



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 10:44 PM UTC

PDB ID : 5GSM / pdb_00005gsm
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

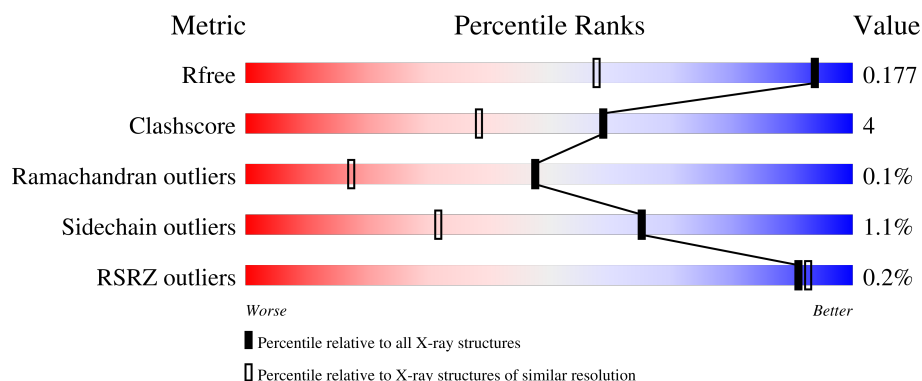
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	808	-	X	-	-
4	PPI	B	810	-	X	X	-
4	PPI	B	811	-	X	X	-
4	PPI	B	812	-	-	X	-
4	PPI	B	813	-	-	X	-
5	B3P	A	811	-	X	-	-

2 Entry composition [i](#)

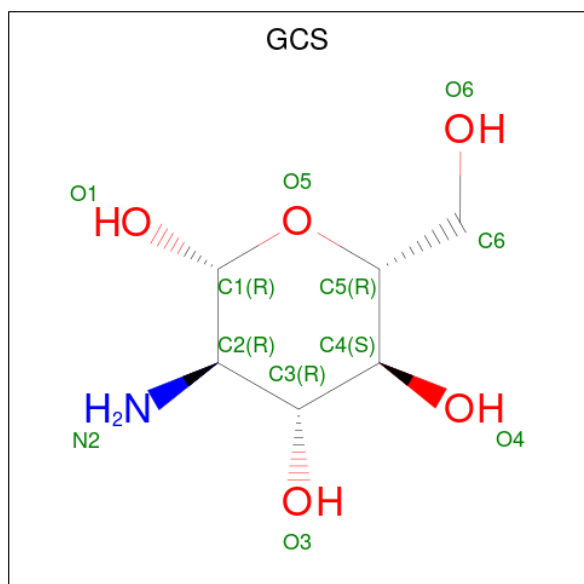
There are 6 unique types of molecules in this entry. The entry contains 14357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

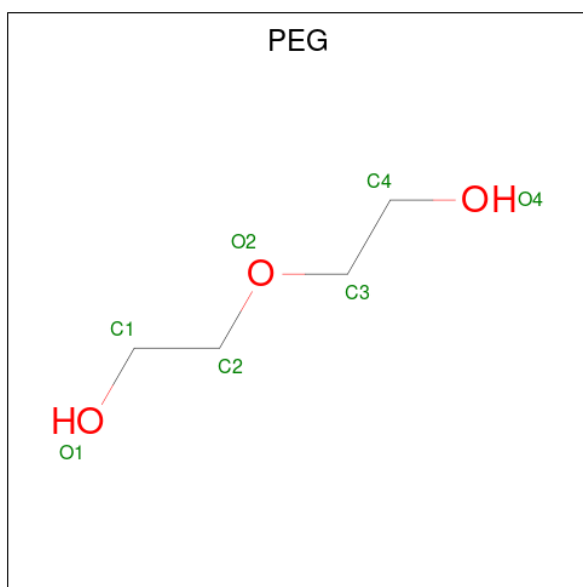
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	786	Total	C	N	O	S	0	7	0
			6446	4191	1064	1176	15			
1	B	786	Total	C	N	O	S	0	8	0
			6457	4197	1070	1174	16			

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



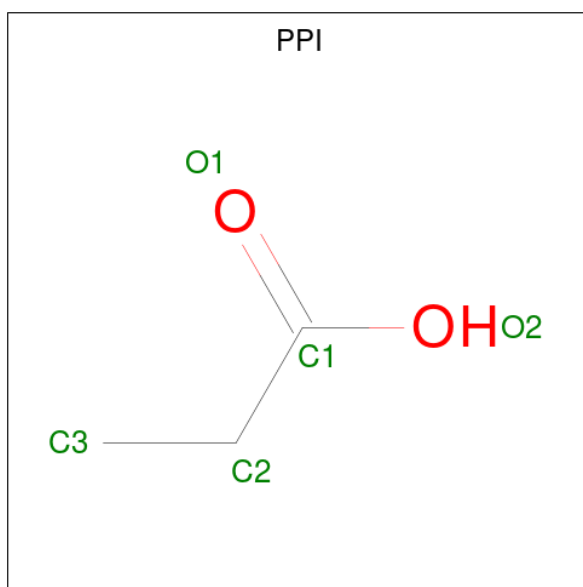
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	1	5		
2	B	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



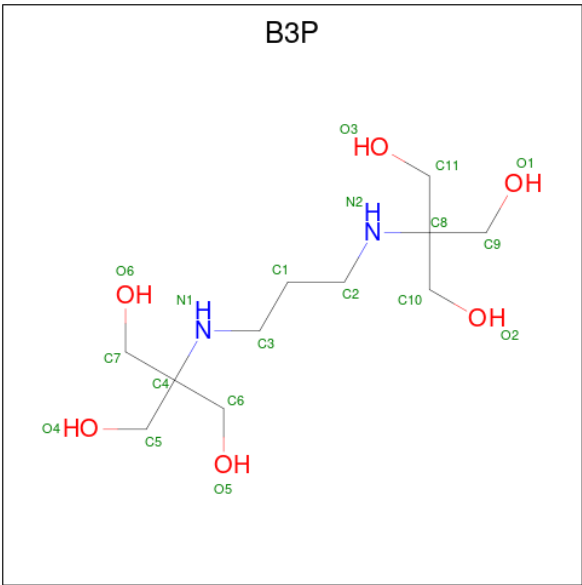
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total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

- Molecule 4 is PROPANOIC ACID (CCD ID: PPI) (formula: C₃H₆O₂).



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

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



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

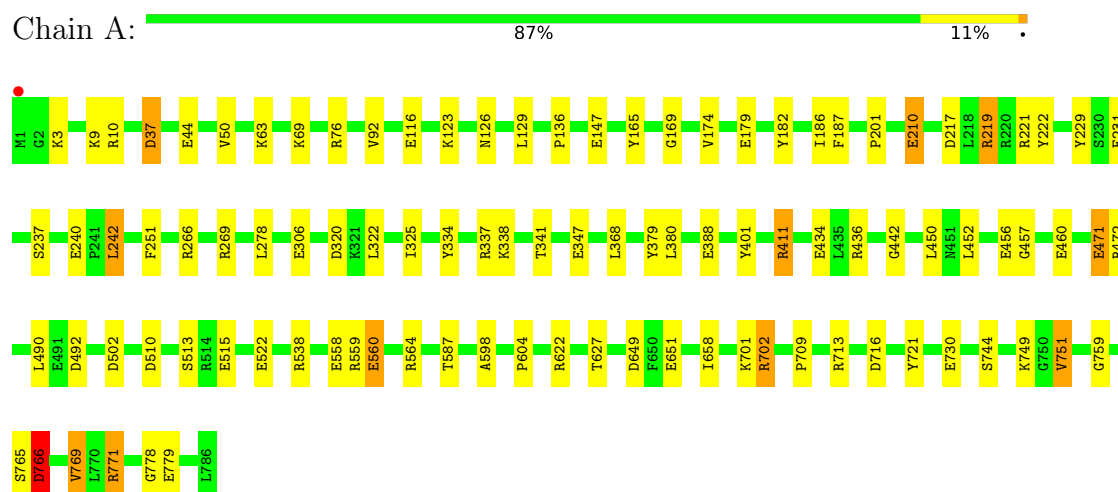
- Molecule 6 is water.

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

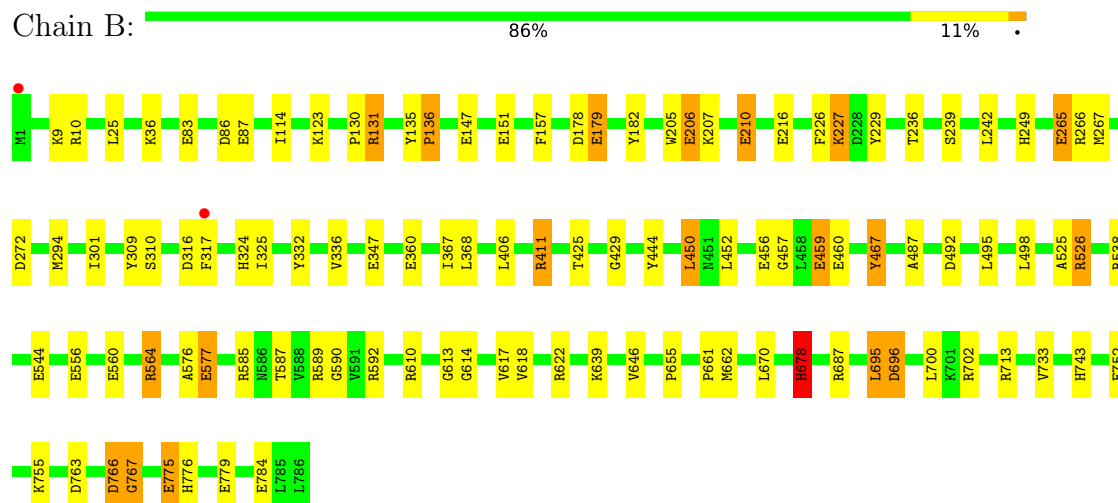
3 Residue-property plots

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



• Molecule 1: Exo-beta-D-glucosaminidase



4 Data and refinement statistics

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 20.00 – 1.27	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-1.27) 92.4 (20.00-1.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.67%)	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 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPI, GCS, PEG, B3P

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	1.64	48/6654 (0.7%)	1.40	32/9046 (0.4%)
1	B	1.62	57/6665 (0.9%)	1.36	36/9060 (0.4%)
All	All	1.63	105/13319 (0.8%)	1.38	68/18106 (0.4%)

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 (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	766	ASP	N-CA	12.42	1.62	1.46
1	A	651	GLU	CD-OE2	-11.12	1.04	1.25
1	A	457	GLY	N-CA	9.87	1.59	1.45
1	A	457	GLY	CA-C	9.67	1.65	1.51
1	A	456	GLU	C-N	-8.72	1.20	1.33
1	B	670	LEU	CB-CG	-8.68	1.36	1.53
1	B	487	ALA	CA-C	-8.57	1.42	1.52
1	B	457	GLY	N-CA	8.19	1.58	1.45
1	B	538	ARG	CZ-NH2	-7.63	1.23	1.33
1	A	559	ARG	NE-CZ	-7.59	1.24	1.33
1	B	662	MET	SD-CE	-7.50	1.60	1.79
1	B	610	ARG	CZ-NH2	-7.43	1.23	1.33
1	B	265	GLU	CD-OE2	7.26	1.39	1.25
1	B	564	ARG	NE-CZ	7.25	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	771	ARG	CZ-NH2	-7.01	1.24	1.33
1	B	114	ILE	CA-CB	6.99	1.63	1.54
1	B	425	THR	CB-OG1	-6.91	1.32	1.43
1	A	716	ASP	CG-OD2	-6.88	1.12	1.25
1	B	564	ARG	CZ-NH1	6.74	1.42	1.32
1	A	210	GLU	CD-OE2	-6.68	1.12	1.25
1	A	564	ARG	CZ-NH2	-6.68	1.24	1.33
1	B	456	GLU	C-N	-6.54	1.26	1.33
1	A	231	GLU	CD-OE1	-6.53	1.12	1.25
1	A	242	LEU	C-O	-6.53	1.18	1.24
1	A	201	PRO	CA-C	6.48	1.60	1.52
1	B	86	ASP	CG-OD2	-6.45	1.13	1.25
1	A	222	TYR	CA-C	6.41	1.61	1.52
1	B	618	VAL	C-O	-6.38	1.17	1.24
1	B	310	SER	CA-CB	6.32	1.64	1.53
1	A	538	ARG	C-O	6.27	1.31	1.23
1	B	411	ARG	CG-CD	-6.25	1.33	1.52
1	A	10	ARG	CD-NE	-6.21	1.37	1.46
1	A	221	ARG	CZ-NH1	6.21	1.41	1.32
1	A	492	ASP	CG-OD2	6.17	1.37	1.25
1	A	37	ASP	CG-OD1	6.16	1.37	1.25
1	B	406	LEU	C-O	6.14	1.31	1.24
1	B	130	PRO	N-CA	6.12	1.54	1.47
1	A	221	ARG	CZ-NH2	6.09	1.41	1.33
1	B	775	GLU	N-CA	6.08	1.53	1.46
1	B	266	ARG	CZ-NH2	6.08	1.41	1.33
1	B	696	ASP	C-O	-6.07	1.16	1.24
1	B	267	MET	N-CA	-6.01	1.39	1.46
1	B	457	GLY	CA-C	5.95	1.61	1.51
1	A	411	ARG	CG-CD	-5.88	1.34	1.52
1	A	778	GLY	N-CA	5.88	1.50	1.44
1	B	696	ASP	CA-CB	5.85	1.63	1.53
1	B	227	LYS	CA-C	5.83	1.60	1.52
1	A	598	ALA	C-O	5.79	1.30	1.23
1	A	649	ASP	CB-CG	-5.78	1.37	1.52
1	B	779	GLU	CD-OE2	-5.77	1.14	1.25
1	A	658	ILE	CA-CB	-5.74	1.47	1.54
1	A	702	ARG	CD-NE	-5.71	1.38	1.46
1	A	123	LYS	CB-CG	-5.70	1.35	1.52
1	B	157	PHE	C-O	-5.69	1.19	1.24
1	B	316	ASP	CA-CB	5.62	1.57	1.53
1	A	76	ARG	N-CA	-5.61	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	ASP	C-N	-5.61	1.27	1.33
1	B	695	LEU	N-CA	-5.59	1.38	1.45
1	B	460	GLU	CD-OE2	-5.56	1.14	1.25
1	B	577	GLU	N-CA	-5.55	1.39	1.46
1	B	538	ARG	CZ-NH1	5.55	1.40	1.32
1	A	240	GLU	CD-OE2	5.54	1.35	1.25
1	A	237	SER	C-O	5.50	1.30	1.23
1	B	452	LEU	CB-CG	-5.50	1.42	1.53
1	B	492	ASP	CG-OD2	5.46	1.35	1.25
1	B	206	GLU	N-CA	-5.45	1.39	1.46
1	A	174	VAL	C-O	-5.43	1.18	1.24
1	A	126	ASN	CA-C	-5.37	1.46	1.52
1	A	515	GLU	CA-C	5.36	1.59	1.52
1	A	771	ARG	CZ-NH1	-5.36	1.25	1.32
1	A	730	GLU	CD-OE2	5.33	1.35	1.25
1	B	450	LEU	CG-CD2	-5.33	1.34	1.52
1	A	749	LYS	CA-C	-5.32	1.46	1.52
1	B	444	TYR	CA-C	-5.31	1.46	1.52
1	B	83	GLU	CG-CD	-5.30	1.38	1.52
1	A	502	ASP	CG-OD2	-5.30	1.15	1.25
1	B	239	SER	C-O	5.30	1.31	1.23
1	A	778	GLY	CA-C	-5.30	1.47	1.52
1	B	429	GLY	CA-C	5.29	1.59	1.51
1	A	513	SER	CA-C	5.28	1.60	1.53
1	B	776	HIS	CA-C	-5.27	1.48	1.52
1	A	604	PRO	CA-CB	-5.25	1.46	1.53
1	B	216	GLU	CD-OE2	-5.25	1.15	1.25
1	B	10	ARG	NE-CZ	-5.21	1.27	1.33
1	A	771	ARG	NE-CZ	-5.19	1.27	1.33
1	A	744	SER	CA-C	-5.18	1.46	1.52
1	B	763	ASP	N-CA	-5.17	1.39	1.46
1	A	471	GLU	CG-CD	5.15	1.65	1.52
1	B	661	PRO	C-O	-5.14	1.18	1.23
1	B	130	PRO	CA-C	5.14	1.58	1.52
1	A	147	GLU	CG-CD	5.13	1.64	1.52
1	A	266	ARG	CZ-NH1	5.13	1.40	1.32
1	B	590	GLY	CA-C	5.13	1.56	1.52
1	B	525	ALA	C-O	5.12	1.30	1.24
1	B	226	PHE	N-CA	5.11	1.52	1.46
1	A	322	LEU	CA-CB	-5.10	1.45	1.53
1	A	779	GLU	CD-OE2	5.08	1.35	1.25
1	B	655	PRO	N-CA	-5.07	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	459	GLU	CG-CD	5.05	1.64	1.52
1	B	610	ARG	CZ-NH1	-5.05	1.25	1.32
1	B	702	ARG	CZ-NH2	5.02	1.40	1.33
1	A	751	VAL	N-CA	-5.02	1.40	1.46
1	B	617	VAL	CA-CB	-5.02	1.48	1.54
1	B	83	GLU	CD-OE2	5.01	1.34	1.25
1	B	205	TRP	C-O	-5.01	1.18	1.24

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	457	GLY	N-CA-C	12.96	128.78	114.40
1	A	765	SER	CA-C-N	10.29	141.19	121.54
1	A	765	SER	C-N-CA	10.29	141.19	121.54
1	B	266	ARG	NE-CZ-NH2	9.07	127.37	119.20
1	B	564	ARG	NE-CZ-NH1	8.64	130.14	121.50
1	A	456	GLU	O-C-N	-8.55	111.84	122.35
1	B	687	ARG	NE-CZ-NH2	-8.42	111.62	119.20
1	B	678	HIS	CB-CG-CD2	-8.28	120.44	131.20
1	B	678	HIS	CB-CG-ND1	7.95	134.62	122.70
1	B	702	ARG	NE-CZ-NH2	7.76	126.19	119.20
1	A	457	GLY	N-CA-C	7.55	131.08	113.18
1	B	526	ARG	NE-CZ-NH2	7.36	125.82	119.20
1	A	471	GLU	CG-CD-OE2	-7.32	101.56	118.40
1	A	766	ASP	N-CA-C	7.25	126.23	110.80
1	B	36	LYS	CG-CD-CE	7.07	127.56	111.30
1	B	266	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	B	564	ARG	CD-NE-CZ	6.77	133.88	124.40
1	A	456	GLU	CA-C-N	-6.73	108.22	121.41
1	A	456	GLU	C-N-CA	-6.73	108.22	121.41
1	A	522	GLU	CB-CG-CD	-6.63	101.33	112.60
1	B	10	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	A	560	GLU	CA-CB-CG	6.33	126.76	114.10
1	A	558[A]	GLU	CB-CA-C	6.23	120.06	109.72
1	A	558[B]	GLU	CB-CA-C	6.23	120.06	109.72
1	A	559	ARG	NE-CZ-NH1	-6.23	115.27	121.50
1	A	219	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	766	ASP	N-CA-CB	6.19	120.94	110.49
1	B	210	GLU	CG-CD-OE1	-6.02	104.55	118.40
1	A	471	GLU	CG-CD-OE1	6.00	132.21	118.40
1	A	341	THR	CA-C-N	-5.96	114.24	120.38
1	A	341	THR	C-N-CA	-5.96	114.24	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ASP	CB-CA-C	-5.93	98.63	110.42
1	B	179	GLU	CB-CA-C	5.91	115.40	111.20
1	B	411	ARG	CG-CD-NE	-5.90	99.03	112.00
1	B	564	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	A	730	GLU	CB-CG-CD	5.84	122.52	112.60
1	A	759	GLY	CA-C-O	-5.81	115.96	121.60
1	B	36	LYS	CD-CE-NZ	5.81	130.48	111.90
1	A	136	PRO	CA-C-N	-5.79	113.97	119.76
1	A	136	PRO	C-N-CA	-5.79	113.97	119.76
1	A	266	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	B	467	TYR	CA-C-O	-5.77	112.52	119.27
1	B	700	LEU	CB-CG-CD1	5.75	127.95	110.70
1	A	442	GLY	O-C-N	5.72	126.95	123.35
1	A	490	LEU	N-CA-C	5.63	118.19	111.71
1	B	83	GLU	CB-CG-CD	5.62	122.14	112.60
1	B	131	ARG	CG-CD-NE	-5.61	99.67	112.00
1	B	646	VAL	CB-CA-C	-5.60	104.53	111.08
1	B	249	HIS	CA-CB-CG	5.59	119.39	113.80
1	A	242	LEU	CA-C-O	5.58	123.47	118.33
1	B	459	GLU	CB-CG-CD	5.48	121.91	112.60
1	B	136	PRO	CA-C-N	-5.41	114.35	119.76
1	B	136	PRO	C-N-CA	-5.41	114.35	119.76
1	A	251	PHE	N-CA-C	5.39	117.16	111.28
1	B	526	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	B	713	ARG	N-CA-C	5.26	117.19	109.24
1	B	498	LEU	N-CA-C	5.26	116.70	111.07
1	B	702	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	487	ALA	CA-C-O	-5.22	114.72	120.30
1	B	207	LYS	CG-CD-CE	5.21	123.28	111.30
1	B	779	GLU	CA-CB-CG	5.17	124.44	114.10
1	A	492	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	129	LEU	CA-C-N	-5.12	114.68	119.85
1	A	129	LEU	C-N-CA	-5.12	114.68	119.85
1	B	131	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	B	585	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	266	ARG	CG-CD-NE	-5.08	100.83	112.00
1	B	687	ARG	NE-CZ-NH1	5.07	126.57	121.50

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

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	58	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	114	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 (114) 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
1:B:766:ASP:CG	1:B:767:GLY:HA2	1.98	0.87
1:B:317[B]:PHE:HE1	1:B:325[B]:ILE:HD11	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:9:LYS:NZ	4:B:811:PPI:O2	2.38	0.56
1:B:564:ARG:HD2	6:B:1327:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:743[A]:HIS:HE2	1:B:775:GLU:CD	2.22	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
1:B:135:TYR:O	1:B:136:PRO:C	2.59	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:B:613:GLY:C	4:B:813:PPI:H33	2.43	0.44
1:A:9:LYS:HZ2	4:A:810:PPI:C1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HD3	6:A:910:HOH:O	2.14	0.43
1:B:332:TYR:CE1	1:B:336:VAL:HG21	2.53	0.43
1:B:696:ASP:O	1:B:696:ASP:CG	2.62	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:B:25:LEU:C	1:B:25:LEU:HD23	2.44	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:B:178:ASP:O	1:B:179:GLU:C	2.62	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: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: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

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	791/786 (101%)	764 (97%)	26 (3%)	1 (0%)	48	17
1	B	792/786 (101%)	766 (97%)	25 (3%)	1 (0%)	48	17
All	All	1583/1572 (101%)	1530 (97%)	51 (3%)	2 (0%)	48	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	767	GLY
1	A	766	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	689/682 (101%)	679 (98%)	10 (2%)	57	21
1	B	690/682 (101%)	685 (99%)	5 (1%)	76	49
All	All	1379/1364 (101%)	1364 (99%)	15 (1%)	65	32

All (15) 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	320	ASP
1	A	388	GLU
1	A	510	ASP
1	A	713	ARG
1	A	751	VAL
1	A	769	VAL
1	B	182	TYR
1	B	227	LYS
1	B	367	ILE
1	B	678	HIS
1	B	752	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	284	GLN
1	A	451	ASN
1	B	212	ASN
1	B	257	ASN
1	B	284	GLN
1	B	324	HIS
1	B	394	ASN
1	B	529	ASN
1	B	678	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.85	0	5,5,5	1.36	1 (20%)
2	GCS	A	801	-	12,12,12	3.53	7 (58%)	16,17,17	2.84	8 (50%)
3	PEG	B	806	-	6,6,6	0.43	0	5,5,5	1.30	1 (20%)
4	PPI	B	811	-	4,4,4	2.05	2 (50%)	4,4,4	1.77	2 (50%)
4	PPI	B	809	-	4,4,4	0.77	0	4,4,4	1.00	0
3	PEG	B	803	-	6,6,6	0.83	0	5,5,5	2.34	2 (40%)
4	PPI	B	812	-	4,4,4	2.15	1 (25%)	4,4,4	2.89	2 (50%)
4	PPI	B	813	-	4,4,4	1.21	0	4,4,4	1.29	1 (25%)
5	B3P	A	811	-	18,18,18	2.64	8 (44%)	23,23,23	3.60	9 (39%)
3	PEG	B	807	-	6,6,6	0.91	0	5,5,5	1.82	1 (20%)
4	PPI	A	810	-	4,4,4	2.37	1 (25%)	4,4,4	1.69	1 (25%)
3	PEG	A	806	-	6,6,6	0.72	0	5,5,5	0.95	0
3	PEG	A	804	-	6,6,6	0.92	0	5,5,5	0.44	0
4	PPI	A	808	-	4,4,4	2.24	2 (50%)	4,4,4	3.15	2 (50%)
3	PEG	B	805	-	6,6,6	0.63	0	5,5,5	0.64	0
4	PPI	B	808	-	4,4,4	0.81	0	4,4,4	2.83	2 (50%)
3	PEG	B	804	-	6,6,6	1.75	2 (33%)	5,5,5	1.26	0
2	GCS	B	801	-	12,12,12	2.97	6 (50%)	16,17,17	2.60	8 (50%)
4	PPI	A	809	-	4,4,4	1.91	1 (25%)	4,4,4	1.51	1 (25%)
3	PEG	A	807	-	6,6,6	1.70	1 (16%)	5,5,5	1.25	0
3	PEG	A	803	-	6,6,6	0.85	0	5,5,5	0.77	0
4	PPI	B	810	-	4,4,4	3.72	2 (50%)	4,4,4	1.92	2 (50%)
3	PEG	A	802	-	6,6,6	0.81	0	5,5,5	0.82	0
3	PEG	B	802	-	6,6,6	0.85	0	5,5,5	1.45	1 (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
3	PEG	A	805	-	-	3/4/4/4	-
2	GCS	A	801	-	-	0/2/22/22	0/1/1/1
3	PEG	B	806	-	-	1/4/4/4	-
4	PPI	B	811	-	-	0/2/2/2	-
4	PPI	B	809	-	-	2/2/2/2	-
3	PEG	B	803	-	-	3/4/4/4	-
4	PPI	B	812	-	-	0/2/2/2	-
4	PPI	B	813	-	-	2/2/2/2	-
5	B3P	A	811	-	-	14/28/28/28	-
3	PEG	B	807	-	-	3/4/4/4	-
4	PPI	A	810	-	-	2/2/2/2	-
3	PEG	A	806	-	-	2/4/4/4	-
3	PEG	A	804	-	-	3/4/4/4	-
4	PPI	A	808	-	-	2/2/2/2	-
3	PEG	B	805	-	-	3/4/4/4	-
4	PPI	B	808	-	-	2/2/2/2	-
3	PEG	B	804	-	-	2/4/4/4	-
2	GCS	B	801	-	-	0/2/22/22	0/1/1/1
4	PPI	A	809	-	-	0/2/2/2	-
3	PEG	A	807	-	-	1/4/4/4	-
3	PEG	A	803	-	-	2/4/4/4	-
4	PPI	B	810	-	-	2/2/2/2	-
3	PEG	A	802	-	-	2/4/4/4	-
3	PEG	B	802	-	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	811	B3P	C9-C8	8.67	1.63	1.53
2	A	801	GCS	C1-C2	6.95	1.60	1.52
4	B	810	PPI	O2-C1	-6.79	1.08	1.30
2	B	801	GCS	O3-C3	6.60	1.59	1.43
2	A	801	GCS	C2-N2	5.49	1.55	1.47
4	A	810	PPI	O2-C1	-4.54	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
4	B	812	PPI	C3-C2	-4.20	1.33	1.51
2	A	801	GCS	O3-C3	4.05	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GCS	O5-C5	3.64	1.53	1.44
2	B	801	GCS	C2-N2	3.58	1.52	1.47
2	B	801	GCS	O5-C5	3.42	1.52	1.44
4	A	809	PPI	O2-C1	-3.41	1.19	1.30
2	A	801	GCS	O4-C4	3.37	1.51	1.43
5	A	811	B3P	C3-N1	-3.34	1.42	1.46
2	B	801	GCS	O5-C1	3.12	1.50	1.42
4	A	808	PPI	O2-C1	-3.08	1.20	1.30
5	A	811	B3P	C2-N2	3.01	1.50	1.46
4	B	811	PPI	C2-C1	-2.74	1.37	1.50
2	B	801	GCS	O4-C4	2.56	1.49	1.43
4	B	811	PPI	O2-C1	-2.42	1.22	1.30
5	A	811	B3P	C11-C8	2.33	1.56	1.53
4	B	810	PPI	C3-C2	-2.31	1.41	1.51
3	A	807	PEG	C2-C1	2.30	1.61	1.49
5	A	811	B3P	C6-C4	2.25	1.56	1.53
4	A	808	PPI	C2-C1	2.23	1.62	1.50
2	A	801	GCS	O6-C6	2.23	1.51	1.42
5	A	811	B3P	O4-C5	-2.14	1.35	1.42
3	B	804	PEG	O1-C1	2.11	1.52	1.42
3	B	804	PEG	O4-C4	2.10	1.52	1.42
5	A	811	B3P	O1-C9	2.02	1.48	1.42
5	A	811	B3P	C7-C4	2.01	1.55	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	811	B3P	C2-N2-C8	6.97	126.37	116.17
5	A	811	B3P	O1-C9-C8	6.75	125.40	111.68
5	A	811	B3P	C3-N1-C4	6.74	126.03	116.17
2	A	801	GCS	C3-C4-C5	-6.73	98.03	110.23
5	A	811	B3P	C11-C8-C10	-6.58	95.58	110.02
2	B	801	GCS	C3-C4-C5	-5.78	99.76	110.23
5	A	811	B3P	O5-C6-C4	5.53	122.94	111.68
5	A	811	B3P	C7-C4-C5	-5.26	98.48	110.02
4	A	808	PPI	O2-C1-O1	-5.21	109.94	123.33
4	B	812	PPI	O2-C1-C2	4.78	133.57	113.49
2	A	801	GCS	O5-C1-C2	-4.66	104.07	109.51
2	A	801	GCS	O4-C4-C3	-4.15	100.60	110.38
4	B	808	PPI	O2-C1-C2	3.90	129.87	113.49
4	B	808	PPI	O2-C1-O1	-3.74	113.70	123.33
5	A	811	B3P	O4-C5-C4	-3.74	104.08	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	GCS	C4-C3-C2	3.58	116.94	110.99
2	B	801	GCS	O1-C1-O5	-3.58	99.78	110.41
3	B	803	PEG	C3-O2-C2	3.47	128.47	113.26
2	B	801	GCS	O5-C1-C2	-3.46	105.47	109.51
3	B	807	PEG	O2-C2-C1	3.31	124.69	110.11
4	A	808	PPI	O2-C1-C2	3.30	127.36	113.49
2	A	801	GCS	C1-O5-C5	-3.26	107.35	113.65
2	B	801	GCS	C3-C2-N2	-3.09	104.72	111.05
3	B	803	PEG	O2-C2-C1	3.07	123.64	110.11
2	B	801	GCS	O4-C4-C5	3.06	116.87	109.32
2	A	801	GCS	C3-C2-N2	-3.01	104.88	111.05
3	A	805	PEG	C3-O2-C2	2.96	126.19	113.26
4	B	810	PPI	O2-C1-O1	-2.85	115.99	123.33
2	A	801	GCS	O1-C1-O5	-2.84	101.98	110.41
5	A	811	B3P	C10-C8-C9	2.81	116.18	110.02
4	B	812	PPI	O1-C1-C2	-2.78	107.05	123.23
5	A	811	B3P	O2-C10-C8	-2.78	106.04	111.68
4	B	811	PPI	O2-C1-C2	2.67	124.68	113.49
4	A	810	PPI	O2-C1-O1	2.53	129.84	123.33
3	B	802	PEG	O2-C2-C1	2.50	121.14	110.11
2	A	801	GCS	O1-C1-C2	-2.33	104.15	108.96
4	B	810	PPI	C3-C2-C1	-2.30	98.32	113.67
2	B	801	GCS	O5-C5-C4	-2.28	105.59	109.70
3	B	806	PEG	C3-O2-C2	-2.23	103.52	113.26
4	A	809	PPI	O2-C1-C2	2.22	122.83	113.49
4	B	813	PPI	O2-C1-C2	2.13	122.43	113.49
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
4	B	811	PPI	O1-C1-C2	-2.00	111.60	123.23

There are no chirality outliers.

All (53) 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

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Mol	Chain	Res	Type	Atoms
5	A	811	B3P	N2-C8-C9-O1
5	A	811	B3P	C10-C8-C9-O1
5	A	811	B3P	C11-C8-C9-O1
5	A	811	B3P	C3-C1-C2-N2
3	A	806	PEG	O2-C3-C4-O4
3	B	805	PEG	O1-C1-C2-O2
3	B	805	PEG	O2-C3-C4-O4
3	B	807	PEG	O2-C3-C4-O4
5	A	811	B3P	C7-C4-C6-O5
3	A	804	PEG	O1-C1-C2-O2
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
5	A	811	B3P	C11-C8-N2-C2
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
4	A	810	PPI	O1-C1-C2-C3
4	B	810	PPI	O1-C1-C2-C3
4	B	813	PPI	O1-C1-C2-C3
5	A	811	B3P	C9-C8-N2-C2
3	B	807	PEG	C4-C3-O2-C2
3	B	804	PEG	O2-C3-C4-O4
3	A	803	PEG	O2-C3-C4-O4
3	A	803	PEG	C4-C3-O2-C2
3	A	806	PEG	O1-C1-C2-O2
3	A	802	PEG	C1-C2-O2-C3
3	A	805	PEG	C4-C3-O2-C2
3	A	802	PEG	O2-C3-C4-O4
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	804	PEG	C1-C2-O2-C3
3	A	807	PEG	C1-C2-O2-C3
3	B	804	PEG	O1-C1-C2-O2
4	B	808	PPI	O2-C1-C2-C3
4	B	809	PPI	O1-C1-C2-C3

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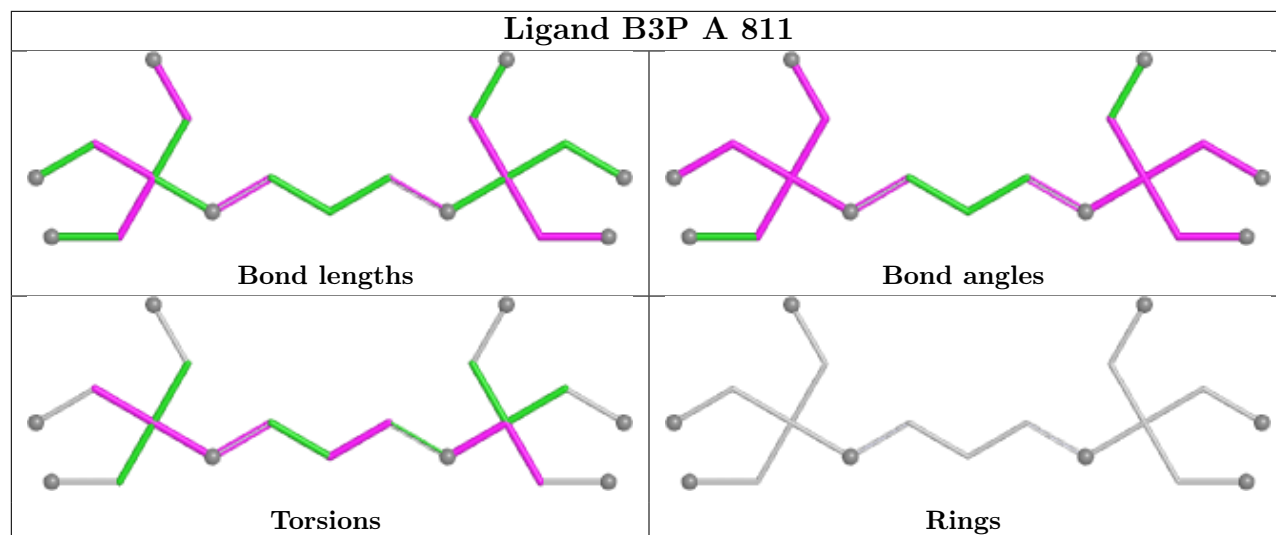
Mol	Chain	Res	Type	Atoms
4	B	809	PPI	O2-C1-C2-C3
3	A	805	PEG	O2-C3-C4-O4
3	B	805	PEG	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 38 short contacts:

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

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



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%)	-0.58	1 (0%) 92 93	4, 12, 29, 65	7 (0%)
1	B	786/786 (100%)	-0.67	2 (0%) 90 92	4, 10, 25, 63	8 (1%)
All	All	1572/1572 (100%)	-0.62	3 (0%) 91 92	4, 11, 28, 65	15 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.6
1	B	1	MET	2.8
1	B	317[A]	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	805	7/7	0.71	0.15	34,43,49,52	0
3	PEG	B	806	7/7	0.79	0.14	34,42,45,63	0

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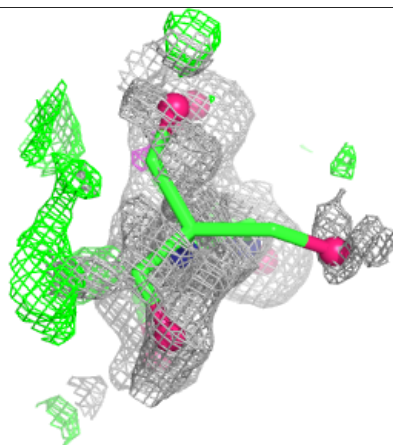
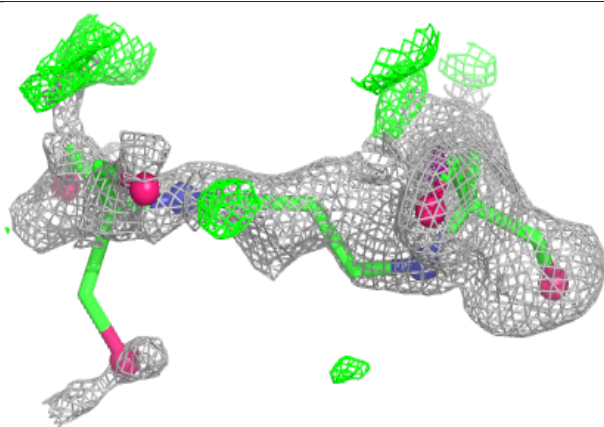
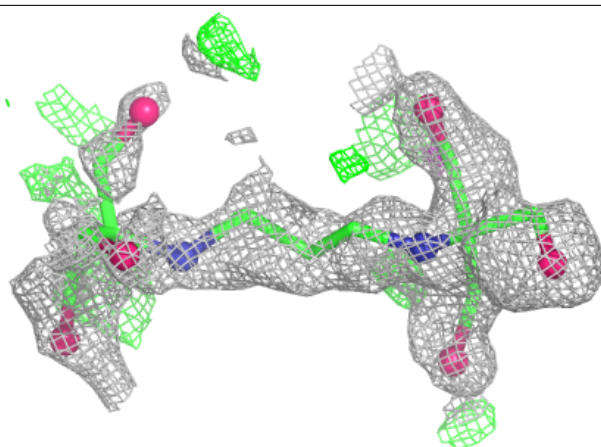
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	B	807	7/7	0.81	0.11	29,31,49,50	0
4	PPI	B	809	5/5	0.81	0.12	39,43,60,62	0
3	PEG	A	807	7/7	0.84	0.11	23,29,37,40	0
3	PEG	A	804	7/7	0.85	0.11	45,46,61,64	0
3	PEG	A	806	7/7	0.85	0.11	31,33,41,41	0
5	B3P	A	811	19/19	0.85	0.11	32,48,75,83	0
3	PEG	B	805	7/7	0.86	0.13	49,55,57,61	0
4	PPI	A	810	5/5	0.86	0.13	20,28,51,65	0
4	PPI	B	811	5/5	0.87	0.16	18,26,56,62	0
3	PEG	A	803	7/7	0.88	0.12	37,43,45,48	0
4	PPI	A	808	5/5	0.88	0.13	32,32,38,40	0
4	PPI	B	812	5/5	0.88	0.12	23,27,35,62	0
3	PEG	B	804	7/7	0.88	0.11	19,23,29,37	0
3	PEG	A	802	7/7	0.90	0.10	27,32,38,56	0
3	PEG	B	803	7/7	0.90	0.10	33,36,44,59	0
3	PEG	B	802	7/7	0.92	0.10	30,32,49,50	0
4	PPI	B	813	5/5	0.93	0.15	14,23,52,113	0
4	PPI	B	808	5/5	0.94	0.08	22,23,32,32	0
2	GCS	A	801	12/12	0.96	0.06	10,17,21,28	0
4	PPI	A	809	5/5	0.96	0.06	19,22,24,27	0
2	GCS	B	801	12/12	0.96	0.06	8,16,23,24	0
4	PPI	B	810	5/5	0.98	0.07	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.