



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:32 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 wwPDB X-ray Structure Validation Summary 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

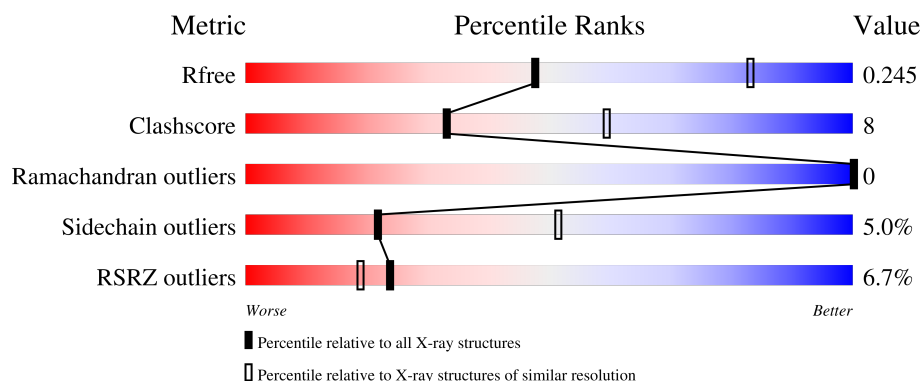
1 Overall quality at a glance

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 $\leq 5\%$. 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	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	248	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	248	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	F	248	<div> <div>11%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	248	
1	H	248	
1	I	248	
1	L	248	
1	M	248	
1	P	248	
2	B	248	
2	E	248	
2	J	248	
2	K	248	
2	N	248	
2	O	248	
3	a	15	
3	b	15	
3	c	15	
3	d	15	
3	e	15	
3	f	15	
3	g	15	
3	h	15	
3	i	15	
3	j	15	
3	k	15	
3	l	15	
3	m	15	

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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

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

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

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

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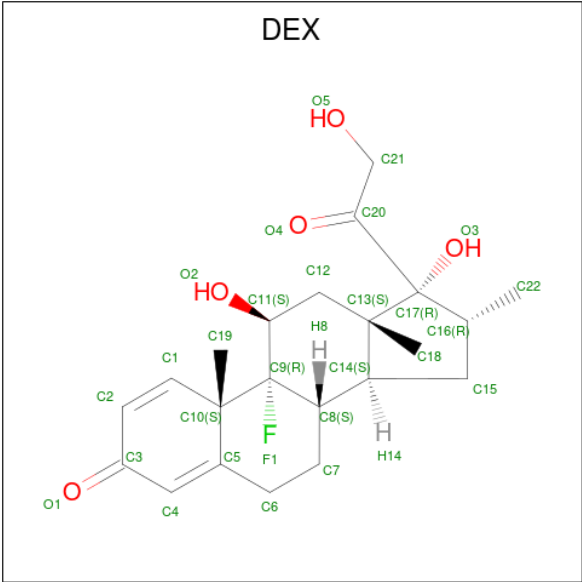
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	245	Total 1997	C 1290	N 327	O 362	S 18	0	2	0
2	O	244	Total 1986	C 1285	N 323	O 360	S 18	0	1	0

- 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 104	C 68	N 17	O 19	0	0	0
3	b	14	Total 104	C 68	N 17	O 19	0	0	0
3	c	14	Total 104	C 68	N 17	O 19	0	0	0
3	d	14	Total 104	C 68	N 17	O 19	0	0	0
3	e	14	Total 104	C 68	N 17	O 19	0	0	0
3	f	13	Total 96	C 62	N 16	O 18	0	0	0
3	g	13	Total 96	C 62	N 16	O 18	0	0	0
3	h	13	Total 96	C 62	N 16	O 18	0	0	0
3	i	15	Total 109	C 71	N 18	O 20	0	0	0
3	j	14	Total 104	C 68	N 17	O 19	0	0	0
3	k	14	Total 104	C 68	N 17	O 19	0	0	0
3	l	14	Total 104	C 68	N 17	O 19	0	0	0
3	m	14	Total 104	C 68	N 17	O 19	0	0	0
3	n	15	Total 109	C 71	N 18	O 20	0	0	0
3	o	14	Total 104	C 68	N 17	O 19	0	0	0
3	p	14	Total 104	C 68	N 17	O 19	0	0	0

- Molecule 4 is DEXAMETHASONE (CCD ID: DEX) (formula: C₂₂H₂₉FO₅).



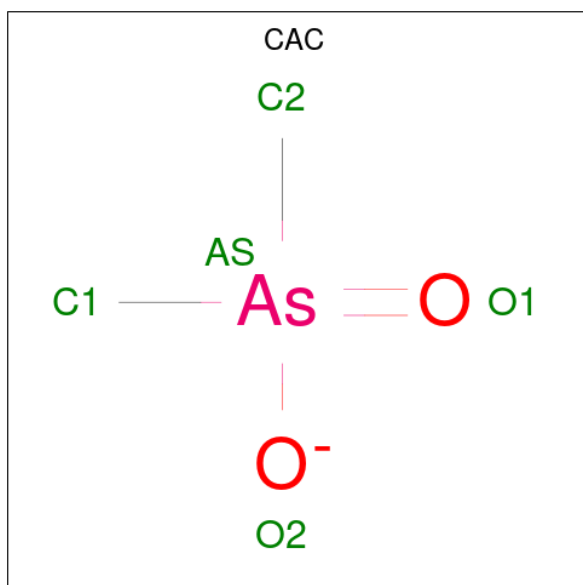
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			28	22	1	5		
4	B	1	Total	C	F	O	0	0
			28	22	1	5		
4	C	1	Total	C	F	O	0	0
			28	22	1	5		
4	D	1	Total	C	F	O	0	0
			28	22	1	5		
4	E	1	Total	C	F	O	0	0
			28	22	1	5		
4	F	1	Total	C	F	O	0	0
			28	22	1	5		
4	G	1	Total	C	F	O	0	0
			28	22	1	5		
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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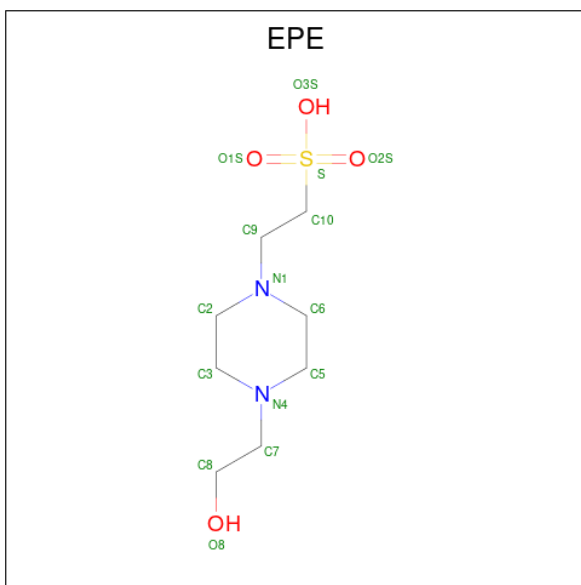
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	O	1	Total	C	F	O	0	0
			28	22	1	5		
4	P	1	Total	C	F	O	0	0
			28	22	1	5		

- 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	0	0
			5	1	2	2		
5	D	1	Total	As	C	O	0	0
			5	1	2	2		
5	E	1	Total	As	C	O	0	0
			5	1	2	2		
5	H	1	Total	As	C	O	0	0
			5	1	2	2		
5	I	1	Total	As	C	O	0	0
			5	1	2	2		
5	K	1	Total	As	C	O	0	0
			5	1	2	2		
5	M	1	Total	As	C	O	0	0
			5	1	2	2		
5	O	1	Total	As	C	O	0	0
			5	1	2	2		

- 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: C₃H₈O₃).



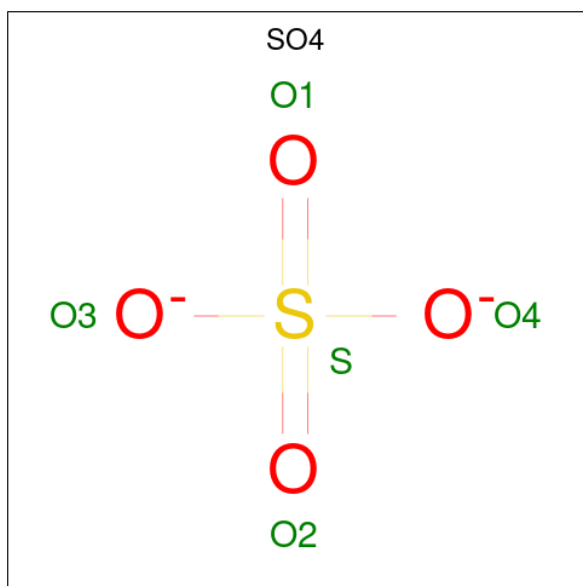
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

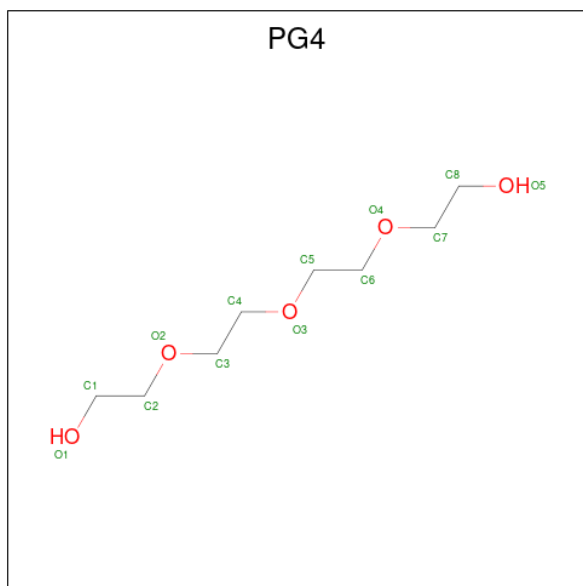


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	J	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



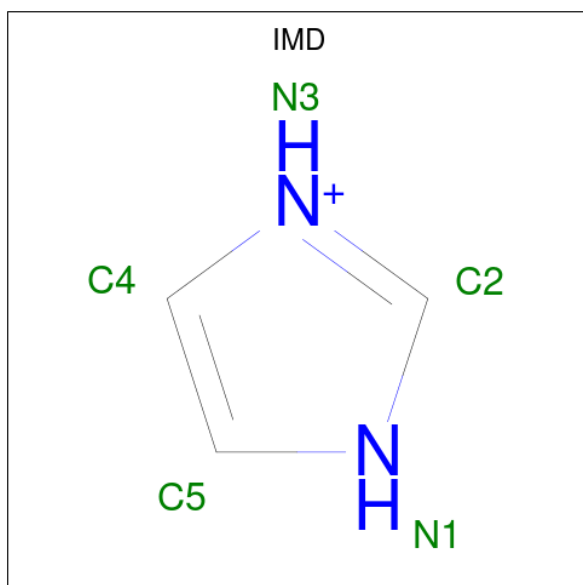
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	8	5		
10	D	1	Total	C	O	0	0
			13	8	5		

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

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



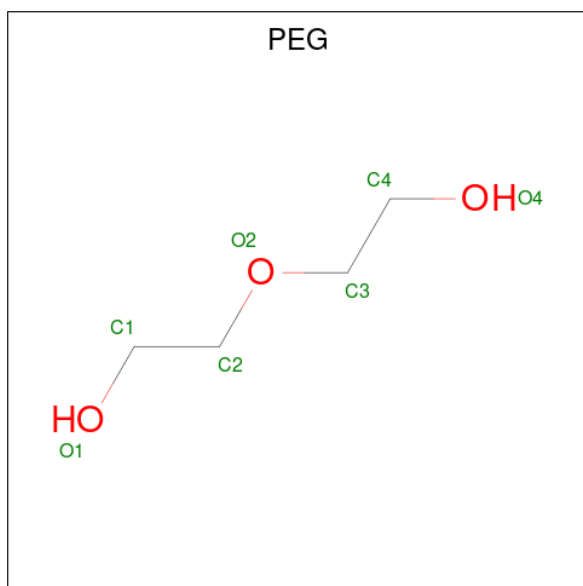
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	N	0	0
			5	3	2		
11	B	1	Total	C	N	0	0
			5	3	2		
11	C	1	Total	C	N	0	0
			5	3	2		
11	E	1	Total	C	N	0	0
			5	3	2		
11	F	1	Total	C	N	0	0
			5	3	2		
11	I	1	Total	C	N	0	0
			5	3	2		
11	J	1	Total	C	N	0	0
			5	3	2		
11	J	1	Total	C	N	0	0
			5	3	2		
11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

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

- 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	0	0
			7	4	3		
12	I	1	Total	C	O	0	0
			7	4	3		
12	K	1	Total	C	O	0	0
			7	4	3		
12	M	1	Total	C	O	0	0
			7	4	3		

- 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	0	0
			10	6	4		

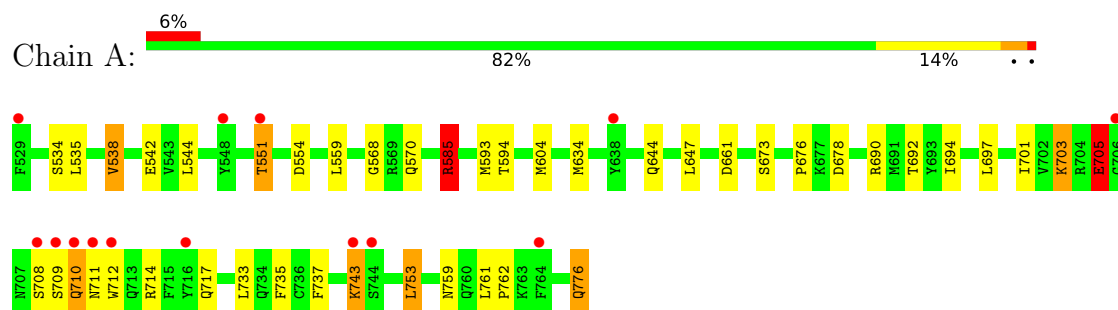
- Molecule 14 is water.

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

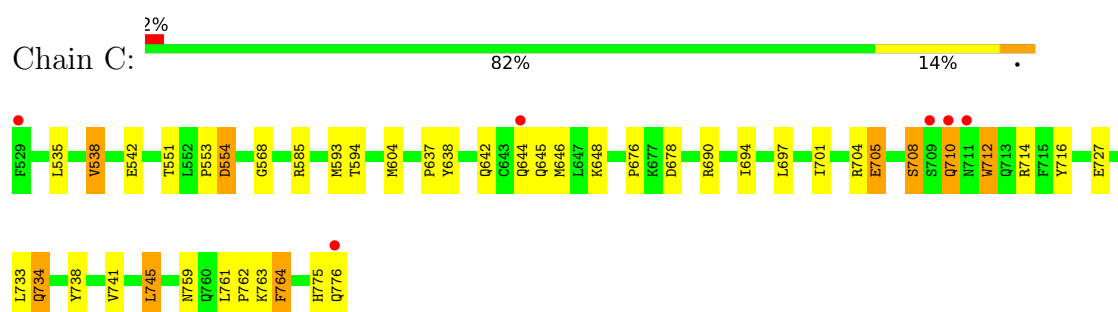
3 Residue-property plots [i](#)

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.

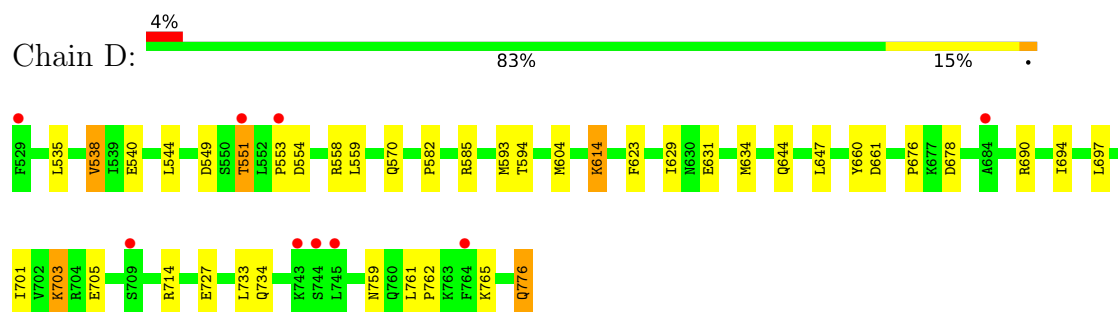
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



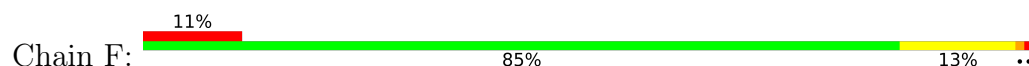
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

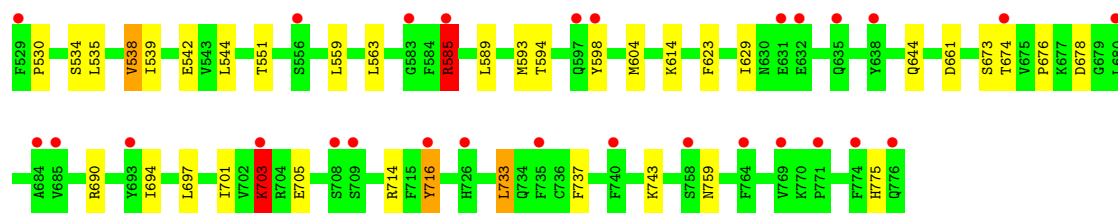


- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

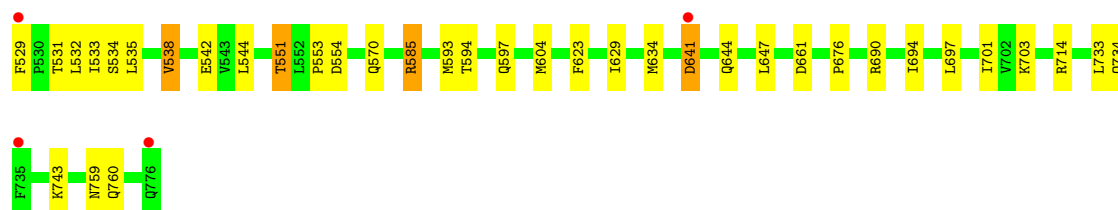
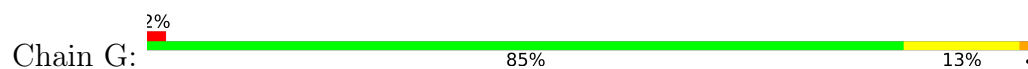


- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

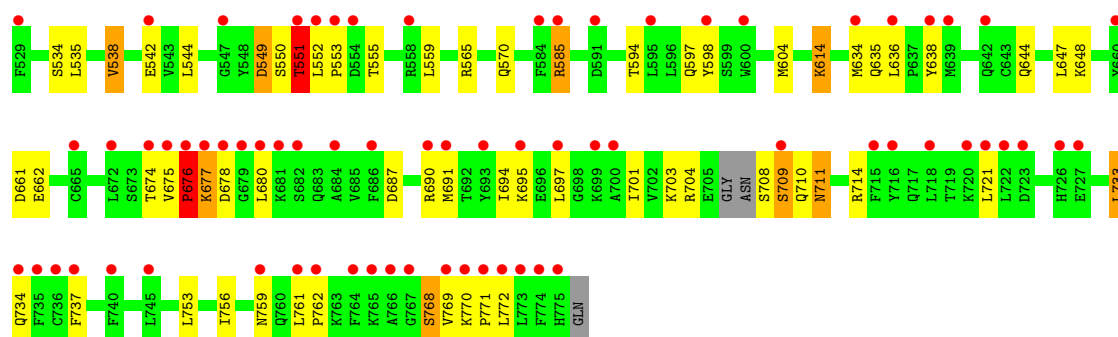
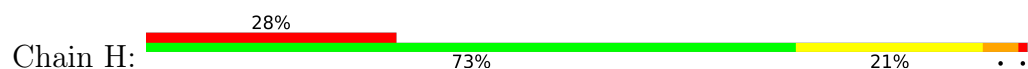




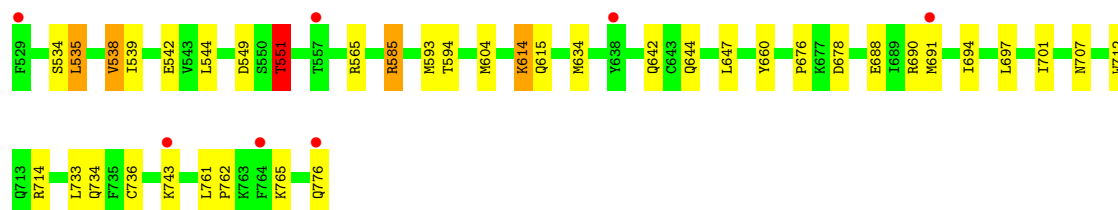
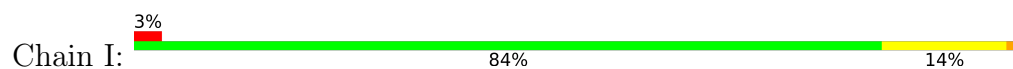
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



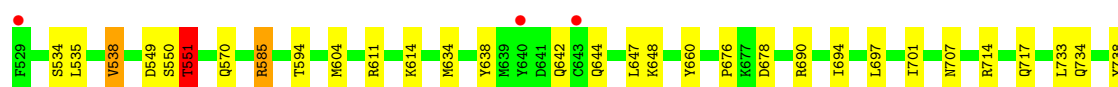
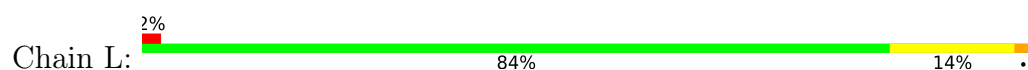
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

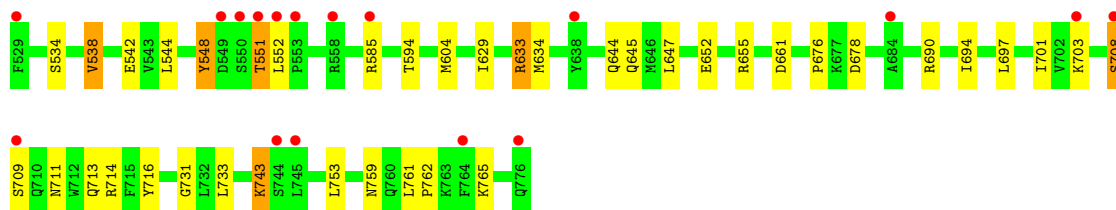
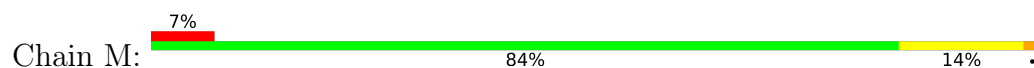


- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain

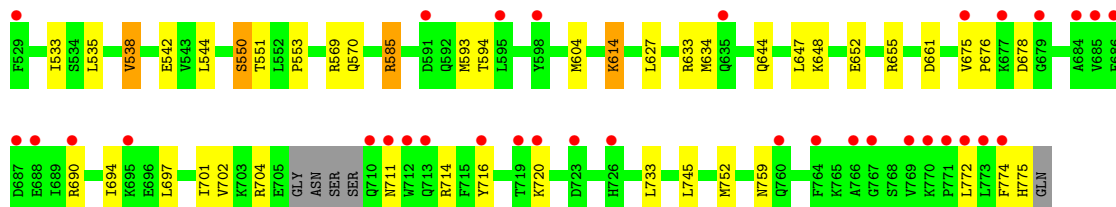
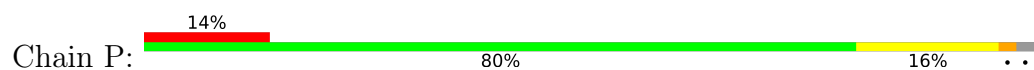




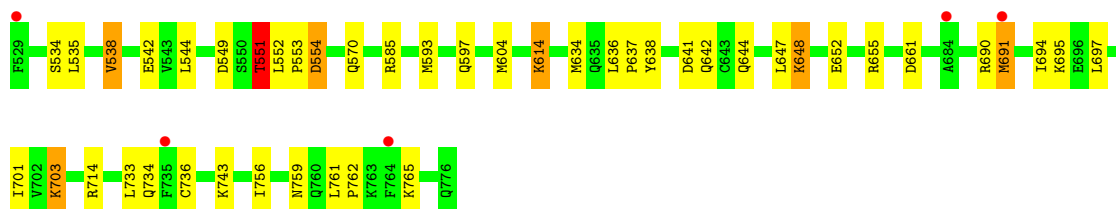
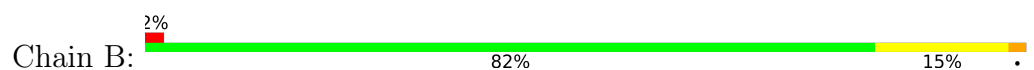
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



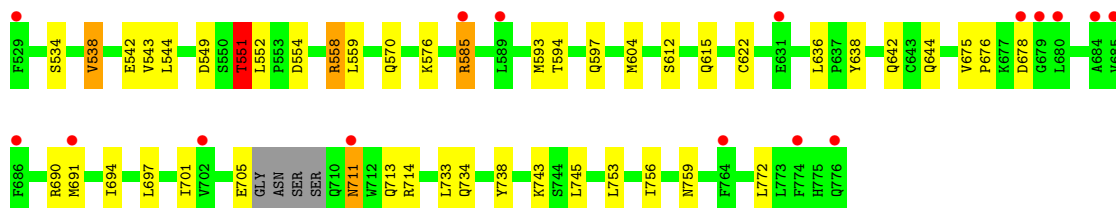
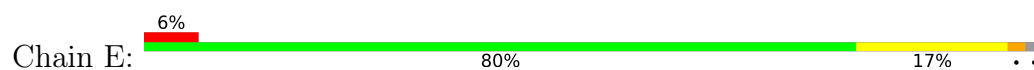
- Molecule 1: Ancestral Glucocorticoid Receptor2 ligand binding domain



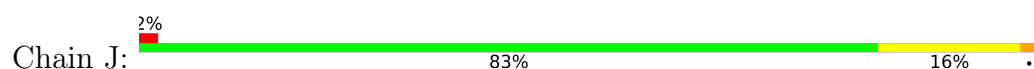
- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

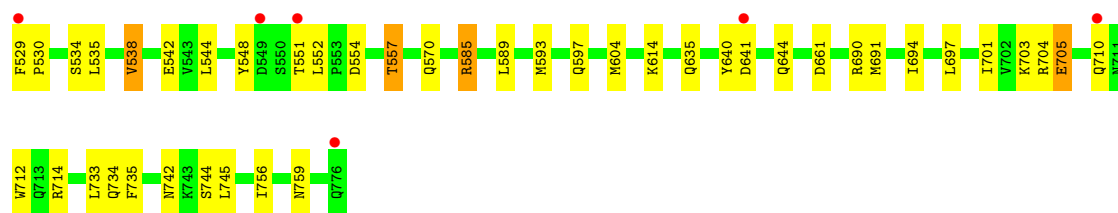


- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

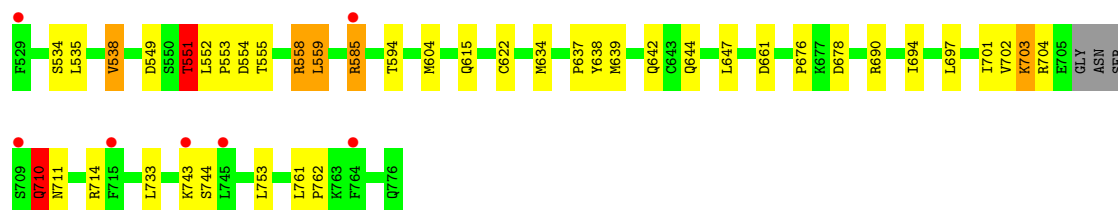
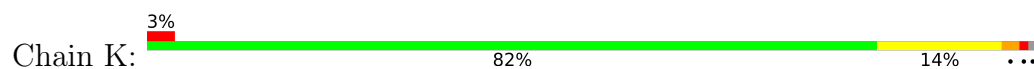


- Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

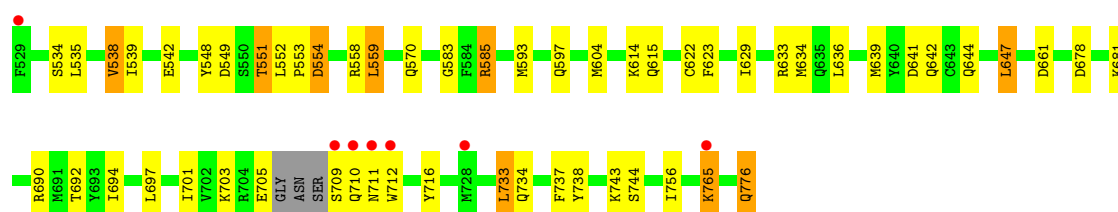
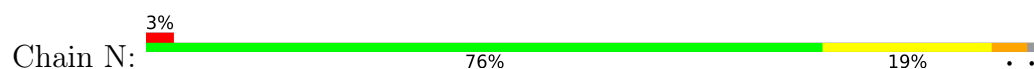




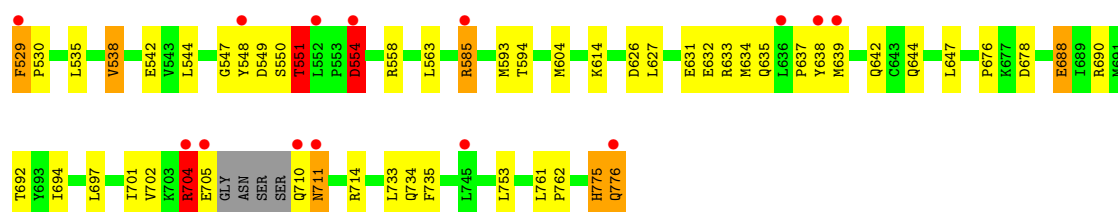
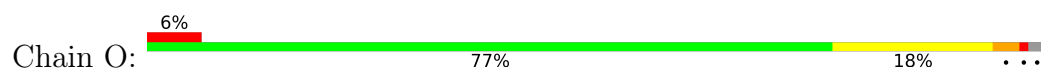
• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain



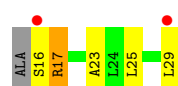
• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain



• Molecule 2: Ancestral Glucocorticoid Receptor2 ligand binding domain

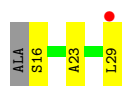


• Molecule 3: Nuclear receptor subfamily 0 group B member 2

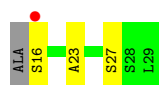
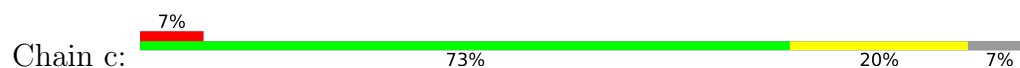


• Molecule 3: Nuclear receptor subfamily 0 group B member 2





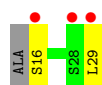
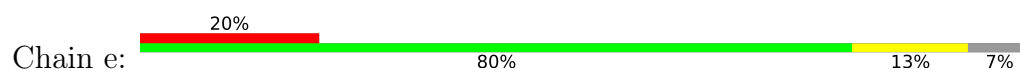
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



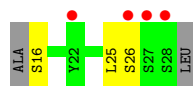
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



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



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



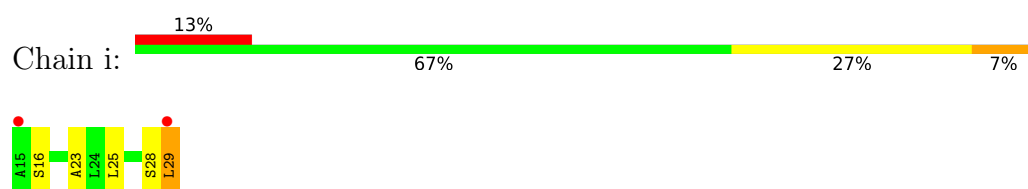
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



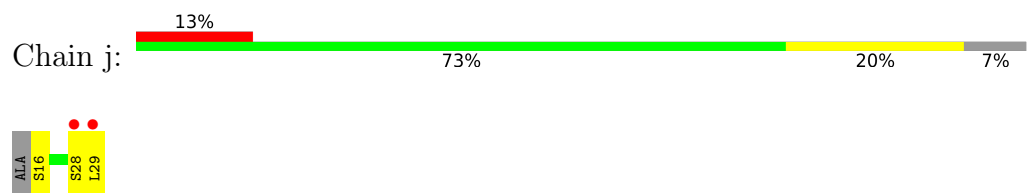
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



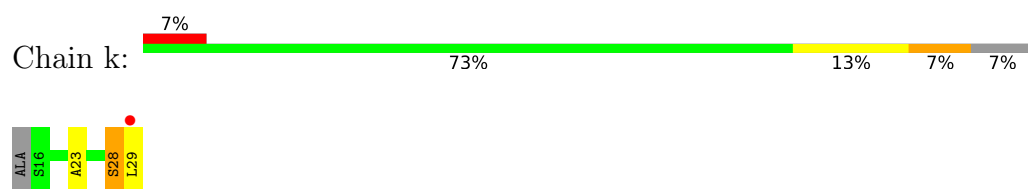
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



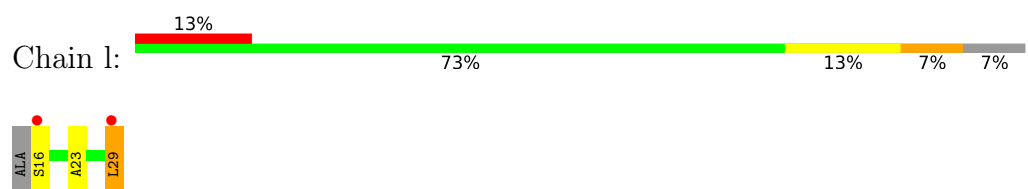
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



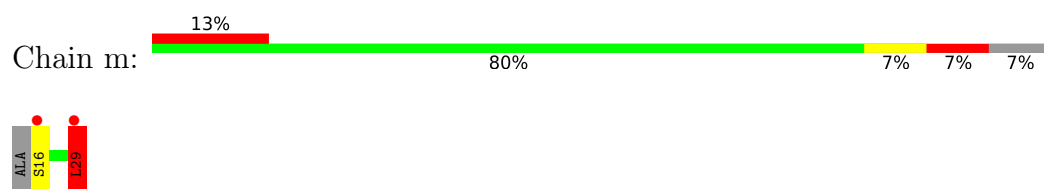
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



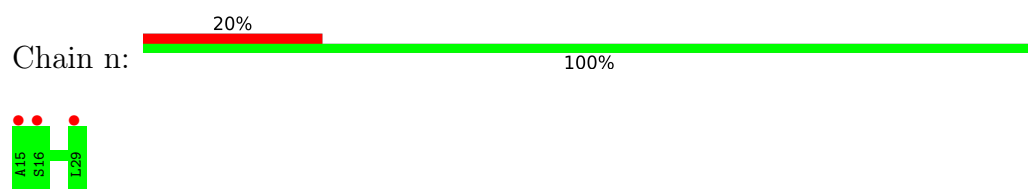
- Molecule 3: Nuclear receptor subfamily 0 group B member 2



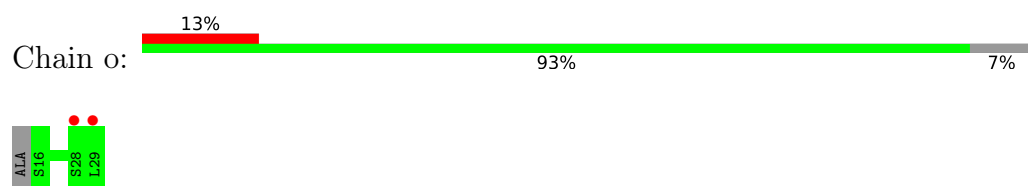
- Molecule 3: Nuclear receptor subfamily 0 group B member 2




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



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



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

Chain p:  27% 80% 13% 7%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

5.2 Too-close contacts ⓘ

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

The worst 5 of 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

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

5.3.1 Protein backbone

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 ⓘ

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3804/3818 (100%)	3612 (95%)	192 (5%)	22	51

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	538	VAL
2	N	538	VAL
2	K	703	LYS
1	L	648	LYS
2	N	681	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	619	ASN
1	L	597	GLN
2	J	645	GLN
2	K	726	HIS
1	M	619	ASN

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.

5 of 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

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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-
12	PEG	F	1002	-	-	1/4/4/4	-
6	EPE	D	804	-	-	2/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	DEX	L	1001	-	-	2/8/84/84	0/4/4/4
7	GOL	J	806	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

There are no ring outliers.

37 monomers are involved in 81 short contacts:

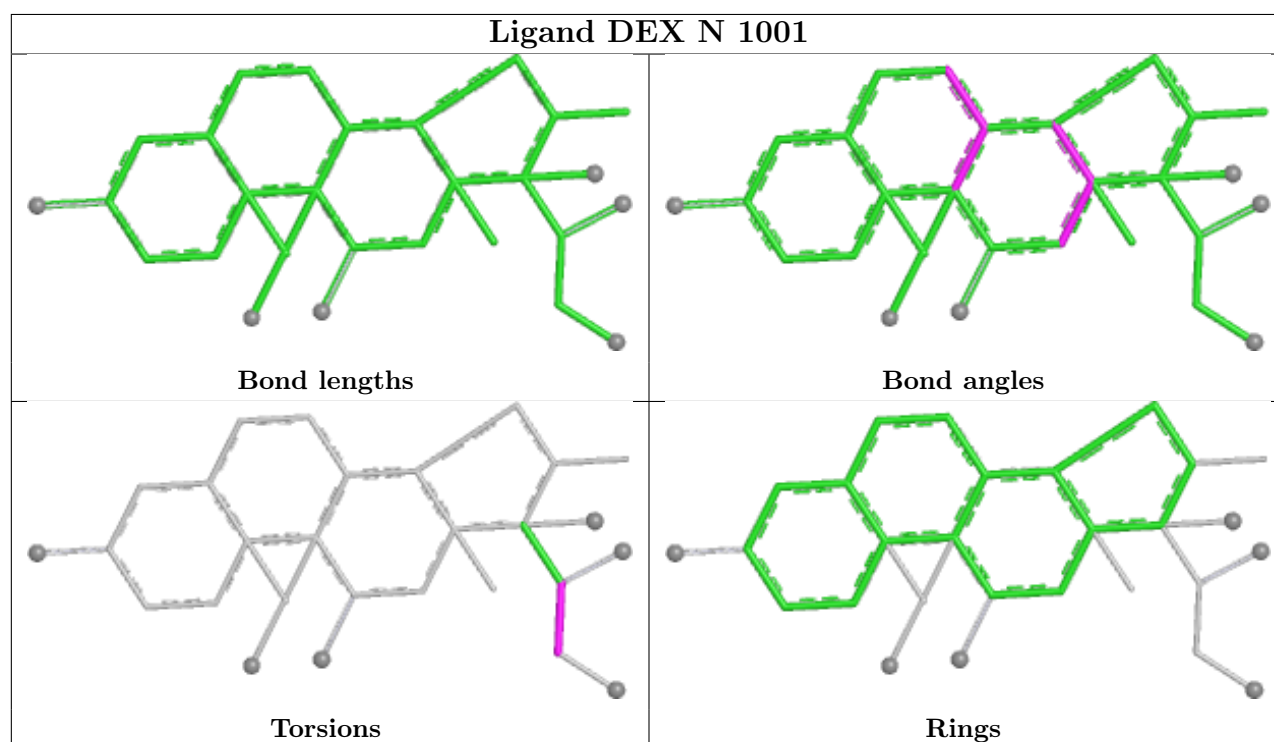
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	804	EPE	1	0
4	N	1001	DEX	2	0
4	M	802	DEX	1	0
4	K	802	DEX	2	0
6	I	1004	EPE	2	0
7	N	1002	GOL	1	0
4	A	1001	DEX	1	0
4	J	802	DEX	2	0
4	B	802	DEX	4	0
7	L	1004	GOL	4	0
6	L	1003	EPE	1	0
12	K	801	PEG	1	0
11	d	101	IMD	4	0
11	N	1003	IMD	2	0
7	C	1003	GOL	3	0
4	I	1001	DEX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

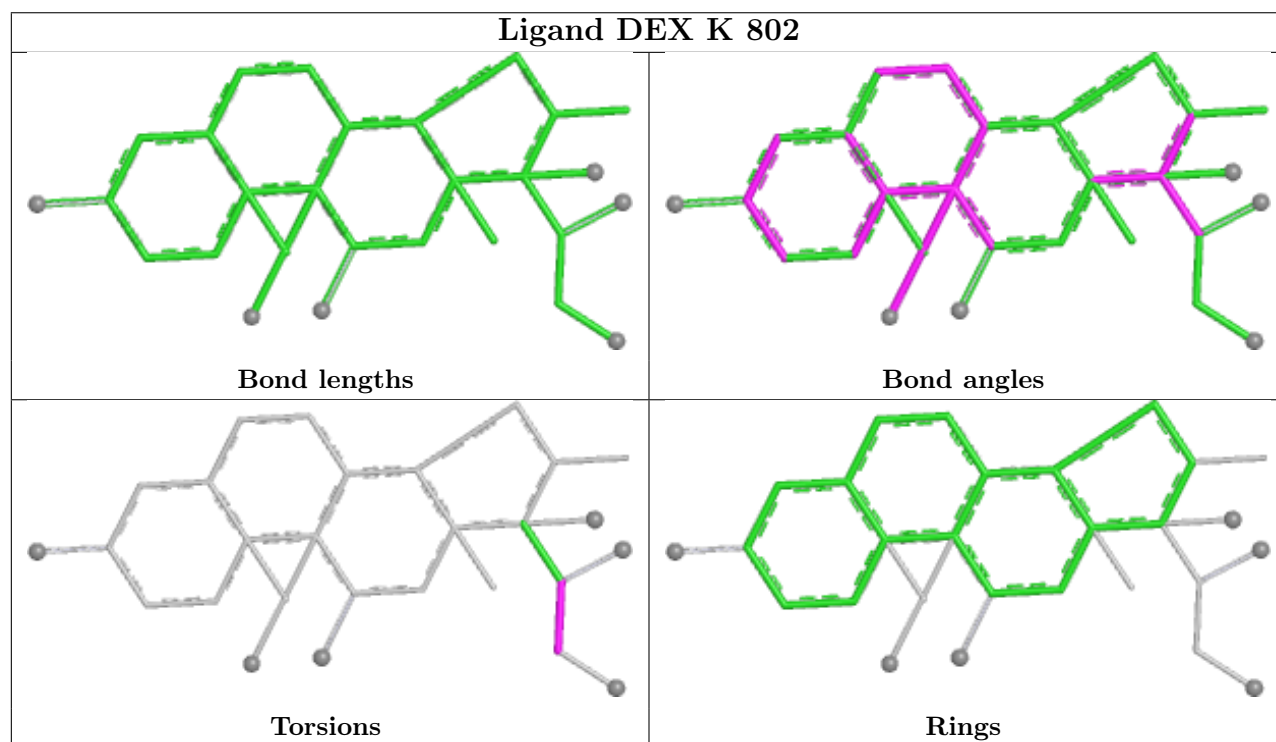
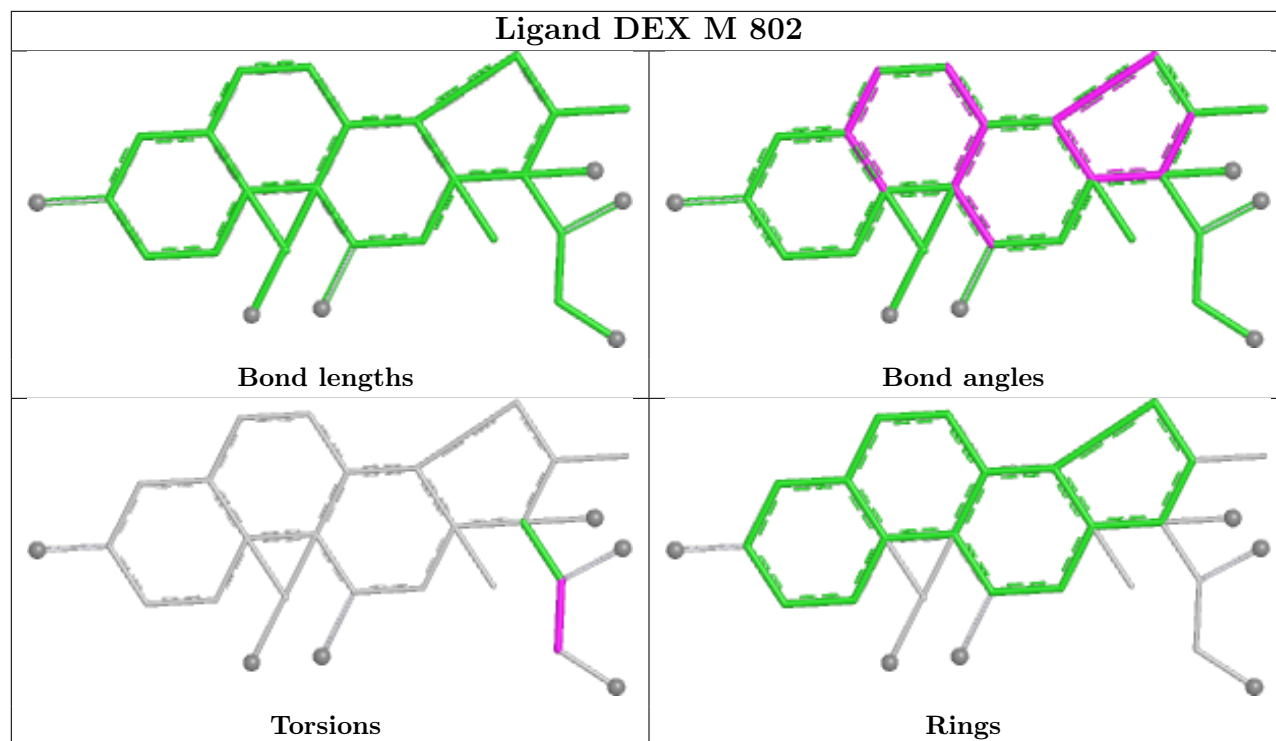
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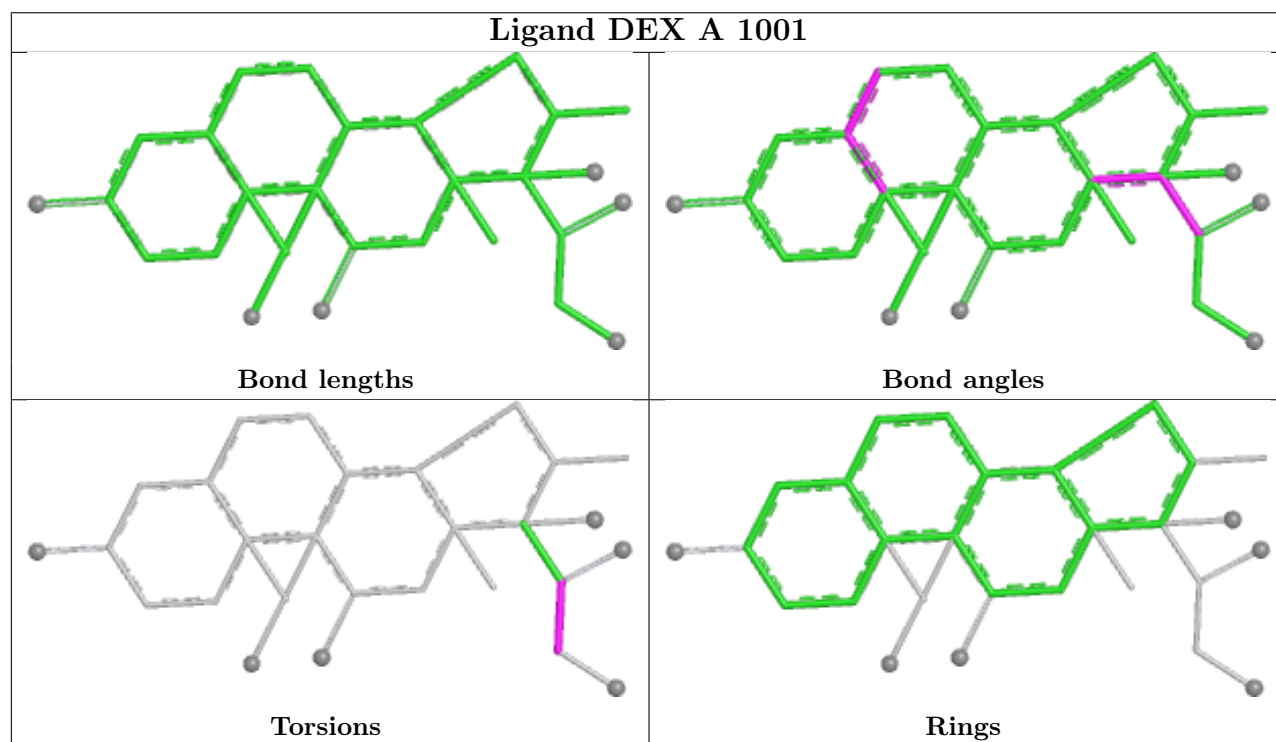
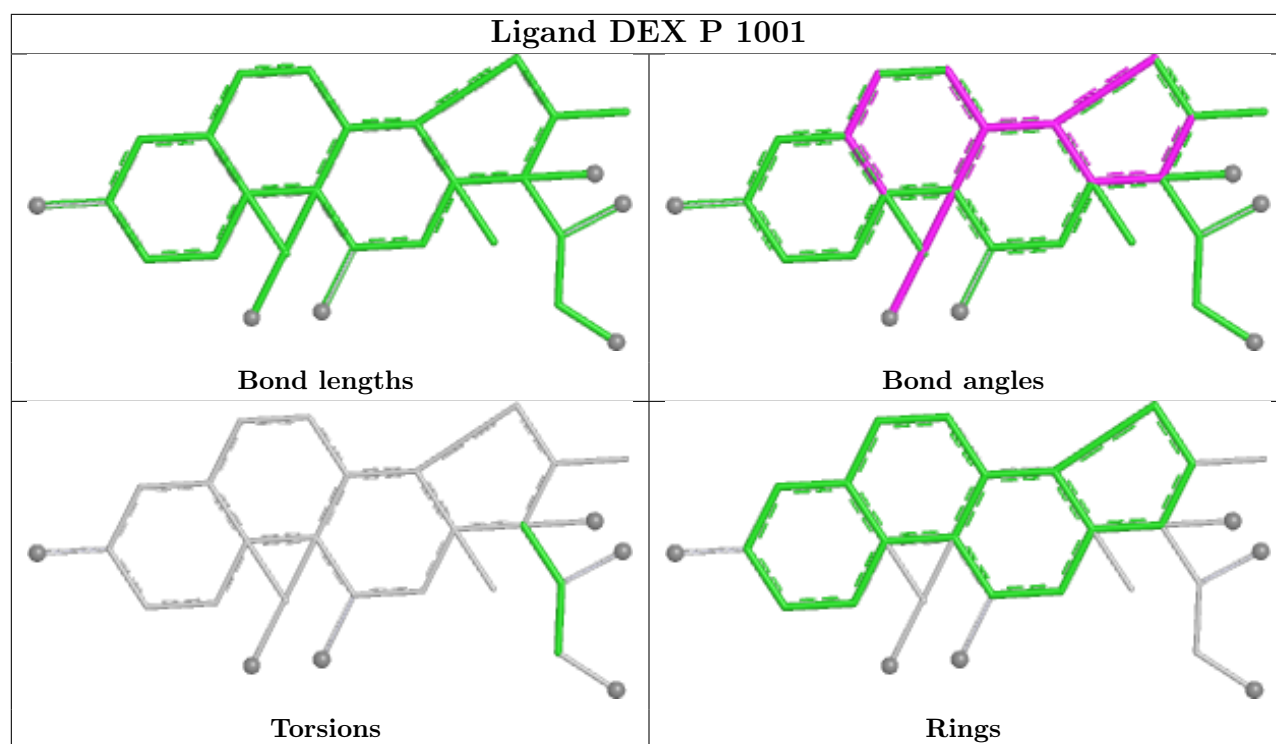
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1005	GOL	1	0
13	M	804	PGE	2	0
4	E	1001	DEX	3	0
6	P	1002	EPE	12	0

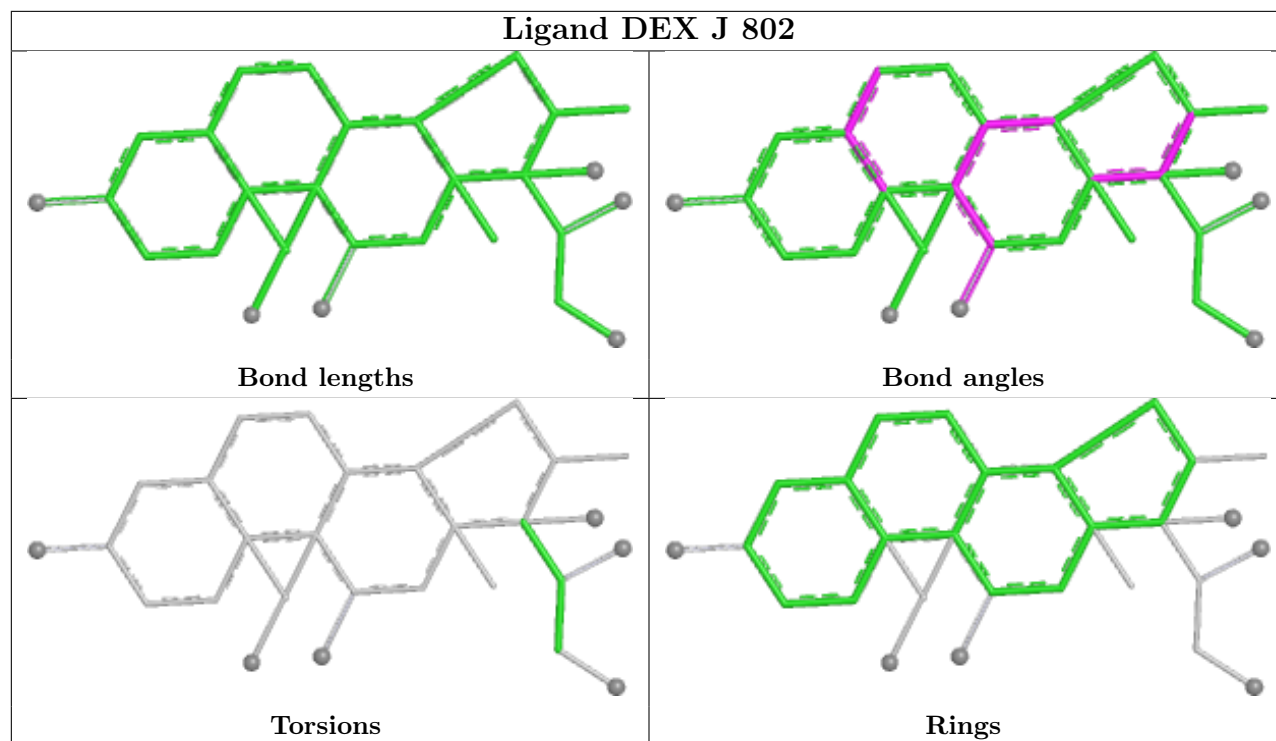
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



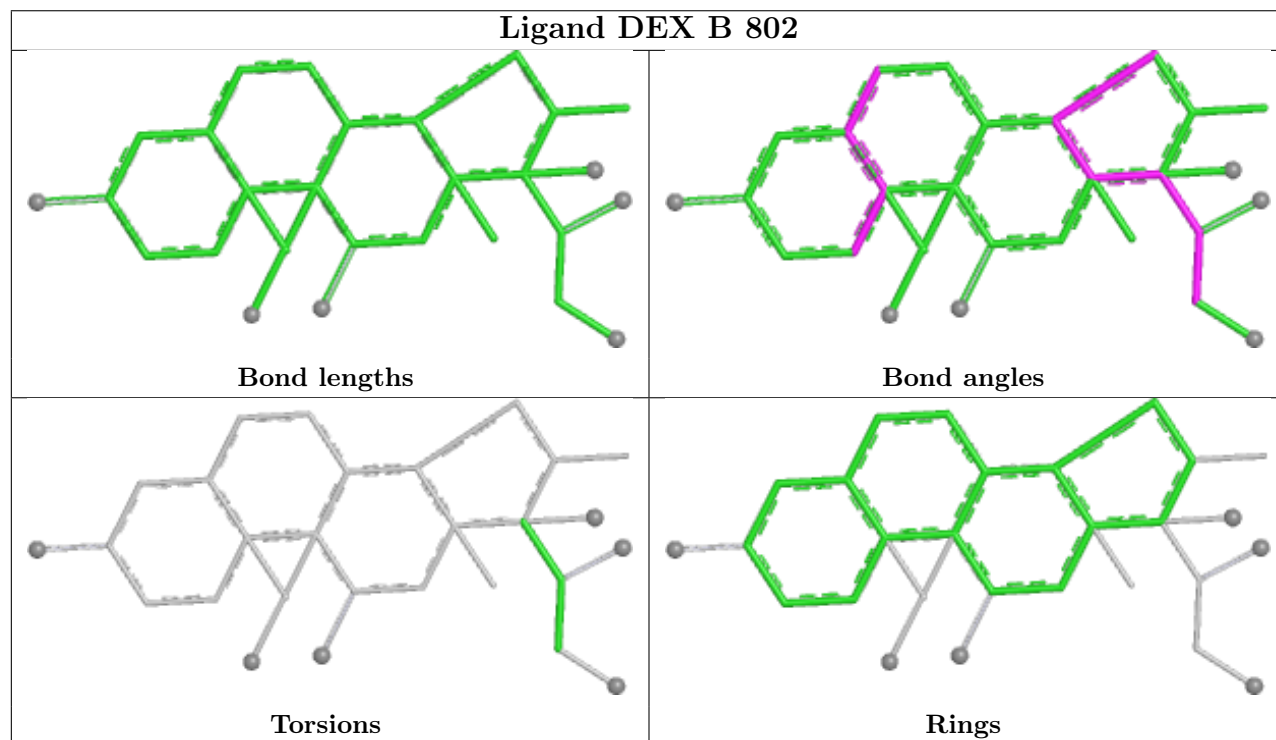


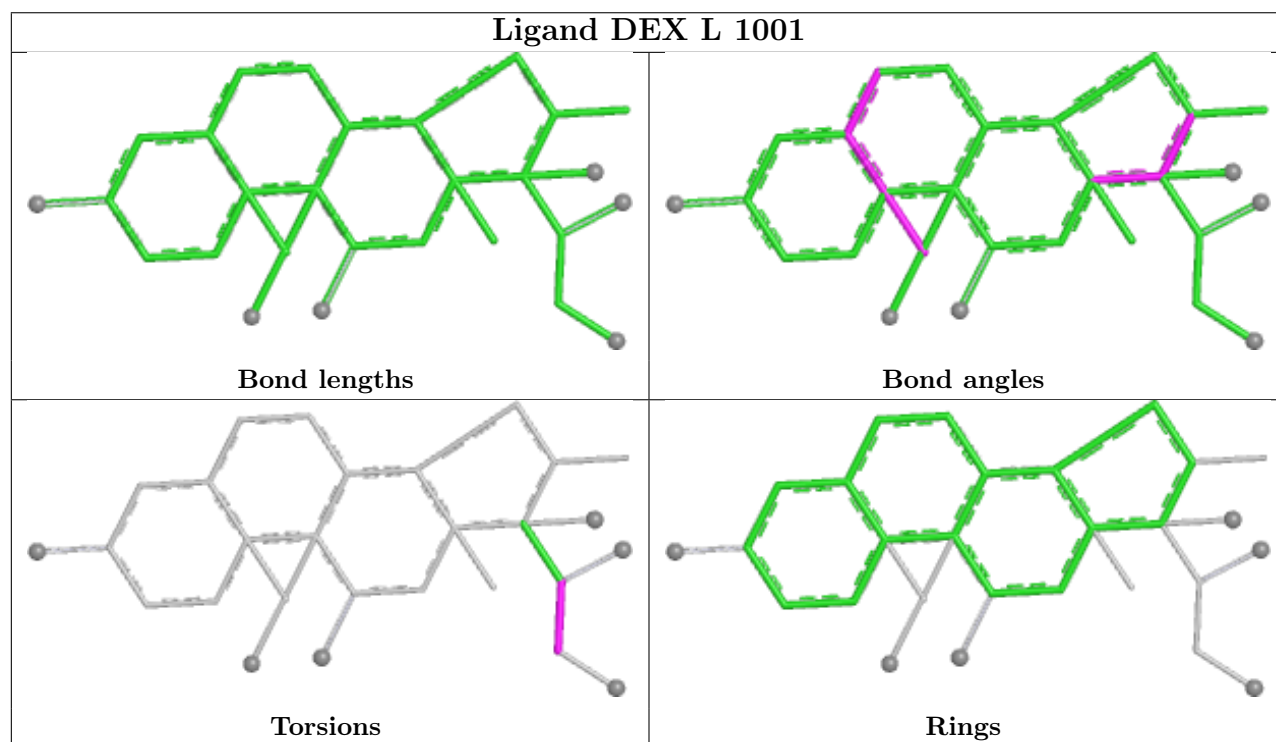
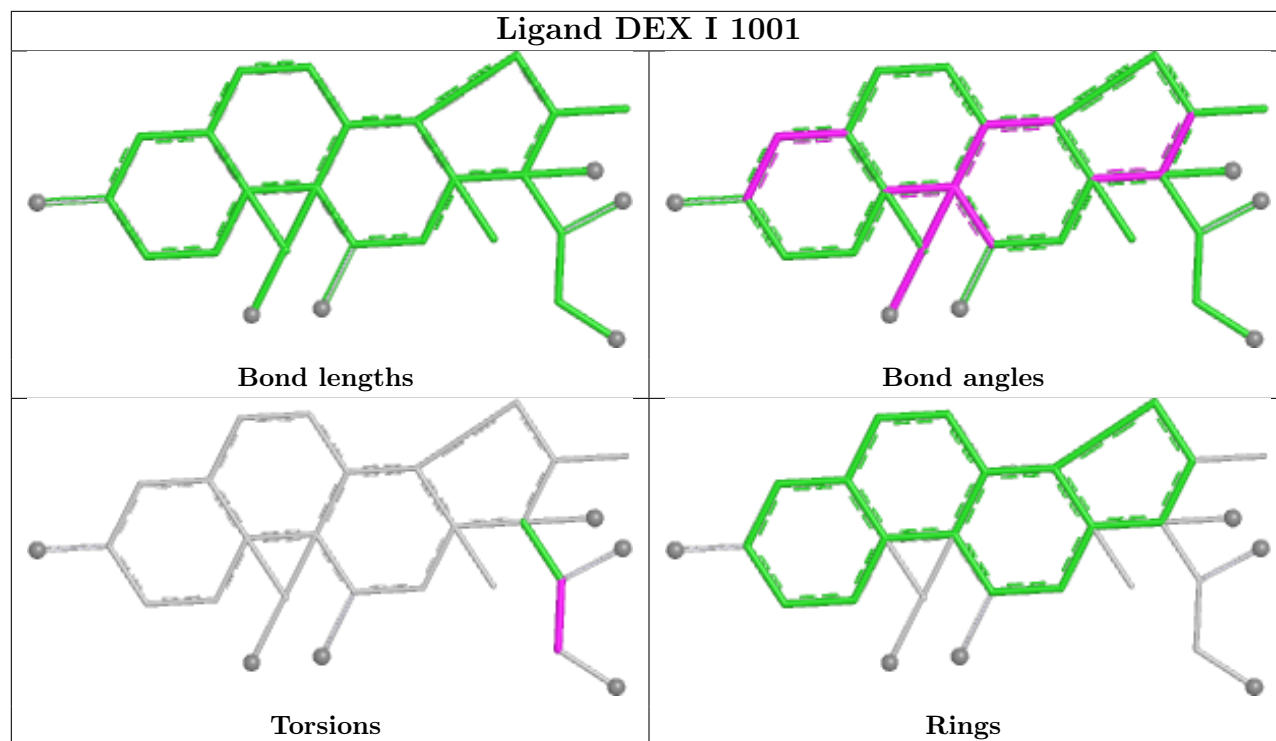


Ligand DEX J 802

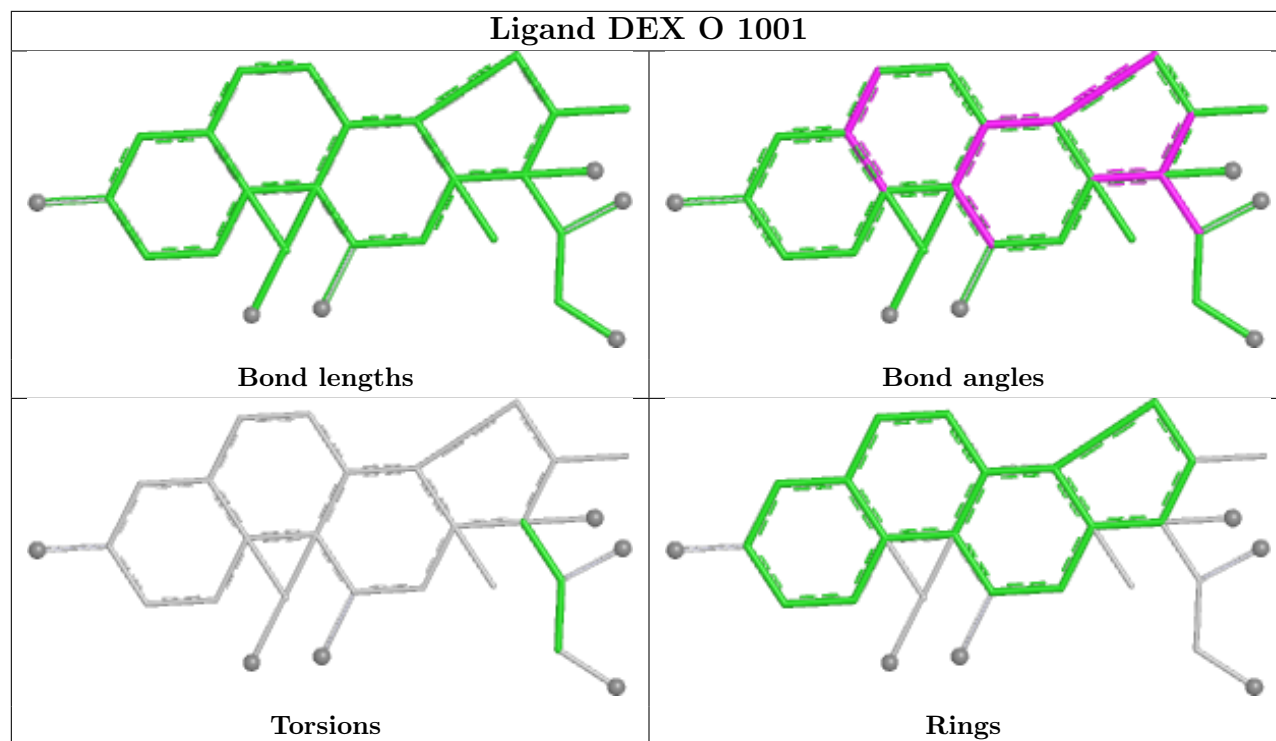


Ligand DEX B 802

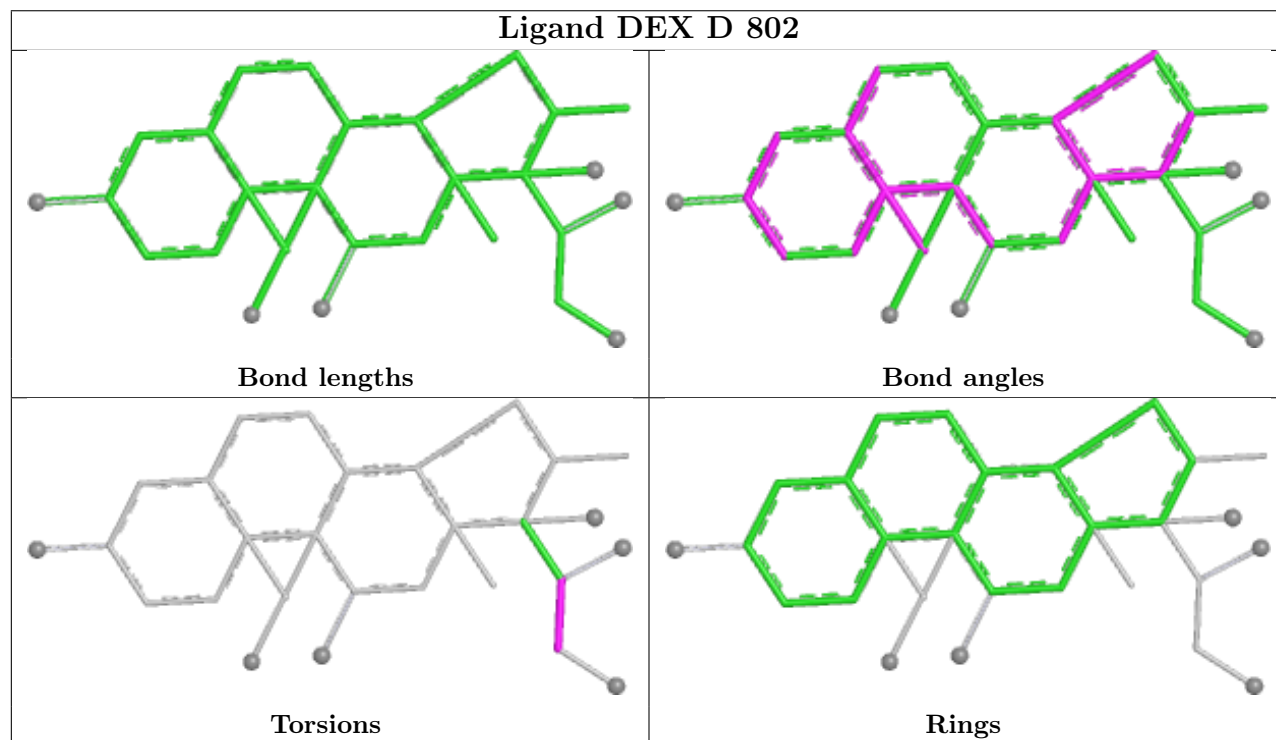


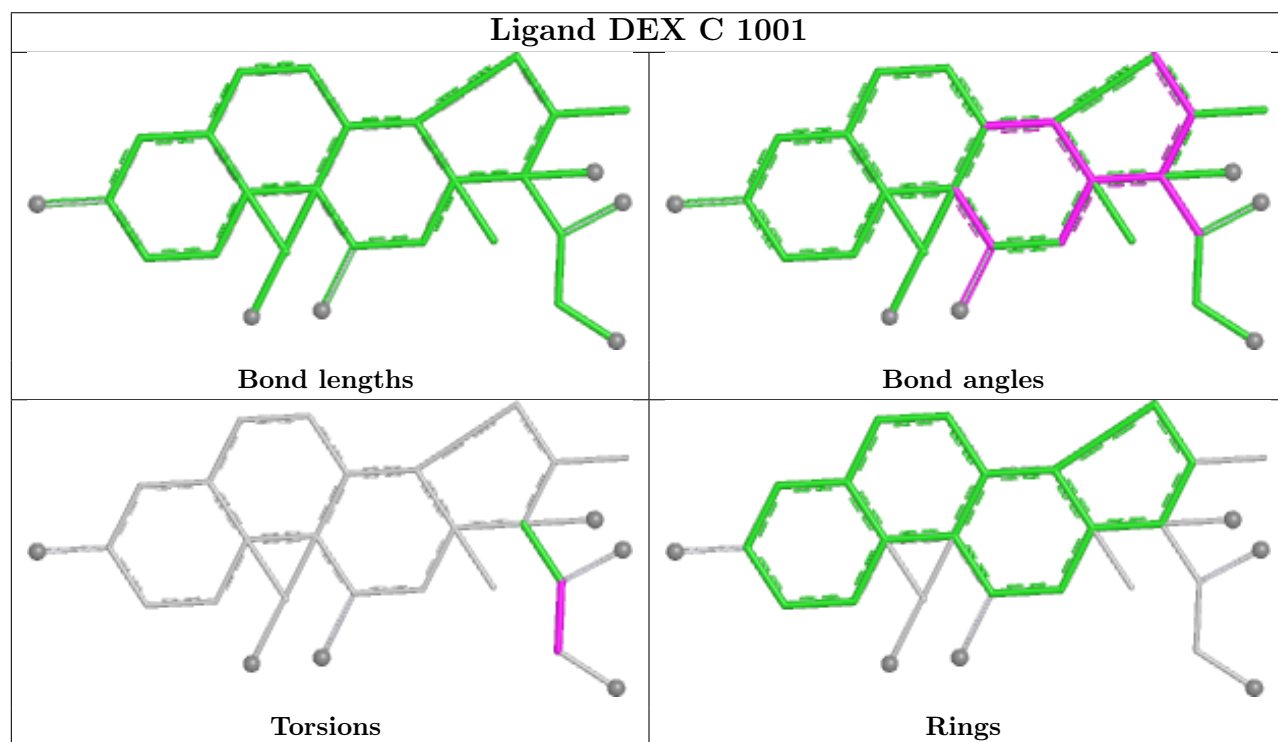
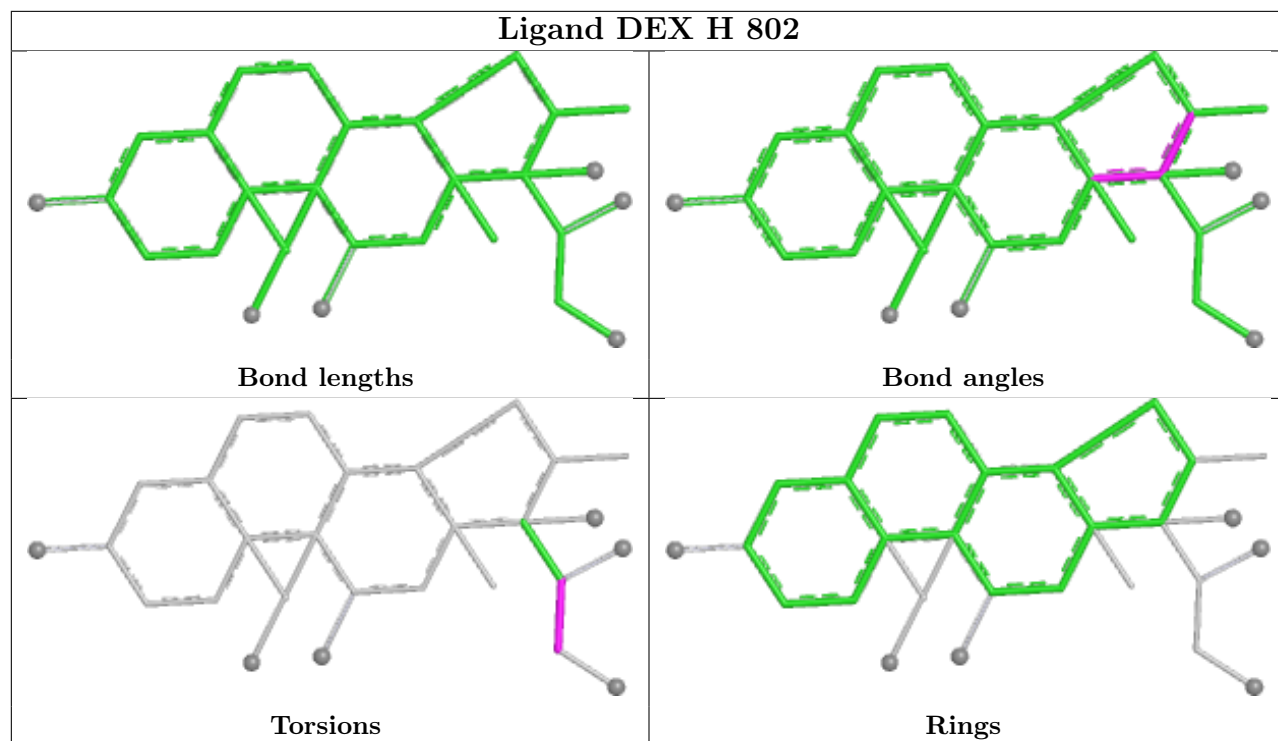


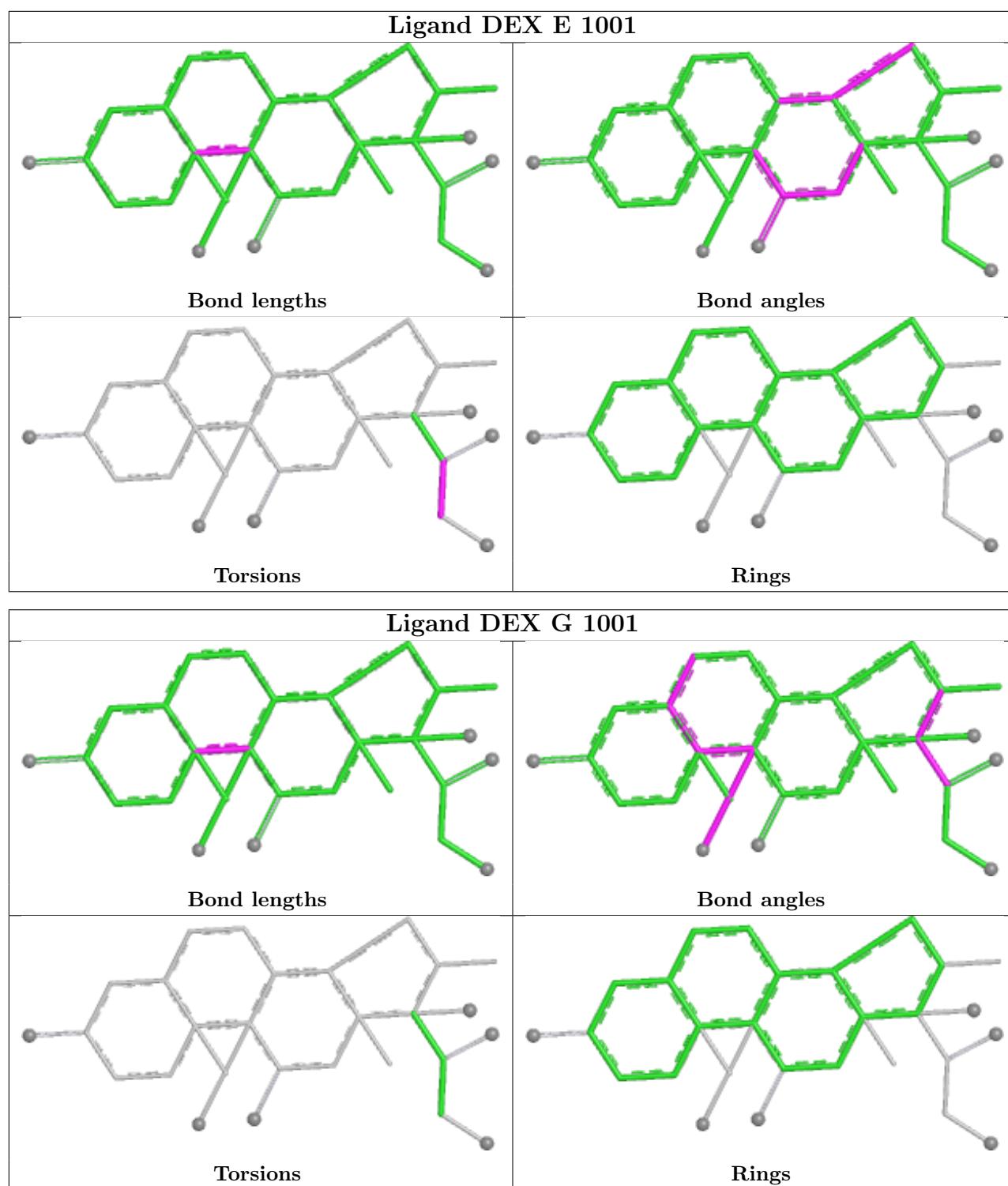
Ligand DEX O 1001



Ligand DEX D 802







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)

The worst 5 of 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

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

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(\AA^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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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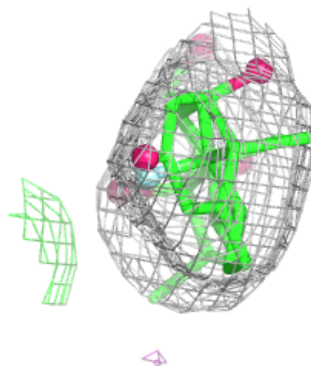
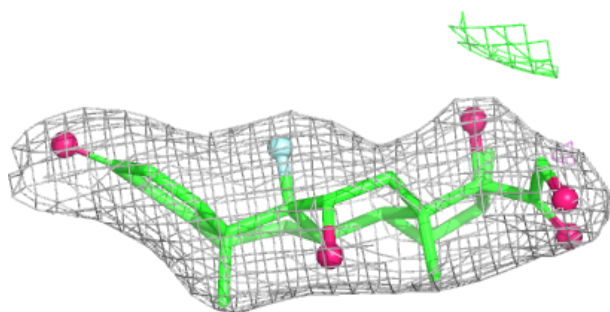
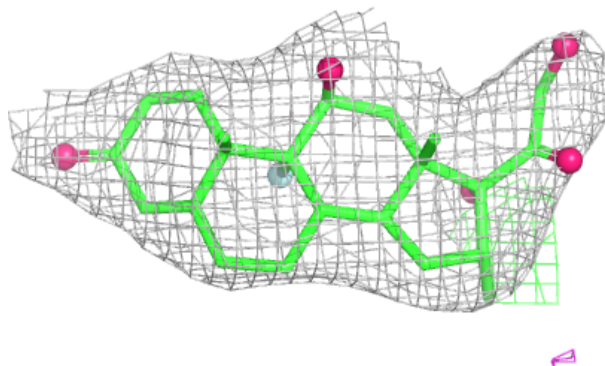
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DEX	F	1001	28/28	0.97	0.07	45,60,68,75	0
4	DEX	E	1001	28/28	0.97	0.07	36,40,47,57	0
4	DEX	K	802	28/28	0.97	0.07	32,44,57,65	0
7	GOL	E	1004	6/6	0.97	0.09	52,56,60,60	0
4	DEX	A	1001	28/28	0.98	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
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

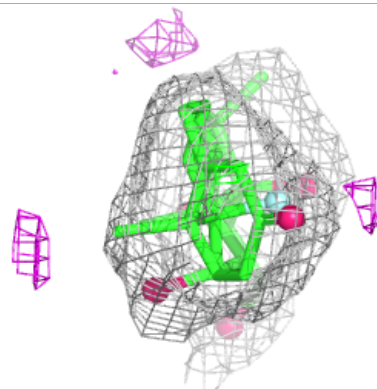
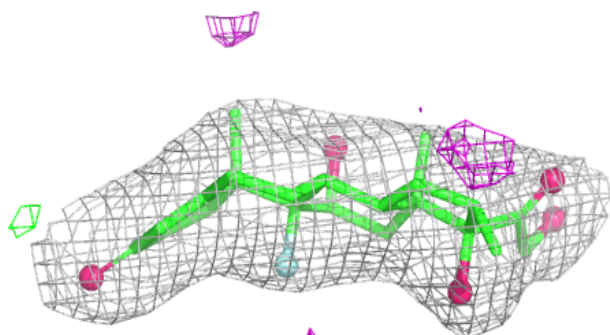
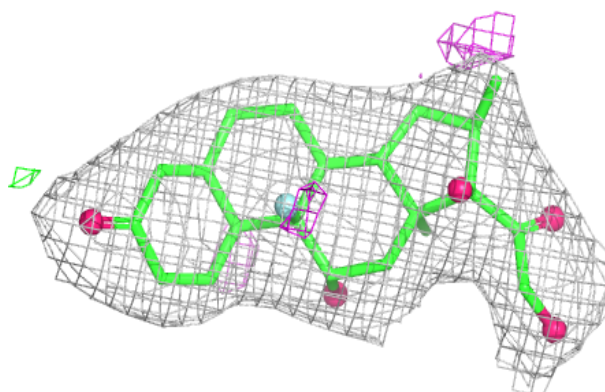
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

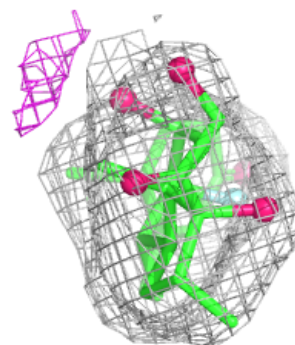
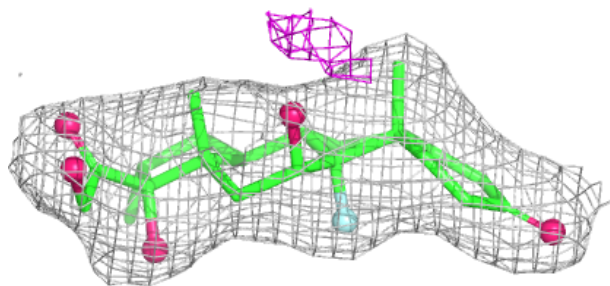
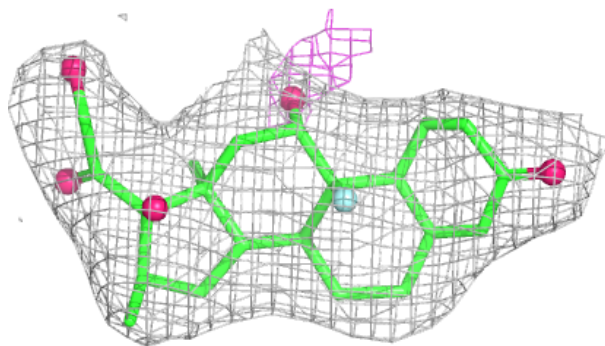
**Electron density around DEX E 1001:**

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

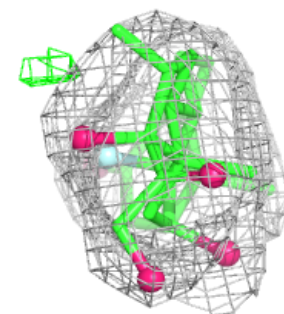
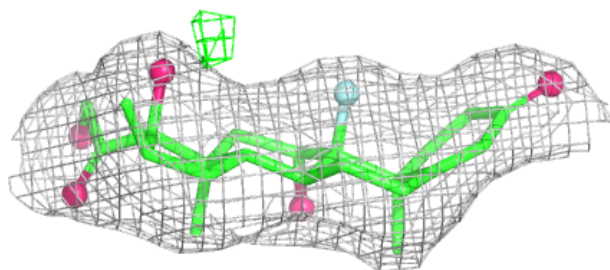
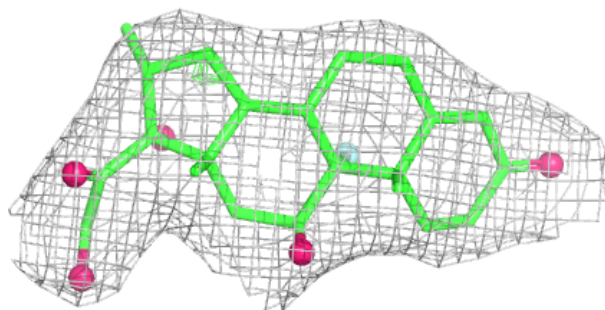


Electron density around DEX K 802:

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

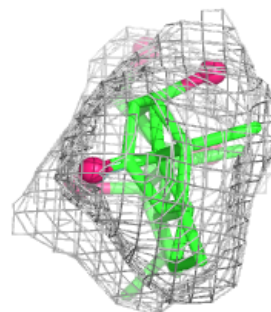
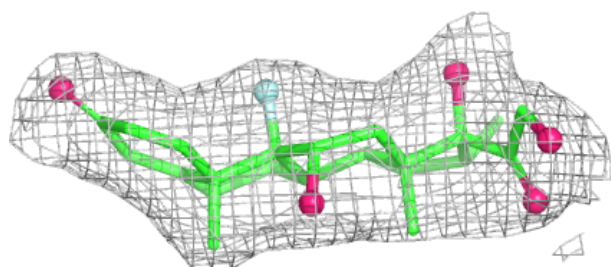
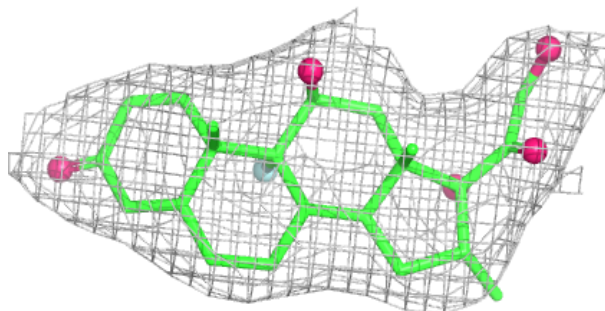
**Electron density around DEX A 1001:**

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

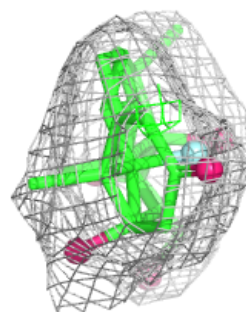
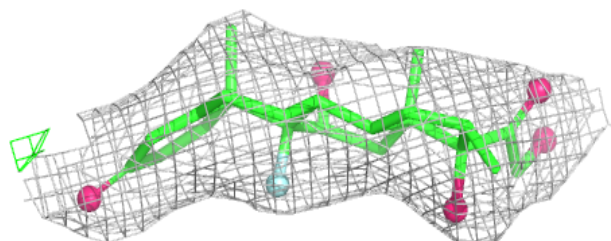
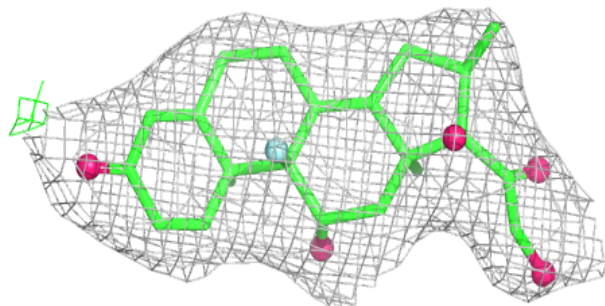


Electron density around DEX B 802:

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

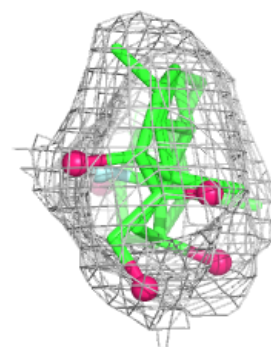
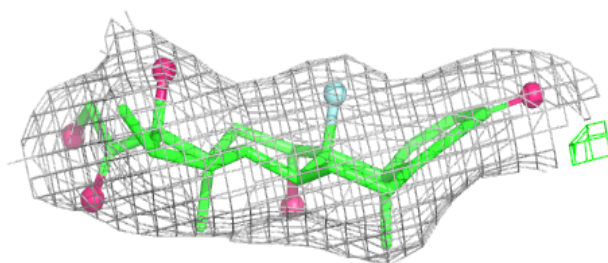
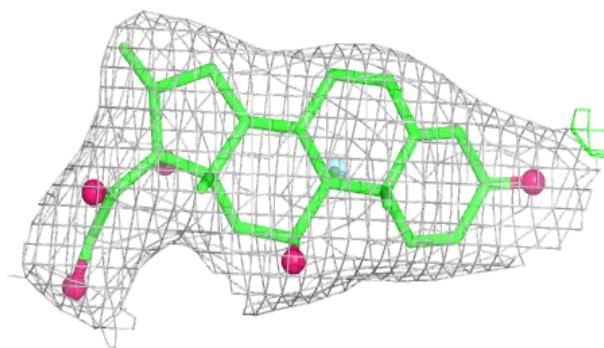
**Electron density around DEX G 1001:**

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

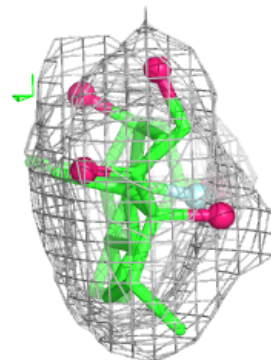
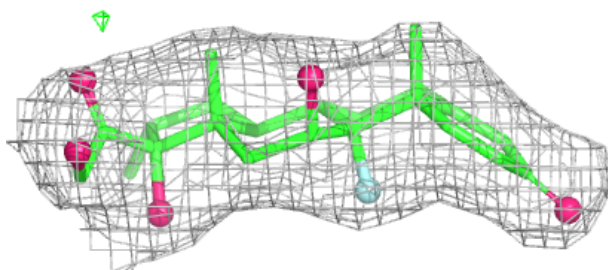
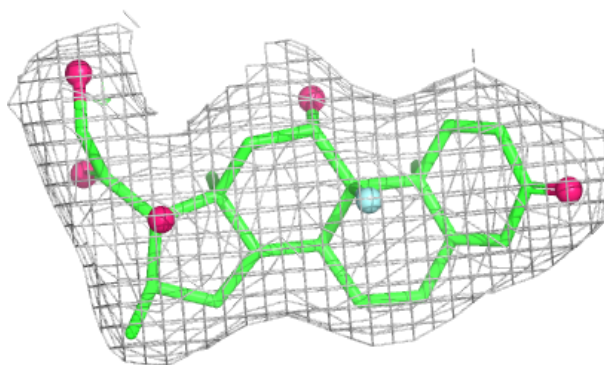


Electron density around DEX C 1001:

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

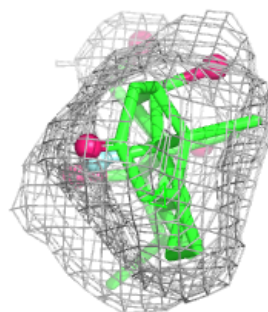
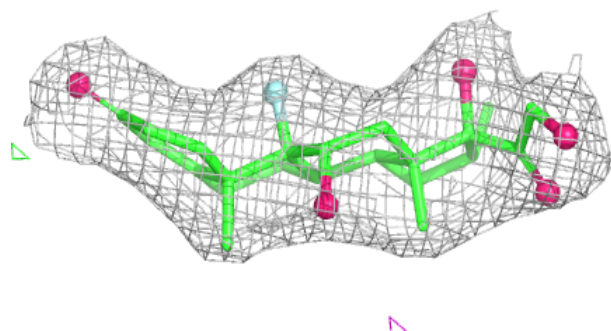
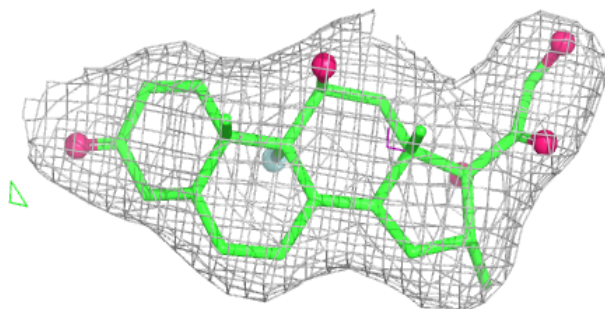
**Electron density around DEX I 1001:**

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

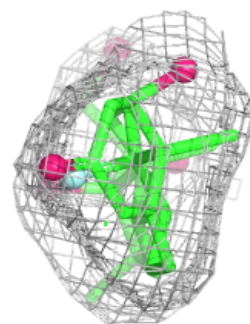
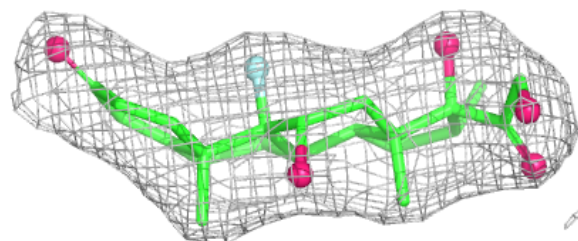
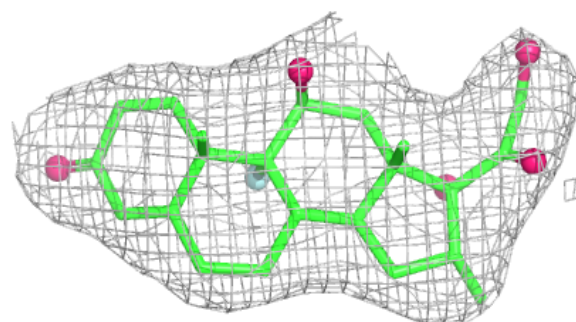


Electron density around DEX J 802:

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

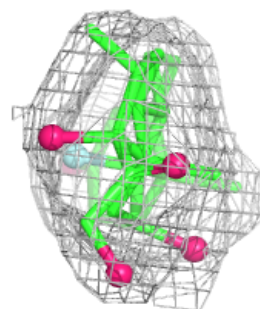
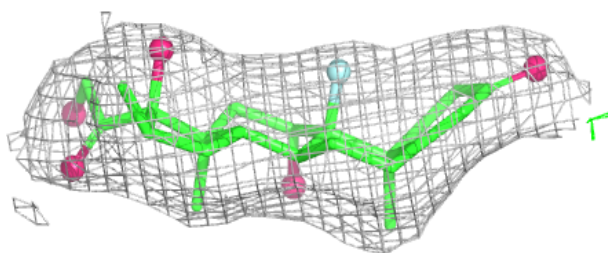
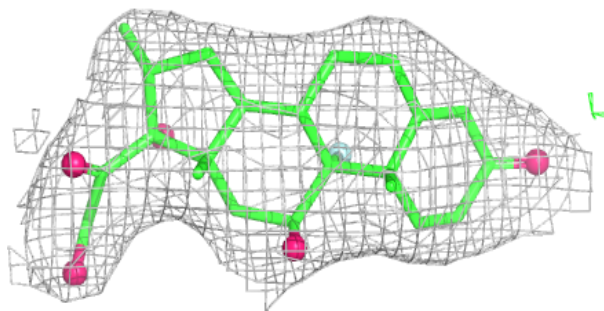
**Electron density around DEX D 802:**

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

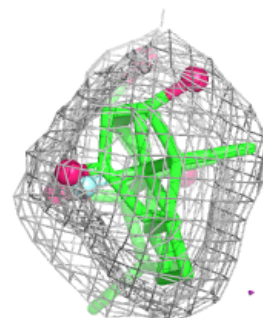
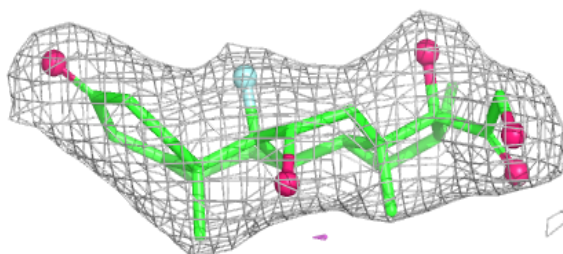
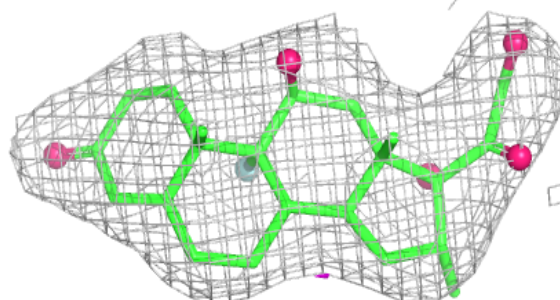


Electron density around DEX L 1001:

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

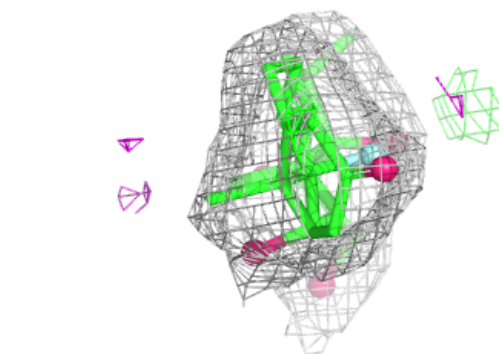
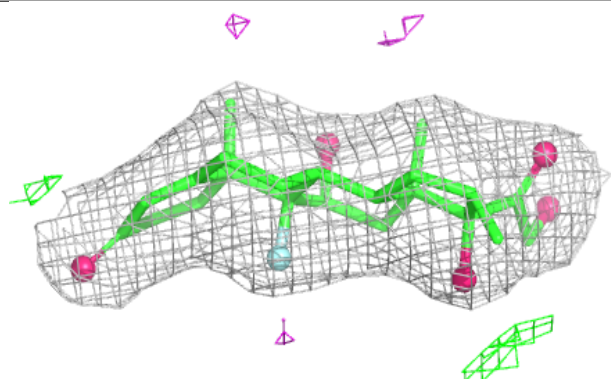
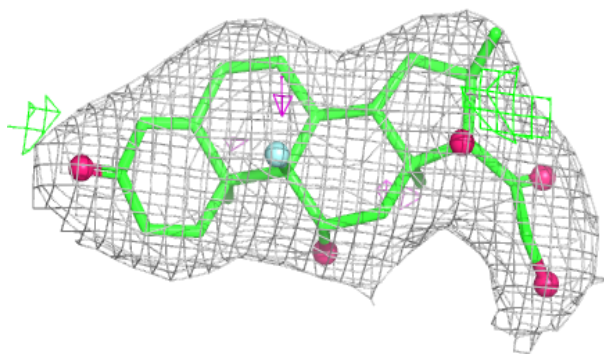
**Electron density around DEX M 802:**

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

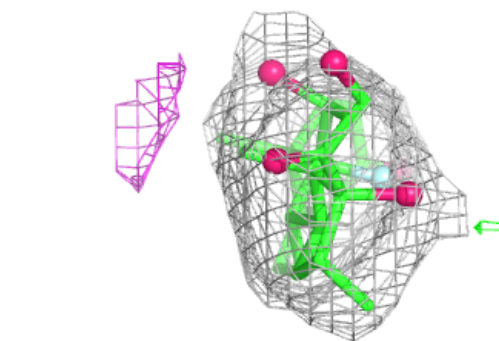
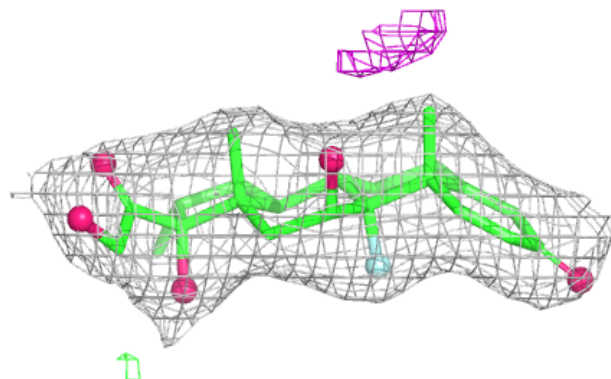


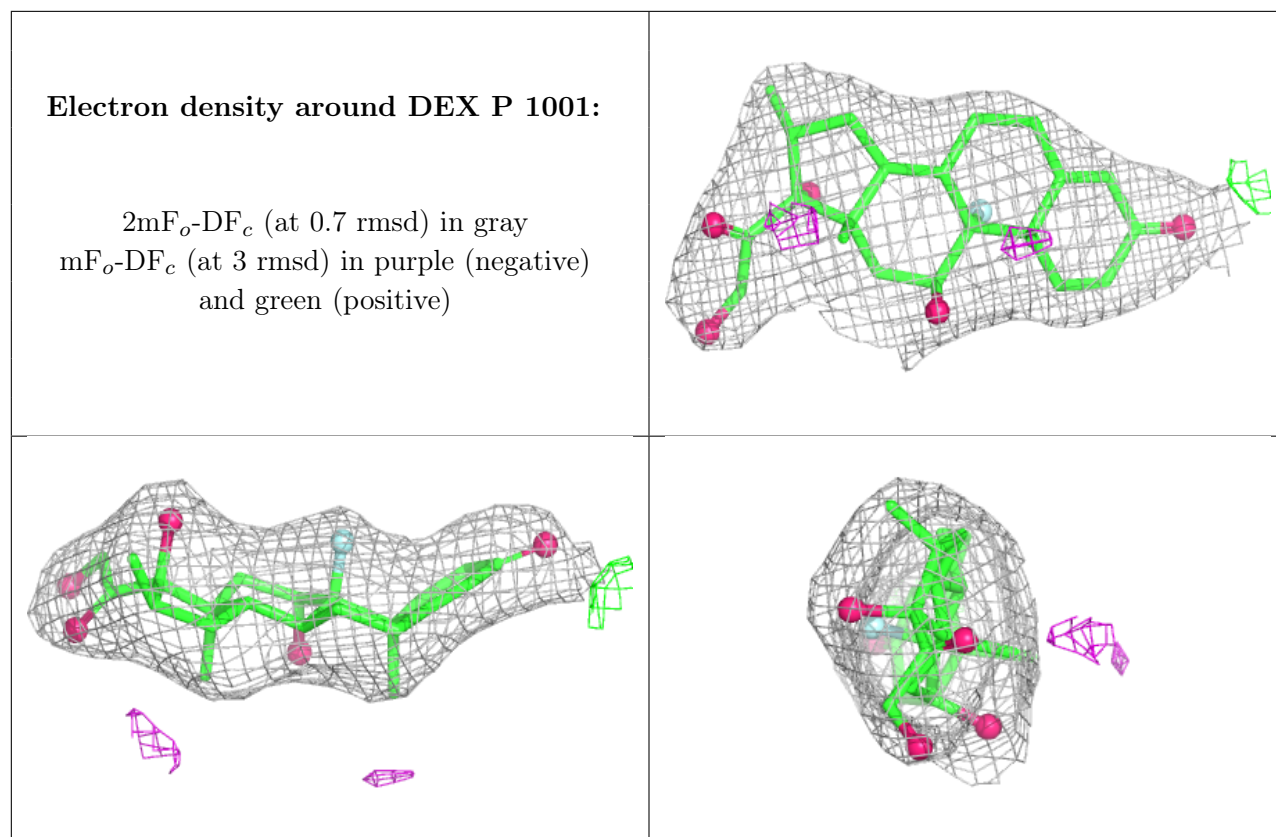
Electron density around DEX N 1001:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.