



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:12 AM UTC

PDB ID : 9Q5G / pdb_00009q5g
Title : Human prolyl endopeptidase (PREP) - apo form
Authors : Fucci, I.J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-20
Resolution : 1.63 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

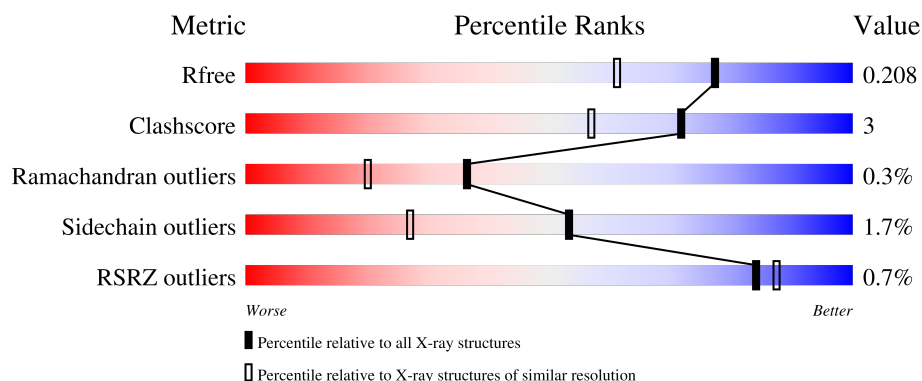
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	711	
1	B	711	
1	C	711	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19676 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.

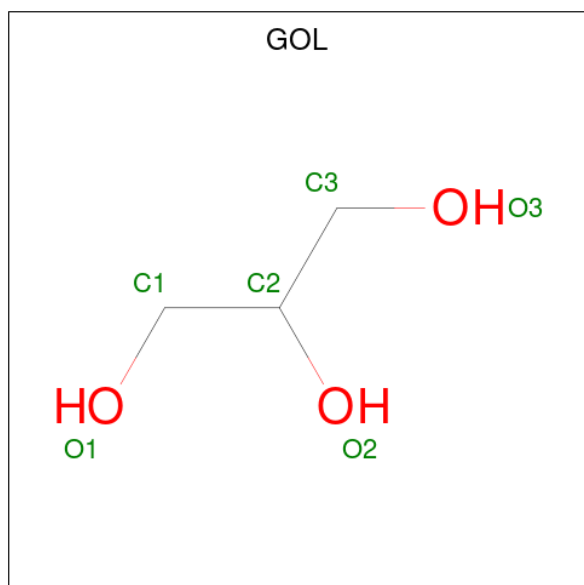
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	15	0
			5743	3692	949	1074	28			
1	B	707	Total	C	N	O	S	0	16	0
			5757	3704	948	1077	28			
1	C	707	Total	C	N	O	S	0	5	0
			5704	3659	946	1072	27			

There are 3 discrepancies between the modelled and reference sequences:

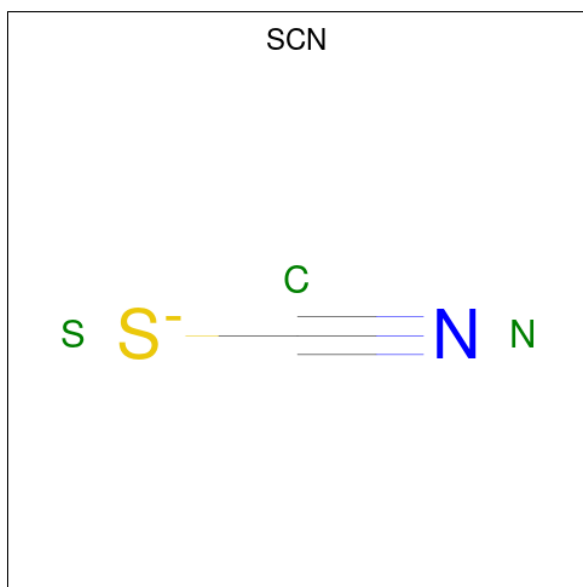
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147
C	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



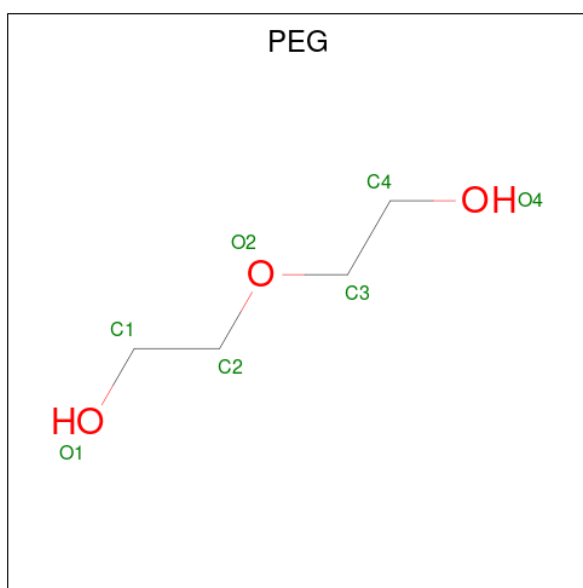
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N S 3 1 1 1	0	0
3	A	1	Total C N S 3 1 1 1	0	0
3	A	1	Total C N S 3 1 1 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		
3	C	1	Total	C	N	S	0	0
			3	1	1	1		
3	C	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



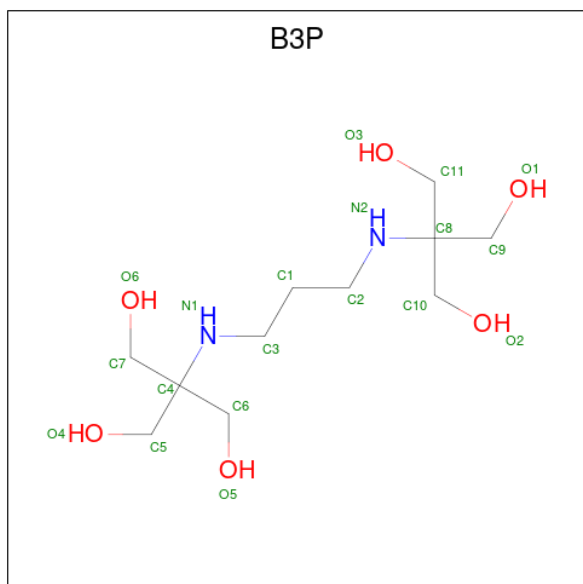
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	1
			14	8	6		
4	B	1	Total	C	O	0	0
			7	4	3		

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

- 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	B	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	895	Total	O	0	4
			899	899		
6	B	871	Total	O	0	5
			876	876		

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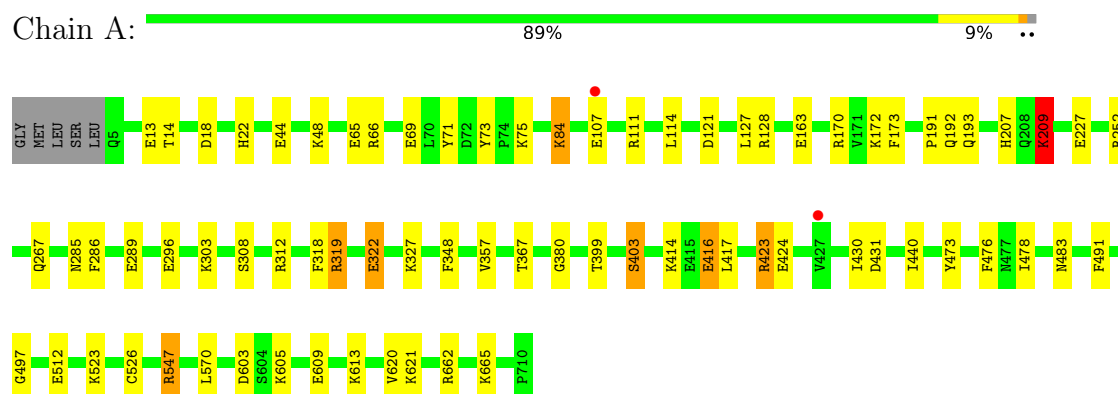
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	518	Total	O	0	0
			518	518		

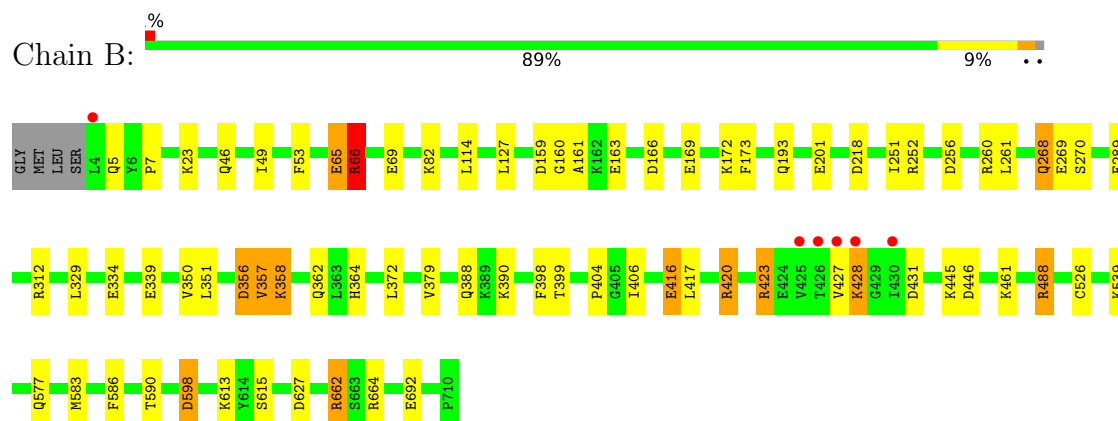
3 Residue-property plots [i](#)

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.

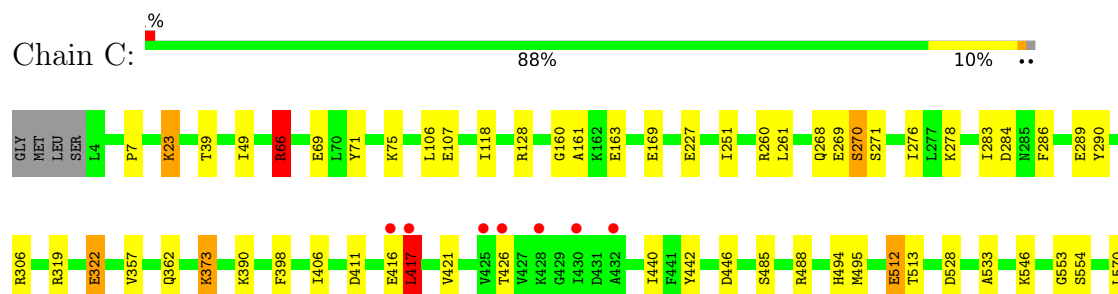
• Molecule 1: Prolyl endopeptidase



• Molecule 1: Prolyl endopeptidase



• Molecule 1: Prolyl endopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.12Å 66.88Å 158.02Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	34.50 – 1.63 34.50 – 1.63	Depositor EDS
% Data completeness (in resolution range)	77.5 (34.50-1.63) 77.9 (34.50-1.63)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.151 , 0.200 0.164 , 0.208	Depositor DCC
R_{free} test set	13544 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19676	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: PEG, GOL, B3P, SCN

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	0.98	2/5940 (0.0%)	1.34	35/8045 (0.4%)
1	B	0.93	1/5957 (0.0%)	1.34	39/8071 (0.5%)
1	C	0.85	1/5871 (0.0%)	1.31	30/7958 (0.4%)
All	All	0.92	4/17768 (0.0%)	1.33	104/24074 (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	1
1	B	0	8
1	C	0	4
All	All	0	13

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	HIS	CG-CD2	-6.36	1.28	1.35
1	A	170	ARG	NE-CZ	-5.87	1.26	1.33
1	B	364	HIS	ND1-CE1	5.34	1.37	1.32
1	C	289	GLU	CD-OE1	5.33	1.35	1.25

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	GLU	CB-CG-CD	11.18	131.60	112.60
1	B	201	GLU	CB-CG-CD	10.25	130.03	112.60
1	B	268	GLN	CB-CA-C	-9.88	92.23	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	GLU	CB-CG-CD	8.82	127.60	112.60
1	A	423	ARG	CD-NE-CZ	-8.64	112.30	124.40
1	C	512	GLU	CB-CG-CD	8.55	127.14	112.60
1	A	267	GLN	CB-CG-CD	8.36	126.81	112.60
1	C	286	PHE	CA-CB-CG	7.84	121.64	113.80
1	B	662	ARG	NE-CZ-NH1	-7.77	113.73	121.50
1	A	547	ARG	CD-NE-CZ	7.72	135.21	124.40
1	C	570	LEU	N-CA-CB	-7.62	98.50	110.46
1	B	428	LYS	CB-CA-C	7.55	122.15	109.84
1	B	423	ARG	CB-CA-C	-7.32	94.51	109.38
1	A	267	GLN	CB-CA-C	7.32	125.10	110.17
1	A	416	GLU	CB-CG-CD	7.20	124.84	112.60
1	C	23	LYS	CB-CA-C	-7.19	97.35	109.65
1	A	322	GLU	CB-CG-CD	7.15	124.76	112.60
1	B	404	PRO	CA-C-N	-7.14	107.42	121.41
1	B	404	PRO	C-N-CA	-7.14	107.42	121.41
1	A	399	THR	OG1-CB-CG2	-7.12	95.07	109.30
1	B	268	GLN	N-CA-CB	7.04	121.20	110.44
1	A	547	ARG	NE-CZ-NH2	6.87	125.39	119.20
1	A	403	SER	CB-CA-C	-6.79	102.34	110.15
1	A	289	GLU	CG-CD-OE2	-6.75	102.88	118.40
1	B	431	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	269	GLU	CB-CG-CD	6.73	124.04	112.60
1	A	367	THR	CA-CB-OG1	-6.65	99.62	109.60
1	B	627	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	339	GLU	CB-CA-C	-6.40	99.00	110.70
1	C	642	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	289	GLU	CG-CD-OE2	-6.35	103.80	118.40
1	A	348	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	13	GLU	CB-CG-CD	6.33	123.35	112.60
1	A	414	LYS	CB-CA-C	-6.29	99.14	109.53
1	B	5	GLN	CB-CA-C	6.28	120.36	110.19
1	A	111	ARG	CG-CD-NE	-6.27	98.20	112.00
1	B	356	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	128	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	A	327	LYS	CG-CD-CE	-6.14	97.17	111.30
1	C	411	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	170	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	C	362	GLN	CB-CA-C	6.02	122.93	109.56
1	C	512	GLU	N-CA-CB	5.98	119.42	110.22
1	C	618	HIS	CA-CB-CG	-5.92	107.88	113.80
1	C	651	LYS	CG-CD-CE	5.92	124.91	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	707	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	416	GLU	CB-CA-C	-5.90	100.66	110.68
1	C	446	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	127	LEU	N-CA-CB	-5.82	101.41	109.97
1	C	289	GLU	CG-CD-OE2	-5.81	105.04	118.40
1	B	169	GLU	CA-CB-CG	-5.80	102.49	114.10
1	A	22	HIS	CA-CB-CG	5.79	119.59	113.80
1	C	686	THR	CA-CB-OG1	-5.76	100.96	109.60
1	C	662	ARG	CD-NE-CZ	5.75	132.45	124.40
1	C	582	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	420	ARG	CA-CB-CG	5.70	125.50	114.10
1	C	639	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	209	LYS	CG-CD-CE	5.62	124.22	111.30
1	A	252	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	A	14	THR	CA-CB-OG1	5.57	117.96	109.60
1	A	289	GLU	CG-CD-OE1	5.54	131.13	118.40
1	C	373	LYS	N-CA-CB	-5.53	102.44	111.24
1	C	528	ASP	CA-CB-CG	5.53	118.12	112.60
1	A	318	PHE	CA-CB-CG	5.51	119.31	113.80
1	C	128	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	414	LYS	CG-CD-CE	-5.49	98.69	111.30
1	C	39	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	66	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	424	GLU	N-CA-CB	-5.44	101.29	111.13
1	B	193	GLN	N-CA-CB	-5.44	102.78	111.43
1	A	111	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	107	GLU	CB-CA-C	5.40	121.17	110.42
1	B	423	ARG	N-CA-CB	5.39	120.78	111.13
1	B	66	ARG	NE-CZ-NH2	-5.36	114.37	119.20
1	B	5	GLN	CA-C-O	5.34	126.08	120.36
1	C	631	PRO	CB-CA-C	-5.34	104.24	111.12
1	B	399	THR	OG1-CB-CG2	-5.33	98.65	109.30
1	C	598	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	127	LEU	N-CA-CB	-5.30	101.82	109.83
1	A	84	LYS	N-CA-C	-5.30	106.12	112.59
1	B	372	LEU	N-CA-CB	5.28	119.21	110.33
1	C	411	ASP	CB-CA-C	-5.25	102.37	111.30
1	A	603	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	626	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	427	VAL	N-CA-CB	5.24	118.27	111.67
1	B	65	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	662	ARG	CD-NE-CZ	5.18	131.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	B	53	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	312	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	380	GLY	CA-C-O	-5.12	117.00	121.04
1	C	278	LYS	N-CA-CB	5.12	117.73	110.46
1	B	446	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	163	GLU	CB-CA-C	-5.10	101.73	109.89
1	C	23	LYS	N-CA-CB	5.09	117.45	109.97
1	B	379	VAL	N-CA-CB	5.08	116.64	110.95
1	B	526[A]	CYS	CB-CA-C	-5.07	102.91	110.88
1	B	526[B]	CYS	CB-CA-C	-5.07	102.91	110.88
1	C	269	GLU	N-CA-CB	5.04	118.08	109.87
1	B	166	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	319	ARG	CB-CG-CD	5.02	122.85	111.30
1	B	159	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	598	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	252	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	547	ARG	Sidechain
1	B	252	ARG	Sidechain
1	B	420	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	488[A]	ARG	Sidechain
1	B	488[B]	ARG	Sidechain
1	B	66	ARG	Sidechain
1	B	662	ARG	Sidechain
1	B	664	ARG	Sidechain
1	C	306	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	66[A]	ARG	Sidechain
1	C	66[B]	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5743	0	5618	44	1
1	B	5757	0	5632	28	0
1	C	5704	0	5530	34	1
2	A	24	0	32	3	0
2	B	30	0	40	4	0
3	A	12	0	0	0	0
3	B	6	0	0	1	0
3	C	6	0	0	0	0
4	A	26	0	35	3	0
4	B	28	0	39	3	0
4	C	28	0	40	5	0
5	B	19	0	26	0	0
6	A	899	0	0	23	2
6	B	876	0	0	12	3
6	C	518	0	0	9	1
All	All	19676	0	16992	112	5

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 3.

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:C:66[B]:ARG:NH2	1:C:69:GLU:OE1	1.72	1.19
1:B:388[B]:GLN:NE2	6:B:901:HOH:O	1.91	1.01
1:C:271:SER:HA	6:C:1209:HOH:O	1.56	1.01
4:C:804:PEG:H21	6:C:1285:HOH:O	1.62	0.99
1:C:268:GLN:NE2	6:C:901:HOH:O	2.04	0.91
1:A:192:GLN:HE21	1:A:193:GLN:H	1.24	0.85
1:C:322:GLU:HG2	6:C:1313:HOH:O	1.84	0.77
1:A:609:GLU:OE1	6:A:901:HOH:O	2.03	0.77
1:A:620:VAL:O	1:A:621[B]:LYS:HD2	1.85	0.75
1:A:227:GLU:OE2	6:A:902:HOH:O	2.07	0.72
1:A:322:GLU:HG3	6:A:1537:HOH:O	1.91	0.70
1:B:362:GLN:HE22	2:B:802:GOL:C1	2.04	0.70
1:A:285:ASN:HD21	2:A:810:GOL:H31	1.59	0.67
1:A:286:PHE:H	1:B:428:LYS:HZ1	1.43	0.66
1:A:69[A]:GLU:HG3	6:A:1042:HOH:O	1.93	0.66
1:C:66[A]:ARG:HD3	1:C:494:HIS:NE2	2.10	0.66
1:B:356:ASP:O	1:B:358:LYS:HE3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ILE:HD12	4:C:805:PEG:H11	1.77	0.65
4:B:810:PEG:H12	6:B:1393:HOH:O	1.95	0.65
1:A:18:ASP:OD2	6:A:903:HOH:O	2.14	0.64
1:A:114:LEU:HD11	6:A:1618:HOH:O	1.98	0.64
4:B:807[B]:PEG:H11	6:B:1549:HOH:O	1.98	0.62
1:A:319:ARG:HG2	6:A:1605:HOH:O	1.98	0.62
2:A:801:GOL:H12	6:A:1358:HOH:O	2.00	0.62
1:C:7:PRO:HD3	1:C:49:ILE:CD1	2.31	0.60
1:A:286:PHE:H	1:B:428:LYS:NZ	2.00	0.59
1:C:7:PRO:HD3	1:C:49:ILE:HD11	1.84	0.59
1:B:329:LEU:O	3:B:806:SCN:S	2.60	0.59
1:B:7:PRO:HD3	1:B:49[B]:ILE:HD11	1.85	0.58
1:C:227:GLU:H	4:C:805:PEG:H12	1.67	0.58
1:A:44[B]:GLU:OE1	6:A:904:HOH:O	2.17	0.58
1:C:66[B]:ARG:CZ	1:C:69:GLU:OE1	2.49	0.57
1:A:285:ASN:HD21	2:A:810:GOL:C3	2.17	0.57
1:A:620:VAL:C	1:A:621[B]:LYS:HD2	2.30	0.56
1:A:71:TYR:CE2	1:A:75:LYS:NZ	2.73	0.56
1:C:625:ALA:HB3	1:C:628:ILE:HD12	1.87	0.56
2:B:803:GOL:H31	6:B:1459:HOH:O	2.05	0.55
1:A:523:LYS:O	1:A:526[B]:CYS:HB3	2.07	0.54
1:A:296:GLU:HG3	6:A:1647:HOH:O	2.08	0.54
1:B:362:GLN:NE2	2:B:802:GOL:O1	2.40	0.54
1:B:334:GLU:OE1	6:B:902:HOH:O	2.19	0.52
1:C:163:GLU:HG3	6:C:1132:HOH:O	2.08	0.52
1:A:473:TYR:CE2	1:A:478[A]:ILE:HD12	2.45	0.51
1:A:322:GLU:HG3	6:B:1623:HOH:O	2.10	0.51
1:A:431:ASP:OD1	6:A:905:HOH:O	2.18	0.51
1:A:303:LYS:HE3	6:A:1485:HOH:O	2.11	0.50
1:C:485:SER:OG	1:C:488:ARG:HD3	2.11	0.50
1:B:69[A]:GLU:HG2	6:B:1351:HOH:O	2.11	0.50
1:C:160:GLY:O	1:C:161:ALA:C	2.55	0.50
1:A:163:GLU:OE2	6:A:906:HOH:O	2.19	0.50
1:A:322:GLU:CG	6:B:1623:HOH:O	2.59	0.50
1:C:513:THR:HG23	6:C:1076:HOH:O	2.11	0.50
1:A:303:LYS:CE	6:A:1485:HOH:O	2.60	0.49
1:A:191:PRO:HG3	1:A:209:LYS:NZ	2.27	0.49
1:A:322:GLU:CD	6:A:955:HOH:O	2.55	0.49
1:C:647:LEU:C	1:C:647:LEU:HD12	2.38	0.49
1:C:546:LYS:HD2	6:C:1292:HOH:O	2.13	0.49
1:A:84:LYS:HE3	6:A:1572:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LYS:NZ	1:C:417:LEU:O	2.32	0.48
1:A:605:LYS:NZ	1:A:609:GLU:OE2	2.46	0.47
4:A:808:PEG:C3	6:A:1596:HOH:O	2.63	0.47
1:C:270:SER:O	1:C:271:SER:OG	2.29	0.47
1:C:691[A]:GLU:HG2	6:C:1202:HOH:O	2.15	0.47
1:A:613:LYS:HE3	6:A:1386:HOH:O	2.14	0.47
1:A:665:LYS:HD2	6:A:1137:HOH:O	2.14	0.47
1:B:358:LYS:NZ	6:B:921:HOH:O	2.44	0.46
1:B:7:PRO:HD3	1:B:49[B]:ILE:CD1	2.44	0.46
1:A:416:GLU:O	1:A:417:LEU:C	2.55	0.46
1:C:440:ILE:C	1:C:440:ILE:HD12	2.41	0.46
1:C:416:GLU:O	1:C:417:LEU:HB2	2.15	0.46
4:A:808:PEG:H31	6:A:1596:HOH:O	2.17	0.45
1:B:398:PHE:HB3	1:B:406:ILE:CG2	2.47	0.45
1:A:423:ARG:HD3	6:A:1157:HOH:O	2.17	0.45
1:B:586:PHE:CD1	1:B:586:PHE:C	2.95	0.45
1:C:227:GLU:OE2	4:C:805:PEG:H42	2.17	0.44
1:B:416:GLU:O	1:B:417:LEU:C	2.60	0.44
4:B:807[A]:PEG:H21	4:B:807[A]:PEG:H41	1.31	0.44
1:A:73:TYR:O	1:A:75:LYS:HE3	2.16	0.44
1:C:406:ILE:HD11	1:C:421:VAL:HG22	1.99	0.44
1:A:491:PHE:CE2	1:A:497:GLY:HA3	2.53	0.44
1:C:283:ILE:HD13	1:C:290:TYR:CE2	2.53	0.44
1:B:362:GLN:HE22	2:B:802:GOL:H12	1.81	0.43
1:B:577:GLN:NE2	1:B:692[A]:GLU:OE1	2.51	0.43
1:C:260:ARG:NH1	1:C:284:ASP:OD1	2.50	0.43
1:C:583:MET:HB2	1:C:615:SER:HB2	1.99	0.43
1:A:308[A]:SER:OG	1:A:312:ARG:HD3	2.18	0.43
1:B:160:GLY:O	1:B:161:ALA:C	2.62	0.43
1:A:44[A]:GLU:HG2	6:A:991:HOH:O	2.19	0.43
1:C:71:TYR:CZ	1:C:75:LYS:HE2	2.54	0.42
1:B:46:GLN:O	1:B:49[A]:ILE:HG12	2.20	0.42
1:C:705:ASN:ND2	6:C:934:HOH:O	2.52	0.42
1:A:84:LYS:H	1:A:84:LYS:HG2	1.77	0.42
1:C:251:ILE:HB	1:C:260:ARG:HB2	2.00	0.42
1:A:44[B]:GLU:HG2	1:A:48:LYS:HE3	1.99	0.42
1:A:476:PHE:CZ	4:A:807:PEG:H21	2.55	0.42
1:B:65:GLU:OE2	1:B:66:ARG:HD2	2.20	0.42
1:C:442:TYR:CZ	1:C:533:ALA:HB2	2.55	0.42
1:B:461:LYS:N	1:B:461:LYS:HD3	2.35	0.42
1:A:440:ILE:C	1:A:440:ILE:HD12	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HD3	1:B:173:PHE:CE2	2.54	0.42
1:C:398:PHE:HB3	1:C:406:ILE:HG23	2.01	0.41
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.56	0.41
1:B:256:ASP:HB2	6:B:1024:HOH:O	2.19	0.41
1:A:69[A]:GLU:CG	6:A:1042:HOH:O	2.59	0.41
1:B:350:VAL:C	1:B:351:LEU:HD12	2.46	0.41
1:A:65:GLU:O	1:A:69[A]:GLU:HG3	2.21	0.41
1:B:583:MET:HB2	1:B:615:SER:HB2	2.02	0.41
1:C:495:MET:HE3	1:C:701:ALA:HB2	2.02	0.41
1:C:553:GLY:O	4:C:804:PEG:O1	2.36	0.40
1:B:613:LYS:HE3	6:B:1008:HOH:O	2.21	0.40
1:B:251:ILE:HB	1:B:260:ARG:HB2	2.04	0.40
1:B:82:LYS:NZ	6:B:939:HOH:O	2.50	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121[A]:ASP:OD2	1:C:664:ARG:NH1[2_556]	2.08	0.12
6:A:1132:HOH:O	6:B:1554:HOH:O[2_555]	2.12	0.08
6:A:1615:HOH:O	6:A:1693:HOH:O[2_555]	2.17	0.03
6:B:1134:HOH:O	6:C:1324:HOH:O[2_545]	2.17	0.03
6:B:1654:HOH:O	6:B:1666:HOH:O[1_565]	2.18	0.02

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	719/711 (101%)	694 (96%)	24 (3%)	1 (0%)	48	29
1	B	721/711 (101%)	702 (97%)	17 (2%)	2 (0%)	36	20
1	C	710/711 (100%)	683 (96%)	24 (3%)	3 (0%)	30	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2150/2133 (101%)	2079 (97%)	65 (3%)	6 (0%)	36	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	554	SER
1	C	417	LEU
1	B	590	THR
1	C	357	VAL
1	B	357	VAL
1	A	357	VAL

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	628/617 (102%)	621 (99%)	7 (1%)	65	44
1	B	630/617 (102%)	614 (98%)	16 (2%)	42	14
1	C	619/617 (100%)	606 (98%)	13 (2%)	47	19
All	All	1877/1851 (101%)	1841 (98%)	36 (2%)	53	23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	GLU
1	A	209	LYS
1	A	403	SER
1	A	430	ILE
1	A	483	ASN
1	A	512	GLU
1	A	570	LEU
1	B	23	LYS
1	B	114[A]	LEU
1	B	114[B]	LEU

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Mol	Chain	Res	Type
1	B	218[A]	ASP
1	B	218[B]	ASP
1	B	261	LEU
1	B	268	GLN
1	B	270	SER
1	B	357	VAL
1	B	358	LYS
1	B	390	LYS
1	B	445	LYS
1	B	488[A]	ARG
1	B	488[B]	ARG
1	B	539	LYS
1	B	598	ASP
1	C	23	LYS
1	C	66[A]	ARG
1	C	66[B]	ARG
1	C	106	LEU
1	C	118	ILE
1	C	169	GLU
1	C	261	LEU
1	C	270	SER
1	C	390	LYS
1	C	417	LEU
1	C	426	THR
1	C	512	GLU
1	C	598	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	103	GLN
1	A	192	GLN
1	A	268	GLN
1	A	397	GLN
1	A	483	ASN
1	A	503	ASN
1	A	531	GLN
1	A	551	ASN
1	A	577	GLN
1	B	17	GLN
1	B	267	GLN

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Mol	Chain	Res	Type
1	B	362	GLN
1	B	439	GLN
1	B	477	ASN
1	B	503	ASN
1	B	524	GLN
1	B	531	GLN
1	B	551	ASN
1	B	566	GLN
1	B	577	GLN
1	B	606	GLN
1	B	705	ASN
1	C	103	GLN
1	C	388	GLN
1	C	397	GLN
1	C	551	ASN
1	C	577	GLN
1	C	705	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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	SCN	B	806	-	1,2,2	0.12	0	0,1,1	-	-
2	GOL	B	803	-	5,5,5	0.29	0	5,5,5	1.04	0
3	SCN	A	809	-	1,2,2	0.48	0	0,1,1	-	-
5	B3P	B	801	-	18,18,18	0.85	0	23,23,23	1.33	2 (8%)
3	SCN	A	802	-	1,2,2	2.02	1 (100%)	0,1,1	-	-
4	PEG	C	805	-	6,6,6	0.41	0	5,5,5	0.18	0
4	PEG	C	801	-	6,6,6	0.82	0	5,5,5	0.62	0
2	GOL	B	804	-	5,5,5	0.12	0	5,5,5	0.40	0
3	SCN	C	806	-	1,2,2	2.34	1 (100%)	0,1,1	-	-
4	PEG	A	806	-	6,6,6	0.42	0	5,5,5	0.39	0
2	GOL	B	811	-	5,5,5	0.38	0	5,5,5	1.01	0
2	GOL	B	802	-	5,5,5	0.70	0	5,5,5	1.85	2 (40%)
4	PEG	C	804	-	6,6,6	0.40	0	5,5,5	0.43	0
4	PEG	B	807[A]	-	6,6,6	0.29	0	5,5,5	0.17	0
3	SCN	A	803	-	1,2,2	0.71	0	0,1,1	-	-
4	PEG	B	807[B]	-	6,6,6	0.75	0	5,5,5	0.43	0
4	PEG	A	812	-	6,6,6	0.32	0	5,5,5	0.40	0
4	PEG	B	809	-	6,6,6	0.47	0	5,5,5	0.50	0
3	SCN	C	803	-	1,2,2	0.35	0	0,1,1	-	-
2	GOL	A	801	-	5,5,5	0.27	0	5,5,5	0.37	0
2	GOL	A	810	-	5,5,5	0.28	0	5,5,5	0.87	0
4	PEG	A	807	-	6,6,6	0.46	0	5,5,5	0.59	0
4	PEG	A	808	-	4,4,6	0.42	0	3,3,5	0.15	0
4	PEG	C	802	-	6,6,6	0.54	0	5,5,5	0.69	0
2	GOL	A	811	-	5,5,5	0.30	0	5,5,5	0.77	0
2	GOL	A	805	-	5,5,5	0.23	0	5,5,5	0.47	0
3	SCN	B	808	-	1,2,2	0.30	0	0,1,1	-	-
3	SCN	A	804	-	1,2,2	4.75	1 (100%)	0,1,1	-	-
4	PEG	B	810	-	6,6,6	0.61	0	5,5,5	0.37	0
2	GOL	B	805	-	5,5,5	0.17	0	5,5,5	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	803	-	-	3/4/4/4	-
5	B3P	B	801	-	-	0/28/28/28	-
4	PEG	C	805	-	-	2/4/4/4	-
4	PEG	C	801	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	804	-	-	3/4/4/4	-
4	PEG	A	806	-	-	2/4/4/4	-
2	GOL	B	811	-	-	1/4/4/4	-
2	GOL	B	802	-	-	0/4/4/4	-
4	PEG	C	804	-	-	2/4/4/4	-
4	PEG	B	807[A]	-	-	4/4/4/4	-
4	PEG	B	807[B]	-	-	3/4/4/4	-
4	PEG	A	812	-	-	2/4/4/4	-
4	PEG	B	809	-	-	1/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-
2	GOL	A	810	-	-	2/4/4/4	-
4	PEG	A	807	-	-	1/4/4/4	-
4	PEG	A	808	-	-	2/2/2/4	-
4	PEG	C	802	-	-	3/4/4/4	-
2	GOL	A	811	-	-	2/4/4/4	-
2	GOL	A	805	-	-	1/4/4/4	-
4	PEG	B	810	-	-	3/4/4/4	-
2	GOL	B	805	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	SCN	C-N	4.75	1.31	1.15
3	C	806	SCN	C-N	2.34	1.23	1.15
3	A	802	SCN	C-N	2.02	1.22	1.15

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	GOL	O2-C2-C3	3.44	123.44	109.18
5	B	801	B3P	O5-C6-C4	-2.60	106.39	111.68
5	B	801	B3P	C7-C4-C6	-2.29	105.00	110.02
2	B	802	GOL	C3-C2-C1	-2.19	103.77	111.80

There are no chirality outliers.

All (42) torsion outliers are listed below:

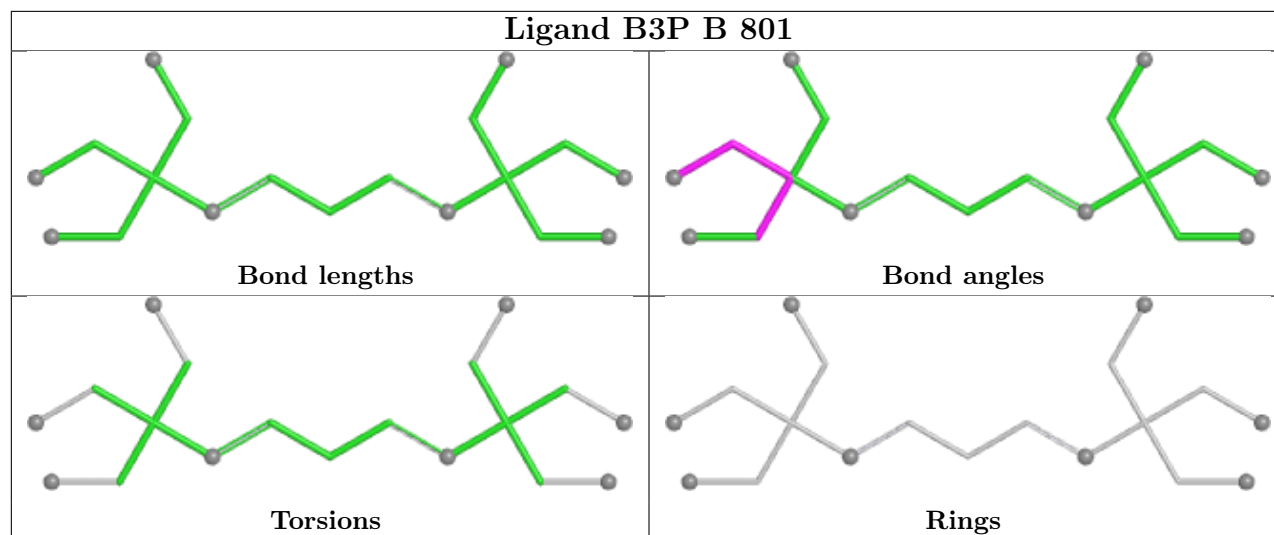
Mol	Chain	Res	Type	Atoms
2	A	810	GOL	O1-C1-C2-C3
2	A	811	GOL	O1-C1-C2-O2
2	A	811	GOL	O1-C1-C2-C3
4	B	807[A]	PEG	C4-C3-O2-C2
4	A	806	PEG	O2-C3-C4-O4
4	C	802	PEG	O2-C3-C4-O4
4	B	807[A]	PEG	O1-C1-C2-O2
4	C	801	PEG	O1-C1-C2-O2
2	B	803	GOL	C1-C2-C3-O3
2	B	804	GOL	O1-C1-C2-C3
2	B	805	GOL	C1-C2-C3-O3
4	A	806	PEG	O1-C1-C2-O2
4	A	808	PEG	O2-C3-C4-O4
2	B	803	GOL	O2-C2-C3-O3
4	A	812	PEG	O1-C1-C2-O2
4	B	807[A]	PEG	O2-C3-C4-O4
4	B	807[B]	PEG	O2-C3-C4-O4
2	A	810	GOL	O1-C1-C2-O2
2	B	803	GOL	O1-C1-C2-O2
2	B	804	GOL	O1-C1-C2-O2
4	B	807[B]	PEG	C4-C3-O2-C2
2	B	805	GOL	O2-C2-C3-O3
4	A	808	PEG	C4-C3-O2-C2
2	A	805	GOL	O2-C2-C3-O3
4	B	809	PEG	O1-C1-C2-O2
4	C	805	PEG	O2-C3-C4-O4
4	C	804	PEG	C4-C3-O2-C2
4	A	812	PEG	C1-C2-O2-C3
4	A	807	PEG	O2-C3-C4-O4
4	B	810	PEG	O2-C3-C4-O4
4	B	807[A]	PEG	C1-C2-O2-C3
4	C	805	PEG	C1-C2-O2-C3
4	C	802	PEG	C1-C2-O2-C3
4	B	810	PEG	O1-C1-C2-O2
2	B	811	GOL	C1-C2-C3-O3
4	C	804	PEG	C1-C2-O2-C3
4	B	810	PEG	C1-C2-O2-C3
4	C	802	PEG	O1-C1-C2-O2
4	C	801	PEG	C1-C2-O2-C3
4	B	807[B]	PEG	C1-C2-O2-C3
4	C	801	PEG	O2-C3-C4-O4
2	B	804	GOL	O2-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	806	SCN	1	0
2	B	803	GOL	1	0
4	C	805	PEG	3	0
2	B	802	GOL	3	0
4	C	804	PEG	2	0
4	B	807[A]	PEG	1	0
4	B	807[B]	PEG	1	0
2	A	801	GOL	1	0
2	A	810	GOL	2	0
4	A	807	PEG	1	0
4	A	808	PEG	2	0
4	B	810	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	706/711 (99%)	-0.56	2 (0%) 90 91	7, 15, 30, 53	15 (2%)
1	B	707/711 (99%)	-0.51	6 (0%) 82 86	7, 16, 32, 62	16 (2%)
1	C	707/711 (99%)	-0.07	7 (0%) 79 84	12, 24, 48, 101	5 (0%)
All	All	2120/2133 (99%)	-0.38	15 (0%) 84 87	7, 18, 41, 101	36 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	ILE	3.9
1	C	425	VAL	3.6
1	C	417	LEU	2.8
1	A	427	VAL	2.8
1	C	426	THR	2.5
1	B	425	VAL	2.5
1	B	428	LYS	2.4
1	B	4	LEU	2.3
1	B	426	THR	2.3
1	C	416	GLU	2.2
1	B	430	ILE	2.2
1	A	107	GLU	2.1
1	C	428	LYS	2.1
1	C	432	ALA	2.0
1	B	427	VAL	2.0

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 ⓘ

There are no oligosaccharides in this entry.

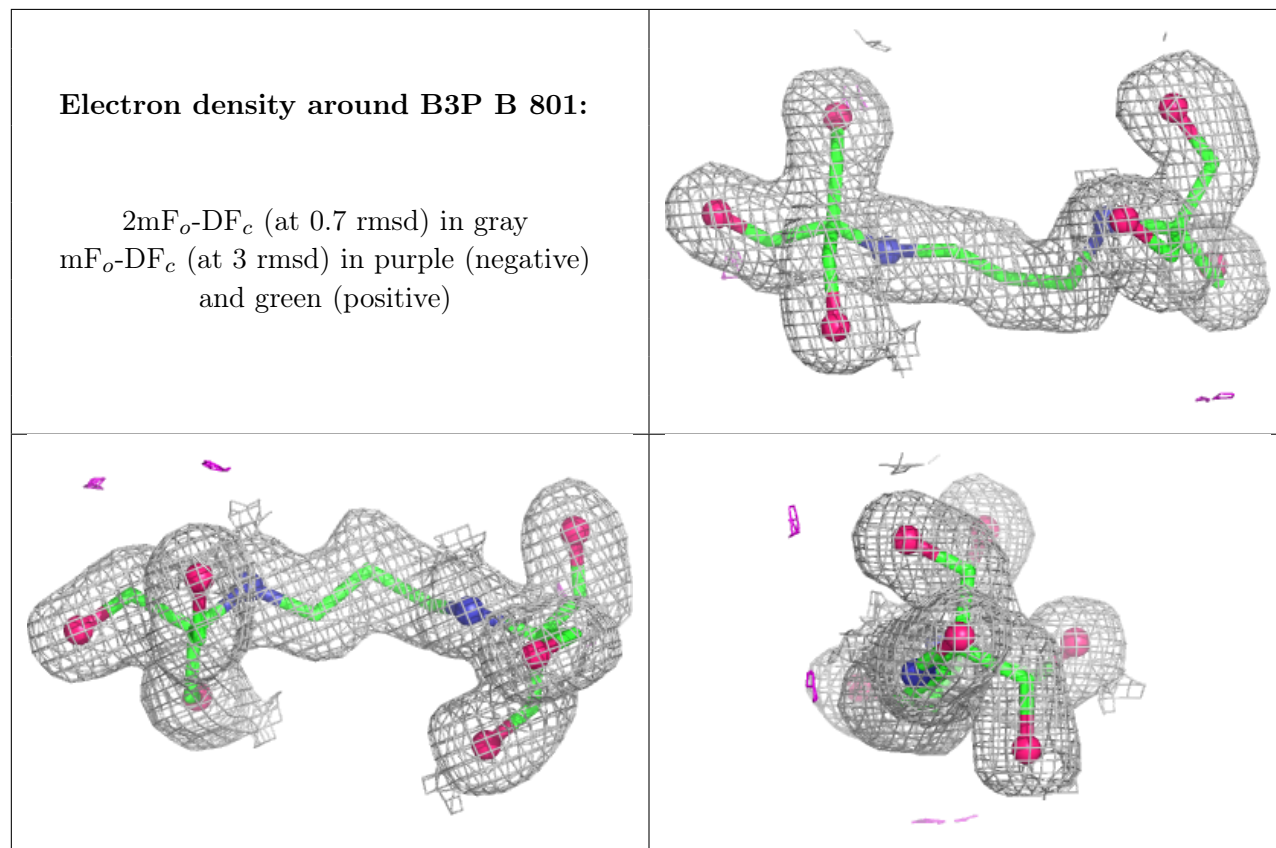
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	C	804	7/7	0.76	0.17	41,47,51,54	0
4	PEG	B	807[B]	7/7	0.79	0.17	15,25,31,32	7
4	PEG	B	807[A]	7/7	0.79	0.17	35,40,47,49	7
2	GOL	A	810	6/6	0.81	0.15	33,45,52,54	0
4	PEG	C	801	7/7	0.83	0.15	31,38,44,50	0
4	PEG	B	809	7/7	0.84	0.13	38,40,45,49	0
3	SCN	B	808	3/3	0.84	0.12	38,38,44,63	0
4	PEG	A	812	7/7	0.84	0.14	38,39,52,53	0
3	SCN	C	803	3/3	0.86	0.13	37,37,39,55	0
2	GOL	A	805	6/6	0.87	0.12	26,42,46,47	0
2	GOL	A	801	6/6	0.87	0.12	28,43,48,60	0
4	PEG	A	806	7/7	0.87	0.14	28,37,47,51	0
4	PEG	C	805	7/7	0.87	0.13	22,36,56,57	0
2	GOL	B	804	6/6	0.88	0.12	29,44,49,53	0
4	PEG	B	810	7/7	0.89	0.11	24,26,32,35	0
2	GOL	B	802	6/6	0.89	0.11	19,28,31,35	0
2	GOL	B	811	6/6	0.89	0.10	29,39,42,47	0
2	GOL	B	803	6/6	0.89	0.12	29,36,36,47	0
4	PEG	A	808	5/7	0.90	0.11	34,35,37,38	0
2	GOL	A	811	6/6	0.90	0.10	30,39,42,43	0
2	GOL	B	805	6/6	0.90	0.12	30,47,51,64	0
4	PEG	C	802	7/7	0.92	0.09	31,33,38,41	0
4	PEG	A	807	7/7	0.92	0.08	23,25,28,31	0
3	SCN	A	803	3/3	0.92	0.17	28,28,37,39	0
3	SCN	A	804	3/3	0.94	0.12	24,24,26,29	0
3	SCN	B	806	3/3	0.94	0.10	18,18,21,27	0
3	SCN	C	806	3/3	0.94	0.15	36,36,39,41	0
3	SCN	A	809	3/3	0.97	0.13	25,25,27,30	0
5	B3P	B	801	19/19	0.97	0.05	11,14,16,18	0
3	SCN	A	802	3/3	0.98	0.09	24,24,29,33	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.