



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 04:16 PM EDT

PDB ID : 9Q6I / pdb_00009q6i
Title : Human prolyl endopeptidase (PREP) - complex with JP-6-1-7
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-22
Resolution : 1.73 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

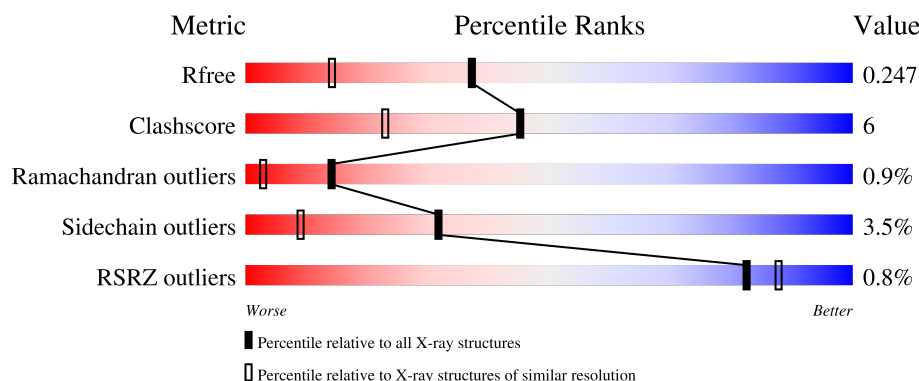
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	<div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	B	711	<div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	C	711	<div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div>

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
3	GOL	B	802	-	-	X	-

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.

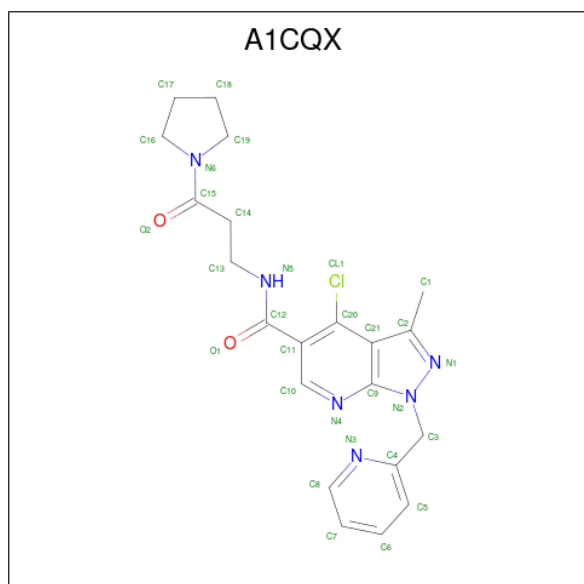
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	707	Total 11208	C 3646	H 5524	N 941	O 1070	S 27	177	2	0
1	B	707	Total 11187	C 3639	H 5514	N 941	O 1066	S 27	177	0	0
1	C	707	Total 11224	C 3650	H 5539	N 941	O 1066	S 28	178	3	0

There are 3 discrepancies between the modelled and reference sequences:

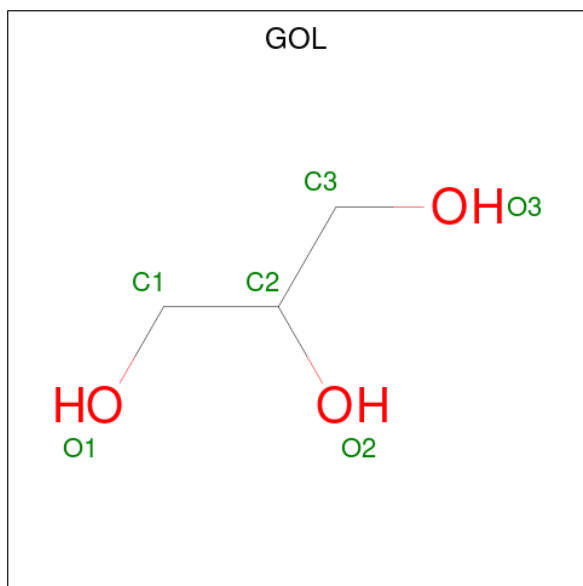
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147
C	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is 3-methyl-N-[3-oxo-3-(pyrrolidin-1-yl)propyl]-1-[(pyridin-2-yl)methyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQX) (formula: $C_{21}H_{23}ClN_6O_2$) (labeled as "Ligand of Interest" by depositor).



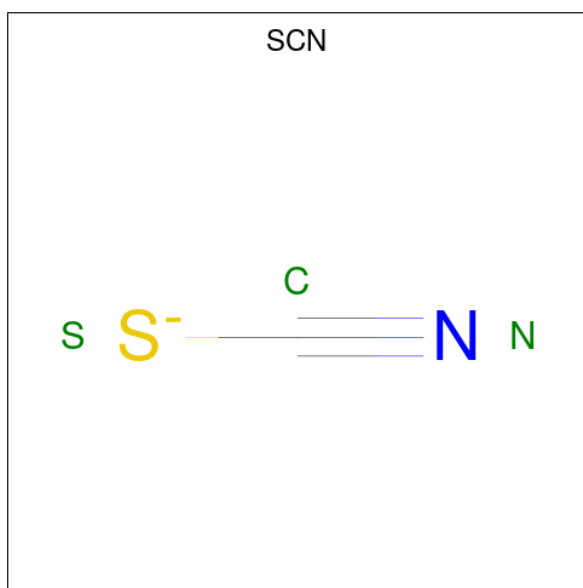
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	3	0
			52	21	23	6	2		
2	B	1	Total	C	H	N	O	3	0
			52	21	23	6	2		
2	C	1	Total	C	H	N	O	3	0
			52	21	23	6	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



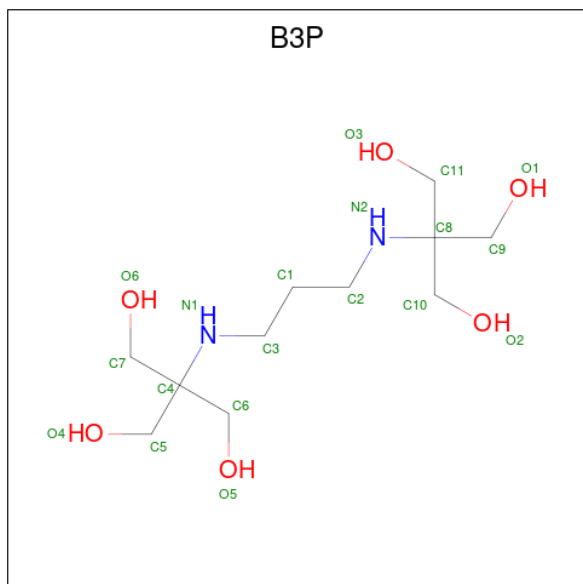
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	C	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 4 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



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

- 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	C	1	Total	C	H	N	O	8	0
			45	11	26	2	6		

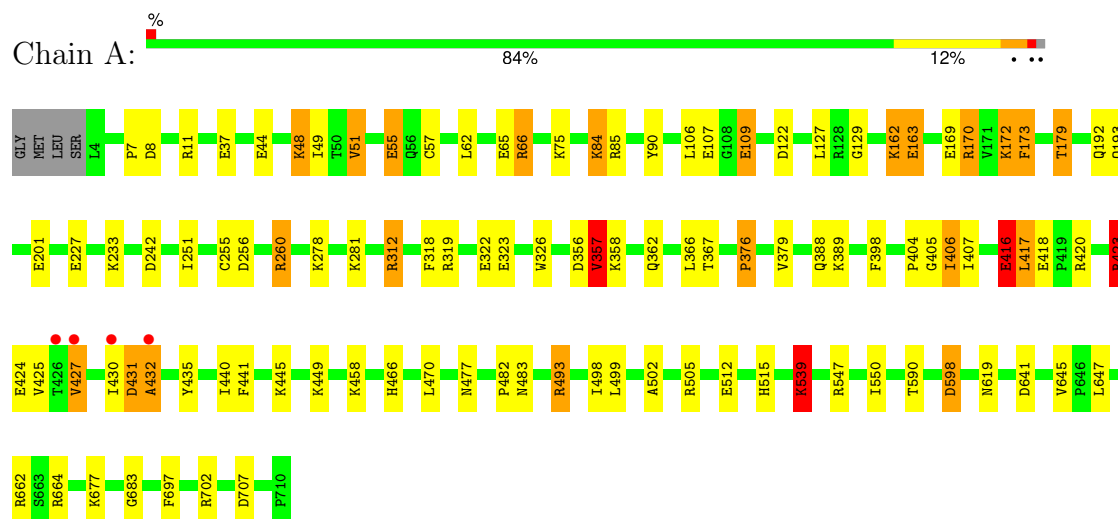
- Molecule 6 is water.

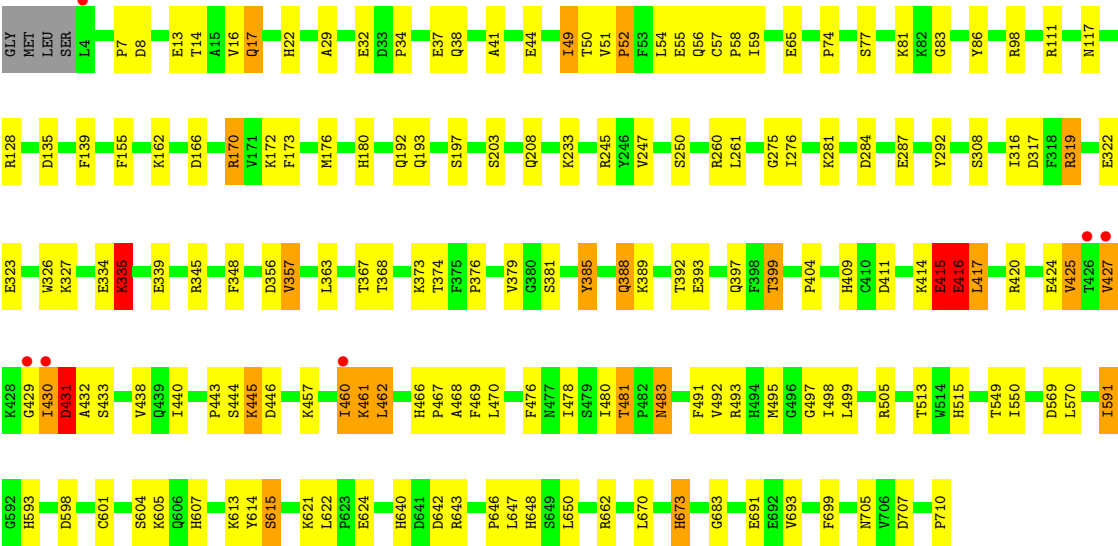
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	564	Total	O	0	1
			565	565		
6	B	360	Total	O	0	1
			361	361		
6	C	395	Total	O	0	1
			396	396		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.35Å 66.88Å 157.49Å 90.00° 99.34° 90.00°	Depositor
Resolution (Å)	43.90 – 1.73 43.90 – 1.73	Depositor EDS
% Data completeness (in resolution range)	65.5 (43.90-1.73) 65.5 (43.90-1.73)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.180 , 0.247 0.181 , 0.247	Depositor DCC
R_{free} test set	11284 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	35307	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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: GOL, SCN, A1CQX, 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	1.10	6/5842 (0.1%)	1.59	59/7920 (0.7%)
1	B	1.02	9/5825 (0.2%)	1.63	62/7897 (0.8%)
1	C	1.05	9/5846 (0.2%)	1.60	70/7926 (0.9%)
All	All	1.06	24/17513 (0.1%)	1.61	191/23743 (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	5
1	B	0	7
1	C	0	7
All	All	0	19

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CD-OE1	6.82	1.38	1.25
1	C	250	SER	CA-CB	-6.72	1.44	1.53
1	B	648	HIS	ND1-CE1	6.42	1.39	1.32
1	B	648	HIS	CG-CD2	6.21	1.42	1.35
1	C	22	HIS	CG-CD2	6.11	1.42	1.35
1	C	29	ALA	C-O	-6.08	1.16	1.24
1	A	172	LYS	CD-CE	-6.02	1.34	1.52
1	A	51	VAL	CA-CB	6.01	1.57	1.54
1	B	618	HIS	CE1-NE2	5.92	1.38	1.32
1	C	203	SER	CA-CB	-5.86	1.44	1.53
1	B	260	ARG	NE-CZ	-5.60	1.26	1.33
1	B	174	SER	CA-CB	-5.53	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	515	HIS	CE1-NE2	5.39	1.38	1.32
1	C	197	SER	C-O	-5.36	1.17	1.23
1	C	77	SER	CA-CB	-5.33	1.45	1.53
1	C	515	HIS	CG-CD2	5.30	1.41	1.35
1	B	593	HIS	CG-CD2	-5.22	1.30	1.35
1	A	482	PRO	CA-CB	-5.13	1.47	1.53
1	C	176	MET	C-O	-5.12	1.17	1.24
1	C	640	HIS	ND1-CE1	5.10	1.37	1.32
1	B	505	ARG	CZ-NH2	5.05	1.40	1.33
1	B	167	VAL	C-O	-5.04	1.19	1.24
1	A	163	GLU	C-O	-5.02	1.18	1.23
1	A	515	HIS	CE1-NE2	-5.00	1.27	1.32

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	165	PRO	CB-CA-C	-11.22	95.73	112.11
1	B	335	LYS	CB-CA-C	10.87	126.08	109.13
1	B	335	LYS	N-CA-CB	-10.18	97.45	111.00
1	C	322	GLU	CB-CG-CD	10.13	129.82	112.60
1	A	418	GLU	CB-CA-C	9.76	124.47	111.01
1	C	339	GLU	CB-CA-C	-9.17	93.92	110.70
1	A	389	LYS	CG-CD-CE	8.87	131.69	111.30
1	A	66	ARG	CG-CD-NE	-8.75	92.74	112.00
1	C	8	ASP	CB-CA-C	-8.74	94.70	109.65
1	C	52	PRO	CB-CA-C	-8.65	98.72	112.21
1	B	65	GLU	CB-CG-CD	8.57	127.17	112.60
1	A	423	ARG	CB-CA-C	-8.51	90.67	109.56
1	B	265	ASP	CA-CB-CG	8.38	120.98	112.60
1	A	66	ARG	NE-CZ-NH1	-8.29	113.21	121.50
1	C	388	GLN	N-CA-CB	-8.29	98.00	110.60
1	C	480	ILE	N-CA-CB	-8.16	104.14	112.06
1	B	334	GLU	N-CA-CB	8.05	122.08	110.16
1	B	414	LYS	N-CA-CB	7.95	122.07	110.06
1	B	66	ARG	N-CA-CB	-7.90	98.47	110.16
1	C	549	THR	CA-CB-OG1	7.88	121.43	109.60
1	A	322	GLU	CG-CD-OE2	-7.87	100.30	118.40
1	A	423	ARG	N-CA-CB	7.86	126.15	111.53
1	C	513	THR	OG1-CB-CG2	-7.84	93.61	109.30
1	A	62	LEU	N-CA-CB	-7.84	98.59	110.12
1	C	8	ASP	N-CA-CB	7.83	121.48	109.97
1	B	603	ASP	CA-CB-CG	7.78	120.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	GLU	CB-CA-C	-7.76	97.76	110.79
1	C	499	LEU	N-CA-CB	-7.70	98.44	110.06
1	C	247	VAL	N-CA-CB	7.53	120.02	111.21
1	C	416	GLU	N-CA-CB	-7.47	97.86	110.49
1	A	8	ASP	CB-CA-C	-7.45	97.98	109.89
1	C	505	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	C	481	THR	OG1-CB-CG2	-7.35	94.60	109.30
1	C	139	PHE	N-CA-CB	-7.33	98.11	110.80
1	C	705	ASN	CA-CB-CG	-7.21	105.39	112.60
1	A	65	GLU	CB-CG-CD	7.17	124.79	112.60
1	B	172	LYS	N-CA-CB	-7.12	98.25	111.13
1	B	705	ASN	CA-CB-CG	-6.97	105.63	112.60
1	C	691	GLU	CG-CD-OE2	-6.92	102.48	118.40
1	A	445	LYS	CB-CA-C	-6.90	98.95	110.68
1	A	109	GLU	CB-CG-CD	6.86	124.25	112.60
1	C	56	GLN	CB-CA-C	-6.84	96.34	109.95
1	C	14	THR	CA-CB-OG1	-6.80	99.39	109.60
1	B	512	GLU	CB-CA-C	6.78	123.16	110.63
1	B	414	LYS	CB-CA-C	-6.73	98.15	109.53
1	A	502	ALA	CA-C-O	6.71	127.54	120.36
1	C	327	LYS	CB-CA-C	-6.69	98.25	109.48
1	A	431	ASP	CA-C-N	-6.68	116.37	126.86
1	A	431	ASP	C-N-CA	-6.68	116.37	126.86
1	A	417	LEU	N-CA-CB	6.67	121.77	110.49
1	A	664	ARG	CA-CB-CG	-6.62	100.86	114.10
1	C	691	GLU	CG-CD-OE1	6.58	133.53	118.40
1	B	705	ASN	CB-CA-C	-6.54	97.42	110.42
1	C	591	ILE	N-CA-CB	-6.47	104.81	112.39
1	C	135	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	707	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	697	PHE	CA-CB-CG	-6.42	107.39	113.80
1	A	48	LYS	CA-CB-CG	-6.41	101.28	114.10
1	A	598	ASP	CA-CB-CG	6.38	118.97	112.60
1	B	461	LYS	CB-CA-C	-6.37	98.62	109.51
1	C	155	PHE	CA-CB-CG	6.36	120.16	113.80
1	A	483	ASN	CA-CB-CG	-6.34	106.25	112.60
1	C	260	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	B	336	ASP	CB-CA-C	6.26	120.06	109.80
1	C	385	TYR	CA-C-O	-6.26	113.74	120.75
1	B	391	ASP	CA-C-O	-6.25	114.75	121.94
1	B	481	THR	OG1-CB-CG2	-6.25	96.81	109.30
1	C	399	THR	CA-CB-OG1	-6.22	100.27	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	66	ARG	CA-CB-CG	-6.21	101.68	114.10
1	C	155	PHE	N-CA-CB	-6.17	101.62	111.43
1	B	505	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	C	476	PHE	CA-CB-CG	-6.13	107.67	113.80
1	C	505	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	C	335	LYS	N-CA-CB	-6.10	100.17	110.49
1	B	311	TYR	N-CA-CB	6.10	120.80	110.49
1	A	169	GLU	N-CA-CB	-6.08	101.92	111.05
1	B	69	GLU	N-CA-CB	-6.08	101.25	110.07
1	A	179	THR	CA-CB-OG1	6.00	118.59	109.60
1	B	608	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	367	THR	OG1-CB-CG2	-5.99	97.32	109.30
1	B	44	GLU	CB-CA-C	-5.97	101.51	110.88
1	C	424	GLU	CA-C-N	-5.97	114.91	122.37
1	C	424	GLU	C-N-CA	-5.97	114.91	122.37
1	C	469	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	362	GLN	CG-CD-NE2	-5.96	107.46	116.40
1	B	416	GLU	CB-CA-C	-5.96	98.55	110.42
1	B	50	THR	OG1-CB-CG2	5.96	121.22	109.30
1	B	247	VAL	N-CA-CB	5.96	117.80	111.00
1	A	170	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	B	202	THR	OG1-CB-CG2	5.89	121.08	109.30
1	B	456	HIS	CA-CB-CG	5.89	119.69	113.80
1	B	281	LYS	N-CA-CB	5.87	117.10	110.35
1	C	287	GLU	N-CA-CB	5.86	119.67	110.46
1	A	515	HIS	CA-CB-CG	5.84	119.64	113.80
1	A	416	GLU	CB-CA-C	-5.83	101.68	110.90
1	A	11	ARG	CD-NE-CZ	5.82	132.54	124.40
1	C	379	VAL	N-CA-CB	-5.81	105.25	111.46
1	C	284	ASP	CA-CB-CG	-5.78	106.82	112.60
1	C	368	THR	CA-CB-OG1	-5.75	100.97	109.60
1	C	374	THR	CA-CB-OG1	-5.74	101.00	109.60
1	B	306	ARG	CB-CA-C	5.72	118.40	110.16
1	B	598	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	170	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	A	66	ARG	N-CA-CB	-5.66	101.81	110.01
1	C	376	PRO	O-C-N	5.65	130.00	123.06
1	B	155	PHE	N-CA-CB	-5.65	101.09	111.37
1	A	641	ASP	N-CA-CB	5.64	118.47	110.46
1	B	128	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	B	413	THR	CA-CB-OG1	-5.63	101.15	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	643	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	C	281	LYS	CB-CA-C	5.62	120.56	112.12
1	C	208	GLN	CB-CA-C	-5.62	100.39	109.72
1	B	348	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	281	LYS	N-CA-CB	-5.61	104.07	110.35
1	A	66	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	C	44	GLU	N-CA-CB	-5.59	101.97	110.07
1	A	55	GLU	CB-CA-C	-5.59	101.52	110.79
1	B	339	GLU	N-CA-CB	5.55	118.34	110.13
1	A	398	PHE	N-CA-CB	-5.54	101.98	110.85
1	A	260	ARG	CG-CD-NE	-5.53	99.83	112.00
1	B	267	GLN	CB-CA-C	-5.52	101.26	110.81
1	C	8	ASP	N-CA-C	-5.52	102.11	110.28
1	A	539	LYS	CB-CA-C	5.52	120.84	110.63
1	C	367	THR	CA-CB-OG1	-5.52	101.33	109.60
1	C	335	LYS	CB-CA-C	5.50	121.36	110.42
1	A	170	ARG	CD-NE-CZ	5.49	132.09	124.40
1	C	117	ASN	CA-CB-CG	-5.48	107.12	112.60
1	B	128	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	B	437	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	658	TYR	N-CA-CB	5.47	118.00	110.07
1	C	260	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	162	LYS	CB-CA-C	5.46	118.76	109.80
1	A	201	GLU	CB-CG-CD	5.43	121.82	112.60
1	A	256	ASP	CA-C-O	5.41	125.27	120.02
1	A	499	LEU	CB-CA-C	5.39	118.64	109.75
1	B	540	GLU	CB-CA-C	5.38	119.70	110.01
1	C	673	HIS	CB-CA-C	5.38	119.07	109.65
1	B	426	THR	CA-CB-OG1	-5.38	101.54	109.60
1	B	507	GLY	O-C-N	-5.37	118.19	122.81
1	A	318	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	312	ARG	CB-CG-CD	-5.36	98.97	111.30
1	A	66	ARG	CD-NE-CZ	5.34	131.88	124.40
1	A	458	LYS	CB-CA-C	-5.33	99.73	109.54
1	B	318	PHE	N-CA-CB	-5.33	102.07	110.06
1	C	615	SER	CA-C-N	5.32	124.78	119.24
1	C	615	SER	C-N-CA	5.32	124.78	119.24
1	B	385	TYR	CA-C-O	-5.31	115.05	120.89
1	C	37	GLU	CB-CG-CD	-5.31	103.58	112.60
1	B	176	MET	CG-SD-CE	-5.30	89.23	100.90
1	C	461	LYS	CB-CA-C	-5.30	100.79	109.53
1	A	173	PHE	N-CA-CB	-5.26	103.71	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLU	CG-CD-OE1	5.25	130.49	118.40
1	A	107	GLU	CB-CA-C	-5.25	100.64	110.36
1	B	453	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	492	VAL	N-CA-CB	5.25	117.29	110.57
1	C	642	ASP	CA-CB-CG	5.25	117.84	112.60
1	B	530	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	621	LYS	CB-CA-C	5.24	120.84	110.42
1	B	81	LYS	CB-CA-C	5.23	118.78	109.72
1	C	128	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	441	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	619	ASN	CA-CB-CG	-5.23	107.37	112.60
1	B	119	LEU	N-CA-C	-5.21	106.70	113.16
1	C	693	VAL	N-CA-CB	5.17	117.57	110.54
1	C	446	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	449	LYS	CG-CD-CE	5.16	123.17	111.30
1	C	49	ILE	N-CA-C	-5.15	106.66	111.45
1	A	109	GLU	CG-CD-OE1	5.14	130.23	118.40
1	C	322	GLU	CB-CA-C	-5.14	101.42	109.70
1	A	502	ALA	O-C-N	-5.14	117.36	123.22
1	B	231	GLU	CG-CD-OE2	-5.12	106.61	118.40
1	C	483	ASN	CA-CB-CG	-5.12	107.48	112.60
1	C	415	GLU	N-CA-CB	5.12	117.49	110.07
1	B	441	PHE	CA-CB-CG	-5.11	108.69	113.80
1	C	98	ARG	CB-CA-C	5.11	120.22	109.65
1	A	127	LEU	N-CA-CB	-5.10	102.25	109.85
1	C	670	LEU	N-CA-CB	-5.08	102.59	110.87
1	C	287	GLU	N-CA-C	-5.08	107.09	113.28
1	A	493	ARG	CA-CB-CG	5.06	124.22	114.10
1	B	164	LEU	N-CA-CB	-5.06	103.78	109.49
1	B	580	VAL	CB-CA-C	-5.06	106.44	111.80
1	C	180	HIS	CB-CA-C	5.05	120.56	109.99
1	B	89	PHE	N-CA-CB	5.05	118.81	110.69
1	A	505	ARG	CD-NE-CZ	5.04	131.46	124.40
1	C	56	GLN	N-CA-CB	5.04	118.88	110.41
1	B	170	ARG	CD-NE-CZ	5.04	131.45	124.40
1	B	543	THR	CA-CB-OG1	5.03	117.15	109.60
1	A	376	PRO	CB-CA-C	5.02	117.93	110.85
1	C	613	LYS	CB-CG-CD	-5.02	99.75	111.30
1	B	623	PRO	CB-CA-C	5.02	117.55	110.98

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain
1	A	312	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	432	ALA	Peptide
1	B	170	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	345	ARG	Sidechain
1	B	416	GLU	Peptide
1	B	488	ARG	Sidechain
1	B	643	ARG	Sidechain
1	B	664	ARG	Sidechain
1	C	111	ARG	Sidechain
1	C	245	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	415	GLU	Peptide
1	C	420	ARG	Sidechain
1	C	431	ASP	Peptide
1	C	643	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	5684	5524	5501	54	0
1	B	5673	5514	5490	76	0
1	C	5685	5539	5515	69	0
2	A	29	23	0	1	0
2	B	29	23	0	0	0
2	C	29	23	0	0	0
3	A	24	32	32	2	0
3	B	24	32	32	7	0
3	C	6	8	8	0	0
4	A	18	0	0	2	0
4	B	9	0	0	0	0
4	C	12	0	0	2	0
5	C	19	26	26	0	0
6	A	565	0	0	19	0
6	B	361	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	396	0	0	12	0
All	All	18563	16744	16604	201	0

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 6.

All (201) 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:A:255:CYS:SG	2:A:801:A1CQX:C20	2.07	1.42
1:C:416:GLU:O	1:C:417:LEU:O	1.79	0.99
1:C:17:GLN:HB2	4:C:807:SCN:S	2.08	0.94
1:C:493:ARG:NH2	1:C:710:PRO:O	1.99	0.94
1:B:431:ASP:OD2	1:B:433:SER:OG	1.94	0.85
1:A:432:ALA:HA	1:A:435:TYR:HD2	1.43	0.82
3:B:804:GOL:H31	6:B:1184:HOH:O	1.81	0.80
1:B:76:TYR:CD1	1:B:423:ARG:HD3	2.16	0.80
1:C:569:ASP:OD1	6:C:901:HOH:O	2.00	0.79
1:B:291:ASP:OD1	6:B:901:HOH:O	2.00	0.78
1:C:192:GLN:HE21	1:C:193:GLN:H	1.30	0.77
1:A:424:GLU:O	6:A:901:HOH:O	2.02	0.77
1:A:547:ARG:HD3	6:A:1101:HOH:O	1.85	0.76
1:B:229:PRO:HD2	3:B:802:GOL:O3	1.85	0.76
1:B:245:ARG:HD2	1:B:267:GLN:NE2	2.00	0.75
1:B:56:GLN:OE1	6:B:902:HOH:O	2.02	0.75
3:A:803:GOL:H2	6:A:1361:HOH:O	1.85	0.75
1:C:38:GLN:HG2	6:C:1267:HOH:O	1.87	0.72
1:A:431:ASP:O	1:A:432:ALA:HB3	1.90	0.71
1:C:416:GLU:C	1:C:417:LEU:O	2.35	0.70
1:A:432:ALA:HA	1:A:435:TYR:CD2	2.24	0.69
1:A:416:GLU:HA	1:A:416:GLU:OE1	1.92	0.69
1:A:423:ARG:HH21	1:A:423:ARG:HG3	1.57	0.69
1:C:335:LYS:HE2	6:C:1181:HOH:O	1.93	0.69
1:A:493:ARG:O	6:A:903:HOH:O	2.13	0.66
1:A:512:GLU:OE1	6:A:902:HOH:O	2.13	0.66
1:B:57:CYS:HB3	6:B:1195:HOH:O	1.95	0.65
1:C:388:GLN:O	1:C:389:LYS:C	2.37	0.65
1:C:492:VAL:HG13	1:C:497:GLY:O	1.95	0.65
1:B:52:PRO:HB2	6:B:935:HOH:O	1.96	0.65
1:C:404:PRO:CD	1:C:427:VAL:HG22	2.27	0.65
1:C:233:LYS:HE2	1:C:593:HIS:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:OE2	1:B:37:GLU:HA	1.95	0.65
1:A:404:PRO:HB2	1:A:425:VAL:HG23	1.79	0.64
1:B:462:LEU:HA	1:B:541:GLY:O	1.98	0.64
1:B:623:PRO:O	1:B:665:LYS:NZ	2.29	0.63
1:B:431:ASP:O	1:B:432:ALA:CB	2.46	0.63
1:B:488:ARG:HD3	1:B:499:LEU:HD13	1.81	0.62
1:A:404:PRO:HB2	1:A:425:VAL:CG2	2.29	0.62
1:B:54:LEU:HA	1:B:57:CYS:SG	2.40	0.62
1:C:292:TYR:O	6:C:902:HOH:O	2.16	0.62
1:A:466:HIS:HB2	1:A:498:ILE:HD12	1.82	0.61
1:A:242:ASP:OD2	6:A:904:HOH:O	2.16	0.61
1:A:367:THR:O	6:A:905:HOH:O	2.16	0.61
1:A:440:ILE:C	1:A:440:ILE:HD12	2.27	0.60
1:B:51:VAL:HB	1:B:52:PRO:HD3	1.83	0.59
1:B:495:MET:HE3	1:B:701:ALA:HB2	1.85	0.59
1:B:416:GLU:HA	1:B:416:GLU:OE1	2.03	0.59
1:A:129:GLY:N	4:A:809:SCN:N	2.43	0.58
1:C:397:GLN:NE2	6:C:909:HOH:O	2.36	0.58
1:A:84:LYS:HG3	6:A:1402:HOH:O	2.03	0.57
1:B:229:PRO:HD2	3:B:802:GOL:HO3	1.70	0.57
1:C:348:PHE:CD2	1:C:363:LEU:HD21	2.40	0.57
1:C:683:GLY:HA2	6:C:1198:HOH:O	2.04	0.57
1:C:467:PRO:O	1:C:497:GLY:HA2	2.04	0.56
1:C:81:LYS:HE2	1:C:83:GLY:O	2.05	0.56
1:A:423:ARG:HH21	1:A:423:ARG:CG	2.18	0.56
1:B:230:ASP:HB2	3:B:802:GOL:H31	1.87	0.56
1:A:539:LYS:HE2	6:A:1165:HOH:O	2.06	0.56
1:C:440:ILE:C	1:C:440:ILE:HD12	2.31	0.56
1:B:166:ASP:O	6:B:904:HOH:O	2.18	0.55
1:B:269:GLU:OE2	1:B:278:LYS:HB2	2.06	0.55
1:A:122:ASP:OD2	1:A:677:LYS:NZ	2.33	0.55
1:A:547:ARG:CD	6:A:1101:HOH:O	2.47	0.55
1:B:247:VAL:O	1:B:263:TYR:HA	2.07	0.55
1:A:407:ILE:HD12	1:A:423:ARG:HD3	1.88	0.55
1:C:54:LEU:HA	1:C:57:CYS:SG	2.46	0.55
1:A:7:PRO:HD3	1:A:49:ILE:CD1	2.37	0.54
1:B:393:GLU:OE1	1:B:409:HIS:NE2	2.33	0.54
1:B:647:LEU:C	1:B:647:LEU:HD12	2.32	0.54
1:A:44:GLU:OE2	1:A:48:LYS:NZ	2.37	0.54
1:B:207:HIS:CE1	1:B:232:PRO:HG3	2.43	0.54
1:B:66:ARG:NH2	1:B:69:GLU:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLU:OE1	1:B:416:GLU:CA	2.53	0.53
1:B:473:TYR:CZ	1:B:555:ASN:HB3	2.43	0.53
1:A:192:GLN:HE21	1:A:193:GLN:H	1.54	0.53
1:C:466:HIS:HB2	1:C:498:ILE:HD12	1.90	0.53
1:B:50:THR:HG21	1:B:673:HIS:HB2	1.90	0.53
1:A:683:GLY:HA2	6:A:1166:HOH:O	2.09	0.53
1:A:431:ASP:O	1:A:432:ALA:CB	2.55	0.52
1:B:522:ASN:HB3	1:B:525:ASN:ND2	2.25	0.52
1:B:51:VAL:O	1:B:52:PRO:C	2.52	0.52
1:A:227:GLU:O	3:A:803:GOL:H12	2.10	0.51
1:C:173:PHE:CE2	1:C:591:ILE:HG12	2.45	0.51
1:C:373:LYS:HE3	1:C:417:LEU:HB2	1.91	0.51
1:C:444:SER:O	1:C:445:LYS:C	2.52	0.51
1:A:539:LYS:CE	6:A:1165:HOH:O	2.58	0.51
1:B:128:ARG:HB2	6:B:1121:HOH:O	2.11	0.50
1:C:345:ARG:HG3	1:C:392:THR:HA	1.92	0.50
1:A:388:GLN:HA	6:A:1194:HOH:O	2.12	0.49
1:C:7:PRO:HD3	1:C:49:ILE:HD11	1.94	0.49
1:C:261:LEU:C	1:C:261:LEU:HD13	2.37	0.49
1:C:356:ASP:C	1:C:357:VAL:HG23	2.38	0.49
1:B:607:HIS:CD2	1:B:610:TRP:CH2	3.01	0.49
1:B:404:PRO:HB2	1:B:425:VAL:HG11	1.94	0.49
1:C:491:PHE:O	1:C:495:MET:HB2	2.12	0.49
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.95	0.48
1:A:405:GLY:O	1:A:425:VAL:HG22	2.13	0.48
1:C:393:GLU:OE1	1:C:409:HIS:NE2	2.41	0.48
1:A:406:ILE:HG23	1:A:424:GLU:HB2	1.94	0.48
1:C:13:GLU:HA	1:C:13:GLU:OE1	2.13	0.48
1:B:265:ASP:OD1	1:B:267:GLN:HG3	2.13	0.48
1:A:477:ASN:ND2	6:A:902:HOH:O	2.47	0.48
1:B:172:LYS:NZ	1:B:205:ASN:HD21	2.11	0.48
1:C:170:ARG:HD3	6:C:1241:HOH:O	2.12	0.47
1:B:445:LYS:HB2	1:B:445:LYS:HE3	1.34	0.47
1:C:457:LYS:O	1:C:460:ILE:HG12	2.15	0.47
1:B:184:GLY:HA3	1:B:212:TYR:CZ	2.50	0.47
1:C:317:ASP:OD2	1:C:319:ARG:NH1	2.48	0.47
1:B:229:PRO:CD	3:B:802:GOL:O3	2.59	0.46
1:B:60:ARG:HG2	1:B:60:ARG:HH11	1.80	0.46
1:B:323:GLU:HA	1:B:326:TRP:CE2	2.51	0.46
1:C:32:GLU:O	1:C:34:PRO:HD3	2.16	0.46
1:B:622:LEU:HD11	1:B:663:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LEU:O	1:B:705:ASN:C	2.57	0.46
1:B:431:ASP:O	1:B:432:ALA:HB2	2.16	0.46
1:B:233:LYS:HE2	6:B:1039:HOH:O	2.14	0.45
1:C:662:ARG:NH1	6:C:946:HOH:O	2.49	0.45
1:B:347:ASN:N	1:B:347:ASN:OD1	2.48	0.45
1:B:260:ARG:HD3	1:B:284:ASP:OD1	2.15	0.45
1:B:404:PRO:HB2	1:B:425:VAL:CG1	2.47	0.45
1:C:570:LEU:HD23	1:C:570:LEU:HA	1.75	0.45
1:B:275:GLY:O	1:B:276:ILE:C	2.58	0.45
1:B:625:ALA:HB3	1:B:628:ILE:CG1	2.46	0.45
1:A:51:VAL:O	1:A:55:GLU:HG3	2.17	0.45
1:C:162:LYS:HB3	1:C:162:LYS:HE2	1.78	0.45
1:C:468:ALA:HA	1:C:498:ILE:O	2.16	0.45
1:C:348:PHE:CE2	1:C:363:LEU:HD21	2.52	0.45
1:C:399:THR:HG23	1:C:483:ASN:HA	1.99	0.44
1:B:166:ASP:HA	6:B:1156:HOH:O	2.17	0.44
1:B:158:VAL:O	1:B:159:ASP:C	2.59	0.44
1:B:462:LEU:CA	1:B:541:GLY:O	2.64	0.44
1:A:7:PRO:HD3	1:A:49:ILE:HD11	2.00	0.44
1:B:114:LEU:HD21	1:B:141:TYR:CD2	2.53	0.44
1:B:512:GLU:HG3	1:B:516:LYS:HD2	2.00	0.44
1:C:74:PRO:O	1:C:425:VAL:HG11	2.18	0.44
1:B:536:TYR:OH	6:B:903:HOH:O	2.06	0.43
1:A:233:LYS:NZ	6:A:949:HOH:O	2.50	0.43
1:A:645:VAL:HG23	1:A:647:LEU:HG	2.00	0.43
1:A:379:VAL:HG23	6:A:1323:HOH:O	2.18	0.43
1:B:300:PHE:HB3	1:B:302:PHE:CE1	2.54	0.43
1:C:647:LEU:HD12	1:C:648:HIS:N	2.33	0.43
1:C:275:GLY:O	1:C:276:ILE:C	2.60	0.43
1:C:50:THR:HG21	1:C:673:HIS:HB2	2.01	0.43
1:C:162:LYS:NZ	6:C:952:HOH:O	2.51	0.43
1:C:172:LYS:HD3	1:C:173:PHE:CE2	2.53	0.43
1:B:158:VAL:O	1:B:160:GLY:N	2.52	0.43
1:C:462:LEU:HD23	1:C:462:LEU:N	2.34	0.43
1:C:614:TYR:O	1:C:615:SER:C	2.62	0.43
1:A:85:ARG:NE	6:A:910:HOH:O	2.41	0.42
1:C:411:ASP:OD2	1:C:414:LYS:HE2	2.18	0.42
1:A:470:LEU:HB3	1:A:550:ILE:HG22	2.01	0.42
1:C:81:LYS:HD2	1:C:86:TYR:CZ	2.54	0.42
1:C:605:LYS:HB2	1:C:605:LYS:HE2	1.77	0.42
1:A:57:CYS:HA	1:A:702:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:O	4:A:805:SCN:S	2.78	0.42
1:C:58:PRO:HD2	6:C:1216:HOH:O	2.19	0.42
1:C:646:PRO:O	1:C:650:LEU:HG	2.20	0.42
1:B:428:LYS:O	1:B:429:GLY:C	2.62	0.42
1:C:385:TYR:CD2	1:C:385:TYR:C	2.96	0.42
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.97	0.42
1:A:662:ARG:NH2	6:A:950:HOH:O	2.50	0.42
1:B:106:LEU:HD23	1:B:106:LEU:HA	1.80	0.42
1:A:677:LYS:HE2	1:A:677:LYS:HB3	1.85	0.41
1:B:434:ASP:HB2	1:B:435:TYR:CE2	2.55	0.41
1:A:163:GLU:HG2	6:A:1048:HOH:O	2.19	0.41
1:B:226:ALA:HA	3:B:804:GOL:O2	2.20	0.41
1:B:405:GLY:C	1:B:406:ILE:HG13	2.45	0.41
1:A:323:GLU:HA	1:A:326:TRP:CE2	2.54	0.41
1:C:430:ILE:O	1:C:431:ASP:HB3	2.20	0.41
1:B:99:VAL:HG13	1:B:115:ASP:HA	2.02	0.41
1:B:631:PRO:O	1:B:633:MET:HG3	2.20	0.41
1:B:645:VAL:HG23	1:B:647:LEU:HG	2.02	0.41
1:C:316:ILE:HG12	1:C:326:TRP:CD1	2.55	0.41
1:C:323:GLU:HA	1:C:326:TRP:CE2	2.55	0.41
1:C:491:PHE:CE2	1:C:497:GLY:HA3	2.55	0.41
1:A:84:LYS:H	1:A:84:LYS:HG2	1.47	0.41
1:B:325:LYS:HA	1:B:325:LYS:HD3	1.89	0.41
1:C:41:ALA:HB1	4:C:806:SCN:S	2.60	0.41
1:B:536:TYR:CD1	1:B:536:TYR:C	2.98	0.41
1:B:622:LEU:HD11	1:B:663:SER:CB	2.51	0.41
1:A:75:LYS:O	1:A:90:TYR:HA	2.21	0.41
1:B:267:GLN:HA	3:B:801:GOL:O3	2.20	0.41
1:C:443:PRO:HB3	6:C:1203:HOH:O	2.20	0.41
1:C:601:CYS:O	1:C:607:HIS:HB2	2.20	0.41
1:A:431:ASP:OD1	1:A:431:ASP:C	2.60	0.41
1:B:231:GLU:HG3	1:B:234:TRP:CZ2	2.56	0.41
1:C:51:VAL:N	1:C:52:PRO:HD2	2.36	0.41
1:B:240:LEU:HD13	1:B:240:LEU:HA	1.92	0.40
1:B:283:ILE:HG21	1:B:290:TYR:CE2	2.56	0.40
1:B:406:ILE:HG12	1:B:424:GLU:HG3	2.03	0.40
1:B:440:ILE:HD12	1:B:440:ILE:C	2.46	0.40
1:C:404:PRO:HD3	1:C:427:VAL:HG22	2.00	0.40
1:C:381:SER:OG	1:C:481:THR:HB	2.22	0.40
1:C:470:LEU:HD23	1:C:550:ILE:HG22	2.04	0.40
1:A:172:LYS:HD3	1:A:173:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASP:C	1:A:357:VAL:HG23	2.45	0.40
1:B:653:ILE:O	1:B:657:GLN:HG3	2.21	0.40
1:C:52:PRO:HA	1:C:55:GLU:OE1	2.22	0.40
1:C:647:LEU:HD12	1:C:647:LEU:C	2.45	0.40
1:C:192:GLN:OE1	6:C:903:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	707/711 (99%)	678 (96%)	25 (4%)	4 (1%)	21	8
1	B	705/711 (99%)	658 (93%)	40 (6%)	7 (1%)	12	2
1	C	708/711 (100%)	665 (94%)	35 (5%)	8 (1%)	11	2
All	All	2120/2133 (99%)	2001 (94%)	100 (5%)	19 (1%)	14	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	VAL
1	C	416	GLU
1	C	417	LEU
1	C	432	ALA
1	B	429	GLY
1	B	430	ILE
1	B	432	ALA
1	C	429	GLY
1	C	431	ASP
1	A	590	THR
1	B	159	ASP
1	A	417	LEU

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Mol	Chain	Res	Type
1	B	357	VAL
1	B	423	ARG
1	B	554	SER
1	C	357	VAL
1	C	427	VAL
1	C	430	ILE
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	616/617 (100%)	599 (97%)	17 (3%)	38	15
1	B	614/617 (100%)	589 (96%)	25 (4%)	27	6
1	C	617/617 (100%)	593 (96%)	24 (4%)	28	7
All	All	1847/1851 (100%)	1781 (96%)	66 (4%)	32	9

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	66	ARG
1	A	84	LYS
1	A	109	GLU
1	A	162	LYS
1	A	179	THR
1	A	278	LYS
1	A	357	VAL
1	A	358	LYS
1	A	376	PRO
1	A	406	ILE
1	A	416	GLU
1	A	423	ARG
1	A	427	VAL
1	A	430	ILE

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Mol	Chain	Res	Type
1	A	539	LYS
1	A	598	ASP
1	B	23	LYS
1	B	37	GLU
1	B	44	GLU
1	B	48	LYS
1	B	59	ILE
1	B	66	ARG
1	B	106	LEU
1	B	111	ARG
1	B	162	LYS
1	B	169	GLU
1	B	170	ARG
1	B	230	ASP
1	B	267	GLN
1	B	287	GLU
1	B	335	LYS
1	B	418	GLU
1	B	426	THR
1	B	427	VAL
1	B	445	LYS
1	B	449	LYS
1	B	547	ARG
1	B	598	ASP
1	B	604	SER
1	B	605	LYS
1	B	664	ARG
1	C	16[A]	VAL
1	C	16[B]	VAL
1	C	17	GLN
1	C	59	ILE
1	C	65	GLU
1	C	166	ASP
1	C	308	SER
1	C	334	GLU
1	C	335	LYS
1	C	415	GLU
1	C	425	VAL
1	C	433	SER
1	C	438	VAL
1	C	445	LYS
1	C	460	ILE

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Mol	Chain	Res	Type
1	C	461	LYS
1	C	462	LEU
1	C	478[A]	ILE
1	C	478[B]	ILE
1	C	598	ASP
1	C	604	SER
1	C	622	LEU
1	C	624	GLU
1	C	707	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	103	GLN
1	A	192	GLN
1	A	193	GLN
1	A	205	ASN
1	A	477	ASN
1	B	38	GLN
1	B	56	GLN
1	B	103	GLN
1	B	193	GLN
1	B	205	ASN
1	B	362	GLN
1	B	397	GLN
1	B	525	ASN
1	B	607	HIS
1	C	17	GLN
1	C	192	GLN
1	C	205	ASN
1	C	388	GLN
1	C	397	GLN
1	C	503	ASN
1	C	577	GLN
1	C	607	HIS

5.3.3 RNA ⓘ

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](#)

26 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	GOL	A	803	-	5,5,5	0.69	0	5,5,5	0.72	0
4	SCN	B	807	-	1,2,2	0.33	0	0,1,1	-	-
5	B3P	C	802	-	18,18,18	0.89	0	23,23,23	1.19	1 (4%)
3	GOL	C	804	-	5,5,5	0.27	0	5,5,5	1.06	0
2	A1CQX	B	803	1	32,32,33	1.48	2 (6%)	42,44,46	1.87	6 (14%)
3	GOL	B	804	-	5,5,5	0.15	0	5,5,5	0.43	0
4	SCN	C	807	-	1,2,2	0.56	0	0,1,1	-	-
4	SCN	B	808	-	1,2,2	0.99	0	0,1,1	-	-
4	SCN	C	805	-	1,2,2	1.59	0	0,1,1	-	-
4	SCN	A	810	-	1,2,2	0.24	0	0,1,1	-	-
3	GOL	A	807	-	5,5,5	0.32	0	5,5,5	1.14	1 (20%)
4	SCN	A	809	-	1,2,2	1.90	0	0,1,1	-	-
4	SCN	C	806	-	1,2,2	0.16	0	0,1,1	-	-
4	SCN	A	805	-	1,2,2	1.09	0	0,1,1	-	-
4	SCN	C	803	-	1,2,2	3.22	1 (100%)	0,1,1	-	-
3	GOL	A	802	-	5,5,5	0.31	0	5,5,5	0.71	0
3	GOL	B	801	-	5,5,5	0.44	0	5,5,5	1.00	0
3	GOL	B	802	-	5,5,5	0.24	0	5,5,5	0.53	0
3	GOL	A	808	-	5,5,5	0.24	0	5,5,5	0.63	0
3	GOL	B	806	-	5,5,5	0.37	0	5,5,5	0.23	0
2	A1CQX	C	801	1	32,32,33	1.55	5 (15%)	42,44,46	1.91	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SCN	A	811	-	1,2,2	0.15	0	0,1,1	-	-
4	SCN	A	804	-	1,2,2	0.60	0	0,1,1	-	-
2	A1CQX	A	801	-	32,32,33	1.15	2 (6%)	42,44,46	2.18	11 (26%)
4	SCN	A	806	-	1,2,2	1.00	0	0,1,1	-	-
4	SCN	B	805	-	1,2,2	1.35	0	0,1,1	-	-

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	A1CQX	C	801	1	-	4/18/25/25	0/4/4/4
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	A	803	-	-	2/4/4/4	-
3	GOL	B	801	-	-	3/4/4/4	-
5	B3P	C	802	-	-	0/28/28/28	-
3	GOL	B	802	-	-	2/4/4/4	-
3	GOL	C	804	-	-	1/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
2	A1CQX	B	803	1	-	4/18/25/25	0/4/4/4
3	GOL	B	806	-	-	0/4/4/4	-
3	GOL	B	804	-	-	2/4/4/4	-
2	A1CQX	A	801	-	-	6/18/25/25	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	803	A1CQX	C2-N1	5.43	1.37	1.32
2	C	801	A1CQX	C2-N1	5.21	1.37	1.32
2	B	803	A1CQX	C9-N2	3.96	1.39	1.35
2	C	801	A1CQX	C9-N2	3.50	1.38	1.35
4	C	803	SCN	C-N	3.22	1.26	1.15
2	C	801	A1CQX	N2-N1	3.20	1.43	1.36
2	A	801	A1CQX	C13-C14	-3.12	1.41	1.51
2	A	801	A1CQX	C10-C11	2.79	1.43	1.39
2	C	801	A1CQX	C18-C19	-2.35	1.43	1.51
2	C	801	A1CQX	C10-C11	2.03	1.42	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	A1CQX	C14-C13-N5	8.36	129.78	112.00
2	B	803	A1CQX	C21-C2-N1	-6.63	108.16	110.76
2	C	801	A1CQX	C9-C21-C2	5.45	106.90	105.15
2	A	801	A1CQX	C13-N5-C12	-5.31	110.10	122.11
2	C	801	A1CQX	C3-N2-C9	5.01	130.99	127.81
2	B	803	A1CQX	C3-N2-C9	4.53	130.68	127.81
2	C	801	A1CQX	C21-C2-N1	-4.51	108.99	110.76
2	A	801	A1CQX	C20-C21-C2	3.69	140.60	136.72
2	B	803	A1CQX	C2-N1-N2	3.65	109.08	104.97
2	A	801	A1CQX	C9-N2-N1	3.45	112.99	111.05
2	C	801	A1CQX	O1-C12-C11	3.42	127.68	120.90
2	A	801	A1CQX	O1-C12-N5	-3.39	115.98	122.59
2	A	801	A1CQX	C20-C21-C9	-3.27	114.38	117.67
5	C	802	B3P	O5-C6-C4	-3.24	105.09	111.68
2	B	803	A1CQX	C9-C21-C2	3.04	106.12	105.15
2	C	801	A1CQX	C20-C21-C9	-3.02	114.63	117.67
2	B	803	A1CQX	C9-N2-N1	-2.96	109.39	111.05
2	C	801	A1CQX	C21-C9-N4	-2.66	123.85	127.01
2	C	801	A1CQX	O1-C12-N5	-2.59	117.54	122.59
2	B	803	A1CQX	O2-C15-N6	-2.50	117.66	122.12
2	A	801	A1CQX	C1-C2-C21	2.49	131.87	127.56
2	A	801	A1CQX	C14-C15-N6	-2.43	114.41	118.09
2	C	801	A1CQX	N4-C9-N2	2.33	128.97	125.34
2	A	801	A1CQX	C20-C11-C10	-2.27	115.59	117.92
2	A	801	A1CQX	C1-C2-N1	-2.14	117.05	119.93
2	C	801	A1CQX	C1-C2-C21	2.12	131.23	127.56
2	A	801	A1CQX	C3-C4-C5	-2.07	116.90	121.26
3	A	807	GOL	C3-C2-C1	2.05	119.30	111.80
2	C	801	A1CQX	C14-C13-N5	2.01	116.28	112.00
2	C	801	A1CQX	C20-C11-C10	-2.01	115.86	117.92

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	GOL	C1-C2-C3-O3
3	A	808	GOL	O1-C1-C2-O2
3	A	808	GOL	O1-C1-C2-C3
3	B	801	GOL	C1-C2-C3-O3
3	B	802	GOL	O1-C1-C2-C3
3	B	804	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	803	A1CQX	C20-C11-C12-O1
2	C	801	A1CQX	C20-C11-C12-O1
2	C	801	A1CQX	C20-C11-C12-N5
2	A	801	A1CQX	C10-C11-C12-O1
2	A	801	A1CQX	C20-C11-C12-N5
2	B	803	A1CQX	C20-C11-C12-N5
2	A	801	A1CQX	C20-C11-C12-O1
2	B	803	A1CQX	C10-C11-C12-N5
2	B	803	A1CQX	C10-C11-C12-O1
2	C	801	A1CQX	C10-C11-C12-O1
2	A	801	A1CQX	C10-C11-C12-N5
2	C	801	A1CQX	C10-C11-C12-N5
2	A	801	A1CQX	C11-C12-N5-C13
3	A	802	GOL	C1-C2-C3-O3
3	A	807	GOL	O1-C1-C2-C3
3	C	804	GOL	O1-C1-C2-C3
3	A	803	GOL	O2-C2-C3-O3
3	A	807	GOL	O1-C1-C2-O2
3	B	802	GOL	O1-C1-C2-O2
3	B	804	GOL	O2-C2-C3-O3
2	A	801	A1CQX	O1-C12-N5-C13
3	B	801	GOL	O2-C2-C3-O3
3	B	801	GOL	O1-C1-C2-O2
3	A	802	GOL	O2-C2-C3-O3

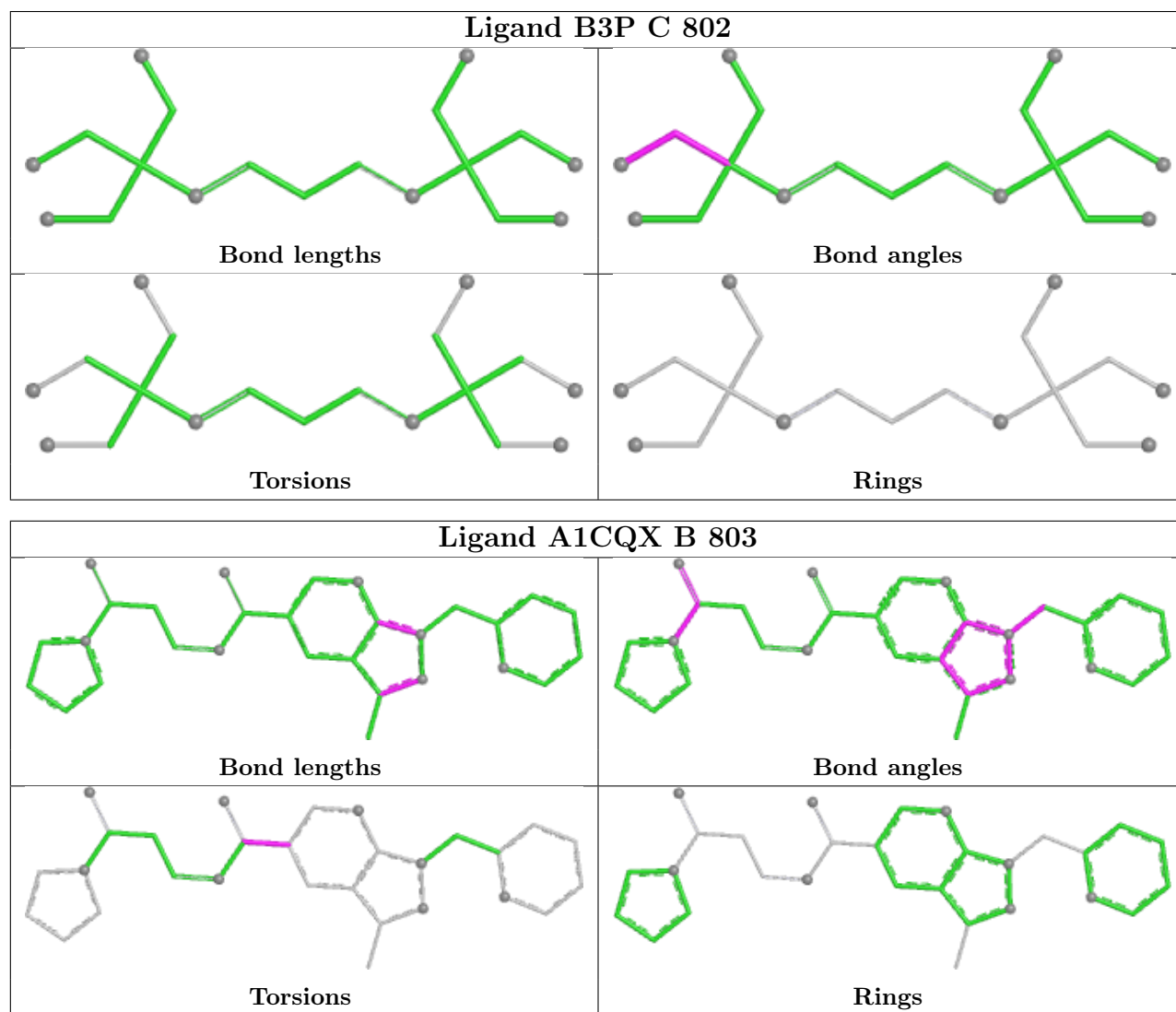
There are no ring outliers.

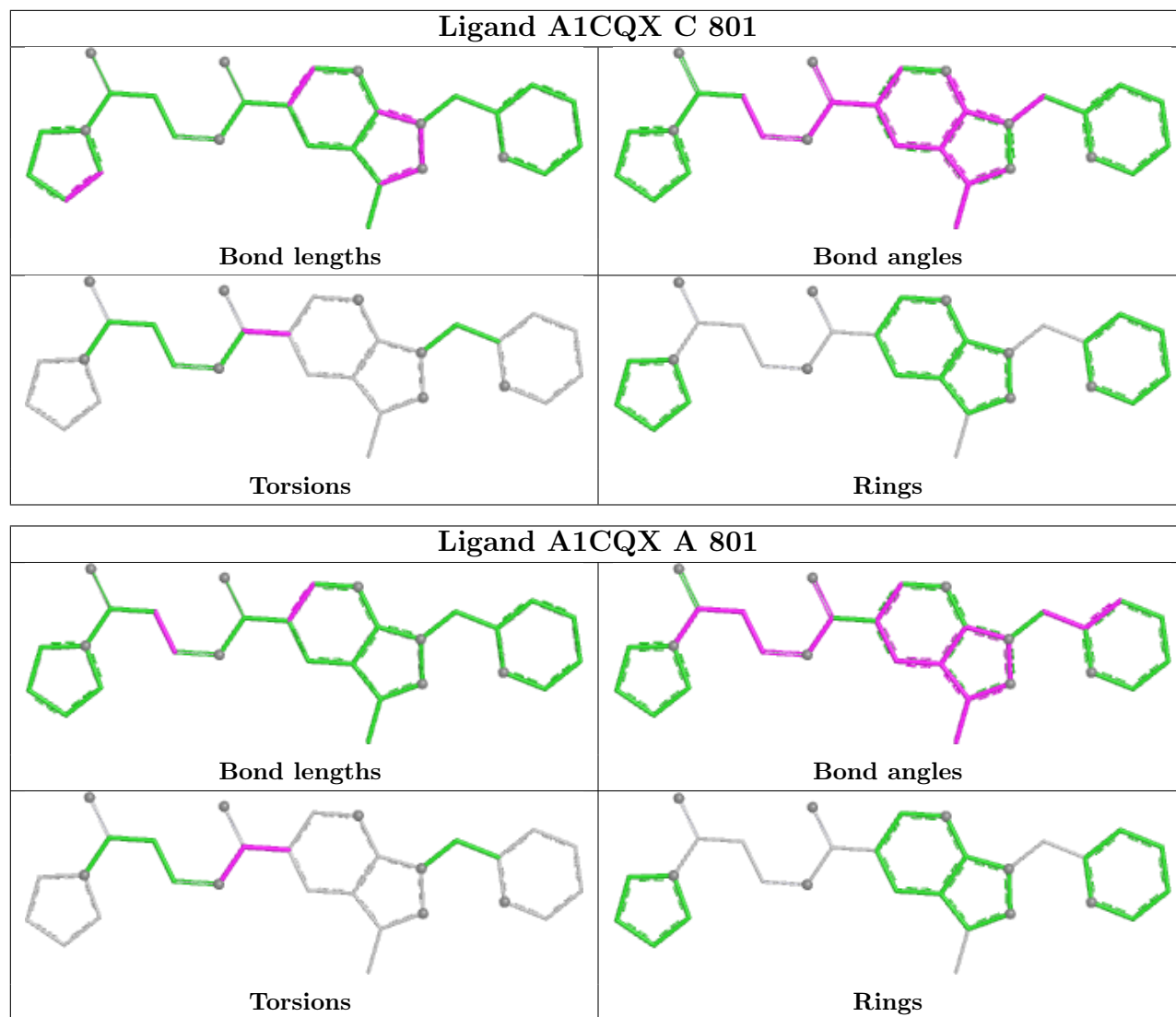
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	GOL	2	0
3	B	804	GOL	2	0
4	C	807	SCN	1	0
4	A	809	SCN	1	0
4	C	806	SCN	1	0
4	A	805	SCN	1	0
3	B	801	GOL	1	0
3	B	802	GOL	4	0
2	A	801	A1CQX	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	707/711 (99%)	-0.79	4 (0%) 85 90	7, 18, 36, 67	2 (0%)
1	B	707/711 (99%)	-0.35	8 (1%) 78 84	11, 25, 48, 109	0
1	C	707/711 (99%)	-0.30	6 (0%) 82 88	8, 27, 52, 81	3 (0%)
All	All	2121/2133 (99%)	-0.48	18 (0%) 82 88	7, 23, 48, 109	5 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	VAL	6.8
1	C	427	VAL	4.5
1	B	429	GLY	3.1
1	B	272	GLY	3.0
1	A	427	VAL	2.9
1	B	270	SER	2.9
1	C	4	LEU	2.9
1	A	426	THR	2.8
1	A	432	ALA	2.7
1	B	4	LEU	2.5
1	B	428	LYS	2.5
1	C	430	ILE	2.5
1	C	429	GLY	2.4
1	B	430	ILE	2.4
1	B	426	THR	2.2
1	C	460	ILE	2.2
1	A	430	ILE	2.2
1	C	426	THR	2.1

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 ⓘ

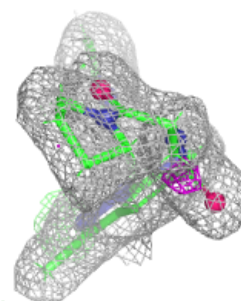
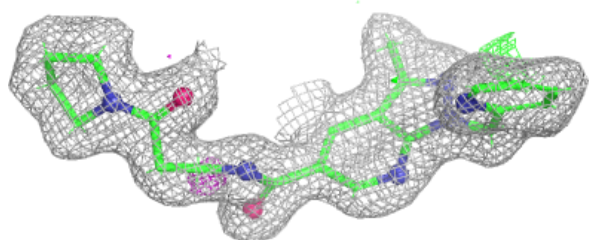
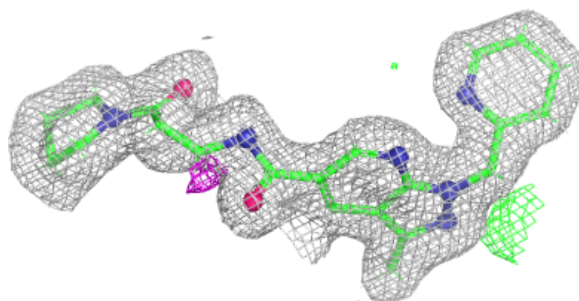
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	807	6/6	0.87	0.09	28,41,43,45	3
3	GOL	B	801	6/6	0.88	0.10	32,39,42,45	3
4	SCN	C	807	3/3	0.88	0.12	40,40,43,57	0
4	SCN	B	808	3/3	0.89	0.14	49,49,51,55	0
4	SCN	A	810	3/3	0.90	0.12	34,34,36,52	0
3	GOL	A	803	6/6	0.90	0.12	23,35,41,41	3
3	GOL	B	802	6/6	0.90	0.09	32,38,41,47	3
4	SCN	A	811	3/3	0.93	0.10	38,38,43,56	0
4	SCN	B	807	3/3	0.93	0.11	35,35,40,49	0
4	SCN	A	809	3/3	0.93	0.10	30,30,31,49	0
3	GOL	A	808	6/6	0.93	0.09	25,40,44,51	3
3	GOL	B	804	6/6	0.94	0.09	26,40,43,46	3
4	SCN	C	805	3/3	0.94	0.07	25,25,27,53	0
4	SCN	A	805	3/3	0.94	0.10	17,17,21,34	0
4	SCN	C	806	3/3	0.95	0.08	29,29,32,50	0
4	SCN	C	803	3/3	0.95	0.11	19,19,24,33	0
4	SCN	A	806	3/3	0.96	0.08	21,21,29,44	0
4	SCN	B	805	3/3	0.96	0.08	23,23,36,39	0
3	GOL	C	804	6/6	0.96	0.08	15,22,41,41	3
3	GOL	B	806	6/6	0.96	0.07	17,29,41,42	3
3	GOL	A	802	6/6	0.97	0.05	16,24,41,41	3
2	A1CQX	A	801	29/30	0.97	0.05	11,15,30,41	3
2	A1CQX	B	803	29/30	0.97	0.06	14,23,36,41	3
5	B3P	C	802	19/19	0.97	0.04	10,14,41,41	8
4	SCN	A	804	3/3	0.98	0.07	30,30,38,44	0
2	A1CQX	C	801	29/30	0.98	0.04	12,17,29,41	3

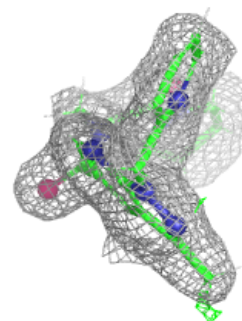
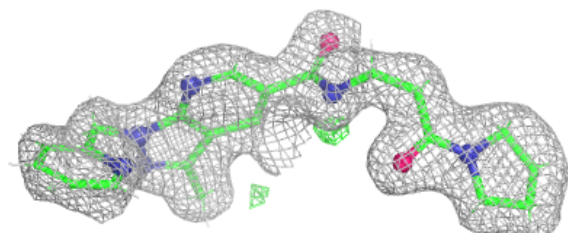
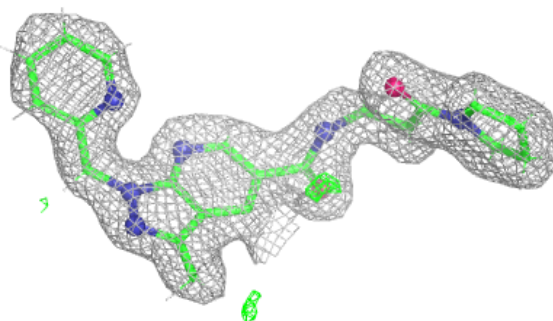
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CQX A 801:

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

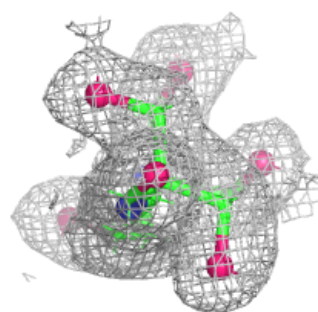
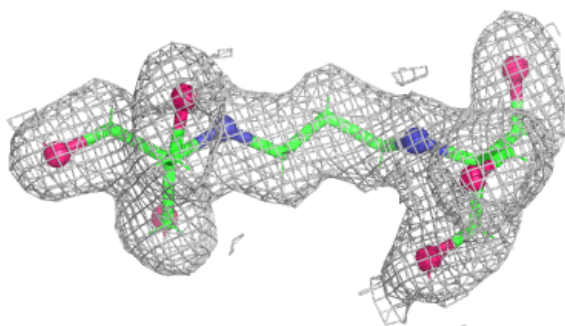
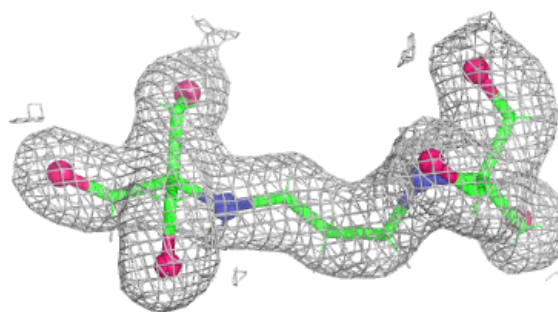
**Electron density around A1CQX B 803:**

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

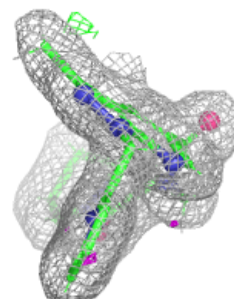
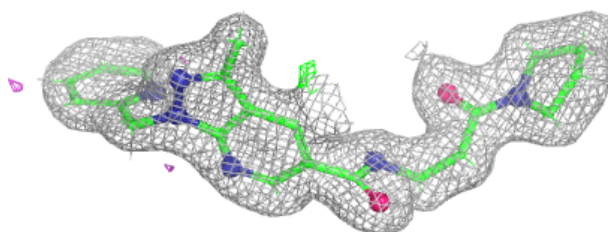
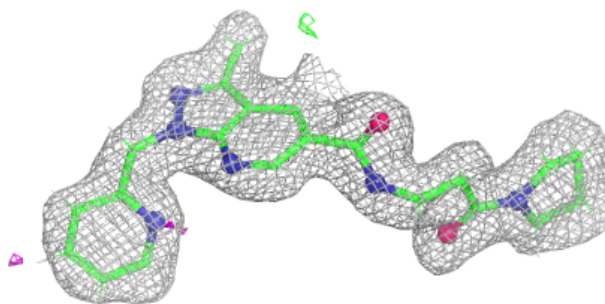


Electron density around B3P C 802:

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

**Electron density around A1CQX C 801:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.