



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:52 AM UTC

PDB ID : 9Q65 / pdb_00009q65
Title : Human prolyl endopeptidase (PREP) - complex with KT-2-75
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-21
Resolution : 1.89 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

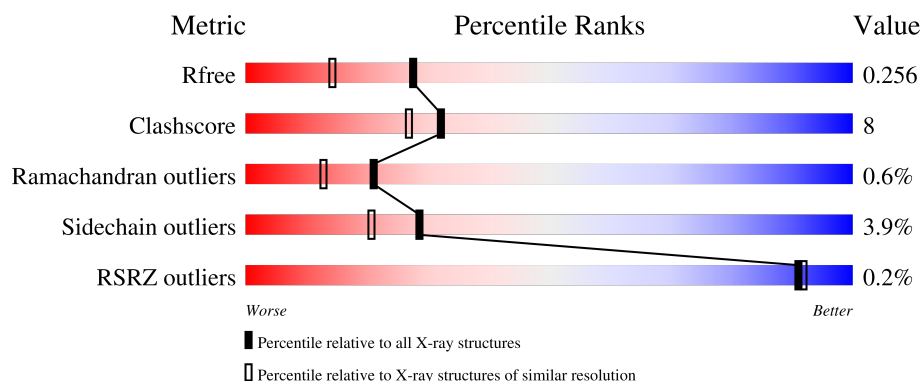
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	B	711	
1	D	711	
1	F	711	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 34283 atoms, of which 16687 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.

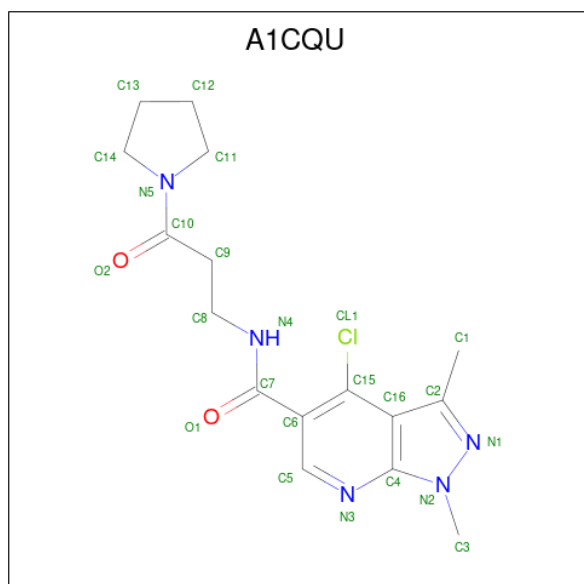
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	706	Total	C	H	N	O	S	179	1	0
			11173	3635	5504	940	1067	27			
1	D	706	Total	C	H	N	O	S	179	4	0
			11190	3640	5510	942	1071	27			
1	F	706	Total	C	H	N	O	S	179	1	0
			11183	3637	5513	941	1065	27			

There are 3 discrepancies between the modelled and reference sequences:

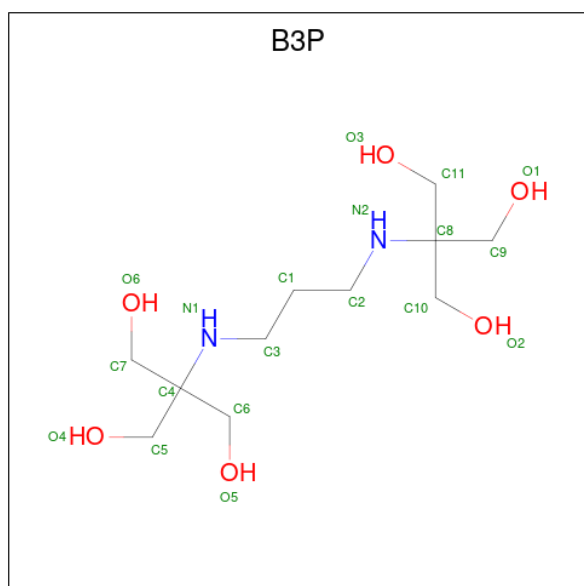
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P48147
D	0	GLY	-	expression tag	UNP P48147
F	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is 4-chloro-1,3-dimethyl-N-[3-oxo-3-(pyrrolidin-1-yl)propyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQU) (formula: C₁₆H₂₀ClN₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	6	0
			43	16	20	5	2		
2	D	1	Total	C	H	N	O	6	0
			43	16	20	5	2		
2	F	1	Total	C	H	N	O	6	0
			43	16	20	5	2		

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



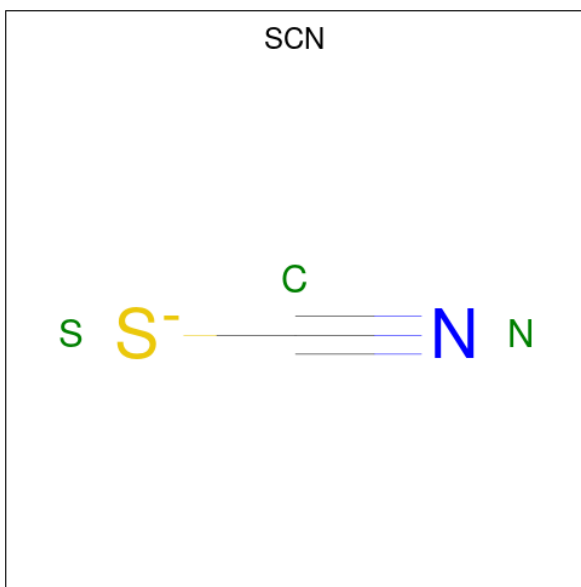
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	8	0
			45	11	26	2	6		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		
5	B	1	Total	C	N	S	0	0
			3	1	1	1		
5	D	1	Total	C	N	S	0	0
			3	1	1	1		
5	F	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	H	O	2	0
			17	4	10	3		

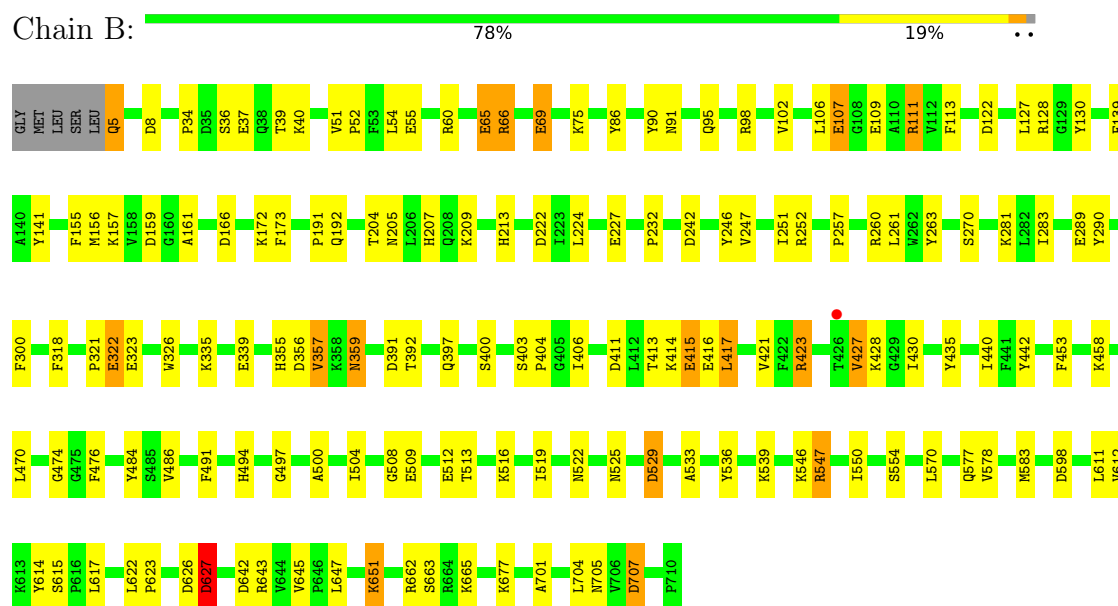
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	179	Total	O	0	0
			179	179		
7	D	109	Total	O	0	0
			109	109		
7	F	128	Total	O	0	0
			128	128		

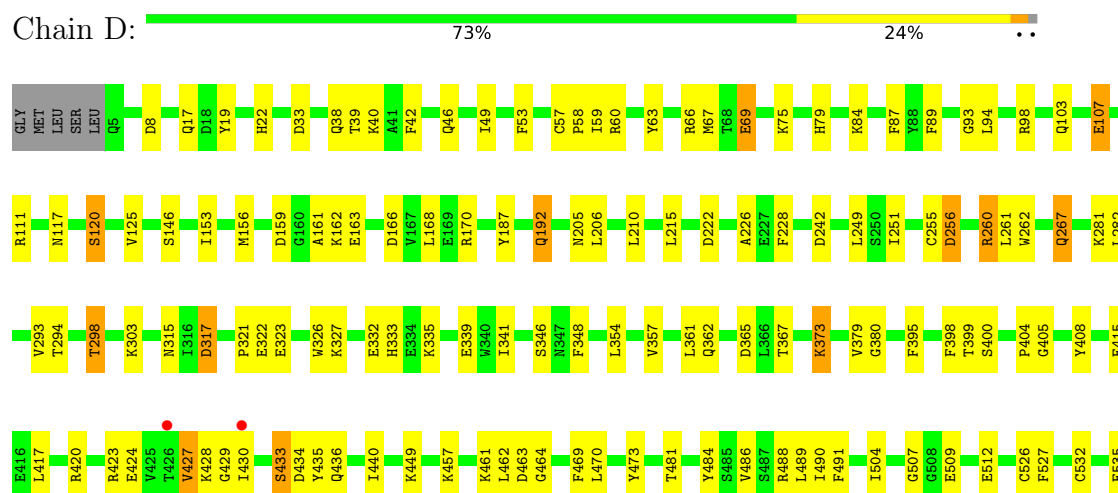
3 Residue-property plots

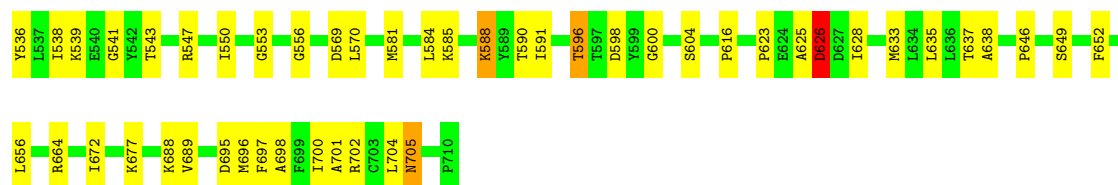
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Prolyl endopeptidase



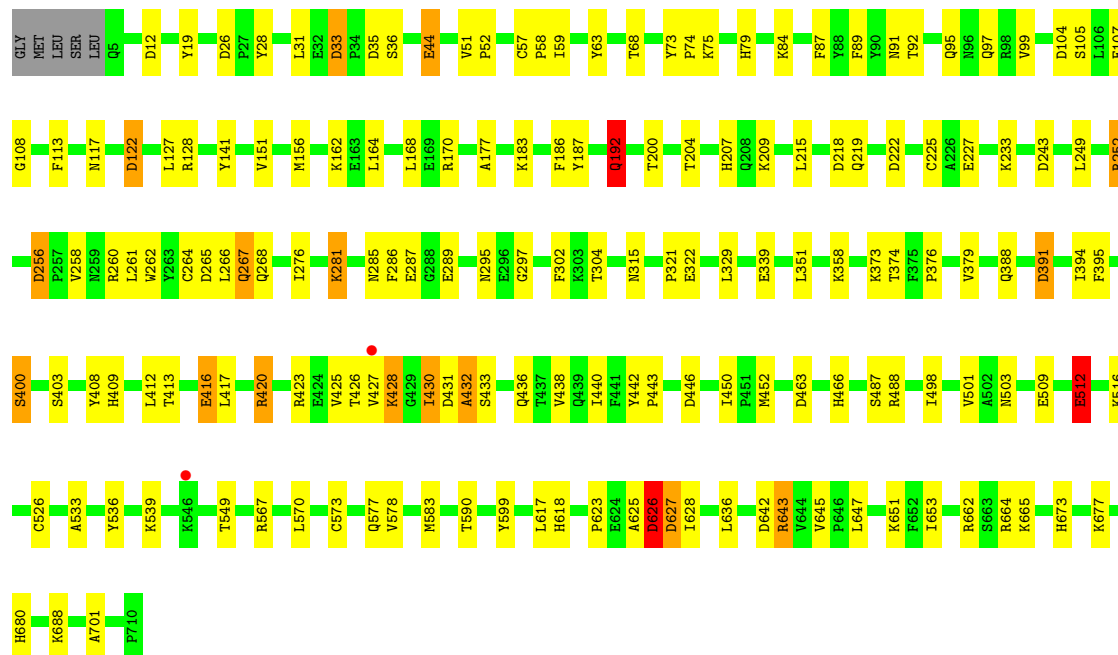
• Molecule 1: Prolyl endopeptidase





• Molecule 1: Prolyl endopeptidase

Chain F: 76% 21% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.52Å 65.99Å 159.33Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	34.60 – 1.89 34.60 – 1.89	Depositor EDS
% Data completeness (in resolution range)	69.7 (34.60-1.89) 70.0 (34.60-1.89)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.218 , 0.295 0.188 , 0.256	Depositor DCC
R_{free} test set	58737 reflections (33.81%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34283	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, SCN, GOL, A1CQU, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.79	1/5824 (0.0%)	1.34	22/7896 (0.3%)
1	D	0.78	0/5849	1.36	36/7931 (0.5%)
1	F	0.73	0/5825	1.36	27/7896 (0.3%)
All	All	0.77	1/17498 (0.0%)	1.36	85/23723 (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	B	0	5
1	D	0	5
1	F	0	8
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	651	LYS	C-O	-5.22	1.18	1.24

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	627	ASP	CA-CB-CG	9.93	122.53	112.60
1	F	35	ASP	CA-CB-CG	9.29	121.89	112.60
1	B	339	GLU	CB-CA-C	-8.42	97.59	110.90
1	D	527	PHE	CA-CB-CG	8.03	121.83	113.80
1	B	322	GLU	CB-CG-CD	7.91	126.04	112.60
1	B	65	GLU	CB-CA-C	7.67	122.92	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	354	LEU	N-CA-CB	-7.31	98.50	110.42
1	F	68	THR	CA-CB-OG1	-7.31	98.64	109.60
1	F	526	CYS	CB-CA-C	-7.12	98.75	110.85
1	D	298	THR	CA-CB-OG1	-7.07	99.00	109.60
1	F	281	LYS	N-CA-CB	-7.04	102.46	110.35
1	B	107	GLU	CB-CA-C	-6.91	97.94	109.55
1	F	512	GLU	CB-CG-CD	6.88	124.29	112.60
1	B	391	ASP	CA-CB-CG	6.68	119.28	112.60
1	F	642	ASP	CA-CB-CG	6.68	119.28	112.60
1	D	695	ASP	CA-CB-CG	6.60	119.20	112.60
1	F	443	PRO	CB-CA-C	-6.55	105.44	111.40
1	B	662	ARG	CD-NE-CZ	6.51	133.52	124.40
1	D	436	GLN	N-CA-CB	-6.51	99.48	111.13
1	D	348	PHE	CA-CB-CG	6.43	120.23	113.80
1	D	317	ASP	CA-CB-CG	6.43	119.03	112.60
1	D	40	LYS	CB-CA-C	-6.38	99.83	110.68
1	D	87	PHE	CA-CB-CG	6.36	120.16	113.80
1	D	267	GLN	N-CA-CB	6.36	119.58	110.16
1	D	481	THR	CA-CB-OG1	-6.35	100.07	109.60
1	B	242	ASP	CA-CB-CG	6.22	118.82	112.60
1	F	183	LYS	CB-CA-C	-6.21	99.11	109.55
1	F	339	GLU	CB-CA-C	-6.19	101.12	110.90
1	D	623	PRO	CB-CA-C	6.14	119.38	111.64
1	B	623	PRO	CB-CA-C	6.03	119.24	111.46
1	B	707	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	365	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	53	PHE	N-CA-CB	5.96	118.98	110.16
1	B	428	LYS	CB-CA-C	-5.88	99.82	109.53
1	F	192	GLN	CB-CA-C	5.87	119.47	109.72
1	F	33	ASP	CA-CB-CG	5.83	118.44	112.60
1	B	204	THR	CA-CB-OG1	-5.80	100.89	109.60
1	F	391	ASP	CA-CB-CG	5.77	118.37	112.60
1	F	374	THR	CA-CB-OG1	-5.76	100.96	109.60
1	F	249	LEU	N-CA-CB	-5.74	101.75	110.77
1	F	243	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	476	PHE	CA-CB-CG	-5.74	108.06	113.80
1	D	434	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	8	ASP	CA-CB-CG	5.72	118.32	112.60
1	F	200	THR	CA-CB-OG1	-5.67	101.09	109.60
1	D	584	LEU	N-CA-C	-5.66	106.50	113.41
1	D	159	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	318	PHE	N-CA-CB	-5.61	101.01	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	HIS	CB-CA-C	5.57	119.52	110.22
1	D	117	ASN	CA-C-N	-5.56	115.36	122.26
1	D	117	ASN	C-N-CA	-5.56	115.36	122.26
1	D	449	LYS	CA-C-N	-5.54	118.51	123.33
1	D	449	LYS	C-N-CA	-5.54	118.51	123.33
1	D	170	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	B	642	ASP	CA-CB-CG	5.50	118.10	112.60
1	F	645	VAL	CB-CA-C	5.50	117.01	110.68
1	F	26	ASP	CA-CB-CG	5.49	118.09	112.60
1	D	33	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	395	PHE	CA-CB-CG	5.48	119.28	113.80
1	F	626	ASP	CB-CA-C	5.43	121.22	110.42
1	D	590	THR	CA-CB-OG1	5.38	117.67	109.60
1	D	379	VAL	N-CA-CB	-5.37	104.68	110.53
1	D	424	GLU	CG-CD-OE2	-5.34	106.13	118.40
1	F	122	ASP	CB-CA-C	-5.33	101.48	110.44
1	F	436	GLN	N-CA-CB	-5.32	101.87	110.81
1	D	163	GLU	CB-CA-C	-5.32	102.28	110.26
1	B	570	LEU	N-CA-CB	-5.32	102.61	110.53
1	F	618	HIS	CA-CB-CG	-5.32	108.48	113.80
1	D	596	THR	CA-CB-OG1	-5.27	101.69	109.60
1	D	69	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	281	LYS	CB-CA-C	5.25	120.00	112.12
1	F	413	THR	CA-CB-OG1	-5.25	101.72	109.60
1	B	69	GLU	CB-CG-CD	5.23	121.49	112.60
1	B	65	GLU	N-CA-CB	-5.22	102.44	110.01
1	D	367	THR	CA-CB-OG1	-5.19	101.82	109.60
1	B	529	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	159	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	256	ASP	CA-CB-CG	5.16	117.76	112.60
1	F	688	LYS	CA-C-N	5.08	126.96	120.56
1	F	688	LYS	C-N-CA	5.08	126.96	120.56
1	D	192	GLN	CB-CA-C	5.07	118.88	109.54
1	D	473	TYR	CB-CA-C	5.05	120.47	110.42
1	D	547	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	B	627	ASP	CA-CB-CG	5.03	117.63	112.60
1	F	19	TYR	CB-CA-C	-5.00	102.61	111.22

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	ARG	Sidechain
1	B	128	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	547	ARG	Sidechain
1	B	643	ARG	Sidechain
1	D	111	ARG	Sidechain
1	D	260	ARG	Sidechain
1	D	488	ARG	Sidechain
1	D	60	ARG	Sidechain
1	D	664	ARG	Sidechain
1	F	128	ARG	Sidechain
1	F	170	ARG	Sidechain
1	F	252	ARG	Sidechain
1	F	302	PHE	Peptide
1	F	488	ARG	Sidechain
1	F	643	ARG	Sidechain
1	F	662	ARG	Sidechain
1	F	664	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	B	5669	5504	5478	78	0
1	D	5680	5510	5465	96	0
1	F	5670	5513	5487	96	0
2	B	23	20	0	0	0
2	D	23	20	0	2	0
2	F	23	20	0	0	0
3	B	19	26	26	0	0
4	B	30	40	40	0	0
4	D	18	24	24	3	0
5	B	12	0	0	1	0
5	D	3	0	0	1	0
5	F	3	0	0	1	0
6	F	7	10	10	1	0
7	B	179	0	0	8	0
7	D	109	0	0	1	0
7	F	128	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17596	16687	16530	269	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 8.

All (269) 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:D:255:CYS:SG	2:D:801:A1CQU:C15	2.01	1.46
1:B:66:ARG:NH2	1:B:69:GLU:OE2	1.94	0.99
1:F:420:ARG:HG3	1:F:420:ARG:HH11	1.35	0.90
1:D:404:PRO:CD	1:D:427:VAL:HG22	2.04	0.87
1:F:260:ARG:NH2	7:F:901:HOH:O	2.06	0.87
1:D:66:ARG:NH2	1:D:69:GLU:OE2	2.13	0.81
1:D:427:VAL:HG12	1:D:430:ILE:HB	1.62	0.81
1:D:404:PRO:CG	1:D:427:VAL:HG22	2.11	0.79
1:D:404:PRO:HD3	1:D:427:VAL:HG22	1.65	0.79
1:B:322:GLU:HG2	7:B:1054:HOH:O	1.87	0.73
1:D:697:PHE:HA	1:D:700:ILE:HD12	1.75	0.68
1:B:546:LYS:O	1:B:704:LEU:HD22	1.93	0.67
1:B:37:GLU:HG2	7:B:943:HOH:O	1.93	0.67
1:D:206:LEU:H	4:D:803:GOL:H2	1.58	0.67
1:F:625:ALA:C	1:F:626:ASP:O	2.38	0.66
1:B:494:HIS:NE2	7:B:903:HOH:O	2.30	0.64
1:F:420:ARG:HG3	1:F:420:ARG:NH1	2.09	0.64
1:B:491:PHE:CE2	1:B:497:GLY:HA3	2.34	0.63
1:F:192:GLN:HA	1:F:192:GLN:NE2	2.15	0.62
1:F:463:ASP:OD1	1:F:463:ASP:C	2.40	0.62
1:B:102:VAL:HG12	1:B:113:PHE:HB2	1.82	0.62
1:D:635:LEU:HB2	1:D:672:ILE:HG13	1.82	0.61
1:D:404:PRO:HD3	1:D:427:VAL:CG2	2.30	0.61
1:D:107:GLU:H	1:D:107:GLU:CD	2.09	0.61
1:F:122:ASP:OD2	1:F:677:LYS:NZ	2.33	0.60
1:F:623:PRO:O	1:F:665:LYS:NZ	2.35	0.60
1:D:261:LEU:HD12	1:D:282:LEU:HD23	1.83	0.60
1:B:5:GLN:HA	1:B:5:GLN:HE21	1.66	0.60
1:D:156:MET:CE	1:D:161:ALA:HB1	2.32	0.59
1:D:625:ALA:C	1:D:626:ASP:O	2.41	0.59
1:B:166:ASP:O	7:B:901:HOH:O	2.17	0.59
1:F:431:ASP:O	1:F:432:ALA:C	2.45	0.59
1:B:172:LYS:HD3	1:B:173:PHE:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:GLU:HG3	1:D:326:TRP:CZ3	2.38	0.58
1:F:388:GLN:O	1:F:391:ASP:HB2	2.04	0.58
1:B:127:LEU:HD11	1:B:141:TYR:HB2	1.84	0.58
1:D:532:CYS:HA	1:D:535:GLU:OE1	2.04	0.58
1:F:431:ASP:O	1:F:433:SER:N	2.37	0.57
1:F:623:PRO:HB2	1:F:628:ILE:O	2.03	0.57
1:F:549:THR:HA	1:F:573:CYS:O	2.03	0.57
1:D:461:LYS:O	1:D:463:ASP:N	2.36	0.57
1:F:567:ARG:HH21	1:F:570:LEU:HD13	1.70	0.57
1:F:12:ASP:C	1:F:12:ASP:OD1	2.48	0.57
1:F:73:TYR:O	1:F:75:LYS:HE3	2.03	0.57
1:F:260:ARG:HG3	1:F:286:PHE:CE1	2.40	0.57
1:D:404:PRO:CD	1:D:427:VAL:CG2	2.82	0.56
1:D:536:TYR:HA	1:D:539:LYS:HD3	1.87	0.56
1:D:17:GLN:HG2	1:D:19:TYR:CE1	2.41	0.56
1:F:394:ILE:HG23	1:F:412:LEU:HD11	1.86	0.56
1:F:285:ASN:O	7:F:902:HOH:O	2.18	0.56
1:D:440:ILE:HD12	1:D:440:ILE:C	2.30	0.55
1:F:187:TYR:OH	1:F:222:ASP:OD2	2.20	0.55
1:B:191:PRO:O	1:B:192:GLN:C	2.49	0.55
1:D:404:PRO:HG2	1:D:427:VAL:HG22	1.88	0.55
1:B:156:MET:CE	1:B:161:ALA:HB1	2.36	0.55
1:B:251:ILE:HB	1:B:260:ARG:HB2	1.89	0.55
1:B:484:TYR:HE2	1:B:486:VAL:HG22	1.71	0.55
1:D:688:LYS:O	1:D:689:VAL:C	2.49	0.55
1:F:28:TYR:HB3	1:F:31:LEU:HD12	1.89	0.55
1:F:446:ASP:C	1:F:446:ASP:OD1	2.51	0.54
1:B:435:TYR:O	1:B:458:LYS:HE3	2.08	0.54
1:B:508:GLY:O	1:B:509:GLU:C	2.50	0.54
1:B:484:TYR:CE2	1:B:486:VAL:HG22	2.42	0.54
1:D:323:GLU:HG3	1:D:326:TRP:CE3	2.43	0.54
1:F:51:VAL:HB	1:F:52:PRO:HD3	1.90	0.54
1:F:567:ARG:NH2	1:F:570:LEU:HD13	2.23	0.54
1:D:153:ILE:HB	1:D:168:LEU:HB2	1.90	0.53
1:D:205:ASN:HA	4:D:803:GOL:C3	2.38	0.53
1:F:256:ASP:HB3	1:F:258:VAL:HG22	1.89	0.53
1:D:107:GLU:CD	1:D:107:GLU:N	2.66	0.53
1:D:146:SER:HB3	1:D:677:LYS:HA	1.90	0.52
1:B:65:GLU:O	1:B:69:GLU:HG3	2.09	0.52
1:D:469:PHE:HB2	1:D:491:PHE:CE2	2.45	0.52
1:B:645:VAL:HG23	1:B:647:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:PHE:O	1:D:405:GLY:HA2	2.10	0.52
1:B:440:ILE:HD12	1:B:440:ILE:C	2.35	0.51
1:F:512:GLU:HG2	1:F:516:LYS:HD2	1.91	0.51
1:D:38:GLN:CD	1:D:38:GLN:H	2.18	0.51
1:F:79:HIS:HA	1:F:87:PHE:O	2.11	0.51
1:F:59:ILE:HG12	1:F:701:ALA:CB	2.40	0.51
1:F:452:MET:HA	1:F:501:VAL:O	2.11	0.51
1:B:51:VAL:HB	1:B:52:PRO:HD3	1.93	0.50
1:D:323:GLU:HA	1:D:326:TRP:CE2	2.46	0.50
1:F:209:LYS:HE2	7:F:958:HOH:O	2.09	0.50
1:B:516:LYS:HA	1:B:519:ILE:HG12	1.93	0.50
1:D:373:LYS:HD3	1:D:417:LEU:O	2.11	0.50
1:B:172:LYS:NZ	1:B:205:ASN:OD1	2.45	0.50
1:F:89:PHE:HA	1:F:99:VAL:O	2.12	0.50
1:F:162:LYS:HE2	1:F:164:LEU:CD2	2.42	0.50
1:D:428:LYS:O	1:D:430:ILE:N	2.44	0.50
1:B:283:ILE:HG21	1:B:290:TYR:CE2	2.47	0.50
1:B:626:ASP:O	1:B:627:ASP:HB2	2.12	0.49
1:F:431:ASP:C	1:F:433:SER:N	2.70	0.49
1:F:577:GLN:O	1:F:578:VAL:C	2.55	0.49
1:B:5:GLN:HA	1:B:5:GLN:NE2	2.26	0.49
1:D:470:LEU:HB3	1:D:550:ILE:HG22	1.94	0.49
1:B:614:TYR:O	1:B:615:SER:C	2.54	0.49
1:B:207:HIS:CE1	1:B:232:PRO:HB3	2.47	0.49
1:D:652:PHE:CE2	1:D:656:LEU:HD11	2.47	0.49
1:B:34:PRO:HA	1:B:39:THR:HG21	1.94	0.49
1:B:192:GLN:HA	1:B:192:GLN:NE2	2.27	0.49
1:D:486:VAL:O	1:D:490:ILE:HG13	2.12	0.49
1:D:581:MET:O	1:D:616:PRO:HD2	2.12	0.49
1:F:267:GLN:HG2	7:F:988:HOH:O	2.13	0.49
1:F:503:ASN:HB3	1:F:509:GLU:HG2	1.93	0.49
1:F:322:GLU:HB3	7:F:937:HOH:O	2.13	0.49
1:D:93:GLY:O	1:D:94:LEU:HD23	2.13	0.48
1:B:397:GLN:NE2	7:B:916:HOH:O	2.45	0.48
1:F:265:ASP:OD1	1:F:265:ASP:C	2.55	0.48
1:B:257:PRO:O	1:B:289:GLU:HB2	2.13	0.48
1:D:380:GLY:HA3	1:D:398:PHE:CE1	2.48	0.48
1:B:54:LEU:O	1:B:55:GLU:C	2.55	0.48
1:D:205:ASN:HA	4:D:803:GOL:H32	1.93	0.48
1:D:315:ASN:HB2	1:D:327:LYS:HB2	1.95	0.48
1:D:303:LYS:HE2	1:D:339:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:HE2	1:B:227:GLU:OE1	2.13	0.48
1:F:267:GLN:HG3	7:F:978:HOH:O	2.13	0.48
1:B:522:ASN:O	1:B:525:ASN:HB2	2.14	0.48
1:B:246:TYR:CD2	1:B:300:PHE:HZ	2.32	0.48
1:D:362:GLN:HE22	5:D:805:SCN:C	2.27	0.48
1:D:484:TYR:CE1	1:D:489:LEU:CD1	2.97	0.47
1:F:376:PRO:O	1:F:376:PRO:HG2	2.14	0.47
1:B:224:LEU:N	7:B:908:HOH:O	2.38	0.47
1:F:127:LEU:HD11	1:F:141:TYR:HB2	1.96	0.47
1:F:626:ASP:O	1:F:628:ILE:N	2.47	0.47
1:F:395:PHE:HA	1:F:408:TYR:O	2.15	0.47
1:F:295:ASN:ND2	1:F:297:GLY:O	2.46	0.47
1:F:79:HIS:CE1	1:F:423:ARG:HH22	2.33	0.47
1:F:252:ARG:NH2	1:F:258:VAL:O	2.48	0.47
1:B:36:SER:O	1:B:40:LYS:HG3	2.15	0.47
1:D:156:MET:HE2	1:D:161:ALA:HB1	1.96	0.47
1:D:262:TRP:CD1	1:D:281:LYS:HA	2.50	0.47
1:D:585:LYS:O	1:D:588:LYS:HG3	2.15	0.47
1:F:287:GLU:HB2	7:F:966:HOH:O	2.13	0.47
1:B:91:ASN:OD1	1:B:95:GLN:HB2	2.15	0.46
1:B:701:ALA:O	1:B:705:ASN:N	2.48	0.46
1:D:569:ASP:N	1:D:569:ASP:OD1	2.47	0.46
1:F:177:ALA:HB3	1:F:186:PHE:HB2	1.97	0.46
1:B:247:VAL:O	1:B:263:TYR:HA	2.15	0.46
1:B:577:GLN:C	1:B:578:VAL:HG22	2.39	0.46
1:F:192:GLN:HA	1:F:192:GLN:HE21	1.79	0.46
1:D:75:LYS:NZ	1:D:93:GLY:O	2.48	0.46
1:D:210:LEU:HD22	1:D:249:LEU:HD13	1.96	0.46
1:D:251:ILE:HB	1:D:260:ARG:HB2	1.97	0.46
1:D:428:LYS:C	1:D:430:ILE:H	2.22	0.46
1:D:704:LEU:O	1:D:705:ASN:C	2.57	0.46
1:F:209:LYS:HD2	1:F:227:GLU:HB3	1.98	0.46
1:B:60:ARG:O	1:B:60:ARG:HG2	2.14	0.46
1:F:636:LEU:CD2	1:F:673:HIS:HB3	2.45	0.46
1:B:130:TYR:HB2	1:B:139:PHE:CE1	2.50	0.46
1:B:513:THR:HG23	7:B:978:HOH:O	2.15	0.46
1:D:464:GLY:N	1:D:541:GLY:O	2.49	0.46
1:F:105:SER:OG	1:F:108:GLY:HA3	2.16	0.46
1:B:86:TYR:CE1	1:B:106:LEU:HD13	2.51	0.45
1:B:415:GLU:HG3	1:B:416:GLU:N	2.30	0.45
1:B:617:LEU:CD2	1:B:651:LYS:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:LEU:HA	1:F:219:GLN:OE1	2.16	0.45
1:D:242:ASP:OD2	1:D:294:THR:OG1	2.25	0.45
1:F:625:ALA:O	1:F:626:ASP:O	2.34	0.45
1:F:626:ASP:C	1:F:628:ILE:H	2.23	0.45
1:B:536:TYR:HA	1:B:539:LYS:HD2	1.99	0.45
1:D:504:ILE:HD12	1:D:526:CYS:HB3	1.99	0.45
1:D:538:ILE:HA	1:D:543:THR:O	2.15	0.45
1:B:416:GLU:O	1:B:417:LEU:HB2	2.17	0.45
1:B:663:SER:O	5:B:807:SCN:S	2.74	0.45
1:D:79:HIS:HE1	1:D:423:ARG:HH22	1.65	0.45
1:D:626:ASP:C	1:D:628[B]:ILE:H	2.25	0.45
1:B:421:VAL:HB	1:D:322:GLU:HG2	1.99	0.45
1:D:646:PRO:HD2	7:D:956:HOH:O	2.16	0.44
1:F:204:THR:O	1:F:204:THR:HG23	2.17	0.44
1:D:57:CYS:SG	1:D:702:ARG:HD3	2.58	0.44
1:D:187:TYR:OH	1:D:222:ASP:OD2	2.34	0.44
1:F:92:THR:OG1	1:F:95:GLN:HG3	2.17	0.44
1:F:442:TYR:CZ	1:F:533:ALA:HB2	2.53	0.44
1:B:583:MET:HB3	1:B:611:LEU:HD22	1.98	0.44
1:D:633:MET:HE2	1:D:633:MET:HB3	1.88	0.44
1:F:218:ASP:O	1:F:219:GLN:C	2.61	0.44
1:B:323:GLU:HG3	1:B:326:TRP:CE3	2.53	0.44
1:D:255:CYS:HB3	2:D:801:A1CQU:O1	2.17	0.44
1:F:59:ILE:HG12	1:F:701:ALA:HB3	1.98	0.44
1:D:591:ILE:O	1:D:591:ILE:HG13	2.17	0.44
1:D:63:TYR:CD1	1:D:63:TYR:C	2.96	0.43
1:B:442:TYR:OH	1:B:533:ALA:HB2	2.18	0.43
1:D:39:THR:O	1:D:42:PHE:HB3	2.19	0.43
1:D:120:SER:HB2	1:D:125:VAL:HG23	1.99	0.43
1:F:262:TRP:CZ3	1:F:281:LYS:HE2	2.52	0.43
1:D:361:LEU:HD12	1:D:361:LEU:HA	1.89	0.43
1:F:97:GLN:O	1:F:117:ASN:ND2	2.32	0.43
1:F:420:ARG:NH1	1:F:420:ARG:CG	2.80	0.43
1:D:701:ALA:O	1:D:702:ARG:C	2.61	0.43
1:F:653:ILE:HD12	1:F:653:ILE:HA	1.91	0.43
1:B:617:LEU:HD21	1:B:651:LYS:HE2	2.01	0.43
1:D:293:VAL:HG22	1:D:341:ILE:HG23	1.99	0.43
1:D:435:TYR:HD1	1:D:457:LYS:HA	1.83	0.43
1:F:44:GLU:N	1:F:44:GLU:OE2	2.52	0.43
1:F:225:CYS:C	1:F:276:ILE:HD13	2.43	0.43
1:F:583:MET:HE1	1:F:599:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:SER:HB3	1:B:403:SER:HB2	2.00	0.43
1:F:315:ASN:HD21	1:F:329:LEU:HD13	1.84	0.43
1:B:355:HIS:O	1:B:356:ASP:C	2.62	0.43
1:F:266:LEU:C	1:F:268:GLN:H	2.27	0.43
1:F:440:ILE:HD13	1:F:536:TYR:CZ	2.54	0.43
1:B:323:GLU:HG3	1:B:326:TRP:CZ3	2.54	0.42
1:B:404:PRO:CD	1:B:427:VAL:HG22	2.49	0.42
1:B:411:ASP:OD2	1:B:414:LYS:HE2	2.19	0.42
1:D:298:THR:O	1:D:317:ASP:HA	2.19	0.42
1:F:267:GLN:CB	7:F:988:HOH:O	2.67	0.42
1:F:466:HIS:HB2	1:F:498:ILE:HD12	2.01	0.42
1:D:637:THR:OG1	1:D:638:ALA:N	2.53	0.42
1:F:289:GLU:O	1:F:304:THR:HA	2.19	0.42
1:B:359:ASN:HD22	1:B:359:ASN:HA	1.76	0.42
1:D:332:GLU:HG2	1:D:333:HIS:N	2.34	0.42
1:D:553:GLY:O	1:D:556:GLY:N	2.48	0.42
1:D:57:CYS:HB3	1:D:698:ALA:HB1	2.01	0.42
1:D:507:GLY:HA3	1:D:509:GLU:OE1	2.19	0.42
1:B:157:LYS:NZ	7:B:902:HOH:O	2.29	0.42
1:B:321:PRO:O	1:B:322:GLU:C	2.63	0.42
1:B:470:LEU:HB3	1:B:550:ILE:HG22	2.02	0.42
1:D:408:TYR:HA	1:D:420:ARG:O	2.19	0.42
1:B:257:PRO:C	1:B:289:GLU:HB2	2.45	0.42
1:F:400:SER:HB3	1:F:403:SER:HB3	2.00	0.42
1:F:617:LEU:HD11	1:F:651:LYS:HB3	2.01	0.42
1:F:51:VAL:N	1:F:52:PRO:CD	2.82	0.42
1:F:63:TYR:OH	1:F:487:SER:HA	2.19	0.42
1:F:626:ASP:O	1:F:627:ASP:HB2	2.20	0.42
1:F:74:PRO:HA	1:F:91:ASN:O	2.19	0.42
1:F:395:PHE:CD2	1:F:409:HIS:HB2	2.55	0.42
1:B:577:GLN:C	1:B:578:VAL:CG2	2.93	0.42
1:D:79:HIS:CE1	1:D:423:ARG:HH22	2.38	0.42
1:F:151:VAL:O	5:F:801:SCN:S	2.77	0.42
1:B:626:ASP:O	1:B:627:ASP:CB	2.68	0.42
1:D:57:CYS:HA	1:D:58:PRO:HD3	1.72	0.42
1:F:113:PHE:O	1:F:156:MET:HE1	2.20	0.42
1:B:474:GLY:HA3	1:B:504:ILE:HG13	2.01	0.41
1:D:596:THR:O	1:D:600:GLY:N	2.46	0.41
1:F:416:GLU:CD	1:F:416:GLU:C	2.88	0.41
1:F:351:LEU:HD12	1:F:351:LEU:N	2.35	0.41
1:B:98:ARG:HH11	1:B:98:ARG:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:PHE:HB3	1:D:98:ARG:HD2	2.01	0.41
1:D:210:LEU:HD22	1:D:249:LEU:CD1	2.50	0.41
1:F:428:LYS:C	1:F:430:ILE:H	2.28	0.41
1:D:66:ARG:NH2	1:D:69:GLU:CD	2.79	0.41
1:D:67:MET:HA	1:D:490:ILE:CD1	2.51	0.41
1:F:647:LEU:HD12	1:F:647:LEU:C	2.45	0.41
1:F:373:LYS:NZ	1:F:417:LEU:O	2.49	0.41
1:B:213:HIS:ND1	1:B:222:ASP:OD1	2.54	0.41
1:F:57:CYS:HA	1:F:58:PRO:HD3	1.92	0.41
1:F:321:PRO:O	1:F:322:GLU:C	2.63	0.41
1:D:210:LEU:HB3	1:D:226:ALA:HB3	2.03	0.41
1:B:122:ASP:OD2	1:B:677:LYS:NZ	2.50	0.41
1:D:156:MET:HA	1:D:162:LYS:O	2.21	0.41
1:D:166:ASP:OD2	1:D:215:LEU:HA	2.21	0.41
1:D:626:ASP:C	1:D:628[A]:ILE:H	2.26	0.41
1:F:358:LYS:HD2	1:F:379:VAL:HG13	2.03	0.41
1:B:75:LYS:O	1:B:90:TYR:HA	2.21	0.40
1:D:166:ASP:OD2	1:D:215:LEU:HD12	2.21	0.40
1:B:139:PHE:O	1:B:155:PHE:HA	2.21	0.40
1:B:504:ILE:HG22	1:B:529:ASP:HB3	2.03	0.40
1:F:104:ASP:OD2	6:F:803:PEG:H31	2.22	0.40
1:F:207:HIS:O	1:F:209:LYS:HE3	2.21	0.40
1:B:392:THR:HB	1:B:413:THR:HG23	2.03	0.40
1:B:453:PHE:O	1:B:500:ALA:HA	2.22	0.40
1:D:46:GLN:HB3	1:D:672:ILE:HG22	2.01	0.40
1:D:484:TYR:CE1	1:D:489:LEU:HD11	2.57	0.40
1:D:696:MET:HE2	1:D:696:MET:HB3	1.90	0.40
1:F:162:LYS:HE2	1:F:164:LEU:HD23	2.03	0.40
1:F:442:TYR:CZ	1:F:450:ILE:HB	2.56	0.40
1:F:643:ARG:HG2	1:F:680:HIS:CD2	2.57	0.40
1:F:33:ASP:OD2	1:F:36:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

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	B	705/711 (99%)	663 (94%)	39 (6%)	3 (0%)	30	22
1	D	708/711 (100%)	664 (94%)	38 (5%)	6 (1%)	16	8
1	F	705/711 (99%)	653 (93%)	49 (7%)	3 (0%)	30	22
All	All	2118/2133 (99%)	1980 (94%)	126 (6%)	12 (1%)	21	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	626	ASP
1	B	417	LEU
1	B	627	ASP
1	D	427	VAL
1	D	429	GLY
1	D	462	LEU
1	D	705	ASN
1	F	432	ALA
1	D	626	ASP
1	D	433	SER
1	F	590	THR
1	B	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	B	613/617 (99%)	589 (96%)	24 (4%)	28	21
1	D	616/617 (100%)	589 (96%)	27 (4%)	25	17
1	F	613/617 (99%)	592 (97%)	21 (3%)	32	25
All	All	1842/1851 (100%)	1770 (96%)	72 (4%)	28	21

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

Mol	Chain	Res	Type
1	B	5	GLN
1	B	66	ARG
1	B	107	GLU
1	B	109	GLU
1	B	111	ARG
1	B	252	ARG
1	B	261	LEU
1	B	270	SER
1	B	335	LYS
1	B	357	VAL
1	B	359	ASN
1	B	406	ILE
1	B	415	GLU
1	B	423	ARG
1	B	427	VAL
1	B	430	ILE
1	B	512	GLU
1	B	547	ARG
1	B	554	SER
1	B	598	ASP
1	B	612	VAL
1	B	622	LEU
1	B	665	LYS
1	B	707	ASP
1	D	8	ASP
1	D	49	ILE
1	D	59	ILE
1	D	84	LYS
1	D	103	GLN
1	D	107	GLU
1	D	120	SER
1	D	192	GLN
1	D	228	PHE
1	D	256	ASP
1	D	267	GLN
1	D	321	PRO
1	D	335	LYS
1	D	346	SER
1	D	357	VAL
1	D	373	LYS
1	D	399	THR
1	D	400	SER
1	D	415	GLU

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Mol	Chain	Res	Type
1	D	433	SER
1	D	512	GLU
1	D	570	LEU
1	D	588	LYS
1	D	598	ASP
1	D	604	SER
1	D	626	ASP
1	D	649	SER
1	F	44	GLU
1	F	84	LYS
1	F	107	GLU
1	F	192	GLN
1	F	215	LEU
1	F	233	LYS
1	F	256	ASP
1	F	261	LEU
1	F	264	CYS
1	F	267	GLN
1	F	400	SER
1	F	416	GLU
1	F	420	ARG
1	F	425	VAL
1	F	426	THR
1	F	427	VAL
1	F	428	LYS
1	F	430	ILE
1	F	438	VAL
1	F	512	GLU
1	F	539	LYS

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

Mol	Chain	Res	Type
1	B	5	GLN
1	B	180	HIS
1	B	192	GLN
1	B	397	GLN
1	B	524	GLN
1	B	531	GLN
1	B	566	GLN
1	D	103	GLN
1	D	193	GLN

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Mol	Chain	Res	Type
1	D	267	GLN
1	D	362	GLN
1	D	397	GLN
1	D	439	GLN
1	D	483	ASN
1	D	551	ASN
1	D	668	ASN
1	F	22	HIS
1	F	79	HIS
1	F	192	GLN
1	F	362	GLN
1	F	388	GLN
1	F	397	GLN
1	F	503	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](#)

19 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	B3P	B	802	-	18,18,18	0.52	0	23,23,23	1.19	1 (4%)
4	GOL	B	805	-	5,5,5	0.11	0	5,5,5	0.38	0
5	SCN	B	807	-	1,2,2	0.73	0	0,1,1	-	-
5	SCN	F	801	-	1,2,2	0.29	0	0,1,1	-	-
4	GOL	B	804	-	5,5,5	0.13	0	5,5,5	0.45	0
5	SCN	B	811	-	1,2,2	0.27	0	0,1,1	-	-
2	A1CQU	D	801	-	25,25,26	1.06	1 (4%)	31,35,37	1.29	3 (9%)
4	GOL	B	809	-	5,5,5	0.19	0	5,5,5	0.25	0
4	GOL	B	803	-	5,5,5	0.10	0	5,5,5	0.25	0
4	GOL	D	804	-	5,5,5	0.13	0	5,5,5	0.40	0
2	A1CQU	F	802	1	25,25,26	0.89	2 (8%)	31,35,37	0.97	2 (6%)
5	SCN	B	808	-	1,2,2	0.36	0	0,1,1	-	-
2	A1CQU	B	801	1	25,25,26	1.27	2 (8%)	31,35,37	1.15	2 (6%)
6	PEG	F	803	-	6,6,6	0.24	0	5,5,5	0.25	0
5	SCN	D	805	-	1,2,2	0.57	0	0,1,1	-	-
4	GOL	D	802	-	5,5,5	0.14	0	5,5,5	0.36	0
4	GOL	B	810	-	5,5,5	0.21	0	5,5,5	0.38	0
5	SCN	B	806	-	1,2,2	0.23	0	0,1,1	-	-
4	GOL	D	803	-	5,5,5	0.10	0	5,5,5	0.34	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
6	PEG	F	803	-	-	3/4/4/4	-
2	A1CQU	D	801	-	-	10/14/21/21	0/3/3/3
3	B3P	B	802	-	-	12/28/28/28	-
4	GOL	D	802	-	-	2/4/4/4	-
4	GOL	B	809	-	-	4/4/4/4	-
4	GOL	B	810	-	-	3/4/4/4	-
2	A1CQU	F	802	1	-	5/14/21/21	0/3/3/3
4	GOL	B	805	-	-	0/4/4/4	-
4	GOL	B	803	-	-	0/4/4/4	-
4	GOL	D	803	-	-	1/4/4/4	-
2	A1CQU	B	801	1	-	6/14/21/21	0/3/3/3
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	D	804	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1CQU	C2-N1	5.40	1.37	1.32
2	D	801	A1CQU	C2-N1	4.28	1.36	1.32
2	F	802	A1CQU	C16-C4	-2.61	1.37	1.41
2	F	802	A1CQU	C2-N1	2.26	1.34	1.32
2	B	801	A1CQU	C5-C6	2.13	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1CQU	C16-C2-N1	-3.68	109.32	110.76
3	B	802	B3P	C3-N1-C4	3.50	121.28	116.17
2	D	801	A1CQU	C16-C2-N1	-3.43	109.41	110.76
2	F	802	A1CQU	C16-C4-N3	-2.65	123.87	127.01
2	D	801	A1CQU	C9-C8-N4	2.28	116.86	112.00
2	D	801	A1CQU	O2-C10-C9	-2.24	115.21	121.26
2	F	802	A1CQU	C15-C6-C5	-2.21	115.66	117.92
2	B	801	A1CQU	C15-C16-C2	2.08	138.91	136.72

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	A1CQU	O2-C10-N5-C11
2	D	801	A1CQU	C9-C10-N5-C11
2	D	801	A1CQU	C9-C10-N5-C14
2	D	801	A1CQU	O2-C10-N5-C11
2	D	801	A1CQU	O2-C10-N5-C14
2	F	802	A1CQU	O2-C10-N5-C14
3	B	802	B3P	C5-C4-N1-C3
3	B	802	B3P	C6-C4-N1-C3
3	B	802	B3P	C7-C4-N1-C3
3	B	802	B3P	N2-C8-C9-O1
3	B	802	B3P	C11-C8-C9-O1
4	B	804	GOL	O1-C1-C2-O2
4	B	804	GOL	O1-C1-C2-C3
4	B	809	GOL	O1-C1-C2-C3
4	B	810	GOL	C1-C2-C3-O3
4	B	810	GOL	O2-C2-C3-O3
4	D	802	GOL	O1-C1-C2-C3
4	D	804	GOL	C1-C2-C3-O3
2	F	802	A1CQU	C15-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
2	F	802	A1CQU	C15-C6-C7-N4
2	F	802	A1CQU	C5-C6-C7-O1
2	D	801	A1CQU	C15-C6-C7-N4
2	D	801	A1CQU	C5-C6-C7-N4
2	F	802	A1CQU	C5-C6-C7-N4
2	D	801	A1CQU	C5-C6-C7-O1
2	D	801	A1CQU	C15-C6-C7-O1
3	B	802	B3P	C2-C1-C3-N1
4	D	802	GOL	O1-C1-C2-O2
3	B	802	B3P	C1-C2-N2-C8
3	B	802	B3P	C1-C3-N1-C4
2	B	801	A1CQU	C15-C6-C7-N4
4	B	809	GOL	C1-C2-C3-O3
4	B	810	GOL	O1-C1-C2-C3
6	F	803	PEG	O1-C1-C2-O2
4	B	809	GOL	O1-C1-C2-O2
4	B	809	GOL	O2-C2-C3-O3
4	D	804	GOL	O2-C2-C3-O3
3	B	802	B3P	O3-C11-C8-C9
2	B	801	A1CQU	N4-C8-C9-C10
2	B	801	A1CQU	C15-C6-C7-O1
2	D	801	A1CQU	N5-C10-C9-C8
4	D	804	GOL	O1-C1-C2-O2
6	F	803	PEG	C1-C2-O2-C3
6	F	803	PEG	C4-C3-O2-C2
2	B	801	A1CQU	C5-C6-C7-N4
2	D	801	A1CQU	O2-C10-C9-C8
3	B	802	B3P	C10-C8-C9-O1
3	B	802	B3P	O3-C11-C8-C10
3	B	802	B3P	O3-C11-C8-N2
4	D	803	GOL	C1-C2-C3-O3
2	B	801	A1CQU	C5-C6-C7-O1

There are no ring outliers.

6 monomers are involved in 9 short contacts:

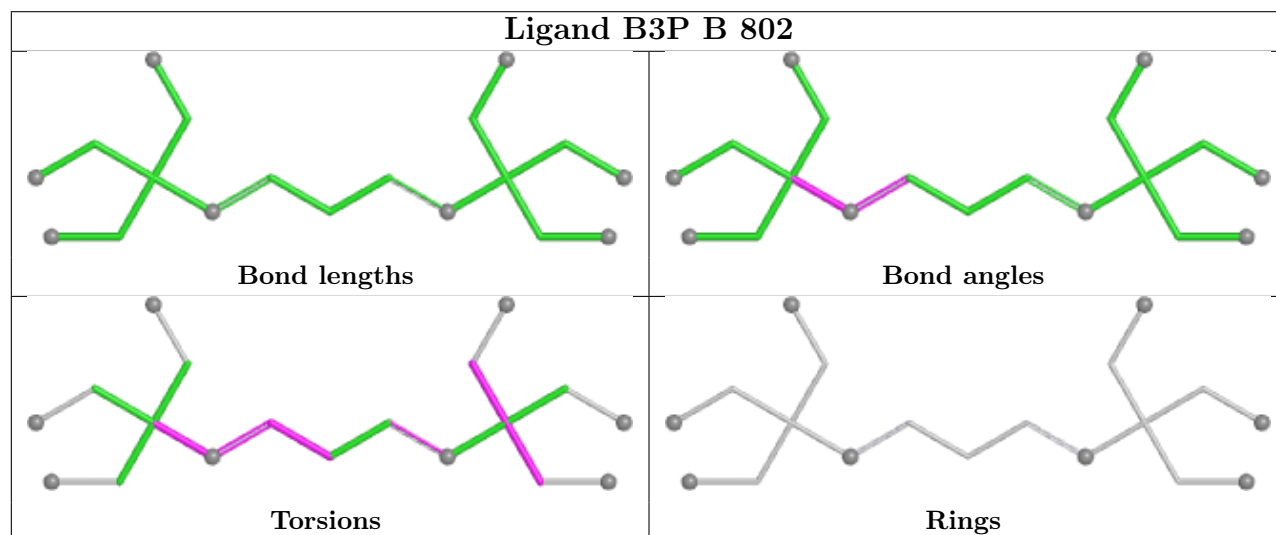
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	807	SCN	1	0
5	F	801	SCN	1	0
2	D	801	A1CQU	2	0
6	F	803	PEG	1	0
5	D	805	SCN	1	0

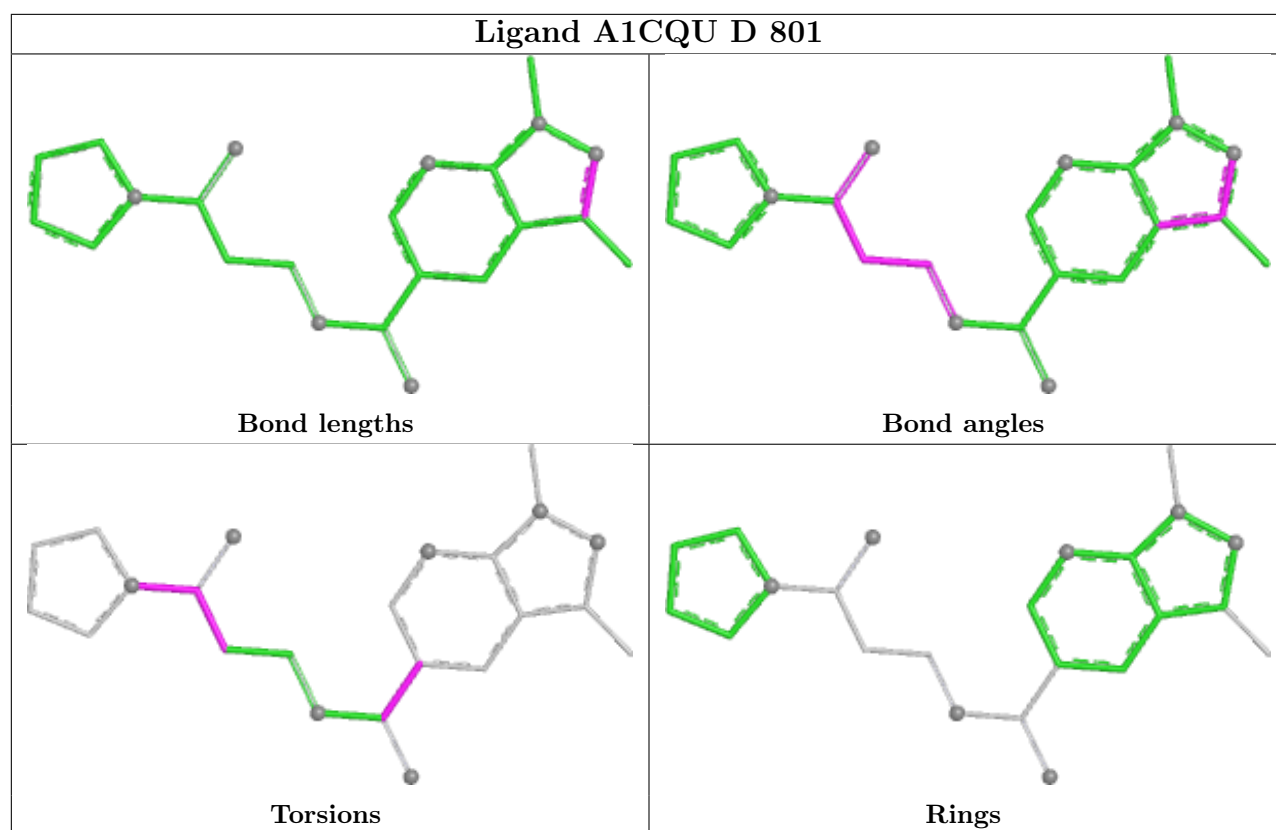
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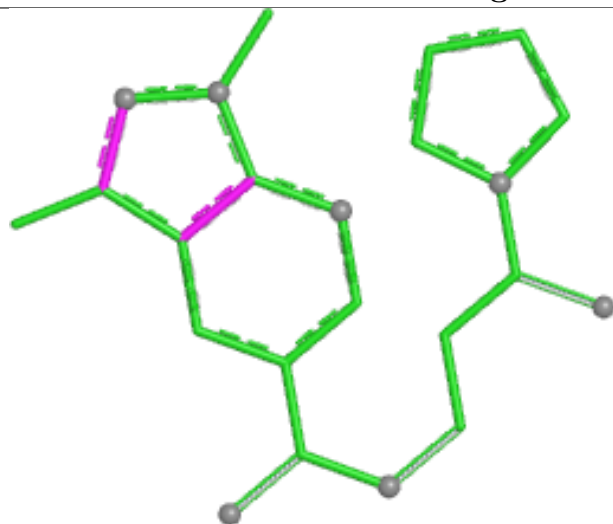
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	GOL	3	0

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.

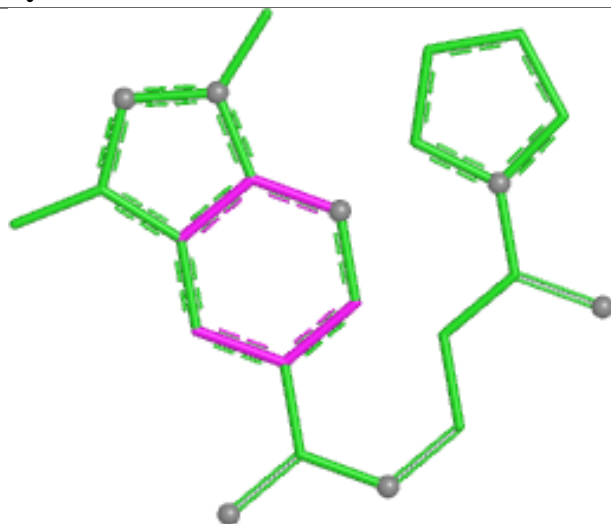




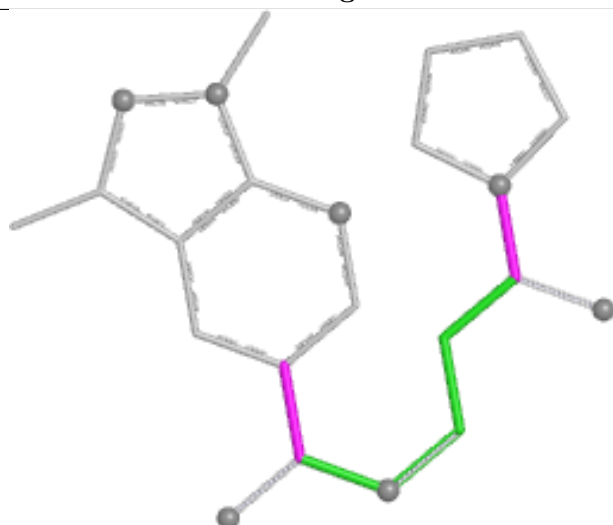
Ligand A1CQU F 802



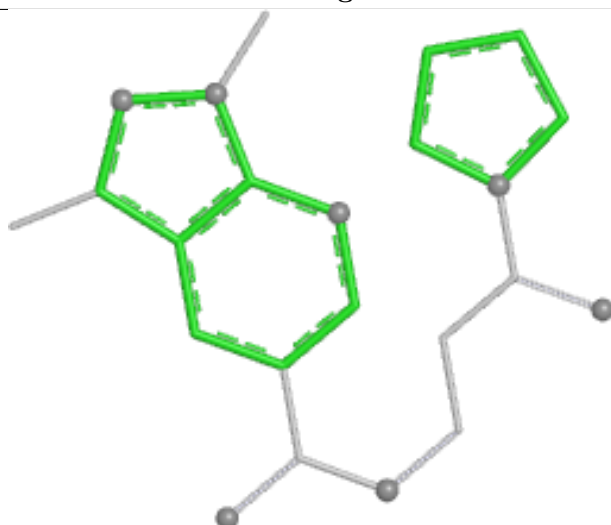
Bond lengths



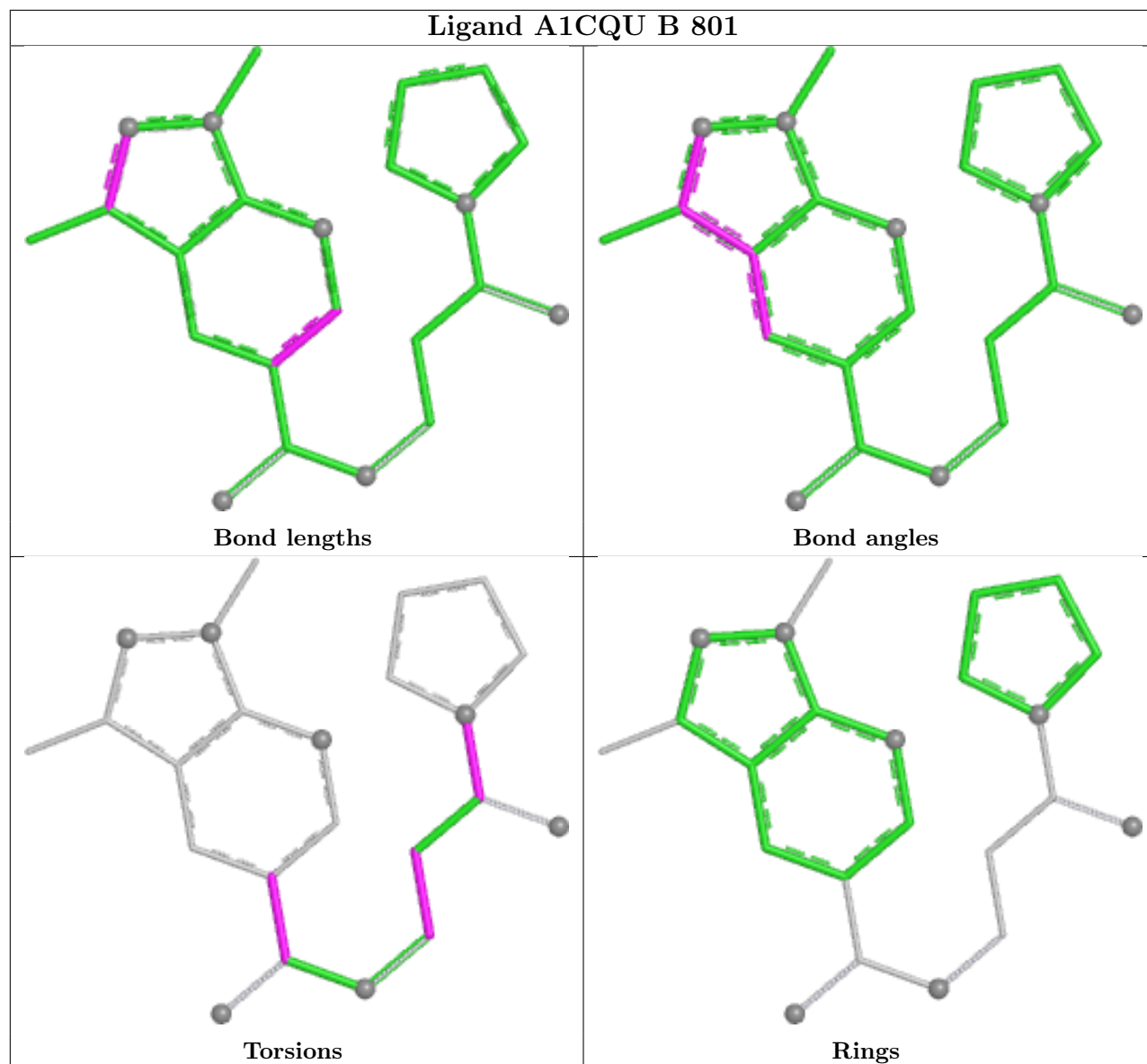
Bond angles



Torsions



Rings



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	B	706/711 (99%)	-0.39	1 (0%)	92 92	10, 15, 22, 31	1 (0%)
1	D	706/711 (99%)	-0.23	2 (0%)	90 91	9, 18, 25, 35	2 (0%)
1	F	706/711 (99%)	-0.28	2 (0%)	90 91	11, 18, 25, 36	1 (0%)
All	All	2118/2133 (99%)	-0.30	5 (0%)	91 92	9, 17, 25, 36	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	426	THR	2.7
1	D	430	ILE	2.6
1	B	426	THR	2.4
1	F	427	VAL	2.3
1	F	546	LYS	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

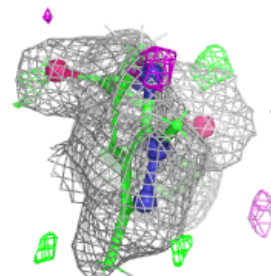
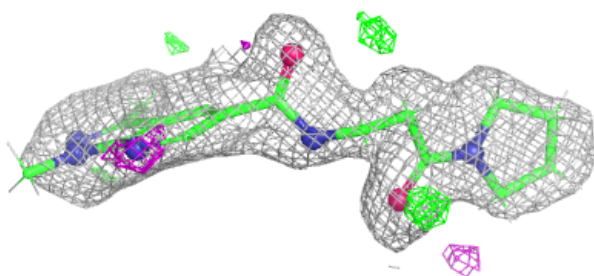
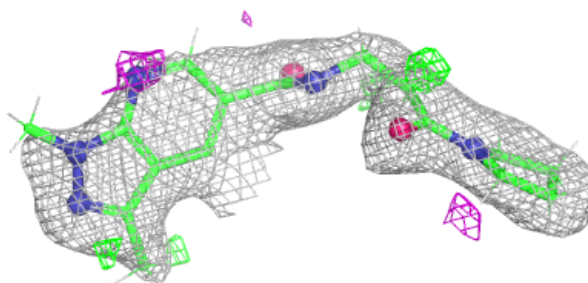
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	810	6/6	0.55	0.31	17,18,31,31	14
4	GOL	B	809	6/6	0.60	0.26	14,15,31,31	14
5	SCN	D	805	3/3	0.62	0.30	16,16,18,23	3
4	GOL	D	804	6/6	0.72	0.31	18,20,31,31	14
4	GOL	D	803	6/6	0.75	0.30	18,19,31,31	14
6	PEG	F	803	7/7	0.82	0.25	17,19,31,31	17
5	SCN	B	811	3/3	0.85	0.28	20,20,21,23	3
2	A1CQU	F	802	23/24	0.87	0.10	19,21,31,31	6
5	SCN	B	806	3/3	0.91	0.12	24,24,24,26	0
5	SCN	B	808	3/3	0.92	0.12	23,23,25,28	0
4	GOL	D	802	6/6	0.92	0.07	17,18,31,31	3
4	GOL	B	805	6/6	0.92	0.10	17,20,31,31	3
5	SCN	B	807	3/3	0.92	0.22	12,12,13,16	3
2	A1CQU	B	801	23/24	0.94	0.07	14,16,31,31	6
3	B3P	B	802	19/19	0.94	0.06	14,16,31,31	8
4	GOL	B	804	6/6	0.94	0.06	17,20,31,31	3
4	GOL	B	803	6/6	0.95	0.08	13,15,31,31	3
2	A1CQU	D	801	23/24	0.95	0.06	15,18,31,31	6
5	SCN	F	801	3/3	0.97	0.07	19,19,22,23	0

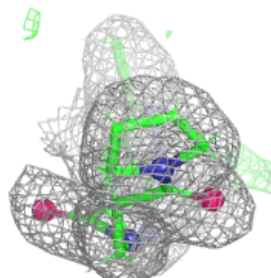
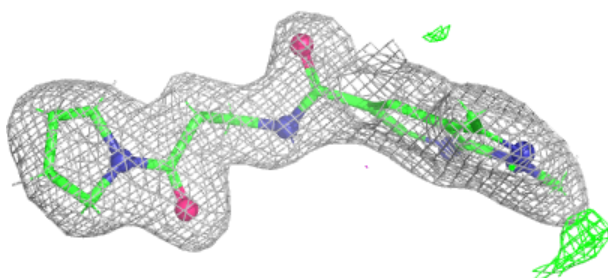
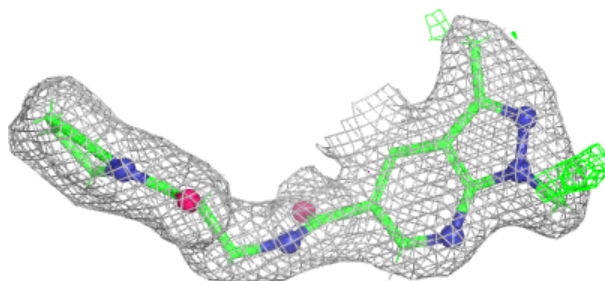
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CQU F 802:

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

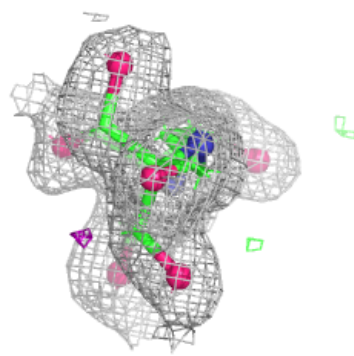
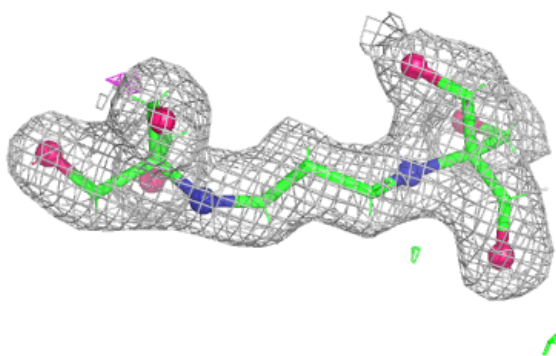
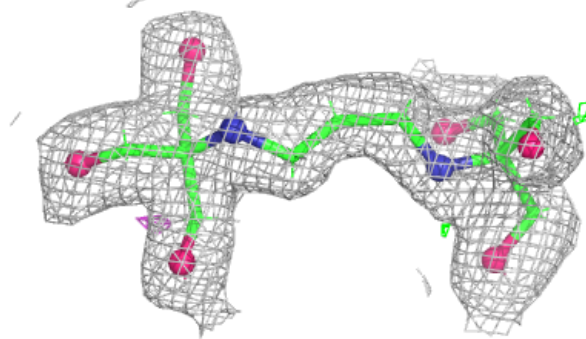
**Electron density around A1CQU B 801:**

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

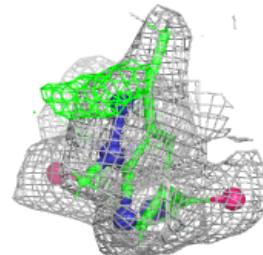
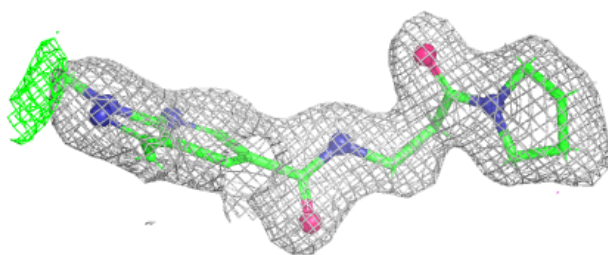
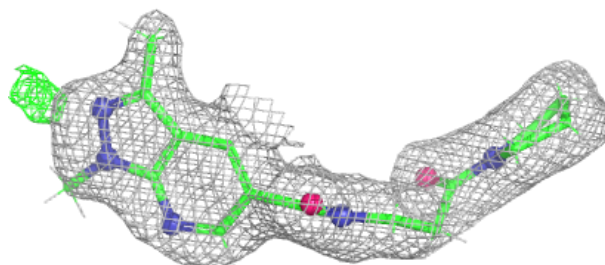


Electron density around B3P B 802:

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

**Electron density around A1CQU D 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.