Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 10:18 PM EDT

PDB ID	:	6TEP
Title	:	Crystal structure of a galactokinase from Bifidobacterium infantis in complex with ADP
Authors	:	Keenan, T.; Parmeggiani, F.; Fontenelle, C.Q.; Malassis, J.; Vendeville, J.; Offen, W.A.; Both, P.; Huang, K.; Marchesi, A.; Heyam, A.; Young, C.; Charnock, S.; Davies, G.J.; Linclau, B.; Flitsch, S.L.; Fascione, M.A.
Deposited on	:	2019-11-12
Resolution	:	1.45 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 (1)) were used in the production of this report:

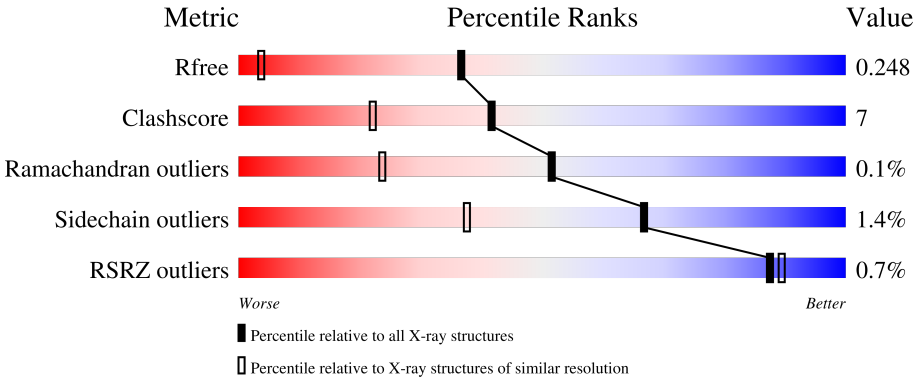
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.45 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}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	429	86% 10% • •
1	B	429	86% 11% •
1	C	429	89% 8% •
1	D	429	2% 84% 12% • •

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
2	PEG	B	501	-	-	X	-
2	PEG	B	503	-	-	-	X
2	PEG	D	503	-	-	X	-
3	GOL	A	502	-	-	X	-
3	GOL	B	506	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14438 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 Galactokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	15	0
			3193	1988	562	629	14			
1	D	413	Total	C	N	O	S	0	16	0
			3194	1991	559	630	14			
1	C	415	Total	C	N	O	S	0	12	0
			3161	1972	552	623	14			
1	B	416	Total	C	N	O	S	0	11	0
			3154	1961	553	628	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LYS	-	expression tag	UNP B7GUI0
A	418	LEU	-	expression tag	UNP B7GUI0
A	419	ALA	-	expression tag	UNP B7GUI0
A	420	ALA	-	expression tag	UNP B7GUI0
A	421	ALA	-	expression tag	UNP B7GUI0
A	422	LEU	-	expression tag	UNP B7GUI0
A	423	GLU	-	expression tag	UNP B7GUI0
A	424	HIS	-	expression tag	UNP B7GUI0
A	425	HIS	-	expression tag	UNP B7GUI0
A	426	HIS	-	expression tag	UNP B7GUI0
A	427	HIS	-	expression tag	UNP B7GUI0
A	428	HIS	-	expression tag	UNP B7GUI0
A	429	HIS	-	expression tag	UNP B7GUI0
D	417	LYS	-	expression tag	UNP B7GUI0
D	418	LEU	-	expression tag	UNP B7GUI0
D	419	ALA	-	expression tag	UNP B7GUI0
D	420	ALA	-	expression tag	UNP B7GUI0
D	421	ALA	-	expression tag	UNP B7GUI0
D	422	LEU	-	expression tag	UNP B7GUI0
D	423	GLU	-	expression tag	UNP B7GUI0
D	424	HIS	-	expression tag	UNP B7GUI0

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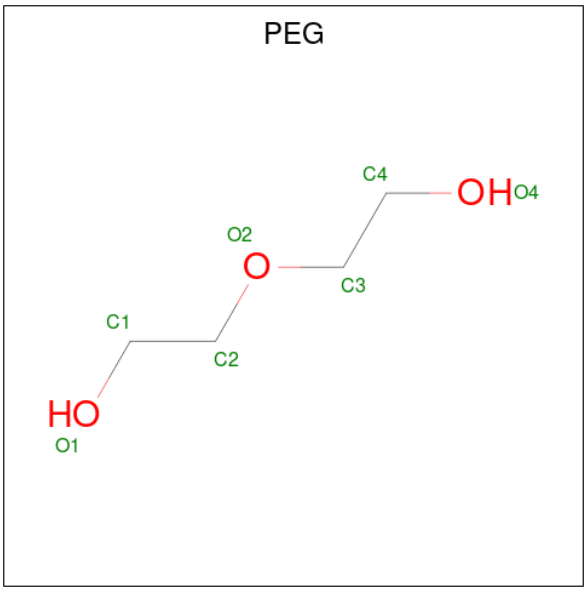
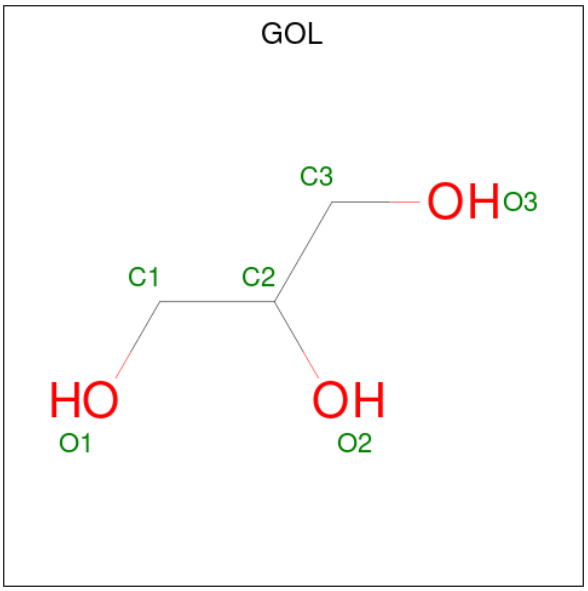
Chain	Residue	Modelled	Actual	Comment	Reference
D	425	HIS	-	expression tag	UNP B7GUI0
D	426	HIS	-	expression tag	UNP B7GUI0
D	427	HIS	-	expression tag	UNP B7GUI0
D	428	HIS	-	expression tag	UNP B7GUI0
D	429	HIS	-	expression tag	UNP B7GUI0
C	417	LYS	-	expression tag	UNP B7GUI0
C	418	LEU	-	expression tag	UNP B7GUI0
C	419	ALA	-	expression tag	UNP B7GUI0
C	420	ALA	-	expression tag	UNP B7GUI0
C	421	ALA	-	expression tag	UNP B7GUI0
C	422	LEU	-	expression tag	UNP B7GUI0
C	423	GLU	-	expression tag	UNP B7GUI0
C	424	HIS	-	expression tag	UNP B7GUI0
C	425	HIS	-	expression tag	UNP B7GUI0
C	426	HIS	-	expression tag	UNP B7GUI0
C	427	HIS	-	expression tag	UNP B7GUI0
C	428	HIS	-	expression tag	UNP B7GUI0
C	429	HIS	-	expression tag	UNP B7GUI0
B	417	LYS	-	expression tag	UNP B7GUI0
B	418	LEU	-	expression tag	UNP B7GUI0
B	419	ALA	-	expression tag	UNP B7GUI0
B	420	ALA	-	expression tag	UNP B7GUI0
B	421	ALA	-	expression tag	UNP B7GUI0
B	422	LEU	-	expression tag	UNP B7GUI0
B	423	GLU	-	expression tag	UNP B7GUI0
B	424	HIS	-	expression tag	UNP B7GUI0
B	425	HIS	-	expression tag	UNP B7GUI0
B	426	HIS	-	expression tag	UNP B7GUI0
B	427	HIS	-	expression tag	UNP B7GUI0
B	428	HIS	-	expression tag	UNP B7GUI0
B	429	HIS	-	expression tag	UNP B7GUI0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



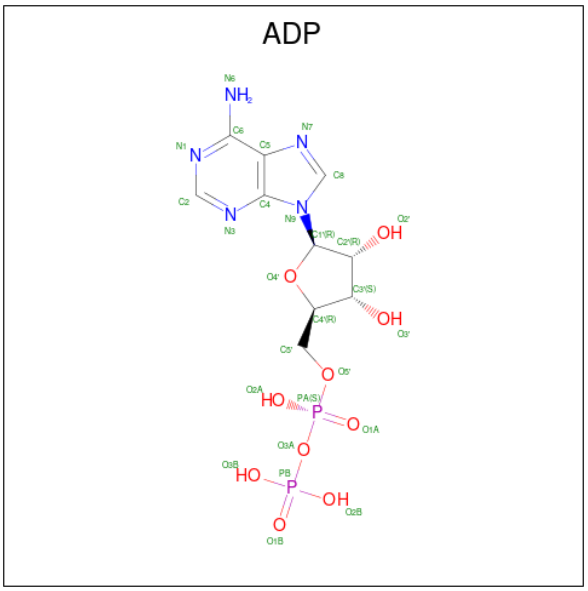
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	D	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	C	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0
2	B	1	Total C O 7 4 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	D	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

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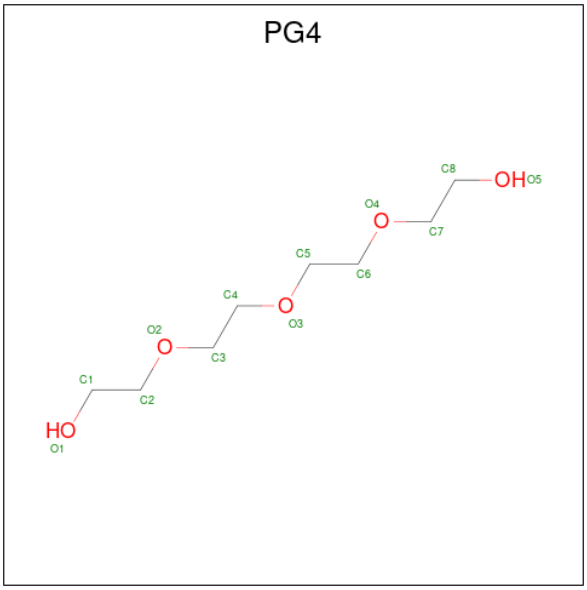
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

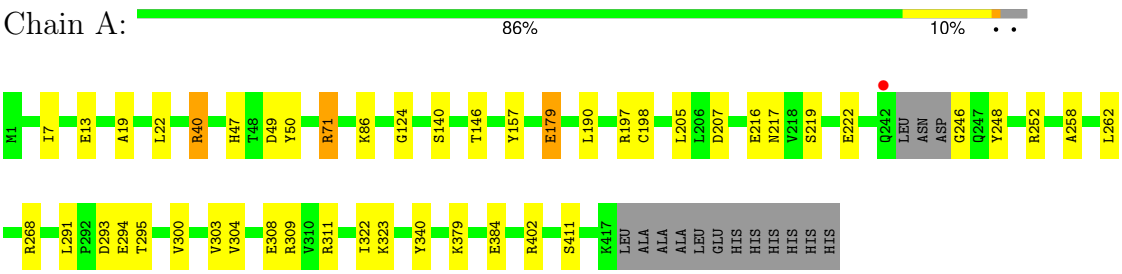
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	354	Total O 354 354	0	0
8	D	345	Total O 345 345	0	0
8	C	380	Total O 380 380	0	0
8	B	396	Total O 396 396	0	0

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.

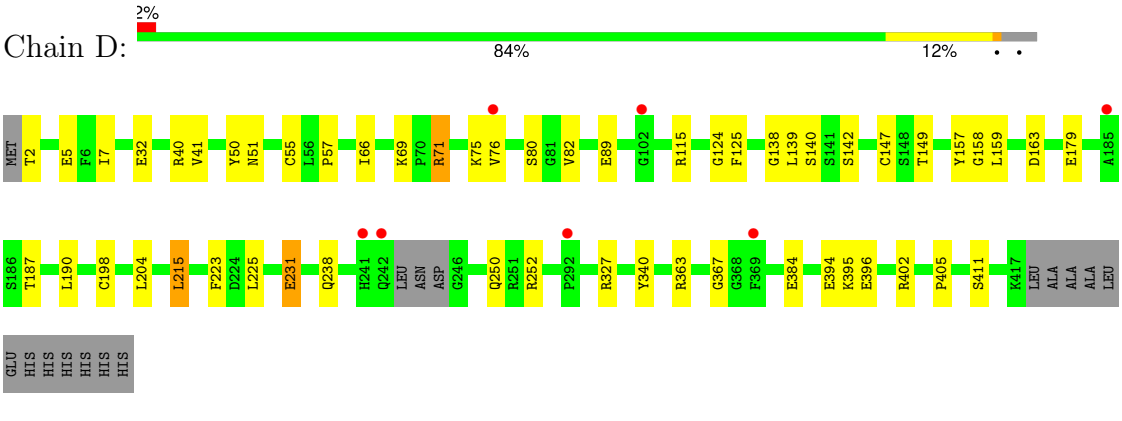
• Molecule 1: Galactokinase

Chain A:



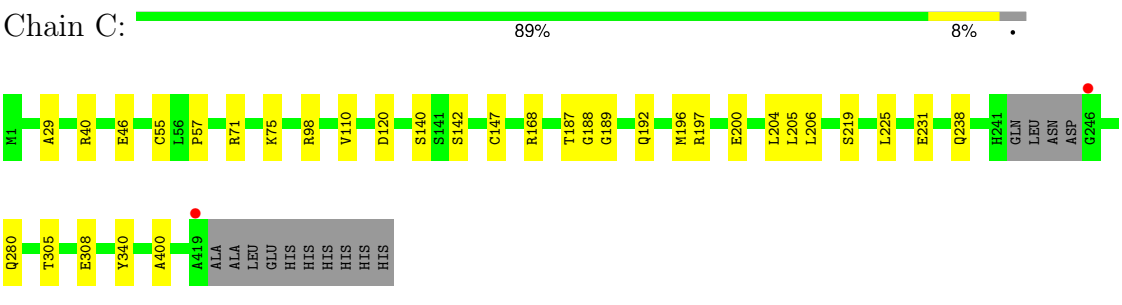
• Molecule 1: Galactokinase

Chain D:



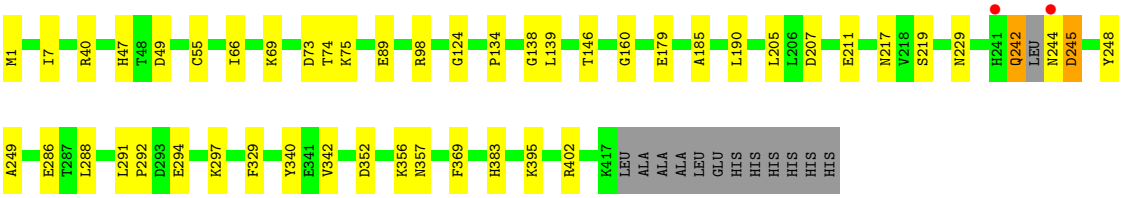
• Molecule 1: Galactokinase

Chain C:



• Molecule 1: Galactokinase

Chain B:


M1 I7 R40 H47 T48 D49 C55 I66 K69 D73 T74 K75 E89 R98 G124 P134 G138 L139 T146 G160 E179 A185 L190 L205 L206 D207 E211 N217 V218 S219 N229 H241 Q242 LEU N244 D245 Y248
A249 E266 T287 L288 L291 P292 D293 E294 K297 F329 Y340 E341 V342 D352 K356 N357 F369 H383 K395 R402 K417 LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	52.27Å 164.50Å 115.87Å 90.00° 95.80° 90.00°	Depositor
Resolution (Å)	94.58 – 1.45 94.40 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.3 (94.58-1.45) 98.3 (94.40-1.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.184 , 0.245 0.189 , 0.248	Depositor DCC
R_{free} test set	16932 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14438	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.17% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, ADP, PG4, PEG, CL

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	1.02	7/3251 (0.2%)	1.07	10/4407 (0.2%)
1	B	0.99	5/3208 (0.2%)	1.03	4/4352 (0.1%)
1	C	0.98	5/3218 (0.2%)	1.02	1/4363 (0.0%)
1	D	0.98	3/3249 (0.1%)	1.02	4/4403 (0.1%)
All	All	0.99	20/12926 (0.2%)	1.04	19/17525 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	CD-OE2	7.97	1.34	1.25
1	B	73	ASP	C-O	7.21	1.37	1.23
1	A	179[A]	GLU	CD-OE2	-7.18	1.17	1.25
1	A	179[B]	GLU	CD-OE2	-7.18	1.17	1.25
1	A	216	GLU	CD-OE1	7.02	1.33	1.25
1	A	13	GLU	CD-OE1	6.57	1.32	1.25
1	A	124	GLY	C-O	6.56	1.34	1.23
1	B	211	GLU	CD-OE2	6.45	1.32	1.25
1	C	308	GLU	CD-OE1	-6.42	1.18	1.25
1	C	147	CYS	C-O	6.08	1.34	1.23
1	D	149	THR	C-O	6.08	1.34	1.23
1	C	110	VAL	C-O	5.98	1.34	1.23
1	C	46	GLU	CD-OE1	5.62	1.31	1.25
1	A	308	GLU	CD-OE2	-5.50	1.19	1.25
1	D	147	CYS	C-O	5.45	1.33	1.23
1	B	286	GLU	CD-OE1	-5.43	1.19	1.25
1	C	280	GLN	C-O	-5.29	1.13	1.23
1	B	74	THR	C-O	5.28	1.33	1.23
1	D	51	ASN	C-O	5.19	1.33	1.23
1	B	160	GLY	C-O	5.07	1.31	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	363	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	311[A]	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	311[B]	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	311[A]	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	311[B]	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	71	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	98	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	268	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	B	329	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	A	309	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	248	TYR	CB-CA-C	5.74	121.87	110.40
1	A	71	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	157	TYR	CB-CG-CD2	5.57	124.34	121.00
1	D	115	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	329	PHE	CB-CG-CD1	5.41	124.59	120.80
1	D	327	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	197	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	197	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	71	ARG	NE-CZ-NH1	5.13	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3193	0	3109	43	1
1	B	3154	0	3044	46	0
1	C	3161	0	3083	26	0
1	D	3194	0	3104	52	0
2	A	7	0	10	1	0
2	B	35	0	50	12	0
2	C	14	0	20	2	0
2	D	21	0	30	11	0
3	A	12	0	16	9	0
3	B	18	0	24	13	0
3	C	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	1	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	1	0
5	A	2	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	C	13	0	18	2	0
8	A	354	0	0	9	0
8	B	396	0	0	18	0
8	C	380	0	0	14	0
8	D	345	0	0	20	1
All	All	14438	0	12588	180	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 7.

All (180) 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)
2:C:503:PEG:H31	8:C:831:HOH:O	1.26	1.26
1:D:225[B]:LEU:HD11	8:D:860:HOH:O	1.25	1.26
2:B:501:PEG:H12	8:B:602:HOH:O	1.36	1.22
1:D:252:ARG:HG2	8:D:618:HOH:O	1.43	1.18
1:D:231[A]:GLU:OE2	8:D:601:HOH:O	1.68	1.11
1:B:294[B]:GLU:OE1	2:B:501:PEG:H32	1.51	1.10
1:B:294[A]:GLU:OE1	8:B:601:HOH:O	1.66	1.08
1:C:225[A]:LEU:HD13	8:C:635:HOH:O	1.57	1.03
1:C:305:THR:CG2	8:C:916:HOH:O	2.08	1.01
1:D:66:ILE:HD11	8:D:915:HOH:O	1.63	0.97
1:A:293[B]:ASP:OD2	8:A:602:HOH:O	1.84	0.94
1:C:225[A]:LEU:CD1	8:C:635:HOH:O	2.11	0.92
1:D:187[B]:THR:HG22	8:D:692:HOH:O	1.72	0.90
1:B:294[A]:GLU:OE2	8:B:602:HOH:O	1.90	0.89
1:B:244:ASN:OD1	1:B:245:ASP:N	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200[B]:GLU:OE1	8:C:602:HOH:O	1.94	0.86
1:D:7:ILE:HD11	1:D:402:ARG:HD2	1.56	0.85
1:B:291:LEU:O	3:B:506:GOL:C1	2.24	0.85
1:A:300:VAL:O	1:A:303[B]:VAL:HG12	1.77	0.84
1:A:262[A]:LEU:HD11	1:A:291:LEU:HD21	1.58	0.84
1:B:244:ASN:CG	1:B:245:ASP:H	1.81	0.83
1:D:5[B]:GLU:HG3	8:D:869:HOH:O	1.81	0.81
1:A:262[A]:LEU:CD1	1:A:291:LEU:HD21	2.11	0.81
1:B:294[B]:GLU:OE2	8:B:603:HOH:O	1.98	0.80
1:C:305:THR:HG21	8:C:916:HOH:O	1.76	0.78
1:A:300:VAL:O	1:A:303[B]:VAL:CG1	2.31	0.77
1:D:396:GLU:OE1	8:D:604:HOH:O	2.00	0.77
1:D:394[B]:GLU:OE1	8:D:603:HOH:O	2.00	0.77
1:A:19:ALA:HA	8:A:655:HOH:O	1.84	0.75
1:C:140[B]:SER:OG	8:C:603:HOH:O	2.06	0.74
1:C:168:ARG:HD3	1:C:196[A]:MET:HE3	1.68	0.74
1:D:384:GLU:HG3	8:D:856:HOH:O	1.87	0.73
1:D:367:GLY:H	2:D:503:PEG:C4	2.01	0.73
1:D:140[B]:SER:OG	8:D:602:HOH:O	1.99	0.73
1:D:394[A]:GLU:OE1	8:D:605:HOH:O	2.08	0.71
1:D:367:GLY:H	2:D:503:PEG:H42	1.57	0.70
1:A:22:LEU:HB3	8:A:655:HOH:O	1.94	0.68
1:D:2:THR:N	8:D:613:HOH:O	2.27	0.68
5:A:506:CL:CL	8:A:847:HOH:O	2.48	0.67
1:A:293[A]:ASP:CG	8:A:702:HOH:O	2.33	0.67
1:D:225[B]:LEU:CD1	8:D:860:HOH:O	2.05	0.67
2:B:501:PEG:H41	8:B:603:HOH:O	1.95	0.67
1:B:297:LYS:NZ	3:B:506:GOL:H31	2.10	0.66
1:D:163[B]:ASP:OD1	8:D:607:HOH:O	2.14	0.66
2:D:503:PEG:H31	8:D:606:HOH:O	1.95	0.66
1:B:291:LEU:O	3:B:506:GOL:H12	1.96	0.66
1:C:187[B]:THR:HG22	8:C:711:HOH:O	1.95	0.66
1:C:142:SER:OG	8:C:603:HOH:O	2.13	0.65
1:B:89:GLU:OE1	8:B:605:HOH:O	2.15	0.65
1:B:395[B]:LYS:NZ	8:B:604:HOH:O	2.07	0.64
1:A:303[B]:VAL:HG13	1:A:304:VAL:N	2.12	0.64
1:B:291:LEU:O	3:B:506:GOL:O2	2.13	0.64
1:B:249:ALA:HB3	8:B:685:HOH:O	1.97	0.64
2:B:503:PEG:H12	8:B:613:HOH:O	1.97	0.64
1:D:142:SER:OG	8:D:602:HOH:O	2.15	0.63
1:B:1:MET:CB	8:B:666:HOH:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395[B]:LYS:CE	8:B:604:HOH:O	2.44	0.62
1:B:294[A]:GLU:OE2	2:B:501:PEG:H12	2.00	0.62
1:A:293[B]:ASP:OD2	1:A:295:THR:N	2.26	0.61
1:D:367:GLY:N	2:D:503:PEG:H42	2.15	0.61
1:D:215:LEU:HD12	1:D:215:LEU:N	2.16	0.61
1:B:244:ASN:CG	1:B:245:ASP:N	2.54	0.60
1:C:400:ALA:HB3	3:C:504:GOL:O3	2.03	0.59
1:A:258:ALA:O	1:A:262[A]:LEU:HD13	2.02	0.59
1:A:293[B]:ASP:CG	8:A:602:HOH:O	2.30	0.58
1:A:293[A]:ASP:CB	8:A:702:HOH:O	2.50	0.58
1:B:356:LYS:O	3:B:507:GOL:H11	2.03	0.58
1:C:168:ARG:CD	1:C:196[A]:MET:HE3	2.33	0.58
1:C:238:GLN:HG3	3:C:504:GOL:O2	2.04	0.57
1:B:179[B]:GLU:HG2	1:B:185:ALA:O	2.04	0.57
1:D:138:GLY:HA2	2:D:503:PEG:O4	2.05	0.57
1:C:305:THR:HB	8:C:916:HOH:O	2.03	0.56
1:B:146:THR:HG21	1:B:179[A]:GLU:HG3	1.88	0.56
1:A:293[B]:ASP:CG	1:A:294[B]:GLU:N	2.59	0.56
1:A:323:LYS:H	3:A:502:GOL:C3	2.19	0.56
1:B:291:LEU:O	3:B:506:GOL:C2	2.54	0.56
1:A:7:ILE:HD11	1:A:402:ARG:HD2	1.89	0.55
1:D:75[B]:LYS:HE3	1:D:89:GLU:OE2	2.07	0.55
1:B:294[B]:GLU:HG2	8:B:601:HOH:O	2.06	0.55
1:D:367:GLY:H	2:D:503:PEG:H41	1.70	0.55
1:A:323:LYS:HG3	3:A:502:GOL:H31	1.88	0.54
1:B:47:HIS:HA	3:B:508:GOL:O1	2.06	0.54
1:B:291:LEU:O	3:B:506:GOL:H11	2.04	0.54
1:B:297:LYS:HZ3	3:B:506:GOL:H31	1.71	0.54
1:A:146:THR:HG21	1:A:179[B]:GLU:HG3	1.91	0.53
1:D:158:GLY:HA3	2:D:502:PEG:H22	1.91	0.53
1:A:293[B]:ASP:OD2	1:A:294[B]:GLU:N	2.42	0.53
1:B:294[B]:GLU:OE1	2:B:501:PEG:C3	2.42	0.52
1:A:300:VAL:C	1:A:303[B]:VAL:HG12	2.30	0.52
1:D:250:GLN:HG3	8:D:826:HOH:O	2.09	0.51
1:A:222:GLU:OE1	8:A:603:HOH:O	2.19	0.51
1:B:288:LEU:O	1:B:297:LYS:HE2	2.10	0.51
1:A:293[B]:ASP:CG	1:A:294[B]:GLU:H	2.14	0.51
2:B:501:PEG:C1	8:B:602:HOH:O	2.20	0.51
1:D:7:ILE:HD11	1:D:402:ARG:CD	2.32	0.51
1:D:32:GLU:HG3	2:D:501:PEG:H21	1.92	0.51
1:A:300:VAL:HA	1:A:303[B]:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:N	3:A:502:GOL:H32	2.26	0.50
1:D:215:LEU:H	1:D:215:LEU:CD1	2.24	0.50
1:A:323:LYS:H	3:A:502:GOL:H32	1.75	0.50
1:C:57:PRO:HD2	1:C:204:LEU:O	2.11	0.50
1:B:294[B]:GLU:OE1	2:B:501:PEG:H22	2.11	0.50
1:C:75:LYS:NZ	1:C:75:LYS:HB3	2.26	0.50
1:A:300:VAL:HA	1:A:303[B]:VAL:HG12	1.92	0.50
1:B:356:LYS:HD2	8:B:670:HOH:O	2.11	0.50
1:D:5[A]:GLU:CD	8:D:615:HOH:O	2.50	0.49
1:C:205:LEU:HB3	1:C:219[B]:SER:OG	2.13	0.49
1:D:215:LEU:N	1:D:215:LEU:CD1	2.76	0.48
1:D:238:GLN:OE1	1:D:402:ARG:CZ	2.61	0.48
1:B:205:LEU:HB3	1:B:219:SER:HB3	1.94	0.48
1:C:29:ALA:HB3	1:B:242:GLN:HG3	1.96	0.48
1:C:187[A]:THR:HG23	1:C:188:GLY:O	2.14	0.48
1:D:187[B]:THR:CG2	8:D:692:HOH:O	2.45	0.47
2:B:504:PEG:H12	2:B:504:PEG:H31	1.43	0.47
1:A:71:ARG:HA	2:A:501:PEG:H32	1.97	0.47
1:D:140[B]:SER:HA	4:D:505:ADP:O1B	2.14	0.47
1:B:342:VAL:HG12	1:B:369:PHE:CZ	2.49	0.47
1:A:248:TYR:CD2	1:A:252[A]:ARG:NH2	2.82	0.47
1:B:352:ASP:OD2	1:B:356:LYS:HE2	2.14	0.47
1:A:205:LEU:HB3	1:A:219[B]:SER:HB3	1.97	0.47
1:D:157:TYR:O	2:D:502:PEG:C2	2.62	0.47
1:B:66:ILE:O	1:B:66:ILE:HG23	2.14	0.47
2:D:503:PEG:H21	3:D:504:GOL:C1	2.46	0.46
1:A:190:LEU:C	1:A:190:LEU:HD23	2.35	0.46
1:C:231[B]:GLU:HB2	8:C:638:HOH:O	2.15	0.46
1:D:69:LYS:HG3	2:D:501:PEG:H12	1.98	0.46
1:C:71:ARG:O	8:C:604:HOH:O	2.21	0.46
1:C:71:ARG:HD3	1:C:75:LYS:O	2.15	0.46
1:B:297:LYS:HZ1	3:B:506:GOL:H31	1.78	0.46
1:B:49:ASP:OD1	3:B:508:GOL:H11	2.16	0.45
1:D:55[B]:CYS:SG	1:D:190:LEU:HD13	2.56	0.45
1:C:305:THR:HG22	8:C:916:HOH:O	1.93	0.45
1:B:134:PRO:HG2	1:B:139:LEU:HD12	1.99	0.45
1:A:293[B]:ASP:CB	8:A:702:HOH:O	2.64	0.45
1:D:179:GLU:CD	1:D:187[A]:THR:HG21	2.37	0.45
1:A:323:LYS:CG	3:A:502:GOL:H31	2.47	0.45
1:D:75[B]:LYS:O	1:D:124:GLY:HA3	2.17	0.45
1:D:41[A]:VAL:HG12	1:D:139:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LYS:O	1:B:124:GLY:HA3	2.16	0.45
1:B:207:ASP:O	1:B:217:ASN:HB2	2.16	0.45
1:D:57:PRO:HD2	1:D:204:LEU:O	2.17	0.44
1:A:40:ARG:CZ	1:A:140[A]:SER:OG	2.66	0.44
1:C:187[A]:THR:HG21	1:C:192:GLN:HE22	1.81	0.44
1:A:207:ASP:O	1:A:217:ASN:HB2	2.16	0.44
1:A:300:VAL:O	1:A:303[B]:VAL:HG13	2.13	0.44
7:C:501:PG4:H22	7:C:501:PG4:H42	1.70	0.44
1:A:323:LYS:HG3	3:A:502:GOL:H12	2.00	0.44
1:D:215:LEU:HD12	1:D:215:LEU:H	1.80	0.43
1:D:198:CYS:O	1:D:411:SER:HB3	2.18	0.43
1:B:383:HIS:HE1	8:B:935:HOH:O	2.01	0.43
1:A:49:ASP:OD1	3:A:503:GOL:H32	2.18	0.43
2:B:503:PEG:O1	2:B:503:PEG:C3	2.66	0.43
1:C:55[A]:CYS:SG	1:C:206:LEU:HD23	2.59	0.43
1:C:187[B]:THR:HG22	1:C:188:GLY:O	2.18	0.43
1:B:357:ASN:C	3:B:507:GOL:H32	2.38	0.43
7:C:501:PG4:H31	8:C:636:HOH:O	2.19	0.43
1:A:50:TYR:CD1	1:A:252[B]:ARG:HG2	2.54	0.43
1:C:189:GLY:N	2:C:503:PEG:O1	2.38	0.42
1:D:75[B]:LYS:HB2	1:D:75[B]:LYS:NZ	2.34	0.42
1:A:47:HIS:HA	3:A:503:GOL:O3	2.19	0.42
1:D:80:SER:OG	1:D:82:VAL:HG12	2.19	0.42
1:D:50:TYR:CD1	1:D:252:ARG:HG3	2.55	0.42
1:D:76:VAL:HA	1:D:125:PHE:O	2.20	0.42
2:B:503:PEG:O1	2:B:503:PEG:H32	2.20	0.42
2:B:502:PEG:H32	2:B:502:PEG:H12	1.53	0.42
1:B:7:ILE:HD11	1:B:402:ARG:HD2	2.01	0.41
1:A:198:CYS:O	1:A:411:SER:HB3	2.20	0.41
1:A:300:VAL:CA	1:A:303[B]:VAL:HG12	2.51	0.41
1:D:223:PHE:CZ	1:D:225[B]:LEU:HD21	2.55	0.41
1:B:55:CYS:CB	1:B:190[A]:LEU:HD23	2.50	0.41
1:B:138:GLY:HA3	8:B:711:HOH:O	2.21	0.41
1:B:292:PRO:HA	3:B:506:GOL:H11	2.02	0.41
1:A:323:LYS:H	3:A:502:GOL:H31	1.83	0.41
1:D:7:ILE:O	1:D:405:PRO:HD2	2.21	0.41
1:D:138:GLY:HA3	8:D:608:HOH:O	2.21	0.41
1:D:395:LYS:HE2	8:B:713:HOH:O	2.20	0.41
1:D:71:ARG:HD3	1:D:75[A]:LYS:O	2.21	0.40
1:B:69:LYS:NZ	8:B:633:HOH:O	2.53	0.40
1:D:71:ARG:NH2	1:D:75[B]:LYS:HD2	2.37	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:A:246:GLY:N	8:D:716:HOH:O[2_447]	1.44	0.76

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	425/429 (99%)	418 (98%)	7 (2%)	0	100 100
1	B	423/429 (99%)	416 (98%)	6 (1%)	1 (0%)	47 22
1	C	423/429 (99%)	417 (99%)	6 (1%)	0	100 100
1	D	425/429 (99%)	417 (98%)	8 (2%)	0	100 100
All	All	1696/1716 (99%)	1668 (98%)	27 (2%)	1 (0%)	51 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	ASP

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	323/326 (99%)	319 (99%)	4 (1%)	71 43
1	B	316/326 (97%)	312 (99%)	4 (1%)	69 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	319/326 (98%)	315 (99%)	4 (1%)	69 40
1	D	323/326 (99%)	317 (98%)	6 (2%)	57 23
All	All	1281/1304 (98%)	1263 (99%)	18 (1%)	67 37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	86	LYS
1	A	340	TYR
1	A	379	LYS
1	D	40	ARG
1	D	159	LEU
1	D	215	LEU
1	D	231[A]	GLU
1	D	231[B]	GLU
1	D	340	TYR
1	C	40	ARG
1	C	98	ARG
1	C	120	ASP
1	C	340	TYR
1	B	40	ARG
1	B	229	ASN
1	B	242	GLN
1	B	340	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	241	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 9 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
3	GOL	B	508	-	5,5,5	0.23	0	5,5,5	0.56	0
3	GOL	B	507	-	5,5,5	0.20	0	5,5,5	0.40	0
3	GOL	A	503	-	5,5,5	0.54	0	5,5,5	0.64	0
2	PEG	A	501	-	6,6,6	0.29	0	5,5,5	0.32	0
3	GOL	C	505	-	5,5,5	0.75	0	5,5,5	1.29	0
2	PEG	C	503	-	6,6,6	0.24	0	5,5,5	0.39	0
3	GOL	C	504	-	5,5,5	0.18	0	5,5,5	0.45	0
4	ADP	C	507	6	24,29,29	0.85	0	29,45,45	0.96	2 (6%)
4	ADP	A	504	6	24,29,29	0.82	0	29,45,45	0.83	1 (3%)
2	PEG	B	503	-	6,6,6	0.25	0	5,5,5	0.21	0
2	PEG	B	504	-	6,6,6	0.45	0	5,5,5	0.28	0
2	PEG	D	502	-	6,6,6	0.34	0	5,5,5	0.54	0
2	PEG	B	501	-	6,6,6	0.23	0	5,5,5	0.32	0
4	ADP	B	509	6	24,29,29	0.77	0	29,45,45	1.06	2 (6%)
3	GOL	D	504	-	5,5,5	0.53	0	5,5,5	1.11	0
3	GOL	A	502	-	5,5,5	0.33	0	5,5,5	0.75	0
7	PG4	C	501	-	12,12,12	0.26	0	11,11,11	0.23	0
2	PEG	D	503	-	6,6,6	0.55	0	5,5,5	0.53	0
2	PEG	D	501	-	6,6,6	0.15	0	5,5,5	0.13	0
2	PEG	B	505	-	6,6,6	0.25	0	5,5,5	0.15	0
2	PEG	C	502	-	6,6,6	0.14	0	5,5,5	0.13	0
3	GOL	C	506	-	5,5,5	0.27	0	5,5,5	0.48	0
2	PEG	B	502	-	6,6,6	0.25	0	5,5,5	0.31	0
3	GOL	B	506	-	5,5,5	0.06	0	5,5,5	0.53	0
4	ADP	D	505	6	24,29,29	0.75	0	29,45,45	0.94	1 (3%)

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
3	GOL	B	508	-	-	2/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
2	PEG	A	501	-	-	1/4/4/4	-
3	GOL	C	505	-	-	0/4/4/4	-
2	PEG	C	503	-	-	1/4/4/4	-
3	GOL	C	504	-	-	2/4/4/4	-
4	ADP	C	507	6	-	3/12/32/32	0/3/3/3
4	ADP	A	504	6	-	3/12/32/32	0/3/3/3
2	PEG	B	503	-	-	1/4/4/4	-
2	PEG	B	504	-	-	3/4/4/4	-
2	PEG	D	502	-	-	2/4/4/4	-
2	PEG	B	501	-	-	3/4/4/4	-
4	ADP	B	509	6	-	2/12/32/32	0/3/3/3
3	GOL	D	504	-	-	0/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
7	PG4	C	501	-	-	6/10/10/10	-
2	PEG	D	503	-	-	2/4/4/4	-
2	PEG	D	501	-	-	3/4/4/4	-
2	PEG	B	505	-	-	3/4/4/4	-
2	PEG	C	502	-	-	3/4/4/4	-
3	GOL	C	506	-	-	0/4/4/4	-
2	PEG	B	502	-	-	3/4/4/4	-
3	GOL	B	506	-	-	2/4/4/4	-
4	ADP	D	505	6	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	507	ADP	C5-C6-N6	3.14	125.09	120.31
4	A	504	ADP	C5-C6-N6	3.11	125.05	120.31
4	D	505	ADP	C5-C6-N6	2.73	124.47	120.31
4	B	509	ADP	C5-C6-N6	2.64	124.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	507	ADP	O2A-PA-O1A	2.34	123.35	112.44
4	B	509	ADP	O4'-C1'-N9	-2.27	105.74	108.75

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	C	504	GOL	C1-C2-C3-O3
3	B	506	GOL	O1-C1-C2-C3
4	A	504	ADP	PA-O3A-PB-O2B
4	A	504	ADP	PA-O3A-PB-O3B
4	C	507	ADP	PA-O3A-PB-O2B
2	B	504	PEG	C1-C2-O2-C3
2	D	502	PEG	C4-C3-O2-C2
7	C	501	PG4	O2-C3-C4-O3
3	A	502	GOL	O1-C1-C2-O2
3	B	506	GOL	O1-C1-C2-O2
2	B	503	PEG	O1-C1-C2-O2
2	B	504	PEG	O1-C1-C2-O2
2	B	504	PEG	O2-C3-C4-O4
7	C	501	PG4	O1-C1-C2-O2
2	B	502	PEG	C1-C2-O2-C3
2	D	502	PEG	O1-C1-C2-O2
2	D	503	PEG	O2-C3-C4-O4
2	B	501	PEG	O2-C3-C4-O4
2	B	502	PEG	O1-C1-C2-O2
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	B	507	GOL	O1-C1-C2-C3
3	B	508	GOL	C1-C2-C3-O3
7	C	501	PG4	O3-C5-C6-O4
3	A	502	GOL	O2-C2-C3-O3
3	C	504	GOL	O2-C2-C3-O3
2	C	502	PEG	O1-C1-C2-O2
2	D	503	PEG	O1-C1-C2-O2
2	B	505	PEG	O2-C3-C4-O4
7	C	501	PG4	C4-C3-O2-C2
2	D	501	PEG	O1-C1-C2-O2
3	B	508	GOL	O2-C2-C3-O3
2	D	501	PEG	C1-C2-O2-C3
3	B	507	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	C	501	PG4	C5-C6-O4-C7
4	B	509	ADP	PA-O3A-PB-O2B
2	A	501	PEG	O2-C3-C4-O4
2	D	501	PEG	O2-C3-C4-O4
2	B	501	PEG	C1-C2-O2-C3
2	B	505	PEG	C4-C3-O2-C2
2	B	501	PEG	O1-C1-C2-O2
2	C	503	PEG	O1-C1-C2-O2
2	B	502	PEG	O2-C3-C4-O4
2	C	502	PEG	O2-C3-C4-O4
7	C	501	PG4	C6-C5-O3-C4
4	B	509	ADP	PA-O3A-PB-O1B
3	A	503	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
2	B	505	PEG	C1-C2-O2-C3
2	C	502	PEG	C1-C2-O2-C3
4	C	507	ADP	PA-O3A-PB-O1B
4	D	505	ADP	PA-O3A-PB-O3B
4	C	507	ADP	PA-O3A-PB-O3B
4	A	504	ADP	PA-O3A-PB-O1B

There are no ring outliers.

18 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	508	GOL	2	0
3	B	507	GOL	2	0
3	A	503	GOL	2	0
2	A	501	PEG	1	0
2	C	503	PEG	2	0
3	C	504	GOL	2	0
2	B	503	PEG	3	0
2	B	504	PEG	1	0
2	D	502	PEG	2	0
2	B	501	PEG	7	0
3	D	504	GOL	1	0
3	A	502	GOL	7	0
7	C	501	PG4	2	0
2	D	503	PEG	7	0
2	D	501	PEG	2	0
2	B	502	PEG	1	0
3	B	506	GOL	9	0

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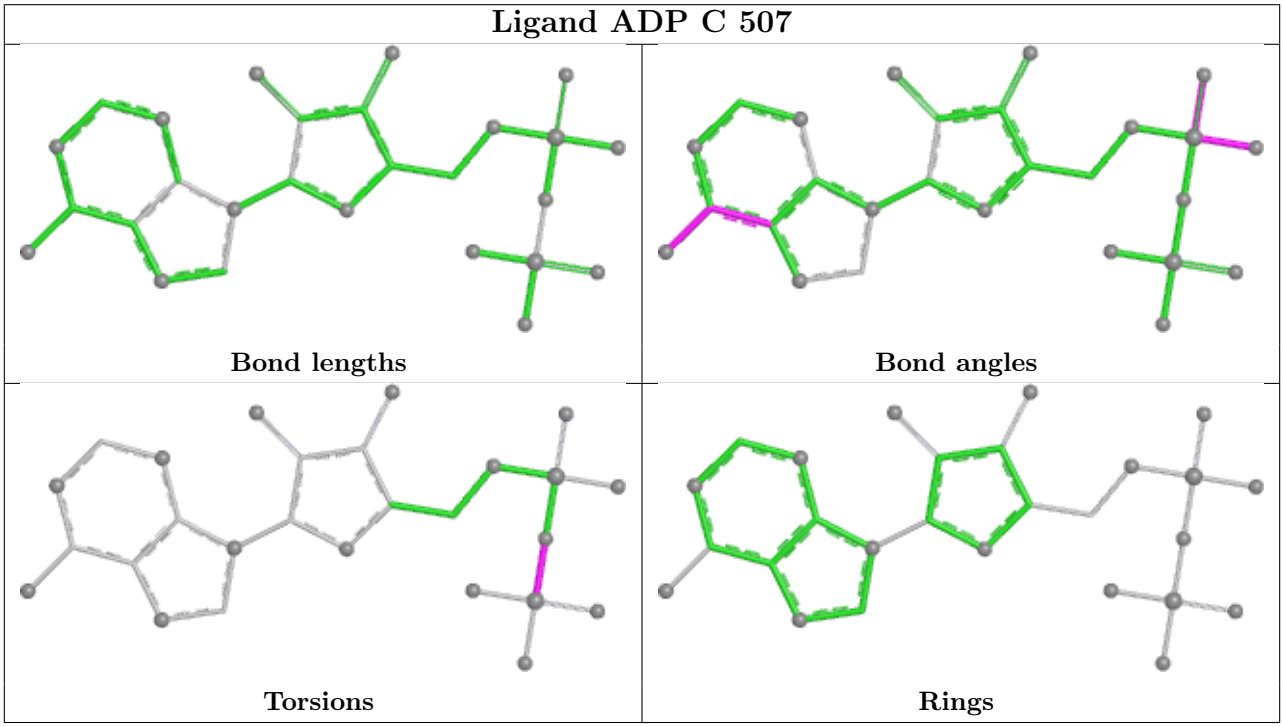
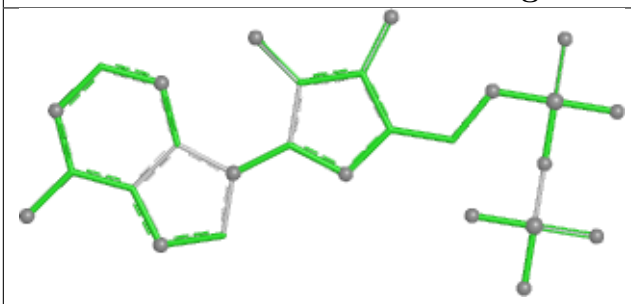
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	505	ADP	1	0

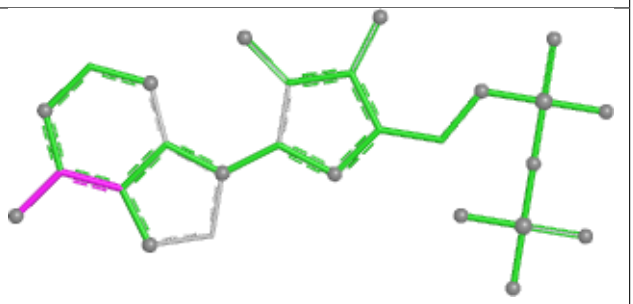
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



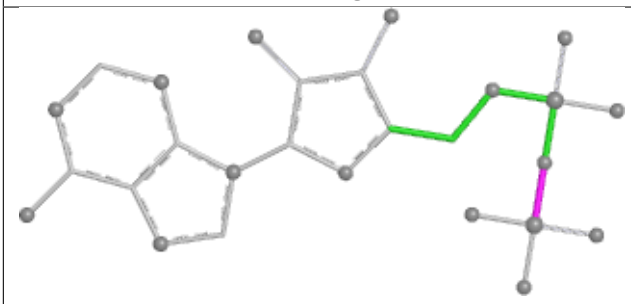
Ligand ADP A 504



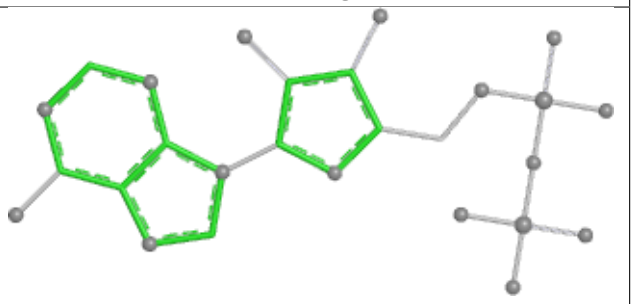
Bond lengths



Bond angles

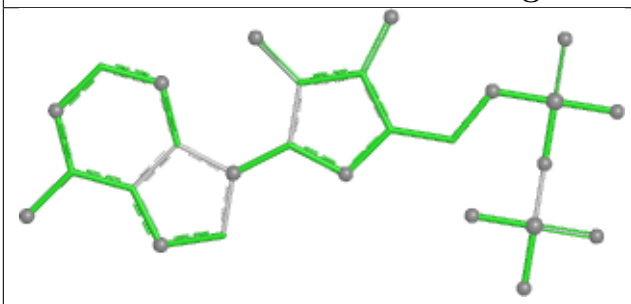


Torsions

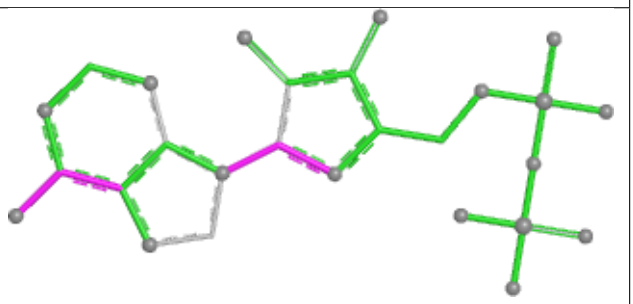


Rings

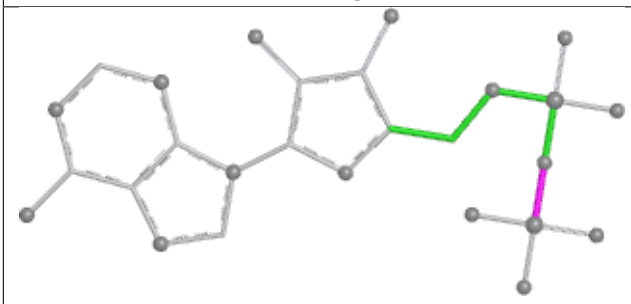
Ligand ADP B 509



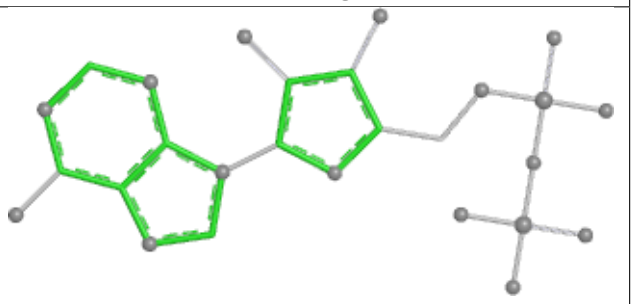
Bond lengths



Bond angles

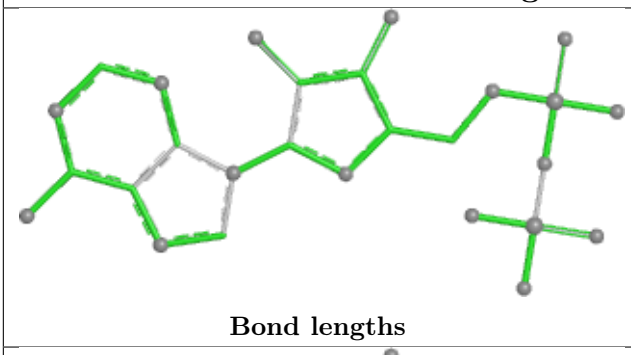


Torsions

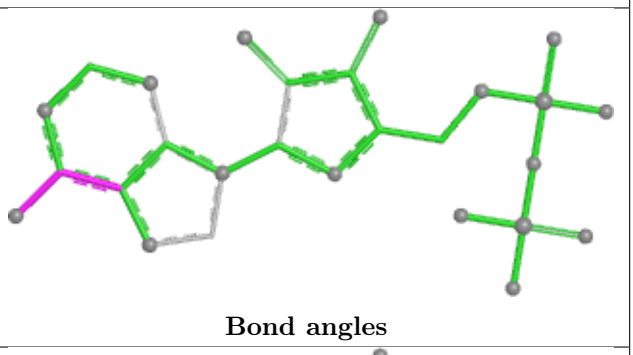


Rings

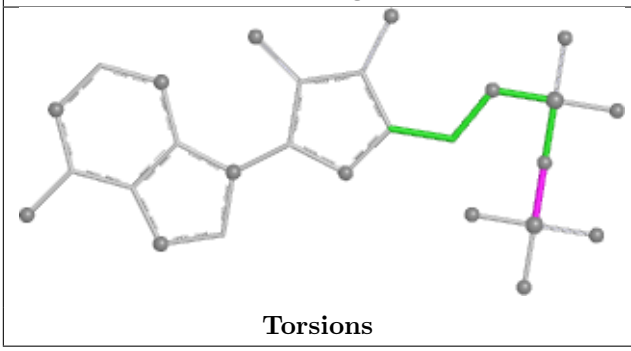
Ligand ADP D 505



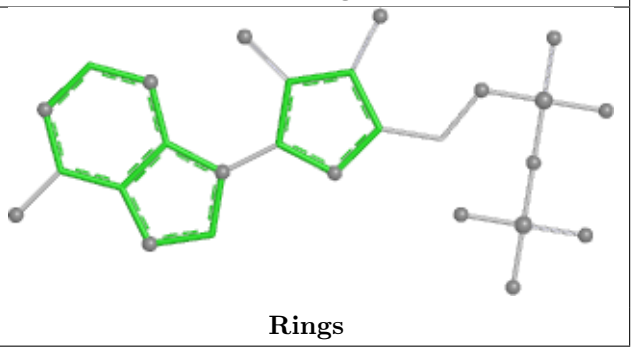
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	414/429 (96%)	-0.14	1 (0%)	95	95	9, 15, 27, 44	14 (3%)
1	B	416/429 (96%)	-0.16	2 (0%)	91	93	10, 17, 29, 50	8 (1%)
1	C	415/429 (96%)	-0.11	2 (0%)	91	93	10, 16, 30, 46	10 (2%)
1	D	413/429 (96%)	-0.03	7 (1%)	70	70	12, 19, 33, 49	17 (4%)
All	All	1658/1716 (96%)	-0.11	12 (0%)	87	89	9, 17, 30, 50	49 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	GLN	6.4
1	B	241	HIS	3.9
1	D	241	HIS	3.3
1	B	244	ASN	2.8
1	A	242	GLN	2.7
1	C	419	ALA	2.6
1	D	102	GLY	2.5
1	D	185	ALA	2.4
1	D	369	PHE	2.3
1	D	292	PRO	2.3
1	D	76	VAL	2.3
1	C	246	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} 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.

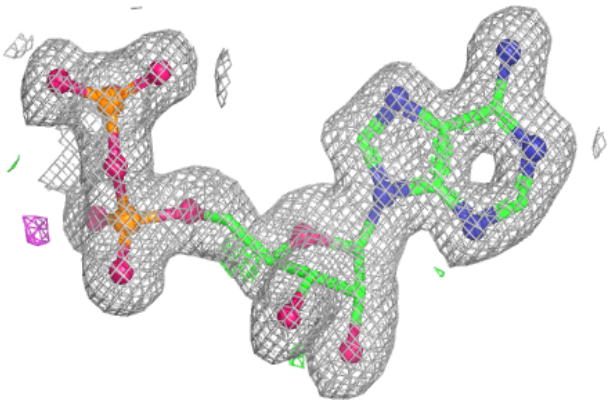
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	504	6/6	0.67	0.31	24,26,32,45	6
3	GOL	C	506	6/6	0.74	0.29	37,60,67,75	0
2	PEG	B	503	7/7	0.77	0.49	29,38,43,43	7
2	PEG	B	504	7/7	0.77	0.21	19,21,27,28	7
2	PEG	C	502	7/7	0.78	0.32	33,39,47,52	7
2	PEG	D	503	7/7	0.79	0.23	27,27,29,29	7
7	PG4	C	501	13/13	0.80	0.21	20,22,30,34	13
3	GOL	B	506	6/6	0.81	0.20	25,26,27,29	6
2	PEG	D	501	7/7	0.82	0.19	32,34,39,42	6
2	PEG	B	505	7/7	0.82	0.26	29,30,42,52	7
2	PEG	B	501	7/7	0.83	0.23	24,25,27,29	7
2	PEG	B	502	7/7	0.84	0.24	32,34,41,49	7
3	GOL	B	507	6/6	0.85	0.35	36,40,57,57	6
2	PEG	A	501	7/7	0.87	0.34	27,28,34,48	7
2	PEG	D	502	7/7	0.88	0.15	48,56,60,62	0
3	GOL	A	503	6/6	0.89	0.18	14,19,22,22	0
2	PEG	C	503	7/7	0.92	0.15	18,20,23,24	7
3	GOL	D	504	6/6	0.93	0.09	18,21,22,22	0
3	GOL	C	505	6/6	0.93	0.14	15,22,29,36	0
3	GOL	B	508	6/6	0.95	0.16	13,24,32,35	1
3	GOL	A	502	6/6	0.96	0.12	20,30,37,41	2
4	ADP	B	509	27/27	0.97	0.08	14,18,21,22	0
4	ADP	D	505	27/27	0.97	0.11	19,23,26,33	0
4	ADP	A	504	27/27	0.98	0.06	13,16,18,19	0
5	CL	A	506	1/1	0.98	0.04	57,57,57,57	0
6	MG	D	507	1/1	0.98	0.07	24,24,24,24	0
4	ADP	C	507	27/27	0.98	0.08	14,17,20,24	0
6	MG	B	511	1/1	0.99	0.07	17,17,17,17	0
5	CL	D	506	1/1	0.99	0.07	19,19,19,19	0
6	MG	A	507	1/1	1.00	0.07	17,17,17,17	0
5	CL	A	505	1/1	1.00	0.06	21,21,21,21	0
6	MG	C	509	1/1	1.00	0.08	18,18,18,18	0
5	CL	C	508	1/1	1.00	0.07	16,16,16,16	0
5	CL	B	510	1/1	1.00	0.05	22,22,22,22	0

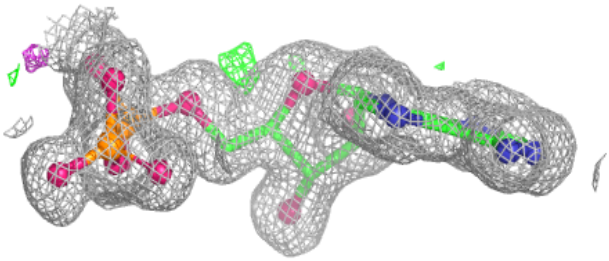
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

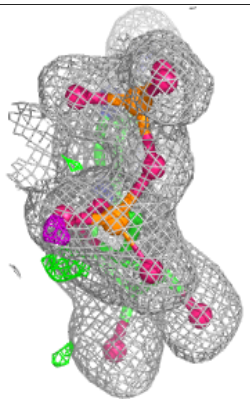
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 509:

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

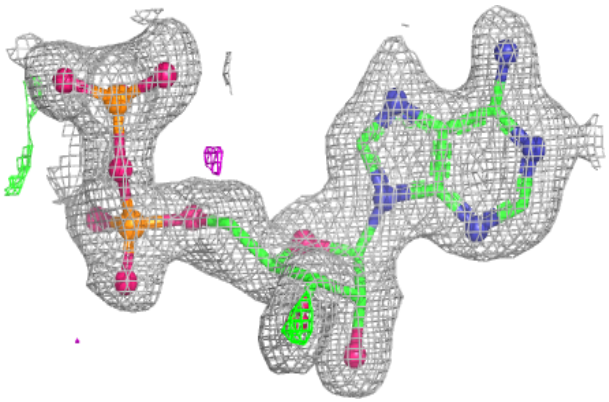


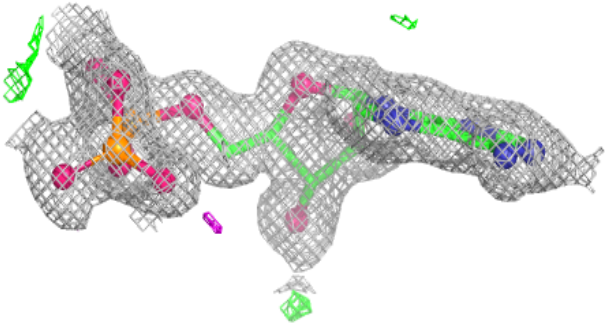


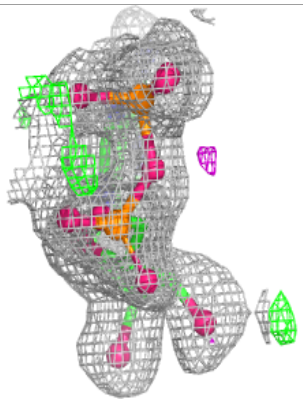


Electron density around ADP D 505:

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

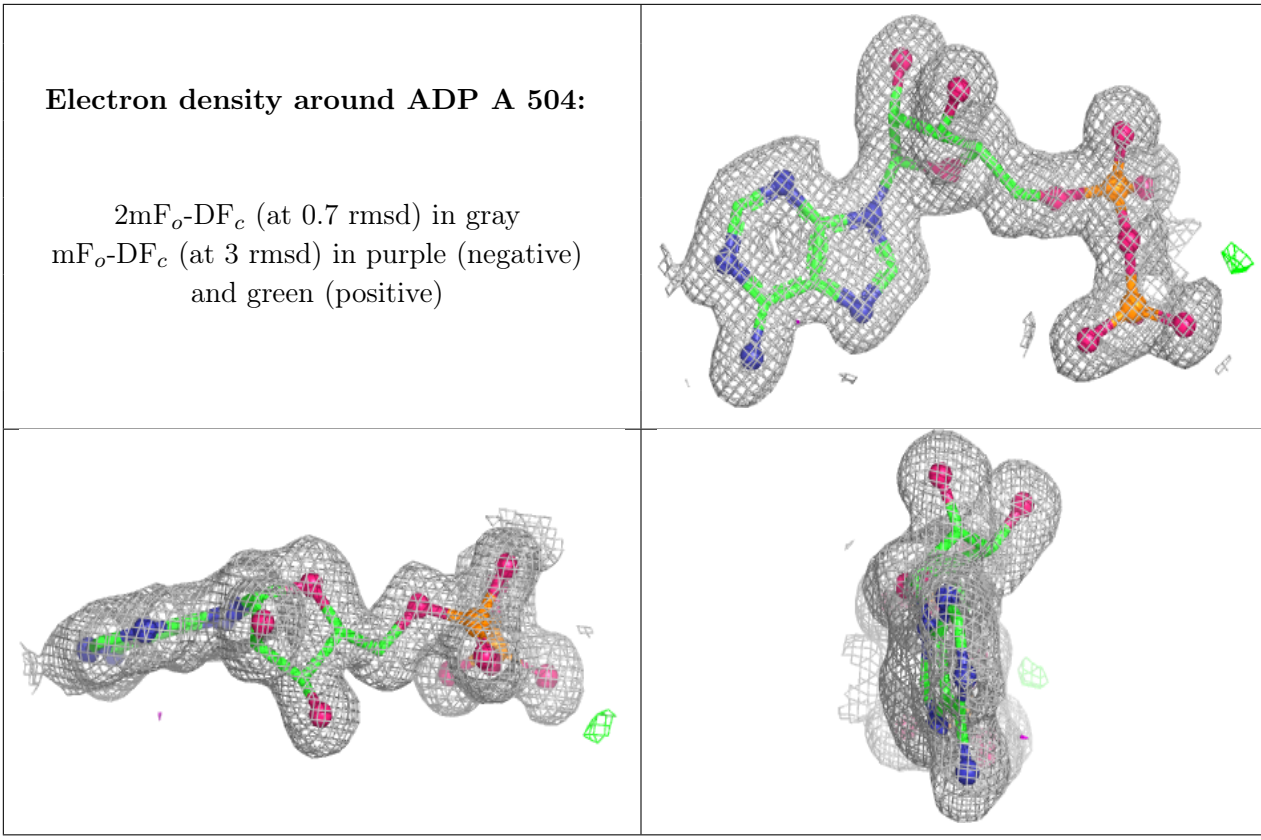






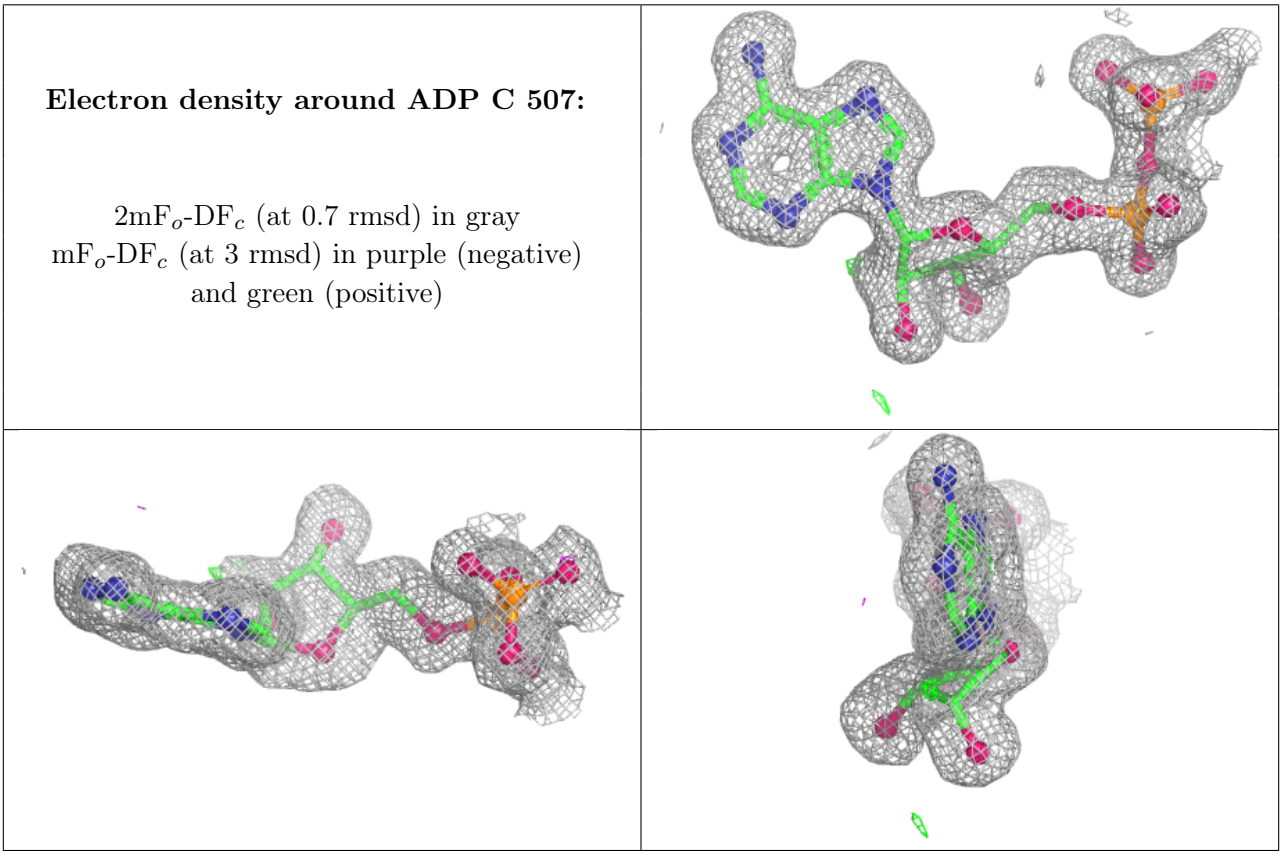
Electron density around ADP A 504:

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



Electron density around ADP C 507:

$2mF_o$-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.