



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:39 PM UTC

PDB ID : 9Q66 / pdb_00009q66
Title : Human prolyl endopeptidase (PREP) - complex with JP-4-1-7
Authors : Fucci, I.J.; Thakur, K.; Pandian, J.; Yoo, E.; Monteiro, D.C.F.
Deposited on : 2025-08-21
Resolution : 2.01 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

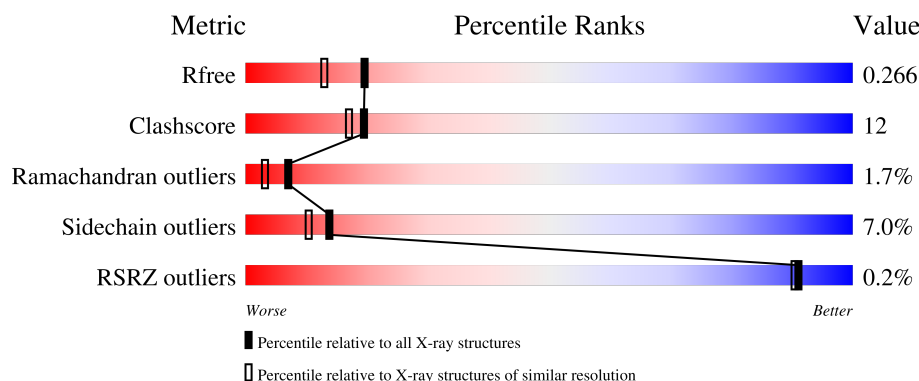
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	74% 21% . ..
1	B	711	56% 34% 8% ..
1	C	711	57% 33% 7% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	803	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34673 atoms, of which 16734 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.

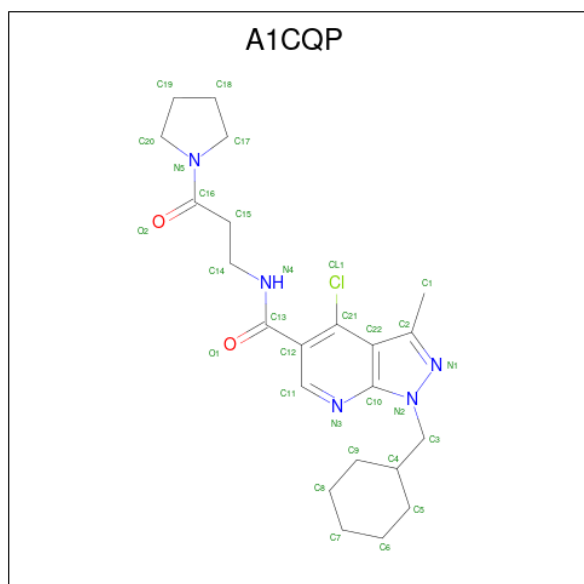
- Molecule 1 is a protein called Prolyl endopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	707	Total	C	H	N	O	S	176	2	0
			11249	3654	5552	950	1066	27			
1	B	707	Total	C	H	N	O	S	176	0	0
			11186	3639	5513	941	1066	27			
1	C	707	Total	C	H	N	O	S	176	0	0
			11186	3639	5513	941	1066	27			

There are 3 discrepancies between the modelled and reference sequences:

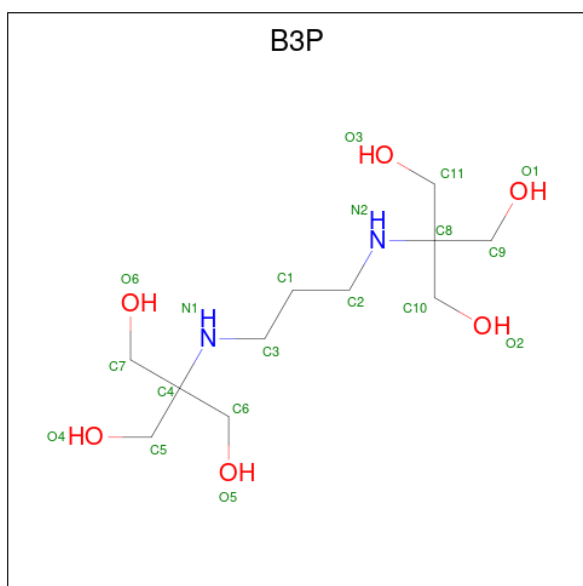
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P48147
B	0	GLY	-	expression tag	UNP P48147
C	0	GLY	-	expression tag	UNP P48147

- Molecule 2 is 4-chloro-1-(cyclohexylmethyl)-3-methyl-N-[3-oxo-3-(pyrrolidin-1-yl)propyl]-1H-pyrazolo[3,4-b]pyridine-5-carboxamide (CCD ID: A1CQP) (formula: C₂₂H₃₀ClN₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	3	0
			59	22	30	5	2		
2	B	1	Total	C	H	N	O	3	0
			59	22	30	5	2		
2	C	1	Total	C	H	N	O	3	0
			59	22	30	5	2		

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



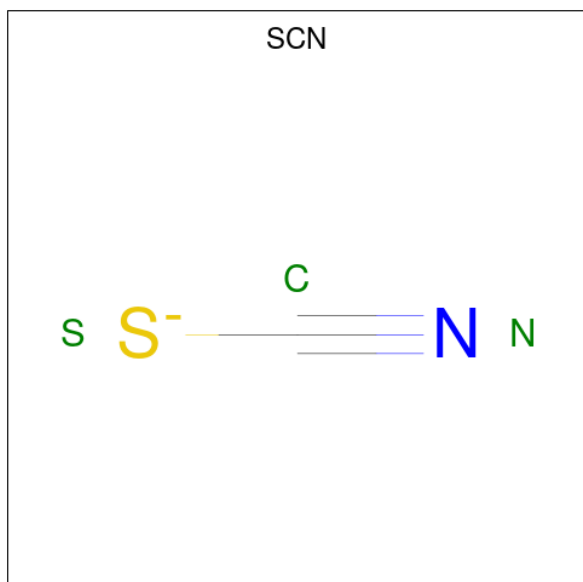
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	8	0
			45	11	26	2	6		

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



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

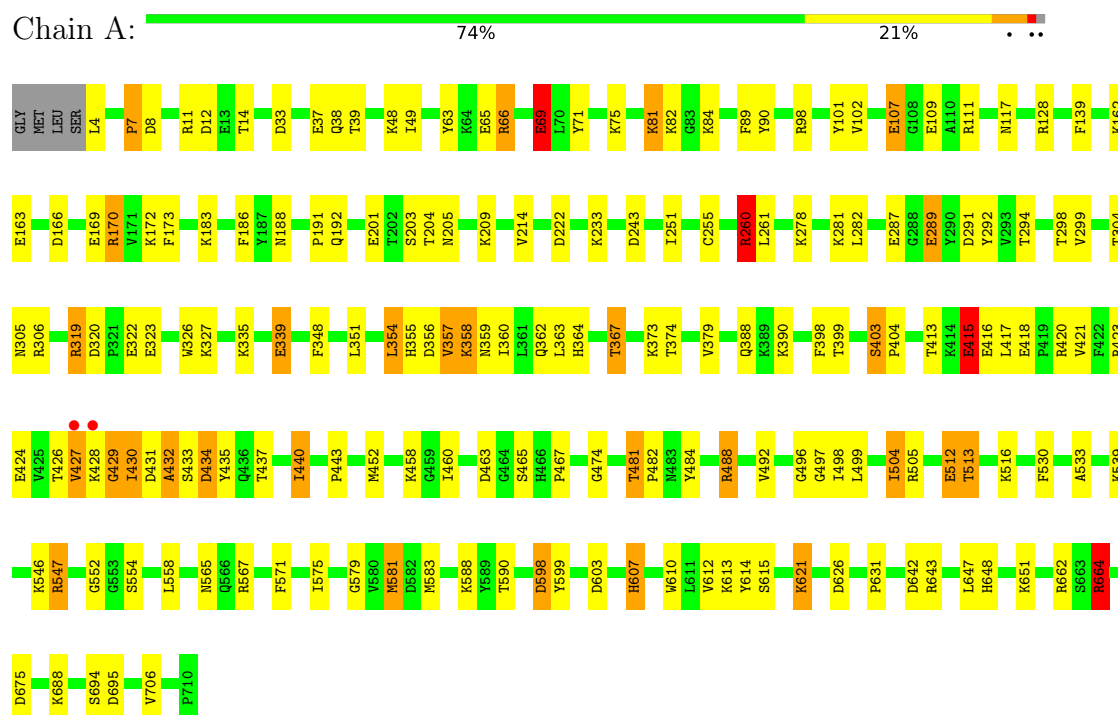
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	421	Total O 421 421	0	0
6	B	188	Total O 188 188	0	0
6	C	130	Total O 130 130	0	0

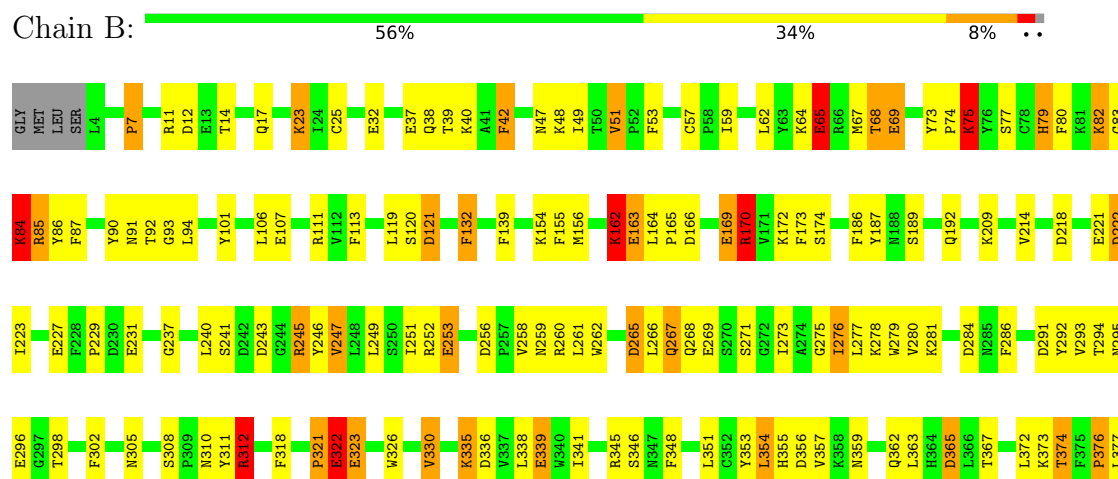
3 Residue-property plots

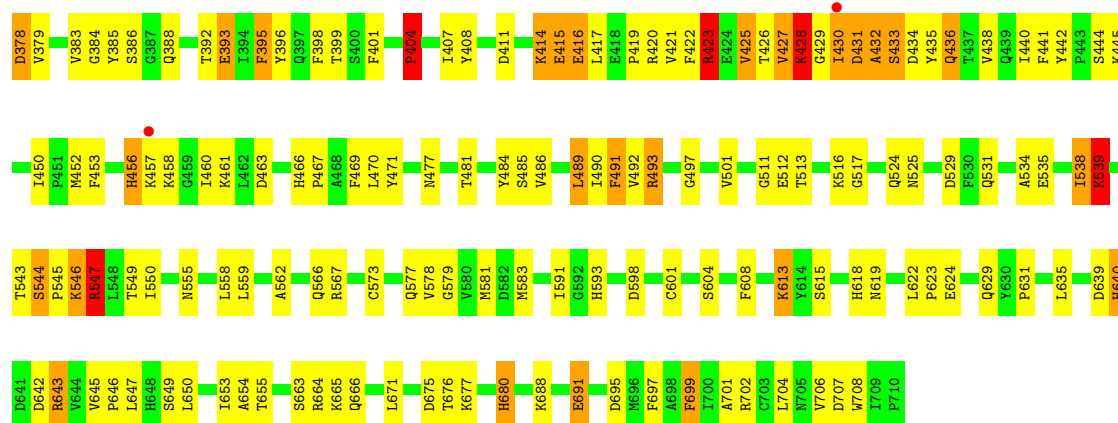
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



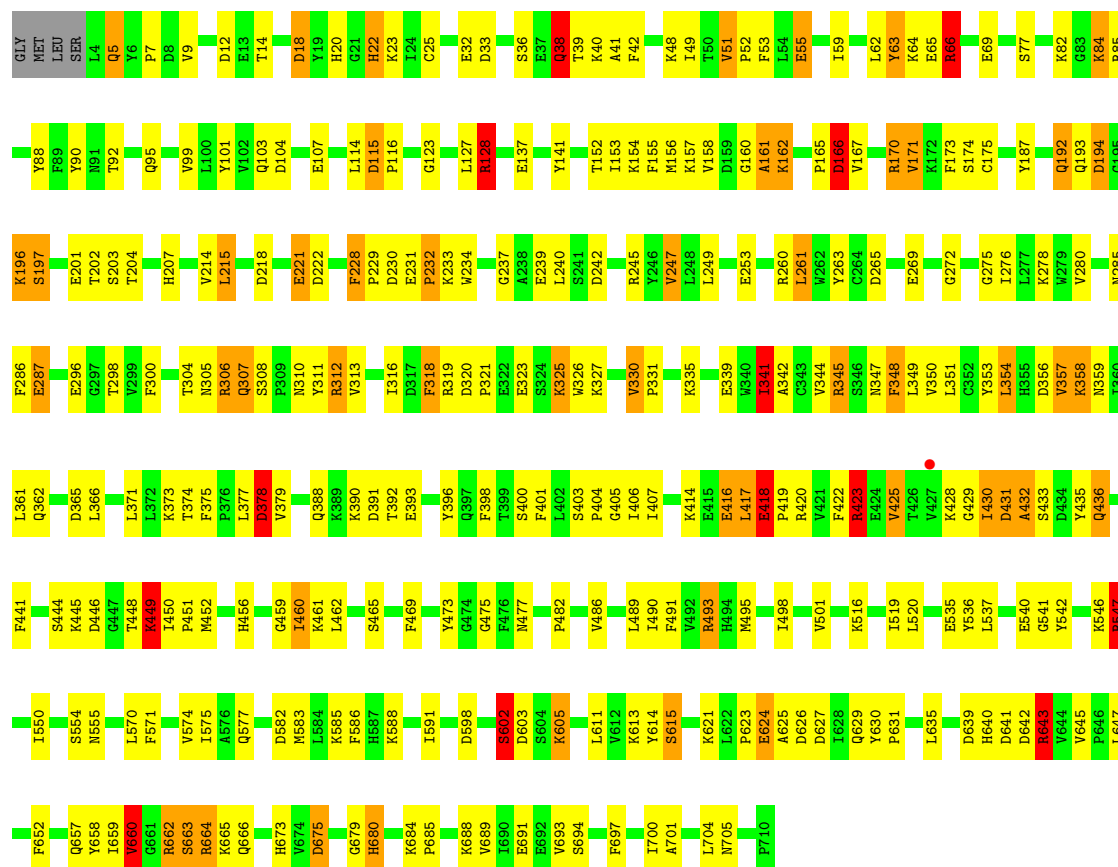
• Molecule 1: Prolyl endopeptidase





• Molecule 1: Prolyl endopeptidase

Chain C: 57% 33% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.85Å 67.29Å 158.02Å 90.00° 99.11° 90.00°	Depositor
Resolution (Å)	44.00 – 2.01 44.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	73.4 (44.00-2.01) 73.4 (44.00-2.01)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.184 , 0.266 0.185 , 0.266	Depositor DCC
R_{free} test set	7315 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34673	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% 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: A1CQP, B3P, SCN, GOL

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	1.14	8/5858 (0.1%)	1.76	104/7939 (1.3%)
1	B	1.02	5/5825 (0.1%)	1.78	118/7897 (1.5%)
1	C	0.95	2/5825 (0.0%)	1.78	136/7897 (1.7%)
All	All	1.04	15/17508 (0.1%)	1.77	358/23733 (1.5%)

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	12
1	B	0	15
1	C	0	6
All	All	0	33

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	618	HIS	CE1-NE2	6.37	1.39	1.32
1	C	615	SER	CA-CB	-6.09	1.43	1.53
1	B	555	ASN	C-O	-5.97	1.16	1.24
1	A	581	MET	C-O	-5.89	1.16	1.24
1	A	567	ARG	NE-CZ	5.86	1.39	1.33
1	B	189	SER	CA-CB	-5.70	1.43	1.54
1	A	37	GLU	CD-OE1	5.65	1.36	1.25
1	A	37	GLU	CD-OE2	5.39	1.35	1.25
1	B	174	SER	CA-CB	-5.38	1.44	1.53
1	A	363	LEU	C-O	-5.21	1.17	1.24
1	A	482	PRO	CA-CB	-5.16	1.47	1.53
1	A	203	SER	CA-CB	-5.14	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	646	PRO	CA-CB	-5.12	1.46	1.53
1	A	452	MET	C-O	-5.09	1.18	1.23
1	C	308	SER	CA-CB	-5.02	1.47	1.53

All (358) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	624	GLU	N-CA-CB	12.79	129.33	110.53
1	B	339	GLU	CB-CA-C	-11.35	88.66	110.11
1	A	513	THR	CA-CB-OG1	-10.65	93.63	109.60
1	B	339	GLU	N-CA-CB	10.63	126.09	110.26
1	C	378	ASP	CA-CB-CG	-10.35	102.25	112.60
1	C	603	ASP	CA-CB-CG	10.26	122.86	112.60
1	A	499	LEU	N-CA-CB	-9.91	95.02	110.57
1	C	449	LYS	CB-CA-C	-9.85	94.14	110.29
1	A	320	ASP	CA-CB-CG	9.54	122.14	112.60
1	A	374	THR	CA-CB-OG1	-9.42	95.47	109.60
1	B	322	GLU	CB-CG-CD	9.14	128.14	112.60
1	A	443	PRO	CB-CA-C	8.94	119.54	111.40
1	C	416	GLU	CB-CA-C	-8.85	96.22	110.81
1	C	540	GLU	CB-CA-C	8.83	124.83	110.09
1	B	367	THR	CA-CB-OG1	-8.82	96.38	109.60
1	C	449	LYS	N-CA-CB	8.78	124.18	109.87
1	C	38	GLN	N-CA-CB	8.77	122.73	110.01
1	A	14	THR	CA-CB-OG1	-8.77	96.45	109.60
1	A	512	GLU	N-CA-CB	8.67	123.07	110.06
1	C	204	THR	CA-CB-OG1	-8.57	96.75	109.60
1	C	331	PRO	CB-CA-C	8.54	122.16	110.98
1	A	367	THR	CA-CB-OG1	-8.36	97.06	109.60
1	B	425	VAL	N-CA-CB	8.33	119.80	110.72
1	A	373	LYS	CB-CA-C	-8.31	95.17	110.62
1	A	428	LYS	N-CA-CB	8.30	122.99	109.88
1	B	113	PHE	CA-CB-CG	-8.28	105.52	113.80
1	B	269	GLU	CB-CG-CD	8.25	126.63	112.60
1	B	139	PHE	N-CA-CB	-8.20	97.41	110.77
1	B	697	PHE	CA-CB-CG	-8.18	105.62	113.80
1	A	434	ASP	CB-CA-C	-8.07	97.40	110.79
1	A	65	GLU	CB-CG-CD	7.99	126.18	112.60
1	B	404	PRO	CA-C-N	-7.92	116.55	122.33
1	B	404	PRO	C-N-CA	-7.92	116.55	122.33
1	B	420	ARG	CB-CA-C	7.91	124.14	110.45
1	C	422	PHE	N-CA-CB	-7.89	97.08	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	LYS	N-CA-CB	7.87	121.93	110.20
1	C	418	GLU	CB-CG-CD	7.83	125.92	112.60
1	A	163	GLU	CB-CA-C	-7.83	96.29	109.53
1	C	356	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	81	LYS	N-CA-CB	-7.66	97.82	110.23
1	C	374	THR	CA-CB-OG1	-7.62	98.17	109.60
1	B	549	THR	CA-CB-OG1	7.59	120.99	109.60
1	C	388	GLN	N-CA-CB	-7.59	99.06	110.60
1	C	201	GLU	CB-CG-CD	7.53	125.40	112.60
1	C	166	ASP	CA-CB-CG	7.41	120.01	112.60
1	C	247	VAL	N-CA-CB	7.38	119.42	111.00
1	B	422	PHE	CB-CA-C	7.36	123.19	110.23
1	B	163	GLU	CB-CG-CD	-7.36	100.10	112.60
1	C	577	GLN	CB-CA-C	7.35	121.85	109.80
1	B	75	LYS	CB-CA-C	7.34	123.89	109.35
1	A	69	GLU	N-CA-CB	-7.34	99.26	110.20
1	B	593	HIS	CA-CB-CG	7.32	121.12	113.80
1	A	37	GLU	CB-CA-C	-7.29	98.28	110.68
1	A	413	THR	CA-CB-OG1	7.27	120.51	109.60
1	B	23	LYS	CB-CA-C	7.27	121.81	109.53
1	A	496	GLY	CA-C-N	-7.26	113.98	122.77
1	A	496	GLY	C-N-CA	-7.26	113.98	122.77
1	C	461	LYS	CB-CA-C	-7.26	96.31	109.38
1	A	243	ASP	CA-CB-CG	7.25	119.85	112.60
1	C	540	GLU	N-CA-CB	-7.23	99.79	110.49
1	B	408	TYR	CB-CA-C	-7.22	95.65	109.66
1	C	40	LYS	N-CA-CB	7.17	120.41	110.01
1	C	318	PHE	N-CA-CB	-7.14	99.63	110.12
1	C	320	ASP	CA-CB-CG	7.11	119.71	112.60
1	B	214	VAL	N-CA-CB	7.09	118.89	110.95
1	B	310	ASN	CB-CA-C	-7.07	98.61	110.56
1	C	705	ASN	CA-CB-CG	-7.06	105.54	112.60
1	A	664	ARG	CA-CB-CG	7.05	128.19	114.10
1	B	65	GLU	N-CA-CB	-7.03	99.78	110.12
1	C	664	ARG	CB-CA-C	7.03	122.60	110.79
1	C	697	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	463	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	63	TYR	N-CA-CB	7.00	120.37	109.94
1	B	291	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	469	PHE	CA-CB-CG	6.98	120.78	113.80
1	C	451	PRO	CB-CA-C	-6.98	101.93	111.21
1	A	552	GLY	O-C-N	6.96	130.04	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	ASP	CB-CA-C	6.95	123.59	109.76
1	B	695	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	388	GLN	N-CA-CB	-6.84	99.49	110.51
1	B	396	TYR	CA-CB-CG	6.84	126.20	113.90
1	A	117	ASN	CA-CB-CG	-6.81	105.79	112.60
1	B	642	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	107	GLU	CB-CA-C	6.78	123.10	111.45
1	B	286	PHE	N-CA-CB	-6.74	100.11	111.17
1	B	14	THR	CA-CB-OG1	-6.73	99.50	109.60
1	A	98	ARG	CB-CA-C	6.72	121.91	109.54
1	C	18	ASP	CA-CB-CG	6.72	119.33	112.60
1	C	448	THR	OG1-CB-CG2	-6.71	95.87	109.30
1	C	577	GLN	N-CA-CB	-6.70	99.10	110.16
1	C	242	ASP	CA-CB-CG	6.69	119.29	112.60
1	C	613	LYS	N-CA-CB	-6.67	100.31	110.12
1	C	624	GLU	CB-CA-C	-6.67	97.15	109.29
1	A	424	GLU	N-CA-CB	-6.67	99.20	111.13
1	C	626	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	481	THR	CA-CB-OG1	-6.66	99.61	109.60
1	C	306	ARG	CD-NE-CZ	6.65	133.71	124.40
1	A	287	GLU	CB-CG-CD	6.63	123.87	112.60
1	C	202	THR	CA-CB-OG1	-6.62	99.67	109.60
1	B	383	VAL	N-CA-CB	-6.62	103.72	112.26
1	A	139	PHE	N-CA-CB	-6.61	99.70	110.81
1	C	318	PHE	CB-CA-C	6.61	121.75	110.79
1	A	173	PHE	N-CA-CB	-6.59	102.19	111.62
1	C	645	VAL	N-CA-CB	6.59	116.21	110.08
1	C	23	LYS	N-CA-CB	-6.58	99.57	110.23
1	B	362	GLN	CB-CA-C	-6.57	98.13	110.16
1	C	362	GLN	CB-CA-C	-6.57	96.32	110.45
1	C	85	ARG	CD-NE-CZ	6.56	133.58	124.40
1	B	84	LYS	CB-CA-C	-6.55	99.86	110.74
1	C	12	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	192	GLN	CB-CA-C	6.48	120.25	109.89
1	A	664	ARG	CD-NE-CZ	6.48	133.47	124.40
1	C	416	GLU	CB-CG-CD	-6.47	101.61	112.60
1	C	33	ASP	CB-CA-C	-6.46	102.65	110.08
1	C	652	PHE	CA-CB-CG	6.45	120.25	113.80
1	C	171	VAL	N-CA-CB	6.44	117.74	110.72
1	B	293	VAL	N-CA-CB	-6.43	104.34	111.41
1	C	449	LYS	CA-CB-CG	6.43	126.95	114.10
1	A	339	GLU	CB-CA-C	-6.40	98.02	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	GLU	CB-CG-CD	-6.39	101.74	112.60
1	C	419	PRO	CB-CA-C	-6.38	103.22	111.46
1	A	7	PRO	CB-CA-C	6.37	119.33	110.98
1	B	121	ASP	CB-CA-C	-6.37	97.27	109.95
1	C	296	GLU	CG-CD-OE2	-6.35	103.80	118.40
1	A	335	LYS	N-CA-CB	-6.33	101.44	110.81
1	A	109	GLU	N-CA-C	-6.33	101.06	110.23
1	A	424	GLU	CA-C-N	-6.33	114.64	122.93
1	A	424	GLU	C-N-CA	-6.33	114.64	122.93
1	C	396	TYR	CA-C-N	-6.33	114.08	123.00
1	C	396	TYR	C-N-CA	-6.33	114.08	123.00
1	A	403	SER	CB-CA-C	-6.31	102.82	110.08
1	C	348	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	89	PHE	O-C-N	6.29	130.11	123.06
1	C	423	ARG	N-CA-CB	6.29	121.38	110.81
1	C	39	THR	CA-CB-OG1	-6.29	100.17	109.60
1	B	335	LYS	N-CA-CB	-6.23	99.97	110.49
1	B	330	VAL	N-CA-CB	6.22	119.91	111.21
1	C	547	ARG	CB-CG-CD	6.20	125.55	111.30
1	C	392	THR	CA-CB-OG1	6.19	118.89	109.60
1	C	335	LYS	CB-CA-C	6.19	121.53	111.26
1	B	296	GLU	N-CA-C	-6.17	97.66	110.80
1	C	642	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	434	ASP	N-CA-C	6.16	118.00	111.28
1	A	90	TYR	N-CA-CB	-6.15	100.08	111.52
1	B	376	PRO	O-C-N	6.15	130.42	123.04
1	C	128	ARG	NE-CZ-NH1	-6.15	115.35	121.50
1	C	341	ILE	CA-C-O	-6.15	114.86	121.19
1	A	186	PHE	N-CA-CB	6.12	120.39	110.41
1	A	291	ASP	N-CA-CB	-6.11	101.12	110.65
1	C	40	LYS	CB-CA-C	-6.09	101.33	110.88
1	C	491	PHE	N-CA-CB	-6.07	101.19	110.12
1	A	39	THR	N-CA-C	-6.04	104.78	111.36
1	A	222	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	469	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	39	THR	OG1-CB-CG2	-6.03	97.25	109.30
1	A	163	GLU	CB-CG-CD	-6.03	102.36	112.60
1	B	68	THR	CA-CB-OG1	-6.02	100.57	109.60
1	C	475	GLY	CA-C-N	6.01	130.92	122.08
1	C	475	GLY	C-N-CA	6.01	130.92	122.08
1	A	435	TYR	N-CA-CB	-6.01	101.28	110.42
1	A	299	VAL	N-CA-CB	6.01	118.70	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	PRO	CB-CA-C	-6.01	103.32	111.85
1	C	680	HIS	CB-CA-C	6.00	121.06	110.85
1	B	69	GLU	CB-CA-C	-5.99	99.74	110.70
1	B	675	ASP	CB-CA-C	5.98	121.66	109.76
1	B	25	CYS	CB-CA-C	5.97	119.44	109.89
1	B	312	ARG	CD-NE-CZ	-5.96	116.06	124.40
1	C	689	VAL	N-CA-CB	5.96	117.11	110.62
1	B	529	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	132	PHE	CA-C-O	-5.94	114.45	121.16
1	C	325	LYS	CB-CA-C	-5.94	100.69	110.72
1	C	242	ASP	N-CA-C	-5.93	105.30	112.54
1	A	48	LYS	N-CA-CB	5.93	119.35	110.22
1	C	603	ASP	CB-CA-C	-5.92	97.23	110.21
1	A	102	VAL	N-CA-CB	5.92	120.16	111.52
1	B	253	GLU	N-CA-CB	5.91	120.43	110.69
1	B	456	HIS	CA-CB-CG	5.91	119.71	113.80
1	C	327	LYS	N-CA-CB	5.90	120.04	110.43
1	B	426	THR	OG1-CB-CG2	-5.88	97.53	109.30
1	B	423	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	C	304	THR	CA-CB-OG1	5.86	118.39	109.60
1	C	300	PHE	N-CA-CB	-5.86	100.88	110.43
1	A	322	GLU	N-CA-CB	5.85	118.67	109.83
1	B	170	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	A	499	LEU	CB-CA-C	5.83	119.81	109.72
1	A	512	GLU	CB-CA-C	-5.83	100.76	110.68
1	B	680	HIS	CA-CB-CG	-5.82	107.98	113.80
1	B	577	GLN	N-CA-CB	-5.80	100.98	110.43
1	C	393	GLU	CB-CG-CD	5.77	122.41	112.60
1	B	166	ASP	CB-CA-C	5.77	118.49	109.84
1	B	302	PHE	CB-CA-C	-5.76	97.98	109.79
1	C	582	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	169	GLU	CB-CA-C	5.76	120.61	110.36
1	C	115	ASP	CA-C-N	5.75	125.43	119.56
1	C	115	ASP	C-N-CA	5.75	125.43	119.56
1	C	535	GLU	CB-CG-CD	-5.75	102.82	112.60
1	A	166	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	14	THR	N-CA-CB	5.74	119.22	110.44
1	A	567	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	358	LYS	CG-CD-CE	5.71	124.44	111.30
1	B	209	LYS	CG-CD-CE	-5.71	98.18	111.30
1	C	287	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	642	ASP	CA-CB-CG	5.70	118.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	GLU	N-CA-CB	5.69	118.74	110.26
1	A	607	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	335	LYS	CB-CA-C	5.68	119.26	109.15
1	C	194	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	92	THR	OG1-CB-CG2	5.68	120.66	109.30
1	C	489	LEU	N-CA-C	-5.67	105.24	111.82
1	A	427	VAL	CA-C-N	-5.67	112.43	122.07
1	A	427	VAL	C-N-CA	-5.67	112.43	122.07
1	B	608	PHE	CA-CB-CG	-5.67	108.13	113.80
1	C	305	ASN	N-CA-C	-5.66	104.94	113.89
1	B	374	THR	OG1-CB-CG2	-5.66	97.98	109.30
1	C	366	LEU	N-CA-CB	-5.66	100.99	110.39
1	C	287	GLU	CB-CA-C	5.64	121.00	109.55
1	C	32	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	11	ARG	CD-NE-CZ	5.62	132.27	124.40
1	C	66	ARG	CB-CA-C	5.62	120.39	110.85
1	B	111	ARG	CA-CB-CG	5.61	125.31	114.10
1	B	539	LYS	N-CA-CB	-5.59	101.04	110.49
1	A	481	THR	N-CA-CB	-5.58	101.96	109.88
1	A	255	CYS	N-CA-CB	5.58	118.70	110.56
1	B	640	HIS	CA-CB-CG	5.57	119.37	113.80
1	A	603	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	664	ARG	N-CA-C	-5.56	105.30	111.36
1	B	378	ASP	N-CA-CB	-5.56	102.00	110.45
1	C	420	ARG	CD-NE-CZ	5.55	132.18	124.40
1	A	89	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	214	VAL	N-CA-CB	5.53	117.15	110.95
1	B	241	SER	CA-C-N	5.53	127.96	120.38
1	B	241	SER	C-N-CA	5.53	127.96	120.38
1	C	477	ASN	CB-CA-C	5.53	120.38	111.36
1	A	488	ARG	N-CA-CB	5.52	118.61	110.33
1	C	419	PRO	N-CA-C	5.52	119.75	111.14
1	A	170	ARG	CD-NE-CZ	5.51	132.12	124.40
1	B	489	LEU	N-CA-CB	5.51	118.71	110.22
1	B	162	LYS	N-CA-CB	-5.51	101.07	110.16
1	B	258	VAL	CA-C-O	-5.51	115.93	121.49
1	A	565	ASN	N-CA-C	-5.49	105.22	111.14
1	C	207	HIS	CB-CA-C	-5.49	103.94	111.73
1	B	94	LEU	CA-C-N	-5.48	112.92	120.71
1	B	94	LEU	C-N-CA	-5.48	112.92	120.71
1	C	162	LYS	N-CA-CB	-5.48	101.47	110.68
1	C	104	ASP	CA-CB-CG	5.48	118.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ILE	N-CA-C	-5.48	105.76	110.74
1	C	127	LEU	N-CA-CB	-5.47	101.69	109.85
1	B	119	LEU	N-CA-CB	-5.47	101.55	110.42
1	A	255	CYS	N-CA-C	-5.47	106.20	112.92
1	C	222	ASP	CA-CB-CG	-5.46	107.14	112.60
1	B	393	GLU	N-CA-CB	-5.46	102.78	111.62
1	B	452	MET	CG-SD-CE	5.46	112.90	100.90
1	C	575	ILE	O-C-N	5.45	127.88	122.97
1	C	630	TYR	N-CA-C	5.45	115.87	109.60
1	B	414	LYS	CB-CA-C	-5.45	100.87	109.80
1	A	505	ARG	CD-NE-CZ	5.44	132.02	124.40
1	C	643	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	662	ARG	N-CA-CB	-5.44	101.84	110.22
1	A	588	LYS	CB-CG-CD	5.43	123.78	111.30
1	C	51	VAL	N-CA-CB	5.43	114.68	110.45
1	C	38	GLN	N-CA-C	-5.42	105.27	111.07
1	C	664	ARG	N-CA-C	-5.42	104.78	111.40
1	C	675	ASP	CB-CA-C	5.41	120.74	110.51
1	A	33	ASP	CA-CB-CG	5.39	118.00	112.60
1	A	626	ASP	CB-CA-C	-5.38	101.53	110.68
1	A	415	GLU	CB-CG-CD	5.37	121.73	112.60
1	A	348	PHE	CA-CB-CG	5.36	119.16	113.80
1	C	84	LYS	CB-CA-C	-5.36	101.14	110.09
1	C	345	ARG	CD-NE-CZ	5.36	131.90	124.40
1	C	330	VAL	N-CA-CB	5.36	118.71	111.21
1	A	204	THR	CA-CB-OG1	-5.35	101.58	109.60
1	C	391	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	437	THR	OG1-CB-CG2	-5.33	98.64	109.30
1	B	65	GLU	CB-CA-C	5.33	119.63	110.79
1	A	398	PHE	CA-CB-CG	-5.32	108.48	113.80
1	C	280	VAL	N-CA-CB	5.30	117.05	111.00
1	B	567	ARG	CD-NE-CZ	5.30	131.82	124.40
1	A	675	ASP	CB-CA-C	5.29	120.53	109.68
1	A	233	LYS	CG-CD-CE	-5.29	99.14	111.30
1	C	358	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	327	LYS	CB-CA-C	5.27	118.87	109.38
1	B	252	ARG	CD-NE-CZ	5.27	131.78	124.40
1	B	280	VAL	N-CA-CB	-5.27	104.66	110.99
1	B	573	CYS	CB-CA-C	5.27	120.12	109.68
1	C	53	PHE	N-CA-C	-5.27	105.70	111.82
1	B	252	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	C	675	ASP	CA-CB-CG	5.26	117.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	LEU	CA-C-O	-5.26	115.76	121.44
1	A	399	THR	CA-CB-OG1	-5.25	101.73	109.60
1	C	657	GLN	O-C-N	5.24	127.68	122.12
1	B	531	GLN	N-CA-CB	-5.22	102.22	110.06
1	B	42	PHE	CB-CA-C	5.22	119.08	110.88
1	B	691	GLU	CG-CD-OE1	5.22	130.41	118.40
1	A	260	ARG	CG-CD-NE	-5.22	100.52	112.00
1	A	598	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	231	GLU	N-CA-CB	-5.21	104.63	111.09
1	C	689	VAL	CB-CA-C	-5.21	105.30	111.81
1	B	51	VAL	N-CA-CB	5.21	114.51	110.45
1	B	17	GLN	N-CA-CB	-5.20	102.19	111.08
1	A	621	LYS	CD-CE-NZ	-5.20	95.27	111.90
1	C	253	GLU	CG-CD-OE2	-5.20	106.45	118.40
1	A	139	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	671	LEU	CB-CG-CD1	-5.19	95.13	110.70
1	B	80	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	319	ARG	CG-CD-NE	-5.17	100.62	112.00
1	B	491	PHE	N-CA-CB	-5.17	101.75	110.49
1	C	269	GLU	CB-CA-C	5.17	118.35	109.51
1	B	186	PHE	CB-CA-C	-5.17	99.47	109.76
1	A	662	ARG	CA-CB-CG	-5.17	103.77	114.10
1	B	613	LYS	CA-C-N	-5.15	114.14	122.23
1	B	613	LYS	C-N-CA	-5.15	114.14	122.23
1	C	375	PHE	CA-C-O	-5.15	115.94	119.29
1	B	79	HIS	CA-CB-CG	5.15	118.95	113.80
1	B	265	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	55	GLU	CB-CA-C	5.14	120.73	109.99
1	C	228	PHE	CA-C-N	5.14	124.80	119.56
1	C	228	PHE	C-N-CA	5.14	124.80	119.56
1	B	247	VAL	N-CA-CB	5.14	116.86	111.00
1	C	660	VAL	N-CA-CB	-5.13	105.26	112.35
1	A	516	LYS	CA-CB-CG	-5.13	103.83	114.10
1	B	676	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	201	GLU	CA-C-O	-5.13	116.04	121.94
1	C	170	ARG	CB-CA-C	5.12	119.01	111.73
1	A	416	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	477	ASN	CB-CA-C	5.12	119.70	111.36
1	C	306	ARG	CG-CD-NE	-5.12	100.75	112.00
1	A	63	TYR	N-CA-C	-5.11	105.62	111.14
1	B	39	THR	OG1-CB-CG2	-5.11	99.08	109.30
1	B	267	GLN	N-CA-CB	5.11	119.32	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ASP	CB-CA-C	5.10	118.17	109.75
1	B	649	SER	CA-C-N	5.10	127.07	120.44
1	B	649	SER	C-N-CA	5.10	127.07	120.44
1	C	652	PHE	N-CA-CB	5.10	117.70	110.16
1	B	477	ASN	N-CA-C	-5.08	106.66	112.86
1	B	399	THR	CA-CB-OG1	-5.08	101.98	109.60
1	C	331	PRO	N-CA-CB	-5.08	98.61	103.33
1	A	416	GLU	CB-CA-C	-5.07	101.42	110.70
1	A	651	LYS	N-CA-C	-5.07	105.84	112.23
1	C	239	GLU	CB-CA-C	5.07	119.97	109.38
1	C	77	SER	CA-C-N	-5.07	112.98	121.39
1	C	77	SER	C-N-CA	-5.07	112.98	121.39
1	C	14	THR	N-CA-CB	-5.06	102.55	110.44
1	A	289	GLU	O-C-N	5.06	128.91	123.10
1	B	547	ARG	N-CA-C	-5.06	104.94	111.71
1	C	23	LYS	CB-CA-C	5.06	117.87	109.53
1	B	32	GLU	CB-CG-CD	5.05	121.19	112.60
1	B	688	LYS	CB-CG-CD	-5.05	99.67	111.30
1	B	218	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	186	PHE	CA-C-O	-5.05	115.86	121.81
1	C	221	GLU	CB-CA-C	-5.04	99.46	109.99
1	B	699	PHE	N-CA-C	-5.04	106.30	112.90
1	A	101	TYR	CE1-CZ-OH	-5.03	104.81	119.90
1	B	655	THR	N-CA-C	-5.03	105.71	111.14
1	C	406	ILE	CB-CA-C	5.03	118.07	110.63
1	B	535	GLU	O-C-N	5.02	127.44	122.12
1	C	5	GLN	CB-CA-C	-5.02	102.59	111.22
1	C	365	ASP	CB-CA-C	-5.02	101.57	109.80
1	B	336	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain
1	A	260	ARG	Sidechain
1	A	306	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	488	ARG	Sidechain
1	A	547[A]	ARG	Sidechain
1	A	547[B]	ARG	Sidechain
1	A	547[C]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	612	VAL	Mainchain
1	A	66[A]	ARG	Sidechain
1	A	66[B]	ARG	Sidechain
1	A	664	ARG	Sidechain
1	B	11	ARG	Sidechain
1	B	170	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	259	ASN	Peptide
1	B	312	ARG	Sidechain
1	B	345	ARG	Sidechain
1	B	376	PRO	Peptide
1	B	493	ARG	Sidechain
1	B	57	CYS	Peptide
1	B	631	PRO	Peptide
1	B	643	ARG	Sidechain
1	B	664	ARG	Sidechain
1	B	7	PRO	Peptide
1	B	82	LYS	Peptide
1	B	85	ARG	Sidechain
1	C	312	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	417	LEU	Peptide
1	C	493	ARG	Sidechain
1	C	643	ARG	Sidechain
1	C	662	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5697	5552	5529	64	0
1	B	5673	5513	5490	167	0
1	C	5673	5513	5490	161	1
2	A	29	30	0	0	0
2	B	29	30	0	0	0
2	C	29	30	0	0	0
3	A	19	26	26	1	0
4	A	12	16	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	16	16	4	0
4	C	6	8	8	1	0
5	A	9	0	0	0	0
5	B	6	0	0	1	0
5	C	6	0	0	0	0
6	A	421	0	0	11	1
6	B	188	0	0	11	1
6	C	130	0	0	8	0
All	All	17939	16734	16575	392	2

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 12.

All (392) 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:192:GLN:OE1	1:C:192:GLN:HA	1.53	1.03
1:B:69:GLU:HG2	1:C:287:GLU:OE2	1.75	0.87
1:B:107:GLU:OE1	6:B:901:HOH:O	1.94	0.85
1:B:339:GLU:OE2	1:B:354:LEU:CD2	2.24	0.85
1:C:192:GLN:OE1	1:C:192:GLN:CA	2.27	0.82
1:C:128:ARG:HB2	6:C:1005:HOH:O	1.80	0.81
1:C:428:LYS:O	1:C:430:ILE:N	2.12	0.81
1:C:38:GLN:OE1	1:C:38:GLN:N	2.14	0.80
1:B:339:GLU:OE2	1:B:354:LEU:HD21	1.81	0.80
1:B:431:ASP:CG	1:B:432:ALA:H	1.90	0.78
1:C:400:SER:OG	1:C:403:SER:HB3	1.84	0.78
1:C:417:LEU:HA	1:C:418:GLU:OE2	1.84	0.78
1:C:306:ARG:NH2	1:C:323:GLU:OE1	2.15	0.77
1:C:196:LYS:O	1:C:197:SER:HB2	1.83	0.77
1:B:470:LEU:HD23	1:B:550:ILE:HG22	1.67	0.77
1:B:86:TYR:OH	1:B:393:GLU:OE2	2.02	0.76
1:C:358:LYS:HD2	1:C:379:VAL:HG13	1.69	0.76
1:C:22:HIS:NE2	6:C:901:HOH:O	2.13	0.75
1:A:539:LYS:HD3	6:A:1183:HOH:O	1.86	0.74
1:C:643:ARG:NH1	4:C:803:GOL:H32	2.02	0.74
1:C:350:VAL:CG1	1:C:361:LEU:HD11	2.18	0.73
1:B:339:GLU:HG2	1:B:354:LEU:HD22	1.70	0.72
1:C:7:PRO:HD3	1:C:49:ILE:CD1	2.19	0.72
1:B:534:ALA:O	1:B:538:ILE:HG13	1.90	0.71
1:B:40:LYS:O	6:B:902:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ASP:OD2	1:B:434:ASP:N	2.25	0.70
1:A:339:GLU:OE2	1:A:354:LEU:HD13	1.92	0.70
1:B:273:ILE:O	6:B:903:HOH:O	2.10	0.70
1:C:245:ARG:NE	1:C:265:ASP:OD2	2.22	0.69
1:B:268:GLN:HB3	1:B:278:LYS:NZ	2.08	0.69
1:B:431:ASP:CG	1:B:432:ALA:N	2.49	0.69
1:A:433:SER:HB2	6:A:1266:HOH:O	1.92	0.68
1:A:66[B]:ARG:NH1	1:A:69:GLU:HG2	2.08	0.68
1:C:436:GLN:HA	6:C:959:HOH:O	1.92	0.68
1:B:38:GLN:N	1:B:38:GLN:OE1	2.27	0.68
1:B:543:THR:OG1	1:B:544:SER:N	2.26	0.68
1:B:7:PRO:HD3	1:B:49:ILE:HD11	1.75	0.68
1:C:66:ARG:HH22	1:C:69:GLU:HG2	1.58	0.67
1:B:613:LYS:CE	6:B:916:HOH:O	2.43	0.67
1:A:7:PRO:HD3	1:A:49:ILE:HD11	1.76	0.67
1:A:539:LYS:HE3	6:A:1183:HOH:O	1.95	0.67
1:B:440:ILE:HD12	1:B:440:ILE:C	2.20	0.67
1:C:306:ARG:HH21	1:C:323:GLU:CD	2.00	0.67
1:B:276:ILE:HG23	4:B:803:GOL:H12	1.76	0.66
1:C:7:PRO:HD3	1:C:49:ILE:HD11	1.78	0.65
1:C:22:HIS:CE1	6:C:901:HOH:O	2.48	0.65
1:A:440:ILE:C	1:A:440:ILE:HD12	2.21	0.64
1:B:156:MET:HA	1:B:162:LYS:O	1.97	0.64
1:C:684:LYS:HG3	1:C:685:PRO:HD2	1.79	0.64
1:B:90:TYR:HB3	1:B:101:TYR:CE1	2.32	0.63
1:B:339:GLU:OE2	1:B:354:LEU:HD22	1.96	0.63
1:B:613:LYS:HE2	6:B:916:HOH:O	1.97	0.63
1:C:639:ASP:OD1	1:C:640:HIS:ND1	2.27	0.63
1:B:75:LYS:HB2	6:B:1046:HOH:O	1.98	0.63
1:B:516:LYS:O	6:B:904:HOH:O	2.15	0.63
1:C:431:ASP:OD2	1:C:433:SER:OG	2.16	0.63
1:B:490:ILE:O	1:B:491:PHE:C	2.40	0.63
1:A:128:ARG:HG3	6:A:1185:HOH:O	1.99	0.63
4:A:806:GOL:H11	6:A:1229:HOH:O	1.98	0.62
1:B:7:PRO:HD3	1:B:49:ILE:CD1	2.28	0.62
1:B:164:LEU:HB3	1:B:165:PRO:HD2	1.81	0.62
1:B:639:ASP:OD1	1:B:640:HIS:ND1	2.27	0.62
1:B:471:TYR:HB3	1:B:501:VAL:HG22	1.81	0.62
1:A:539:LYS:CD	6:A:1183:HOH:O	2.45	0.61
1:A:547[B]:ARG:NH1	1:A:706:VAL:HG22	2.16	0.61
1:C:196:LYS:O	1:C:197:SER:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:VAL:HG12	1:B:427:VAL:O	2.00	0.61
1:B:260:ARG:NH1	1:B:284:ASP:OD1	2.34	0.61
1:B:579:GLY:HA3	1:B:581:MET:HE2	1.83	0.60
1:A:356:ASP:C	1:A:357:VAL:HG23	2.27	0.60
1:B:245:ARG:HH21	1:B:267:GLN:HB3	1.65	0.60
1:C:310:ASN:O	1:C:311:TYR:HB2	2.00	0.59
1:B:53:PHE:O	1:B:702:ARG:NH1	2.35	0.59
1:B:417:LEU:O	1:B:419:PRO:HD3	2.03	0.59
1:B:268:GLN:HB3	1:B:278:LYS:HZ1	1.66	0.59
1:B:591:ILE:O	1:B:591:ILE:HG13	2.02	0.59
1:B:411:ASP:OD2	1:B:414:LYS:HE2	2.03	0.58
1:C:66:ARG:HH22	1:C:69:GLU:CG	2.15	0.58
1:B:262:TRP:CZ2	1:B:281:LYS:HD3	2.37	0.58
1:C:537:LEU:O	1:C:542:TYR:HB2	2.04	0.58
1:C:431:ASP:O	1:C:432:ALA:CB	2.52	0.58
1:A:188:ASN:HA	1:A:209:LYS:O	2.03	0.58
1:C:192:GLN:OE1	1:C:193:GLN:N	2.37	0.58
1:A:431:ASP:O	1:A:432:ALA:CB	2.52	0.57
1:C:547:ARG:HB2	1:C:547:ARG:NH1	2.20	0.57
1:A:251:ILE:HB	1:A:260:ARG:HB2	1.86	0.57
1:A:613:LYS:HE3	6:A:1011:HOH:O	2.05	0.57
1:B:624:GLU:OE2	1:B:624:GLU:HA	2.04	0.57
1:B:246:TYR:CE2	1:B:265:ASP:HB2	2.40	0.57
1:A:539:LYS:CE	6:A:1183:HOH:O	2.51	0.56
1:A:292:TYR:CZ	1:A:294:THR:HA	2.40	0.56
1:B:64:LYS:HE3	1:B:691:GLU:OE2	2.04	0.56
1:C:405:GLY:O	1:C:425:VAL:HG13	2.04	0.56
1:C:550:ILE:CG1	1:C:574:VAL:HG22	2.34	0.56
1:C:114:LEU:HD21	1:C:141:TYR:CE2	2.40	0.56
1:B:73:TYR:HB2	1:B:74:PRO:HD2	1.87	0.56
1:C:123:GLY:O	1:C:685:PRO:HB3	2.06	0.56
1:C:345:ARG:NH2	1:C:347:ASN:OD1	2.36	0.56
1:A:513:THR:HG22	6:A:1257:HOH:O	2.06	0.56
1:B:62:LEU:HD13	1:B:708:TRP:CD1	2.40	0.56
1:B:613:LYS:HE3	6:B:916:HOH:O	2.05	0.56
1:C:9:VAL:HB	6:C:961:HOH:O	2.05	0.56
1:C:114:LEU:HD21	1:C:141:TYR:CD2	2.40	0.56
1:A:358:LYS:HD2	1:A:379:VAL:HG13	1.88	0.55
1:B:339:GLU:CG	1:B:354:LEU:HD22	2.36	0.55
1:C:473:TYR:CZ	1:C:555:ASN:HB3	2.41	0.55
1:C:218:ASP:O	1:C:221:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:LYS:HD3	1:C:325:LYS:N	2.20	0.55
1:C:175:CYS:O	1:C:187:TYR:HA	2.06	0.55
1:B:245:ARG:NE	1:B:265:ASP:OD1	2.37	0.55
1:C:90:TYR:CZ	1:C:92:THR:HA	2.42	0.55
1:C:141:TYR:O	1:C:153:ILE:HA	2.07	0.55
1:B:154:LYS:C	1:B:155:PHE:CD1	2.85	0.55
1:B:292:TYR:OH	1:B:295:ASN:OD1	2.21	0.55
1:A:431:ASP:O	1:A:432:ALA:HB3	2.07	0.55
1:C:431:ASP:O	1:C:432:ALA:HB3	2.06	0.54
1:B:154:LYS:O	1:B:155:PHE:CD1	2.60	0.54
1:C:441:PHE:O	1:C:449:LYS:HD3	2.07	0.54
1:B:323:GLU:HA	1:B:326:TRP:CE2	2.43	0.54
1:C:371:LEU:HD11	1:C:373:LYS:O	2.07	0.54
1:C:660:VAL:O	1:C:663:SER:HB3	2.07	0.54
1:C:446:ASP:C	1:C:446:ASP:OD1	2.50	0.54
1:C:341:ILE:HD11	1:C:349:LEU:HD22	1.90	0.54
1:A:571:PHE:O	1:A:631:PRO:HB3	2.08	0.54
1:C:154:LYS:C	1:C:155:PHE:CD1	2.86	0.54
1:C:114:LEU:HD13	1:C:156:MET:SD	2.49	0.53
1:C:547:ARG:HH11	1:C:547:ARG:CB	2.21	0.53
1:B:73:TYR:HB2	1:B:74:PRO:CD	2.39	0.53
1:C:92:THR:HG23	1:C:95:GLN:OE1	2.09	0.53
1:C:173:PHE:CE2	1:C:591:ILE:HG12	2.43	0.53
1:A:460:ILE:CD1	1:A:498:ILE:HD11	2.38	0.53
1:C:428:LYS:C	1:C:430:ILE:H	2.15	0.53
1:C:99:VAL:HG13	1:C:115:ASP:HA	1.91	0.53
1:B:276:ILE:HD12	4:B:803:GOL:H11	1.91	0.53
1:B:547:ARG:HA	1:B:704:LEU:HD13	1.91	0.53
1:C:462:LEU:HA	1:C:541:GLY:O	2.09	0.53
1:B:404:PRO:HB2	1:B:425:VAL:CG2	2.39	0.52
1:B:292:TYR:CZ	1:B:294:THR:HA	2.44	0.52
1:B:434:ASP:O	1:B:458:LYS:N	2.40	0.52
1:B:524:GLN:O	1:B:525:ASN:C	2.48	0.52
1:C:583:MET:HB3	1:C:611:LEU:HD22	1.91	0.52
1:B:74:PRO:O	1:B:425:VAL:HG11	2.09	0.52
1:C:90:TYR:OH	1:C:92:THR:HA	2.10	0.52
1:B:298:THR:HB	1:B:318:PHE:HB2	1.91	0.52
1:C:341:ILE:HG12	1:C:342:ALA:N	2.23	0.52
1:B:615:SER:O	1:B:619:ASN:ND2	2.36	0.52
1:B:271:SER:O	1:B:271:SER:OG	2.21	0.52
1:B:275:GLY:O	1:B:276:ILE:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:GLN:HB2	1:C:666:GLN:OE1	2.09	0.52
1:C:373:LYS:HD3	1:C:417:LEU:HB2	1.92	0.52
1:A:351:LEU:HD13	1:A:364:HIS:CD2	2.45	0.51
1:B:251:ILE:HB	1:B:260:ARG:HB2	1.91	0.51
1:B:404:PRO:HB2	1:B:425:VAL:HG23	1.92	0.51
1:B:276:ILE:HD12	4:B:803:GOL:C1	2.41	0.51
1:B:276:ILE:CG2	4:B:803:GOL:H12	2.40	0.51
1:B:411:ASP:C	1:B:411:ASP:OD1	2.51	0.51
1:C:441:PHE:HA	1:C:450:ILE:O	2.10	0.51
1:B:546:LYS:O	1:B:704:LEU:HD22	2.10	0.51
1:B:578:VAL:CG2	1:B:680:HIS:CE1	2.94	0.51
1:B:227:GLU:HG3	1:B:229:PRO:HD3	1.93	0.51
1:B:221:GLU:O	1:B:222:ASP:C	2.53	0.51
1:B:398:PHE:C	1:B:398:PHE:CD1	2.89	0.51
1:C:233:LYS:HB2	6:C:990:HOH:O	2.10	0.51
1:C:160:GLY:O	1:C:161:ALA:HB3	2.09	0.50
1:B:277:LEU:HD12	1:B:279:TRP:CZ2	2.47	0.50
1:C:298:THR:HB	1:C:318:PHE:HB2	1.93	0.50
1:A:404:PRO:HB3	1:A:484:TYR:CE2	2.47	0.50
1:B:538:ILE:HD13	1:B:545:PRO:HD3	1.93	0.50
1:C:673:HIS:CE1	1:C:675:ASP:HB2	2.46	0.50
1:A:427:VAL:O	1:A:429:GLY:N	2.45	0.50
1:B:395:PHE:N	1:B:395:PHE:CD1	2.80	0.50
1:C:339:GLU:OE1	1:C:354:LEU:HD22	2.12	0.50
1:A:474:GLY:HA3	1:A:504:ILE:HD11	1.94	0.50
1:B:172:LYS:HD3	1:B:173:PHE:CE2	2.46	0.50
1:B:321:PRO:O	1:B:322:GLU:C	2.55	0.50
1:C:170:ARG:NH1	6:C:908:HOH:O	2.45	0.50
1:B:373:LYS:HE3	1:B:417:LEU:HB2	1.93	0.49
1:C:339:GLU:CD	1:C:354:LEU:HD22	2.36	0.49
1:C:407:ILE:HD12	1:C:423:ARG:HD2	1.93	0.49
1:B:407:ILE:HD12	1:B:423:ARG:HD2	1.95	0.49
1:B:73:TYR:O	1:B:93:GLY:HA2	2.12	0.49
1:A:421:VAL:HB	1:B:322:GLU:HG2	1.95	0.49
1:C:344:VAL:O	1:C:348:PHE:HB2	2.13	0.49
1:C:585:LYS:O	1:C:586:PHE:C	2.52	0.49
1:C:662:ARG:O	1:C:663:SER:C	2.56	0.49
1:B:650:LEU:O	1:B:653:ILE:HG22	2.13	0.49
1:C:237:GLY:O	1:C:249:LEU:HA	2.12	0.49
1:C:456:HIS:HB3	1:C:498:ILE:HG12	1.95	0.49
1:A:323:GLU:HA	1:A:326:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:O	1:B:68:THR:C	2.56	0.48
1:C:430:ILE:HG22	1:C:430:ILE:O	2.13	0.48
1:A:664:ARG:CZ	1:A:664:ARG:HB3	2.43	0.48
1:B:267:GLN:O	1:B:267:GLN:HG2	2.12	0.48
1:C:354:LEU:HD13	1:C:359:ASN:ND2	2.27	0.48
1:A:111:ARG:NH1	1:A:111:ARG:HG3	2.29	0.48
1:B:90:TYR:HB3	1:B:101:TYR:CD1	2.48	0.48
1:C:66:ARG:NH2	1:C:69:GLU:HB3	2.28	0.48
1:C:614:TYR:O	1:C:615:SER:C	2.56	0.48
1:A:643:ARG:NH1	4:A:803:GOL:H32	2.29	0.48
1:A:172:LYS:NZ	1:A:205:ASN:HD21	2.11	0.48
1:C:602:SER:HB3	6:C:967:HOH:O	2.14	0.48
1:B:84:LYS:HB3	1:B:85:ARG:HG3	1.96	0.48
1:C:444:SER:OG	1:C:445:LYS:N	2.47	0.48
1:C:350:VAL:HG12	1:C:361:LEU:HD11	1.96	0.47
1:B:378:ASP:OD1	1:B:378:ASP:N	2.47	0.47
1:B:427:VAL:HG13	1:B:484:TYR:OH	2.14	0.47
1:C:625:ALA:O	1:C:665:LYS:NZ	2.46	0.47
1:B:645:VAL:HG23	1:B:647:LEU:HG	1.96	0.47
1:C:342:ALA:O	1:C:349:LEU:HA	2.14	0.47
1:A:431:ASP:C	1:A:431:ASP:OD1	2.57	0.47
1:B:246:TYR:CD2	1:B:265:ASP:HB2	2.50	0.47
1:B:384:GLY:HA2	6:B:1051:HOH:O	2.14	0.47
1:C:519:ILE:HD12	1:C:520:LEU:HD12	1.96	0.47
1:A:71:TYR:CE2	1:A:75:LYS:HE2	2.50	0.47
1:B:12:ASP:OD1	1:B:12:ASP:C	2.55	0.47
1:B:305:ASN:HB3	1:B:311:TYR:CE2	2.49	0.47
1:C:231:GLU:HG3	1:C:234:TRP:CZ2	2.50	0.47
1:B:433:SER:O	1:B:458:LYS:HG3	2.15	0.47
1:C:627:ASP:OD1	1:C:627:ASP:C	2.57	0.47
1:A:191:PRO:HG3	1:A:209:LYS:HE2	1.97	0.46
1:A:281:LYS:O	1:A:282:LEU:C	2.57	0.46
1:B:374:THR:O	1:B:374:THR:HG22	2.15	0.46
1:C:228:PHE:N	1:C:229:PRO:CD	2.78	0.46
1:B:339:GLU:CD	1:B:354:LEU:HD22	2.40	0.46
1:B:351:LEU:N	1:B:351:LEU:HD12	2.31	0.46
1:B:492:VAL:HG22	1:B:497:GLY:O	2.14	0.46
1:C:316:ILE:HG23	1:C:326:TRP:CD1	2.50	0.46
1:C:341:ILE:HG13	1:C:351:LEU:HD12	1.98	0.46
1:C:643:ARG:HB3	1:C:680:HIS:CG	2.51	0.46
1:B:268:GLN:HB3	1:B:278:LYS:HZ3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LEU:HD23	1:B:550:ILE:CG2	2.42	0.46
1:B:538:ILE:O	1:B:539:LYS:C	2.58	0.46
1:C:166:ASP:C	1:C:167:VAL:HG23	2.41	0.46
1:B:323:GLU:OE2	1:B:326:TRP:CZ3	2.69	0.46
1:A:289:GLU:O	1:A:304:THR:HA	2.16	0.46
1:C:62:LEU:O	1:C:66:ARG:HB2	2.16	0.46
1:C:658:TYR:CD2	1:C:659:ILE:HD13	2.50	0.46
1:A:360:ILE:CG2	1:A:362:GLN:HE21	2.29	0.46
1:B:348:PHE:CE1	1:B:363:LEU:HD21	2.51	0.46
1:C:99:VAL:HB	1:C:101:TYR:CE1	2.51	0.46
1:C:495:MET:HE3	1:C:701:ALA:HB2	1.98	0.46
1:B:431:ASP:O	1:B:432:ALA:CB	2.64	0.45
1:B:435:TYR:OH	1:B:493:ARG:HD3	2.16	0.45
1:B:365:ASP:HB2	1:B:372:LEU:HD11	1.97	0.45
1:B:440:ILE:HD12	1:B:441:PHE:N	2.31	0.45
1:C:22:HIS:CD2	1:C:22:HIS:C	2.93	0.45
1:C:214:VAL:HG12	1:C:215:LEU:O	2.16	0.45
1:B:65:GLU:O	1:B:69:GLU:HG3	2.15	0.45
1:C:623:PRO:O	1:C:665:LYS:NZ	2.49	0.45
1:C:685:PRO:HG2	1:C:688:LYS:HG3	1.98	0.45
1:B:47:ASN:O	1:B:51:VAL:HG23	2.17	0.45
1:B:245:ARG:NH2	1:B:267:GLN:HE21	2.14	0.45
1:C:417:LEU:H	1:C:417:LEU:HD22	1.81	0.45
1:A:647:LEU:HD12	1:A:648:HIS:N	2.31	0.45
1:C:261:LEU:HD13	1:C:261:LEU:C	2.42	0.45
1:A:614:TYR:O	1:A:615:SER:C	2.60	0.45
1:B:643:ARG:HG2	1:B:680:HIS:CD2	2.52	0.45
1:B:663:SER:OG	1:B:665:LYS:HG2	2.16	0.45
1:A:579:GLY:HA3	1:A:581:MET:HE2	1.98	0.45
1:B:385:TYR:CG	1:B:386:SER:N	2.85	0.45
1:C:171:VAL:HG13	1:C:174:SER:HB2	1.99	0.45
1:C:486:VAL:O	1:C:490:ILE:HG13	2.17	0.45
1:A:460:ILE:HD12	1:A:498:ILE:HD11	1.99	0.44
1:B:227:GLU:HG3	1:B:229:PRO:CD	2.47	0.44
1:B:353:TYR:O	1:B:359:ASN:HA	2.18	0.44
1:B:414:LYS:CB	1:B:416:GLU:HG2	2.47	0.44
1:C:66:ARG:HH22	1:C:69:GLU:CB	2.30	0.44
1:B:429:GLY:O	1:B:430:ILE:C	2.60	0.44
1:C:41:ALA:O	1:C:42:PHE:C	2.60	0.44
1:B:355:HIS:O	1:B:356:ASP:C	2.59	0.44
1:C:547:ARG:NH1	1:C:547:ARG:CB	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:HB2	1:B:87:PHE:HE1	1.83	0.44
1:B:629:GLN:HB2	1:B:666:GLN:OE1	2.16	0.44
1:C:285:ASN:OD1	1:C:287:GLU:HB2	2.18	0.44
1:C:378:ASP:HB2	1:C:398:PHE:CZ	2.53	0.44
1:B:243:ASP:C	1:B:243:ASP:OD1	2.61	0.44
1:C:88:TYR:HE2	1:C:103:GLN:OE1	2.00	0.44
1:A:467:PRO:HA	1:A:547[C]:ARG:HB2	2.00	0.44
1:C:137:GLU:C	1:C:158:VAL:HG23	2.43	0.44
1:C:230:ASP:C	1:C:232:PRO:HD3	2.43	0.44
1:C:428:LYS:C	1:C:430:ILE:N	2.76	0.44
1:C:65:GLU:C	1:C:65:GLU:CD	2.86	0.43
1:B:312:ARG:HB2	1:B:330:VAL:O	2.18	0.43
1:C:20:HIS:CD2	1:C:605:LYS:HA	2.52	0.43
1:C:312:ARG:HB2	1:C:330:VAL:O	2.17	0.43
1:C:401:PHE:CD2	1:C:482:PRO:HB3	2.53	0.43
1:A:111:ARG:HG3	1:A:111:ARG:HH11	1.83	0.43
1:A:430:ILE:HG22	1:A:430:ILE:O	2.18	0.43
1:B:354:LEU:HD13	1:B:359:ASN:ND2	2.34	0.43
1:B:444:SER:OG	1:B:445:LYS:N	2.50	0.43
1:B:558:LEU:O	1:B:559:LEU:C	2.60	0.43
1:A:8:ASP:N	6:A:932:HOH:O	2.50	0.43
1:B:431:ASP:O	1:B:432:ALA:HB2	2.18	0.43
1:C:275:GLY:O	1:C:276:ILE:C	2.60	0.43
1:B:517:GLY:O	1:B:525:ASN:ND2	2.43	0.43
1:B:677:LYS:HB3	1:B:677:LYS:HE2	1.87	0.43
1:B:79:HIS:HE1	1:B:423:ARG:NH1	2.17	0.43
1:B:415:GLU:HG2	1:B:416:GLU:OE1	2.19	0.43
1:C:473:TYR:CE1	1:C:555:ASN:HB3	2.54	0.43
1:C:554:SER:HB2	1:C:680:HIS:NE2	2.33	0.43
1:A:530:PHE:O	1:A:533:ALA:HB3	2.19	0.43
1:A:298:THR:HG21	1:A:319:ARG:CZ	2.49	0.43
1:C:570:LEU:HB3	1:C:571:PHE:CE1	2.53	0.43
1:B:170:ARG:HD3	5:B:804:SCN:N	2.34	0.43
1:C:165:PRO:O	1:C:167:VAL:HG23	2.19	0.43
1:C:663:SER:HB3	1:C:666:GLN:HB3	2.01	0.43
1:A:465:SER:C	1:A:547[C]:ARG:HD2	2.44	0.42
1:B:427:VAL:O	1:B:428:LYS:C	2.62	0.42
1:B:486:VAL:O	1:B:490:ILE:HG13	2.18	0.42
1:B:436:GLN:HG3	1:B:456:HIS:CE1	2.54	0.42
1:C:310:ASN:O	1:C:311:TYR:CB	2.65	0.42
1:B:622:LEU:HA	1:B:623:PRO:HD3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:VAL:CG1	1:C:174:SER:HB2	2.49	0.42
1:C:353:TYR:O	1:C:359:ASN:HA	2.19	0.42
1:C:435:TYR:OH	1:C:493:ARG:HD3	2.18	0.42
1:C:137:GLU:O	1:C:158:VAL:HG23	2.20	0.42
1:C:570:LEU:HD23	1:C:570:LEU:HA	1.88	0.42
1:A:81:LYS:C	1:A:82:LYS:HG2	2.44	0.42
1:C:673:HIS:HE1	1:C:675:ASP:HB2	1.83	0.42
1:B:601:CYS:HB3	6:B:1004:HOH:O	2.20	0.42
1:B:82:LYS:HG3	1:B:132:PHE:CD2	2.55	0.42
1:C:449:LYS:HE3	1:C:449:LYS:HA	2.01	0.42
1:B:192:GLN:HA	1:B:192:GLN:OE1	2.19	0.42
1:B:240:LEU:HD13	1:B:240:LEU:HA	1.87	0.42
1:B:416:GLU:O	1:B:417:LEU:HB2	2.19	0.42
1:B:701:ALA:HA	1:B:706:VAL:HB	2.02	0.42
1:C:571:PHE:O	1:C:631:PRO:HB3	2.20	0.42
1:C:700:ILE:HG23	1:C:704:LEU:HD12	2.02	0.42
1:B:91:ASN:OD1	1:B:93:GLY:N	2.44	0.42
1:B:467:PRO:HA	1:B:547:ARG:O	2.20	0.42
1:C:63:TYR:CD2	1:C:694:SER:HA	2.55	0.42
1:C:192:GLN:OE1	1:C:192:GLN:C	2.63	0.42
1:A:355:HIS:O	1:A:356:ASP:C	2.63	0.41
1:B:268:GLN:CB	1:B:278:LYS:NZ	2.80	0.41
1:B:442:TYR:CZ	1:B:450:ILE:HB	2.55	0.41
1:C:66:ARG:NH2	1:C:69:GLU:CB	2.83	0.41
1:C:260:ARG:HG3	1:C:286:PHE:CE1	2.55	0.41
1:B:253:GLU:HB3	6:B:928:HOH:O	2.20	0.41
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.53	0.41
1:B:305:ASN:HB3	1:B:311:TYR:CD2	2.56	0.41
1:A:38:GLN:OE1	1:A:38:GLN:N	2.49	0.41
1:C:493:ARG:NH1	1:C:493:ARG:HG3	2.34	0.41
1:A:440:ILE:C	1:A:440:ILE:CD1	2.93	0.41
1:A:492:VAL:HA	1:A:497:GLY:O	2.21	0.41
1:A:607:HIS:CD2	1:A:610:TRP:CH2	3.07	0.41
1:C:416:GLU:O	1:C:418:GLU:HG3	2.19	0.41
1:C:516:LYS:HA	1:C:519:ILE:HG12	2.02	0.41
1:C:641:ASP:N	1:C:679:GLY:HA2	2.35	0.41
1:B:511:GLY:O	1:B:513:THR:N	2.53	0.41
1:A:12:ASP:OD1	1:A:12:ASP:C	2.62	0.41
1:A:278:LYS:HB2	1:A:278:LYS:HE3	1.69	0.41
1:B:262:TRP:N	1:B:262:TRP:CD1	2.85	0.41
1:C:586:PHE:C	1:C:586:PHE:CD1	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:SER:O	1:B:545:PRO:C	2.62	0.41
1:B:653:ILE:HG23	1:B:654:ALA:N	2.35	0.41
1:B:187:TYR:OH	1:B:222:ASP:OD2	2.36	0.41
1:C:82:LYS:HA	1:C:82:LYS:HD3	1.92	0.41
1:C:339:GLU:CG	1:C:354:LEU:HD22	2.51	0.41
1:A:694:SER:O	1:A:695:ASP:C	2.64	0.41
3:A:802:B3P:H101	3:A:802:B3P:H22	1.73	0.41
1:B:91:ASN:OD1	1:B:91:ASN:C	2.63	0.41
1:B:338:LEU:HB2	1:B:353:TYR:CE2	2.55	0.41
1:B:415:GLU:CG	1:B:416:GLU:OE1	2.69	0.41
1:C:459:GLY:O	1:C:460:ILE:C	2.60	0.41
1:C:663:SER:HB3	1:C:666:GLN:CB	2.51	0.41
1:C:64:LYS:NZ	1:C:691:GLU:OE2	2.43	0.41
1:C:247:VAL:O	1:C:263:TYR:HA	2.20	0.41
1:C:459:GLY:O	1:C:460:ILE:O	2.38	0.41
1:A:434:ASP:O	1:A:458:LYS:HG3	2.20	0.40
1:B:414:LYS:HB3	1:B:416:GLU:OE1	2.22	0.40
1:C:51:VAL:HB	1:C:52:PRO:HD3	2.03	0.40
1:C:63:TYR:HE2	1:C:693:VAL:HG23	1.86	0.40
1:A:354:LEU:HD12	1:A:359:ASN:ND2	2.35	0.40
1:B:401:PHE:HE2	1:B:453:PHE:CD2	2.39	0.40
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.68	0.40
1:B:583:MET:HB3	1:B:583:MET:HE3	1.91	0.40
1:C:51:VAL:N	1:C:52:PRO:HD2	2.36	0.40
1:C:536:TYR:CD1	1:C:536:TYR:C	2.99	0.40
1:B:237:GLY:O	1:B:249:LEU:HD12	2.21	0.40
1:B:562:ALA:O	1:B:566:GLN:HG3	2.22	0.40
1:C:658:TYR:HD2	1:C:659:ILE:HD13	1.87	0.40
1:A:583:MET:HB2	1:A:615:SER:HB2	2.03	0.40
1:B:79:HIS:HE1	1:B:423:ARG:HH11	1.69	0.40
1:C:306:ARG:HG3	1:C:307:GLN:N	2.36	0.40
1:C:452:MET:HA	1:C:501:VAL:O	2.21	0.40
1:C:591:ILE:O	1:C:591:ILE:HG23	2.21	0.40
1:A:172:LYS:NZ	1:A:205:ASN:ND2	2.70	0.40
1:A:305:ASN:HB2	6:A:1075:HOH:O	2.22	0.40
1:A:583:MET:HE1	1:A:599:TYR:CD2	2.55	0.40
1:B:430:ILE:HD13	1:B:489:LEU:HB3	2.03	0.40
1:C:313:VAL:CG2	1:C:330:VAL:HB	2.52	0.40
1:C:404:PRO:HB2	1:C:425:VAL:HG22	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1320:HOH:O	6:B:1086:HOH:O[2_546]	2.07	0.13
1:C:25:CYS:H	1:C:194:ASP:OD1[2_647]	1.53	0.07

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	708/711 (100%)	672 (95%)	29 (4%)	7 (1%)	12	8
1	B	705/711 (99%)	634 (90%)	57 (8%)	14 (2%)	6	2
1	C	705/711 (99%)	644 (91%)	47 (7%)	14 (2%)	6	2
All	All	2118/2133 (99%)	1950 (92%)	133 (6%)	35 (2%)	7	3

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	PRO
1	B	430	ILE
1	B	431	ASP
1	C	196	LYS
1	C	197	SER
1	C	429	GLY
1	C	460	ILE
1	C	602	SER
1	A	415	GLU
1	A	432	ALA
1	B	83	GLY
1	B	432	ALA
1	B	707	ASP
1	C	161	ALA
1	C	272	GLY
1	C	307	GLN
1	C	357	VAL
1	C	432	ALA

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Mol	Chain	Res	Type
1	A	429	GLY
1	A	554	SER
1	B	276	ILE
1	C	663	SER
1	A	357	VAL
1	A	417	LEU
1	A	590	THR
1	B	415	GLU
1	B	539	LYS
1	C	377	LEU
1	C	431	ASP
1	B	222	ASP
1	B	322	GLU
1	B	427	VAL
1	B	428	LYS
1	B	357	VAL
1	C	418	GLU

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	617/617 (100%)	589 (96%)	28 (4%)	24	23
1	B	614/617 (100%)	561 (91%)	53 (9%)	10	6
1	C	614/617 (100%)	566 (92%)	48 (8%)	11	8
All	All	1845/1851 (100%)	1716 (93%)	129 (7%)	14	10

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	69	GLU
1	A	84	LYS
1	A	107	GLU
1	A	162	LYS

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Mol	Chain	Res	Type
1	A	169	GLU
1	A	183	LYS
1	A	261	LEU
1	A	354	LEU
1	A	358	LYS
1	A	367	THR
1	A	390	LYS
1	A	403	SER
1	A	415	GLU
1	A	418	GLU
1	A	423	ARG
1	A	426	THR
1	A	430	ILE
1	A	440	ILE
1	A	481	THR
1	A	504	ILE
1	A	512	GLU
1	A	546	LYS
1	A	558	LEU
1	A	575	ILE
1	A	598	ASP
1	A	621	LYS
1	A	664	ARG
1	B	23	LYS
1	B	42	PHE
1	B	48	LYS
1	B	59	ILE
1	B	65	GLU
1	B	75	LYS
1	B	77	SER
1	B	84	LYS
1	B	106	LEU
1	B	120	SER
1	B	121	ASP
1	B	162	LYS
1	B	163	GLU
1	B	169	GLU
1	B	223	ILE
1	B	247	VAL
1	B	256	ASP
1	B	261	LEU
1	B	308	SER

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Mol	Chain	Res	Type
1	B	321	PRO
1	B	322	GLU
1	B	323	GLU
1	B	335	LYS
1	B	341	ILE
1	B	346	SER
1	B	354	LEU
1	B	365	ASP
1	B	377	LEU
1	B	379	VAL
1	B	388	GLN
1	B	392	THR
1	B	395	PHE
1	B	416	GLU
1	B	421	VAL
1	B	423	ARG
1	B	428	LYS
1	B	433	SER
1	B	436	GLN
1	B	438	VAL
1	B	457	LYS
1	B	460	ILE
1	B	461	LYS
1	B	463	ASP
1	B	466	HIS
1	B	485	SER
1	B	512	GLU
1	B	544	SER
1	B	546	LYS
1	B	547	ARG
1	B	598	ASP
1	B	604	SER
1	B	635	LEU
1	B	699	PHE
1	C	5	GLN
1	C	18	ASP
1	C	22	HIS
1	C	36	SER
1	C	38	GLN
1	C	48	LYS
1	C	55	GLU
1	C	59	ILE

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Mol	Chain	Res	Type
1	C	66	ARG
1	C	84	LYS
1	C	107	GLU
1	C	128	ARG
1	C	152	THR
1	C	157	LYS
1	C	162	LYS
1	C	166	ASP
1	C	192	GLN
1	C	203	SER
1	C	232	PRO
1	C	240	LEU
1	C	261	LEU
1	C	278	LYS
1	C	321	PRO
1	C	341	ILE
1	C	354	LEU
1	C	357	VAL
1	C	378	ASP
1	C	390	LYS
1	C	414	LYS
1	C	418	GLU
1	C	423	ARG
1	C	425	VAL
1	C	430	ILE
1	C	436	GLN
1	C	449	LYS
1	C	465	SER
1	C	546	LYS
1	C	547	ARG
1	C	588	LYS
1	C	598	ASP
1	C	602	SER
1	C	605	LYS
1	C	621	LYS
1	C	624	GLU
1	C	635	LEU
1	C	647	LEU
1	C	660	VAL
1	C	664	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	205	ASN
1	A	267	GLN
1	A	362	GLN
1	A	397	GLN
1	A	551	ASN
1	A	577	GLN
1	B	79	HIS
1	B	205	ASN
1	B	267	GLN
1	B	436	GLN
1	B	456	HIS
1	B	503	ASN
1	C	46	GLN
1	C	56	GLN
1	C	193	GLN
1	C	205	ASN
1	C	307	GLN
1	C	355	HIS
1	C	436	GLN
1	C	477	ASN
1	C	524	GLN
1	C	531	GLN
1	C	566	GLN
1	C	657	GLN
1	C	673	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

16 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
5	SCN	A	805	-	1,2,2	0.59	0	0,1,1	-	-
5	SCN	A	807	-	1,2,2	2.33	1 (100%)	0,1,1	-	-
5	SCN	C	802	-	1,2,2	0.36	0	0,1,1	-	-
5	SCN	A	804	-	1,2,2	0.17	0	0,1,1	-	-
3	B3P	A	802	-	18,18,18	0.93	1 (5%)	23,23,23	1.51	5 (21%)
4	GOL	C	803	-	5,5,5	0.50	0	5,5,5	1.16	0
2	A1CQP	B	801	1	32,32,33	0.94	1 (3%)	43,44,46	2.62	15 (34%)
4	GOL	B	803	-	5,5,5	0.33	0	5,5,5	0.35	0
5	SCN	B	805	-	1,2,2	0.00	0	0,1,1	-	-
2	A1CQP	A	801	1	32,32,33	1.40	5 (15%)	43,44,46	3.02	10 (23%)
4	GOL	A	803	-	5,5,5	0.30	0	5,5,5	1.16	0
2	A1CQP	C	801	1	32,32,33	1.08	3 (9%)	43,44,46	1.62	8 (18%)
4	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.44	0
5	SCN	B	804	-	1,2,2	0.33	0	0,1,1	-	-
5	SCN	C	804	-	1,2,2	0.73	0	0,1,1	-	-
4	GOL	A	806	-	5,5,5	0.24	0	5,5,5	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B3P	A	802	-	-	6/28/28/28	-
4	GOL	C	803	-	-	1/4/4/4	-
2	A1CQP	B	801	1	-	9/18/33/33	0/4/4/4
4	GOL	B	803	-	-	2/4/4/4	-
2	A1CQP	A	801	1	-	7/18/33/33	0/4/4/4
4	GOL	A	803	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1CQP	C	801	1	-	7/18/33/33	0/4/4/4
4	GOL	B	802	-	-	0/4/4/4	-
4	GOL	A	806	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1CQP	C11-C12	3.34	1.44	1.39
2	A	801	A1CQP	C21-C12	3.06	1.44	1.39
3	A	802	B3P	C11-C8	-3.02	1.50	1.53
2	C	801	A1CQP	C22-C10	3.01	1.45	1.41
2	C	801	A1CQP	C2-N1	2.87	1.35	1.32
2	C	801	A1CQP	C11-C12	2.68	1.43	1.39
2	A	801	A1CQP	C21-C22	2.60	1.43	1.39
2	A	801	A1CQP	C19-C20	-2.45	1.43	1.51
2	A	801	A1CQP	N2-N1	2.45	1.41	1.36
5	A	807	SCN	C-N	-2.33	1.07	1.15
2	B	801	A1CQP	C2-N1	2.13	1.34	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	A1CQP	C4-C3-N2	16.76	123.18	112.03
2	B	801	A1CQP	C4-C3-N2	9.29	118.21	112.03
2	B	801	A1CQP	C15-C14-N4	5.96	124.68	112.00
2	B	801	A1CQP	C21-C12-C11	4.86	122.91	117.92
2	B	801	A1CQP	C14-N4-C13	-4.64	111.61	122.11
2	A	801	A1CQP	C21-C22-C2	4.45	141.40	136.72
2	C	801	A1CQP	C21-C22-C2	4.44	141.39	136.72
2	B	801	A1CQP	C22-C2-N1	-4.37	109.05	110.76
2	B	801	A1CQP	C10-N2-N1	3.96	113.28	111.05
2	A	801	A1CQP	C21-C22-C10	-3.70	113.95	117.67
2	C	801	A1CQP	C21-C22-C10	-3.66	113.99	117.67
2	C	801	A1CQP	C10-N2-N1	3.38	112.95	111.05
2	C	801	A1CQP	C22-C2-N1	-3.20	109.50	110.76
2	B	801	A1CQP	C22-C10-N2	-3.17	105.21	107.18
2	A	801	A1CQP	C15-C14-N4	3.12	118.64	112.00
2	C	801	A1CQP	C22-C10-N2	-3.00	105.32	107.18
2	B	801	A1CQP	O2-C16-N5	2.94	127.36	122.12
2	B	801	A1CQP	C21-C22-C10	-2.92	114.72	117.67
2	B	801	A1CQP	C10-C22-C2	2.90	106.08	105.15
2	B	801	A1CQP	O2-C16-C15	-2.88	113.47	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	B3P	C10-C8-C9	2.75	116.06	110.02
2	A	801	A1CQP	C18-C19-C20	-2.69	97.65	105.10
3	A	802	B3P	C2-N2-C8	-2.51	112.49	116.17
2	B	801	A1CQP	C3-N2-C10	2.46	131.07	127.89
2	C	801	A1CQP	O2-C16-N5	-2.43	117.80	122.12
2	B	801	A1CQP	C15-C16-N5	-2.37	114.50	118.09
2	B	801	A1CQP	C21-C22-C2	2.35	139.19	136.72
2	C	801	A1CQP	C2-N1-N2	2.35	107.62	104.97
3	A	802	B3P	O1-C9-C8	-2.29	107.03	111.68
3	A	802	B3P	O3-C11-C8	-2.27	107.07	111.68
2	A	801	A1CQP	C11-C12-C13	-2.25	113.40	120.58
2	A	801	A1CQP	C1-C2-C22	2.24	131.44	127.56
3	A	802	B3P	C11-C8-C9	-2.20	105.20	110.02
2	A	801	A1CQP	O2-C16-N5	-2.16	118.27	122.12
2	A	801	A1CQP	C3-N2-C10	-2.15	125.09	127.89
2	A	801	A1CQP	C18-C17-N5	-2.11	99.89	103.44
2	C	801	A1CQP	C1-C2-C22	2.11	131.21	127.56
2	B	801	A1CQP	C19-C18-C17	-2.00	99.55	105.10

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1CQP	N2-C3-C4-C5
2	A	801	A1CQP	N2-C3-C4-C9
2	B	801	A1CQP	C15-C16-N5-C17
2	B	801	A1CQP	C15-C16-N5-C20
3	A	802	B3P	O2-C10-C8-N2
3	A	802	B3P	O2-C10-C8-C9
3	A	802	B3P	O2-C10-C8-C11
4	A	803	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-O2
4	A	806	GOL	O1-C1-C2-C3
4	B	803	GOL	C1-C2-C3-O3
2	B	801	A1CQP	C21-C12-C13-O1
2	C	801	A1CQP	C21-C12-C13-O1
2	A	801	A1CQP	C21-C12-C13-O1
2	B	801	A1CQP	C21-C12-C13-N4
2	C	801	A1CQP	C11-C12-C13-O1
2	A	801	A1CQP	C21-C12-C13-N4
2	C	801	A1CQP	C21-C12-C13-N4
2	C	801	A1CQP	C11-C12-C13-N4

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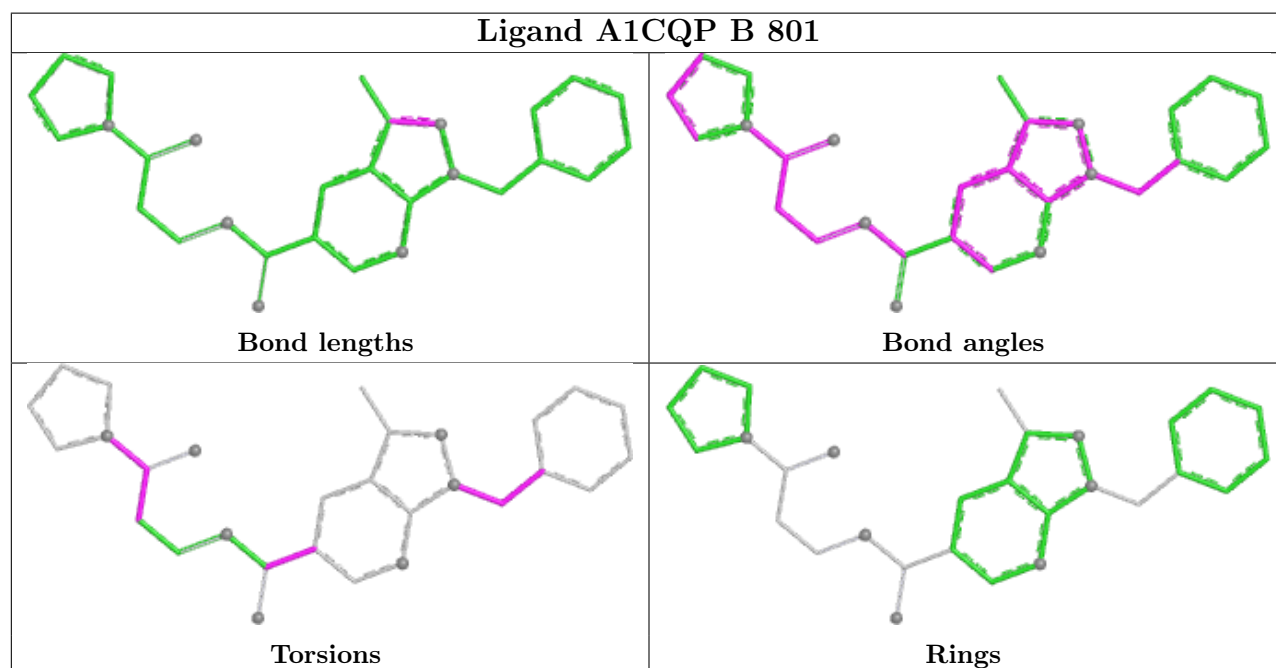
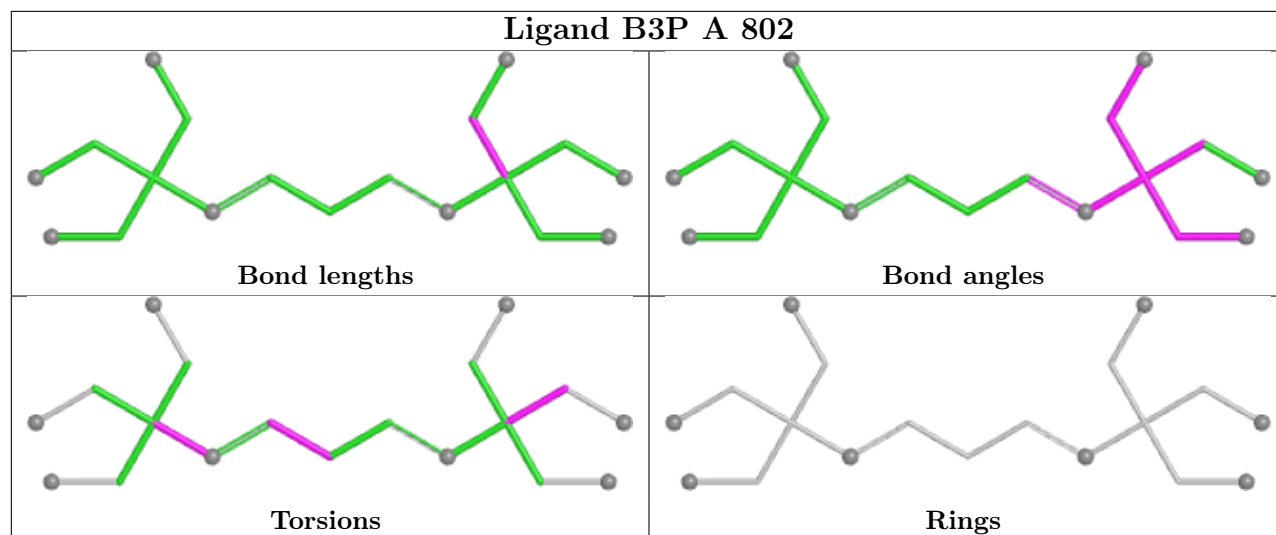
Mol	Chain	Res	Type	Atoms
2	B	801	A1CQP	C11-C12-C13-O1
2	B	801	A1CQP	C11-C12-C13-N4
2	A	801	A1CQP	C11-C12-C13-O1
2	A	801	A1CQP	C11-C12-C13-N4
4	B	803	GOL	O2-C2-C3-O3
3	A	802	B3P	C2-C1-C3-N1
4	A	803	GOL	O2-C2-C3-O3
3	A	802	B3P	C7-C4-N1-C3
2	B	801	A1CQP	C14-C15-C16-O2
4	A	806	GOL	O2-C2-C3-O3
4	C	803	GOL	O2-C2-C3-O3
2	A	801	A1CQP	N4-C14-C15-C16
2	C	801	A1CQP	N2-C3-C4-C5
3	A	802	B3P	C6-C4-N1-C3
2	C	801	A1CQP	C12-C13-N4-C14
2	C	801	A1CQP	N2-C3-C4-C9
2	B	801	A1CQP	N2-C3-C4-C9
2	B	801	A1CQP	C4-C3-N2-N1

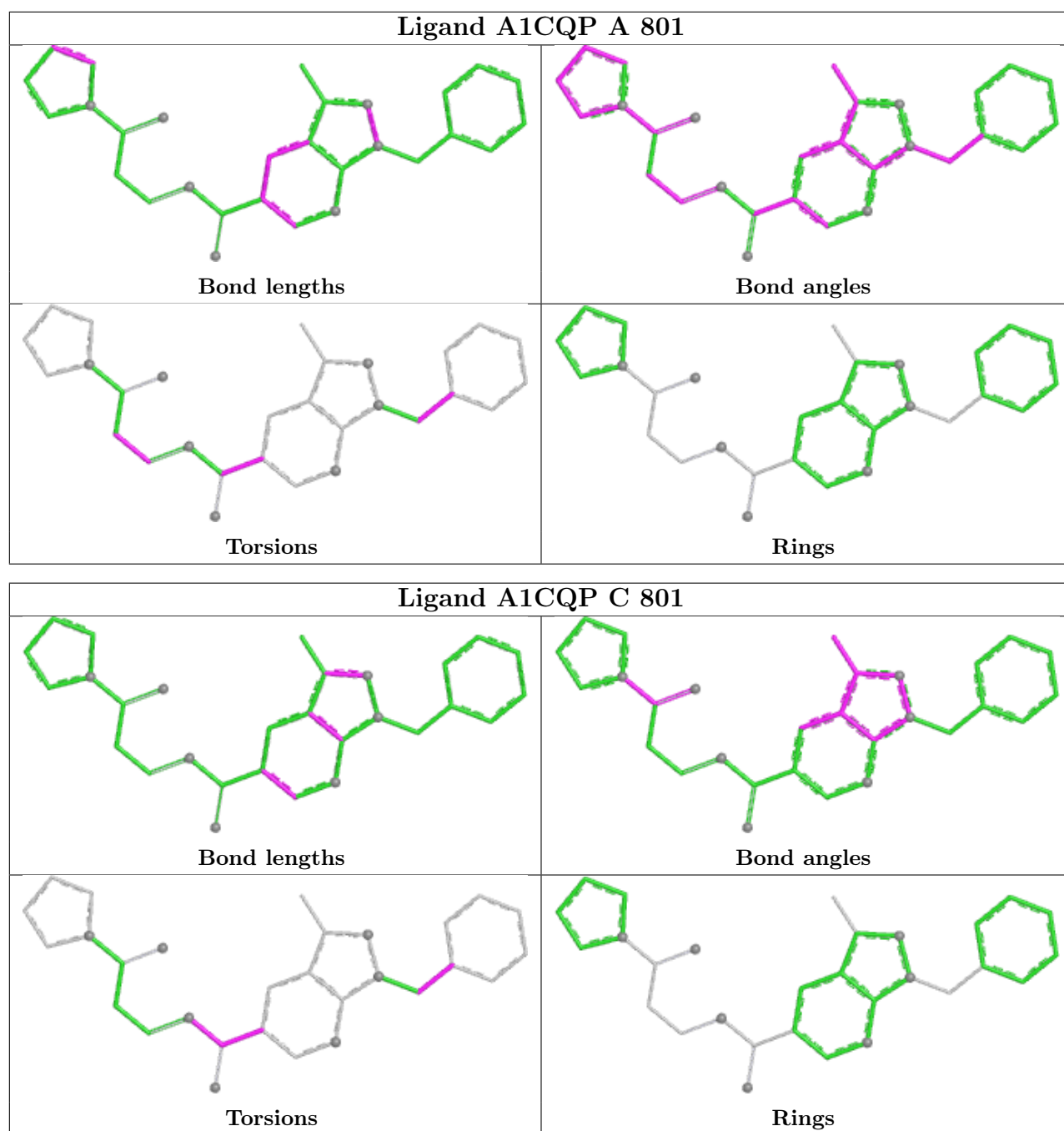
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	B3P	1	0
4	C	803	GOL	1	0
4	B	803	GOL	4	0
4	A	803	GOL	1	0
5	B	804	SCN	1	0
4	A	806	GOL	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%)	-1.04	2 (0%) 90 89	9, 22, 42, 86	2 (0%)
1	B	707/711 (99%)	-0.44	2 (0%) 90 89	10, 37, 68, 96	0
1	C	707/711 (99%)	-0.39	1 (0%) 92 91	19, 39, 63, 92	0
All	All	2121/2133 (99%)	-0.62	5 (0%) 91 90	9, 32, 62, 96	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	427	VAL	2.8
1	B	430	ILE	2.7
1	B	457	LYS	2.3
1	A	428	LYS	2.2
1	A	427	VAL	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](#)

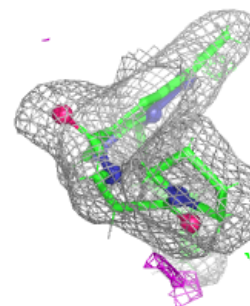
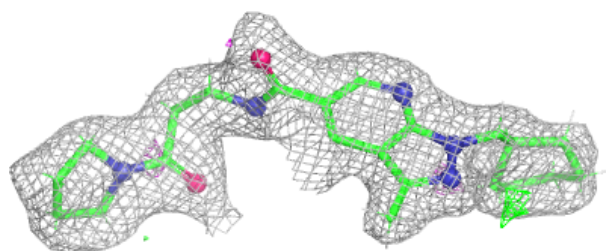
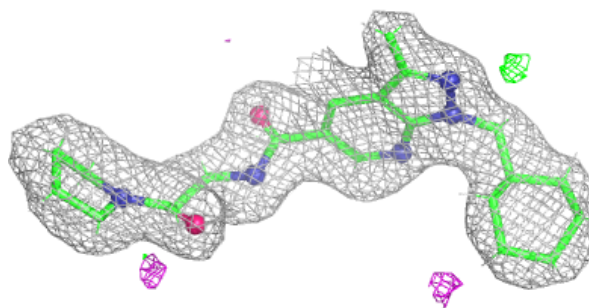
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	A	806	6/6	0.87	0.12	30,52,57,61	3
5	SCN	B	805	3/3	0.89	0.13	33,33,57,62	0
4	GOL	C	803	6/6	0.91	0.10	30,39,42,43	3
5	SCN	C	802	3/3	0.92	0.11	47,47,55,72	0
5	SCN	B	804	3/3	0.93	0.09	39,39,49,59	0
5	SCN	A	805	3/3	0.94	0.12	24,24,30,50	0
4	GOL	B	803	6/6	0.94	0.08	30,37,45,50	3
5	SCN	C	804	3/3	0.94	0.08	39,39,44,53	0
5	SCN	A	807	3/3	0.95	0.08	30,30,32,60	0
4	GOL	A	803	6/6	0.96	0.06	18,26,33,39	3
5	SCN	A	804	3/3	0.96	0.09	34,34,42,45	0
2	A1CQP	B	801	29/30	0.96	0.06	15,24,31,32	3
2	A1CQP	C	801	29/30	0.96	0.06	25,33,40,41	3
4	GOL	B	802	6/6	0.97	0.05	17,26,31,35	3
3	B3P	A	802	19/19	0.97	0.04	13,18,30,30	8
2	A1CQP	A	801	29/30	0.98	0.04	9,20,25,30	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.

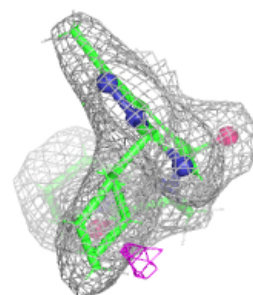
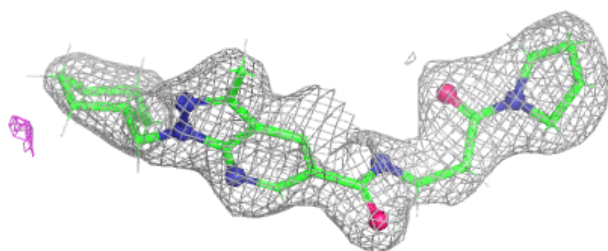
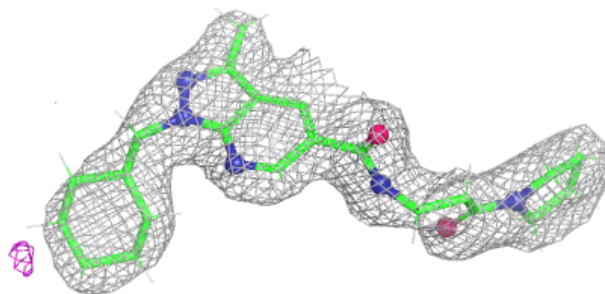
Electron density around A1CQP B 801:

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

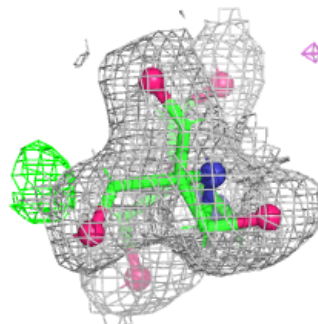
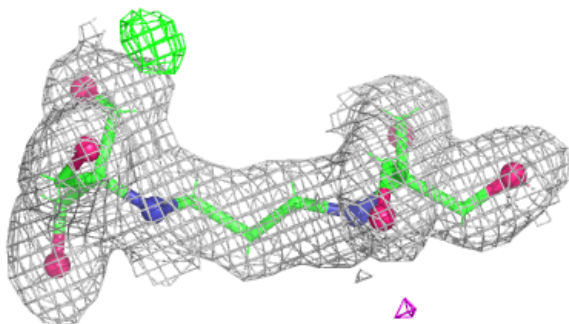
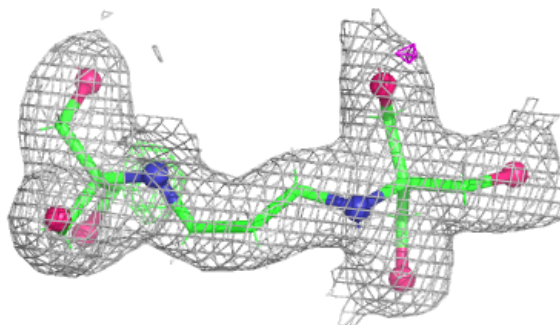


Electron density around A1CQP C 801:

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

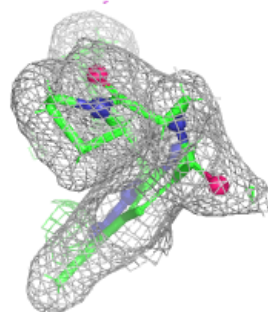
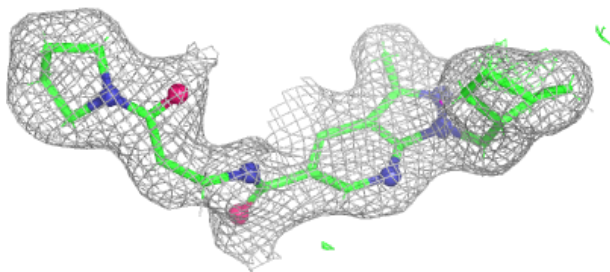
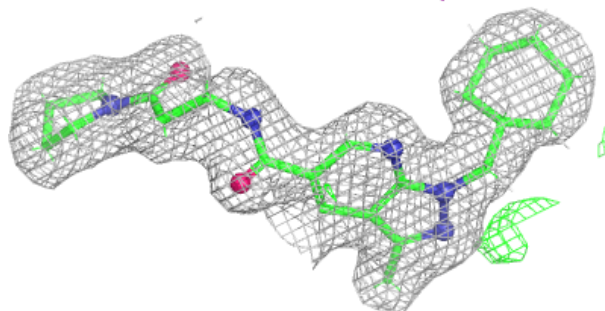
**Electron density around B3P A 802:**

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



Electron density around A1CQP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.