



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:00 PM UTC

PDB ID : 5Z5L / pdb_00005z5l
Title : Crystal structure of ConA-R5M
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Deposited on : 2018-01-18
Resolution : 2.30 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

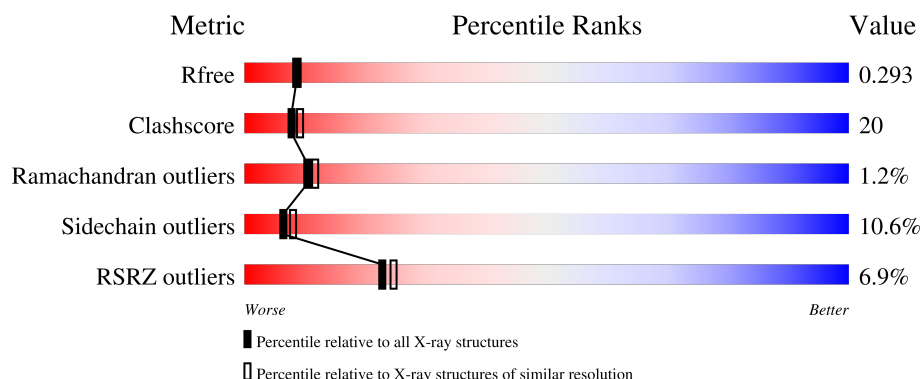
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	237	5% 65% 26% 5% ••
1	B	237	7% 59% 27% 9% •
1	C	237	8% 59% 28% 8% ••
1	D	237	6% 59% 30% 8% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7155 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Concanavalin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	17	0
			1794	1132	293	365	4			
1	B	227	Total	C	N	O	S	0	17	0
			1740	1100	287	350	3			
1	C	229	Total	C	N	O	S	5	16	0
			1756	1110	293	350	3			
1	D	230	Total	C	N	O	S	0	16	0
			1771	1119	291	357	4			

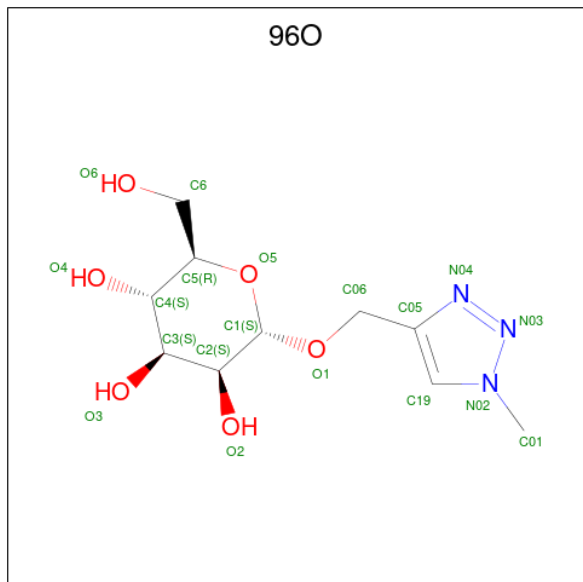
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (1-methyl-1H-1,2,3-triazol-4-yl)methyl α -D-mannopyranoside (CCD ID: 96O) (formula: $C_{10}H_{17}N_3O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			19	10	3	6		

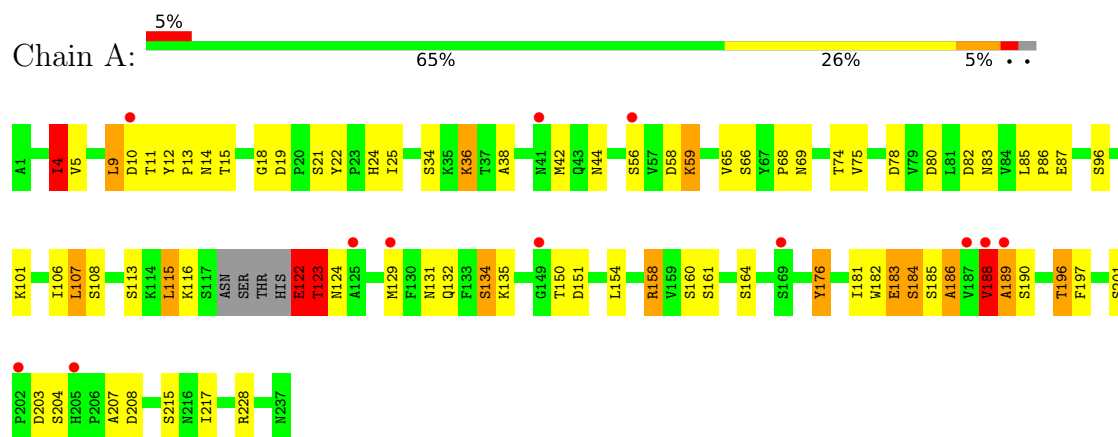
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	20	Total	O	0	0
			20	20		
5	C	9	Total	O	0	0
			9	9		
5	D	22	Total	O	0	0
			22	22		

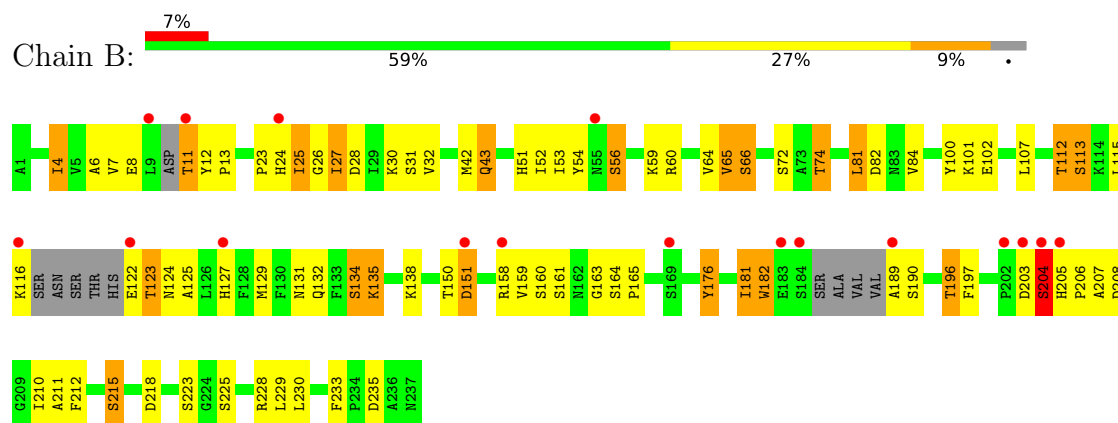
3 Residue-property plots

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.

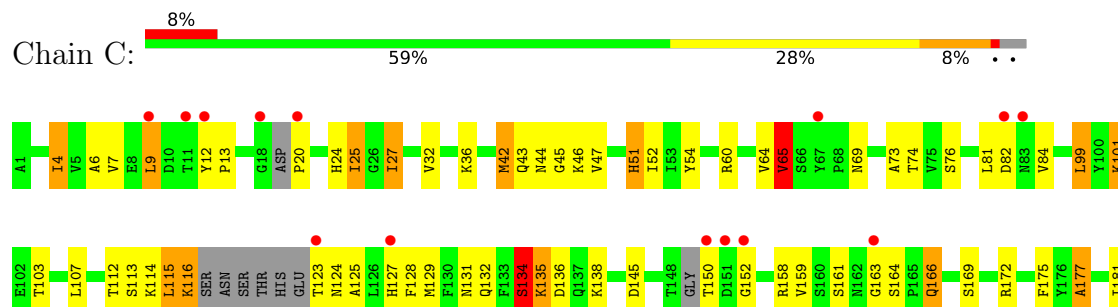
• Molecule 1: Concanavalin-A

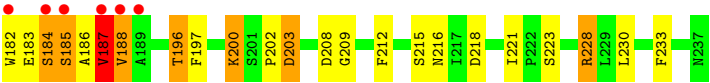


• Molecule 1: Concanavalin-A

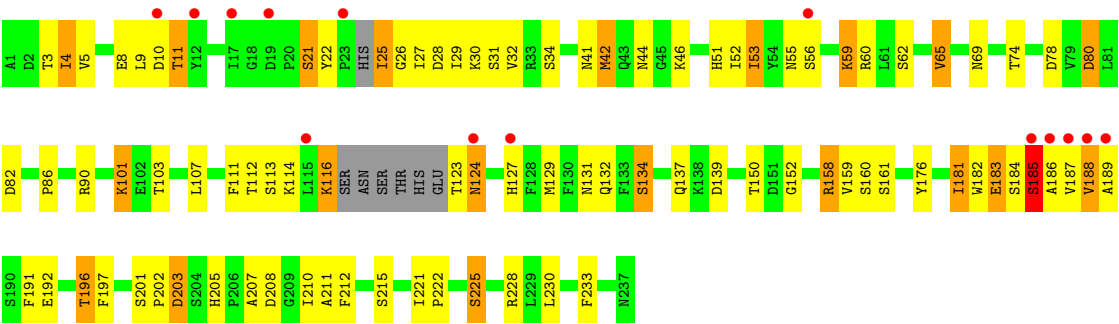


• Molecule 1: Concanavalin-A





● Molecule 1: Concanavalin-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.41Å 64.09Å 126.11Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	125.94 – 2.30 125.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (125.94-2.30) 96.3 (125.94-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.201 , 0.277 0.225 , 0.293	Depositor DCC
R_{free} test set	1937 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7155	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: MN, 96O, CA

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	2.04	18/1924 (0.9%)	1.56	45/2619 (1.7%)
1	B	2.24	31/1869 (1.7%)	1.76	43/2539 (1.7%)
1	C	1.97	24/1881 (1.3%)	1.43	30/2558 (1.2%)
1	D	2.37	21/1892 (1.1%)	1.51	31/2573 (1.2%)
All	All	2.16	94/7566 (1.2%)	1.57	149/10289 (1.4%)

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	D	2	0

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185[A]	SER	CB-OG	42.25	2.26	1.42
1	D	185[B]	SER	CB-OG	42.25	2.26	1.42
1	A	160[A]	SER	CB-OG	-24.69	0.92	1.42
1	A	160[B]	SER	CB-OG	-24.69	0.92	1.42
1	B	113[A]	SER	CB-OG	-21.75	0.98	1.42
1	B	113[B]	SER	CB-OG	-21.75	0.98	1.42
1	D	113[A]	SER	CB-OG	-18.31	1.05	1.42
1	D	113[B]	SER	CB-OG	-18.31	1.05	1.42
1	D	160[A]	SER	CB-OG	-17.93	1.06	1.42
1	D	160[B]	SER	CB-OG	-17.93	1.06	1.42
1	A	161[A]	SER	CB-OG	-16.32	1.09	1.42
1	A	161[B]	SER	CB-OG	-16.32	1.09	1.42
1	C	113[A]	SER	CB-OG	-16.05	1.10	1.42
1	C	113[B]	SER	CB-OG	-16.05	1.10	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161[A]	SER	CB-OG	-15.56	1.11	1.42
1	C	161[B]	SER	CB-OG	-15.56	1.11	1.42
1	B	129[A]	MET	CG-SD	-15.09	1.43	1.80
1	B	129[B]	MET	CG-SD	-15.09	1.43	1.80
1	B	25[A]	ILE	CA-CB	14.17	1.70	1.54
1	B	25[B]	ILE	CA-CB	14.17	1.70	1.54
1	C	166[A]	GLN	CG-CD	-14.01	1.17	1.52
1	C	166[B]	GLN	CG-CD	-14.01	1.17	1.52
1	A	113[A]	SER	CB-OG	-13.85	1.14	1.42
1	A	113[B]	SER	CB-OG	-13.85	1.14	1.42
1	B	215[A]	SER	CB-OG	-12.93	1.16	1.42
1	B	215[B]	SER	CB-OG	-12.93	1.16	1.42
1	B	160[A]	SER	CB-OG	-12.17	1.17	1.42
1	B	160[B]	SER	CB-OG	-12.17	1.17	1.42
1	B	161[A]	SER	CB-OG	-12.06	1.18	1.42
1	B	161[B]	SER	CB-OG	-12.06	1.18	1.42
1	B	27[A]	ILE	CG1-CD1	-12.00	1.04	1.51
1	B	27[B]	ILE	CG1-CD1	-12.00	1.04	1.51
1	C	9[A]	LEU	CB-CG	10.96	1.75	1.53
1	C	9[B]	LEU	CB-CG	10.96	1.75	1.53
1	D	134[A]	SER	CB-OG	-10.35	1.21	1.42
1	D	134[B]	SER	CB-OG	-10.35	1.21	1.42
1	C	27[A]	ILE	CG1-CD1	-10.34	1.11	1.51
1	C	27[B]	ILE	CG1-CD1	-10.34	1.11	1.51
1	B	132[A]	GLN	CG-CD	-10.23	1.26	1.52
1	B	132[B]	GLN	CG-CD	-10.23	1.26	1.52
1	B	218[A]	ASP	CB-CG	-9.18	1.29	1.52
1	B	218[B]	ASP	CB-CG	-9.18	1.29	1.52
1	B	151[A]	ASP	CB-CG	-9.05	1.29	1.52
1	B	151[B]	ASP	CB-CG	-9.05	1.29	1.52
1	C	223[A]	SER	CB-OG	-8.71	1.24	1.42
1	C	223[B]	SER	CB-OG	-8.71	1.24	1.42
1	A	78[A]	ASP	CB-CG	-8.32	1.31	1.52
1	A	78[B]	ASP	CB-CG	-8.32	1.31	1.52
1	D	78[A]	ASP	CB-CG	-8.30	1.31	1.52
1	D	78[B]	ASP	CB-CG	-8.30	1.31	1.52
1	B	164[A]	SER	CB-OG	-8.19	1.25	1.42
1	B	164[B]	SER	CB-OG	-8.19	1.25	1.42
1	A	42[A]	MET	CB-CG	-7.88	1.28	1.52
1	A	42[B]	MET	CB-CG	-7.88	1.28	1.52
1	D	161[A]	SER	CB-OG	-7.68	1.26	1.42
1	D	161[B]	SER	CB-OG	-7.68	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	42[A]	MET	CB-CG	-7.25	1.30	1.52
1	D	42[B]	MET	CB-CG	-7.25	1.30	1.52
1	A	15[A]	THR	CA-CB	-6.89	1.41	1.53
1	A	15[B]	THR	CA-CB	-6.89	1.41	1.53
1	A	134[A]	SER	CB-OG	-6.75	1.28	1.42
1	A	134[B]	SER	CB-OG	-6.75	1.28	1.42
1	A	129[A]	MET	CG-SD	-6.62	1.64	1.80
1	A	129[B]	MET	CG-SD	-6.62	1.64	1.80
1	D	11	THR	N-CA	-6.42	1.37	1.46
1	D	25[A]	ILE	CA-CB	-6.31	1.37	1.54
1	D	25[B]	ILE	CA-CB	-6.31	1.37	1.54
1	B	134[A]	SER	CB-OG	-6.12	1.29	1.42
1	B	134[B]	SER	CB-OG	-6.12	1.29	1.42
1	A	11	THR	N-CA	-5.90	1.38	1.46
1	B	135[A]	LYS	CD-CE	5.76	1.69	1.52
1	B	135[B]	LYS	CD-CE	5.76	1.69	1.52
1	D	129[A]	MET	CG-SD	-5.69	1.66	1.80
1	D	129[B]	MET	CG-SD	-5.69	1.66	1.80
1	B	24	HIS	N-CA	-5.59	1.39	1.46
1	B	24	HIS	C-N	-5.58	1.25	1.33
1	C	134[A]	SER	CB-OG	-5.47	1.31	1.42
1	C	134[B]	SER	CB-OG	-5.47	1.31	1.42
1	C	132[A]	GLN	CG-CD	-5.43	1.38	1.52
1	C	132[B]	GLN	CG-CD	-5.43	1.38	1.52
1	C	47	VAL	C-O	-5.41	1.18	1.24
1	C	64	VAL	C-O	-5.39	1.18	1.24
1	B	8	GLU	CA-C	-5.21	1.46	1.52
1	A	10	ASP	CA-CB	5.17	1.59	1.52
1	D	65[A]	VAL	C-O	-5.16	1.18	1.24
1	D	65[B]	VAL	C-O	-5.16	1.18	1.24
1	C	128	PHE	C-O	-5.15	1.17	1.23
1	C	65	VAL	C-O	-5.10	1.18	1.24
1	C	129[A]	MET	CG-SD	-5.09	1.68	1.80
1	C	129[B]	MET	CG-SD	-5.09	1.68	1.80
1	B	223[A]	SER	CB-OG	-5.07	1.32	1.42
1	B	223[B]	SER	CB-OG	-5.07	1.32	1.42
1	C	164[A]	SER	CB-OG	-5.04	1.32	1.42
1	C	164[B]	SER	CB-OG	-5.04	1.32	1.42

All (149) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25[A]	ILE	N-CA-CB	24.03	138.40	111.00
1	B	25[B]	ILE	N-CA-CB	24.03	138.40	111.00
1	A	78[A]	ASP	CA-CB-CG	20.00	132.60	112.60
1	A	78[B]	ASP	CA-CB-CG	20.00	132.60	112.60
1	B	151[A]	ASP	CA-CB-CG	18.98	131.58	112.60
1	B	151[B]	ASP	CA-CB-CG	18.98	131.58	112.60
1	D	78[A]	ASP	CA-CB-CG	18.95	131.54	112.60
1	D	78[B]	ASP	CA-CB-CG	18.95	131.54	112.60
1	D	185[A]	SER	CA-CB-OG	-18.80	73.50	111.10
1	D	185[B]	SER	CA-CB-OG	-18.80	73.50	111.10
1	B	23	PRO	O-C-N	17.43	142.62	123.10
1	C	161[A]	SER	CA-CB-OG	15.33	141.76	111.10
1	C	161[B]	SER	CA-CB-OG	15.33	141.76	111.10
1	C	27[A]	ILE	CB-CG1-CD1	14.77	144.81	113.80
1	C	27[B]	ILE	CB-CG1-CD1	14.77	144.81	113.80
1	A	123	THR	N-CA-C	14.12	130.12	110.35
1	B	218[A]	ASP	CA-CB-CG	13.79	126.39	112.60
1	B	218[B]	ASP	CA-CB-CG	13.79	126.39	112.60
1	B	161[A]	SER	CA-CB-OG	12.72	136.53	111.10
1	B	161[B]	SER	CA-CB-OG	12.72	136.53	111.10
1	B	27[A]	ILE	CB-CG1-CD1	12.38	139.80	113.80
1	B	27[B]	ILE	CB-CG1-CD1	12.38	139.80	113.80
1	C	166[A]	GLN	CB-CG-CD	12.20	133.33	112.60
1	C	166[B]	GLN	CB-CG-CD	12.20	133.33	112.60
1	D	25[A]	ILE	N-CA-CB	11.33	130.76	111.50
1	D	25[B]	ILE	N-CA-CB	11.33	130.76	111.50
1	B	23	PRO	CA-C-N	10.43	137.70	122.99
1	B	23	PRO	C-N-CA	10.43	137.70	122.99
1	A	9[A]	LEU	CA-C-N	10.00	138.37	122.17
1	A	9[A]	LEU	C-N-CA	10.00	138.37	122.17
1	A	9[B]	LEU	CA-C-N	10.00	138.37	122.17
1	A	9[B]	LEU	C-N-CA	10.00	138.37	122.17
1	C	114[A]	LYS	CD-CE-NZ	9.70	142.93	111.90
1	C	114[B]	LYS	CD-CE-NZ	9.70	142.93	111.90
1	D	161[A]	SER	CA-CB-OG	9.66	130.43	111.10
1	D	161[B]	SER	CA-CB-OG	9.66	130.43	111.10
1	B	24	HIS	CA-C-N	9.58	134.34	122.37
1	B	24	HIS	C-N-CA	9.58	134.34	122.37
1	B	25[A]	ILE	CB-CA-C	-9.15	99.89	110.96
1	B	25[B]	ILE	CB-CA-C	-9.15	99.89	110.96
1	B	135[A]	LYS	CG-CD-CE	9.13	132.31	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135[B]	LYS	CG-CD-CE	9.13	132.31	111.30
1	A	9[A]	LEU	CA-CB-CG	8.91	147.50	116.30
1	A	9[B]	LEU	CA-CB-CG	8.91	147.50	116.30
1	D	9	LEU	CA-C-N	8.42	135.81	122.17
1	D	9	LEU	C-N-CA	8.42	135.81	122.17
1	B	24	HIS	CA-C-O	8.32	129.34	120.36
1	C	218[A]	ASP	CA-CB-CG	8.13	120.73	112.60
1	C	218[B]	ASP	CA-CB-CG	8.13	120.73	112.60
1	A	160[A]	SER	CA-CB-OG	8.06	127.22	111.10
1	A	160[B]	SER	CA-CB-OG	8.06	127.22	111.10
1	C	6	ALA	N-CA-C	7.96	120.82	108.96
1	A	161[A]	SER	CA-CB-OG	7.90	126.90	111.10
1	A	161[B]	SER	CA-CB-OG	7.90	126.90	111.10
1	A	185	SER	N-CA-C	-7.40	105.13	112.97
1	D	11	THR	CA-C-N	-7.22	112.88	122.56
1	D	11	THR	C-N-CA	-7.22	112.88	122.56
1	A	42[A]	MET	CA-CB-CG	7.18	128.46	114.10
1	A	42[B]	MET	CA-CB-CG	7.18	128.46	114.10
1	D	5	VAL	N-CA-C	-7.16	98.17	108.48
1	A	122	GLU	CA-C-N	7.02	131.78	121.31
1	A	122	GLU	C-N-CA	7.02	131.78	121.31
1	B	129[A]	MET	CB-CG-SD	6.98	133.63	112.70
1	B	129[B]	MET	CB-CG-SD	6.98	133.63	112.70
1	B	230	LEU	N-CA-C	6.81	120.89	111.90
1	A	22	TYR	N-CA-C	6.73	114.06	108.07
1	D	26	GLY	N-CA-C	6.66	120.82	111.10
1	B	23	PRO	CA-C-O	-6.62	113.49	121.03
1	A	158	ARG	N-CA-C	6.51	119.81	110.10
1	C	138	LYS	N-CA-C	6.46	120.26	112.38
1	B	26	GLY	N-CA-C	6.45	123.36	110.97
1	A	4	ILE	N-CA-C	6.42	117.72	108.48
1	B	205	HIS	CA-C-N	-6.29	114.17	120.21
1	B	205	HIS	C-N-CA	-6.29	114.17	120.21
1	C	230	LEU	N-CA-C	6.29	120.27	112.47
1	D	10	ASP	N-CA-CB	-6.26	101.16	110.24
1	B	66	SER	N-CA-C	6.18	117.63	108.60
1	A	10	ASP	N-CA-CB	-6.15	101.32	110.24
1	A	96	SER	N-CA-C	6.09	118.10	108.79
1	D	27[A]	ILE	CB-CG1-CD1	6.08	126.57	113.80
1	D	27[B]	ILE	CB-CG1-CD1	6.08	126.57	113.80
1	C	101	LYS	N-CA-C	6.08	116.30	108.34
1	C	103	THR	N-CA-C	-6.07	101.50	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ASP	N-CA-CB	-6.06	100.25	110.49
1	D	101	LYS	N-CA-C	6.05	118.15	109.14
1	D	4	ILE	N-CA-C	6.03	116.55	108.11
1	A	15[A]	THR	N-CA-CB	6.02	120.66	110.49
1	A	15[B]	THR	N-CA-CB	6.02	120.66	110.49
1	D	10	ASP	N-CA-C	5.93	118.44	108.23
1	D	34	SER	N-CA-C	5.87	118.87	110.24
1	A	164[A]	SER	CA-CB-OG	5.87	122.83	111.10
1	A	164[B]	SER	CA-CB-OG	5.87	122.83	111.10
1	C	73	ALA	N-CA-C	-5.83	100.38	109.72
1	D	230	LEU	N-CA-C	5.83	119.97	112.86
1	D	176	TYR	N-CA-C	5.81	117.61	111.28
1	A	189	ALA	N-CA-C	-5.80	94.76	111.00
1	B	190	SER	N-CA-C	5.80	119.41	110.42
1	A	24	HIS	N-CA-C	5.80	117.06	108.60
1	B	158	ARG	N-CA-C	5.77	118.61	109.96
1	A	66	SER	N-CA-C	5.74	117.52	108.96
1	A	11	THR	CA-C-N	-5.71	114.90	122.56
1	A	11	THR	C-N-CA	-5.71	114.90	122.56
1	C	84	VAL	N-CA-C	5.71	116.72	111.81
1	C	125	ALA	N-CA-C	5.70	117.85	109.24
1	C	212	PHE	N-CA-C	-5.70	100.41	109.76
1	A	15[A]	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	15[B]	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	123	THR	CB-CA-C	-5.65	100.68	109.61
1	C	216	ASN	N-CA-C	-5.64	102.55	110.50
1	C	152	GLY	N-CA-C	5.62	122.51	115.21
1	D	212	PHE	N-CA-C	-5.62	100.09	109.24
1	D	197	PHE	N-CA-C	5.60	117.70	109.24
1	C	187	VAL	N-CA-C	-5.57	95.41	111.00
1	A	5	VAL	N-CA-C	-5.55	99.55	107.77
1	A	34	SER	N-CA-C	5.53	118.36	110.24
1	A	197	PHE	N-CA-C	5.51	117.57	109.24
1	C	4	ILE	N-CA-C	5.51	116.42	108.48
1	C	158	ARG	N-CA-C	5.49	118.19	109.96
1	D	65[A]	VAL	CA-CB-CG1	5.42	119.61	110.40
1	D	65[B]	VAL	CA-CB-CG1	5.42	119.61	110.40
1	B	6	ALA	N-CA-C	5.38	116.98	108.96
1	A	176	TYR	N-CA-C	5.35	117.11	111.28
1	B	132[A]	GLN	CG-CD-NE2	-5.34	108.39	116.40
1	B	132[B]	GLN	CG-CD-NE2	-5.34	108.39	116.40
1	B	138	LYS	N-CA-C	5.34	119.28	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	LEU	O-C-N	5.34	128.28	122.20
1	B	81	LEU	CA-C-N	5.32	131.71	121.54
1	B	81	LEU	C-N-CA	5.32	131.71	121.54
1	D	11	THR	N-CA-CB	-5.31	102.31	110.44
1	B	212	PHE	N-CA-C	-5.31	101.05	109.76
1	C	197	PHE	N-CA-C	5.31	117.48	109.41
1	C	177	ALA	N-CA-C	5.27	116.30	109.65
1	A	59	LYS	N-CA-C	-5.26	104.03	111.56
1	A	87	GLU	N-CA-C	5.24	118.93	112.54
1	C	184	SER	N-CA-C	-5.20	99.72	110.80
1	D	103	THR	N-CA-C	-5.18	102.81	110.48
1	A	188	VAL	CA-C-N	5.14	130.95	121.70
1	A	188	VAL	C-N-CA	5.14	130.95	121.70
1	C	209	GLY	N-CA-C	5.14	117.54	111.63
1	B	125	ALA	N-CA-C	5.13	116.99	109.24
1	B	182	TRP	N-CA-C	5.09	116.15	108.46
1	C	25[A]	ILE	N-CA-CB	5.07	120.59	111.21
1	C	25[B]	ILE	N-CA-CB	5.07	120.59	111.21
1	D	158	ARG	N-CA-C	5.07	117.65	110.10
1	B	197	PHE	N-CA-C	5.06	116.89	109.24
1	B	176	TYR	N-CA-C	5.05	116.78	111.28
1	A	18	GLY	N-CA-C	5.03	121.45	114.92
1	A	217	ILE	N-CA-C	5.02	116.34	110.62
1	D	90	ARG	N-CA-C	-5.02	101.75	109.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	25[A]	ILE	CA
1	D	25[B]	ILE	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1794	0	1736	62	0
1	B	1740	0	1679	54	0
1	C	1756	0	1691	79	0
1	D	1771	0	1731	100	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	19	0	0	0	0
5	A	16	0	0	0	0
5	B	20	0	0	3	0
5	C	9	0	0	1	0
5	D	22	0	0	0	0
All	All	7155	0	6837	280	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 20.

All (280) 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:184:SER:CB	1:D:185[A]:SER:HB2	1.59	1.30
1:D:184:SER:CB	1:D:185[B]:SER:HB2	1.59	1.30
1:C:186:ALA:HA	1:C:187:VAL:CB	1.52	1.26
1:C:116:LYS:HG2	1:C:123:THR:CG2	1.81	1.09
1:D:184:SER:HB2	1:D:185[A]:SER:HB2	1.17	1.07
1:D:184:SER:HB2	1:D:185[B]:SER:HB2	1.17	1.07
1:B:107:LEU:HB2	1:B:196:THR:HG22	1.37	1.06
1:D:184:SER:N	1:D:185[A]:SER:HB3	1.69	1.05
1:D:184:SER:N	1:D:185[B]:SER:HB3	1.69	1.05
1:C:116:LYS:HG2	1:C:123:THR:HG22	1.40	1.03
1:D:107:LEU:HB2	1:D:196:THR:CG2	1.93	0.99
1:D:184:SER:CA	1:D:185[A]:SER:HB2	1.94	0.96
1:D:184:SER:CA	1:D:185[B]:SER:HB2	1.94	0.96
1:C:186:ALA:CA	1:C:187:VAL:CB	2.43	0.95
1:A:59:LYS:HD3	1:A:80:ASP:OD1	1.67	0.94
1:D:59:LYS:HD3	1:D:80:ASP:OD1	1.70	0.92
1:B:116:LYS:HG2	1:B:123:THR:HG23	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:O	1:A:184:SER:OG	1.89	0.90
1:C:202:PRO:HD2	1:C:203:ASP:OD1	1.72	0.89
1:A:56:SER:HB2	1:A:188:VAL:HA	1.55	0.89
1:C:107:LEU:HB2	1:C:196:THR:HG22	1.53	0.87
1:B:56:SER:HG	1:B:189:ALA:N	1.73	0.86
1:D:11:THR:HG22	1:D:42[B]:MET:HE2	1.56	0.86
1:C:182:TRP:HA	1:C:186:ALA:HB3	1.57	0.85
1:C:116:LYS:HG2	1:C:123:THR:HG21	1.57	0.83
1:B:113[A]:SER:HB2	5:B:403:HOH:O	1.77	0.83
1:B:113[B]:SER:HB2	5:B:403:HOH:O	1.77	0.83
1:C:196:THR:HG21	5:C:408:HOH:O	1.79	0.82
1:D:107:LEU:HB2	1:D:196:THR:HG22	1.62	0.82
1:A:131:ASN:H	1:B:124:ASN:ND2	1.77	0.82
1:A:59:LYS:CD	1:A:80:ASP:OD1	2.28	0.81
1:C:183:GLU:O	1:C:186:ALA:HB2	1.81	0.81
1:C:112:THR:HG1	1:C:127:HIS:CE1	2.00	0.80
1:B:11:THR:HG21	1:B:102:GLU:OE1	1.82	0.79
1:C:182:TRP:CA	1:C:186:ALA:HB3	2.12	0.79
1:B:107:LEU:HB2	1:B:196:THR:CG2	2.12	0.78
1:B:25[B]:ILE:HG21	1:B:65:VAL:HG11	1.66	0.78
1:C:25[B]:ILE:HG21	1:C:65:VAL:HG11	1.66	0.77
1:C:124:ASN:ND2	1:D:131:ASN:H	1.82	0.77
1:C:183:GLU:H	1:C:186:ALA:CB	1.98	0.76
1:A:189:ALA:HB1	1:A:190:SER:O	1.86	0.76
1:B:60:ARG:NH2	1:C:60:ARG:HH21	1.83	0.75
1:A:107:LEU:HB2	1:A:196:THR:HG22	1.68	0.75
1:D:184:SER:H	1:D:185[B]:SER:HB3	1.52	0.75
1:D:184:SER:H	1:D:185[A]:SER:HB3	1.52	0.75
1:C:116:LYS:HB2	1:C:188:VAL:HB	1.70	0.74
1:A:68:PRO:O	1:A:69:ASN:HB2	1.88	0.73
1:D:4:ILE:HD13	1:D:215[B]:SER:OG	1.88	0.73
1:C:112:THR:OG1	1:C:127:HIS:ND1	2.21	0.70
1:D:187:VAL:O	1:D:188:VAL:HG23	1.91	0.70
1:A:188:VAL:HG12	1:A:190:SER:HB2	1.73	0.70
1:D:181:ILE:HD12	1:D:182:TRP:CD1	2.26	0.70
1:A:131:ASN:H	1:B:124:ASN:HD21	1.36	0.70
1:B:4:ILE:HD13	1:B:215[B]:SER:OG	1.92	0.69
1:D:11:THR:HG22	1:D:42[B]:MET:CE	2.22	0.69
1:B:42:MET:HE1	1:B:206:PRO:HG2	1.75	0.69
1:B:116:LYS:HG2	1:B:123:THR:CG2	2.23	0.68
1:B:203:ASP:O	1:B:204:SER:HB3	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25[B]:ILE:HD13	1:D:65[B]:VAL:HG12	1.76	0.68
1:A:107:LEU:HD23	1:A:107:LEU:N	2.09	0.67
1:C:135:LYS:HD2	1:C:135:LYS:C	2.19	0.67
1:D:187:VAL:O	1:D:188:VAL:CG2	2.42	0.67
1:C:9[B]:LEU:HD23	1:C:25[B]:ILE:HG22	1.76	0.67
1:C:131:ASN:H	1:D:124:ASN:ND2	1.94	0.66
1:C:135:LYS:HD2	1:C:136:ASP:N	2.10	0.66
1:D:42[A]:MET:HE1	1:D:44:ASN:HA	1.78	0.65
1:C:183:GLU:N	1:C:186:ALA:CB	2.59	0.65
1:D:203:ASP:OD1	1:D:203:ASP:N	2.30	0.64
1:C:116:LYS:HA	1:C:123:THR:HG22	1.80	0.63
1:C:183:GLU:N	1:C:186:ALA:HB3	2.13	0.63
1:C:159:VAL:CG1	1:C:163:GLY:HA2	2.29	0.63
1:C:184:SER:O	1:C:186:ALA:N	2.31	0.63
1:D:202:PRO:C	1:D:203:ASP:OD1	2.42	0.63
1:D:51:HIS:HE1	1:D:192:GLU:OE1	1.83	0.61
1:C:25[B]:ILE:HG21	1:C:65:VAL:CG1	2.31	0.61
1:A:82:ASP:HA	1:A:182:TRP:CD1	2.36	0.61
1:C:150:THR:HG23	1:C:150:THR:O	2.01	0.60
1:A:107:LEU:HB2	1:A:196:THR:CG2	2.31	0.60
1:D:184:SER:N	1:D:185[B]:SER:HB2	2.06	0.60
1:A:14:ASN:H	1:A:19:ASP:CB	2.14	0.60
1:D:201:SER:C	1:D:203:ASP:H	2.10	0.60
1:A:124:ASN:ND2	1:B:131:ASN:H	2.00	0.59
1:A:150:THR:O	1:A:151:ASP:HB2	2.02	0.59
1:D:187:VAL:C	1:D:188:VAL:HG23	2.28	0.58
1:D:80:ASP:OD1	1:D:82:ASP:OD1	2.21	0.58
1:C:42:MET:HE2	1:C:43:GLN:C	2.29	0.58
1:D:82:ASP:HA	1:D:182:TRP:CD1	2.39	0.58
1:D:183:GLU:HB2	1:D:186:ALA:HB2	1.85	0.58
1:B:196:THR:HG21	5:B:420:HOH:O	2.03	0.57
1:B:150:THR:HG22	1:B:151[B]:ASP:OD2	2.05	0.57
1:C:203:ASP:OD1	1:C:203:ASP:N	2.36	0.57
1:C:112:THR:OG1	1:C:127:HIS:CE1	2.57	0.56
1:A:68:PRO:O	1:A:69:ASN:CB	2.51	0.56
1:A:85:LEU:HB3	1:A:86:PRO:HD2	1.87	0.56
1:B:60:ARG:NH2	1:C:60:ARG:NH2	2.52	0.56
1:C:20:PRO:HD2	1:C:24:HIS:CE1	2.41	0.55
1:C:131:ASN:H	1:D:124:ASN:HD21	1.54	0.55
1:A:181:ILE:HD13	1:A:182:TRP:CD1	2.42	0.55
1:C:145:ASP:OD2	1:C:169:SER:OG	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LEU:HB2	1:D:196:THR:HG21	1.87	0.55
1:C:107:LEU:HB2	1:C:196:THR:CG2	2.30	0.55
1:B:25[A]:ILE:HD12	1:B:65:VAL:HG12	1.89	0.55
1:B:25[B]:ILE:HG21	1:B:65:VAL:CG1	2.34	0.55
1:D:51:HIS:CE1	1:D:192:GLU:OE1	2.60	0.55
1:B:30:LYS:HE2	1:B:84:VAL:HG13	1.88	0.54
1:A:188:VAL:HB	1:A:189:ALA:HA	1.88	0.54
1:D:183:GLU:O	1:D:184:SER:C	2.50	0.54
1:C:183:GLU:H	1:C:186:ALA:HB2	1.70	0.54
1:C:25[B]:ILE:HD13	1:C:65:VAL:HG12	1.90	0.54
1:C:42:MET:HE1	1:C:44:ASN:HA	1.89	0.53
1:D:107:LEU:CB	1:D:196:THR:HG22	2.38	0.53
1:B:11:THR:HG22	1:B:208:ASP:C	2.35	0.52
1:D:11:THR:HG22	1:D:42[B]:MET:SD	2.49	0.52
1:A:80:ASP:HB3	1:A:82:ASP:OD1	2.10	0.52
1:A:108:SER:OG	1:A:196:THR:HB	2.09	0.52
1:C:82:ASP:HA	1:C:182:TRP:CD1	2.44	0.52
1:C:9[B]:LEU:CD2	1:C:25[B]:ILE:HG22	2.40	0.51
1:D:184:SER:N	1:D:185[A]:SER:HB2	2.06	0.51
1:A:188:VAL:C	1:A:189:ALA:O	2.50	0.51
1:B:150:THR:HG22	1:B:151[A]:ASP:OD2	2.11	0.51
1:D:11:THR:CG2	1:D:42[B]:MET:HE2	2.34	0.51
1:A:14:ASN:H	1:A:19:ASP:HB2	1.73	0.51
1:D:222:PRO:HD2	1:D:225:SER:OG	2.10	0.51
1:A:14:ASN:N	1:A:19:ASP:HB2	2.26	0.50
1:C:124:ASN:HD21	1:D:131:ASN:H	1.57	0.50
1:B:64:VAL:HG22	1:B:74:THR:HB	1.94	0.50
1:B:210:ILE:HG22	1:B:211:ALA:N	2.26	0.50
1:C:182:TRP:C	1:C:186:ALA:HB3	2.36	0.50
1:D:8:GLU:OE1	1:D:28:ASP:OD2	2.30	0.50
1:A:106:ILE:C	1:A:107:LEU:HD23	2.37	0.50
1:A:122:GLU:HG3	1:A:123:THR:OG1	2.12	0.50
1:B:100:TYR:HB2	1:B:207:ALA:CB	2.42	0.49
1:B:7:VAL:HG22	1:B:27[A]:ILE:HD13	1.94	0.49
1:C:159:VAL:HG11	1:C:163:GLY:HA2	1.94	0.49
1:C:135:LYS:C	1:C:135:LYS:CD	2.85	0.49
1:B:32:VAL:HB	1:B:233:PHE:CD2	2.47	0.49
1:C:183:GLU:H	1:C:186:ALA:HB3	1.75	0.49
1:C:184:SER:C	1:C:186:ALA:N	2.71	0.49
1:D:183:GLU:C	1:D:185[A]:SER:HB3	2.34	0.49
1:B:159[A]:VAL:CG1	1:B:163:GLY:HA2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:GLU:C	1:D:185[B]:SER:HB3	2.35	0.49
1:A:181:ILE:CD1	1:A:182:TRP:CD1	2.96	0.48
1:B:100:TYR:HB2	1:B:207:ALA:HB3	1.94	0.48
1:D:53:ILE:HD11	1:D:62:SER:HB2	1.94	0.48
1:D:183:GLU:HB3	1:D:185[A]:SER:HB3	1.94	0.48
1:B:7:VAL:HG22	1:B:27[B]:ILE:HD13	1.95	0.48
1:D:114:LYS:HB2	1:D:114:LYS:HE3	1.61	0.48
1:A:189:ALA:HB1	1:A:190:SER:C	2.38	0.48
1:B:159[B]:VAL:CG1	1:B:163:GLY:HA2	2.43	0.48
1:B:181:ILE:HD12	1:B:182:TRP:HD1	1.78	0.48
1:D:116:LYS:HB3	1:D:187:VAL:CG1	2.43	0.47
1:A:188:VAL:HB	1:A:189:ALA:CA	2.42	0.47
1:D:183:GLU:HB3	1:D:185[B]:SER:HB3	1.95	0.47
1:B:66:SER:HB3	1:B:72:SER:HB3	1.96	0.47
1:A:131:ASN:O	1:B:122:GLU:OE2	2.32	0.47
1:A:116:LYS:HG2	1:A:123:THR:HG23	1.96	0.47
1:B:7:VAL:HG21	1:B:52:ILE:HG12	1.95	0.47
1:C:116:LYS:CG	1:C:123:THR:HG22	2.29	0.47
1:D:28:ASP:HB3	1:D:31:SER:O	2.15	0.47
1:D:181:ILE:O	1:D:189:ALA:HB1	2.15	0.47
1:A:25:ILE:HG22	1:A:38:ALA:HB3	1.97	0.46
1:B:54:TYR:CZ	1:B:81:LEU:HG	2.50	0.46
1:C:4:ILE:HD13	1:C:215[B]:SER:OG	2.15	0.46
1:C:12:TYR:HA	1:C:13:PRO:HD3	1.74	0.46
1:C:25[B]:ILE:CG2	1:C:65:VAL:HG11	2.43	0.46
1:C:32:VAL:HG22	1:C:32:VAL:O	2.16	0.46
1:A:181:ILE:HD13	1:A:182:TRP:HD1	1.80	0.46
1:D:183:GLU:OE2	1:D:185[A]:SER:HB3	2.15	0.46
1:D:183:GLU:OE2	1:D:185[B]:SER:HB3	2.15	0.46
1:A:201:SER:C	1:A:203:ASP:H	2.23	0.46
1:D:150:THR:C	1:D:152:GLY:H	2.23	0.46
1:A:176:TYR:CE2	1:B:176:TYR:CE1	3.04	0.46
1:A:183:GLU:HB2	1:A:186:ALA:HB3	1.98	0.46
1:D:22:TYR:CD1	1:D:22:TYR:C	2.93	0.45
1:D:210:ILE:HG22	1:D:211:ALA:N	2.30	0.45
1:C:183:GLU:N	1:C:186:ALA:HB2	2.29	0.45
1:D:86:PRO:O	1:D:181:ILE:HD11	2.15	0.45
1:C:182:TRP:O	1:C:182:TRP:CE3	2.70	0.45
1:D:158:ARG:HA	1:D:158:ARG:HD3	1.80	0.45
1:D:203:ASP:C	1:D:205:HIS:N	2.74	0.45
1:A:115:LEU:CD2	1:A:188:VAL:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:HD12	1:B:182:TRP:CD1	2.52	0.45
1:A:58:ASP:O	1:A:59:LYS:HB2	2.17	0.45
1:A:207:ALA:HA	1:A:208:ASP:HA	1.86	0.45
1:D:32:VAL:HB	1:D:233:PHE:CD2	2.52	0.45
1:D:150:THR:C	1:D:152:GLY:N	2.74	0.45
1:D:181:ILE:H	1:D:181:ILE:HG13	1.61	0.45
1:A:82:ASP:OD1	1:A:83:ASN:N	2.50	0.45
1:A:12:TYR:HA	1:A:13:PRO:HD3	1.76	0.45
1:A:107:LEU:CB	1:A:196:THR:HG22	2.42	0.45
1:C:45:GLY:HA2	1:C:200:LYS:HG2	1.98	0.44
1:A:158:ARG:HA	1:A:158:ARG:HD3	1.80	0.44
1:A:25:ILE:HD12	1:A:65[B]:VAL:HG12	2.00	0.44
1:B:28:ASP:HB3	1:B:31:SER:O	2.18	0.44
1:B:116:LYS:NZ	1:C:51:HIS:CE1	2.86	0.44
1:C:135:LYS:HD2	1:C:136:ASP:HB2	2.00	0.44
1:B:42:MET:HG2	1:B:43:GLN:N	2.32	0.44
1:C:182:TRP:HA	1:C:186:ALA:CB	2.38	0.43
1:C:172:ARG:HG3	1:C:221:ILE:HD11	2.00	0.43
1:A:124:ASN:HD21	1:B:131:ASN:H	1.66	0.43
1:D:221:ILE:HA	1:D:222:PRO:HD3	1.91	0.43
1:A:4:ILE:HD13	1:A:215[B]:SER:OG	2.19	0.43
1:A:86:PRO:O	1:A:181:ILE:HD11	2.18	0.43
1:D:11:THR:HG22	1:D:42[A]:MET:HG3	1.99	0.43
1:D:183:GLU:CB	1:D:186:ALA:HB2	2.48	0.43
1:D:111:PHE:O	1:D:127:HIS:ND1	2.52	0.43
1:A:131:ASN:N	1:B:124:ASN:HD21	2.11	0.43
1:A:122:GLU:HG3	1:A:123:THR:H	1.84	0.43
1:B:12:TYR:HA	1:B:13:PRO:HD3	1.74	0.42
1:C:32:VAL:HB	1:C:233:PHE:CD2	2.54	0.42
1:B:112:THR:HG23	1:B:127:HIS:HB2	2.01	0.42
1:D:187:VAL:C	1:D:188:VAL:CG2	2.90	0.42
1:A:56:SER:HB3	1:A:188:VAL:HG13	2.01	0.42
1:A:25:ILE:HD12	1:A:65[A]:VAL:HG12	2.01	0.42
1:A:181:ILE:HD12	1:A:181:ILE:C	2.44	0.42
1:D:32:VAL:O	1:D:32:VAL:HG22	2.18	0.42
1:D:187:VAL:O	1:D:187:VAL:HG22	2.17	0.42
1:B:229:LEU:HD22	1:B:235:ASP:O	2.19	0.42
1:C:159:VAL:HG12	1:C:163:GLY:HA2	2.01	0.42
1:D:56:SER:CB	1:D:189:ALA:H	2.33	0.42
1:A:201:SER:C	1:A:203:ASP:N	2.76	0.42
1:D:107:LEU:CB	1:D:196:THR:CG2	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:TYR:CZ	1:C:81:LEU:HG	2.55	0.42
1:A:115:LEU:HD23	1:A:188:VAL:HG23	2.02	0.41
1:A:122:GLU:HG3	1:A:123:THR:N	2.35	0.41
1:D:11:THR:CG2	1:D:42[B]:MET:CE	2.97	0.41
1:D:137:GLN:HG3	1:D:139:ASP:OD1	2.20	0.41
1:A:14:ASN:H	1:A:19:ASP:CG	2.28	0.41
1:D:4:ILE:HD13	1:D:215[A]:SER:HB3	2.01	0.41
1:D:207:ALA:HA	1:D:208:ASP:HA	1.86	0.41
1:D:3:THR:HG23	1:D:30:LYS:HD3	2.02	0.41
1:A:36:LYS:HD2	1:A:75:VAL:CG2	2.50	0.41
1:C:183:GLU:O	1:C:184:SER:CB	2.69	0.41
1:B:116:LYS:HZ3	1:C:51:HIS:CE1	2.38	0.41
1:C:99:LEU:C	1:C:99:LEU:CD1	2.93	0.41
1:D:53:ILE:O	1:D:53:ILE:HG12	2.21	0.41
1:A:44:ASN:HD21	1:A:201:SER:H	1.68	0.41
1:A:181:ILE:HD12	1:A:182:TRP:N	2.36	0.41
1:C:134[A]:SER:OG	1:C:135:LYS:N	2.52	0.41
1:C:185:SER:O	1:C:185:SER:OG	2.33	0.40
1:D:53:ILE:CD1	1:D:62:SER:HB2	2.51	0.40
1:A:106:ILE:HB	1:A:154:LEU:HB3	2.03	0.40
1:C:115:LEU:HD21	1:C:186:ALA:HB1	2.02	0.40
1:C:175:PHE:CE2	1:C:177:ALA:HB3	2.56	0.40
1:C:7:VAL:HG21	1:C:52:ILE:HG12	2.04	0.40
1:C:9[B]:LEU:HD23	1:C:25[B]:ILE:CG2	2.48	0.40
1:D:112:THR:O	1:D:191:PHE:HA	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	A	246/237 (104%)	223 (91%)	18 (7%)	5 (2%)	6 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	236/237 (100%)	220 (93%)	14 (6%)	2 (1%)	16	20
1	C	237/237 (100%)	218 (92%)	17 (7%)	2 (1%)	16	20
1	D	239/237 (101%)	221 (92%)	13 (5%)	5 (2%)	5	4
All	All	958/948 (101%)	882 (92%)	62 (6%)	14 (2%)	10	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	SER
1	B	204	SER
1	C	187	VAL
1	D	21[A]	SER
1	D	21[B]	SER
1	D	185[A]	SER
1	D	185[B]	SER
1	D	188	VAL
1	A	186	ALA
1	A	21[A]	SER
1	A	21[B]	SER
1	B	225	SER
1	A	188	VAL
1	C	228	ARG

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	212/203 (104%)	193 (91%)	19 (9%)	9	12
1	B	203/203 (100%)	184 (91%)	19 (9%)	8	11
1	C	204/203 (100%)	179 (88%)	25 (12%)	4	5
1	D	209/203 (103%)	184 (88%)	25 (12%)	5	5
All	All	828/812 (102%)	740 (89%)	88 (11%)	6	8

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9[A]	LEU
1	A	9[B]	LEU
1	A	36	LYS
1	A	74	THR
1	A	101	LYS
1	A	107	LEU
1	A	115	LEU
1	A	122	GLU
1	A	123	THR
1	A	132	GLN
1	A	134[A]	SER
1	A	134[B]	SER
1	A	135	LYS
1	A	183	GLU
1	A	188	VAL
1	A	196	THR
1	A	204	SER
1	A	228	ARG
1	B	4	ILE
1	B	11	THR
1	B	43	GLN
1	B	51	HIS
1	B	53	ILE
1	B	56	SER
1	B	59	LYS
1	B	65	VAL
1	B	74	THR
1	B	101	LYS
1	B	112	THR
1	B	115	LEU
1	B	123	THR
1	B	134[A]	SER
1	B	134[B]	SER
1	B	181	ILE
1	B	196	THR
1	B	204	SER
1	B	228	ARG
1	C	27[A]	ILE
1	C	27[B]	ILE
1	C	36	LYS
1	C	42	MET

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Mol	Chain	Res	Type
1	C	46	LYS
1	C	51	HIS
1	C	65	VAL
1	C	69	ASN
1	C	74	THR
1	C	76	SER
1	C	99	LEU
1	C	101	LYS
1	C	115	LEU
1	C	116	LYS
1	C	134[A]	SER
1	C	134[B]	SER
1	C	135	LYS
1	C	181	ILE
1	C	185	SER
1	C	188	VAL
1	C	196	THR
1	C	200	LYS
1	C	203	ASP
1	C	208	ASP
1	C	228	ARG
1	D	29	ILE
1	D	46	LYS
1	D	52	ILE
1	D	53	ILE
1	D	55	ASN
1	D	59	LYS
1	D	60	ARG
1	D	69	ASN
1	D	74	THR
1	D	80	ASP
1	D	101	LYS
1	D	116	LYS
1	D	123	THR
1	D	124	ASN
1	D	132[A]	GLN
1	D	132[B]	GLN
1	D	134[A]	SER
1	D	134[B]	SER
1	D	159	VAL
1	D	181	ILE
1	D	183	GLU

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Mol	Chain	Res	Type
1	D	196	THR
1	D	203	ASP
1	D	225	SER
1	D	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	GLN
1	A	104	ASN
1	A	124	ASN
1	A	162	ASN
1	B	43	GLN
1	B	104	ASN
1	B	124	ASN
1	C	41	ASN
1	C	43	GLN
1	C	51	HIS
1	C	124	ASN
1	C	180	HIS
1	C	205	HIS
1	D	41	ASN
1	D	43	GLN
1	D	104	ASN
1	D	124	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

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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$
4	96O	B	303	-	20,20,20	1.73	5 (25%)	27,28,28	2.12	10 (37%)

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
4	96O	B	303	-	-	6/7/27/27	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	96O	N04-N03	3.63	1.37	1.32
4	B	303	96O	O5-C5	2.71	1.51	1.44
4	B	303	96O	O5-C1	2.68	1.48	1.41
4	B	303	96O	C06-C05	2.51	1.53	1.49
4	B	303	96O	O1-C06	-2.27	1.39	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	96O	C01-N02-N03	5.12	127.28	121.32
4	B	303	96O	C19-N02-N03	-4.55	107.64	111.88
4	B	303	96O	C2-C3-C4	2.94	115.99	110.83
4	B	303	96O	C01-N02-C19	-2.86	125.07	127.94
4	B	303	96O	C06-C05-N04	2.78	126.10	121.49
4	B	303	96O	O1-C06-C05	-2.63	104.24	110.27
4	B	303	96O	C05-C19-N02	2.39	108.64	105.33
4	B	303	96O	C06-C05-C19	-2.30	126.25	130.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	96O	O4-C4-C3	-2.19	105.22	110.38
4	B	303	96O	O5-C1-O1	-2.05	105.19	110.04

There are no chirality outliers.

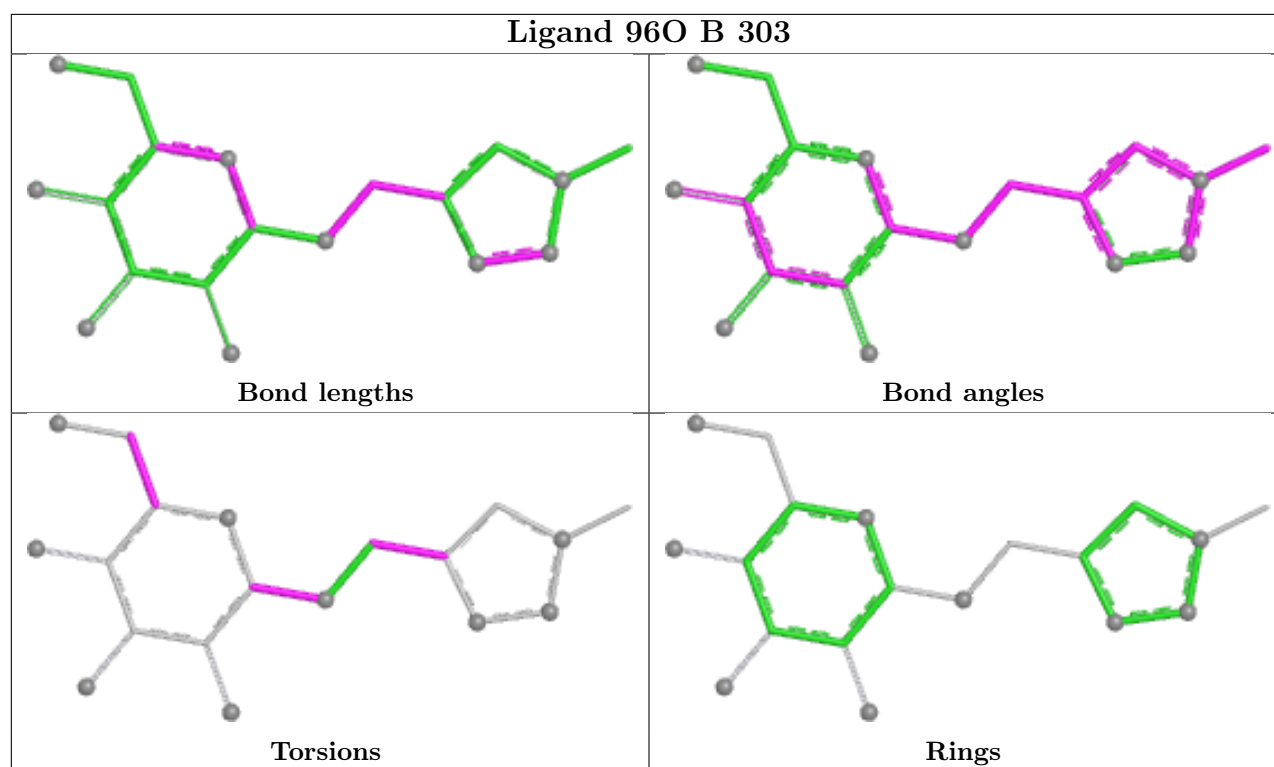
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	96O	C2-C1-O1-C06
4	B	303	96O	O5-C1-O1-C06
4	B	303	96O	C4-C5-C6-O6
4	B	303	96O	N04-C05-C06-O1
4	B	303	96O	C19-C05-C06-O1
4	B	303	96O	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	233/237 (98%)	0.47	12 (5%) 33 34	33, 48, 85, 124	16 (6%)
1	B	227/237 (95%)	0.64	17 (7%) 20 22	30, 50, 81, 111	16 (7%)
1	C	228/237 (96%)	0.67	20 (8%) 15 17	30, 51, 90, 137	15 (6%)
1	D	230/237 (97%)	0.56	14 (6%) 27 29	31, 51, 86, 123	16 (6%)
All	All	918/948 (96%)	0.58	63 (6%) 23 25	30, 50, 87, 137	63 (6%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	6.1
1	B	203	ASP	5.6
1	B	184	SER	4.9
1	C	187	VAL	4.6
1	C	152	GLY	4.5
1	B	205	HIS	4.3
1	C	188	VAL	4.1
1	D	188	VAL	4.0
1	A	189	ALA	4.0
1	D	56	SER	4.0
1	B	24	HIS	4.0
1	C	150	THR	3.7
1	D	23	PRO	3.4
1	A	187	VAL	3.4
1	D	127	HIS	3.2
1	C	18	GLY	3.2
1	D	187	VAL	3.2
1	D	189	ALA	3.1
1	C	12	TYR	3.1
1	B	122	GLU	3.0
1	B	11	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	67	TYR	3.0
1	B	116	LYS	2.9
1	A	205	HIS	2.8
1	B	189	ALA	2.8
1	D	186	ALA	2.8
1	D	10	ASP	2.8
1	B	127	HIS	2.7
1	C	184	SER	2.7
1	A	149	GLY	2.7
1	D	12	TYR	2.6
1	A	129[A]	MET	2.5
1	C	11	THR	2.5
1	B	151[A]	ASP	2.5
1	C	189	ALA	2.4
1	B	183	GLU	2.4
1	A	125	ALA	2.4
1	C	163	GLY	2.4
1	C	185	SER	2.4
1	D	185[A]	SER	2.3
1	B	158	ARG	2.3
1	A	202	PRO	2.3
1	D	17	ILE	2.3
1	A	41	ASN	2.3
1	C	82	ASP	2.3
1	A	169	SER	2.3
1	C	127	HIS	2.3
1	C	9[A]	LEU	2.3
1	C	20	PRO	2.3
1	D	124	ASN	2.2
1	B	9	LEU	2.2
1	D	115	LEU	2.2
1	B	169	SER	2.2
1	B	204	SER	2.2
1	C	151	ASP	2.1
1	B	202	PRO	2.1
1	D	19	ASP	2.1
1	C	182	TRP	2.1
1	B	55	ASN	2.1
1	C	123	THR	2.0
1	A	10	ASP	2.0
1	A	56	SER	2.0
1	C	83	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

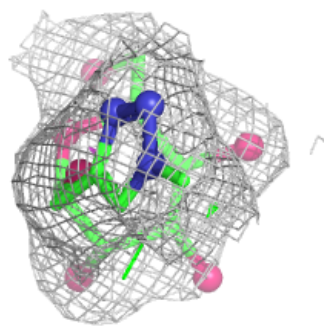
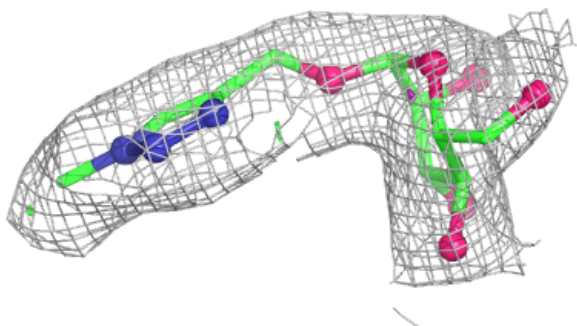
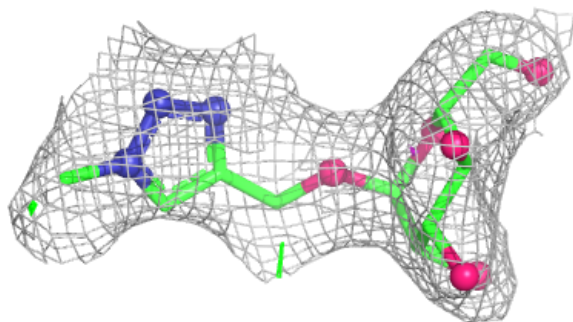
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	96O	B	303	19/19	0.81	0.11	48,56,82,84	0
2	MN	D	301	1/1	0.86	0.15	50,50,50,50	0
2	MN	C	301	1/1	0.86	0.09	47,47,47,47	0
3	CA	C	302	1/1	0.88	0.09	51,51,51,51	0
3	CA	A	302	1/1	0.88	0.07	45,45,45,45	0
2	MN	B	301	1/1	0.89	0.08	50,50,50,50	0
3	CA	D	302	1/1	0.92	0.07	49,49,49,49	0
3	CA	B	302	1/1	0.95	0.07	50,50,50,50	0
2	MN	A	301	1/1	0.95	0.09	46,46,46,46	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 96O B 303:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.