20	0.70	0
5	CAC	H	801	-	2,4,4	3.20	2 (100%)	4,6,6	5.33	3 (75%)
10	PG4	H	803	-	12,12,12	0.34	0	11,11,11	0.19	0
11	IMD	b	101	-	5,5,5	0.28	0	5,5,5	0.54	0
7	GOL	J	805	-	5,5,5	0.14	0	5,5,5	0.36	0
5	CAC	O	1002	-	2,4,4	3.22	2 (100%)	4,6,6	8.97	2 (50%)
11	IMD	E	1006	-	5,5,5	0.31	0	5,5,5	0.54	0
8	SO4	C	1005	-	4,4,4	0.32	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	C	1006	-	4,4,4	0.38	0	6,6,6	0.05	0
4	DEX	L	1001	-	31,31,31	0.49	0	53,53,53	1.06	3 (5%)
6	EPE	J	803	-	15,15,15	0.64	1 (6%)	19,20,20	0.65	0
8	SO4	A	1006	-	4,4,4	0.31	0	6,6,6	0.07	0
4	DEX	O	1001	-	31,31,31	0.61	0	53,53,53	1.18	5 (9%)
7	GOL	L	1005	-	5,5,5	0.11	0	5,5,5	0.37	0
11	IMD	F	1003	-	5,5,5	0.31	0	5,5,5	0.59	0
4	DEX	D	802	-	31,31,31	0.49	0	53,53,53	1.33	8 (15%)
4	DEX	H	802	-	31,31,31	0.46	0	53,53,53	0.98	1 (1%)
11	IMD	I	1006	-	5,5,5	0.25	0	5,5,5	0.58	0
11	IMD	O	1004	-	5,5,5	0.35	0	5,5,5	0.73	0
7	GOL	C	1002	-	5,5,5	0.33	0	5,5,5	1.16	0
4	DEX	C	1001	-	31,31,31	0.67	0	53,53,53	1.08	5 (9%)
7	GOL	I	1005	-	5,5,5	0.18	0	5,5,5	0.53	0
7	GOL	E	1005	-	5,5,5	0.16	0	5,5,5	0.54	0
13	PGE	M	804	-	9,9,9	0.17	0	8,8,8	0.15	0
7	GOL	K	805	-	5,5,5	0.10	0	5,5,5	0.35	0
7	GOL	B	805	-	5,5,5	0.19	0	5,5,5	0.54	0
4	DEX	E	1001	-	31,31,31	0.67	1 (3%)	53,53,53	0.93	3 (5%)
11	IMD	J	807	-	5,5,5	0.33	0	5,5,5	0.64	0
4	DEX	G	1001	-	31,31,31	0.62	1 (3%)	53,53,53	1.01	3 (5%)
6	EPE	P	1002	-	15,15,15	0.69	1 (6%)	19,20,20	0.68	0
7	GOL	M	801	-	5,5,5	0.09	0	5,5,5	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DEX	F	1001	-	-	0/8/84/84	0/4/4/4
7	GOL	A	1005	-	-	2/4/4/4	-
12	PEG	K	801	-	-	1/4/4/4	-
4	DEX	H	802	-	-	2/8/84/84	0/4/4/4
11	IMD	d	101	-	-	-	0/1/1/1
11	IMD	I	1006	-	-	-	0/1/1/1
6	EPE	A	1003	-	-	3/9/19/19	0/1/1/1
7	GOL	P	1003	-	-	2/4/4/4	-
12	PEG	M	805	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEG	F	1002	-	-	1/4/4/4	-
6	EPE	D	804	-	-	2/9/19/19	0/1/1/1
7	GOL	A	1004	-	-	4/4/4/4	-
11	IMD	M	806	-	-	-	0/1/1/1
4	DEX	N	1001	-	-	2/8/84/84	0/4/4/4
11	IMD	C	1004	-	-	-	0/1/1/1
11	IMD	N	1003	-	-	-	0/1/1/1
11	IMD	J	808	-	-	-	0/1/1/1
7	GOL	C	1003	-	-	4/4/4/4	-
11	IMD	B	806	-	-	-	0/1/1/1
11	IMD	O	1004	-	-	-	0/1/1/1
6	EPE	B	804	-	-	5/9/19/19	0/1/1/1
7	GOL	E	1004	-	-	0/4/4/4	-
4	DEX	M	802	-	-	2/8/84/84	0/4/4/4
7	GOL	C	1002	-	-	2/4/4/4	-
4	DEX	K	802	-	-	2/8/84/84	0/4/4/4
7	GOL	E	1003	-	-	2/4/4/4	-
10	PG4	H	803	-	-	5/10/10/10	-
4	DEX	C	1001	-	-	2/8/84/84	0/4/4/4
7	GOL	I	1005	-	-	2/4/4/4	-
10	PG4	L	1002	-	-	4/10/10/10	-
11	IMD	b	101	-	-	-	0/1/1/1
6	EPE	I	1004	-	-	6/9/19/19	0/1/1/1
10	PG4	B	803	-	-	8/10/10/10	-
7	GOL	J	805	-	-	2/4/4/4	-
7	GOL	N	1002	-	-	1/4/4/4	-
7	GOL	E	1005	-	-	2/4/4/4	-
4	DEX	P	1001	-	-	0/8/84/84	0/4/4/4
4	DEX	A	1001	-	-	2/8/84/84	0/4/4/4
13	PGE	M	804	-	-	3/7/7/7	-
11	IMD	E	1006	-	-	-	0/1/1/1
7	GOL	K	805	-	-	2/4/4/4	-
7	GOL	B	805	-	-	2/4/4/4	-
7	GOL	J	804	-	-	4/4/4/4	-
4	DEX	I	1001	-	-	2/8/84/84	0/4/4/4
4	DEX	J	802	-	-	0/8/84/84	0/4/4/4
4	DEX	B	802	-	-	0/8/84/84	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DEX	L	1001	-	-	2/8/84/84	0/4/4/4
7	GOL	J	806	-	-	0/4/4/4	-
4	DEX	E	1001	-	-	2/8/84/84	0/4/4/4
6	EPE	J	803	-	-	2/9/19/19	0/1/1/1
11	IMD	J	807	-	-	-	0/1/1/1
4	DEX	G	1001	-	-	0/8/84/84	0/4/4/4
7	GOL	K	804	-	-	2/4/4/4	-
11	IMD	L	1007	-	-	-	0/1/1/1
4	DEX	O	1001	-	-	0/8/84/84	0/4/4/4
6	EPE	P	1002	-	-	4/9/19/19	0/1/1/1
11	IMD	B	807	-	-	-	0/1/1/1
7	GOL	L	1004	-	-	2/4/4/4	-
7	GOL	L	1005	-	-	0/4/4/4	-
12	PEG	I	1003	-	-	2/4/4/4	-
11	IMD	F	1003	-	-	-	0/1/1/1
11	IMD	L	1006	-	-	-	0/1/1/1
10	PG4	D	803	-	-	7/10/10/10	-
7	GOL	M	801	-	-	1/4/4/4	-
6	EPE	L	1003	-	-	8/9/19/19	0/1/1/1
7	GOL	O	1003	-	-	0/4/4/4	-
4	DEX	D	802	-	-	2/8/84/84	0/4/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1002	CAC	AS-C1	4.42	2.00	1.90
5	A	1002	CAC	AS-C1	4.06	1.99	1.90
5	K	803	CAC	AS-C1	4.00	1.99	1.90
5	D	801	CAC	AS-C1	3.69	1.99	1.90
5	K	803	CAC	AS-C2	3.56	1.98	1.90
5	H	801	CAC	AS-C1	3.53	1.98	1.90
5	O	1002	CAC	AS-C1	3.36	1.98	1.90
5	I	1002	CAC	AS-C1	3.28	1.98	1.90
5	D	801	CAC	AS-C2	3.26	1.98	1.90
5	E	1002	CAC	AS-C2	3.23	1.97	1.90
5	O	1002	CAC	AS-C2	3.07	1.97	1.90
5	I	1002	CAC	AS-C2	3.06	1.97	1.90
5	M	803	CAC	AS-C2	2.94	1.97	1.90
5	M	803	CAC	AS-C1	2.89	1.97	1.90
5	H	801	CAC	AS-C2	2.83	1.97	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	CAC	AS-C2	2.77	1.96	1.90
6	I	1004	EPE	O3S-S	2.32	1.55	1.47
6	P	1002	EPE	O3S-S	2.29	1.55	1.47
6	L	1003	EPE	O3S-S	2.27	1.55	1.47
6	B	804	EPE	O3S-S	2.27	1.55	1.47
6	D	804	EPE	O3S-S	2.24	1.55	1.47
6	J	803	EPE	O3S-S	2.21	1.55	1.47
6	A	1003	EPE	O3S-S	2.16	1.55	1.47
4	G	1001	DEX	C10-C9	-2.06	1.55	1.57
4	E	1001	DEX	C10-C9	-2.03	1.55	1.57

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	1002	CAC	O1-AS-C1	-12.95	95.40	111.50
5	O	1002	CAC	O1-AS-C2	12.26	126.75	111.50
5	M	803	CAC	O1-AS-C2	11.58	125.90	111.50
5	M	803	CAC	O1-AS-C1	-10.36	98.62	111.50
5	A	1002	CAC	O1-AS-C2	9.72	123.58	111.50
5	D	801	CAC	O2-AS-C1	8.34	126.05	105.84
5	K	803	CAC	O2-AS-C2	7.36	123.67	105.84
5	H	801	CAC	O1-AS-C2	-7.33	102.39	111.50
5	K	803	CAC	O1-AS-C1	-7.09	102.69	111.50
5	A	1002	CAC	O1-AS-C1	-6.80	103.04	111.50
5	H	801	CAC	O2-AS-C2	6.22	120.91	105.84
5	E	1002	CAC	O1-AS-C2	-5.76	104.33	111.50
5	I	1002	CAC	O1-AS-C1	-5.59	104.54	111.50
5	H	801	CAC	O1-AS-C1	-4.41	106.01	111.50
4	B	802	DEX	C6-C5-C10	4.28	118.52	115.70
5	D	801	CAC	O1-AS-C2	-4.28	106.18	111.50
5	K	803	CAC	O1-AS-C2	-3.77	106.81	111.50
4	I	1001	DEX	C9-C8-C14	3.76	112.64	109.34
5	I	1002	CAC	O1-AS-C2	-3.69	106.91	111.50
4	O	1001	DEX	C6-C5-C10	3.64	118.10	115.70
5	D	801	CAC	O1-AS-C1	-3.58	107.05	111.50
4	K	802	DEX	C13-C17-C16	3.55	105.93	102.85
4	D	802	DEX	C6-C5-C10	3.52	118.02	115.70
4	D	802	DEX	C1-C10-C5	-3.27	110.42	112.33
4	B	802	DEX	C13-C17-C20	-3.25	108.62	112.86
4	P	1001	DEX	C13-C17-C16	3.17	105.61	102.85
4	O	1001	DEX	C15-C14-C8	-3.14	116.12	119.08
4	G	1001	DEX	C6-C5-C10	2.95	117.64	115.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1001	DEX	C13-C14-C8	-2.94	111.29	113.76
4	I	1001	DEX	F1-C9-C10	-2.90	101.64	104.16
4	N	1001	DEX	C12-C13-C14	-2.87	105.44	108.03
4	I	1001	DEX	C13-C17-C16	2.86	105.34	102.85
4	N	1001	DEX	C7-C8-C9	-2.86	107.75	110.98
5	E	1002	CAC	O1-AS-C1	-2.83	107.98	111.50
4	H	802	DEX	C13-C17-C16	2.75	105.24	102.85
4	G	1001	DEX	F1-C9-C10	-2.74	101.78	104.16
4	J	802	DEX	C13-C17-C16	2.72	105.22	102.85
4	O	1001	DEX	C13-C17-C16	2.70	105.19	102.85
4	P	1001	DEX	C17-C13-C14	-2.70	96.92	99.35
4	A	1001	DEX	C6-C5-C10	2.65	117.45	115.70
4	M	802	DEX	C13-C17-C16	2.63	105.14	102.85
4	K	802	DEX	C10-C9-C11	2.60	117.34	115.49
6	I	1004	EPE	C10-C9-N1	2.58	122.14	112.36
4	L	1001	DEX	C13-C17-C16	2.58	105.09	102.85
4	I	1001	DEX	C10-C9-C11	2.57	117.31	115.49
4	D	802	DEX	C19-C10-C5	2.56	111.01	107.70
4	D	802	DEX	C13-C17-C16	2.50	105.02	102.85
4	I	1001	DEX	C5-C4-C3	-2.44	120.50	122.72
4	K	802	DEX	F1-C9-C11	-2.44	99.23	102.58
4	B	802	DEX	C21-C20-C17	-2.41	115.60	117.63
4	D	802	DEX	C12-C13-C14	-2.39	105.87	108.03
4	J	802	DEX	C6-C5-C10	2.39	117.28	115.70
4	E	1001	DEX	O2-C11-C9	-2.38	105.59	109.04
4	J	802	DEX	C9-C8-C14	2.36	111.41	109.34
5	E	1002	CAC	O2-AS-C1	-2.36	100.13	105.84
4	P	1001	DEX	C15-C14-C8	-2.34	116.88	119.08
6	A	1003	EPE	O3S-S-C10	-2.34	101.43	106.00
4	B	802	DEX	C15-C14-C13	2.32	106.39	103.98
4	C	1001	DEX	C15-C16-C17	2.32	106.65	105.10
4	D	802	DEX	C2-C3-C4	-2.31	114.78	117.12
4	O	1001	DEX	C13-C17-C20	-2.30	109.86	112.86
4	L	1001	DEX	C6-C5-C10	2.29	117.21	115.70
4	K	802	DEX	C6-C7-C8	2.20	115.98	111.70
4	E	1001	DEX	C15-C14-C8	-2.20	117.01	119.08
4	K	802	DEX	C13-C17-C20	-2.19	110.00	112.86
4	M	802	DEX	C7-C8-C9	-2.19	108.50	110.98
4	O	1001	DEX	C8-C9-C11	2.19	117.15	114.58
4	D	802	DEX	C15-C14-C13	2.18	106.24	103.98
4	G	1001	DEX	C16-C17-C20	2.18	117.85	113.49
4	K	802	DEX	C8-C9-C11	2.17	117.14	114.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	802	DEX	C15-C14-C13	-2.17	101.74	103.98
4	C	1001	DEX	C13-C17-C20	-2.16	110.05	112.86
4	P	1001	DEX	C6-C5-C10	2.15	117.12	115.70
6	D	804	EPE	O2S-S-O1S	2.10	120.65	113.82
4	M	802	DEX	C8-C9-C11	2.09	117.04	114.58
4	B	802	DEX	C1-C10-C5	-2.09	111.11	112.33
4	C	1001	DEX	C12-C13-C17	-2.09	113.81	115.65
4	A	1001	DEX	C13-C17-C20	-2.09	110.14	112.86
4	E	1001	DEX	C13-C12-C11	-2.09	110.21	113.20
4	K	802	DEX	C1-C10-C5	-2.08	111.12	112.33
4	M	802	DEX	C6-C5-C10	2.08	117.07	115.70
4	D	802	DEX	C10-C9-C11	2.05	116.95	115.49
4	C	1001	DEX	O2-C11-C9	-2.05	106.08	109.04
4	K	802	DEX	C2-C3-C4	-2.04	115.05	117.12
4	J	802	DEX	O2-C11-C9	-2.04	106.09	109.04
4	P	1001	DEX	C7-C8-C9	-2.03	108.68	110.98
4	P	1001	DEX	F1-C9-C8	-2.03	104.08	105.96
4	L	1001	DEX	C19-C10-C5	2.01	110.29	107.70

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	DEX	C17-C20-C21-O5
4	A	1001	DEX	O4-C20-C21-O5
4	D	802	DEX	C17-C20-C21-O5
4	D	802	DEX	O4-C20-C21-O5
4	H	802	DEX	C17-C20-C21-O5
4	I	1001	DEX	C17-C20-C21-O5
4	I	1001	DEX	O4-C20-C21-O5
4	K	802	DEX	C17-C20-C21-O5
4	K	802	DEX	O4-C20-C21-O5
4	L	1001	DEX	C17-C20-C21-O5
4	L	1001	DEX	O4-C20-C21-O5
4	M	802	DEX	C17-C20-C21-O5
4	M	802	DEX	O4-C20-C21-O5
6	A	1003	EPE	C8-C7-N4-C5
6	B	804	EPE	C10-C9-N1-C2
6	B	804	EPE	C10-C9-N1-C6
6	B	804	EPE	S-C10-C9-N1
6	I	1004	EPE	C9-C10-S-O1S
6	L	1003	EPE	C10-C9-N1-C6

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Mol	Chain	Res	Type	Atoms
6	P	1002	EPE	C8-C7-N4-C5
7	A	1004	GOL	O1-C1-C2-C3
7	A	1005	GOL	C1-C2-C3-O3
7	B	805	GOL	C1-C2-C3-O3
7	C	1003	GOL	O1-C1-C2-C3
7	E	1003	GOL	O1-C1-C2-C3
7	E	1005	GOL	C1-C2-C3-O3
7	I	1005	GOL	C1-C2-C3-O3
7	J	804	GOL	O1-C1-C2-C3
7	J	804	GOL	C1-C2-C3-O3
7	J	805	GOL	O1-C1-C2-C3
7	K	804	GOL	C1-C2-C3-O3
7	K	805	GOL	C1-C2-C3-O3
7	P	1003	GOL	O1-C1-C2-C3
10	D	803	PG4	O2-C3-C4-O3
10	B	803	PG4	O2-C3-C4-O3
7	K	804	GOL	O2-C2-C3-O3
10	H	803	PG4	O1-C1-C2-O2
12	F	1002	PEG	O1-C1-C2-O2
6	L	1003	EPE	C9-C10-S-O3S
6	D	804	EPE	N4-C7-C8-O8
10	B	803	PG4	O1-C1-C2-O2
10	D	803	PG4	O1-C1-C2-O2
10	L	1002	PG4	O4-C7-C8-O5
7	A	1004	GOL	C1-C2-C3-O3
7	C	1002	GOL	O1-C1-C2-C3
7	C	1003	GOL	C1-C2-C3-O3
10	B	803	PG4	O4-C7-C8-O5
7	A	1004	GOL	O2-C2-C3-O3
7	B	805	GOL	O2-C2-C3-O3
7	C	1002	GOL	O1-C1-C2-O2
7	E	1005	GOL	O2-C2-C3-O3
7	I	1005	GOL	O2-C2-C3-O3
7	J	804	GOL	O2-C2-C3-O3
7	K	805	GOL	O2-C2-C3-O3
7	P	1003	GOL	O1-C1-C2-O2
10	L	1002	PG4	O3-C5-C6-O4
12	M	805	PEG	O1-C1-C2-O2
4	H	802	DEX	O4-C20-C21-O5
6	I	1004	EPE	C9-C10-S-O3S
4	C	1001	DEX	C17-C20-C21-O5
6	A	1003	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
7	A	1005	GOL	O2-C2-C3-O3
7	E	1003	GOL	O1-C1-C2-O2
7	J	805	GOL	O1-C1-C2-O2
7	L	1004	GOL	O2-C2-C3-O3
6	L	1003	EPE	C10-C9-N1-C2
6	P	1002	EPE	C10-C9-N1-C6
10	B	803	PG4	O3-C5-C6-O4
7	C	1003	GOL	O1-C1-C2-O2
7	C	1003	GOL	O2-C2-C3-O3
7	J	804	GOL	O1-C1-C2-O2
7	L	1004	GOL	O1-C1-C2-O2
7	M	801	GOL	O2-C2-C3-O3
10	D	803	PG4	O4-C7-C8-O5
6	I	1004	EPE	N4-C7-C8-O8
6	L	1003	EPE	C8-C7-N4-C3
6	J	803	EPE	N4-C7-C8-O8
7	N	1002	GOL	O1-C1-C2-O2
6	D	804	EPE	C9-C10-S-O2S
6	I	1004	EPE	C9-C10-S-O2S
6	L	1003	EPE	C9-C10-S-O1S
6	L	1003	EPE	C9-C10-S-O2S
10	B	803	PG4	C6-C5-O3-C4
10	D	803	PG4	C8-C7-O4-C6
10	H	803	PG4	C1-C2-O2-C3
10	B	803	PG4	C5-C6-O4-C7
4	N	1001	DEX	C17-C20-C21-O5
6	A	1003	EPE	S-C10-C9-N1
6	J	803	EPE	S-C10-C9-N1
10	L	1002	PG4	C3-C4-O3-C5
10	D	803	PG4	C6-C5-O3-C4
12	I	1003	PEG	C4-C3-O2-C2
10	B	803	PG4	C4-C3-O2-C2
10	H	803	PG4	C8-C7-O4-C6
10	D	803	PG4	C4-C3-O2-C2
7	A	1004	GOL	O1-C1-C2-O2
12	K	801	PEG	O1-C1-C2-O2
6	I	1004	EPE	C8-C7-N4-C3
6	L	1003	EPE	C8-C7-N4-C5
6	P	1002	EPE	C10-C9-N1-C2
13	M	804	PGE	C6-C5-O3-C4
4	C	1001	DEX	O4-C20-C21-O5
4	N	1001	DEX	O4-C20-C21-O5

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Mol	Chain	Res	Type	Atoms
6	L	1003	EPE	N4-C7-C8-O8
6	I	1004	EPE	C8-C7-N4-C5
13	M	804	PGE	C3-C4-O3-C5
12	M	805	PEG	C4-C3-O2-C2
12	I	1003	PEG	C1-C2-O2-C3
10	B	803	PG4	C3-C4-O3-C5
4	E	1001	DEX	C17-C20-C21-O5
10	L	1002	PG4	O2-C3-C4-O3
10	H	803	PG4	O3-C5-C6-O4
4	E	1001	DEX	O4-C20-C21-O5
10	D	803	PG4	O3-C5-C6-O4
13	M	804	PGE	O3-C5-C6-O4
10	H	803	PG4	O2-C3-C4-O3
6	B	804	EPE	C8-C7-N4-C3
6	B	804	EPE	C8-C7-N4-C5
6	P	1002	EPE	C8-C7-N4-C3

There are no ring outliers.

37 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	804	EPE	1	0
4	N	1001	DEX	2	0
4	M	802	DEX	1	0
4	K	802	DEX	2	0
6	I	1004	EPE	2	0
7	N	1002	GOL	1	0
4	A	1001	DEX	1	0
4	J	802	DEX	2	0
4	B	802	DEX	4	0
7	L	1004	GOL	4	0
6	L	1003	EPE	1	0
12	K	801	PEG	1	0
11	d	101	IMD	4	0
11	N	1003	IMD	2	0
7	C	1003	GOL	3	0
4	I	1001	DEX	2	0
11	L	1007	IMD	2	0
10	D	803	PG4	1	0
4	F	1001	DEX	2	0
7	A	1005	GOL	1	0
7	P	1003	GOL	4	0

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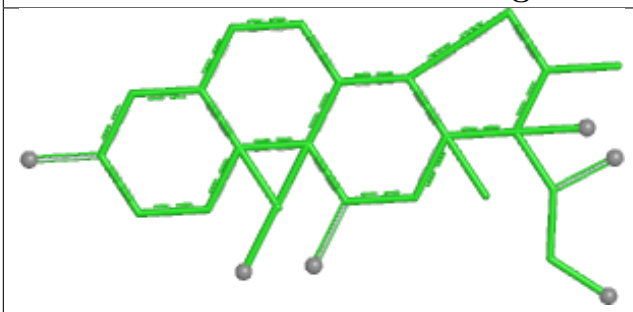
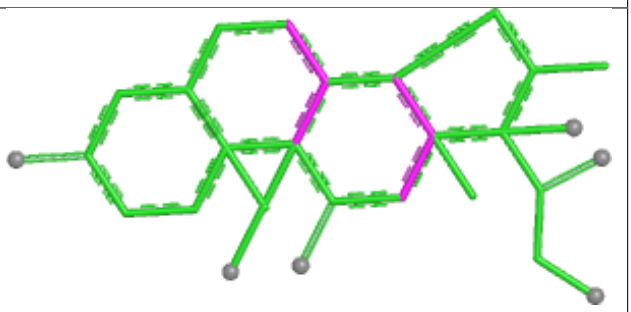
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	804	EPE	1	0
5	H	801	CAC	1	0
10	H	803	PG4	1	0
8	C	1006	SO4	3	0
4	L	1001	DEX	1	0
8	A	1006	SO4	1	0
4	O	1001	DEX	2	0
7	L	1005	GOL	1	0
4	H	802	DEX	1	0
11	O	1004	IMD	1	0
7	C	1002	GOL	5	0
4	C	1001	DEX	3	0
7	I	1005	GOL	1	0
13	M	804	PGE	2	0
4	E	1001	DEX	3	0
6	P	1002	EPE	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

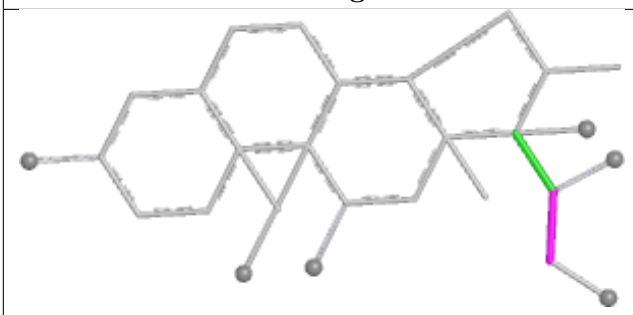
Ligand DEX N 1001



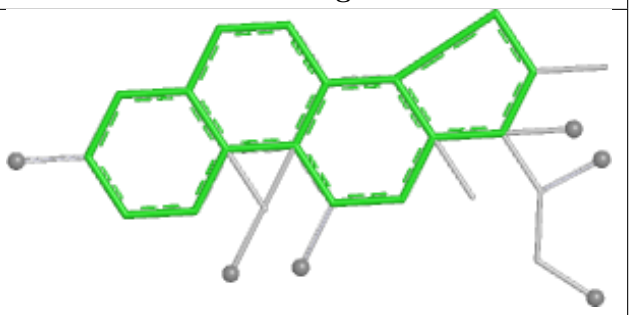
Bond lengths



Bond angles

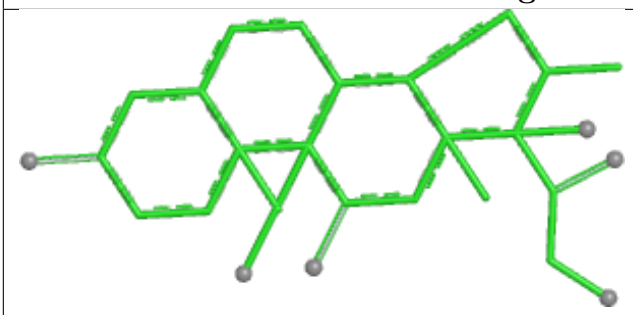


Torsions

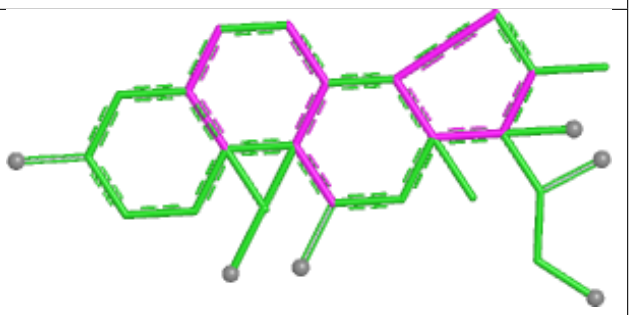


Rings

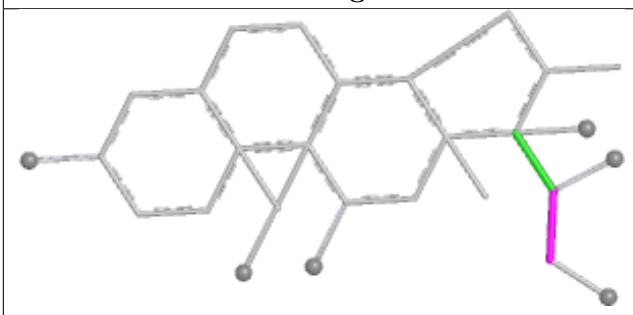
Ligand DEX M 802



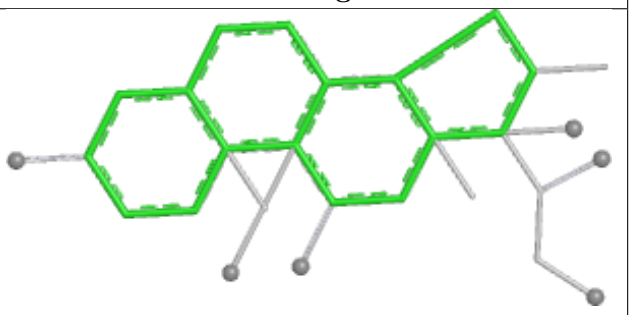
Bond lengths



Bond angles

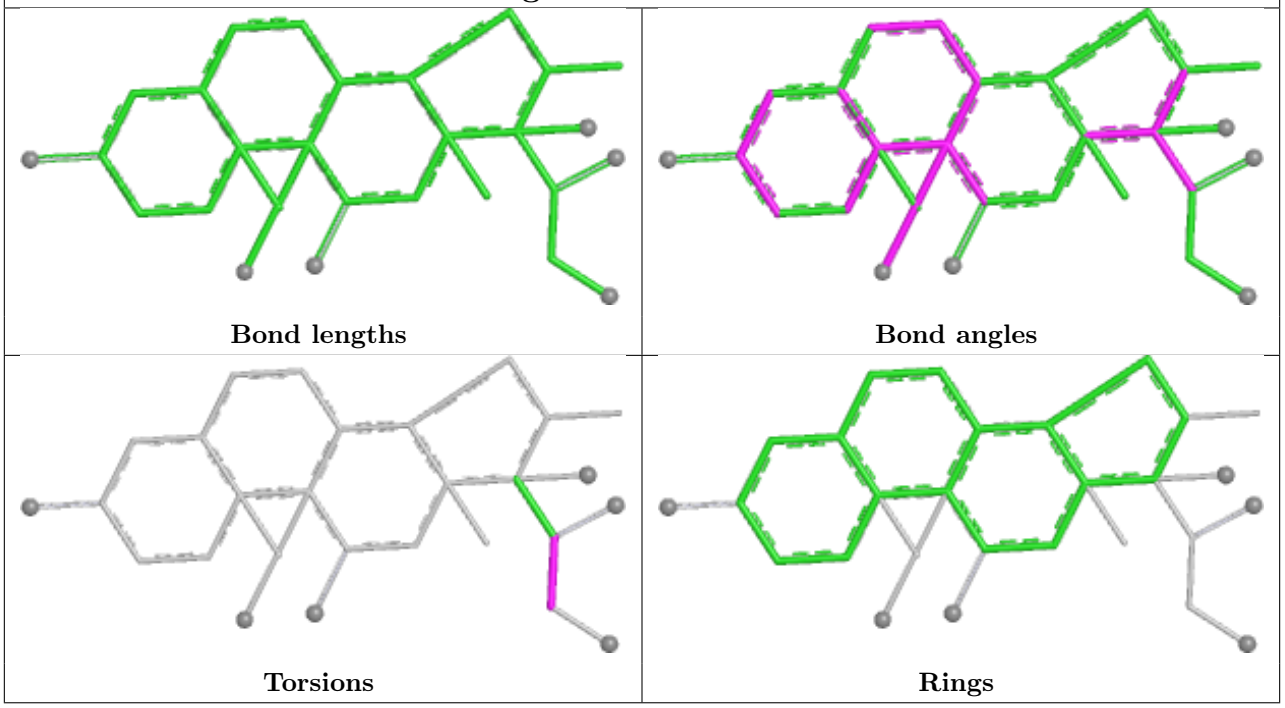


Torsions



Rings

Ligand DEX K 802



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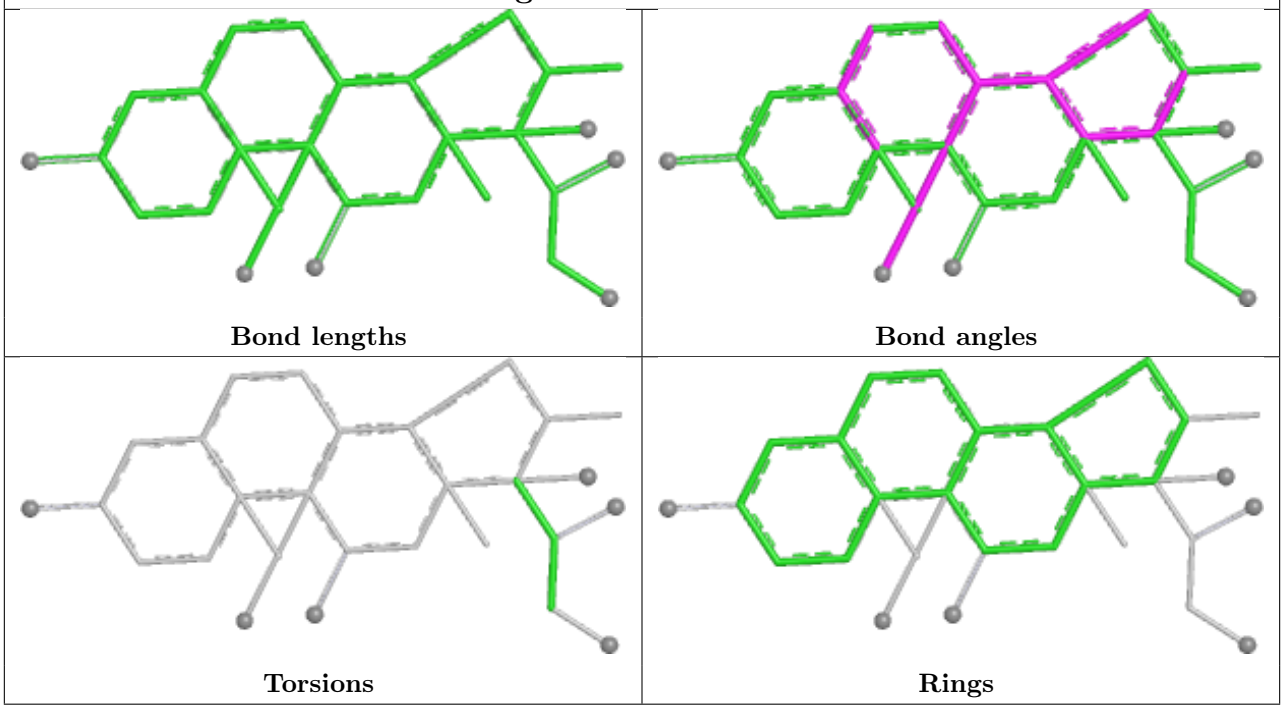
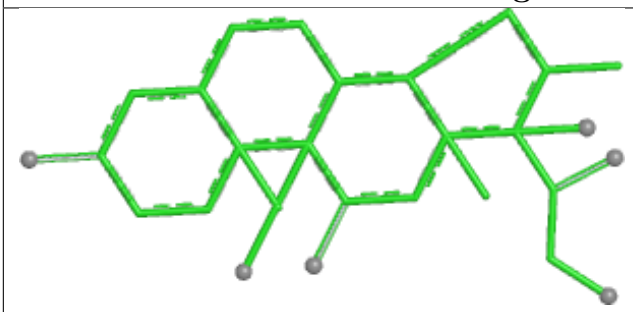
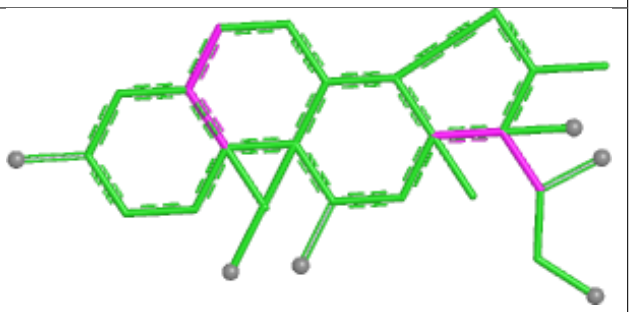


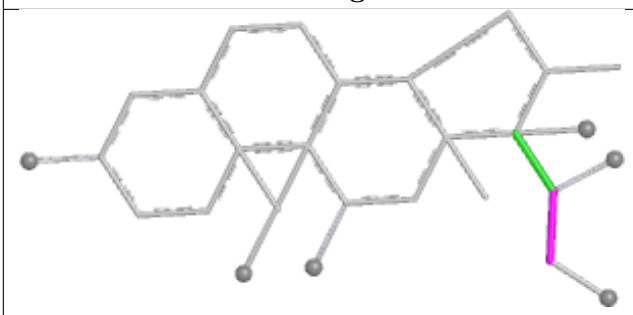
Ligand DEX A 1001



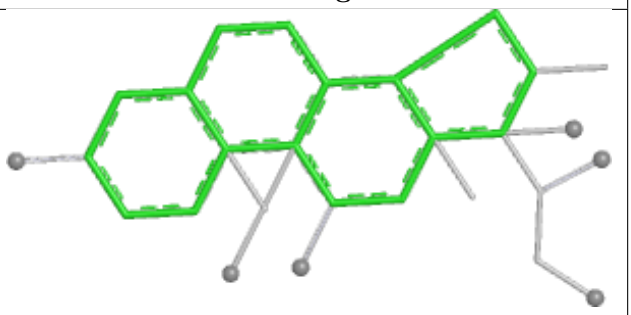
Bond lengths



Bond angles

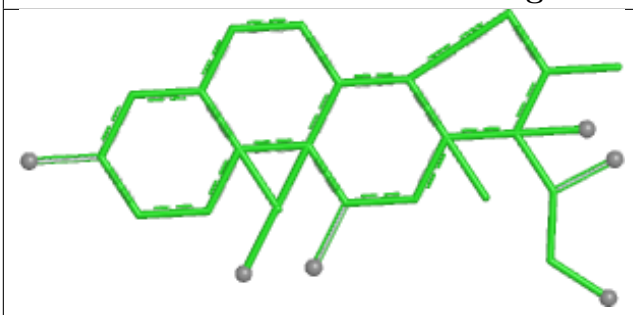


Torsions

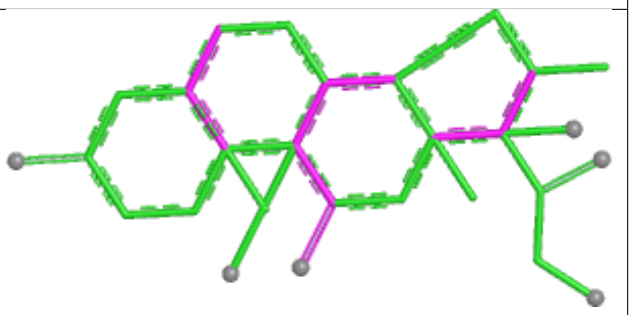


Rings

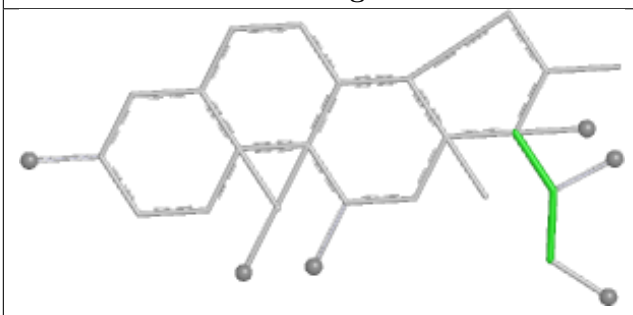
Ligand DEX J 802



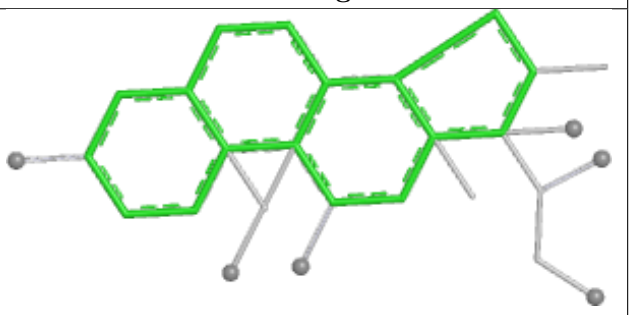
Bond lengths



Bond angles

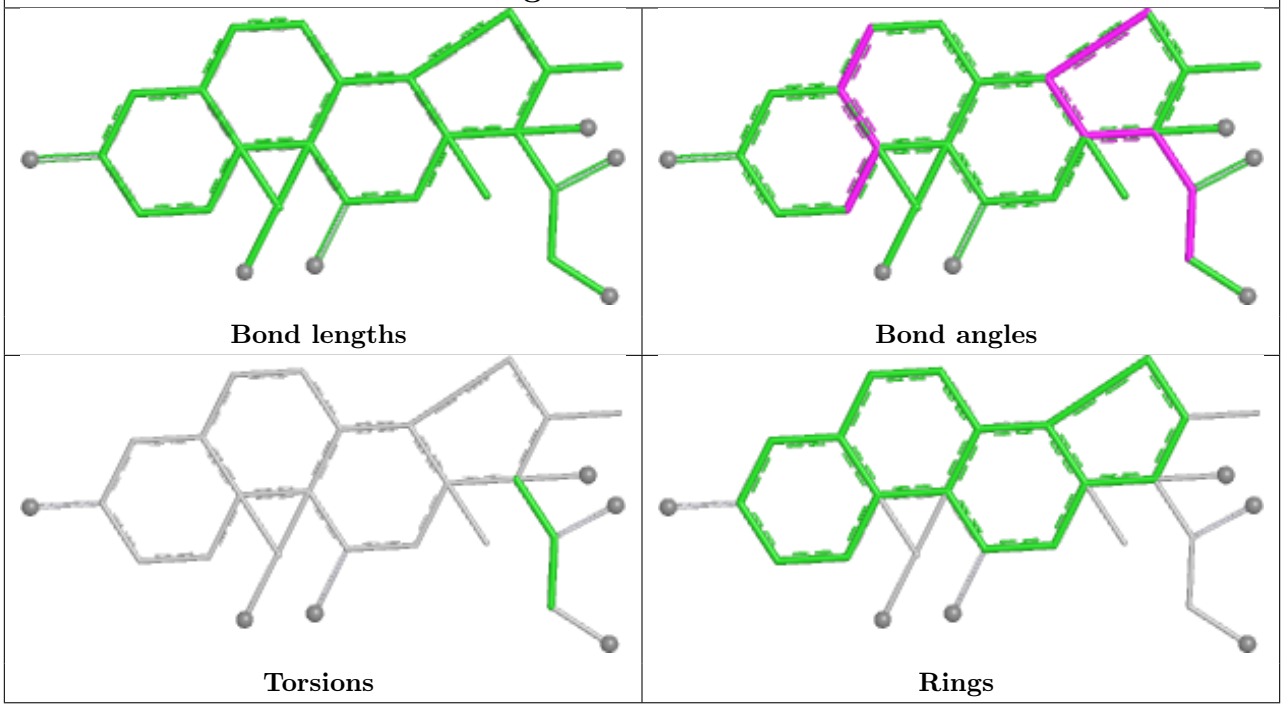


Torsions

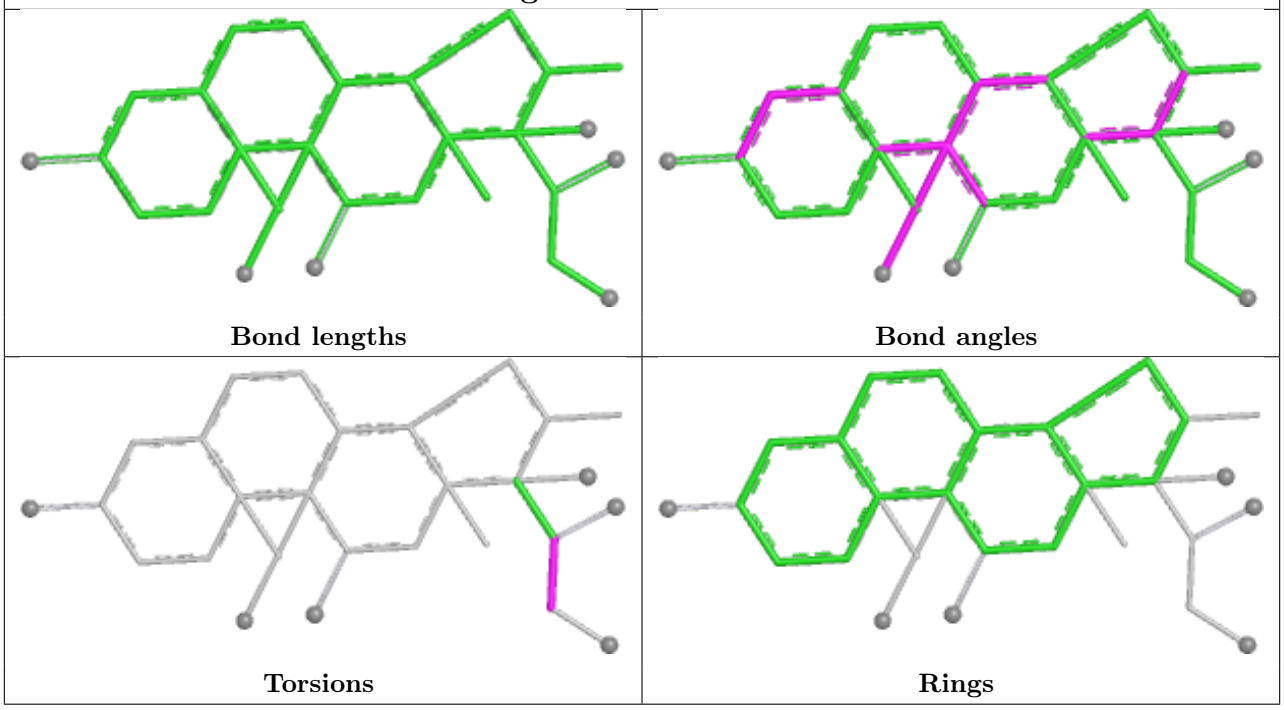


Rings

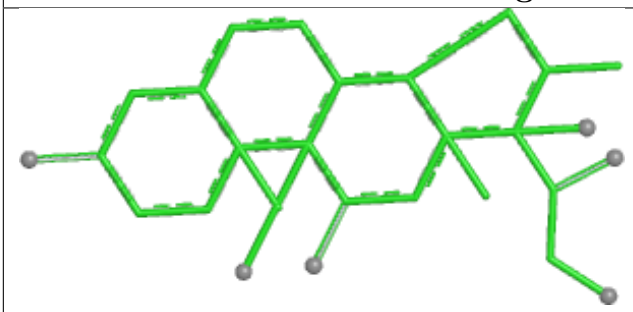
Ligand DEX B 802



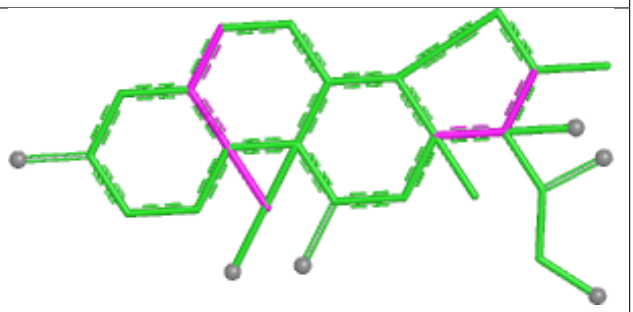
Ligand DEX I 1001



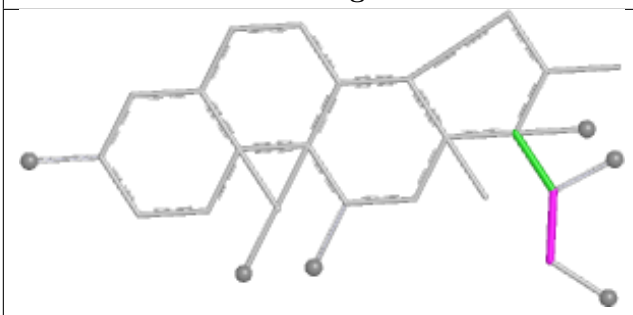
Ligand DEX L 1001



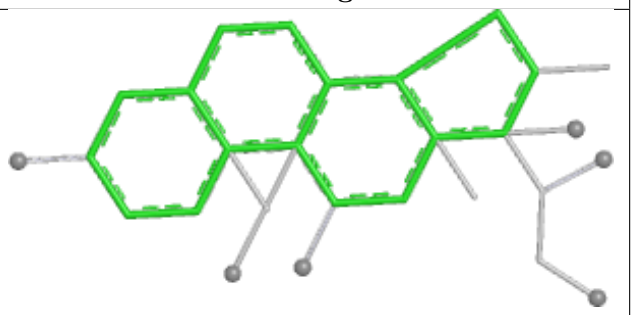
Bond lengths



Bond angles

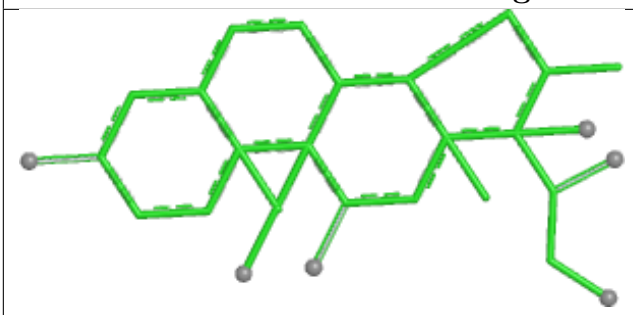


Torsions

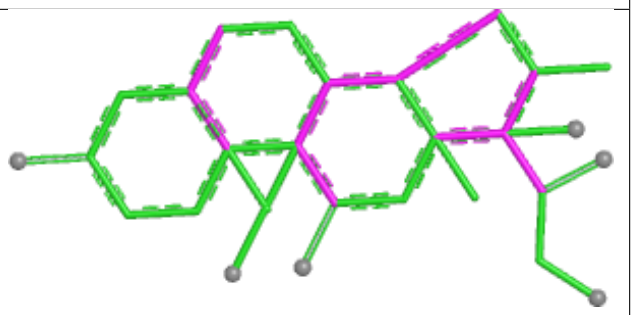


Rings

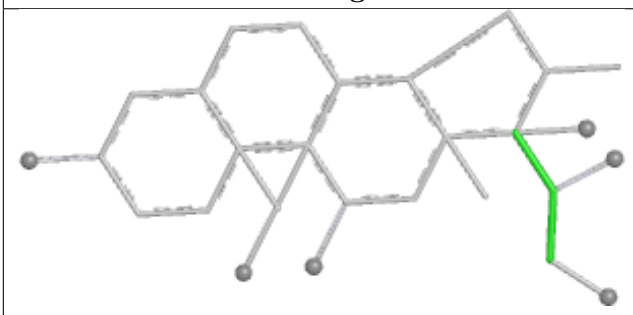
Ligand DEX O 1001



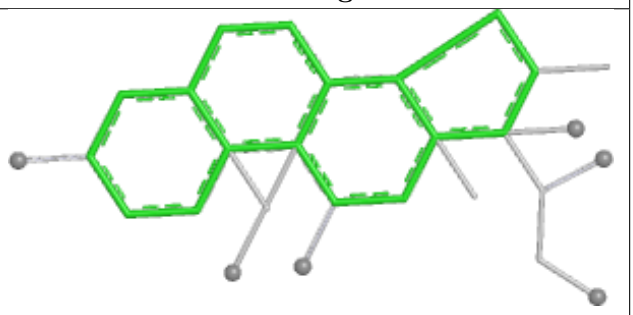
Bond lengths



Bond angles

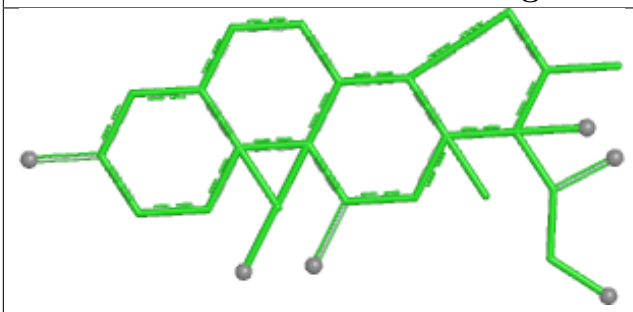


Torsions

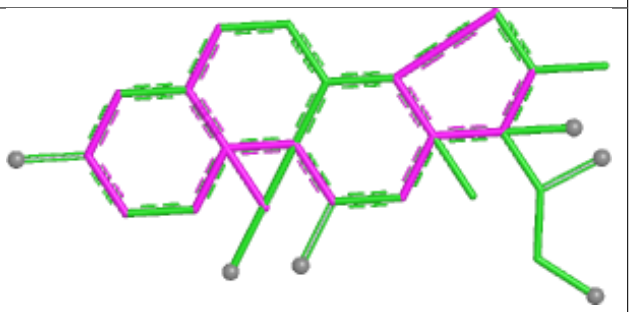


Rings

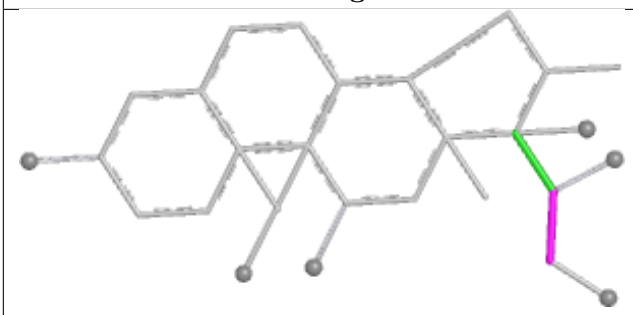
Ligand DEX D 802



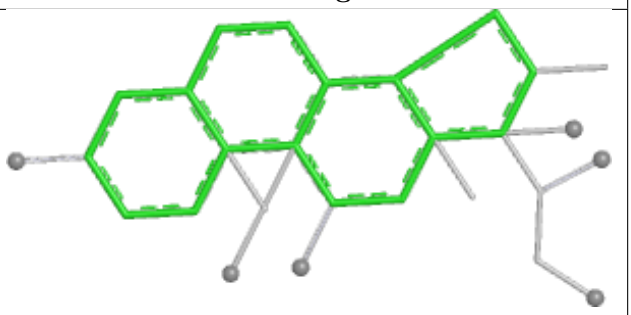
Bond lengths



Bond angles

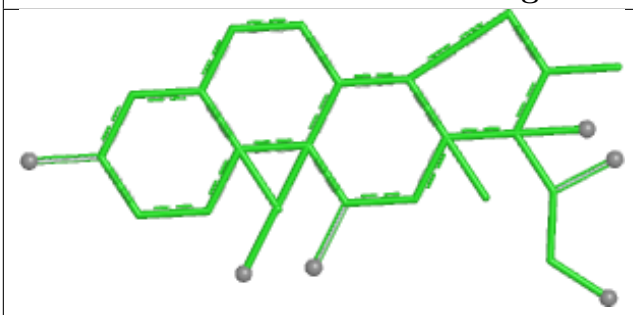


Torsions

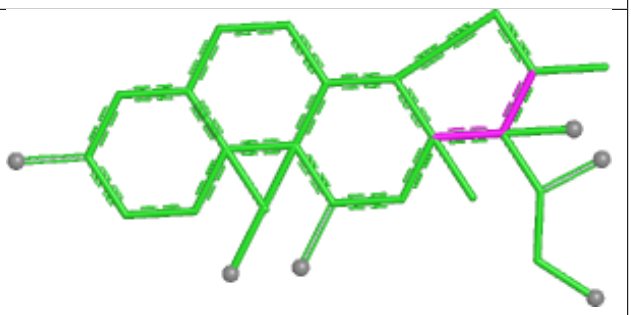


Rings

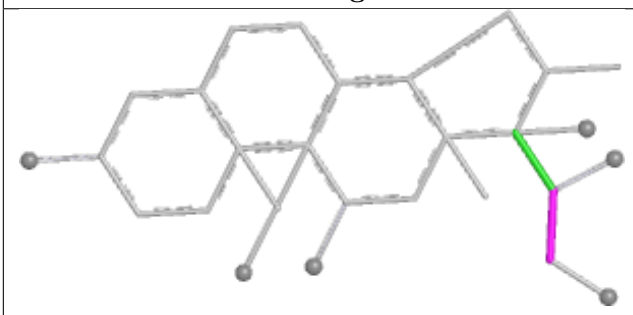
Ligand DEX H 802



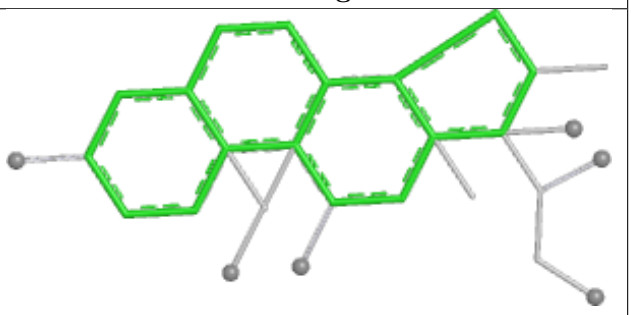
Bond lengths



Bond angles

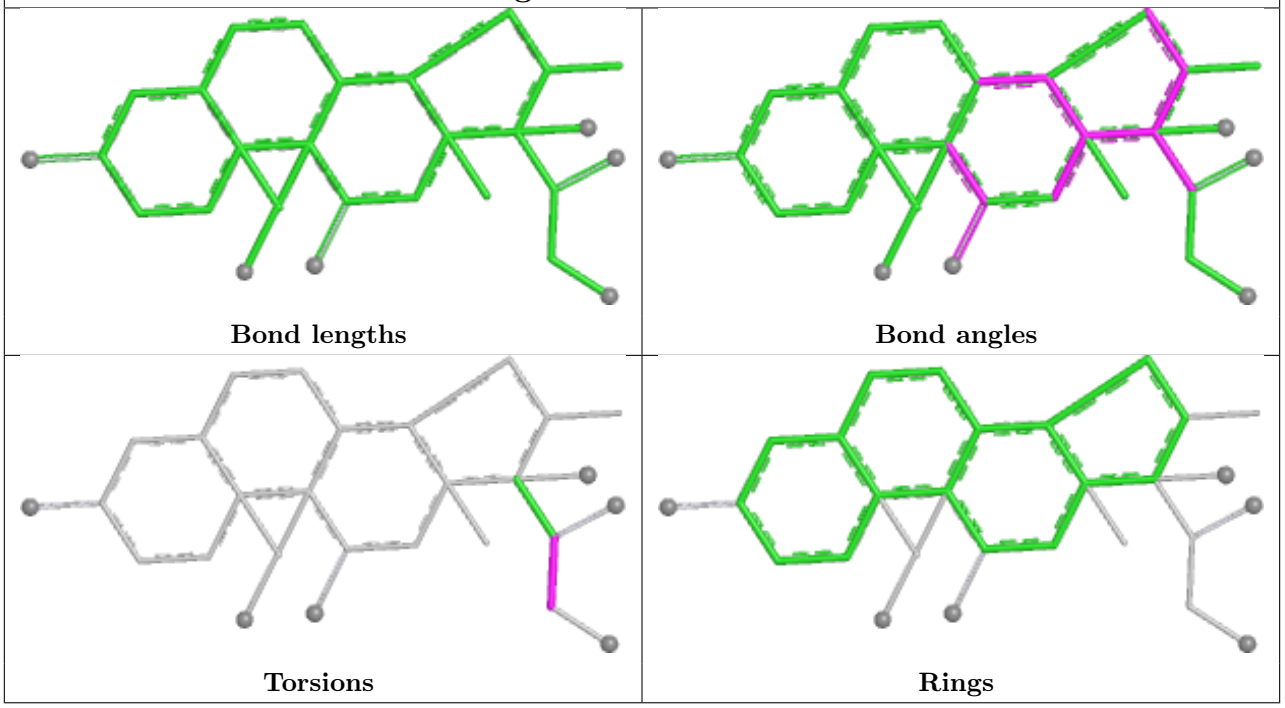


Torsions

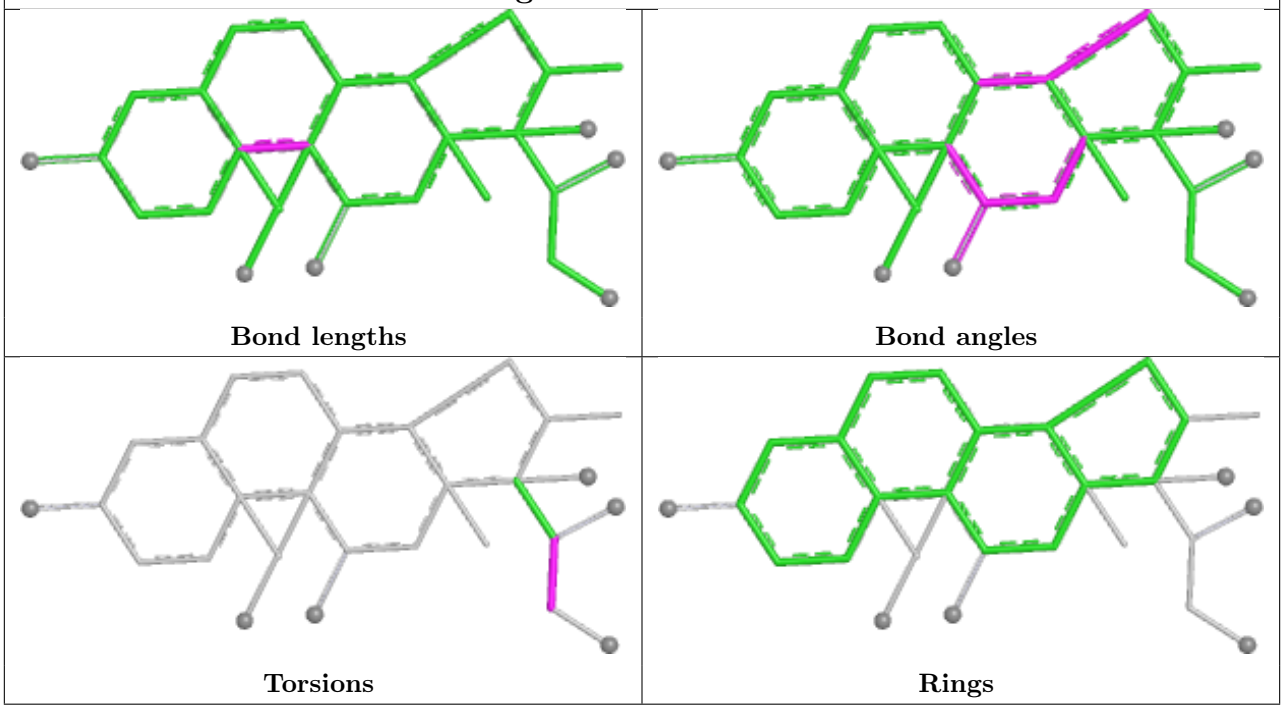


Rings

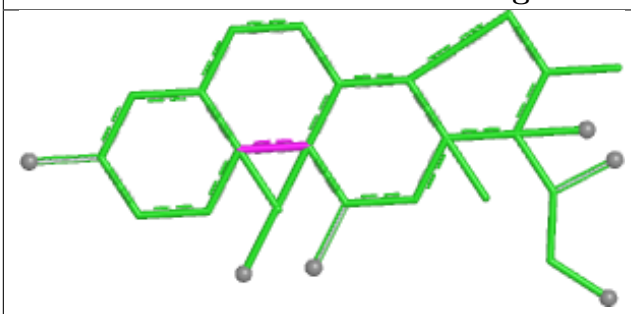
Ligand DEX C 1001



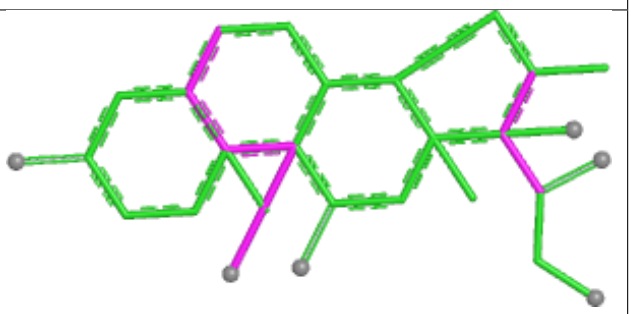
Ligand DEX E 1001



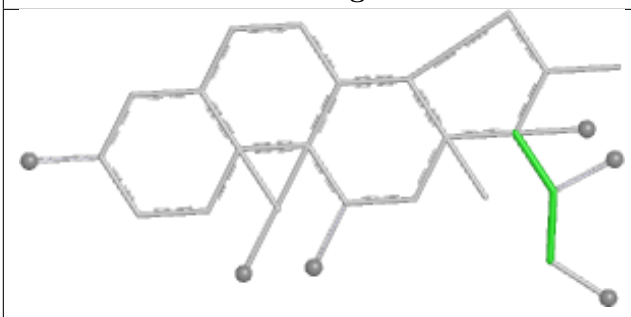
Ligand DEX G 1001



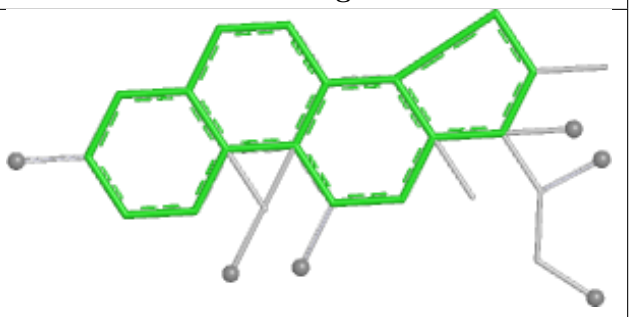
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	248/248 (100%)	0.20	14 (5%) 30 25	33, 63, 108, 155	0
1	C	248/248 (100%)	-0.11	6 (2%) 59 52	29, 51, 83, 126	0
1	D	248/248 (100%)	0.04	9 (3%) 46 39	33, 57, 109, 141	0
1	F	248/248 (100%)	0.83	28 (11%) 10 8	44, 76, 122, 156	1 (0%)
1	G	248/248 (100%)	0.16	4 (1%) 70 63	37, 67, 111, 155	1 (0%)
1	H	245/248 (98%)	1.51	70 (28%) 1 1	44, 95, 146, 196	0
1	I	248/248 (100%)	-0.14	7 (2%) 55 47	33, 55, 95, 140	0
1	L	248/248 (100%)	-0.11	5 (2%) 65 58	34, 54, 89, 135	0
1	M	248/248 (100%)	0.40	17 (6%) 23 18	38, 67, 117, 166	0
1	P	243/248 (97%)	0.69	34 (13%) 6 5	37, 70, 115, 159	0
2	B	247/248 (99%)	-0.14	5 (2%) 65 58	30, 53, 96, 127	0
2	E	243/248 (97%)	0.46	16 (6%) 24 19	38, 63, 104, 140	1 (0%)
2	J	247/248 (99%)	-0.10	6 (2%) 59 52	29, 54, 94, 138	1 (0%)
2	K	244/248 (98%)	0.06	7 (2%) 53 46	36, 63, 100, 150	0
2	N	244/248 (98%)	-0.02	7 (2%) 53 46	32, 60, 97, 134	1 (0%)
2	O	243/248 (97%)	0.32	14 (5%) 29 24	37, 65, 103, 129	0
3	a	14/15 (93%)	0.25	2 (14%) 6 5	41, 53, 115, 115	0
3	b	14/15 (93%)	0.18	1 (7%) 22 17	39, 55, 103, 117	0
3	c	14/15 (93%)	0.35	1 (7%) 22 17	43, 56, 114, 114	0
3	d	14/15 (93%)	0.45	1 (7%) 22 17	47, 63, 120, 126	0
3	e	14/15 (93%)	1.01	3 (21%) 2 2	53, 74, 130, 134	0
3	f	13/15 (86%)	1.53	4 (30%) 1 1	72, 96, 130, 135	0
3	g	13/15 (86%)	0.72	1 (7%) 19 15	50, 62, 120, 133	0
3	h	13/15 (86%)	1.28	1 (7%) 19 15	71, 94, 119, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	i	15/15 (100%)	0.58	2 (13%) 7 6	45, 61, 115, 125	0
3	j	14/15 (93%)	0.42	2 (14%) 6 5	40, 55, 106, 124	0
3	k	14/15 (93%)	0.38	1 (7%) 22 17	49, 60, 116, 129	0
3	l	14/15 (93%)	0.42	2 (14%) 6 5	48, 59, 109, 135	0
3	m	14/15 (93%)	0.55	2 (14%) 6 5	60, 72, 129, 137	0
3	n	15/15 (100%)	0.48	3 (20%) 3 2	47, 66, 120, 145	0
3	o	14/15 (93%)	1.08	2 (14%) 6 5	53, 78, 122, 140	0
3	p	14/15 (93%)	1.25	4 (28%) 1 1	59, 80, 123, 143	0
All	All	4163/4208 (98%)	0.27	281 (6%) 24 19	29, 63, 115, 196	5 (0%)

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	553	PRO	8.6
1	H	716	TYR	6.4
1	H	774	PHE	5.6
2	O	529	PHE	5.2
1	H	675	VAL	5.1
2	E	529	PHE	5.0
1	M	552	LEU	5.0
1	H	552	LEU	4.8
1	H	775	HIS	4.8
3	i	29	LEU	4.7
1	H	680	LEU	4.5
1	D	553	PRO	4.5
1	A	712	TRP	4.5
1	P	774	PHE	4.5
1	H	529	PHE	4.4
2	K	745	LEU	4.3
1	A	529	PHE	4.3
1	H	553	PRO	4.2
1	H	737	PHE	4.2
1	C	529	PHE	4.2
1	H	766	ALA	4.1
1	P	529	PHE	4.1
2	K	743	LYS	4.1
1	D	529	PHE	4.1
1	H	709	SER	4.1
1	P	773	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	769	VAL	4.0
2	K	709	SER	4.0
3	g	28	SER	4.0
2	E	764	PHE	4.0
3	j	29	LEU	3.9
1	H	686	PHE	3.9
1	G	529	PHE	3.8
1	A	744	SER	3.8
1	H	690	ARG	3.8
1	P	688	GLU	3.8
1	H	722	LEU	3.8
1	H	726	HIS	3.7
1	F	684	ALA	3.7
1	H	676	PRO	3.7
1	I	743	LYS	3.7
1	H	764	PHE	3.7
1	A	711	ASN	3.6
1	H	679	GLY	3.6
1	P	771	PRO	3.6
2	N	728	MET	3.6
1	M	529	PHE	3.6
1	H	772	LEU	3.6
1	H	639	MET	3.6
1	F	529	PHE	3.6
1	H	642	GLN	3.5
1	M	764	PHE	3.5
2	O	638	TYR	3.5
1	F	709	SER	3.5
1	H	761	LEU	3.5
2	K	529	PHE	3.5
3	h	22	TYR	3.4
3	p	28	SER	3.4
1	P	679	GLY	3.4
1	F	735	PHE	3.4
2	B	529	PHE	3.4
1	H	767	GLY	3.3
1	H	773	LEU	3.3
3	f	26	SER	3.3
1	F	680	LEU	3.3
1	M	745	LEU	3.3
2	O	711	ASN	3.3
3	b	29	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	708	SER	3.2
1	H	591	ASP	3.2
1	H	674	THR	3.2
2	E	679	GLY	3.2
2	E	585	ARG	3.2
1	P	675	VAL	3.2
1	M	709	SER	3.2
1	H	723	ASP	3.1
2	B	691	MET	3.1
1	M	551	THR	3.1
1	F	703	LYS	3.1
1	H	551	THR	3.1
2	J	529	PHE	3.1
2	E	711	ASN	3.0
2	N	712	TRP	3.0
1	A	638	TYR	3.0
1	M	684	ALA	3.0
1	P	716	TYR	3.0
1	A	710	GLN	3.0
1	P	770	LYS	3.0
3	p	29	LEU	3.0
3	c	16	SER	3.0
1	H	695	LYS	3.0
2	N	711	ASN	3.0
1	H	598	TYR	3.0
1	H	736	CYS	2.9
1	M	638	TYR	2.9
1	F	585	ARG	2.9
1	M	549	ASP	2.9
1	H	745	LEU	2.9
2	O	552	LEU	2.9
3	n	29	LEU	2.9
3	o	29	LEU	2.9
1	A	743	LYS	2.9
3	o	28	SER	2.9
2	E	691	MET	2.9
1	D	551	THR	2.9
1	F	638	TYR	2.9
1	P	764	PHE	2.9
1	I	691	MET	2.9
1	M	776	GLN	2.9
1	P	710	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	P	677	LYS	2.9
1	F	708	SER	2.8
3	f	28	SER	2.8
1	P	767	GLY	2.8
1	D	745	LEU	2.8
1	H	771	PRO	2.8
1	P	760	GLN	2.8
3	m	16	SER	2.8
3	p	22	TYR	2.8
1	G	735	PHE	2.8
1	I	529	PHE	2.8
1	H	595	LEU	2.8
1	H	735	PHE	2.8
2	O	705	GLU	2.8
1	C	644	GLN	2.8
2	O	745	LEU	2.8
1	P	687	ASP	2.8
1	P	685	VAL	2.8
2	O	548	TYR	2.8
1	H	600	TRP	2.7
1	H	672	LEU	2.7
1	M	744	SER	2.7
2	N	529	PHE	2.7
1	C	711	ASN	2.7
3	d	16	SER	2.7
3	f	27	SER	2.7
1	F	769	VAL	2.7
2	J	551	THR	2.7
3	l	16	SER	2.7
3	a	16	SER	2.6
1	F	740	PHE	2.6
1	H	715	PHE	2.6
3	n	15	ALA	2.6
1	F	597	GLN	2.6
1	H	740	PHE	2.6
1	H	554	ASP	2.6
2	J	549	ASP	2.6
1	H	762	PRO	2.6
1	A	551	THR	2.6
1	P	772	LEU	2.6
1	A	716	TYR	2.6
1	F	598	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	720	LYS	2.6
1	P	726	HIS	2.6
1	I	557	THR	2.5
1	P	695	LYS	2.5
1	F	774	PHE	2.5
1	I	764	PHE	2.5
2	O	639	MET	2.5
1	H	636	LEU	2.5
1	H	697	LEU	2.5
1	H	721	LEU	2.5
1	F	771	PRO	2.5
1	H	691	MET	2.5
1	C	709	SER	2.5
1	F	556	SER	2.5
1	H	585	ARG	2.5
3	e	29	LEU	2.5
1	P	635	GLN	2.5
1	P	769	VAL	2.5
1	H	700	ALA	2.5
2	B	735	PHE	2.5
1	H	665	CYS	2.5
1	M	558	ARG	2.5
2	J	641	ASP	2.5
3	f	22	TYR	2.5
1	L	529	PHE	2.5
1	L	743	LYS	2.4
1	D	709	SER	2.4
1	D	764	PHE	2.4
1	H	770	LYS	2.4
2	J	710	GLN	2.4
1	P	719	THR	2.4
3	a	29	LEU	2.4
1	P	591	ASP	2.4
1	H	542	GLU	2.4
1	H	660	TYR	2.4
1	P	766	ALA	2.4
1	H	759	ASN	2.4
1	D	744	SER	2.4
1	F	632	GLU	2.4
1	P	723	ASP	2.4
1	F	776	GLN	2.4
2	N	710	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	715	PHE	2.4
3	i	15	ALA	2.4
1	F	631	GLU	2.4
1	H	699	LYS	2.4
1	L	643	CYS	2.4
3	p	17	ARG	2.4
1	D	684	ALA	2.4
1	G	641	ASP	2.3
3	j	28	SER	2.3
3	n	16	SER	2.3
2	O	710	GLN	2.3
2	E	685	VAL	2.3
1	H	684	ALA	2.3
1	H	718	LEU	2.3
2	E	589	LEU	2.3
1	H	765	LYS	2.3
2	E	631	GLU	2.3
1	H	547	GLY	2.3
1	P	686	PHE	2.3
1	D	743	LYS	2.3
1	H	677	LYS	2.3
2	O	554	ASP	2.3
3	e	16	SER	2.3
3	e	28	SER	2.3
2	O	585	ARG	2.3
1	F	635	GLN	2.3
1	H	558	ARG	2.3
2	N	709	SER	2.3
1	A	764	PHE	2.3
1	F	716	TYR	2.2
1	P	711	ASN	2.2
1	F	583	GLY	2.2
1	P	712	TRP	2.2
1	F	726	HIS	2.2
1	L	765	LYS	2.2
2	J	776	GLN	2.2
2	O	776	GLN	2.2
1	A	709	SER	2.2
3	k	29	LEU	2.2
1	P	720	LYS	2.2
1	F	764	PHE	2.2
1	C	710	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	776	GLN	2.2
1	H	734	GLN	2.2
1	I	776	GLN	2.2
1	M	550	SER	2.2
2	E	678	ASP	2.2
2	N	765	LYS	2.2
2	O	636	LEU	2.2
3	m	29	LEU	2.2
1	F	685	VAL	2.2
2	K	764	PHE	2.2
1	P	690	ARG	2.2
1	A	548	TYR	2.2
1	H	638	TYR	2.2
1	M	703	LYS	2.2
2	E	680	LEU	2.2
2	E	702	VAL	2.2
1	P	598	TYR	2.1
1	M	708	SER	2.1
2	E	774	PHE	2.1
1	G	776	GLN	2.1
1	L	640	TYR	2.1
3	l	29	LEU	2.1
1	A	706	GLY	2.1
1	H	678	ASP	2.1
1	H	682	SER	2.1
1	P	684	ALA	2.1
1	H	681	LYS	2.1
1	P	595	LEU	2.1
1	I	638	TYR	2.1
2	E	686	PHE	2.1
1	H	727	GLU	2.1
2	B	684	ALA	2.1
1	H	584	PHE	2.1
1	P	713	GLN	2.0
2	E	776	GLN	2.0
1	F	693	TYR	2.0
1	H	693	TYR	2.0
2	B	764	PHE	2.0
2	K	585	ARG	2.0
2	E	684	ALA	2.0
1	F	758	SER	2.0
1	F	674	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	634	MET	2.0
1	M	585	ARG	2.0
2	O	704	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CSO	J	622	7/8	0.93	0.11	48,51,91,103	0
2	CSO	K	622[A]	7/8	0.93	0.11	43,48,57,63	2
2	CSO	K	622[B]	7/8	0.93	0.11	43,48,49,51	2
2	CSO	B	622[B]	7/8	0.94	0.10	40,44,64,67	2
2	CSO	B	622[A]	7/8	0.94	0.10	40,44,50,55	2
2	CSO	O	622[A]	7/8	0.94	0.11	39,44,48,59	2
2	CSO	O	622[B]	7/8	0.94	0.11	39,44,48,48	2
2	CSO	N	622[A]	7/8	0.95	0.10	43,44,50,51	2
2	CSO	N	622[B]	7/8	0.95	0.10	43,47,53,64	2
2	CSO	E	622[B]	7/8	0.96	0.08	39,42,50,58	2
2	CSO	E	622[A]	7/8	0.96	0.08	39,42,45,46	2

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SO4	C	1006	5/5	0.68	0.17	143,144,166,175	0
8	SO4	C	1005	5/5	0.69	0.13	153,158,184,187	0
6	EPE	J	803	15/15	0.71	0.30	99,143,200,200	0
6	EPE	A	1003	15/15	0.72	0.22	112,127,165,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EPE	P	1002	15/15	0.75	0.23	101,131,154,177	0
8	SO4	A	1006	5/5	0.77	0.11	163,165,175,185	0
11	IMD	J	807	5/5	0.77	0.25	103,104,108,117	0
6	EPE	B	804	15/15	0.78	0.22	74,113,165,185	0
6	EPE	L	1003	15/15	0.79	0.26	107,124,148,156	0
8	SO4	J	801	5/5	0.80	0.10	138,151,162,182	0
11	IMD	O	1004	5/5	0.81	0.28	77,92,101,103	0
7	GOL	J	806	6/6	0.83	0.18	74,85,96,97	0
11	IMD	B	807	5/5	0.83	0.26	92,99,101,108	0
11	IMD	F	1003	5/5	0.84	0.24	92,93,104,111	0
11	IMD	I	1006	5/5	0.84	0.23	116,117,126,126	0
7	GOL	O	1003	6/6	0.84	0.22	79,93,99,108	0
8	SO4	B	808	5/5	0.84	0.14	91,120,137,137	0
7	GOL	K	805	6/6	0.85	0.17	93,112,122,128	0
7	GOL	C	1002	6/6	0.85	0.21	63,85,91,99	0
11	IMD	J	808	5/5	0.85	0.26	101,102,112,113	0
11	IMD	L	1006	5/5	0.85	0.31	101,104,116,118	0
6	EPE	D	804	15/15	0.85	0.18	84,116,172,190	0
11	IMD	L	1007	5/5	0.86	0.29	106,112,115,117	0
7	GOL	N	1002	6/6	0.86	0.13	68,86,90,96	0
9	CL	F	1004	1/1	0.87	0.09	83,83,83,83	0
7	GOL	E	1003	6/6	0.87	0.18	98,106,119,123	0
6	EPE	I	1004	15/15	0.87	0.21	103,123,154,159	0
7	GOL	A	1005	6/6	0.88	0.16	59,79,82,86	0
7	GOL	E	1005	6/6	0.88	0.19	82,88,101,103	0
5	CAC	K	803	5/5	0.88	0.21	60,76,116,132	0
10	PG4	H	803	13/13	0.88	0.16	76,93,108,109	0
12	PEG	F	1002	7/7	0.88	0.17	64,82,92,94	0
7	GOL	A	1004	6/6	0.89	0.12	65,84,94,99	0
11	IMD	E	1006	5/5	0.89	0.28	106,106,112,113	0
7	GOL	K	804	6/6	0.89	0.12	87,92,97,98	0
10	PG4	D	803	13/13	0.89	0.18	70,83,95,103	0
11	IMD	b	101	5/5	0.89	0.21	87,93,95,95	0
7	GOL	C	1003	6/6	0.89	0.20	72,93,99,110	0
11	IMD	C	1004	5/5	0.90	0.31	106,116,125,128	0
12	PEG	K	801	7/7	0.90	0.14	47,58,63,65	0
7	GOL	B	805	6/6	0.91	0.12	67,78,89,92	0
11	IMD	M	806	5/5	0.91	0.18	95,97,106,113	0
12	PEG	I	1003	7/7	0.91	0.18	77,80,92,94	0
5	CAC	H	801	5/5	0.91	0.17	62,76,103,114	0
7	GOL	J	804	6/6	0.92	0.17	62,86,91,91	0
11	IMD	d	101	5/5	0.92	0.22	110,110,125,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CL	J	809	1/1	0.92	0.17	81,81,81,81	0
10	PG4	B	803	13/13	0.92	0.19	77,89,98,101	0
7	GOL	J	805	6/6	0.92	0.12	54,76,82,83	0
9	CL	B	809	1/1	0.93	0.11	80,80,80,80	0
9	CL	E	1007	1/1	0.93	0.10	93,93,93,93	0
5	CAC	M	803	5/5	0.93	0.17	62,85,114,118	0
7	GOL	L	1004	6/6	0.93	0.11	51,51,54,57	0
9	CL	N	1004	1/1	0.93	0.14	87,87,87,87	0
7	GOL	M	801	6/6	0.93	0.12	65,65,68,69	0
7	GOL	I	1005	6/6	0.93	0.12	65,76,88,89	0
5	CAC	E	1002	5/5	0.93	0.15	58,63,92,99	0
12	PEG	M	805	7/7	0.93	0.15	66,70,82,88	0
7	GOL	L	1005	6/6	0.94	0.10	60,67,71,85	0
9	CL	B	810	1/1	0.94	0.12	94,94,94,94	0
5	CAC	A	1002	5/5	0.94	0.17	53,58,97,97	0
10	PG4	L	1002	13/13	0.94	0.16	63,75,93,102	0
5	CAC	I	1002	5/5	0.94	0.15	58,61,104,109	0
5	CAC	O	1002	5/5	0.94	0.17	68,93,105,112	0
7	GOL	P	1003	6/6	0.94	0.12	68,89,102,113	0
13	PGE	M	804	10/10	0.94	0.14	75,85,111,114	0
5	CAC	D	801	5/5	0.95	0.15	46,60,99,108	0
11	IMD	B	806	5/5	0.95	0.14	110,112,118,122	0
9	CL	M	807	1/1	0.95	0.09	85,85,85,85	0
11	IMD	N	1003	5/5	0.95	0.15	91,95,98,105	0
9	CL	D	805	1/1	0.96	0.18	82,82,82,82	0
9	CL	L	1008	1/1	0.96	0.08	84,84,84,84	0
4	DEX	H	802	28/28	0.96	0.09	57,68,78,83	0
9	CL	C	1007	1/1	0.96	0.08	75,75,75,75	0
4	DEX	F	1001	28/28	0.97	0.07	45,60,68,75	0
4	DEX	E	1001	28/28	0.97	0.07	36,40,47,57	0
4	DEX	K	802	28/28	0.97	0.07	32,44,57,65	0
7	GOL	E	1004	6/6	0.97	0.09	52,56,60,60	0
4	DEX	A	1001	28/28	0.98	0.06	35,43,60,65	0
4	DEX	B	802	28/28	0.98	0.07	32,41,49,52	0
4	DEX	G	1001	28/28	0.98	0.06	36,41,52,66	0
4	DEX	C	1001	28/28	0.98	0.06	32,39,46,58	0
9	CL	B	801	1/1	0.98	0.09	43,43,43,43	0
4	DEX	I	1001	28/28	0.98	0.06	33,38,50,65	0
4	DEX	J	802	28/28	0.98	0.05	26,34,47,61	0
4	DEX	D	802	28/28	0.98	0.06	36,41,52,63	0
4	DEX	L	1001	28/28	0.98	0.06	29,41,55,66	0
4	DEX	M	802	28/28	0.98	0.06	42,49,59,72	0

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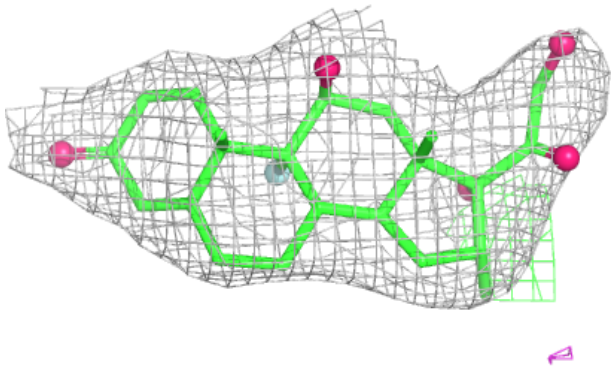
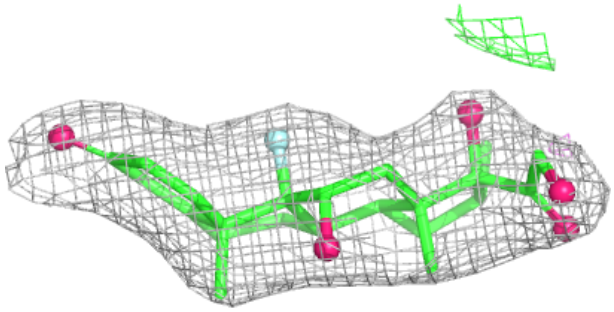
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DEX	N	1001	28/28	0.98	0.06	33,43,51,53	0
4	DEX	O	1001	28/28	0.98	0.07	33,40,57,70	0
4	DEX	P	1001	28/28	0.98	0.07	38,45,56,60	0

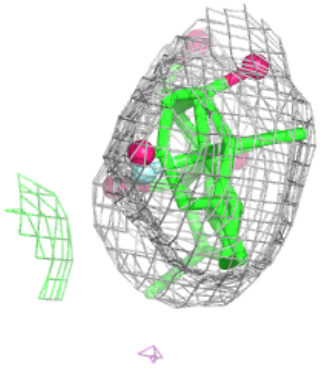
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DEX H 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

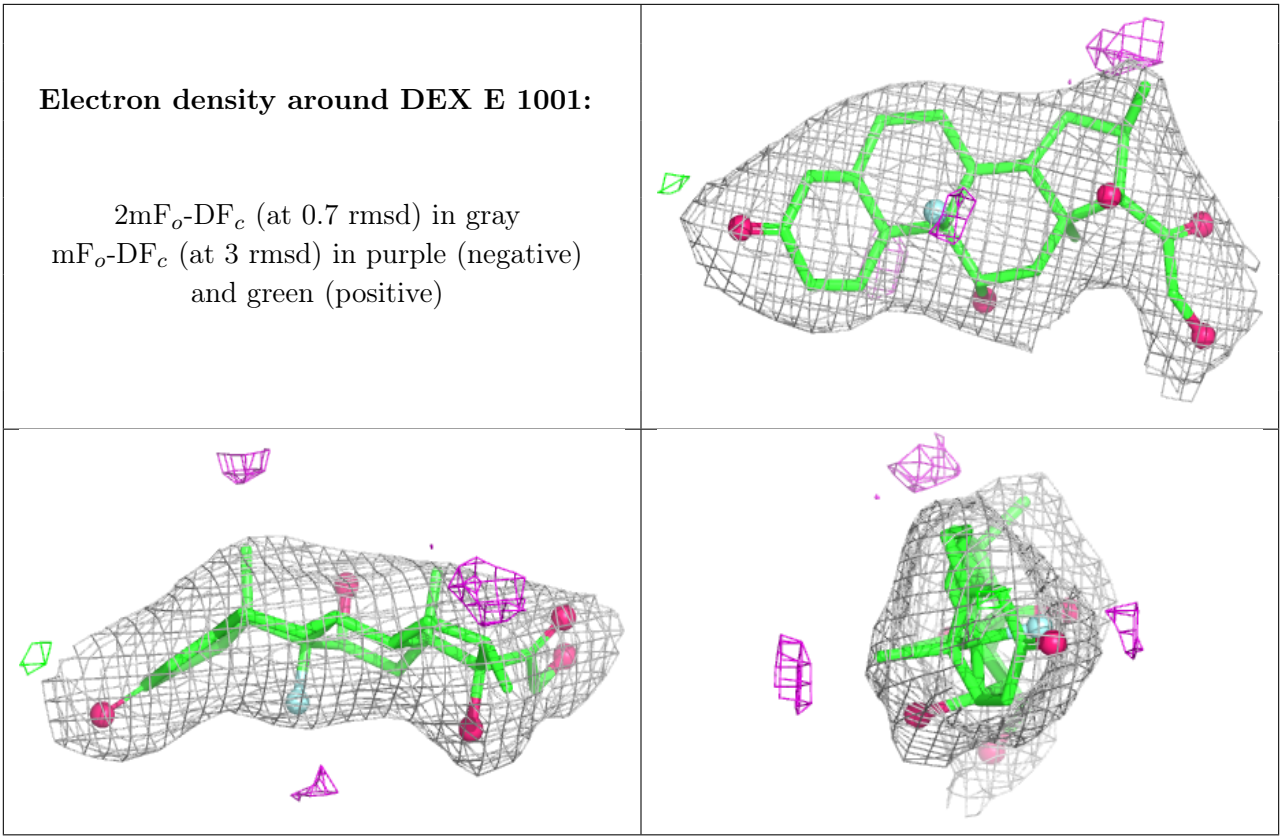






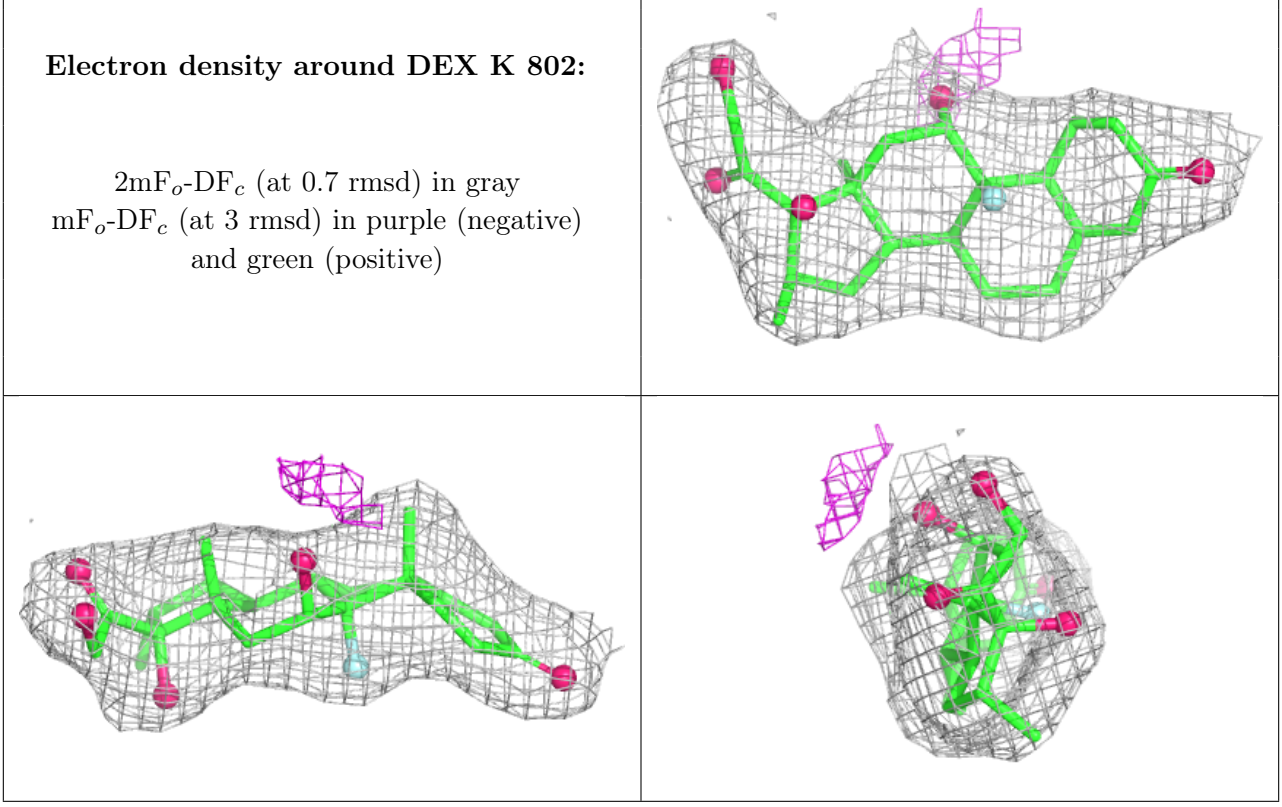
Electron density around DEX E 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



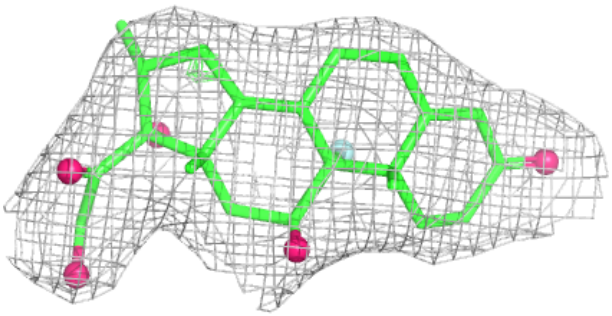
Electron density around DEX K 802:

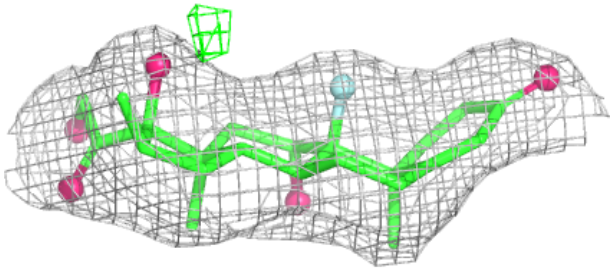
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

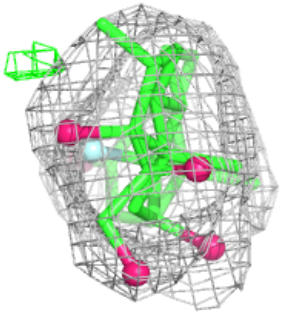


Electron density around DEX A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

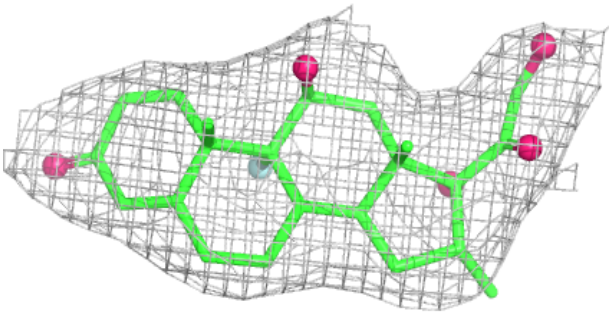


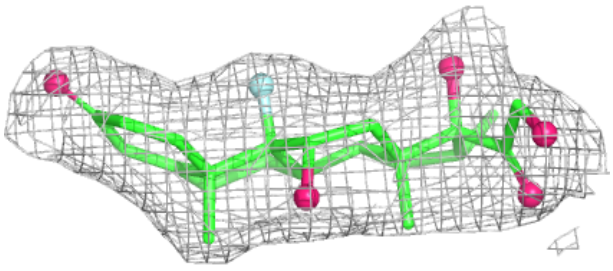


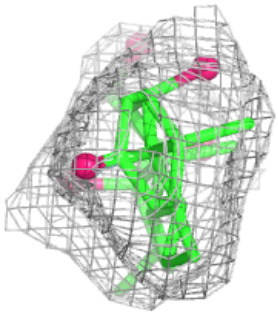


Electron density around DEX B 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

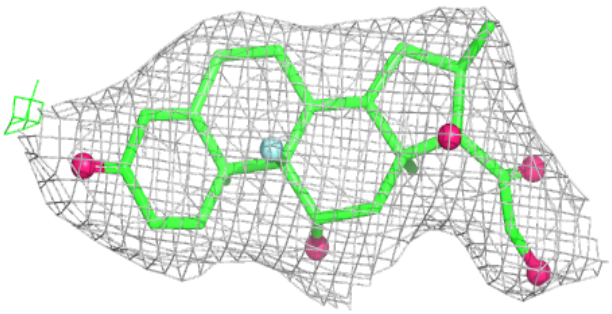


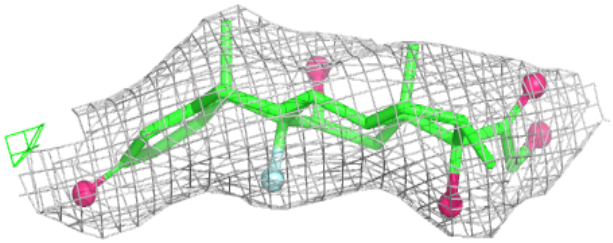


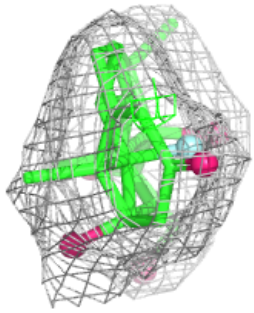


Electron density around DEX G 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

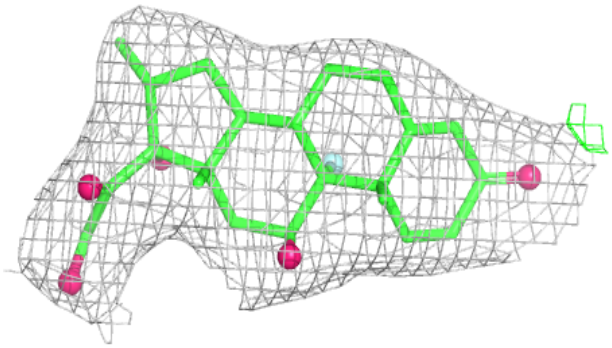


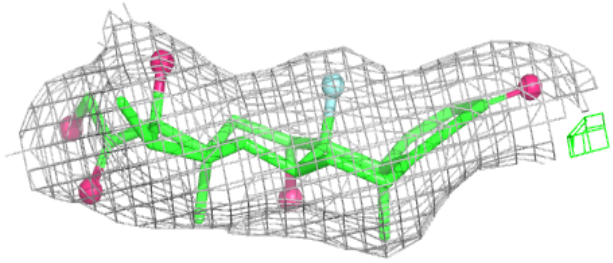


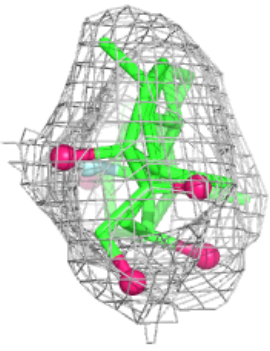


Electron density around DEX C 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

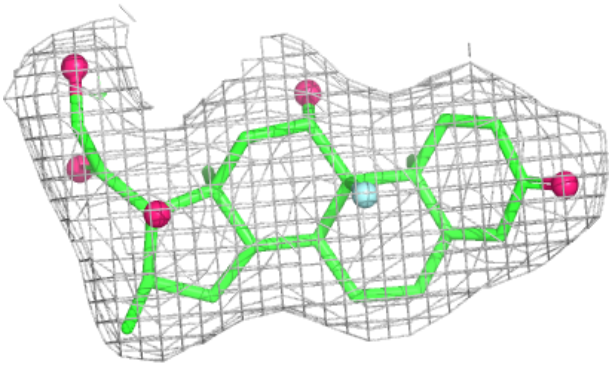


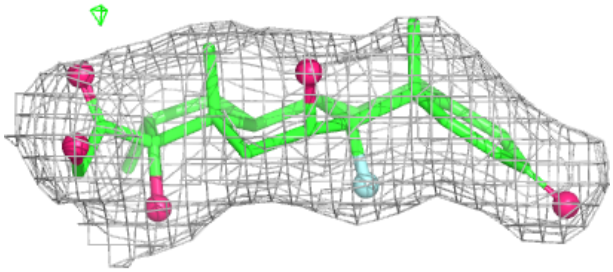


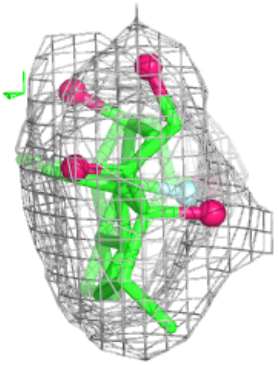


Electron density around DEX I 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

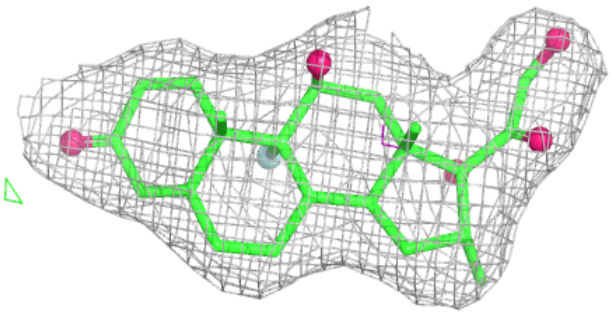


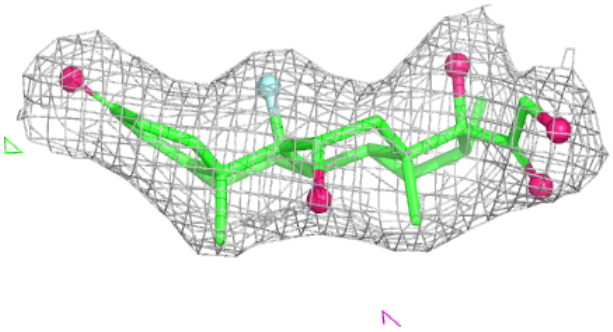


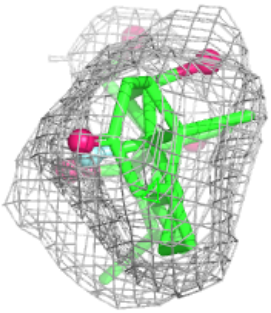


Electron density around DEX J 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

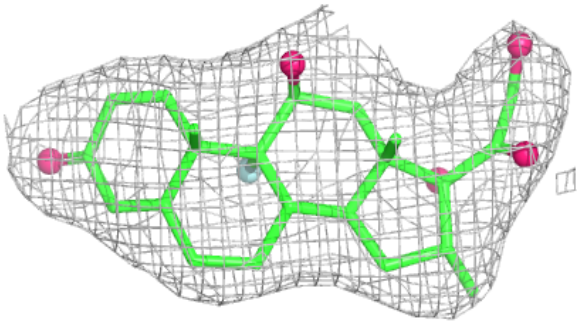


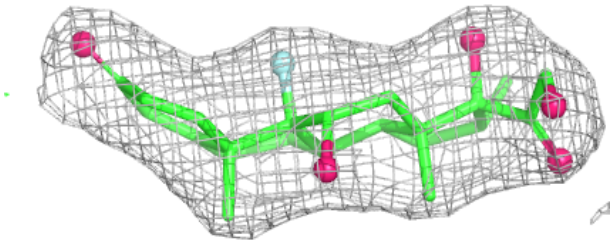


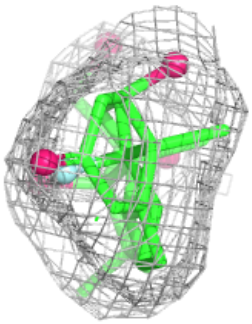


Electron density around DEX D 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

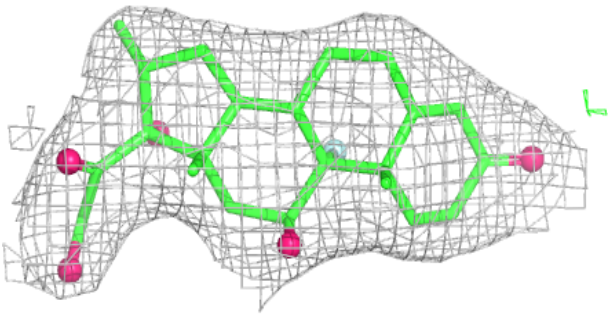


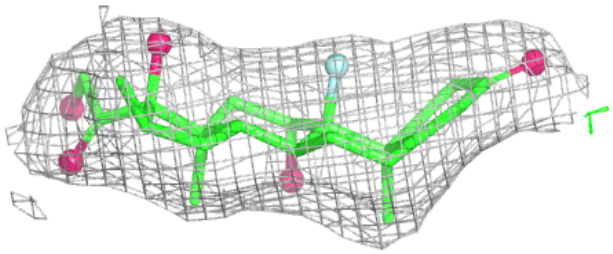


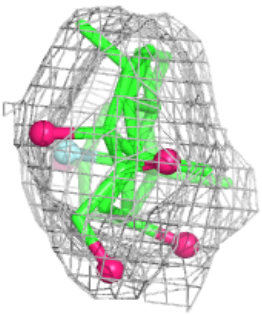


Electron density around DEX L 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

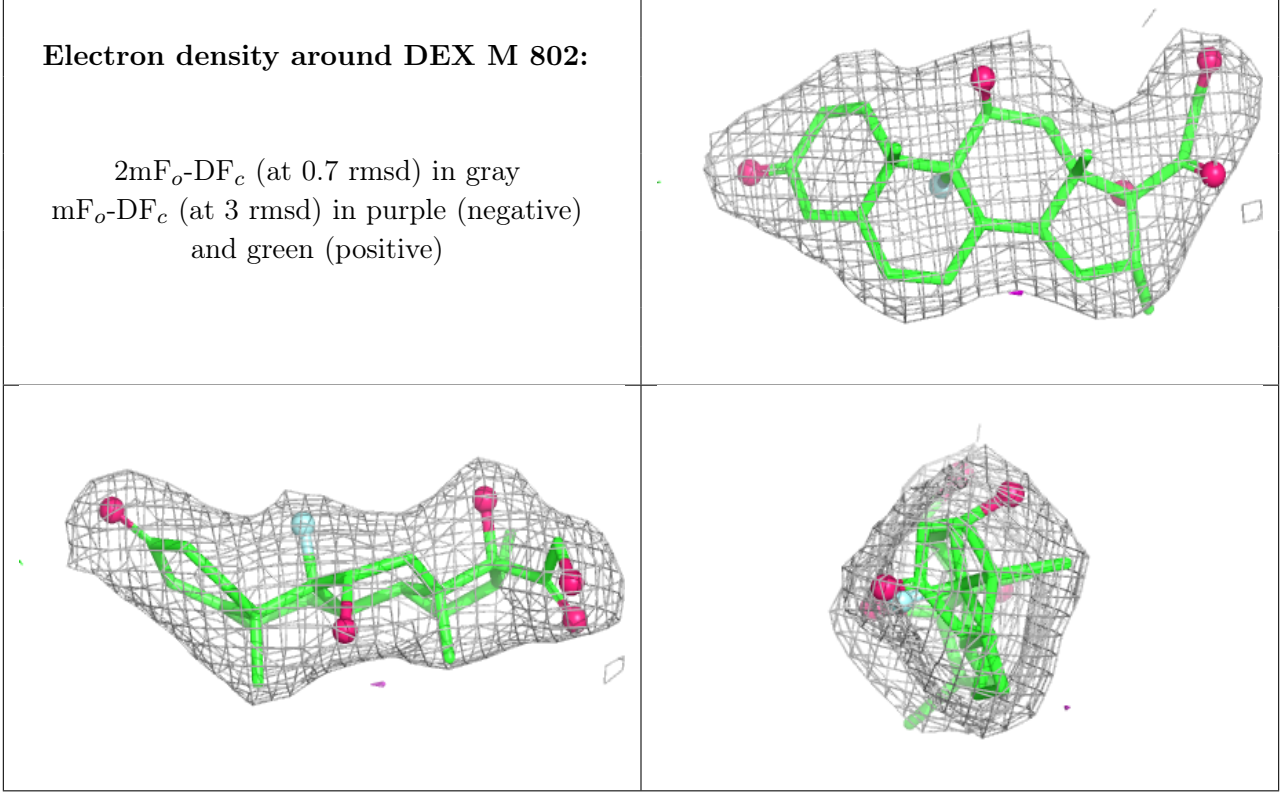






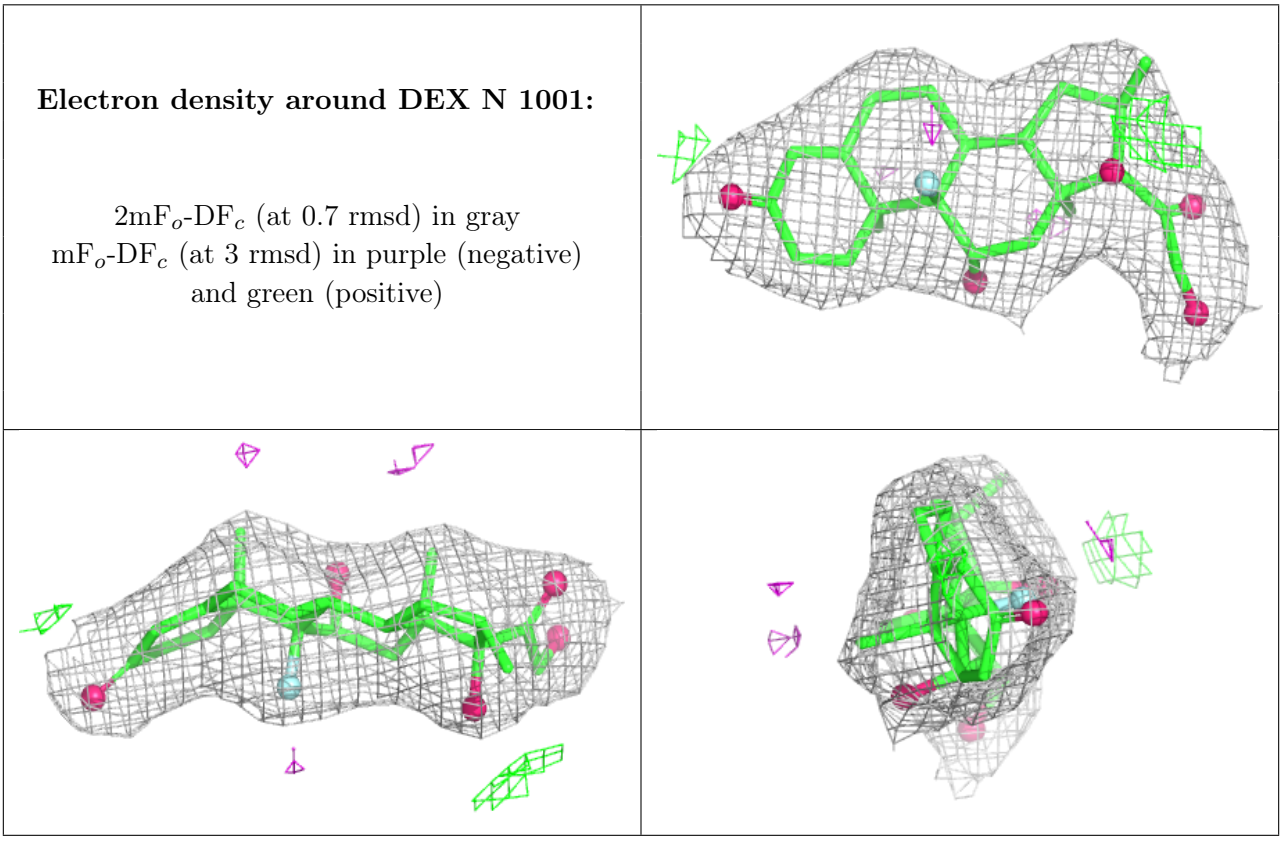
Electron density around DEX M 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



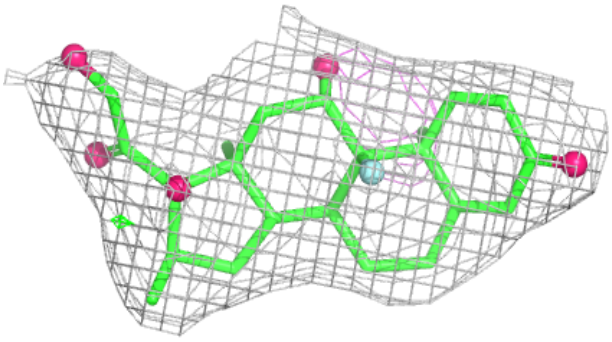
Electron density around DEX N 1001:

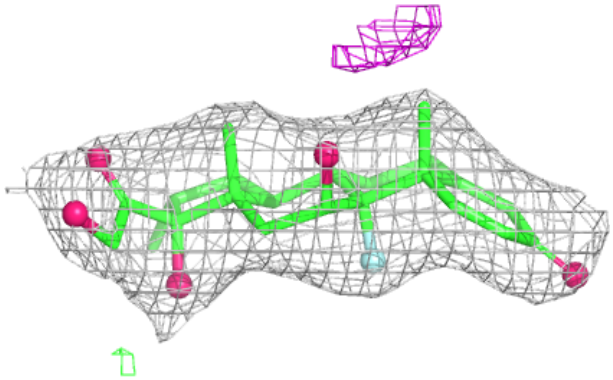
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

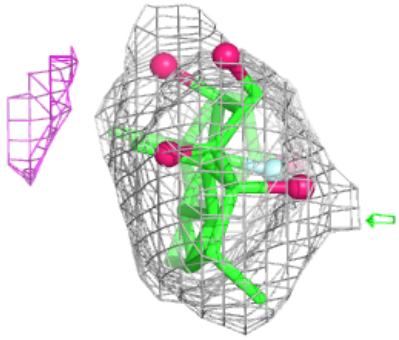


Electron density around DEX O 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

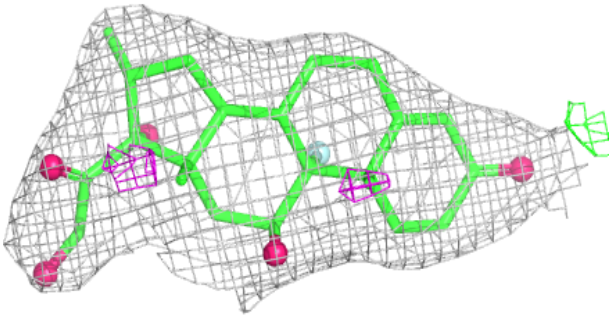


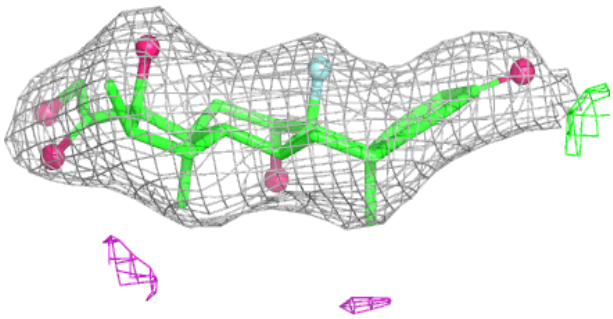


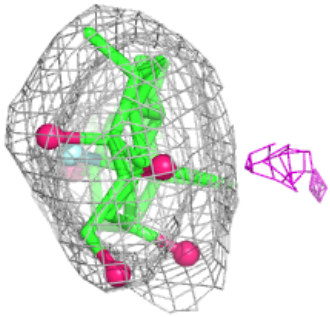


Electron density around DEX P 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.