Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 05:35 PM JST

PDB ID	:	5GSM
Title	:	Glycoside hydrolase B with product
Authors	:	Watanabe, M.; Kamachi, S.; Mine, S.
Deposited on	:	2016-08-16
Resolution	:	1.27 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 (i) 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 (i)) were used in the production of this report:

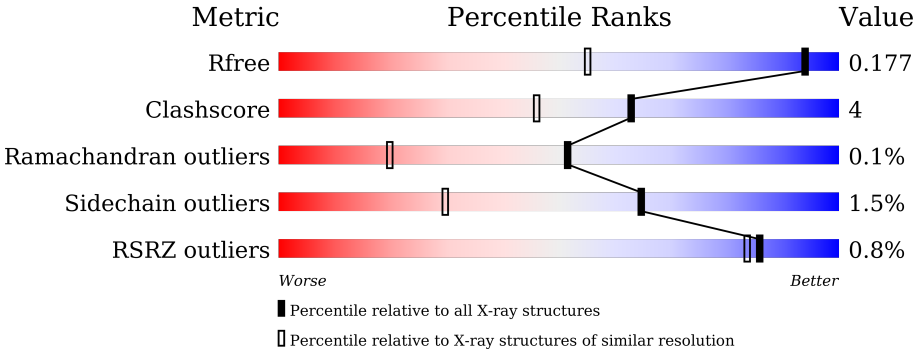
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

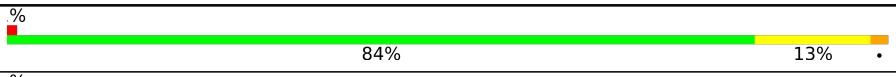
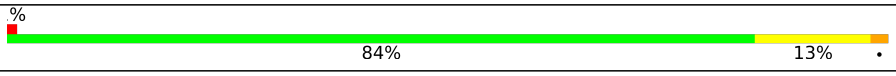
The reported resolution of this entry is 1.27 Å.

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	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	786	
1	B	786	

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	PPI	A	808	-	X	-	-
4	PPI	A	810	-	X	X	-
4	PPI	B	810	-	X	X	-
4	PPI	B	811	-	-	X	-
4	PPI	B	812	-	-	X	-
4	PPI	B	813	-	-	X	-
5	B3P	A	811	-	X	-	-

2 Entry composition (i)

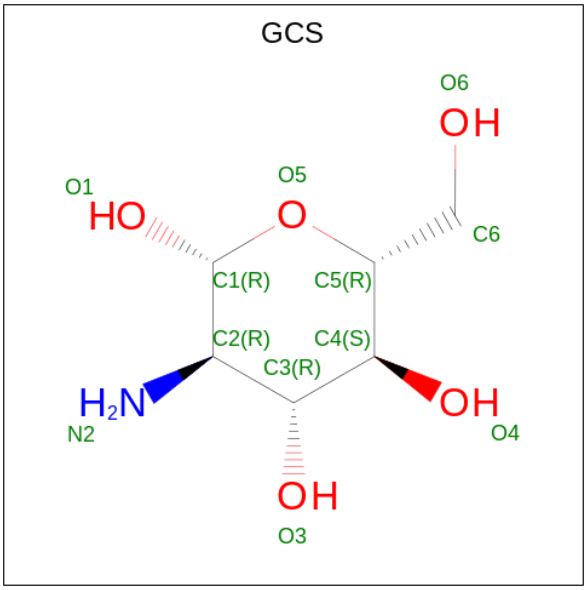
There are 6 unique types of molecules in this entry. The entry contains 14357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exo-beta-D-glucosaminidase.

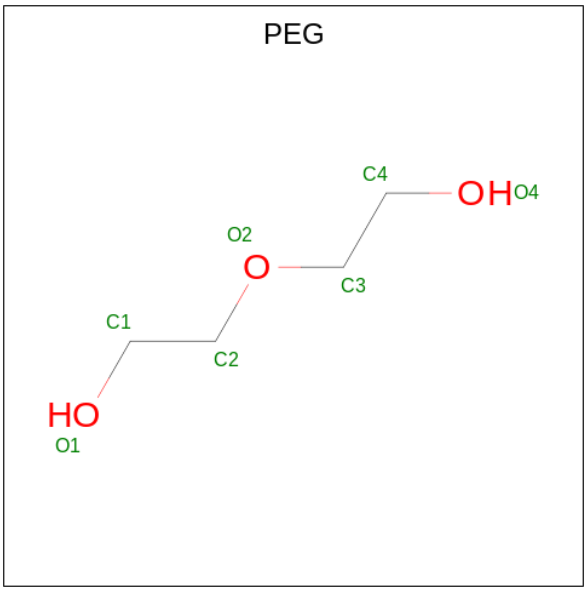
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	786	6446	4191	1064	1176	15	0	7	0
1	B	786	6457	4197	1070	1174	16	0	8	0

- Molecule 2 is 2-amino-2-deoxy-beta-D-glucopyranose (three-letter code: GCS) (formula: $C_6H_{13}NO_5$).



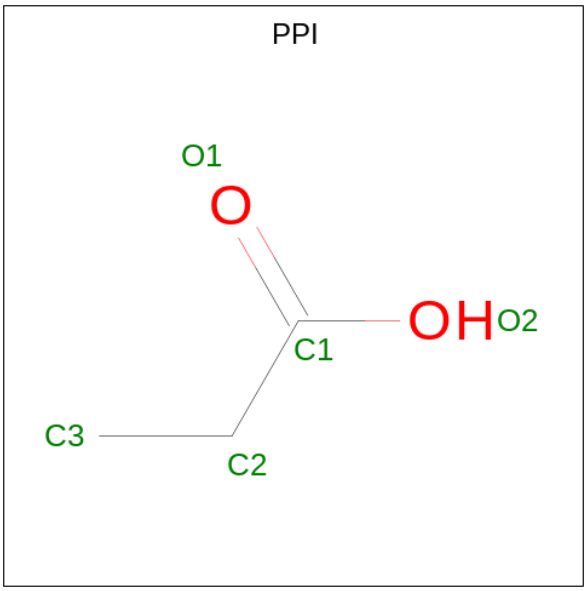
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	6	1	5	0	0
2	B	1	12	6	1	5	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



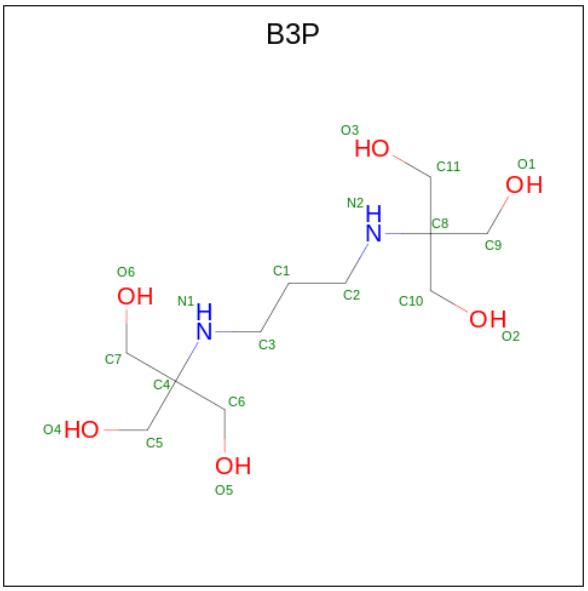
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4	3		0	0
			Total	C	O			
3	B	1	7	4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

- Molecule 4 is PROPANOIC ACID (three-letter code: PPI) (formula: $C_3H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	5	3	2	0	0
4	A	1	5	3	2	0	0
4	A	1	5	3	2	0	0
4	B	1	5	3	2	0	0
4	B	1	5	3	2	0	0
4	B	1	5	3	2	0	0
4	B	1	5	3	2	0	0
4	B	1	5	3	2	0	0
4	B	1	5	3	2	0	0

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	19	11	2	6	0	0

- Molecule 6 is water.

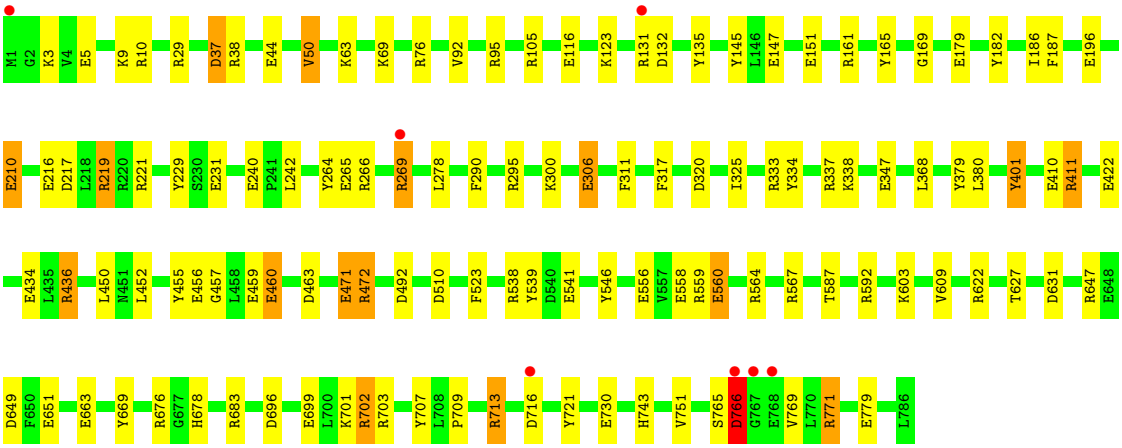
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	608	608	608	0	0
			Total	O		
6	B	674	674	674	0	0

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.

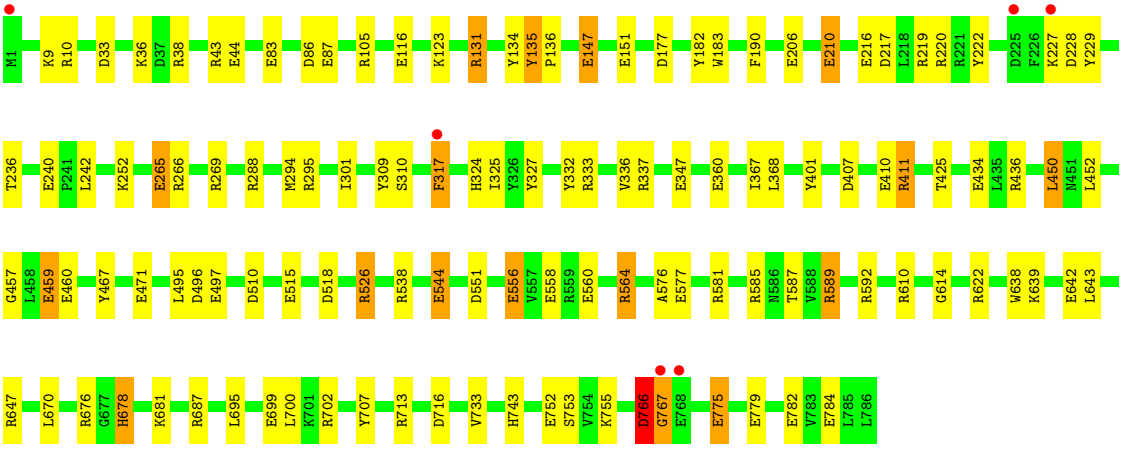
• Molecule 1: Exo-beta-D-glucosaminidase

Chain A:



• Molecule 1: Exo-beta-D-glucosaminidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.58Å 119.99Å 85.90Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	20.00 – 1.27 19.98 – 1.27	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-1.27) 92.4 (19.98-1.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.130 , 0.175 0.131 , 0.177	Depositor DCC
R_{free} test set	18716 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	7.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14357	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GCS, B3P, PPI, 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	1.47	61/6654 (0.9%)	1.36	75/9046 (0.8%)
1	B	1.41	53/6665 (0.8%)	1.37	72/9060 (0.8%)
All	All	1.44	114/13319 (0.9%)	1.37	147/18106 (0.8%)

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	2
1	B	0	1
All	All	0	3

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	651	GLU	CD-OE2	-19.47	1.04	1.25
1	B	265	GLU	CD-OE2	12.26	1.39	1.25
1	A	210	GLU	CD-OE2	-11.82	1.12	1.25
1	A	231	GLU	CD-OE1	-11.55	1.12	1.25
1	A	558[A]	GLU	CD-OE1	11.01	1.37	1.25
1	A	558[B]	GLU	CD-OE1	11.01	1.37	1.25
1	B	779	GLU	CD-OE2	-10.25	1.14	1.25
1	B	460	GLU	CD-OE2	-9.88	1.14	1.25
1	B	216	GLU	CD-OE2	-9.35	1.15	1.25
1	A	240	GLU	CD-OE2	9.29	1.35	1.25
1	A	457	GLY	N-CA	9.09	1.59	1.46
1	A	730	GLU	CD-OE2	8.93	1.35	1.25
1	B	83	GLU	CG-CD	-8.77	1.38	1.51
1	A	471	GLU	CG-CD	8.66	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLU	CG-CD	8.62	1.64	1.51
1	A	457	GLY	CA-C	8.54	1.65	1.51
1	A	779	GLU	CD-OE2	8.51	1.35	1.25
1	B	459	GLU	CG-CD	8.48	1.64	1.51
1	B	83	GLU	CD-OE2	8.39	1.34	1.25
1	A	663	GLU	CD-OE1	-8.37	1.16	1.25
1	B	457	GLY	N-CA	8.30	1.58	1.46
1	A	471	GLU	CD-OE2	-8.01	1.16	1.25
1	A	766	ASP	N-CA	7.93	1.62	1.46
1	A	5	GLU	CD-OE1	7.89	1.34	1.25
1	B	310	SER	CA-CB	7.82	1.64	1.52
1	A	456	GLU	CD-OE2	-7.59	1.17	1.25
1	A	460	GLU	CD-OE2	-7.58	1.17	1.25
1	A	151	GLU	CD-OE2	7.54	1.33	1.25
1	B	642	GLU	CD-OE1	7.53	1.33	1.25
1	B	538	ARG	CZ-NH2	-7.32	1.23	1.33
1	B	411	ARG	CG-CD	-7.30	1.33	1.51
1	A	50	VAL	CB-CG1	-7.27	1.37	1.52
1	B	610	ARG	CZ-NH2	-7.12	1.23	1.33
1	B	564	ARG	CZ-NH1	7.02	1.42	1.33
1	B	134	TYR	CE1-CZ	-7.01	1.29	1.38
1	B	434	GLU	CD-OE2	7.01	1.33	1.25
1	A	422	GLU	CB-CG	6.96	1.65	1.52
1	A	471	GLU	CD-OE1	6.94	1.33	1.25
1	B	410	GLU	CB-CG	-6.94	1.39	1.52
1	B	544	GLU	CD-OE1	6.90	1.33	1.25
1	A	411	ARG	CG-CD	-6.86	1.34	1.51
1	A	456	GLU	C-N	-6.82	1.20	1.33
1	A	649	ASP	CB-CG	-6.74	1.37	1.51
1	A	771	ARG	CZ-NH2	-6.70	1.24	1.33
1	B	471	GLU	CD-OE2	-6.70	1.18	1.25
1	A	539	TYR	CE1-CZ	-6.67	1.29	1.38
1	A	265	GLU	CG-CD	6.58	1.61	1.51
1	B	116	GLU	CD-OE1	6.48	1.32	1.25
1	A	221	ARG	CZ-NH1	6.46	1.41	1.33
1	B	779	GLU	CB-CG	-6.45	1.40	1.52
1	B	779	GLU	CG-CD	6.45	1.61	1.51
1	A	559	ARG	NE-CZ	-6.42	1.24	1.33
1	A	221	ARG	CZ-NH2	6.40	1.41	1.33
1	B	266	ARG	CZ-NH2	6.38	1.41	1.33
1	A	123	LYS	CB-CG	-6.37	1.35	1.52
1	A	564	ARG	CZ-NH2	-6.37	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	GLU	CD-OE2	-6.37	1.18	1.25
1	A	730	GLU	CD-OE1	6.33	1.32	1.25
1	B	497	GLU	CD-OE2	-6.32	1.18	1.25
1	A	663	GLU	CD-OE2	6.25	1.32	1.25
1	B	638	TRP	CG-CD1	6.20	1.45	1.36
1	B	564	ARG	NE-CZ	6.13	1.41	1.33
1	B	36	LYS	CE-NZ	6.01	1.64	1.49
1	A	771	ARG	CZ-NH1	-6.00	1.25	1.33
1	B	337	ARG	CG-CD	5.97	1.66	1.51
1	B	753	SER	CB-OG	-5.96	1.34	1.42
1	A	422	GLU	CG-CD	5.93	1.60	1.51
1	B	457	GLY	CA-C	5.92	1.61	1.51
1	A	216	GLU	CD-OE2	5.85	1.32	1.25
1	A	699	GLU	CD-OE2	5.85	1.32	1.25
1	B	538	ARG	CZ-NH1	5.75	1.40	1.33
1	A	265	GLU	CD-OE2	5.75	1.31	1.25
1	A	609	VAL	CB-CG2	-5.72	1.40	1.52
1	A	716	ASP	CG-OD2	-5.68	1.12	1.25
1	B	782	GLU	CG-CD	5.68	1.60	1.51
1	B	670	LEU	CB-CG	-5.67	1.36	1.52
1	B	610	ARG	CZ-NH1	-5.67	1.25	1.33
1	A	669	TYR	CE2-CZ	-5.60	1.31	1.38
1	B	544	GLU	CG-CD	5.59	1.60	1.51
1	A	538	ARG	CG-CD	5.52	1.65	1.51
1	B	515	GLU	CD-OE2	-5.46	1.19	1.25
1	A	306	GLU	CD-OE1	-5.45	1.19	1.25
1	A	459	GLU	CD-OE2	5.41	1.31	1.25
1	A	145	TYR	CG-CD2	-5.39	1.32	1.39
1	B	766	ASP	CB-CG	5.37	1.63	1.51
1	B	775	GLU	CB-CG	-5.37	1.42	1.52
1	B	86	ASP	CG-OD2	-5.33	1.13	1.25
1	B	702	ARG	CZ-NH2	5.33	1.40	1.33
1	A	265	GLU	CD-OE1	5.33	1.31	1.25
1	A	311	PHE	CG-CD2	-5.31	1.30	1.38
1	B	147	GLU	CD-OE2	5.31	1.31	1.25
1	A	266	ARG	CZ-NH1	5.29	1.40	1.33
1	B	425	THR	CB-OG1	-5.28	1.32	1.43
1	B	265	GLU	CG-CD	5.27	1.59	1.51
1	B	471	GLU	CG-CD	5.26	1.59	1.51
1	A	730	GLU	CG-CD	5.25	1.59	1.51
1	B	558	GLU	CD-OE1	5.24	1.31	1.25
1	A	10	ARG	CD-NE	-5.23	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLU	CD-OE2	5.22	1.31	1.25
1	A	196	GLU	CB-CG	5.17	1.61	1.52
1	B	240	GLU	CD-OE2	5.15	1.31	1.25
1	B	252	LYS	CD-CE	-5.14	1.38	1.51
1	A	266	ARG	CZ-NH2	5.13	1.39	1.33
1	B	36	LYS	CD-CE	5.12	1.64	1.51
1	A	459	GLU	CG-CD	5.12	1.59	1.51
1	B	556	GLU	CD-OE1	5.12	1.31	1.25
1	A	492	ASP	CG-OD2	5.10	1.37	1.25
1	B	699	GLU	CG-CD	5.09	1.59	1.51
1	A	37	ASP	CG-OD1	5.09	1.37	1.25
1	A	707	TYR	CG-CD2	-5.07	1.32	1.39
1	B	317[A]	PHE	CD2-CE2	-5.06	1.29	1.39
1	B	317[B]	PHE	CD2-CE2	-5.06	1.29	1.39
1	A	105	ARG	CG-CD	-5.05	1.39	1.51
1	A	333	ARG	CZ-NH1	-5.03	1.26	1.33

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	564	ARG	NE-CZ-NH1	19.68	130.14	120.30
1	B	687	ARG	NE-CZ-NH2	-17.35	111.62	120.30
1	B	266	ARG	NE-CZ-NH2	14.13	127.37	120.30
1	B	10	ARG	NE-CZ-NH2	-14.08	113.26	120.30
1	B	564	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	A	266	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	B	687	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	B	538	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	B	702	ARG	NE-CZ-NH2	11.77	126.19	120.30
1	A	564	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	B	266	ARG	NE-CZ-NH1	-11.58	114.51	120.30
1	B	131	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	B	526	ARG	NE-CZ-NH2	11.05	125.82	120.30
1	B	131	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	559	ARG	NE-CZ-NH1	-10.05	115.27	120.30
1	A	683	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	592	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	B	700	LEU	CB-CG-CD1	9.97	127.95	111.00
1	A	713	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	76	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	219	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	A	37	ASP	CB-CG-OD2	-8.80	110.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	210	GLU	OE1-CD-OE2	8.62	133.65	123.30
1	A	696	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	A	471	GLU	CG-CD-OE2	-8.37	101.56	118.30
1	B	526	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	B	36	LYS	CD-CE-NZ	8.17	130.48	111.70
1	A	649	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	696	ASP	CB-CG-OD1	8.12	125.61	118.30
1	B	702	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	A	10	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	95	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	716	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	765	SER	C-N-CA	7.79	141.19	121.70
1	B	707	TYR	CB-CG-CD1	7.74	125.64	121.00
1	B	83	GLU	OE1-CD-OE2	7.71	132.56	123.30
1	A	269	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	B	407	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	B	317[A]	PHE	CB-CG-CD1	7.42	125.99	120.80
1	B	317[B]	PHE	CB-CG-CD1	7.42	125.99	120.80
1	B	43	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	134	TYR	CG-CD2-CE2	-7.38	115.40	121.30
1	A	410	GLU	OE1-CD-OE2	7.37	132.15	123.30
1	B	564	ARG	CD-NE-CZ	7.34	133.88	123.60
1	B	288	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	457	GLY	N-CA-C	7.19	131.08	113.10
1	A	221	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	38	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	471	GLU	CG-CD-OE1	6.95	132.21	118.30
1	B	585	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	B	210	GLU	CG-CD-OE1	-6.88	104.55	118.30
1	B	496	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	33	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	86	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	610	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	456	GLU	C-N-CA	-6.70	108.22	122.30
1	B	518	ASP	CB-CG-OD1	6.69	124.33	118.30
1	A	456	GLU	O-C-N	-6.68	111.84	123.20
1	B	288	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	581	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	702	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	472	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	A	131	ARG	NE-CZ-NH1	-6.61	117.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	716	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	452	LEU	CA-CB-CG	6.58	130.43	115.30
1	A	135	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	B	450	LEU	CB-CG-CD2	6.50	122.06	111.00
1	B	228	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	A	135	TYR	CB-CG-CD1	6.45	124.87	121.00
1	A	240	GLU	OE1-CD-OE2	6.44	131.03	123.30
1	B	436	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	558[A]	GLU	CG-CD-OE2	-6.43	105.45	118.30
1	A	558[B]	GLU	CG-CD-OE2	-6.43	105.45	118.30
1	B	220	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	161	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	269	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	681	LYS	CD-CE-NZ	-6.32	97.15	111.70
1	A	631	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	589	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	B	457	GLY	N-CA-C	6.27	128.78	113.10
1	A	290	PHE	CB-CG-CD1	-6.27	116.41	120.80
1	B	219	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	132	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	766	ASP	CB-CG-OD1	-6.24	112.68	118.30
1	A	95	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	564	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	567	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	222	TYR	CB-CG-CD1	6.10	124.66	121.00
1	B	411	ARG	CG-CD-NE	-6.08	99.03	111.80
1	A	560	GLU	CA-CB-CG	6.07	126.76	113.40
1	B	265	GLU	OE1-CD-OE2	6.00	130.50	123.30
1	B	551	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	177	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	B	643	LEU	CB-CG-CD1	-5.96	100.86	111.00
1	B	333	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	766	ASP	CB-CA-C	-5.89	98.63	110.40
1	B	38	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	603	LYS	CD-CE-NZ	-5.86	98.22	111.70
1	B	217	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	B	713	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	779	GLU	OE1-CD-OE2	-5.84	116.30	123.30
1	B	131	ARG	CG-CD-NE	-5.78	99.67	111.80
1	A	766	ASP	N-CA-CB	5.75	120.94	110.60
1	A	295	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	269	ARG	NE-CZ-NH2	-5.65	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	766	ASP	N-CA-C	5.64	126.23	111.00
1	A	300	LYS	CD-CE-NZ	5.62	124.64	111.70
1	A	558[A]	GLU	CB-CA-C	-5.57	99.26	110.40
1	A	558[B]	GLU	CB-CA-C	-5.57	99.26	110.40
1	A	492	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	670	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	523	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	A	264	TYR	CZ-CE2-CD2	5.51	124.76	119.80
1	A	311	PHE	CB-CG-CD1	-5.43	117.00	120.80
1	A	295	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	716	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	702	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	647	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	703	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	38	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	29	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	135	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	37	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	702	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	B	647	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	455	TYR	CB-CG-CD1	5.27	124.16	121.00
1	A	779	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	A	546	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	B	676	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	266	ARG	CG-CD-NE	-5.22	100.83	111.80
1	B	36	LYS	CG-CD-CE	5.22	127.56	111.90
1	B	460	GLU	CG-CD-OE1	5.17	128.64	118.30
1	B	190	PHE	CB-CG-CD1	-5.15	117.20	120.80
1	B	38	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	183	TRP	CG-CD1-NE1	5.13	115.23	110.10
1	A	436	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	463	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	676	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	228	ASP	OD1-CG-OD2	5.04	132.89	123.30
1	B	687	ARG	CG-CD-NE	-5.04	101.22	111.80
1	A	541	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	A	713	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	266	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	B	779	GLU	CA-CB-CG	5.02	124.44	113.40
1	B	105	ARG	NE-CZ-NH2	5.00	122.80	120.30
1	A	556	GLU	CG-CD-OE2	-5.00	108.29	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	GLU	Sidechain
1	A	411	ARG	Sidechain
1	B	766	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6446	0	6312	37	1
1	B	6457	0	6331	56	3
2	A	12	0	12	1	0
2	B	12	0	13	1	0
3	A	42	0	60	1	0
3	B	42	0	60	3	0
4	A	15	0	15	9	0
4	B	30	0	30	20	3
5	A	19	0	25	0	0
6	A	608	0	0	17	7
6	B	674	0	0	21	5
All	All	14357	0	12858	112	14

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 4.

All (112) 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:317[B]:PHE:HZ	1:B:325[B]:ILE:CD1	1.20	1.52
1:B:317[B]:PHE:CZ	1:B:325[B]:ILE:HD11	1.42	1.49
1:B:317[B]:PHE:CZ	1:B:325[B]:ILE:CD1	1.99	1.41
1:B:317[B]:PHE:CE1	1:B:325[B]:ILE:HD11	1.57	1.38
1:A:37:ASP:HB2	6:A:1317:HOH:O	1.22	1.35
1:B:317[B]:PHE:HZ	1:B:325[B]:ILE:HD13	1.32	0.91
6:A:1427:HOH:O	4:B:810:PPI:H31	1.68	0.91
1:B:317[B]:PHE:HZ	1:B:325[B]:ILE:HD12	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317[B]:PHE:HE1	1:B:325[B]:ILE:HD11	1.40	0.85
1:A:337:ARG:HD2	4:A:810:PPI:H31	1.57	0.85
6:A:1427:HOH:O	4:B:810:PPI:C3	2.20	0.85
1:B:766:ASP:CG	1:B:767:GLY:HA2	1.98	0.82
1:B:317[B]:PHE:CZ	1:B:325[B]:ILE:HD12	2.13	0.80
1:B:766:ASP:OD2	1:B:767:GLY:HA2	1.80	0.80
1:A:766:ASP:OD1	1:A:771:ARG:NH1	2.16	0.79
1:B:743[A]:HIS:CD2	1:B:775:GLU:HG2	2.19	0.78
1:B:123:LYS:HE2	6:B:1086:HOH:O	1.86	0.75
4:B:810:PPI:H22	6:B:1485:HOH:O	1.87	0.73
4:B:812:PPI:H32	6:B:1032:HOH:O	1.86	0.73
1:B:743[A]:HIS:NE2	1:B:775:GLU:HG2	2.03	0.73
1:A:766:ASP:HB2	1:A:769:VAL:O	1.91	0.71
1:B:9:LYS:HD2	4:B:811:PPI:O1	1.91	0.71
1:A:187[A]:PHE:HD1	1:A:452:LEU:HD11	1.57	0.70
1:A:219:ARG:CD	6:A:910:HOH:O	2.40	0.69
1:A:401:TYR:OH	1:B:678:HIS:HD2	1.75	0.69
1:B:556:GLU:HG3	1:B:592[A]:ARG:NH2	2.07	0.69
4:A:810:PPI:H33	6:A:1116:HOH:O	1.92	0.68
4:A:810:PPI:O1	6:A:901:HOH:O	2.10	0.68
1:B:123:LYS:CE	6:B:1086:HOH:O	2.42	0.68
4:B:811:PPI:H33	6:B:1189:HOH:O	1.94	0.67
4:B:812:PPI:H31	6:B:1480:HOH:O	1.93	0.66
1:A:187[A]:PHE:CD1	1:A:452:LEU:HD11	2.29	0.66
1:A:9:LYS:NZ	4:A:810:PPI:O2	2.29	0.66
3:A:807:PEG:O4	6:A:902:HOH:O	2.14	0.65
1:A:434:GLU:HA	4:A:810:PPI:O1	1.96	0.65
1:B:265:GLU:HG2	6:B:1307:HOH:O	1.97	0.64
1:B:317[B]:PHE:CE1	1:B:325[B]:ILE:CD1	2.51	0.64
3:B:803:PEG:H21	6:B:1451:HOH:O	1.98	0.63
1:A:219:ARG:HD2	6:A:910:HOH:O	1.99	0.62
1:B:309:TYR:OH	1:B:324:HIS:HD2	1.83	0.60
1:A:44:GLU:HG2	6:A:947:HOH:O	2.01	0.60
1:B:294[B]:MET:SD	1:B:301:ILE:HB	2.42	0.60
1:B:236:THR:O	3:B:807:PEG:H22	2.02	0.59
6:A:1135:HOH:O	4:B:810:PPI:H31	2.03	0.59
4:B:811:PPI:O2	6:B:901:HOH:O	2.17	0.58
1:B:560:GLU:HB3	1:B:587:THR:HG21	1.85	0.58
4:B:812:PPI:C3	6:B:1480:HOH:O	2.50	0.58
1:B:743[A]:HIS:CD2	1:B:775:GLU:CG	2.87	0.58
1:B:210:GLU:HG2	1:B:229:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ARG:HD2	6:B:1327:HOH:O	2.04	0.56
1:B:242:LEU:HD11	1:B:450:LEU:HD21	1.88	0.56
1:B:347:GLU:OE1	2:B:801:GCS:H1	2.07	0.55
4:B:812:PPI:H22	6:B:1420:HOH:O	2.06	0.55
6:A:1135:HOH:O	4:B:810:PPI:C3	2.55	0.54
1:B:743[A]:HIS:NE2	1:B:775:GLU:CG	2.71	0.54
1:A:701:LYS:HE3	1:A:702:ARG:CZ	2.37	0.54
1:A:9:LYS:CE	4:A:810:PPI:O2	2.56	0.54
3:B:803:PEG:C2	6:B:1451:HOH:O	2.54	0.53
1:B:317[B]:PHE:CZ	1:B:325[B]:ILE:HD13	2.17	0.53
1:A:337:ARG:CD	4:A:810:PPI:H31	2.34	0.51
1:B:544:GLU:HG3	6:B:1513:HOH:O	2.09	0.51
1:A:347:GLU:OE1	2:A:801:GCS:H1	2.10	0.51
1:B:495:LEU:HD13	1:B:526:ARG:NH2	2.25	0.51
1:B:9:LYS:HZ1	4:B:811:PPI:C1	2.21	0.51
1:A:325[B]:ILE:HD11	1:A:368:LEU:HD21	1.93	0.51
1:B:324:HIS:HE1	6:B:1130:HOH:O	1.92	0.51
1:B:614:GLY:O	4:B:813:PPI:H21	2.11	0.50
1:B:411:ARG:NH2	4:B:810:PPI:O1	2.44	0.50
1:B:317[A]:PHE:HB2	1:B:360:GLU:HB3	1.94	0.50
1:B:467:TYR:CE1	1:B:622[B]:ARG:HD2	2.47	0.49
4:B:812:PPI:C3	6:B:1032:HOH:O	2.51	0.49
1:B:733:VAL:HG22	1:B:784:GLU:HG2	1.95	0.49
1:B:9:LYS:NZ	4:B:811:PPI:O2	2.38	0.48
4:B:810:PPI:H33	6:B:1047:HOH:O	2.12	0.48
1:A:334:TYR:CZ	1:A:338:LYS:HE3	2.48	0.48
1:B:265:GLU:CG	6:B:1307:HOH:O	2.59	0.48
1:A:460:GLU:OE2	1:A:622[B]:ARG:NH1	2.36	0.47
1:A:334:TYR:CE1	1:A:338:LYS:HE3	2.49	0.47
1:B:210:GLU:HG2	1:B:229:TYR:CD2	2.49	0.47
1:B:147:GLU:OE2	1:B:151:GLU:OE2	2.32	0.47
1:A:3:LYS:HD2	6:A:1413:HOH:O	2.14	0.47
1:A:627:THR:HG23	6:B:1047:HOH:O	2.15	0.47
1:B:265:GLU:HG2	6:B:1537:HOH:O	2.14	0.47
1:B:556:GLU:HG3	1:B:592[A]:ARG:HH22	1.79	0.46
4:A:810:PPI:C3	6:A:1116:HOH:O	2.60	0.45
1:A:269:ARG:HG3	6:A:1029:HOH:O	2.16	0.45
1:A:242:LEU:HD11	1:A:450:LEU:HD21	1.99	0.44
1:B:695:LEU:HD11	1:B:743[B]:HIS:CE1	2.53	0.44
1:A:701:LYS:HE3	1:A:702:ARG:NH1	2.33	0.44
1:A:219:ARG:HD3	6:A:910:HOH:O	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743[A]:HIS:HE2	1:B:775:GLU:CD	2.22	0.43
1:B:332:TYR:CE1	1:B:336:VAL:HG21	2.53	0.43
1:B:459:GLU:HG2	1:B:589:ARG:HH21	1.83	0.43
1:A:165:TYR:HA	1:A:169:GLY:O	2.19	0.43
1:A:179:GLU:HA	1:A:278:LEU:O	2.19	0.42
1:B:206:GLU:HB2	6:B:1381:HOH:O	2.20	0.42
1:A:50:VAL:CG1	1:A:92:VAL:HG22	2.50	0.42
1:A:471:GLU:HG3	1:A:472:ARG:NH1	2.35	0.42
6:A:1427:HOH:O	4:B:810:PPI:H32	2.03	0.42
1:A:186:ILE:CG2	6:A:1382:HOH:O	2.68	0.41
1:A:434:GLU:HB2	1:A:436:ARG:HE	1.84	0.41
1:A:210:GLU:HG2	1:A:229:TYR:CD2	2.55	0.41
1:B:576:ALA:HB1	1:B:639:LYS:HE2	2.02	0.41
1:A:9:LYS:HZ2	4:A:810:PPI:C1	2.30	0.41
1:A:560:GLU:HB3	1:A:587:THR:HG21	2.01	0.41
1:B:325[A]:ILE:HD11	1:B:368:LEU:HD21	2.03	0.41
1:B:560:GLU:CB	1:B:587:THR:HG21	2.50	0.41
1:B:135:TYR:O	1:B:136:PRO:C	2.59	0.41
1:B:614:GLY:O	4:B:813:PPI:C3	2.69	0.41
1:A:379:TYR:HA	1:A:380:LEU:HA	1.96	0.40
1:A:709:PRO:O	1:A:721:TYR:HA	2.21	0.40
1:B:766:ASP:CG	1:B:767:GLY:CA	2.82	0.40

All (14) 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:1398:HOH:O	6:A:1408:HOH:O[1_655]	0.82	1.38
6:B:1007:HOH:O	6:B:1372:HOH:O[2_747]	0.85	1.35
4:B:813:PPI:O2	6:A:1277:HOH:O[2_747]	0.87	1.33
6:B:953:HOH:O	6:B:1199:HOH:O[2_857]	0.98	1.22
6:B:1339:HOH:O	6:B:1412:HOH:O[2_847]	0.98	1.22
6:B:1463:HOH:O	6:B:1539:HOH:O[2_757]	1.14	1.06
6:A:924:HOH:O	6:A:1238:HOH:O[1_455]	1.19	1.01
4:B:813:PPI:C1	6:A:1277:HOH:O[2_747]	1.20	1.00
4:B:813:PPI:O1	6:A:1277:HOH:O[2_747]	1.65	0.55
1:B:131:ARG:NH2	1:B:577:GLU:OE2[2_757]	1.88	0.32
1:B:755:LYS:NZ	6:B:1412:HOH:O[2_847]	1.97	0.23
1:A:63:LYS:O	6:A:1238:HOH:O[1_455]	2.08	0.12
1:B:87:GLU:OE2	1:B:556:GLU:OE2[1_655]	2.16	0.04
6:A:1063:HOH:O	6:A:1432:HOH:O[2_848]	2.17	0.03

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	791/786 (101%)	764 (97%)	26 (3%)	1 (0%)	51	20
1	B	792/786 (101%)	766 (97%)	25 (3%)	1 (0%)	51	20
All	All	1583/1572 (101%)	1530 (97%)	51 (3%)	2 (0%)	51	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	767	GLY
1	A	766	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	689/682 (101%)	676 (98%)	13 (2%)	57	19
1	B	690/682 (101%)	682 (99%)	8 (1%)	71	38
All	All	1379/1364 (101%)	1358 (98%)	21 (2%)	65	30

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	116	GLU
1	A	182	TYR
1	A	217	ASP

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Mol	Chain	Res	Type
1	A	317[A]	PHE
1	A	317[B]	PHE
1	A	320	ASP
1	A	401	TYR
1	A	510	ASP
1	A	678	HIS
1	A	713	ARG
1	A	743	HIS
1	A	751	VAL
1	B	182	TYR
1	B	227	LYS
1	B	327	TYR
1	B	367	ILE
1	B	401	TYR
1	B	510	ASP
1	B	678	HIS
1	B	752	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	257	ASN
1	B	212	ASN
1	B	257	ASN
1	B	324	HIS
1	B	678	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)

24 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	PEG	A	805	-	6,6,6	0.84	0	5,5,5	1.37	1 (20%)
4	PPI	B	812	-	4,4,4	2.05	1 (25%)	4,4,4	2.84	2 (50%)
4	PPI	A	808	-	4,4,4	2.18	2 (50%)	4,4,4	3.20	2 (50%)
3	PEG	A	803	-	6,6,6	0.84	0	5,5,5	0.78	0
3	PEG	A	802	-	6,6,6	0.80	0	5,5,5	0.82	0
3	PEG	B	805	-	6,6,6	0.62	0	5,5,5	0.65	0
3	PEG	A	806	-	6,6,6	0.72	0	5,5,5	0.95	0
2	GCS	A	801	-	12,12,12	3.57	8 (66%)	16,17,17	2.86	8 (50%)
4	PPI	A	809	-	4,4,4	1.86	1 (25%)	4,4,4	1.51	1 (25%)
3	PEG	B	807	-	6,6,6	0.90	0	5,5,5	1.83	1 (20%)
4	PPI	B	811	-	4,4,4	1.98	2 (50%)	4,4,4	1.74	1 (25%)
3	PEG	B	802	-	6,6,6	0.85	0	5,5,5	1.46	1 (20%)
4	PPI	B	809	-	4,4,4	0.75	0	4,4,4	0.99	0
3	PEG	B	803	-	6,6,6	0.83	0	5,5,5	2.36	2 (40%)
4	PPI	B	810	-	4,4,4	3.64	2 (50%)	4,4,4	1.91	2 (50%)
5	B3P	A	811	-	18,18,18	2.57	6 (33%)	21,23,23	3.84	9 (42%)
4	PPI	A	810	-	4,4,4	2.31	1 (25%)	4,4,4	1.70	1 (25%)
2	GCS	B	801	-	12,12,12	3.04	6 (50%)	16,17,17	2.60	8 (50%)
3	PEG	A	804	-	6,6,6	0.91	0	5,5,5	0.45	0
3	PEG	A	807	-	6,6,6	1.69	1 (16%)	5,5,5	1.26	0
4	PPI	B	808	-	4,4,4	0.77	0	4,4,4	2.84	2 (50%)
3	PEG	B	806	-	6,6,6	0.43	0	5,5,5	1.31	1 (20%)
4	PPI	B	813	-	4,4,4	1.19	0	4,4,4	1.27	1 (25%)
3	PEG	B	804	-	6,6,6	1.74	2 (33%)	5,5,5	1.28	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	PEG	A	805	-	-	3/4/4/4	-
4	PPI	B	812	-	-	0/2/2/2	-
4	PPI	A	808	-	-	2/2/2/2	-
3	PEG	A	803	-	-	2/4/4/4	-
3	PEG	A	802	-	-	2/4/4/4	-
3	PEG	B	805	-	-	3/4/4/4	-
3	PEG	A	806	-	-	2/4/4/4	-
2	GCS	A	801	-	-	0/2/22/22	0/1/1/1
4	PPI	A	809	-	-	0/2/2/2	-
3	PEG	B	807	-	-	3/4/4/4	-
4	PPI	B	811	-	-	0/2/2/2	-
3	PEG	B	802	-	-	2/4/4/4	-
4	PPI	B	809	-	-	0/2/2/2	-
3	PEG	B	803	-	-	3/4/4/4	-
4	PPI	B	810	-	-	2/2/2/2	-
5	B3P	A	811	-	-	14/28/28/28	-
4	PPI	A	810	-	-	2/2/2/2	-
2	GCS	B	801	-	-	0/2/22/22	0/1/1/1
3	PEG	A	804	-	-	3/4/4/4	-
3	PEG	A	807	-	-	1/4/4/4	-
4	PPI	B	808	-	-	1/2/2/2	-
3	PEG	B	806	-	-	1/4/4/4	-
4	PPI	B	813	-	-	2/2/2/2	-
3	PEG	B	804	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	811	B3P	C9-C8	8.44	1.63	1.53
2	A	801	GCS	C1-C2	6.95	1.60	1.52
2	B	801	GCS	O3-C3	6.93	1.59	1.43
4	B	810	PPI	O2-C1	-6.65	1.08	1.30
2	A	801	GCS	C2-N2	5.46	1.55	1.47
4	A	810	PPI	O2-C1	-4.44	1.15	1.30
2	B	801	GCS	C3-C2	-4.41	1.48	1.53
2	A	801	GCS	C3-C2	4.35	1.59	1.53
2	A	801	GCS	O3-C3	4.25	1.53	1.43
4	B	812	PPI	C3-C2	-4.01	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GCS	O5-C5	3.68	1.53	1.44
2	B	801	GCS	C2-N2	3.56	1.52	1.47
2	A	801	GCS	O4-C4	3.53	1.51	1.43
2	B	801	GCS	O5-C5	3.46	1.52	1.44
4	A	809	PPI	O2-C1	-3.33	1.19	1.30
5	A	811	B3P	C3-N1	-3.33	1.42	1.46
2	B	801	GCS	O5-C1	3.04	1.50	1.42
4	A	808	PPI	O2-C1	-3.01	1.20	1.30
5	A	811	B3P	C2-N2	2.93	1.50	1.46
2	B	801	GCS	O4-C4	2.68	1.49	1.43
4	B	811	PPI	C2-C1	-2.64	1.37	1.50
4	B	811	PPI	O2-C1	-2.36	1.22	1.30
3	A	807	PEG	C2-C1	2.27	1.61	1.49
5	A	811	B3P	C11-C8	2.27	1.56	1.53
2	A	801	GCS	O6-C6	2.22	1.51	1.42
5	A	811	B3P	C6-C4	2.19	1.56	1.53
4	B	810	PPI	C3-C2	-2.18	1.41	1.51
4	A	808	PPI	C2-C1	2.17	1.62	1.50
3	B	804	PEG	O1-C1	2.08	1.52	1.42
3	B	804	PEG	O4-C4	2.08	1.52	1.42
5	A	811	B3P	O4-C5	-2.04	1.35	1.42
2	A	801	GCS	C4-C5	2.01	1.57	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	811	B3P	C2-N2-C8	7.25	126.37	116.08
5	A	811	B3P	C3-N1-C4	7.01	126.03	116.08
2	A	801	GCS	C3-C4-C5	-6.84	98.03	110.24
5	A	811	B3P	C11-C8-C10	-6.84	95.58	110.04
5	A	811	B3P	O1-C9-C8	6.80	125.40	111.63
2	B	801	GCS	C3-C4-C5	-5.87	99.76	110.24
5	A	811	B3P	O5-C6-C4	5.58	122.94	111.63
5	A	811	B3P	C7-C4-C5	-5.47	98.48	110.04
4	A	808	PPI	O2-C1-O1	-5.36	109.94	123.30
4	B	812	PPI	O2-C1-C2	4.71	133.57	113.35
2	A	801	GCS	O5-C1-C2	-4.66	104.07	109.51
2	A	801	GCS	O4-C4-C3	-4.22	100.60	110.35
4	B	808	PPI	O2-C1-O1	-3.85	113.70	123.30
4	B	808	PPI	O2-C1-C2	3.85	129.87	113.35
5	A	811	B3P	O4-C5-C4	-3.73	104.08	111.63
2	B	801	GCS	O1-C1-O5	-3.53	99.78	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	803	PEG	C3-O2-C2	3.50	128.47	113.29
2	B	801	GCS	O5-C1-C2	-3.46	105.47	109.51
2	B	801	GCS	C4-C3-C2	3.41	116.94	111.07
2	A	801	GCS	C1-O5-C5	-3.34	107.35	113.66
3	B	807	PEG	O2-C2-C1	3.33	124.69	110.07
4	A	808	PPI	O2-C1-C2	3.26	127.36	113.35
2	B	801	GCS	C3-C2-N2	-3.09	104.72	111.05
3	B	803	PEG	O2-C2-C1	3.09	123.64	110.07
2	B	801	GCS	O4-C4-C5	3.05	116.87	109.30
2	A	801	GCS	C3-C2-N2	-3.01	104.88	111.05
3	A	805	PEG	C3-O2-C2	2.98	126.19	113.29
4	B	810	PPI	O2-C1-O1	-2.93	115.99	123.30
5	A	811	B3P	C10-C8-C9	2.90	116.18	110.04
2	A	801	GCS	O1-C1-O5	-2.80	101.98	110.38
5	A	811	B3P	O2-C10-C8	-2.76	106.04	111.63
4	B	812	PPI	O1-C1-C2	-2.69	107.05	123.25
4	B	811	PPI	O2-C1-C2	2.64	124.68	113.35
4	A	810	PPI	O2-C1-O1	2.62	129.84	123.30
3	B	802	PEG	O2-C2-C1	2.52	121.14	110.07
2	A	801	GCS	O1-C1-C2	-2.33	104.15	108.96
2	B	801	GCS	O5-C5-C4	-2.26	105.59	109.69
3	B	806	PEG	C3-O2-C2	-2.25	103.52	113.29
4	A	809	PPI	O2-C1-C2	2.21	122.83	113.35
4	B	810	PPI	C3-C2-C1	-2.19	98.32	113.60
4	B	813	PPI	O2-C1-C2	2.11	122.43	113.35
2	B	801	GCS	O1-C1-C2	2.05	113.19	108.96
2	A	801	GCS	O3-C3-C2	-2.01	106.60	110.22

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	810	PPI	O2-C1-C2-C3
5	A	811	B3P	C1-C3-N1-C4
5	A	811	B3P	C5-C4-N1-C3
5	A	811	B3P	C6-C4-N1-C3
5	A	811	B3P	C7-C4-N1-C3
5	A	811	B3P	N1-C4-C6-O5
5	A	811	B3P	C5-C4-C6-O5
5	A	811	B3P	C10-C8-N2-C2
5	A	811	B3P	N2-C8-C9-O1
5	A	811	B3P	C10-C8-C9-O1

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Mol	Chain	Res	Type	Atoms
5	A	811	B3P	C11-C8-C9-O1
5	A	811	B3P	C3-C1-C2-N2
3	B	805	PEG	O1-C1-C2-O2
3	A	806	PEG	O2-C3-C4-O4
3	B	805	PEG	O2-C3-C4-O4
3	B	807	PEG	O2-C3-C4-O4
3	A	804	PEG	O1-C1-C2-O2
5	A	811	B3P	C7-C4-C6-O5
5	A	811	B3P	C11-C8-N2-C2
3	A	804	PEG	O2-C3-C4-O4
4	A	808	PPI	O2-C1-C2-C3
4	A	810	PPI	O2-C1-C2-C3
4	B	808	PPI	O1-C1-C2-C3
3	B	802	PEG	O1-C1-C2-O2
3	B	803	PEG	O2-C3-C4-O4
3	B	802	PEG	C4-C3-O2-C2
3	B	806	PEG	O1-C1-C2-O2
3	A	805	PEG	O1-C1-C2-O2
3	B	803	PEG	C4-C3-O2-C2
3	B	803	PEG	C1-C2-O2-C3
5	A	811	B3P	C9-C8-N2-C2
3	B	807	PEG	C4-C3-O2-C2
4	A	810	PPI	O1-C1-C2-C3
4	B	810	PPI	O1-C1-C2-C3
4	B	813	PPI	O1-C1-C2-C3
3	B	804	PEG	O2-C3-C4-O4
3	A	803	PEG	C4-C3-O2-C2
3	A	803	PEG	O2-C3-C4-O4
3	A	802	PEG	C1-C2-O2-C3
3	A	805	PEG	C4-C3-O2-C2
3	A	802	PEG	O2-C3-C4-O4
3	A	806	PEG	O1-C1-C2-O2
3	A	804	PEG	C1-C2-O2-C3
4	A	808	PPI	O1-C1-C2-C3
4	B	813	PPI	O2-C1-C2-C3
3	B	807	PEG	C1-C2-O2-C3
3	A	807	PEG	C1-C2-O2-C3
3	B	804	PEG	O1-C1-C2-O2
3	A	805	PEG	O2-C3-C4-O4
3	B	805	PEG	C4-C3-O2-C2

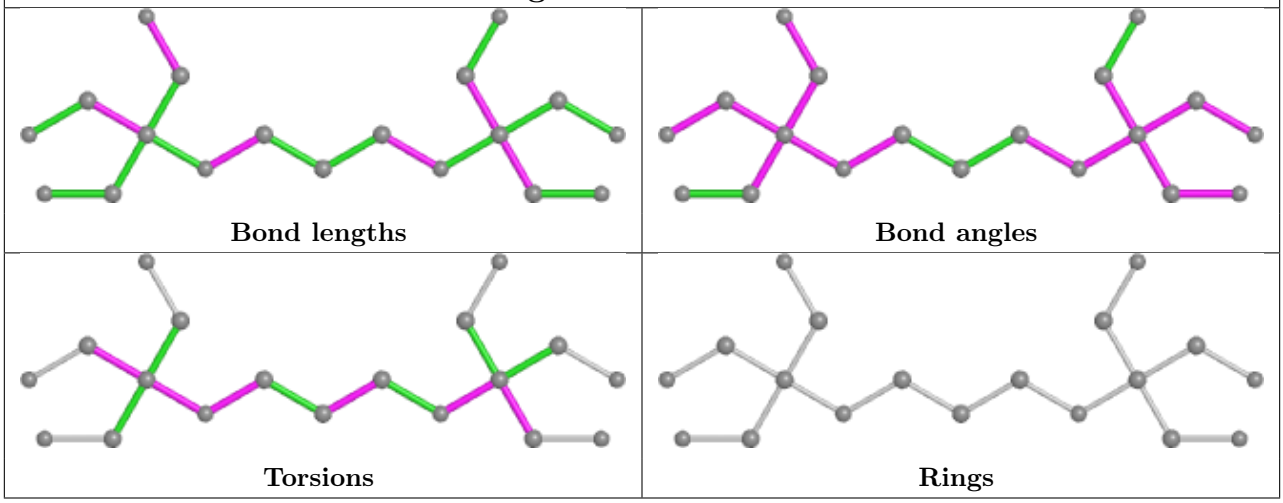
There are no ring outliers.

10 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	812	PPI	5	0
2	A	801	GCS	1	0
3	B	807	PEG	1	0
4	B	811	PPI	5	0
3	B	803	PEG	2	0
4	B	810	PPI	8	0
4	A	810	PPI	9	0
2	B	801	GCS	1	0
3	A	807	PEG	1	0
4	B	813	PPI	2	3

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 B3P A 811



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	786/786 (100%)	-0.63	7 (0%)	84	82	6, 12, 29, 65	0
1	B	786/786 (100%)	-0.71	6 (0%)	86	83	5, 10, 25, 63	0
All	All	1572/1572 (100%)	-0.67	13 (0%)	86	83	5, 11, 28, 65	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	GLY	6.3
1	A	1	MET	4.4
1	A	768	GLU	3.6
1	B	1	MET	3.3
1	B	227	LYS	3.2
1	A	766	ASP	3.2
1	B	767	GLY	3.0
1	B	225	ASP	2.7
1	B	768	GLU	2.6
1	B	317[A]	PHE	2.5
1	A	131	ARG	2.5
1	A	269	ARG	2.2
1	A	716	ASP	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

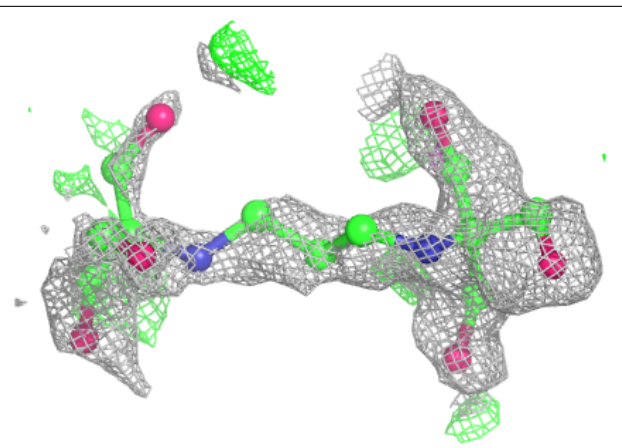
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

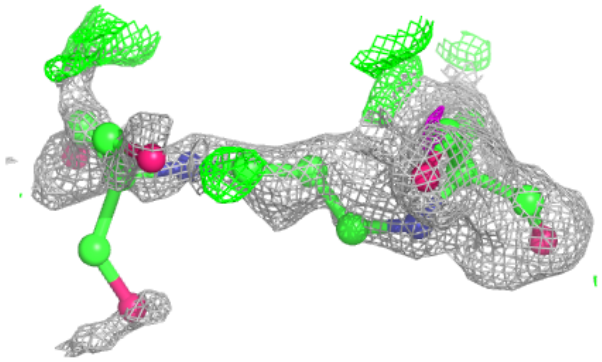
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	805	7/7	0.60	0.35	34,43,49,52	0
3	PEG	A	803	7/7	0.78	0.19	37,43,45,48	0
3	PEG	A	804	7/7	0.79	0.15	45,46,61,64	0
3	PEG	A	806	7/7	0.79	0.14	31,33,41,41	0
3	PEG	B	806	7/7	0.82	0.30	34,42,45,63	0
5	B3P	A	811	19/19	0.82	0.24	32,48,75,83	0
3	PEG	B	805	7/7	0.83	0.17	49,55,57,61	0
3	PEG	B	807	7/7	0.84	0.24	29,31,49,50	0
4	PPI	B	809	5/5	0.84	0.13	39,43,60,62	0
3	PEG	A	807	7/7	0.84	0.14	23,29,37,40	0
3	PEG	B	804	7/7	0.89	0.17	19,23,29,37	0
3	PEG	B	803	7/7	0.89	0.13	33,36,44,59	0
3	PEG	B	802	7/7	0.90	0.12	30,32,49,50	0
4	PPI	A	808	5/5	0.90	0.13	32,32,38,40	0
4	PPI	B	811	5/5	0.91	0.28	18,26,56,62	0
3	PEG	A	802	7/7	0.92	0.11	27,32,38,56	0
4	PPI	B	808	5/5	0.94	0.08	22,23,32,32	0
4	PPI	B	812	5/5	0.94	0.16	23,27,35,62	0
4	PPI	A	810	5/5	0.94	0.27	20,28,51,65	0
2	GCS	B	801	12/12	0.95	0.13	8,16,23,24	0
2	GCS	A	801	12/12	0.95	0.13	10,17,21,28	0
4	PPI	B	813	5/5	0.97	0.22	14,23,52,113	0
4	PPI	A	809	5/5	0.98	0.11	19,22,24,27	0
4	PPI	B	810	5/5	0.99	0.12	13,16,25,58	0

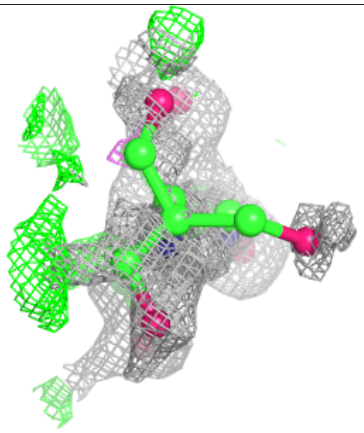
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P A 811:

$2mF_o$-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.