



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:16 PM UTC

PDB ID : 2O6Y / pdb_00002o6y
Title : Tyrosine ammonia-lyase from Rhodobacter sphaeroides
Authors : Louie, G.V.; Bowman, M.E.; Moffitt, M.C.; Baiga, T.J.; Moore, B.S.; Noel, J.P.
Deposited on : 2006-12-09
Resolution : 1.50 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

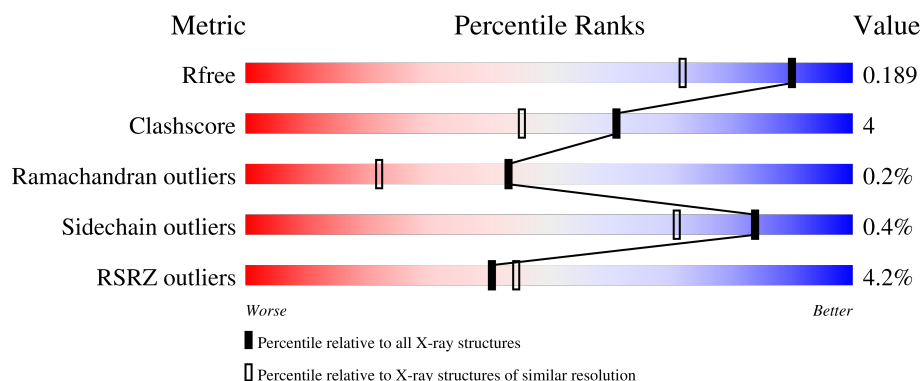
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	521	 5% 90% 8% ..
1	B	521	 3% 87% 12% .
1	C	521	 4% 88% 9% ..
1	D	521	 6% 88% 10% .
1	E	521	 5% 91% 7% ..

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Mol	Chain	Length	Quality of chain
1	F	521	% 90% 7% ..
1	G	521	2% 89% 9% .
1	H	521	7% 87% 10% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34467 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 Putative histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3813	2363	731	705	14			
1	B	515	Total	C	N	O	S	0	0	0
			3813	2363	731	705	14			
1	C	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	D	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	E	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	F	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	G	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			
1	H	514	Total	C	N	O	S	0	0	0
			3806	2358	730	704	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
A	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
B	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
C	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
D	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
E	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
F	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
G	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	ALA	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	SER	SEE REMARK 999	UNP Q3IWB0
H	149	MDO	GLY	SEE REMARK 999	UNP Q3IWB0

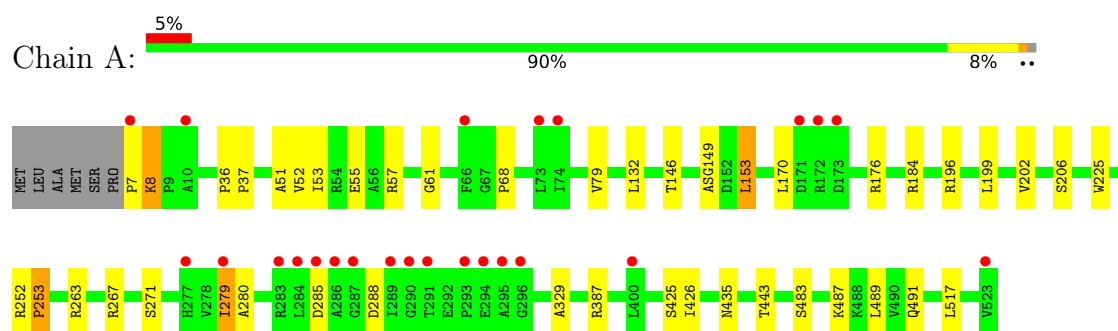
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	458	Total O 458 458	0	0
2	B	487	Total O 487 487	0	0
2	C	496	Total O 496 496	0	0
2	D	494	Total O 494 494	0	0
2	E	498	Total O 498 498	0	0
2	F	586	Total O 586 586	0	0
2	G	523	Total O 523 523	0	0
2	H	463	Total O 463 463	0	0

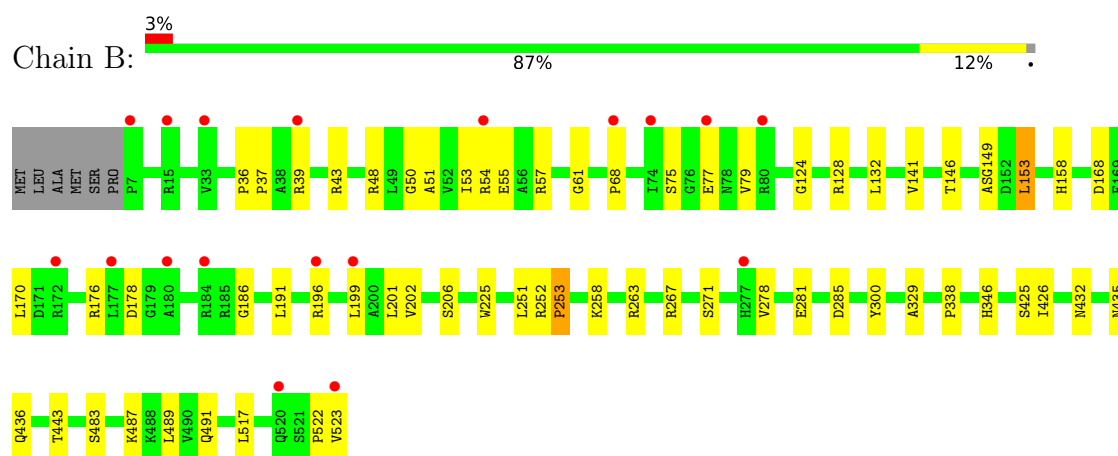
3 Residue-property plots

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.

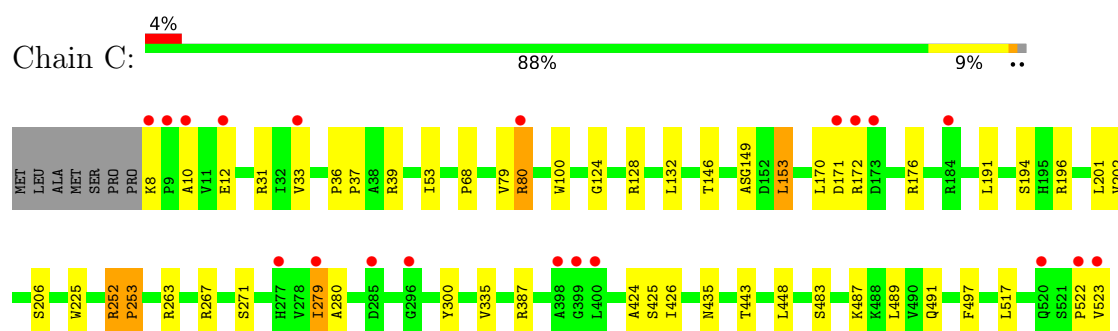
• Molecule 1: Putative histidine ammonia-lyase



• Molecule 1: Putative histidine ammonia-lyase

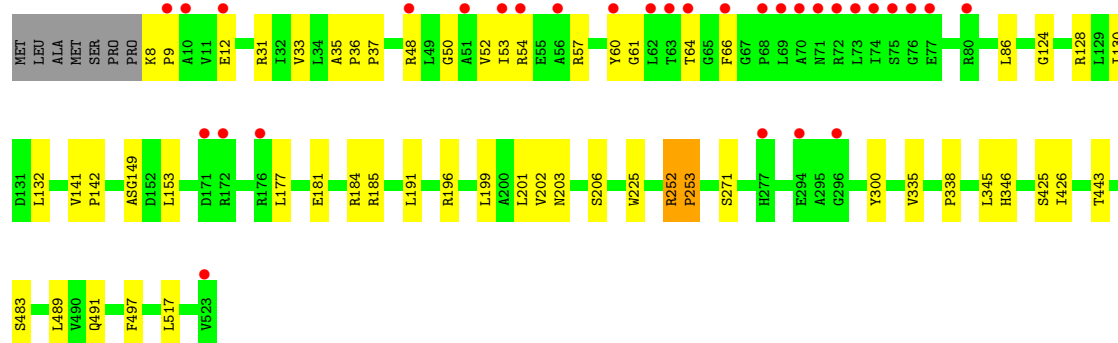


• Molecule 1: Putative histidine ammonia-lyase

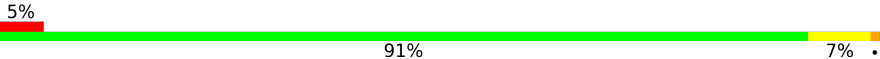


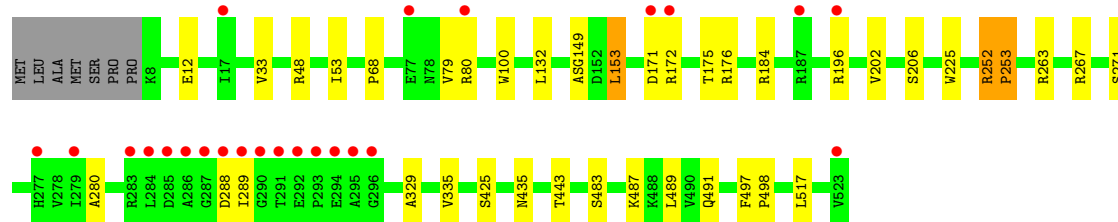
• Molecule 1: Putative histidine ammonia-lyase

Chain D: 

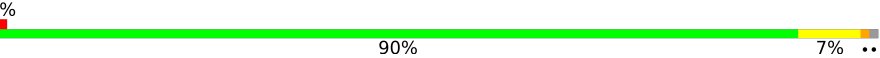


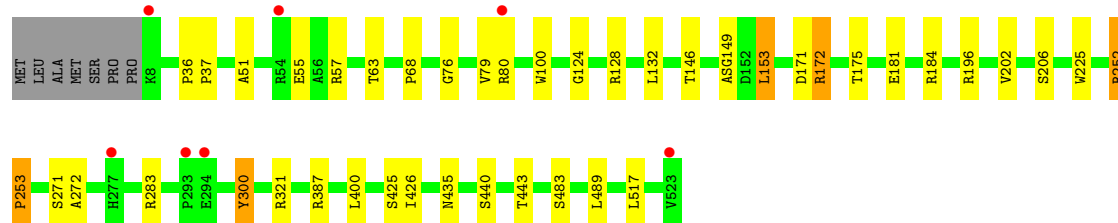
• Molecule 1: Putative histidine ammonia-lyase

Chain E: 



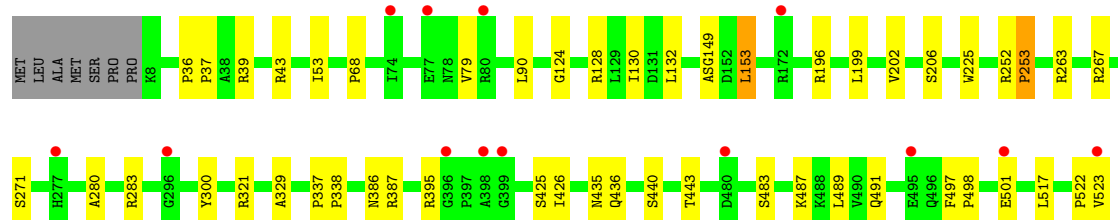
• Molecule 1: Putative histidine ammonia-lyase

Chain F: 

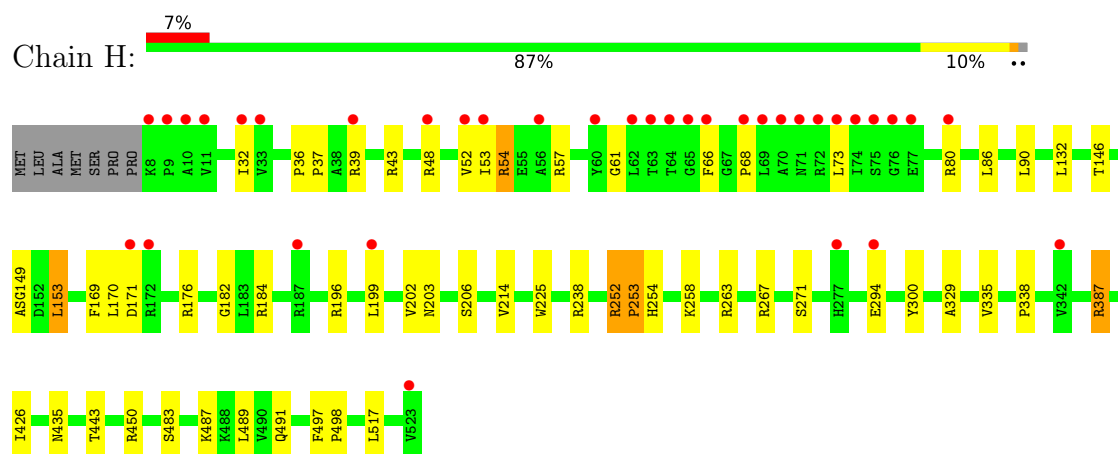


• Molecule 1: Putative histidine ammonia-lyase

Chain G: 



• Molecule 1: Putative histidine ammonia-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.92Å 155.63Å 164.35Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	500.00 – 1.50 163.93 – 1.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (500.00-1.50) 93.2 (163.93-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.189 0.174 , 0.189	Depositor DCC
R_{free} test set	32530 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34467	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: MDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/3862	0.84	8/5253 (0.2%)
1	B	0.33	0/3862	0.84	7/5253 (0.1%)
1	C	0.34	0/3854	0.85	12/5242 (0.2%)
1	D	0.33	0/3854	0.83	6/5242 (0.1%)
1	E	0.33	0/3854	0.84	6/5242 (0.1%)
1	F	0.34	0/3854	0.85	11/5242 (0.2%)
1	G	0.34	0/3854	0.84	10/5242 (0.2%)
1	H	0.33	0/3854	0.82	8/5242 (0.2%)
All	All	0.33	0/30848	0.84	68/41958 (0.2%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	252	ARG	CA-C-N	7.11	128.73	119.84
1	E	252	ARG	C-N-CA	7.11	128.73	119.84
1	C	252	ARG	CA-C-N	6.72	128.24	119.84
1	C	252	ARG	C-N-CA	6.72	128.24	119.84
1	G	206	SER	N-CA-C	6.53	118.40	111.28
1	D	206	SER	N-CA-C	6.39	118.25	111.28
1	F	253	PRO	N-CA-C	6.38	125.62	112.47
1	D	425	SER	N-CA-C	6.29	118.95	111.71
1	C	497	PHE	CA-C-N	6.22	124.20	119.66
1	C	497	PHE	C-N-CA	6.22	124.20	119.66
1	A	252	ARG	CA-C-N	6.22	127.61	119.84
1	A	252	ARG	C-N-CA	6.22	127.61	119.84
1	F	425	SER	N-CA-C	6.21	118.86	111.71
1	G	253	PRO	N-CA-C	6.16	125.15	112.47
1	B	253	PRO	N-CA-C	6.11	125.06	112.47
1	F	206	SER	N-CA-C	6.08	117.91	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	252	ARG	CA-C-N	6.06	127.41	119.84
1	H	252	ARG	C-N-CA	6.06	127.41	119.84
1	C	279	ILE	N-CA-C	6.05	116.80	110.62
1	D	253	PRO	N-CA-C	6.03	124.90	112.47
1	C	425	SER	N-CA-C	6.02	118.64	111.71
1	B	206	SER	N-CA-C	6.00	118.59	111.33
1	G	252	ARG	CA-C-N	5.99	127.33	119.84
1	G	252	ARG	C-N-CA	5.99	127.33	119.84
1	G	425	SER	N-CA-C	5.96	118.57	111.71
1	H	253	PRO	N-CA-C	5.96	124.75	112.47
1	E	425	SER	N-CA-C	5.96	118.56	111.71
1	B	252	ARG	CA-C-N	5.89	127.21	119.84
1	B	252	ARG	C-N-CA	5.89	127.21	119.84
1	B	153	LEU	N-CA-C	5.88	117.37	111.07
1	A	253	PRO	N-CA-C	5.85	124.53	112.47
1	B	300	TYR	N-CA-C	5.80	118.38	111.71
1	C	253	PRO	N-CA-C	5.79	124.39	112.47
1	A	425	SER	N-CA-C	5.74	119.09	111.75
1	F	300	TYR	N-CA-C	5.70	118.27	111.71
1	F	153	LEU	N-CA-C	5.70	117.49	111.28
1	C	153	LEU	N-CA-C	5.68	117.48	111.28
1	A	153	LEU	N-CA-C	5.68	117.47	111.28
1	H	300	TYR	N-CA-C	5.64	118.19	111.71
1	C	206	SER	N-CA-C	5.63	118.14	111.33
1	E	253	PRO	N-CA-C	5.63	124.06	112.47
1	D	252	ARG	CA-C-N	5.61	126.85	119.84
1	D	252	ARG	C-N-CA	5.61	126.85	119.84
1	D	300	TYR	N-CA-C	5.55	118.10	111.71
1	C	171	ASP	N-CA-C	-5.52	102.58	110.59
1	B	425	SER	N-CA-C	5.43	118.70	111.75
1	F	252	ARG	CA-C-N	5.42	126.62	119.84
1	F	252	ARG	C-N-CA	5.42	126.62	119.84
1	H	206	SER	N-CA-C	5.42	117.89	111.33
1	G	300	TYR	N-CA-C	5.41	117.93	111.71
1	A	206	SER	N-CA-C	5.36	117.82	111.33
1	H	387	ARG	N-CA-C	5.33	118.60	111.24
1	G	153	LEU	N-CA-C	5.33	117.09	111.28
1	G	387	ARG	N-CA-C	5.30	118.56	111.24
1	H	153	LEU	N-CA-C	5.26	117.02	111.28
1	C	300	TYR	N-CA-C	5.23	117.72	111.71
1	G	386	ASN	N-CA-C	5.21	118.77	112.93
1	E	206	SER	N-CA-C	5.21	117.64	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	387	ARG	N-CA-C	5.14	118.34	111.24
1	F	387	ARG	N-CA-C	5.09	118.26	111.24
1	E	153	LEU	N-CA-C	5.08	116.81	111.28
1	A	279	ILE	N-CA-C	5.07	116.40	110.62
1	F	440	SER	N-CA-C	5.06	117.92	111.69
1	A	387	ARG	N-CA-C	5.05	118.21	111.24
1	H	254	HIS	N-CA-C	-5.03	103.31	109.65
1	F	272	ALA	N-CA-C	-5.03	106.39	112.88
1	F	400	LEU	N-CA-C	-5.02	106.42	112.54
1	G	440	SER	N-CA-C	5.02	117.86	111.69

There are no chirality outliers.

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	3813	0	3857	25	0
1	B	3813	0	3857	42	0
1	C	3806	0	3849	35	0
1	D	3806	0	3849	34	0
1	E	3806	0	3849	30	0
1	F	3806	0	3849	27	0
1	G	3806	0	3849	28	0
1	H	3806	0	3849	49	0
2	A	458	0	0	3	0
2	B	487	0	0	5	0
2	C	496	0	0	4	0
2	D	494	0	0	4	0
2	E	498	0	0	7	0
2	F	586	0	0	6	0
2	G	523	0	0	4	0
2	H	463	0	0	5	0
All	All	34467	0	30808	255	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 4.

All (255) 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:153:LEU:HD22	1:D:202:VAL:HG12	1.63	0.80
1:B:53:ILE:HG21	1:B:196:ARG:HH11	1.44	0.80
1:H:53:ILE:HG21	1:H:196:ARG:HH11	1.47	0.79
1:H:153:LEU:HD22	1:H:202:VAL:HG12	1.65	0.78
1:E:153:LEU:HD22	1:E:202:VAL:HG12	1.70	0.73
1:E:487:LYS:O	1:E:491:GLN:HG3	1.88	0.73
1:B:153:LEU:HD22	1:B:202:VAL:HG12	1.69	0.73
1:B:487:LYS:O	1:B:491:GLN:HG3	1.89	0.73
1:A:153:LEU:HD22	1:A:202:VAL:HG12	1.70	0.73
1:D:61:GLY:HA3	1:D:199:LEU:HD11	1.70	0.71
1:F:153:LEU:HD22	1:F:202:VAL:HG12	1.72	0.70
1:C:487:LYS:O	1:C:491:GLN:HG3	1.92	0.69
1:E:172:ARG:NH1	2:E:4898:HOH:O	2.24	0.69
1:H:238:ARG:HH11	1:H:387:ARG:NH2	1.91	0.69
1:F:79:VAL:HG11	1:F:196:ARG:HD3	1.76	0.68
1:C:153:LEU:HD22	1:C:202:VAL:HG12	1.76	0.67
1:D:53:ILE:HD13	1:D:196:ARG:HD2	1.78	0.64
1:H:238:ARG:NH1	1:H:387:ARG:NH2	2.47	0.63
1:H:53:ILE:HG21	1:H:196:ARG:NH1	2.14	0.63
1:D:50:GLY:O	1:D:54:ARG:HG3	1.99	0.62
1:H:487:LYS:O	1:H:491:GLN:HG3	2.00	0.62
1:H:214:VAL:HB	1:H:450:ARG:NH2	2.16	0.61
1:F:68:PRO:HG3	1:F:435:ASN:HB2	1.84	0.60
1:G:283:ARG:HD3	2:G:2777:HOH:O	2.00	0.60
1:B:53:ILE:CG2	1:B:196:ARG:HH11	2.14	0.60
1:G:53:ILE:HD13	1:G:196:ARG:HD2	1.83	0.60
1:G:153:LEU:HD22	1:G:202:VAL:HG12	1.83	0.60
1:G:487:LYS:O	1:G:491:GLN:HG3	2.02	0.60
1:B:51:ALA:O	1:B:55:GLU:HG3	2.02	0.59
1:B:79:VAL:HG21	2:B:4884:HOH:O	2.03	0.58
1:B:68:PRO:HG3	1:B:435:ASN:HB2	1.85	0.57
1:F:283:ARG:HD3	2:F:3716:HOH:O	2.04	0.57
1:F:171:ASP:OD2	1:F:175:THR:HB	2.05	0.57
1:H:39:ARG:HG3	1:H:39:ARG:HH11	1.71	0.56
1:E:184:ARG:HD2	2:E:3810:HOH:O	2.06	0.56
1:A:271:SER:HB2	1:A:483:SER:HB3	1.88	0.55
1:H:184:ARG:HG2	1:H:184:ARG:HH11	1.72	0.55
1:A:170:LEU:HD23	1:A:176:ARG:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:VAL:HG13	1:D:57:ARG:HB2	1.88	0.54
1:B:432:ASN:HB2	1:B:436:GLN:HE21	1.72	0.54
1:E:271:SER:HB2	1:E:483:SER:HB3	1.90	0.54
1:C:124:GLY:O	1:C:128:ARG:HG2	2.08	0.54
1:B:61:GLY:HA3	1:B:199:LEU:HD11	1.89	0.53
1:C:176:ARG:HD2	2:C:3285:HOH:O	2.08	0.53
1:H:54:ARG:HG2	1:H:54:ARG:HH11	1.73	0.53
1:E:132:LEU:C	1:E:132:LEU:HD13	2.32	0.53
1:H:271:SER:HB2	1:H:483:SER:HB3	1.90	0.53
1:D:12:GLU:HA	1:D:33:VAL:HG13	1.90	0.53
1:D:36:PRO:HB2	1:D:37:PRO:HD3	1.89	0.53
1:F:124:GLY:O	1:F:128:ARG:HG2	2.09	0.53
1:G:271:SER:HB2	1:G:483:SER:HB3	1.90	0.53
1:H:61:GLY:HA3	1:H:199:LEU:HD21	1.90	0.53
1:A:132:LEU:C	1:A:132:LEU:HD13	2.33	0.53
1:B:53:ILE:HG21	1:B:196:ARG:NH1	2.21	0.53
1:E:225:TRP:CE2	1:E:517:LEU:HD22	2.44	0.53
1:A:279:ILE:HD11	1:D:346:HIS:CE1	2.44	0.52
1:E:79:VAL:HG21	2:E:2045:HOH:O	2.09	0.52
2:A:3436:HOH:O	1:D:426:ILE:HD13	2.09	0.52
1:G:523:VAL:OXT	1:G:523:VAL:HG12	2.08	0.52
1:A:487:LYS:O	1:A:491:GLN:HG3	2.10	0.52
1:C:79:VAL:HG11	1:C:196:ARG:HD3	1.92	0.52
1:C:12:GLU:HA	1:C:33:VAL:HG13	1.92	0.52
1:H:225:TRP:CE2	1:H:517:LEU:HD22	2.45	0.51
1:A:225:TRP:CE2	1:A:517:LEU:HD22	2.46	0.51
2:B:3548:HOH:O	1:C:426:ILE:HD13	2.10	0.51
1:F:426:ILE:HD13	2:G:3571:HOH:O	2.10	0.51
1:H:68:PRO:HG3	1:H:435:ASN:HB2	1.92	0.51
1:B:53:ILE:HD13	1:B:196:ARG:HD2	1.93	0.51
1:A:426:ILE:HD13	2:D:3398:HOH:O	2.10	0.51
1:B:191:LEU:HD21	1:B:201:LEU:CD1	2.40	0.51
1:A:53:ILE:HD13	1:A:196:ARG:HD2	1.92	0.51
1:E:196:ARG:HG3	1:E:196:ARG:HH11	1.75	0.50
1:B:75:SER:HG	1:B:77:GLU:HG2	1.76	0.50
1:B:168:ASP:HB2	1:B:176:ARG:HH21	1.77	0.50
1:D:132:LEU:HD13	1:D:132:LEU:C	2.35	0.50
1:B:124:GLY:O	1:B:128:ARG:HG2	2.11	0.50
1:C:80:ARG:HE	1:C:194:SER:HA	1.77	0.50
1:H:132:LEU:C	1:H:132:LEU:HD13	2.37	0.50
1:A:176:ARG:HD2	2:A:3332:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LYS:HD2	2:B:3514:HOH:O	2.12	0.50
1:A:170:LEU:CD2	1:A:176:ARG:HG2	2.42	0.50
1:G:132:LEU:HD13	1:G:132:LEU:C	2.36	0.50
1:B:251:LEU:HD13	1:C:335:VAL:HG21	1.93	0.50
1:D:66:PHE:CE2	1:D:86:LEU:HB2	2.47	0.50
1:C:132:LEU:C	1:C:132:LEU:HD13	2.37	0.49
1:H:184:ARG:HG2	1:H:184:ARG:NH1	2.28	0.49
1:B:132:LEU:HD13	1:B:132:LEU:C	2.37	0.49
1:C:271:SER:HB2	1:C:483:SER:HB3	1.94	0.49
1:A:61:GLY:HA3	1:A:199:LEU:HD21	1.95	0.49
1:F:225:TRP:CE2	1:F:517:LEU:HD22	2.47	0.49
1:A:7:PRO:O	1:A:8:LYS:C	2.55	0.49
1:B:36:PRO:HB2	1:B:37:PRO:HD3	1.93	0.49
1:D:489:LEU:C	1:D:489:LEU:HD23	2.37	0.49
1:B:39:ARG:HD2	1:B:43:ARG:NH2	2.28	0.49
1:H:66:PHE:CZ	1:H:86:LEU:HD22	2.48	0.49
1:E:263:ARG:O	1:E:267:ARG:HG2	2.13	0.48
1:A:489:LEU:C	1:A:489:LEU:HD23	2.38	0.48
1:A:263:ARG:O	1:A:267:ARG:HG2	2.13	0.48
1:A:280:ALA:O	1:D:57:ARG:HD2	2.13	0.48
1:C:225:TRP:CE2	1:C:517:LEU:HD22	2.48	0.48
1:F:76:GLY:O	1:F:79:VAL:HG23	2.13	0.48
1:A:68:PRO:HG3	1:A:435:ASN:HB2	1.95	0.48
1:D:184:ARG:HG2	1:D:184:ARG:HH11	1.78	0.48
1:D:225:TRP:CE2	1:D:517:LEU:HD22	2.49	0.48
1:E:12:GLU:HA	1:E:33:VAL:HG13	1.95	0.48
1:E:489:LEU:HD23	1:E:489:LEU:C	2.37	0.48
1:B:489:LEU:HD23	1:B:489:LEU:C	2.38	0.48
1:F:171:ASP:C	1:F:171:ASP:OD1	2.57	0.48
1:H:90:LEU:HD13	1:H:153:LEU:HB3	1.96	0.48
1:C:53:ILE:HD13	1:C:196:ARG:HD2	1.94	0.48
1:C:489:LEU:C	1:C:489:LEU:HD23	2.38	0.48
1:A:51:ALA:O	1:A:55:GLU:HG3	2.13	0.48
1:C:39:ARG:NH1	2:C:4878:HOH:O	2.46	0.48
1:B:141:VAL:HG13	1:B:158:HIS:HB2	1.96	0.48
1:C:68:PRO:HG3	1:C:435:ASN:HB2	1.96	0.48
1:G:39:ARG:HD2	1:G:43:ARG:NH2	2.29	0.48
1:E:176:ARG:HD2	2:E:3308:HOH:O	2.13	0.48
1:F:132:LEU:C	1:F:132:LEU:HD13	2.38	0.48
1:G:489:LEU:HD23	1:G:489:LEU:C	2.39	0.48
1:F:79:VAL:CG1	1:F:196:ARG:HD3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:GLY:O	1:G:128:ARG:HG2	2.14	0.47
1:B:278:VAL:HB	1:B:281:GLU:HG3	1.96	0.47
1:C:80:ARG:NE	1:C:194:SER:HA	2.29	0.47
1:G:130:ILE:HD12	2:G:4129:HOH:O	2.13	0.47
1:B:57:ARG:HD2	1:C:280:ALA:O	2.15	0.47
1:H:294:GLU:OE1	1:H:387:ARG:NH2	2.48	0.47
1:B:75:SER:OG	1:B:77:GLU:HG2	2.14	0.47
1:B:523:VAL:OXT	1:B:523:VAL:HG12	2.14	0.47
1:C:36:PRO:HB2	1:C:37:PRO:HD3	1.96	0.47
1:H:52:VAL:HG13	1:H:57:ARG:HB2	1.97	0.47
1:H:450:ARG:HG2	1:H:450:ARG:HH11	1.79	0.47
1:B:225:TRP:CE2	1:B:517:LEU:HD22	2.50	0.47
1:D:497:PHE:HB3	2:D:4227:HOH:O	2.13	0.47
1:A:79:VAL:HG11	1:A:196:ARG:HD3	1.97	0.46
1:C:80:ARG:HH21	1:C:194:SER:CB	2.28	0.46
1:G:225:TRP:CE2	1:G:517:LEU:HD22	2.50	0.46
1:B:329:ALA:HB1	1:C:252:ARG:HA	1.97	0.46
1:F:36:PRO:HB2	1:F:37:PRO:HD3	1.98	0.46
1:F:80:ARG:HG2	2:F:2717:HOH:O	2.14	0.46
2:F:3660:HOH:O	1:G:426:ILE:HD13	2.14	0.46
1:H:36:PRO:N	1:H:37:PRO:HD2	2.29	0.46
1:A:36:PRO:N	1:A:37:PRO:HD2	2.30	0.46
1:F:489:LEU:C	1:F:489:LEU:HD23	2.39	0.46
1:E:48:ARG:HH11	1:E:48:ARG:HG2	1.80	0.46
1:B:50:GLY:O	1:B:54:ARG:HG3	2.16	0.46
1:H:489:LEU:C	1:H:489:LEU:HD23	2.40	0.46
1:H:170:LEU:HD23	1:H:176:ARG:HG2	1.98	0.46
1:E:80:ARG:HG2	2:E:3706:HOH:O	2.16	0.46
1:G:395:ARG:CZ	1:G:501:GLU:HG2	2.46	0.46
1:B:271:SER:HB2	1:B:483:SER:HB3	1.98	0.45
1:D:12:GLU:HG2	1:D:35:ALA:HB2	1.98	0.45
1:F:271:SER:HB2	1:F:483:SER:HB3	1.98	0.45
1:C:170:LEU:HD23	1:C:176:ARG:HG2	1.98	0.45
1:C:225:TRP:CE2	1:C:522:PRO:HG3	2.52	0.45
1:A:329:ALA:HB1	1:D:252:ARG:HA	1.99	0.45
1:B:170:LEU:CD2	1:B:176:ARG:HG2	2.46	0.45
1:E:100:TRP:CZ2	1:E:172:ARG:HG2	2.52	0.45
1:E:171:ASP:OD2	1:E:175:THR:HB	2.15	0.45
1:F:252:ARG:HA	1:G:329:ALA:HB1	1.97	0.45
1:A:52:VAL:HG13	1:A:57:ARG:HB2	1.99	0.45
1:E:288:ASP:O	1:H:73:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:LEU:CD2	1:H:176:ARG:HG2	2.47	0.45
1:H:176:ARG:HD2	2:H:3379:HOH:O	2.16	0.44
1:B:346:HIS:CE1	1:C:279:ILE:HD11	2.52	0.44
1:B:426:ILE:HD13	2:C:3493:HOH:O	2.16	0.44
1:H:39:ARG:O	1:H:43:ARG:HG3	2.16	0.44
1:D:48:ARG:NH2	1:D:338:PRO:O	2.50	0.44
1:G:36:PRO:N	1:G:37:PRO:HD2	2.33	0.44
1:H:238:ARG:NH1	1:H:387:ARG:HH22	2.14	0.44
1:H:146:THR:HG22	2:H:2163:HOH:O	2.18	0.44
1:H:39:ARG:HD3	1:H:43:ARG:HH21	1.83	0.44
1:H:258:LYS:HD2	2:H:3845:HOH:O	2.16	0.44
1:H:335:VAL:HG11	2:H:1982:HOH:O	2.17	0.44
1:B:225:TRP:CE2	1:B:522:PRO:HD3	2.53	0.44
1:G:79:VAL:HG11	1:G:196:ARG:HD3	1.99	0.44
1:H:171:ASP:C	1:H:171:ASP:OD1	2.60	0.44
1:C:12:GLU:HA	1:C:33:VAL:CG1	2.47	0.44
1:E:280:ALA:O	1:H:57:ARG:HD2	2.17	0.44
1:E:196:ARG:HG3	1:E:196:ARG:NH1	2.32	0.43
1:G:68:PRO:HG3	1:G:435:ASN:HB2	2.00	0.43
1:H:214:VAL:HB	1:H:450:ARG:HH21	1.82	0.43
1:D:177:LEU:HD21	1:D:185:ARG:NH1	2.33	0.43
1:D:191:LEU:HD21	1:D:201:LEU:CD1	2.49	0.43
1:H:53:ILE:HD13	1:H:196:ARG:HD2	1.99	0.43
1:C:263:ARG:O	1:C:267:ARG:HG2	2.18	0.43
1:D:271:SER:HB2	1:D:483:SER:HB3	2.00	0.43
1:F:146:THR:HG22	2:F:2088:HOH:O	2.19	0.43
1:H:199:LEU:HD12	1:H:199:LEU:N	2.33	0.43
1:B:48:ARG:NH2	1:B:338:PRO:O	2.51	0.43
1:D:8:LYS:CG	1:D:31:ARG:HG3	2.48	0.43
1:D:66:PHE:CZ	1:D:86:LEU:HD22	2.53	0.43
1:H:199:LEU:O	1:H:203:ASN:HB2	2.19	0.43
1:H:263:ARG:O	1:H:267:ARG:HG2	2.18	0.43
1:D:335:VAL:HG23	1:D:345:LEU:HB2	2.01	0.43
2:E:3348:HOH:O	1:H:426:ILE:HD13	2.18	0.43
1:F:63:THR:HG22	2:F:4294:HOH:O	2.17	0.43
1:G:225:TRP:CE2	1:G:522:PRO:HD3	2.54	0.43
1:B:186:GLY:HA2	2:B:3021:HOH:O	2.19	0.43
1:F:100:TRP:CH2	1:F:172:ARG:HD3	2.54	0.43
1:H:66:PHE:CE2	1:H:86:LEU:HB2	2.54	0.43
1:B:178:ASP:OD2	1:B:178:ASP:C	2.62	0.43
1:B:285:ASP:C	1:B:285:ASP:OD2	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:GLY:O	1:D:128:ARG:HG2	2.19	0.43
1:E:289:ILE:HD11	2:H:4360:HOH:O	2.18	0.43
1:F:181:GLU:OE1	1:F:184:ARG:NH1	2.52	0.43
1:F:321:ARG:HH21	1:G:321:ARG:HH21	1.65	0.43
1:H:169:PHE:CD2	1:H:182:GLY:HA3	2.54	0.43
1:D:199:LEU:O	1:D:203:ASN:HB2	2.19	0.42
1:E:48:ARG:HG2	1:E:48:ARG:NH1	2.34	0.42
1:E:335:VAL:HG11	2:E:1376:HOH:O	2.19	0.42
1:H:80:ARG:HH11	1:H:80:ARG:HG3	1.84	0.42
1:D:184:ARG:HG2	1:D:184:ARG:NH1	2.33	0.42
1:E:252:ARG:HA	1:H:329:ALA:HB1	2.01	0.42
1:F:79:VAL:HG21	2:F:2178:HOH:O	2.19	0.42
1:C:146:THR:HG22	2:C:1832:HOH:O	2.19	0.42
1:B:170:LEU:HD23	1:B:176:ARG:HG2	2.01	0.42
1:C:523:VAL:OXT	1:C:523:VAL:HG12	2.18	0.42
1:D:130:ILE:HD12	2:D:4714:HOH:O	2.19	0.42
1:C:225:TRP:CD2	1:C:522:PRO:HG3	2.54	0.42
1:C:100:TRP:CZ2	1:C:172:ARG:HG2	2.55	0.42
1:D:491:GLN:NE2	2:D:2981:HOH:O	2.52	0.42
1:F:68:PRO:HG3	1:F:435:ASN:CB	2.49	0.42
1:B:263:ARG:O	1:B:267:ARG:HG2	2.19	0.41
1:G:497:PHE:HA	1:G:498:PRO:HD2	1.94	0.41
1:C:8:LYS:HE3	1:C:8:LYS:HB2	1.92	0.41
1:E:171:ASP:OD1	1:E:171:ASP:C	2.61	0.41
1:H:48:ARG:NH2	1:H:338:PRO:O	2.53	0.41
1:H:497:PHE:HA	1:H:498:PRO:HD3	1.91	0.41
1:F:57:ARG:HD2	1:G:280:ALA:O	2.20	0.41
1:H:48:ARG:O	1:H:52:VAL:HG23	2.19	0.41
1:A:146:THR:HG22	2:A:2274:HOH:O	2.20	0.41
1:E:68:PRO:HG3	1:E:435:ASN:HB2	2.01	0.41
1:G:199:LEU:HD23	2:G:4049:HOH:O	2.19	0.41
1:E:53:ILE:HD13	1:E:196:ARG:HD2	2.02	0.41
1:F:51:ALA:O	1:F:55:GLU:HG3	2.20	0.41
1:G:395:ARG:NH1	1:G:501:GLU:HG2	2.35	0.41
1:B:146:THR:HG22	2:B:2492:HOH:O	2.21	0.41
1:F:300:TYR:CZ	1:G:436:GLN:HG2	2.56	0.41
1:G:90:LEU:HD13	1:G:153:LEU:HB3	2.01	0.41
1:C:191:LEU:HD21	1:C:201:LEU:CD1	2.51	0.41
1:A:285:ASP:OD1	1:A:288:ASP:OD2	2.39	0.41
1:B:53:ILE:CG2	1:B:196:ARG:NH1	2.82	0.41
1:C:424:ALA:HB2	1:C:448:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:TYR:HA	1:D:64:THR:OG1	2.21	0.41
1:D:181:GLU:OE1	1:D:181:GLU:HA	2.21	0.41
1:G:337:PRO:HA	1:G:338:PRO:HD3	1.96	0.41
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.86	0.40
1:E:12:GLU:HA	1:E:33:VAL:CG1	2.51	0.40
1:D:141:VAL:HA	1:D:142:PRO:HD3	1.99	0.40
1:G:263:ARG:O	1:G:267:ARG:HG2	2.21	0.40
1:C:10:ALA:HB2	1:C:31:ARG:HH21	1.87	0.40
1:E:329:ALA:HB1	1:H:252:ARG:HA	2.03	0.40
1:E:497:PHE:HA	1:E:498:PRO:HD3	1.91	0.40
1:C:39:ARG:NH1	1:C:39:ARG:HG2	2.36	0.40
1:D:8:LYS:HB2	1:D:9:PRO:HD2	2.04	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	510/521 (98%)	502 (98%)	6 (1%)	2 (0%)	30	12
1	B	510/521 (98%)	505 (99%)	4 (1%)	1 (0%)	43	22
1	C	509/521 (98%)	504 (99%)	4 (1%)	1 (0%)	43	22
1	D	509/521 (98%)	502 (99%)	6 (1%)	1 (0%)	43	22
1	E	509/521 (98%)	502 (99%)	6 (1%)	1 (0%)	43	22
1	F	509/521 (98%)	502 (99%)	6 (1%)	1 (0%)	43	22
1	G	509/521 (98%)	504 (99%)	4 (1%)	1 (0%)	43	22
1	H	509/521 (98%)	502 (99%)	6 (1%)	1 (0%)	43	22
All	All	4074/4168 (98%)	4023 (99%)	42 (1%)	9 (0%)	43	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	253	PRO
1	E	253	PRO
1	B	253	PRO
1	C	253	PRO
1	D	253	PRO
1	F	253	PRO
1	G	253	PRO
1	H	253	PRO

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	384/389 (99%)	383 (100%)	1 (0%)	86	75
1	B	384/389 (99%)	383 (100%)	1 (0%)	86	75
1	C	383/389 (98%)	381 (100%)	2 (0%)	81	66
1	D	383/389 (98%)	382 (100%)	1 (0%)	86	75
1	E	383/389 (98%)	382 (100%)	1 (0%)	86	75
1	F	383/389 (98%)	381 (100%)	2 (0%)	81	66
1	G	383/389 (98%)	382 (100%)	1 (0%)	86	75
1	H	383/389 (98%)	380 (99%)	3 (1%)	73	54
All	All	3066/3112 (98%)	3054 (100%)	12 (0%)	84	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	THR
1	B	443	THR
1	C	80	ARG
1	C	443	THR
1	D	443	THR
1	E	443	THR
1	F	172	ARG

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Mol	Chain	Res	Type
1	F	443	THR
1	G	443	THR
1	H	32	ILE
1	H	54	ARG
1	H	443	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	195	HIS
1	A	353	GLN
1	A	435	ASN
1	A	491	GLN
1	B	164	GLN
1	B	189	GLN
1	B	435	ASN
1	B	436	GLN
1	C	164	GLN
1	C	394	HIS
1	C	435	ASN
1	C	436	GLN
1	D	78	ASN
1	D	164	GLN
1	D	189	GLN
1	D	195	HIS
1	D	394	HIS
1	D	491	GLN
1	E	164	GLN
1	E	189	GLN
1	E	394	HIS
1	E	436	GLN
1	E	520	GLN
1	F	164	GLN
1	F	195	HIS
1	F	394	HIS
1	F	491	GLN
1	F	520	GLN
1	G	164	GLN
1	G	435	ASN
1	H	78	ASN
1	H	164	GLN

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Mol	Chain	Res	Type
1	H	195	HIS
1	H	394	HIS
1	H	435	ASN
1	H	508	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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$
1	MDO	B	149	1	11,13,14	2.42	4 (36%)	15,18,20	2.62	5 (33%)
1	MDO	G	149	1	11,13,14	2.36	4 (36%)	15,18,20	2.79	5 (33%)
1	MDO	C	149	1	11,13,14	2.45	4 (36%)	15,18,20	2.71	5 (33%)
1	MDO	H	149	1	11,13,14	2.44	4 (36%)	15,18,20	2.65	5 (33%)
1	MDO	F	149	1	11,13,14	2.38	4 (36%)	15,18,20	2.72	5 (33%)
1	MDO	A	149	1	11,13,14	2.41	4 (36%)	15,18,20	2.69	5 (33%)
1	MDO	D	149	1	11,13,14	2.40	4 (36%)	15,18,20	2.70	5 (33%)
1	MDO	E	149	1	11,13,14	2.38	4 (36%)	15,18,20	2.76	6 (40%)

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
1	MDO	B	149	1	-	0/4/23/24	0/1/1/1
1	MDO	G	149	1	-	2/4/23/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MDO	C	149	1	-	0/4/23/24	0/1/1/1
1	MDO	H	149	1	-	0/4/23/24	0/1/1/1
1	MDO	F	149	1	-	1/4/23/24	0/1/1/1
1	MDO	A	149	1	-	0/4/23/24	0/1/1/1
1	MDO	D	149	1	-	0/4/23/24	0/1/1/1
1	MDO	E	149	1	-	0/4/23/24	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	MDO	O2-C2	5.19	1.33	1.23
1	B	149	MDO	O2-C2	5.14	1.33	1.23
1	H	149	MDO	O2-C2	5.09	1.33	1.23
1	D	149	MDO	O2-C2	4.97	1.33	1.23
1	A	149	MDO	O2-C2	4.96	1.33	1.23
1	F	149	MDO	O2-C2	4.87	1.33	1.23
1	E	149	MDO	O2-C2	4.86	1.33	1.23
1	G	149	MDO	O2-C2	4.74	1.32	1.23
1	B	149	MDO	C2-N3	-3.82	1.31	1.40
1	C	149	MDO	C2-N3	-3.80	1.31	1.40
1	G	149	MDO	C2-N3	-3.80	1.31	1.40
1	H	149	MDO	C2-N3	-3.78	1.31	1.40
1	E	149	MDO	C2-N3	-3.76	1.31	1.40
1	A	149	MDO	C2-N3	-3.72	1.31	1.40
1	F	149	MDO	C2-N3	-3.63	1.31	1.40
1	D	149	MDO	C2-N3	-3.62	1.31	1.40
1	A	149	MDO	CA2-N2	-2.91	1.34	1.39
1	C	149	MDO	CA2-N2	-2.91	1.34	1.39
1	D	149	MDO	CA2-N2	-2.85	1.34	1.39
1	E	149	MDO	CA2-N2	-2.81	1.34	1.39
1	G	149	MDO	CA2-N2	-2.80	1.34	1.39
1	B	149	MDO	CA2-N2	-2.79	1.34	1.39
1	F	149	MDO	CA2-N2	-2.79	1.34	1.39
1	H	149	MDO	CA2-N2	-2.77	1.34	1.39
1	H	149	MDO	CA2-C2	-2.60	1.38	1.43
1	E	149	MDO	CA2-C2	-2.59	1.38	1.43
1	F	149	MDO	CA2-C2	-2.52	1.38	1.43
1	G	149	MDO	CA2-C2	-2.51	1.38	1.43
1	A	149	MDO	CA2-C2	-2.50	1.38	1.43
1	D	149	MDO	CA2-C2	-2.44	1.38	1.43
1	C	149	MDO	CA2-C2	-2.37	1.38	1.43
1	B	149	MDO	CA2-C2	-2.31	1.38	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	MDO	CA2-C2-N3	7.29	109.62	103.50
1	E	149	MDO	CA2-C2-N3	7.24	109.58	103.50
1	H	149	MDO	CA2-C2-N3	7.14	109.49	103.50
1	C	149	MDO	CA2-C2-N3	7.12	109.48	103.50
1	D	149	MDO	CA2-C2-N3	7.09	109.45	103.50
1	A	149	MDO	CA2-C2-N3	7.04	109.42	103.50
1	F	149	MDO	CA2-C2-N3	7.03	109.41	103.50
1	B	149	MDO	CA2-C2-N3	6.88	109.28	103.50
1	G	149	MDO	O2-C2-CA2	-4.66	128.04	131.02
1	E	149	MDO	O2-C2-CA2	-4.63	128.07	131.02
1	F	149	MDO	O2-C2-CA2	-4.59	128.09	131.02
1	A	149	MDO	O2-C2-CA2	-4.43	128.19	131.02
1	C	149	MDO	O2-C2-CA2	-4.34	128.25	131.02
1	D	149	MDO	O2-C2-CA2	-4.29	128.28	131.02
1	B	149	MDO	O2-C2-CA2	-4.07	128.42	131.02
1	H	149	MDO	O2-C2-CA2	-4.05	128.44	131.02
1	B	149	MDO	C2-CA2-N2	-3.98	106.10	108.95
1	E	149	MDO	C2-CA2-N2	-3.95	106.12	108.95
1	C	149	MDO	C2-CA2-N2	-3.91	106.15	108.95
1	G	149	MDO	C2-CA2-N2	-3.91	106.15	108.95
1	F	149	MDO	C2-CA2-N2	-3.88	106.17	108.95
1	D	149	MDO	C2-CA2-N2	-3.84	106.20	108.95
1	A	149	MDO	C2-CA2-N2	-3.82	106.21	108.95
1	H	149	MDO	C2-CA2-N2	-3.80	106.23	108.95
1	G	149	MDO	N3-C1-N2	-2.75	109.32	111.48
1	H	149	MDO	N3-C1-N2	-2.71	109.34	111.48
1	C	149	MDO	CA2-N2-C1	2.69	107.80	105.39
1	C	149	MDO	N3-C1-N2	-2.66	109.39	111.48
1	D	149	MDO	N3-C1-N2	-2.66	109.39	111.48
1	A	149	MDO	N3-C1-N2	-2.65	109.39	111.48
1	A	149	MDO	CA2-N2-C1	2.65	107.77	105.39
1	F	149	MDO	N3-C1-N2	-2.63	109.41	111.48
1	G	149	MDO	CA2-N2-C1	2.62	107.74	105.39
1	D	149	MDO	CA2-N2-C1	2.61	107.73	105.39
1	E	149	MDO	CA2-N2-C1	2.60	107.72	105.39
1	F	149	MDO	CA2-N2-C1	2.60	107.72	105.39
1	B	149	MDO	CA2-N2-C1	2.59	107.71	105.39
1	E	149	MDO	N3-C1-N2	-2.51	109.51	111.48
1	B	149	MDO	N3-C1-N2	-2.51	109.51	111.48
1	H	149	MDO	CA2-N2-C1	2.50	107.64	105.39
1	E	149	MDO	C2-N3-C1	-2.16	107.07	108.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	149	MDO	N2-C1-CA1-CB
1	G	149	MDO	N2-C1-CA1-CB
1	G	149	MDO	N3-C1-CA1-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	514/521 (98%)	0.28	24 (4%)	36	40	8, 16, 34, 53	0
1	B	514/521 (98%)	0.16	18 (3%)	47	51	7, 15, 31, 48	0
1	C	513/521 (98%)	-0.00	20 (3%)	43	47	7, 13, 28, 41	0
1	D	513/521 (98%)	0.17	31 (6%)	27	30	6, 14, 34, 48	0
1	E	513/521 (98%)	0.07	24 (4%)	36	40	7, 14, 31, 59	0
1	F	513/521 (98%)	-0.22	7 (1%)	73	77	6, 11, 25, 37	0
1	G	513/521 (98%)	-0.08	13 (2%)	58	62	6, 12, 26, 39	0
1	H	513/521 (98%)	0.38	36 (7%)	22	24	7, 16, 36, 52	0
All	All	4106/4168 (98%)	0.10	173 (4%)	40	44	6, 14, 31, 59	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	ILE	8.2
1	H	74	ILE	7.9
1	A	296	GLY	6.5
1	G	523	VAL	6.1
1	A	523	VAL	5.8
1	H	523	VAL	5.7
1	B	523	VAL	5.7
1	A	289	ILE	5.6
1	E	523	VAL	5.4
1	F	523	VAL	5.3
1	H	66	PHE	5.1
1	G	399	GLY	5.0
1	C	523	VAL	5.0
1	B	7	PRO	4.9
1	D	523	VAL	4.9
1	D	70	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	286	ALA	4.8
1	H	73	LEU	4.6
1	H	70	ALA	4.5
1	A	285	ASP	4.5
1	H	69	LEU	4.5
1	D	64	THR	4.4
1	D	66	PHE	4.2
1	H	63	THR	4.1
1	H	75	SER	4.1
1	H	77	GLU	4.1
1	E	289	ILE	4.1
1	A	291	THR	4.0
1	A	7	PRO	4.0
1	C	399	GLY	4.0
1	A	290	GLY	3.9
1	D	75	SER	3.9
1	H	64	THR	3.9
1	H	294	GLU	3.8
1	D	73	LEU	3.8
1	A	172	ARG	3.8
1	H	62	LEU	3.7
1	H	65	GLY	3.7
1	B	172	ARG	3.7
1	E	284	LEU	3.7
1	H	76	GLY	3.7
1	B	184	ARG	3.6
1	H	9	PRO	3.6
1	C	172	ARG	3.6
1	E	290	GLY	3.6
1	E	291	THR	3.6
1	E	295	ALA	3.5
1	E	294	GLU	3.5
1	C	184	ARG	3.5
1	H	277	HIS	3.5
1	E	296	GLY	3.4
1	D	54	ARG	3.4
1	E	172	ARG	3.4
1	A	294	GLU	3.4
1	D	77	GLU	3.4
1	G	398	ALA	3.4
1	D	69	LEU	3.3
1	A	74	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	72	ARG	3.3
1	H	53	ILE	3.3
1	A	293	PRO	3.3
1	D	294	GLU	3.3
1	E	286	ALA	3.3
1	B	277	HIS	3.2
1	D	56	ALA	3.2
1	H	172	ARG	3.2
1	C	296	GLY	3.1
1	F	293	PRO	3.1
1	D	63	THR	3.1
1	E	293	PRO	3.0
1	E	279	ILE	3.0
1	E	277	HIS	3.0
1	B	177	LEU	3.0
1	D	76	GLY	2.9
1	D	277	HIS	2.9
1	D	62	LEU	2.9
1	H	56	ALA	2.9
1	D	60	TYR	2.9
1	B	33	VAL	2.9
1	E	285	ASP	2.9
1	A	279	ILE	2.9
1	F	294	GLU	2.8
1	E	288	ASP	2.8
1	D	71	ASN	2.8
1	C	279	ILE	2.8
1	A	284	LEU	2.8
1	D	9	PRO	2.8
1	C	398	ALA	2.7
1	H	11	VAL	2.7
1	A	287	GLY	2.7
1	G	80	ARG	2.7
1	E	80	ARG	2.7
1	F	277	HIS	2.6
1	G	77	GLU	2.6
1	B	54	ARG	2.6
1	G	74	ILE	2.6
1	F	8	LYS	2.6
1	A	295	ALA	2.6
1	H	80	ARG	2.6
1	B	196	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	10	ALA	2.5
1	H	8	LYS	2.5
1	H	187	ARG	2.5
1	A	277	HIS	2.5
1	H	60	TYR	2.5
1	H	39	ARG	2.5
1	B	180	ALA	2.5
1	H	10	ALA	2.4
1	H	199	LEU	2.4
1	D	80	ARG	2.4
1	E	187	ARG	2.4
1	F	80	ARG	2.4
1	G	172	ARG	2.4
1	D	72	ARG	2.4
1	A	10	ALA	2.4
1	C	10	ALA	2.4
1	H	33	VAL	2.4
1	H	52	VAL	2.4
1	H	342	VAL	2.4
1	D	172	ARG	2.4
1	H	71	ASN	2.4
1	A	171	ASP	2.3
1	B	80	ARG	2.3
1	A	400	LEU	2.3
1	C	400	LEU	2.3
1	C	285	ASP	2.3
1	D	51	ALA	2.3
1	A	66	PHE	2.3
1	C	33	VAL	2.3
1	G	495	GLU	2.3
1	D	68	PRO	2.3
1	B	39	ARG	2.3
1	C	80	ARG	2.3
1	D	176	ARG	2.3
1	D	296	GLY	2.2
1	C	12	GLU	2.2
1	E	292	GLU	2.2
1	D	171	ASP	2.2
1	A	173	ASP	2.2
1	A	73	LEU	2.2
1	D	53	ILE	2.2
1	C	277	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	48	ARG	2.2
1	F	54	ARG	2.2
1	G	277	HIS	2.2
1	B	199	LEU	2.1
1	B	68	PRO	2.1
1	H	32	ILE	2.1
1	H	171	ASP	2.1
1	C	8	LYS	2.1
1	E	283	ARG	2.1
1	C	522	PRO	2.1
1	G	296	GLY	2.1
1	B	15	ARG	2.1
1	H	48	ARG	2.1
1	E	77	GLU	2.1
1	C	173	ASP	2.1
1	G	480	ASP	2.1
1	H	68	PRO	2.1
1	B	74	ILE	2.1
1	E	196	ARG	2.1
1	B	77	GLU	2.1
1	E	287	GLY	2.1
1	G	396	GLY	2.1
1	A	283	ARG	2.0
1	B	520	GLN	2.0
1	C	520	GLN	2.0
1	D	12	GLU	2.0
1	E	17	ILE	2.0
1	C	9	PRO	2.0
1	G	501	GLU	2.0
1	C	171	ASP	2.0
1	E	171	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	MDO	B	149	13/14	0.88	0.10	12,14,20,24	0
1	MDO	E	149	13/14	0.88	0.10	11,12,16,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MDO	D	149	13/14	0.89	0.09	14,16,20,21	0
1	MDO	H	149	13/14	0.89	0.10	12,15,21,23	0
1	MDO	F	149	13/14	0.90	0.09	9,11,17,23	0
1	MDO	A	149	13/14	0.90	0.09	11,13,20,21	0
1	MDO	G	149	13/14	0.91	0.08	9,11,15,21	0
1	MDO	C	149	13/14	0.91	0.08	10,11,18,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.