Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2024 – 04:40 pm BST

PDB ID	:	8RVK
Title	:	Maltodextrin phosphorylase (MalP) in complex with a alpha-1,2-cyclophellitol analogue
Authors	:	Bennett, M.; Ofman, T.P.; Overkleeft, H.S.; Davies, G.J.
Deposited on	:	2024-02-01
Resolution	:	2.18 Å(reported)

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

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

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

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

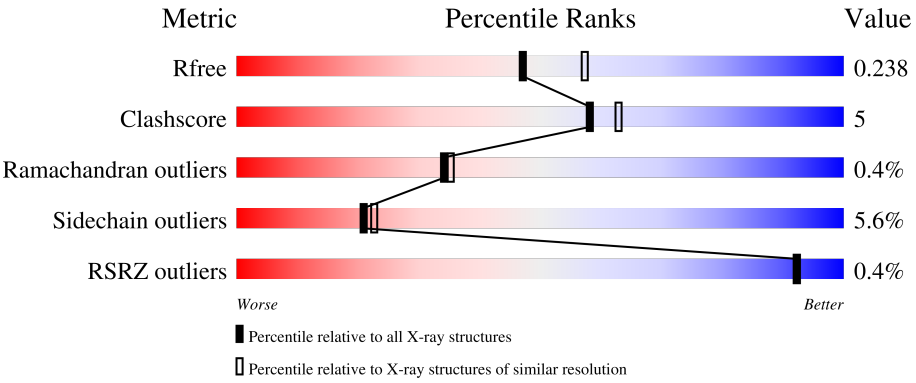
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	797	% 82% 15%
1	B	797	82% 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
4	PEG	B	821	-	-	X	-
5	SO4	A	820	-	-	X	-

2 Entry composition

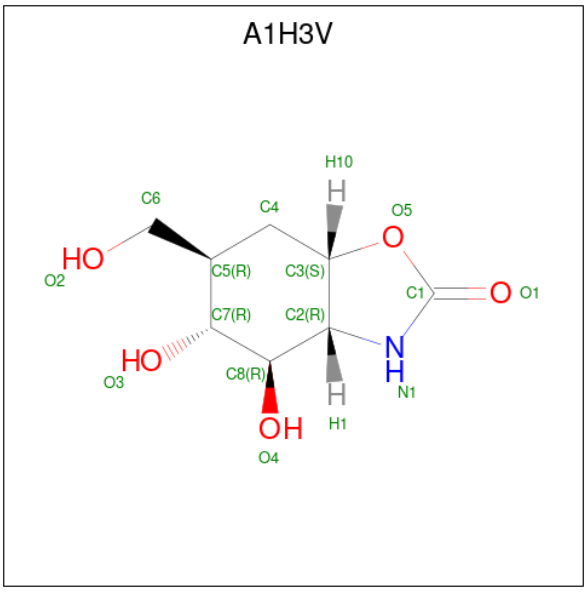
There are 6 unique types of molecules in this entry. The entry contains 13558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Maltodextrin phosphorylase.

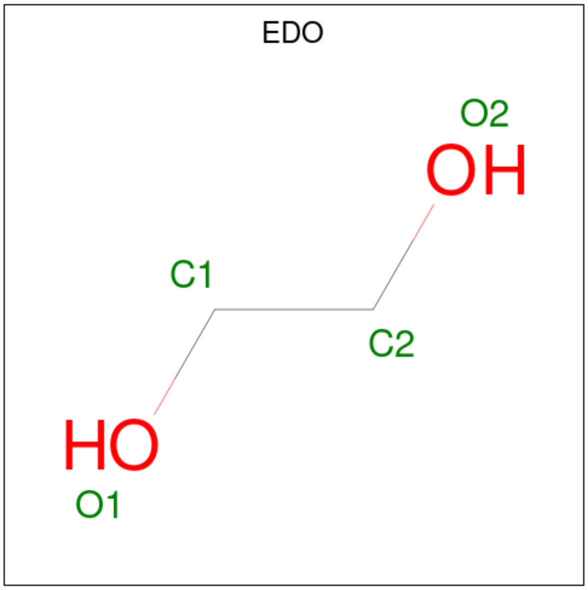
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	P	S	0	0	0
			6332	4045	1103	1163	1	20			
1	B	795	Total	C	N	O	P	S	0	2	0
			6315	4039	1100	1155	1	20			

- Molecule 2 is (3 {a} {R},4 {R},5 {R},6 {R},7 {a} {S})-6-(hydroxymethyl)-4,5-bis(oxidanyl)-3 {a},4,5,6,7,7 {a}-hexahydro-3 {H}-1,3-benzoxazol-2-one (three-letter code: A1H3V) (formula: $C_8H_{13}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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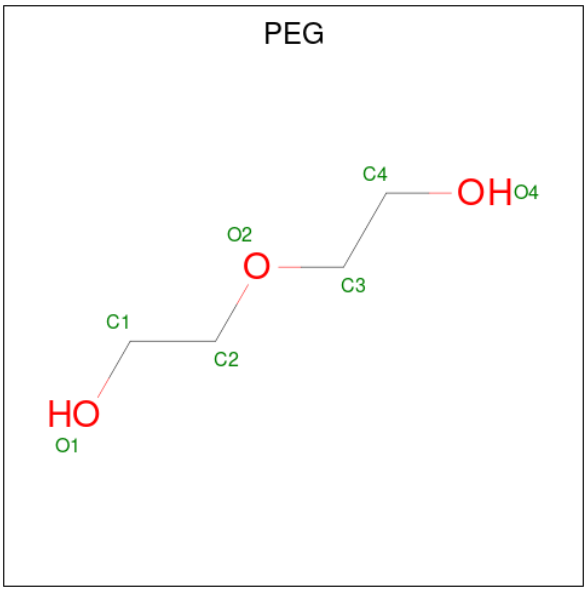
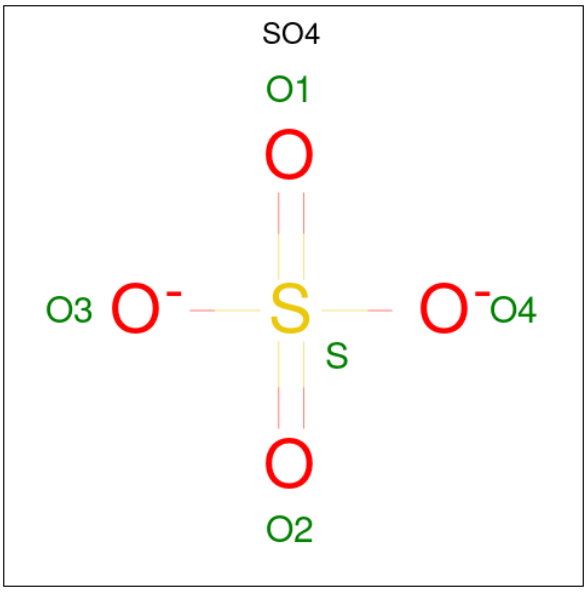
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

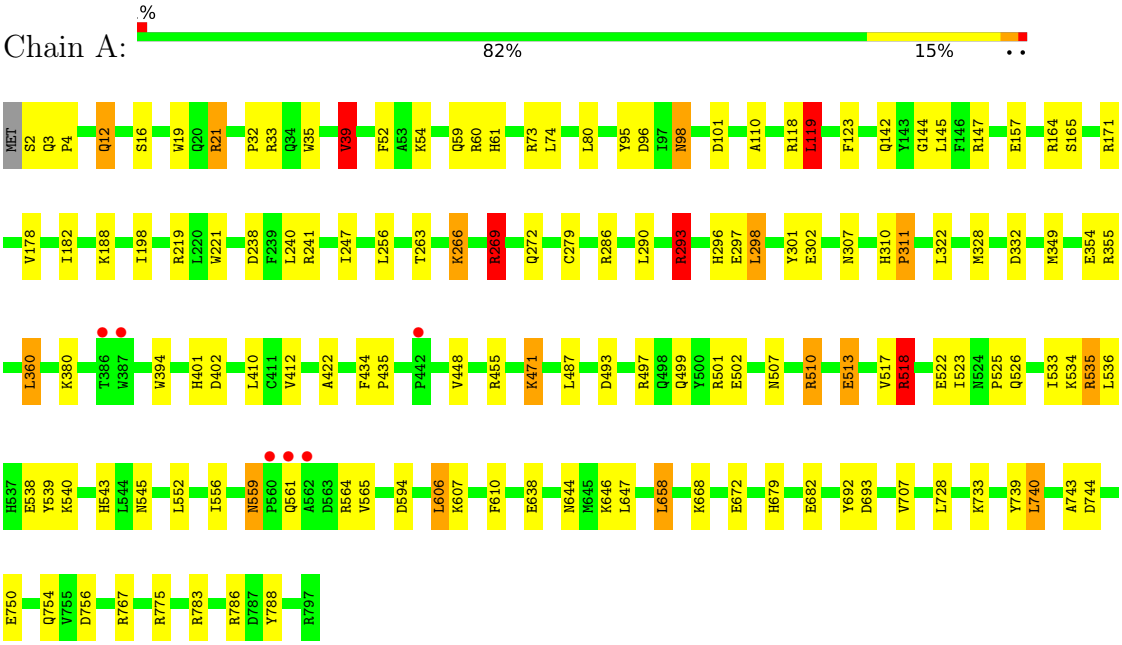
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	320	Total O 320 320	0	0
6	B	309	Total O 309 309	0	0

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.

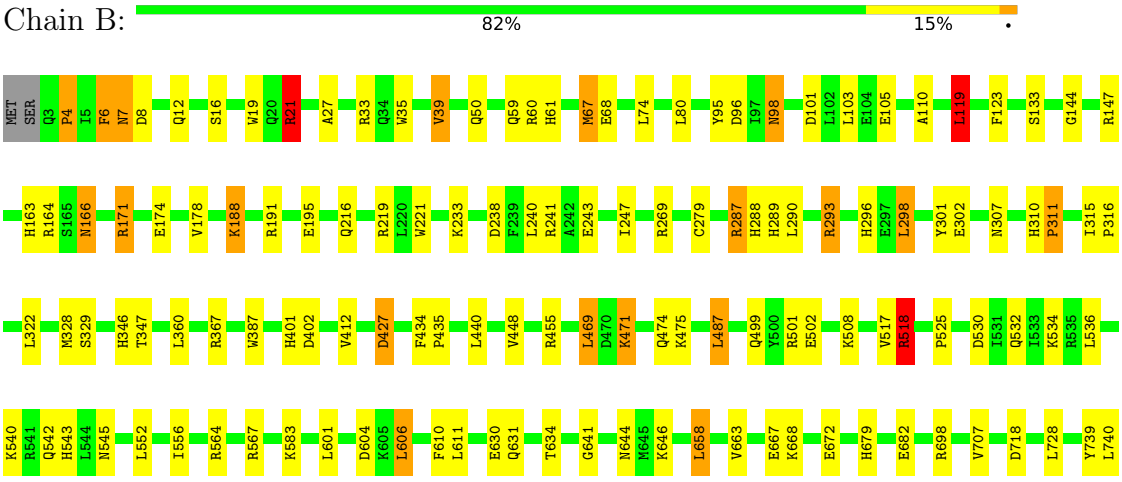
• Molecule 1: Maltodextrin phosphorylase

Chain A:



• Molecule 1: Maltodextrin phosphorylase

Chain B:




D744
D756
V757
L758
Q762
M778
Y788
K796
R797

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.50Å 119.79Å 150.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.50 – 2.18 71.50 – 1.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (71.50-2.18) 99.9 (71.50-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.177 , 0.229 0.186 , 0.238	Depositor DCC
R_{free} test set	2018 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13558	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: A1H3V, EDO, SO4, LLP, PEG

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	0.77	4/6457 (0.1%)	1.30	64/8772 (0.7%)
1	B	0.72	3/6440 (0.0%)	1.23	52/8752 (0.6%)
All	All	0.75	7/12897 (0.1%)	1.27	116/17524 (0.7%)

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	A	0	7
1	B	0	7
All	All	0	14

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	GLU	CD-OE2	7.76	1.34	1.25
1	A	354	GLU	CD-OE1	6.25	1.32	1.25
1	B	243	GLU	CD-OE1	5.94	1.32	1.25
1	B	105	GLU	CD-OE2	-5.45	1.19	1.25
1	A	157	GLU	CD-OE1	-5.42	1.19	1.25
1	A	21	ARG	NE-CZ	5.15	1.39	1.33
1	B	195	GLU	CD-OE1	5.12	1.31	1.25

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	ARG	NE-CZ-NH2	-16.17	112.21	120.30
1	B	171	ARG	NE-CZ-NH2	-12.33	114.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	518	ARG	NE-CZ-NH1	-12.07	114.26	120.30
1	A	293	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	B	21	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	269	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	B	564	ARG	NE-CZ-NH1	-10.47	115.06	120.30
1	A	518	ARG	NE-CZ-NH2	9.99	125.30	120.30
1	B	219	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	60	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	80	LEU	CB-CG-CD1	-9.17	95.41	111.00
1	A	487	LEU	CB-CG-CD1	-9.02	95.66	111.00
1	A	21	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	33	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	518	ARG	NE-CZ-NH1	-8.63	115.99	120.30
1	A	497	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	293	ARG	CD-NE-CZ	8.11	134.95	123.60
1	B	33	ARG	CD-NE-CZ	8.09	134.92	123.60
1	A	80	LEU	CB-CG-CD2	8.03	124.65	111.00
1	A	349	MET	CG-SD-CE	7.97	112.95	100.20
1	A	219	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	564	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	B	33	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	12	GLN	CB-CA-C	-7.76	94.88	110.40
1	A	269	ARG	CD-NE-CZ	7.72	134.41	123.60
1	A	297	GLU	CG-CD-OE1	-7.67	102.97	118.30
1	A	775	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	B	60	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	367	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	219	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	510	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	668	LYS	CD-CE-NZ	-7.12	95.33	111.70
1	A	518	ARG	CD-NE-CZ	7.05	133.47	123.60
1	B	518	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	A	119	LEU	CB-CG-CD2	6.96	122.83	111.00
1	A	658	LEU	CB-CG-CD2	6.95	122.82	111.00
1	A	73	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	21	ARG	CD-NE-CZ	6.94	133.32	123.60
1	A	647	LEU	CB-CG-CD1	6.87	122.68	111.00
1	B	567	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	269	ARG	CG-CD-NE	-6.82	97.49	111.80
1	A	147	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	B	191	ARG	CA-CB-CG	6.78	128.31	113.40
1	B	606	LEU	CB-CG-CD2	6.76	122.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	606	LEU	CB-CG-CD2	6.56	122.15	111.00
1	B	797	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	B	80	LEU	CB-CG-CD2	6.53	122.09	111.00
1	A	502	GLU	N-CA-CB	6.52	122.34	110.60
1	B	796	LYS	CB-CA-C	6.51	123.42	110.40
1	A	290	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	B	427	ASP	CB-CA-C	6.39	123.18	110.40
1	A	535	ARG	CD-NE-CZ	6.33	132.47	123.60
1	A	497	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	658	LEU	CB-CG-CD2	6.25	121.62	111.00
1	B	103	LEU	CB-CG-CD1	-6.17	100.51	111.00
1	B	501	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	559	ASN	CB-CA-C	6.13	122.65	110.40
1	A	607	LYS	N-CA-CB	6.12	121.62	110.60
1	A	354	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	A	740	LEU	CB-CG-CD2	6.07	121.31	111.00
1	A	682	GLU	CB-CA-C	6.05	122.50	110.40
1	B	164	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	B	328	MET	CG-SD-CE	-5.95	90.67	100.20
1	B	601	LEU	CB-CG-CD2	-5.94	100.90	111.00
1	A	502	GLU	CB-CG-CD	5.93	130.22	114.20
1	A	60	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	119	LEU	CB-CG-CD2	5.91	121.04	111.00
1	B	604	ASP	CB-CA-C	5.90	122.20	110.40
1	A	33	ARG	CD-NE-CZ	5.87	131.82	123.60
1	B	241	ARG	CD-NE-CZ	5.81	131.73	123.60
1	B	188	LYS	CD-CE-NZ	-5.79	98.38	111.70
1	A	145	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	B	778	MET	CG-SD-CE	5.71	109.34	100.20
1	A	293	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	269	ARG	CG-CD-NE	5.66	123.69	111.80
1	A	786	ARG	N-CA-CB	5.64	120.75	110.60
1	B	174	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	B	80	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	241	ARG	CD-NE-CZ	5.60	131.45	123.60
1	B	269	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	297	GLU	CG-CD-OE2	5.55	129.40	118.30
1	A	12	GLN	N-CA-CB	5.49	120.48	110.60
1	B	740	LEU	CB-CG-CD2	5.48	120.31	111.00
1	A	502	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	B	698	ARG	NE-CZ-NH1	5.43	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	GLN	N-CA-CB	5.39	120.29	110.60
1	B	8	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	783	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	501	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	487	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	A	518	ARG	CG-CD-NE	5.33	122.98	111.80
1	B	758	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	A	263	THR	CA-CB-OG1	-5.25	97.97	109.00
1	A	164	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	611	LEU	CB-CG-CD1	5.25	119.93	111.00
1	B	698	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	539	TYR	CB-CG-CD2	5.23	124.14	121.00
1	A	256	LEU	CB-CG-CD2	5.22	119.88	111.00
1	B	39	VAL	CA-CB-CG2	5.22	118.73	110.90
1	B	269	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	767	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	39	VAL	CG1-CB-CG2	5.12	119.10	110.90
1	A	59	GLN	CB-CA-C	5.12	120.64	110.40
1	B	21	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	B	59	GLN	CB-CA-C	5.10	120.60	110.40
1	A	513	GLU	CB-CG-CD	5.09	127.95	114.20
1	A	54	LYS	N-CA-CB	5.07	119.72	110.60
1	B	796	LYS	CB-CG-CD	5.07	124.77	111.60
1	B	707	VAL	N-CA-CB	-5.05	100.39	111.50
1	B	601	LEU	N-CA-CB	-5.05	100.31	110.40
1	B	583	LYS	CD-CE-NZ	-5.04	100.10	111.70
1	B	469	LEU	CB-CG-CD2	5.03	119.55	111.00
1	A	307	ASN	CB-CA-C	-5.03	100.34	110.40
1	A	241	ARG	CB-CG-CD	5.01	124.62	111.60
1	A	493	ASP	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	293	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	4	PRO	Peptide
1	A	518	ARG	Sidechain
1	A	564	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	147	ARG	Sidechain
1	B	21	ARG	Sidechain
1	B	287	ARG	Sidechain
1	B	293	ARG	Sidechain
1	B	4	PRO	Peptide
1	B	455	ARG	Sidechain
1	B	518	ARG	Sidechain

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	6332	0	6152	58	0
1	B	6315	0	6117	62	0
2	A	14	0	0	0	0
3	A	56	0	84	7	0
3	B	68	0	102	4	0
4	A	21	0	30	1	0
4	B	28	0	39	7	0
5	A	40	0	0	2	0
5	B	55	0	0	1	0
6	A	320	0	0	11	1
6	B	309	0	0	9	1
All	All	13558	0	12524	121	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 5.

All (121) 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:B:502:GLU:HG3	4:B:821:PEG:H41	1.50	0.93
1:B:289:HIS:HD2	3:B:806:EDO:O1	1.62	0.83
1:A:559:ASN:HA	1:A:561:GLN:NE2	1.95	0.80
1:B:502:GLU:CG	4:B:821:PEG:H41	2.13	0.78
1:A:238:ASP:OD1	6:A:901:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:GLU:HG3	4:B:821:PEG:C4	2.14	0.76
1:B:4:PRO:HB2	1:B:50:GLN:NE2	2.00	0.76
1:A:559:ASN:HA	1:A:561:GLN:HE22	1.52	0.72
1:B:667:GLU:CB	6:B:1204:HOH:O	2.38	0.70
1:B:27:ALA:HB3	3:B:815:EDO:H12	1.75	0.68
1:B:296:HIS:ND1	6:B:903:HOH:O	2.27	0.67
1:B:682[B]:GLU:OE2	6:B:901:HOH:O	2.12	0.66
1:A:561:GLN:H	1:A:561:GLN:CD	1.98	0.66
1:B:4:PRO:HB2	1:B:50:GLN:HE21	1.58	0.66
1:A:401:HIS:HD2	1:A:402:ASP:OD1	1.82	0.63
1:B:401:HIS:HD2	1:B:402:ASP:OD1	1.80	0.63
1:B:289:HIS:CD2	3:B:806:EDO:O1	2.49	0.62
1:B:98:ASN:HD22	1:B:101:ASP:H	1.47	0.62
1:B:110:ALA:HB1	1:B:144:GLY:HA3	1.81	0.61
1:B:12:GLN:NE2	6:B:905:HOH:O	2.31	0.61
1:A:16:SER:HA	1:A:19:TRP:NE1	2.16	0.59
1:B:471:LYS:NZ	1:B:499:GLN:HE22	2.01	0.58
3:A:803:EDO:H21	5:A:820:SO4:O2	2.04	0.58
1:B:469:LEU:CD2	1:B:487:LEU:HD11	2.34	0.58
1:A:52:PHE:HA	6:A:974:HOH:O	2.03	0.57
1:A:559:ASN:OD1	1:A:561:GLN:NE2	2.38	0.57
1:A:182:ILE:HD13	1:A:198:ILE:HD12	1.86	0.57
1:A:32:PRO:HB2	3:A:816:EDO:H11	1.87	0.56
4:B:820:PEG:H32	4:B:820:PEG:O1	2.06	0.56
1:A:35:TRP:O	1:A:39:VAL:HG13	2.06	0.55
1:B:672:GLU:HB3	6:B:1191:HOH:O	2.06	0.55
1:B:508:LYS:HE2	1:B:525:PRO:O	2.06	0.55
1:A:310:HIS:N	1:A:311:PRO:CD	2.70	0.54
1:B:61:HIS:HE1	6:B:935:HOH:O	1.89	0.54
1:A:240:LEU:HD12	1:B:247:ILE:HD13	1.90	0.54
1:B:534:LYS:HE3	1:B:631:GLN:OE1	2.07	0.54
1:B:434:PHE:N	1:B:435:PRO:CD	2.71	0.54
1:A:679:HIS:HD2	1:A:744:ASP:OD1	1.91	0.53
1:B:329:SER:HB2	3:B:814:EDO:H11	1.90	0.53
1:A:328:MET:CE	1:A:332:ASP:HB3	2.39	0.53
1:B:16:SER:HA	1:B:19:TRP:NE1	2.23	0.53
1:B:310:HIS:N	1:B:311:PRO:CD	2.71	0.53
1:B:4:PRO:CB	1:B:50:GLN:HE21	2.20	0.53
1:B:502:GLU:CG	4:B:821:PEG:C4	2.82	0.53
1:A:61:HIS:HE1	6:A:944:HOH:O	1.93	0.52
4:A:804:PEG:H31	6:A:1175:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:HD22	1:A:302:GLU:HB2	1.92	0.51
1:A:638:GLU:O	6:A:902:HOH:O	2.19	0.51
1:B:469:LEU:HD22	1:B:487:LEU:HD11	1.92	0.51
1:B:502:GLU:HB2	4:B:821:PEG:H11	1.92	0.50
1:A:471:LYS:NZ	1:A:499:GLN:HE22	2.09	0.50
1:A:142:GLN:HE21	3:A:802:EDO:H12	1.78	0.49
1:A:434:PHE:N	1:A:435:PRO:CD	2.76	0.49
1:B:401:HIS:CD2	1:B:402:ASP:OD1	2.65	0.49
1:A:247:ILE:HD13	1:B:240:LEU:HD12	1.95	0.48
1:A:98:ASN:HD22	1:A:101:ASP:H	1.61	0.48
1:A:119:LEU:HD22	1:A:123:PHE:CE1	2.48	0.48
1:B:119:LEU:HD22	1:B:123:PHE:CE1	2.48	0.48
1:B:95:TYR:O	1:B:96:ASP:HB2	2.14	0.48
1:B:471:LYS:HZ1	1:B:499:GLN:HE22	1.62	0.48
1:A:538:GLU:HG2	1:A:739:TYR:CD2	2.48	0.48
1:B:35:TRP:O	1:B:39:VAL:HG13	2.14	0.48
1:B:679:HIS:HD2	1:B:744:ASP:OD1	1.96	0.48
1:A:401:HIS:CD2	1:A:402:ASP:OD1	2.66	0.48
1:A:693:ASP:OD1	6:A:903:HOH:O	2.20	0.48
1:B:762:GLN:CG	6:B:1190:HOH:O	2.61	0.48
1:A:221:TRP:CE2	1:A:279:CYS:HB3	2.49	0.47
1:B:434:PHE:N	1:B:435:PRO:HD3	2.29	0.47
1:A:296:HIS:HB3	6:A:1203:HOH:O	2.15	0.47
1:A:266:LYS:CE	6:A:922:HOH:O	2.61	0.47
1:A:266:LYS:HE2	6:A:922:HOH:O	2.14	0.47
1:A:594:ASP:OD2	6:A:904:HOH:O	2.20	0.47
1:B:298:LEU:HD22	1:B:302:GLU:HB2	1.97	0.47
1:B:534:LYS:CE	1:B:631:GLN:OE1	2.63	0.47
1:A:679:HIS:CD2	1:A:744:ASP:OD1	2.68	0.46
1:B:307:ASN:ND2	1:B:346:HIS:NE2	2.63	0.46
1:B:221:TRP:CE2	1:B:279:CYS:HB3	2.51	0.46
1:B:6:PHE:O	1:B:7:ASN:CB	2.63	0.46
1:B:98:ASN:ND2	1:B:101:ASP:H	2.12	0.46
1:A:310:HIS:HB2	1:A:311:PRO:HD3	1.98	0.46
1:B:532:GLN:HE22	1:B:542:GLN:HA	1.80	0.45
1:B:387:TRP:CZ3	1:B:440:LEU:HD21	2.51	0.45
1:A:523:ILE:O	1:A:525:PRO:HD3	2.16	0.45
1:B:475:LYS:NZ	6:B:915:HOH:O	2.41	0.45
1:B:634:THR:OG1	1:B:739:TYR:HB3	2.17	0.44
1:A:518:ARG:HA	1:A:518:ARG:HD2	1.85	0.44
1:B:679:HIS:CD2	1:B:744:ASP:OD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:803:EDO:C2	5:A:820:SO4:O2	2.66	0.44
1:A:32:PRO:HD2	3:A:816:EDO:H21	2.00	0.43
1:A:534:LYS:HD3	1:A:540:LYS:HD3	1.99	0.43
1:B:133:SER:HA	1:B:216:GLN:OE1	2.18	0.43
1:A:171:ARG:HB2	1:B:21:ARG:O	2.19	0.43
1:A:410:LEU:O	1:A:410:LEU:HD12	2.19	0.43
1:A:293:ARG:HD3	1:A:301:TYR:CD1	2.54	0.43
1:A:293:ARG:HD3	1:A:301:TYR:CG	2.53	0.43
1:A:165:SER:OG	3:A:802:EDO:H22	2.20	0.42
1:A:750:GLU:OE2	1:A:754:GLN:NE2	2.53	0.42
1:A:110:ALA:HB1	1:A:144:GLY:HA3	2.00	0.42
1:A:286:ARG:HG2	3:A:807:EDO:H22	2.01	0.42
1:A:692:TYR:CE2	1:A:740:LEU:HD22	2.55	0.42
1:B:530:ASP:OD1	1:B:630:GLU:OE2	2.38	0.42
1:A:328:MET:HE3	1:A:332:ASP:HB3	2.02	0.42
1:B:448:VAL:HG11	1:B:788:TYR:CD2	2.55	0.42
1:A:448:VAL:HG11	1:A:788:TYR:CD2	2.55	0.41
1:A:95:TYR:O	1:A:96:ASP:HB2	2.19	0.41
1:A:380:LYS:HA	1:A:394:TRP:CZ3	2.55	0.41
1:B:233:LYS:HE2	6:B:1177:HOH:O	2.20	0.41
1:B:540:LYS:HE3	5:B:832:SO4:O1	2.20	0.41
1:A:740:LEU:HB3	1:A:743:ALA:HB3	2.02	0.41
1:A:559:ASN:CA	1:A:561:GLN:NE2	2.76	0.41
1:B:293:ARG:HD3	1:B:301:TYR:CG	2.55	0.41
1:B:315:ILE:HB	1:B:316:PRO:CD	2.51	0.41
1:A:221:TRP:CD2	1:A:279:CYS:HB3	2.56	0.41
1:A:360:LEU:HD23	6:A:911:HOH:O	2.20	0.41
1:A:535:ARG:O	1:A:540:LYS:HD2	2.21	0.41
1:B:502:GLU:HG3	4:B:821:PEG:H42	2.01	0.41
1:B:163:HIS:HB3	1:B:166:ASN:ND2	2.35	0.41
1:B:67:MET:HG3	1:B:310:HIS:HB3	2.03	0.40
1:A:533:ILE:O	1:A:534:LYS:HB3	2.21	0.40
1:B:288:HIS:CE1	1:B:298:LEU:HA	2.56	0.40
1:A:507:ASN:OD1	1:A:510:ARG:NH2	2.55	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)
6:A:1165:HOH:O	6:B:1117:HOH:O[4_545]	2.14	0.06

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	793/797 (100%)	760 (96%)	30 (4%)	3 (0%)	34	35
1	B	794/797 (100%)	768 (97%)	22 (3%)	4 (0%)	29	28
All	All	1587/1594 (100%)	1528 (96%)	52 (3%)	7 (0%)	34	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	ASN
1	B	6	PHE
1	A	3	GLN
1	A	422	ALA
1	B	311	PRO
1	A	311	PRO
1	B	641	GLY

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	643/667 (96%)	607 (94%)	36 (6%)	21	23
1	B	635/667 (95%)	599 (94%)	36 (6%)	20	22
All	All	1278/1334 (96%)	1206 (94%)	72 (6%)	21	23

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	12	GLN
1	A	39	VAL
1	A	74	LEU
1	A	98	ASN
1	A	118	ARG
1	A	119	LEU
1	A	178	VAL
1	A	188	LYS
1	A	266	LYS
1	A	269	ARG
1	A	298	LEU
1	A	322	LEU
1	A	360	LEU
1	A	412	VAL
1	A	455	ARG
1	A	471	LYS
1	A	513	GLU
1	A	517	VAL
1	A	518	ARG
1	A	522	GLU
1	A	526	GLN
1	A	536	LEU
1	A	543	HIS
1	A	545	ASN
1	A	552	LEU
1	A	556	ILE
1	A	565	VAL
1	A	606	LEU
1	A	610	PHE
1	A	644	ASN
1	A	658	LEU
1	A	707	VAL
1	A	728	LEU
1	A	733	LYS
1	A	756	ASP
1	B	67	MET
1	B	68	GLU
1	B	74	LEU
1	B	98	ASN
1	B	119	LEU
1	B	166	ASN
1	B	171	ARG

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Mol	Chain	Res	Type
1	B	178	VAL
1	B	188	LYS
1	B	238	ASP
1	B	287	ARG
1	B	290	LEU
1	B	298	LEU
1	B	322	LEU
1	B	347	THR
1	B	360	LEU
1	B	412	VAL
1	B	427	ASP
1	B	471	LYS
1	B	474	GLN
1	B	517	VAL
1	B	518	ARG
1	B	536	LEU
1	B	543	HIS
1	B	545	ASN
1	B	552	LEU
1	B	556	ILE
1	B	606	LEU
1	B	610	PHE
1	B	644	ASN
1	B	658	LEU
1	B	663	VAL
1	B	668	LYS
1	B	718	ASP
1	B	728	LEU
1	B	756	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	61	HIS
1	A	81	ASN
1	A	98	ASN
1	A	401	HIS
1	A	447	ASN
1	A	499	GLN
1	A	526	GLN
1	A	532	GLN

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Mol	Chain	Res	Type
1	A	545	ASN
1	A	679	HIS
1	B	50	GLN
1	B	61	HIS
1	B	98	ASN
1	B	166	ASN
1	B	273	GLN
1	B	289	HIS
1	B	307	ASN
1	B	401	HIS
1	B	406	HIS
1	B	447	ASN
1	B	499	GLN
1	B	532	GLN
1	B	545	ASN
1	B	679	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)

2 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	$\#\|Z\| > 2$
1	LLP	B	646	1	23,24,25	0.91	1 (4%)	25,32,34	1.34	2 (8%)
1	LLP	A	646	1	23,24,25	0.88	1 (4%)	25,32,34	1.74	5 (20%)

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
1	LLP	B	646	1	-	2/16/17/19	0/1/1/1
1	LLP	A	646	1	-	0/16/17/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	646	LLP	P-OP2	-2.92	1.43	1.54
1	B	646	LLP	P-OP2	-2.69	1.44	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	646	LLP	OP2-P-OP4	-4.86	93.80	106.73
1	B	646	LLP	CD-CE-NZ	3.91	120.50	110.93
1	A	646	LLP	OP4-P-OP1	3.56	116.46	106.47
1	A	646	LLP	CD-CE-NZ	3.32	119.06	110.93
1	B	646	LLP	C3-C2-N1	-2.29	117.81	120.77
1	A	646	LLP	OP3-P-OP2	2.20	116.03	107.64
1	A	646	LLP	C3-C2-N1	-2.14	118.01	120.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	646	LLP	C4-C4'-NZ-CE
1	B	646	LLP	C6-C5-C5'-OP4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

58 ligands 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	$\#\|Z\| > 2$
3	EDO	B	804	-	3,3,3	1.45	0	2,2,2	1.12	0
5	SO4	B	828	-	4,4,4	0.65	0	6,6,6	0.64	0
5	SO4	A	826	-	4,4,4	0.23	0	6,6,6	0.29	0
3	EDO	A	811	-	3,3,3	0.67	0	2,2,2	1.02	0
4	PEG	B	820	-	6,6,6	0.71	0	5,5,5	0.55	0
5	SO4	A	825	-	4,4,4	0.49	0	6,6,6	0.50	0
3	EDO	A	809	-	3,3,3	0.52	0	2,2,2	0.57	0
3	EDO	A	807	-	3,3,3	0.55	0	2,2,2	0.52	0
5	SO4	A	821	-	4,4,4	0.29	0	6,6,6	0.26	0
3	EDO	B	805	-	3,3,3	0.23	0	2,2,2	0.27	0
3	EDO	B	812	-	3,3,3	0.31	0	2,2,2	0.36	0
3	EDO	B	810	-	3,3,3	0.22	0	2,2,2	0.19	0
4	PEG	A	804	-	6,6,6	0.54	0	5,5,5	0.56	0
5	SO4	B	827	-	4,4,4	0.17	0	6,6,6	0.29	0
4	PEG	B	819	-	6,6,6	0.32	0	5,5,5	0.28	0
5	SO4	B	824	-	4,4,4	0.14	0	6,6,6	0.29	0
3	EDO	A	805	-	3,3,3	0.59	0	2,2,2	0.87	0
3	EDO	B	815	-	3,3,3	0.56	0	2,2,2	0.89	0
3	EDO	A	817	-	3,3,3	0.22	0	2,2,2	0.34	0
3	EDO	A	815	-	3,3,3	0.55	0	2,2,2	0.14	0
3	EDO	B	813	-	3,3,3	0.68	0	2,2,2	0.44	0
3	EDO	A	810	-	3,3,3	0.16	0	2,2,2	0.18	0
5	SO4	A	824	-	4,4,4	0.43	0	6,6,6	0.53	0
5	SO4	A	822	-	4,4,4	0.37	0	6,6,6	0.47	0
2	A1H3V	A	801	-	15,15,15	1.91	2 (13%)	18,22,22	2.14	6 (33%)
3	EDO	B	814	-	3,3,3	0.71	0	2,2,2	0.42	0
3	EDO	B	802	-	3,3,3	0.86	0	2,2,2	0.80	0
3	EDO	A	802	-	3,3,3	0.93	0	2,2,2	0.04	0
5	SO4	B	832	-	4,4,4	0.54	0	6,6,6	0.46	0
3	EDO	A	814	-	3,3,3	0.87	0	2,2,2	0.76	0
3	EDO	A	808	-	3,3,3	0.47	0	2,2,2	0.74	0
5	SO4	B	825	-	4,4,4	0.34	0	6,6,6	0.22	0
5	SO4	A	820	-	4,4,4	0.32	0	6,6,6	0.26	0
5	SO4	B	826	-	4,4,4	0.29	0	6,6,6	0.06	0
5	SO4	B	823	-	4,4,4	0.22	0	6,6,6	0.44	0
3	EDO	B	818	-	3,3,3	0.32	0	2,2,2	0.47	0
5	SO4	A	823	-	4,4,4	0.48	0	6,6,6	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	B	817	-	3,3,3	0.14	0	2,2,2	0.25	0
5	SO4	B	831	-	4,4,4	0.48	0	6,6,6	0.89	0
3	EDO	B	808	-	3,3,3	0.89	0	2,2,2	0.80	0
4	PEG	A	818	-	6,6,6	0.25	0	5,5,5	0.29	0
5	SO4	A	819	-	4,4,4	0.36	0	6,6,6	0.17	0
3	EDO	A	812	-	3,3,3	0.28	0	2,2,2	0.27	0
5	SO4	B	830	-	4,4,4	0.37	0	6,6,6	0.32	0
5	SO4	B	822	-	4,4,4	0.43	0	6,6,6	0.32	0
4	PEG	B	821	-	6,6,6	0.60	0	5,5,5	0.50	0
3	EDO	A	816	-	3,3,3	0.51	0	2,2,2	0.46	0
3	EDO	A	813	-	3,3,3	0.41	0	2,2,2	0.30	0
3	EDO	B	807	-	3,3,3	0.35	0	2,2,2	0.35	0
3	EDO	B	803	-	3,3,3	0.17	0	2,2,2	0.48	0
3	EDO	B	816	-	3,3,3	0.31	0	2,2,2	0.18	0
4	PEG	A	806	-	6,6,6	0.73	0	5,5,5	0.44	0
5	SO4	B	829	-	4,4,4	0.55	0	6,6,6	0.45	0
3	EDO	B	806	-	3,3,3	0.45	0	2,2,2	0.13	0
3	EDO	B	811	-	3,3,3	0.75	0	2,2,2	0.49	0
3	EDO	A	803	-	3,3,3	0.60	0	2,2,2	0.52	0
3	EDO	B	809	-	3,3,3	0.85	0	2,2,2	0.86	0
4	PEG	B	801	-	6,6,6	0.84	0	5,5,5	0.52	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
3	EDO	B	804	-	-	0/1/1/1	-
3	EDO	A	811	-	-	1/1/1/1	-
4	PEG	B	820	-	-	2/4/4/4	-
3	EDO	A	809	-	-	1/1/1/1	-
3	EDO	A	807	-	-	1/1/1/1	-
3	EDO	B	805	-	-	1/1/1/1	-
3	EDO	B	812	-	-	1/1/1/1	-
3	EDO	B	810	-	-	1/1/1/1	-
4	PEG	A	804	-	-	1/4/4/4	-
4	PEG	B	819	-	-	1/4/4/4	-
3	EDO	A	805	-	-	0/1/1/1	-
3	EDO	B	815	-	-	1/1/1/1	-
3	EDO	A	817	-	-	1/1/1/1	-
3	EDO	A	815	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	813	-	-	1/1/1/1	-
3	EDO	A	810	-	-	1/1/1/1	-
2	A1H3V	A	801	-	-	0/2/30/30	0/2/2/2
3	EDO	B	814	-	-	1/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-
3	EDO	A	802	-	-	1/1/1/1	-
3	EDO	A	814	-	-	0/1/1/1	-
3	EDO	A	808	-	-	0/1/1/1	-
3	EDO	B	818	-	-	1/1/1/1	-
3	EDO	B	817	-	-	0/1/1/1	-
3	EDO	B	808	-	-	1/1/1/1	-
4	PEG	A	818	-	-	3/4/4/4	-
3	EDO	A	812	-	-	0/1/1/1	-
4	PEG	B	821	-	-	3/4/4/4	-
3	EDO	A	816	-	-	1/1/1/1	-
3	EDO	A	813	-	-	0/1/1/1	-
3	EDO	B	807	-	-	0/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-
3	EDO	B	816	-	-	1/1/1/1	-
4	PEG	A	806	-	-	3/4/4/4	-
3	EDO	B	806	-	-	1/1/1/1	-
3	EDO	B	811	-	-	1/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	B	809	-	-	1/1/1/1	-
4	PEG	B	801	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1H3V	C2-N1	6.16	1.56	1.45
2	A	801	A1H3V	C8-C2	2.18	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	A1H3V	C4-C3-C2	5.66	119.54	111.35
2	A	801	A1H3V	C3-O5-C1	3.26	111.87	109.10
2	A	801	A1H3V	O3-C7-C5	-3.22	104.64	110.08
2	A	801	A1H3V	C7-C8-C2	3.09	114.88	110.34
2	A	801	A1H3V	O4-C8-C2	2.76	115.23	109.66
2	A	801	A1H3V	C5-C4-C3	2.12	118.22	112.42

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	PEG	O2-C3-C4-O4
4	B	821	PEG	O2-C3-C4-O4
3	A	809	EDO	O1-C1-C2-O2
3	B	806	EDO	O1-C1-C2-O2
4	B	820	PEG	O2-C3-C4-O4
4	A	806	PEG	O1-C1-C2-O2
3	A	802	EDO	O1-C1-C2-O2
3	B	805	EDO	O1-C1-C2-O2
3	B	808	EDO	O1-C1-C2-O2
3	B	809	EDO	O1-C1-C2-O2
3	B	812	EDO	O1-C1-C2-O2
3	B	816	EDO	O1-C1-C2-O2
3	B	818	EDO	O1-C1-C2-O2
4	A	818	PEG	O2-C3-C4-O4
4	A	804	PEG	O1-C1-C2-O2
3	A	807	EDO	O1-C1-C2-O2
3	A	817	EDO	O1-C1-C2-O2
3	A	810	EDO	O1-C1-C2-O2
3	B	814	EDO	O1-C1-C2-O2
3	B	815	EDO	O1-C1-C2-O2
4	A	818	PEG	O1-C1-C2-O2
4	B	821	PEG	O1-C1-C2-O2
4	A	806	PEG	C4-C3-O2-C2
4	B	819	PEG	C1-C2-O2-C3
4	B	820	PEG	C1-C2-O2-C3
3	A	815	EDO	O1-C1-C2-O2
4	A	818	PEG	C1-C2-O2-C3
4	A	806	PEG	C1-C2-O2-C3
3	B	813	EDO	O1-C1-C2-O2
3	B	810	EDO	O1-C1-C2-O2
4	B	821	PEG	C1-C2-O2-C3
4	B	801	PEG	C1-C2-O2-C3
3	A	811	EDO	O1-C1-C2-O2
3	A	816	EDO	O1-C1-C2-O2
3	B	811	EDO	O1-C1-C2-O2

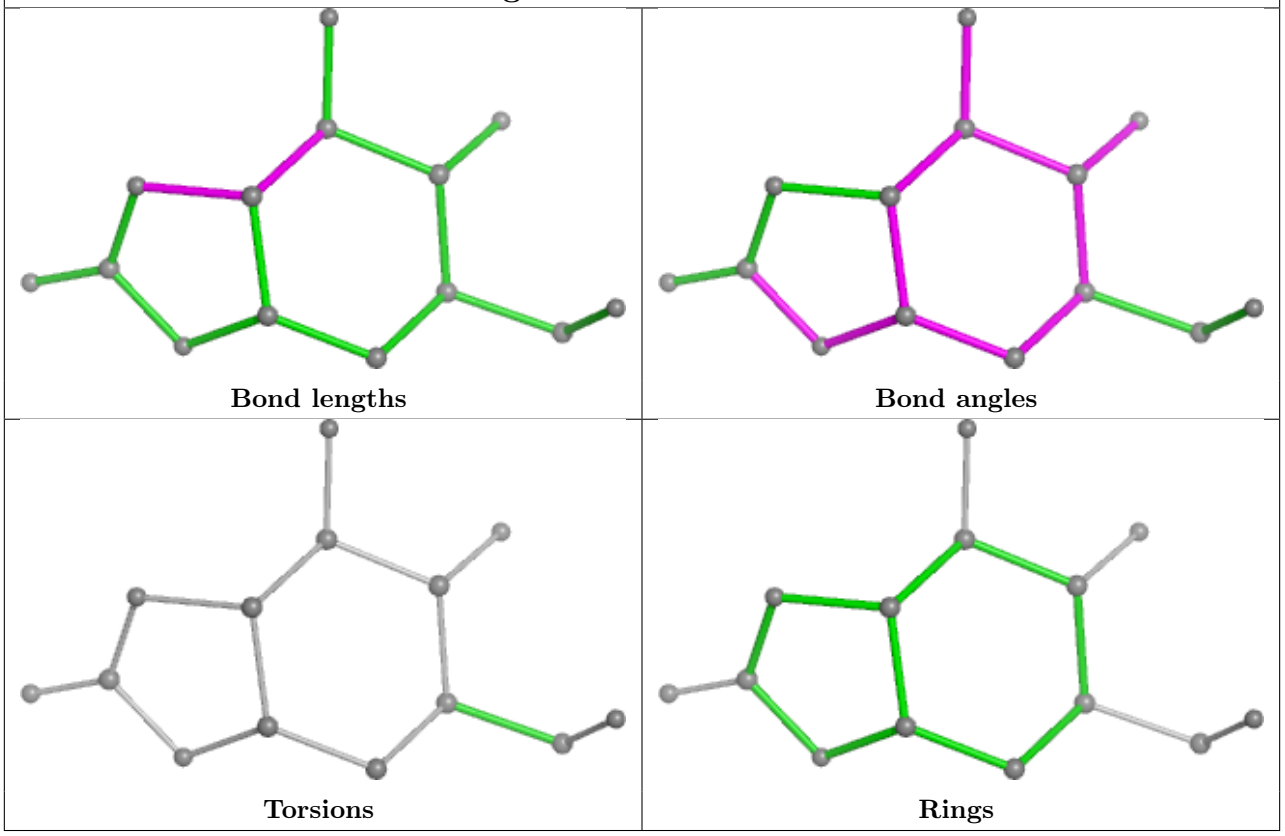
There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	820	PEG	1	0
3	A	807	EDO	1	0
4	A	804	PEG	1	0
3	B	815	EDO	1	0
3	B	814	EDO	1	0
3	A	802	EDO	2	0
5	B	832	SO4	1	0
5	A	820	SO4	2	0
4	B	821	PEG	6	0
3	A	816	EDO	2	0
3	B	806	EDO	2	0
3	A	803	EDO	2	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 A1H3V A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	795/797 (99%)	-0.58	6 (0%) 86 86	23, 33, 56, 91	0
1	B	794/797 (99%)	-0.68	0 100 100	22, 34, 54, 87	0
All	All	1589/1594 (99%)	-0.63	6 (0%) 92 92	22, 34, 55, 91	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	TRP	3.8
1	A	562	ALA	3.4
1	A	560	PRO	3.2
1	A	561	GLN	3.0
1	A	386	THR	3.0
1	A	442	PRO	2.6

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, 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
1	LLP	A	646	24/25	0.97	0.09	22,27,33,38	0
1	LLP	B	646	24/25	0.98	0.09	22,26,35,42	0

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	EDO	B	813	4/4	0.69	0.14	64,65,68,71	0
4	PEG	B	819	7/7	0.73	0.18	62,72,84,85	0
3	EDO	A	815	4/4	0.75	0.22	61,64,67,74	0
3	EDO	A	814	4/4	0.80	0.19	60,63,67,68	0
3	EDO	A	811	4/4	0.81	0.16	59,61,62,65	0
3	EDO	B	812	4/4	0.81	0.11	62,66,66,67	0
4	PEG	B	820	7/7	0.83	0.15	53,63,71,77	0
3	EDO	B	806	4/4	0.84	0.12	50,58,60,60	0
3	EDO	B	810	4/4	0.84	0.12	61,63,69,72	0
3	EDO	A	817	4/4	0.84	0.30	57,60,75,76	0
3	EDO	A	808	4/4	0.85	0.19	49,49,57,58	0
5	SO4	B	826	5/5	0.86	0.44	77,101,121,143	0
3	EDO	B	809	4/4	0.87	0.26	55,57,57,66	0
3	EDO	A	816	4/4	0.87	0.28	43,52,70,73	0
3	EDO	B	816	4/4	0.87	0.13	53,61,63,68	0
4	PEG	B	821	7/7	0.88	0.33	59,72,80,83	0
4	PEG	A	818	7/7	0.88	0.12	56,59,75,80	0
5	SO4	B	827	5/5	0.88	0.20	62,97,120,127	0
3	EDO	B	807	4/4	0.89	0.18	45,64,70,71	0
3	EDO	A	813	4/4	0.89	0.17	54,56,59,62	0
3	EDO	B	814	4/4	0.90	0.16	50,56,66,68	0
3	EDO	A	807	4/4	0.90	0.21	41,41,42,55	0
3	EDO	B	804	4/4	0.91	0.15	41,44,47,55	0
3	EDO	B	815	4/4	0.91	0.20	40,49,52,59	0
3	EDO	B	811	4/4	0.91	0.11	48,55,59,64	0
3	EDO	A	812	4/4	0.92	0.16	59,60,61,62	0
3	EDO	B	818	4/4	0.92	0.13	44,48,50,66	0
4	PEG	A	806	7/7	0.92	0.12	41,59,61,72	0
4	PEG	B	801	7/7	0.93	0.14	38,50,86,88	0
3	EDO	A	809	4/4	0.93	0.09	45,52,57,61	0
5	SO4	B	831	5/5	0.93	0.17	45,54,65,71	0
4	PEG	A	804	7/7	0.94	0.14	44,53,72,76	0
3	EDO	A	805	4/4	0.94	0.11	44,49,59,59	0
5	SO4	A	826	5/5	0.94	0.09	66,67,96,101	0
3	EDO	B	805	4/4	0.94	0.18	41,63,70,84	0
3	EDO	B	817	4/4	0.94	0.24	47,51,52,59	0
3	EDO	B	808	4/4	0.94	0.11	41,42,52,59	0

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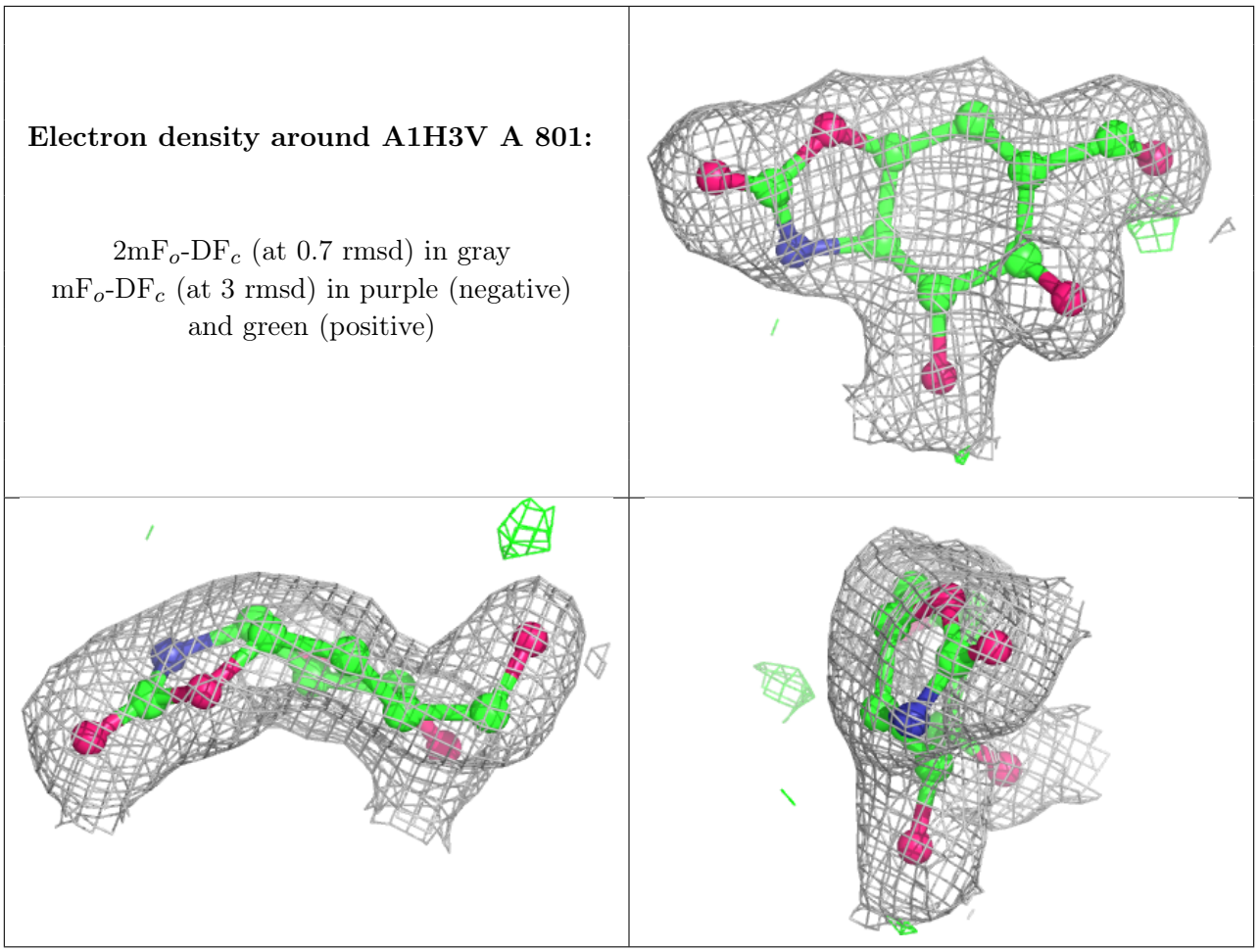
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	802	4/4	0.95	0.18	28,30,34,42	0
5	SO4	A	820	5/5	0.95	0.19	73,79,85,112	0
3	EDO	A	803	4/4	0.95	0.11	36,42,45,49	0
5	SO4	B	823	5/5	0.95	0.14	59,60,78,80	0
5	SO4	B	825	5/5	0.95	0.15	54,68,77,93	0
2	A1H3V	A	801	14/14	0.95	0.09	26,43,48,51	0
3	EDO	B	802	4/4	0.95	0.17	38,39,41,45	0
3	EDO	A	810	4/4	0.95	0.08	51,54,55,57	0
5	SO4	A	821	5/5	0.96	0.08	56,73,74,82	0
5	SO4	A	819	5/5	0.96	0.22	51,68,73,77	0
3	EDO	B	803	4/4	0.96	0.07	42,48,52,71	0
5	SO4	B	824	5/5	0.96	0.10	64,67,69,76	0
5	SO4	A	825	5/5	0.97	0.08	54,55,59,63	0
5	SO4	B	822	5/5	0.97	0.08	38,42,66,69	0
5	SO4	B	832	5/5	0.97	0.08	44,46,48,75	0
5	SO4	A	824	5/5	0.98	0.09	45,46,70,94	0
5	SO4	B	830	5/5	0.98	0.10	43,48,75,81	0
5	SO4	B	829	5/5	0.99	0.09	40,46,58,62	0
5	SO4	A	823	5/5	0.99	0.07	37,42,51,52	0
5	SO4	A	822	5/5	0.99	0.09	38,39,42,43	0
5	SO4	B	828	5/5	0.99	0.07	38,41,44,45	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 A1H3V A 801:

$2mF_o$-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.