



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:45 AM UTC

PDB ID : 2HQF / pdb_00002hqf
Title : Conformation of the AcrB Multidrug Efflux Pump in Mutants of the Putative Proton Relay Pathway
Authors : Su, C.-C.; Li, M.; Gu, R.; Takatsuka, Y.; McDermott, G.; Nikaido, H.; Yu, E.W.
Deposited on : 2006-07-18
Resolution : 3.38 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
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

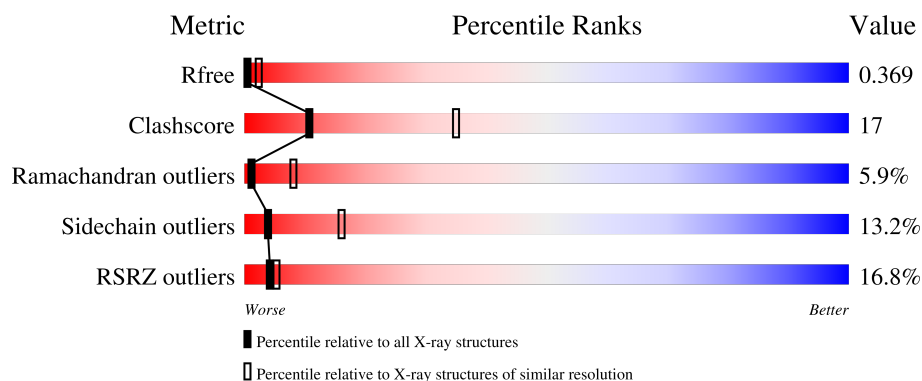
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.38 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	1053	16% 59% 28% 8% ••

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7717 atoms, of which 0 are hydrogens and 0 are deuteriums.

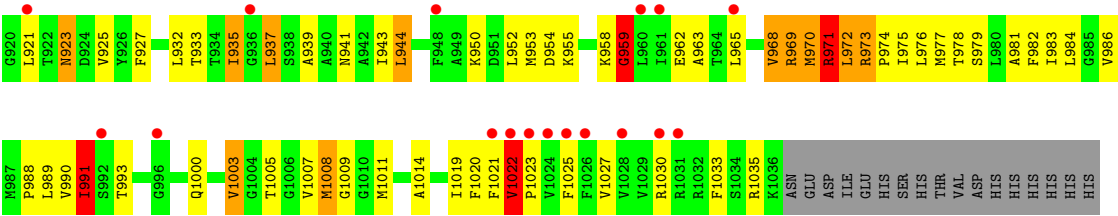
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	0	0	0
			7717	4962	1275	1437	43			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	940	ALA	LYS	engineered mutation	UNP P31224
A	1050	HIS	-	cloning artifact	UNP P31224
A	1051	HIS	-	cloning artifact	UNP P31224
A	1052	HIS	-	cloning artifact	UNP P31224
A	1053	HIS	-	cloning artifact	UNP P31224



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	145.65Å 145.65Å 519.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.38 20.00 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.38) 98.5 (20.00-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.251 , 0.280 0.344 , 0.369	Depositor DCC
R_{free} test set	1768 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7717	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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](#)

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	0.75	10/7860 (0.1%)	0.91	10/10676 (0.1%)

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	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	959	GLY	C-O	18.36	1.48	1.23
1	A	322	LYS	CE-NZ	8.95	1.76	1.49
1	A	959	GLY	C-N	6.95	1.42	1.33
1	A	722	GLU	C-N	6.67	1.43	1.33
1	A	653	ARG	CZ-NH1	6.51	1.41	1.32
1	A	322	LYS	CD-CE	6.31	1.71	1.52
1	A	388	PHE	CA-CB	6.17	1.60	1.53
1	A	106	GLN	CD-OE1	6.12	1.35	1.23
1	A	30	LEU	CG-CD2	6.07	1.72	1.52
1	A	432	ARG	CZ-NH1	5.02	1.39	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	TYR	C-N-CD	-15.95	85.51	120.60
1	A	35	TYR	CA-C-N	15.05	163.11	127.00
1	A	35	TYR	C-N-CA	15.05	163.11	127.00
1	A	426	PRO	N-CA-C	8.60	121.19	110.70
1	A	463	THR	N-CA-C	-6.30	104.63	113.20
1	A	899	PHE	N-CA-C	-6.17	106.72	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	PHE	N-CA-C	5.38	117.16	109.14
1	A	894	SER	N-CA-C	5.31	117.18	110.33
1	A	397	GLY	N-CA-C	-5.28	108.87	114.67
1	A	864	TYR	N-CA-C	5.20	121.88	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	GLN	Peptide
1	A	959	GLY	Mainchain

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	7717	0	7869	260	11
All	All	7717	0	7869	260	11

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 17.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:CE	1:A:322:LYS:NZ	1.76	1.45
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.40	1.01
1:A:680:PHE:HA	1:A:862:MET:HG3	1.45	0.98
1:A:1022:VAL:HB	1:A:1023:PRO:CD	2.02	0.89
1:A:867:ARG:HG3	1:A:868:LEU:H	1.36	0.89
1:A:863:SER:O	1:A:864:TYR:HD2	1.56	0.88
1:A:166:ILE:HG22	1:A:167:SER:H	1.38	0.87
1:A:959:GLY:HA3	1:A:963:ALA:HB3	1.55	0.86
1:A:473:THR:HA	1:A:476:SER:HB2	1.58	0.84
1:A:496:MET:O	1:A:497:LEU:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TYR:HB2	1:A:1022:VAL:HG11	1.64	0.78
1:A:897:ILE:HD13	1:A:897:ILE:H	1.49	0.78
1:A:379:THR:HG21	1:A:473:THR:HG23	1.67	0.77
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.65	0.77
1:A:863:SER:C	1:A:864:TYR:HD2	1.93	0.76
1:A:867:ARG:HG3	1:A:868:LEU:N	2.01	0.76
1:A:466:ILE:HA	1:A:469:GLN:HG2	1.67	0.75
1:A:465:ALA:HB1	1:A:468:ARG:HB3	1.70	0.73
1:A:1003:VAL:O	1:A:1007:VAL:HG23	1.89	0.72
1:A:475:VAL:HA	1:A:478:MET:HG3	1.71	0.72
1:A:470:PHE:CZ	1:A:473:THR:HB	2.25	0.71
1:A:149:MET:HB3	1:A:153:ASP:HB3	1.74	0.70
1:A:864:TYR:HB2	1:A:867:ARG:HG2	1.72	0.70
1:A:394:THR:HB	1:A:470:PHE:CZ	2.27	0.69
1:A:859:TRP:HB3	1:A:863:SER:CB	2.22	0.69
1:A:462:SER:HB2	1:A:867:ARG:HD3	1.73	0.69
1:A:1023:PRO:O	1:A:1027:VAL:HG13	1.93	0.69
1:A:877:TYR:HA	1:A:880:SER:HB2	1.76	0.68
1:A:392:THR:C	1:A:394:THR:H	2.02	0.68
1:A:525:HIS:HA	1:A:529:ASP:HB2	1.76	0.68
1:A:426:PRO:HD2	1:A:427:PRO:HD3	1.74	0.67
1:A:8:ARG:H	1:A:8:ARG:HE	1.42	0.67
1:A:462:SER:C	1:A:464:GLY:H	2.03	0.67
1:A:463:THR:HG22	1:A:867:ARG:HB2	1.77	0.67
1:A:859:TRP:HB3	1:A:863:SER:OG	1.94	0.67
1:A:790:TYR:HB3	1:A:798:MET:HG3	1.77	0.67
1:A:897:ILE:HG12	1:A:898:PRO:HD3	1.76	0.66
1:A:862:MET:C	1:A:864:TYR:H	2.02	0.66
1:A:74:ASN:O	1:A:75:LEU:HB3	1.96	0.65
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.78	0.65
1:A:462:SER:HB2	1:A:867:ARG:CD	2.27	0.64
1:A:156:ASP:HA	1:A:181:GLN:HA	1.79	0.64
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.79	0.64
1:A:1020:PHE:HA	1:A:1025:PHE:HE1	1.63	0.64
1:A:39:ALA:HB2	1:A:672:VAL:HG21	1.80	0.63
1:A:392:THR:HG22	1:A:393:LEU:H	1.64	0.63
1:A:864:TYR:CB	1:A:867:ARG:HG2	2.29	0.63
1:A:131:LYS:HB3	1:A:295:THR:H	1.64	0.62
1:A:488:LEU:O	1:A:490:PRO:HD2	1.99	0.62
1:A:379:THR:HB	1:A:398:MET:HE1	1.81	0.62
1:A:418:ARG:HE	1:A:970:MET:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:VAL:HG13	1:A:887:CYS:HB2	1.82	0.62
1:A:470:PHE:CE1	1:A:473:THR:HB	2.35	0.61
1:A:166:ILE:HG22	1:A:167:SER:N	2.13	0.60
1:A:892:TYR:HB3	1:A:897:ILE:HG13	1.83	0.60
1:A:1020:PHE:HA	1:A:1025:PHE:CE1	2.36	0.60
1:A:188:MET:N	1:A:775:SER:HA	2.18	0.59
1:A:240:LEU:HD22	1:A:245:GLU:HB3	1.84	0.59
1:A:350:LEU:HD12	1:A:984:LEU:HB3	1.84	0.59
1:A:863:SER:O	1:A:864:TYR:CD2	2.47	0.59
1:A:973:ARG:HB2	1:A:974:PRO:HD3	1.84	0.58
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.86	0.57
1:A:574:THR:HA	1:A:665:ALA:HA	1.87	0.57
1:A:863:SER:C	1:A:864:TYR:CD2	2.78	0.57
1:A:339:GLU:HB3	1:A:1000:GLN:HE22	1.69	0.57
1:A:426:PRO:CD	1:A:427:PRO:HD3	2.33	0.57
1:A:1033:PHE:C	1:A:1035:ARG:H	2.12	0.57
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.86	0.57
1:A:680:PHE:HB2	1:A:862:MET:HE3	1.85	0.57
1:A:584:GLN:H	1:A:622:GLN:HE21	1.52	0.57
1:A:939:ALA:O	1:A:943:ILE:HG22	2.05	0.57
1:A:465:ALA:O	1:A:469:GLN:N	2.38	0.56
1:A:691:GLY:H	1:A:694:LYS:HE3	1.70	0.56
1:A:900:SER:HA	1:A:1027:VAL:HB	1.86	0.56
1:A:470:PHE:O	1:A:471:SER:HB2	2.05	0.56
1:A:73:ASP:H	1:A:106:GLN:HE22	1.54	0.56
1:A:470:PHE:O	1:A:471:SER:CB	2.53	0.56
1:A:637:ARG:O	1:A:637:ARG:HG2	2.05	0.55
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.87	0.55
1:A:401:ALA:HB2	1:A:474:ILE:HG13	1.87	0.55
1:A:367:ILE:HG13	1:A:492:LEU:HD22	1.87	0.55
1:A:322:LYS:NZ	1:A:322:LYS:CD	2.68	0.54
1:A:1023:PRO:C	1:A:1027:VAL:HG13	2.32	0.54
1:A:41:PRO:HB2	1:A:94:PHE:HB2	1.89	0.54
1:A:541:TYR:HB3	1:A:1022:VAL:HG13	1.89	0.54
1:A:314:GLU:N	1:A:315:PRO:HD2	2.22	0.54
1:A:367:ILE:HD12	1:A:367:ILE:H	1.72	0.54
1:A:457:ALA:HA	1:A:459:PHE:HD1	1.73	0.54
1:A:973:ARG:HB2	1:A:974:PRO:CD	2.38	0.53
1:A:919:ARG:HD2	1:A:921:LEU:HD13	1.89	0.53
1:A:982:PHE:O	1:A:986:VAL:HG23	2.08	0.53
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:HB3	1:A:978:THR:HG23	1.90	0.53
1:A:41:PRO:HA	1:A:295:THR:HG21	1.91	0.53
1:A:219:LEU:HG	1:A:234:ILE:HD11	1.90	0.53
1:A:479:ALA:O	1:A:483:LEU:HB2	2.09	0.52
1:A:1025:PHE:N	1:A:1027:VAL:HG22	2.24	0.52
1:A:379:THR:CG2	1:A:473:THR:HG23	2.37	0.52
1:A:390:ILE:HG22	1:A:390:ILE:O	2.07	0.52
1:A:901:VAL:O	1:A:904:VAL:HG22	2.09	0.52
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.92	0.52
1:A:959:GLY:HA3	1:A:963:ALA:CB	2.33	0.52
1:A:445:ILE:HG13	1:A:446:ALA:N	2.24	0.52
1:A:569:GLN:HG3	1:A:668:LEU:HB2	1.91	0.52
1:A:713:LEU:HD23	1:A:833:PRO:HD3	1.91	0.52
1:A:140:VAL:HB	1:A:289:LEU:HB2	1.92	0.52
1:A:360:GLN:O	1:A:361:ASN:HB2	2.09	0.52
1:A:300:LEU:HD13	1:A:333:VAL:HG11	1.92	0.52
1:A:815:ARG:HH11	1:A:815:ARG:CG	2.24	0.51
1:A:991:ILE:C	1:A:993:THR:H	2.17	0.51
1:A:392:THR:C	1:A:394:THR:N	2.67	0.51
1:A:986:VAL:HG13	1:A:989:LEU:HD12	1.92	0.51
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.91	0.51
1:A:973:ARG:CB	1:A:974:PRO:HD3	2.40	0.51
1:A:774:MET:O	1:A:775:SER:HB3	2.09	0.51
1:A:527:TYR:HE1	1:A:1020:PHE:HB3	1.75	0.51
1:A:164:ASP:HB3	1:A:767:ARG:HH22	1.74	0.51
1:A:166:ILE:CG2	1:A:167:SER:H	2.17	0.51
1:A:214:VAL:HG22	1:A:237:GLN:HB2	1.93	0.51
1:A:459:PHE:CE1	1:A:468:ARG:HD2	2.46	0.51
1:A:478:MET:HE3	1:A:479:ALA:HB2	1.93	0.50
1:A:482:VAL:HG12	1:A:482:VAL:O	2.11	0.50
1:A:399:VAL:HA	1:A:402:ILE:HB	1.93	0.50
1:A:23:GLY:HA3	1:A:377:LEU:O	2.11	0.50
1:A:831:ALA:O	1:A:832:ALA:HB2	2.10	0.50
1:A:248:LYS:HA	1:A:261:LEU:HD23	1.94	0.50
1:A:1019:ILE:HG23	1:A:1020:PHE:CD2	2.47	0.50
1:A:631:LEU:HD13	1:A:637:ARG:HH12	1.77	0.50
1:A:859:TRP:HB3	1:A:863:SER:HB3	1.93	0.49
1:A:973:ARG:CB	1:A:974:PRO:CD	2.90	0.49
1:A:968:VAL:HG21	1:A:1025:PHE:CZ	2.48	0.49
1:A:178:PHE:HB2	1:A:288:GLY:H	1.78	0.49
1:A:407:ASP:O	1:A:410:ILE:HG22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:HB3	1:A:471:SER:OG	2.13	0.49
1:A:410:ILE:HG12	1:A:977:MET:HE3	1.94	0.49
1:A:166:ILE:C	1:A:168:ARG:H	2.21	0.49
1:A:172:VAL:HG11	1:A:175:VAL:HG23	1.94	0.49
1:A:545:TYR:HB2	1:A:1022:VAL:CG1	2.41	0.49
1:A:634:TRP:HA	1:A:637:ARG:HE	1.78	0.49
1:A:730:ASP:HB3	1:A:806:SER:HB3	1.94	0.49
1:A:462:SER:C	1:A:464:GLY:N	2.67	0.48
1:A:681:ASP:N	1:A:862:MET:SD	2.82	0.48
1:A:968:VAL:HG21	1:A:1025:PHE:CE2	2.48	0.48
1:A:617:PHE:O	1:A:618:ALA:HB3	2.14	0.48
1:A:367:ILE:HG23	1:A:492:LEU:HB3	1.95	0.48
1:A:659:LYS:HG3	1:A:661:ALA:H	1.78	0.48
1:A:673:GLU:HG3	1:A:674:LEU:H	1.78	0.48
1:A:973:ARG:O	1:A:977:MET:HG2	2.14	0.48
1:A:414:GLU:OE2	1:A:418:ARG:NH1	2.46	0.48
1:A:684:LEU:HD13	1:A:702:LEU:HD13	1.95	0.48
1:A:459:PHE:HE1	1:A:468:ARG:HD2	1.78	0.47
1:A:444:GLY:O	1:A:448:VAL:HG22	2.15	0.47
1:A:527:TYR:CE1	1:A:1020:PHE:HB3	2.49	0.47
1:A:380:PHE:HA	1:A:383:LEU:HD12	1.97	0.47
1:A:481:SER:C	1:A:483:LEU:H	2.22	0.47
1:A:36:PRO:HD3	1:A:391:ASN:CG	2.39	0.47
1:A:990:VAL:HG11	1:A:1008:MET:HG2	1.96	0.47
1:A:905:VAL:N	1:A:906:PRO:HD2	2.29	0.47
1:A:366:LEU:O	1:A:370:ILE:HG12	2.14	0.47
1:A:454:VAL:HG13	1:A:475:VAL:HG21	1.97	0.47
1:A:588:GLN:HG2	1:A:613:ASN:HD22	1.80	0.47
1:A:675:GLY:HA3	1:A:867:ARG:NH2	2.29	0.47
1:A:900:SER:CA	1:A:1027:VAL:HB	2.44	0.47
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.97	0.47
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.96	0.46
1:A:438:ILE:HG22	1:A:442:LEU:HD23	1.96	0.46
1:A:549:VAL:O	1:A:552:MET:HG2	2.15	0.46
1:A:134:SER:HA	1:A:292:LYS:HD2	1.98	0.46
1:A:466:ILE:HG22	1:A:925:VAL:HG11	1.96	0.46
1:A:643:LYS:NZ	1:A:645:GLU:HG3	2.30	0.46
1:A:400:LEU:HD13	1:A:1003:VAL:HG22	1.96	0.46
1:A:680:PHE:HA	1:A:862:MET:CG	2.31	0.46
1:A:965:LEU:O	1:A:969:ARG:HB2	2.15	0.46
1:A:897:ILE:HG12	1:A:898:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ASN:HD22	1:A:927:PHE:HD2	1.62	0.46
1:A:327:TYR:CD2	1:A:571:VAL:HG11	2.50	0.46
1:A:971:ARG:HH22	1:A:972:LEU:HB3	1.81	0.46
1:A:184:MET:HE3	1:A:184:MET:HA	1.98	0.45
1:A:188:MET:H	1:A:775:SER:HA	1.82	0.45
1:A:473:THR:HA	1:A:476:SER:CB	2.37	0.45
1:A:445:ILE:HG22	1:A:943:ILE:HG21	1.98	0.45
1:A:452:VAL:HG12	1:A:880:SER:HB3	1.97	0.45
1:A:897:ILE:H	1:A:897:ILE:CD1	2.23	0.45
1:A:937:LEU:HD11	1:A:1011:MET:SD	2.57	0.45
1:A:343:THR:HG23	1:A:988:PRO:HB2	1.99	0.45
1:A:878:ALA:O	1:A:882:ILE:HG12	2.16	0.45
1:A:915:ALA:HB1	1:A:1005:THR:HG22	1.98	0.45
1:A:568:ASP:OD2	1:A:643:LYS:HB2	2.16	0.45
1:A:862:MET:SD	1:A:863:SER:N	2.90	0.45
1:A:389:SER:O	1:A:390:ILE:HB	2.17	0.45
1:A:439:GLN:HG3	1:A:440:GLY:H	1.81	0.45
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.99	0.45
1:A:470:PHE:HD1	1:A:470:PHE:HA	1.71	0.45
1:A:344:LEU:O	1:A:348:ILE:HG12	2.17	0.44
1:A:372:VAL:CG1	1:A:406:VAL:HG22	2.47	0.44
1:A:867:ARG:CG	1:A:868:LEU:H	2.09	0.44
1:A:867:ARG:CG	1:A:868:LEU:N	2.68	0.44
1:A:979:SER:O	1:A:983:ILE:HG12	2.17	0.44
1:A:300:LEU:HD13	1:A:333:VAL:CG1	2.47	0.44
1:A:561:SER:O	1:A:562:SER:HB3	2.18	0.44
1:A:155:SER:HB3	1:A:180:SER:H	1.83	0.44
1:A:407:ASP:OD2	1:A:407:ASP:N	2.51	0.44
1:A:475:VAL:HG13	1:A:478:MET:HE3	1.98	0.44
1:A:723:ASP:HA	1:A:814:PRO:HD3	2.00	0.44
1:A:664:PHE:O	1:A:665:ALA:HB3	2.17	0.43
1:A:375:VAL:HG13	1:A:480:LEU:HB3	2.00	0.43
1:A:456:MET:HG2	1:A:467:TYR:HB3	2.00	0.43
1:A:426:PRO:N	1:A:427:PRO:HD3	2.34	0.43
1:A:222:THR:O	1:A:224:PRO:HD3	2.18	0.43
1:A:142:VAL:HG12	1:A:321:LEU:HD22	2.01	0.43
1:A:617:PHE:O	1:A:618:ALA:CB	2.66	0.43
1:A:953:MET:O	1:A:955:LYS:N	2.51	0.43
1:A:34:GLN:HG3	1:A:35:TYR:H	1.84	0.43
1:A:188:MET:HB2	1:A:775:SER:HB2	1.99	0.43
1:A:542:LEU:HD12	1:A:1030:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:ALA:O	1:A:919:ARG:HB2	2.19	0.43
1:A:702:LEU:HB2	1:A:851:LEU:HD11	2.01	0.43
1:A:1008:MET:HA	1:A:1011:MET:HB3	2.01	0.43
1:A:73:ASP:H	1:A:106:GLN:NE2	2.14	0.43
1:A:944:LEU:HD12	1:A:975:ILE:HD11	2.00	0.43
1:A:38:ILE:H	1:A:38:ILE:HG12	1.70	0.42
1:A:588:GLN:HG2	1:A:613:ASN:ND2	2.34	0.42
1:A:400:LEU:HG	1:A:933:THR:HG21	2.01	0.42
1:A:1025:PHE:H	1:A:1027:VAL:HG22	1.84	0.42
1:A:923:ASN:HA	1:A:927:PHE:HD2	1.83	0.42
1:A:166:ILE:HA	1:A:169:THR:HG22	2.01	0.42
1:A:192:GLU:HG2	1:A:264:ASP:O	2.19	0.42
1:A:862:MET:C	1:A:864:TYR:N	2.73	0.42
1:A:864:TYR:CD2	1:A:865:GLN:HA	2.55	0.42
1:A:68:ASN:O	1:A:110:LYS:HB2	2.19	0.42
1:A:578:LEU:HG	1:A:587:THR:HG22	2.01	0.42
1:A:335:ILE:C	1:A:337:ILE:H	2.28	0.42
1:A:470:PHE:CE2	1:A:473:THR:HB	2.55	0.42
1:A:453:PHE:C	1:A:471:SER:HB3	2.45	0.41
1:A:451:ALA:O	1:A:880:SER:HA	2.20	0.41
1:A:489:THR:O	1:A:490:PRO:C	2.64	0.41
1:A:723:ASP:HA	1:A:813:SER:HA	2.02	0.41
1:A:831:ALA:HB1	1:A:836:SER:HA	2.01	0.41
1:A:110:LYS:H	1:A:110:LYS:HG2	1.63	0.41
1:A:472:ILE:O	1:A:476:SER:N	2.45	0.41
1:A:367:ILE:HD11	1:A:496:MET:HB3	2.02	0.41
1:A:454:VAL:HA	1:A:471:SER:HB3	2.02	0.41
1:A:384:ALA:O	1:A:385:ALA:O	2.38	0.41
1:A:1025:PHE:C	1:A:1027:VAL:N	2.78	0.41
1:A:73:ASP:N	1:A:106:GLN:HE22	2.19	0.41
1:A:15:ILE:HA	1:A:18:ILE:HD12	2.01	0.41
1:A:252:LYS:HE3	1:A:254:ASN:HB3	2.02	0.41
1:A:468:ARG:C	1:A:470:PHE:N	2.79	0.41
1:A:552:MET:HA	1:A:555:LEU:HD12	2.02	0.41
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.80	0.41
1:A:813:SER:HA	1:A:814:PRO:HD3	1.97	0.41
1:A:844:MET:HE3	1:A:844:MET:HA	2.02	0.41
1:A:198:LEU:HD11	1:A:260:VAL:HG11	2.03	0.40
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.50	0.40
1:A:860:THR:HB	1:A:861:GLY:H	1.75	0.40
1:A:454:VAL:HG23	1:A:455:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ALA:C	1:A:941:ASN:H	2.28	0.40
1:A:907:LEU:HD21	1:A:1023:PRO:HD2	2.03	0.40
1:A:1022:VAL:O	1:A:1023:PRO:C	2.65	0.40
1:A:721:LEU:HD23	1:A:722:GLU:N	2.37	0.40

All (11) 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)
1:A:10:ILE:CG2	1:A:893:GLU:OE1[2_545]	0.90	1.30
1:A:113:LEU:CD2	1:A:127:VAL:O[3_655]	1.67	0.53
1:A:14:VAL:CG1	1:A:886:LEU:CD1[2_545]	1.71	0.49
1:A:10:ILE:CG2	1:A:893:GLU:CD[2_545]	1.77	0.43
1:A:51:GLY:O	1:A:216:ALA:O[3_655]	1.90	0.30
1:A:536:ARG:NE	1:A:962:GLU:OE2[16_544]	2.02	0.18
1:A:228:GLN:OE1	1:A:781:MET:CE[2_545]	2.06	0.14
1:A:71:GLY:N	1:A:167:SER:O[3_655]	2.12	0.08
1:A:536:ARG:NE	1:A:962:GLU:CD[16_544]	2.13	0.07
1:A:70:ASN:ND2	1:A:167:SER:OG[3_655]	2.15	0.05
1:A:112:GLN:NE2	1:A:112:GLN:NE2[2_545]	2.16	0.04

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	1012/1053 (96%)	836 (83%)	116 (12%)	60 (6%)	1 8

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	75	LEU

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Mol	Chain	Res	Type
1	A	360	GLN
1	A	385	ALA
1	A	390	ILE
1	A	404	LEU
1	A	459	PHE
1	A	489	THR
1	A	497	LEU
1	A	644	VAL
1	A	671	ILE
1	A	722	GLU
1	A	832	ALA
1	A	971	ARG
1	A	1021	PHE
1	A	1022	VAL
1	A	127	VAL
1	A	217	GLY
1	A	221	GLY
1	A	255	GLN
1	A	256	ASP
1	A	386	PHE
1	A	464	GLY
1	A	674	LEU
1	A	837	THR
1	A	856	GLY
1	A	864	TYR
1	A	893	GLU
1	A	935	ILE
1	A	954	ASP
1	A	959	GLY
1	A	991	ILE
1	A	82	SER
1	A	361	ASN
1	A	432	ARG
1	A	482	VAL
1	A	673	GLU
1	A	677	ALA
1	A	867	ARG
1	A	149	MET
1	A	222	THR
1	A	471	SER
1	A	561	SER
1	A	618	ALA

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Mol	Chain	Res	Type
1	A	778	LYS
1	A	863	SER
1	A	146	ASP
1	A	427	PRO
1	A	453	PHE
1	A	470	PHE
1	A	721	LEU
1	A	169	THR
1	A	665	ALA
1	A	923	ASN
1	A	9	PRO
1	A	461	GLY
1	A	490	PRO
1	A	514	GLY
1	A	675	GLY
1	A	968	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	826/858 (96%)	717 (87%)	109 (13%)	4 16

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	13	TRP
1	A	17	ILE
1	A	30	LEU
1	A	34	GLN
1	A	38	ILE
1	A	45	ILE
1	A	55	LYS
1	A	68	ASN
1	A	76	MET

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Mol	Chain	Res	Type
1	A	84	SER
1	A	110	LYS
1	A	127	VAL
1	A	130	GLU
1	A	143	ILE
1	A	150	THR
1	A	152	GLU
1	A	176	GLN
1	A	177	LEU
1	A	180	SER
1	A	208	LYS
1	A	222	THR
1	A	226	LYS
1	A	234	ILE
1	A	249	ILE
1	A	252	LYS
1	A	278	ILE
1	A	293	LEU
1	A	298	ASN
1	A	306	ILE
1	A	321	LEU
1	A	322	LYS
1	A	337	ILE
1	A	349	ILE
1	A	360	GLN
1	A	366	LEU
1	A	376	LEU
1	A	390	ILE
1	A	393	LEU
1	A	405	LEU
1	A	407	ASP
1	A	415	ASN
1	A	432	ARG
1	A	438	ILE
1	A	442	LEU
1	A	456	MET
1	A	473	THR
1	A	474	ILE
1	A	480	LEU
1	A	483	LEU
1	A	488	LEU
1	A	489	THR

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Mol	Chain	Res	Type
1	A	492	LEU
1	A	498	LYS
1	A	516	PHE
1	A	534	ILE
1	A	547	ILE
1	A	550	VAL
1	A	563	PHE
1	A	578	LEU
1	A	591	LEU
1	A	601	LYS
1	A	632	LYS
1	A	637	ARG
1	A	640	GLU
1	A	643	LYS
1	A	645	GLU
1	A	671	ILE
1	A	672	VAL
1	A	674	LEU
1	A	695	LEU
1	A	696	THR
1	A	697	GLN
1	A	705	GLU
1	A	709	HIS
1	A	760	ASN
1	A	770	LYS
1	A	792	ARG
1	A	797	GLN
1	A	798	MET
1	A	815	ARG
1	A	817	GLU
1	A	846	GLN
1	A	860	THR
1	A	862	MET
1	A	864	TYR
1	A	886	LEU
1	A	888	LEU
1	A	897	ILE
1	A	907	LEU
1	A	913	LEU
1	A	914	LEU
1	A	932	LEU
1	A	935	ILE

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Mol	Chain	Res	Type
1	A	937	LEU
1	A	944	LEU
1	A	950	LYS
1	A	952	LEU
1	A	958	LYS
1	A	969	ARG
1	A	970	MET
1	A	971	ARG
1	A	972	LEU
1	A	973	ARG
1	A	976	LEU
1	A	991	ILE
1	A	1003	VAL
1	A	1008	MET
1	A	1022	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	108	GLN
1	A	123	GLN
1	A	124	GLN
1	A	194	ASN
1	A	284	GLN
1	A	361	ASN
1	A	517	ASN
1	A	604	ASN
1	A	605	ASN
1	A	622	GLN
1	A	687	GLN
1	A	697	GLN
1	A	700	ASN
1	A	760	ASN
1	A	797	GLN
1	A	923	ASN
1	A	1000	GLN
1	A	1001	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1016/1053 (96%)	1.11	171 (16%) 4 5	17, 76, 136, 175	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	PHE	5.7
1	A	868	LEU	5.6
1	A	295	THR	5.3
1	A	294	ALA	4.8
1	A	297	ALA	4.6
1	A	389	SER	4.6
1	A	674	LEU	4.6
1	A	714	THR	4.6
1	A	171	GLY	4.6
1	A	1022	VAL	4.4
1	A	361	ASN	4.3
1	A	149	MET	4.2
1	A	296	GLY	4.2
1	A	303	ALA	4.0
1	A	996	GLY	3.9
1	A	892	TYR	3.9
1	A	833	PRO	3.9
1	A	299	ALA	3.9
1	A	936	GLY	3.9
1	A	170	SER	3.8
1	A	713	LEU	3.8
1	A	676	THR	3.8
1	A	829	GLY	3.7
1	A	31	PRO	3.7
1	A	960	LEU	3.7
1	A	448	VAL	3.7
1	A	860	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	679	GLY	3.6
1	A	563	PHE	3.5
1	A	543	VAL	3.5
1	A	395	MET	3.5
1	A	52	ALA	3.4
1	A	390	ILE	3.4
1	A	425	LEU	3.3
1	A	658	ILE	3.3
1	A	816	LEU	3.3
1	A	444	GLY	3.2
1	A	468	ARG	3.2
1	A	126	GLY	3.2
1	A	1030	ARG	3.2
1	A	869	SER	3.2
1	A	1028	VAL	3.1
1	A	891	LEU	3.1
1	A	306	ILE	3.1
1	A	30	LEU	3.1
1	A	1024	VAL	3.1
1	A	886	LEU	3.0
1	A	817	GLU	3.0
1	A	401	ALA	3.0
1	A	451	ALA	3.0
1	A	678	THR	3.0
1	A	233	SER	2.9
1	A	488	LEU	2.9
1	A	293	LEU	2.9
1	A	435	MET	2.9
1	A	393	LEU	2.9
1	A	59	ASP	2.9
1	A	834	GLY	2.9
1	A	467	TYR	2.8
1	A	535	LEU	2.8
1	A	462	SER	2.8
1	A	385	ALA	2.8
1	A	677	ALA	2.8
1	A	710	PRO	2.8
1	A	173	GLY	2.8
1	A	559	LEU	2.8
1	A	831	ALA	2.8
1	A	1031	ARG	2.8
1	A	426	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.8
1	A	561	SER	2.8
1	A	472	ILE	2.7
1	A	391	ASN	2.7
1	A	443	VAL	2.7
1	A	138	MET	2.7
1	A	705	GLU	2.7
1	A	222	THR	2.7
1	A	379	THR	2.7
1	A	456	MET	2.7
1	A	51	GLY	2.6
1	A	103	ALA	2.6
1	A	172	VAL	2.6
1	A	388	PHE	2.6
1	A	865	GLN	2.6
1	A	400	LEU	2.6
1	A	114	ALA	2.6
1	A	65	ILE	2.6
1	A	675	GLY	2.6
1	A	992	SER	2.5
1	A	887	CYS	2.5
1	A	722	GLU	2.5
1	A	492	LEU	2.5
1	A	387	GLY	2.5
1	A	236	ALA	2.5
1	A	145	THR	2.5
1	A	327	TYR	2.5
1	A	541	TYR	2.5
1	A	898	PRO	2.5
1	A	42	ALA	2.5
1	A	352	PHE	2.5
1	A	470	PHE	2.5
1	A	376	LEU	2.5
1	A	852	PRO	2.5
1	A	622	GLN	2.5
1	A	872	GLN	2.5
1	A	81	ASN	2.4
1	A	404	LEU	2.4
1	A	704	ALA	2.4
1	A	599	LEU	2.4
1	A	921	LEU	2.4
1	A	965	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	455	PRO	2.4
1	A	859	TRP	2.4
1	A	106	GLN	2.4
1	A	375	VAL	2.4
1	A	840	ALA	2.3
1	A	718	PRO	2.3
1	A	702	LEU	2.3
1	A	830	GLN	2.3
1	A	672	VAL	2.3
1	A	873	ALA	2.3
1	A	310	LEU	2.3
1	A	151	GLN	2.3
1	A	90	ILE	2.3
1	A	523	SER	2.3
1	A	292	LYS	2.3
1	A	36	PRO	2.2
1	A	476	SER	2.2
1	A	778	LYS	2.2
1	A	38	ILE	2.2
1	A	72	ILE	2.2
1	A	874	PRO	2.2
1	A	524	THR	2.2
1	A	542	LEU	2.2
1	A	876	LEU	2.2
1	A	302	THR	2.2
1	A	473	THR	2.2
1	A	571	VAL	2.2
1	A	897	ILE	2.2
1	A	76	MET	2.2
1	A	78	MET	2.2
1	A	519	MET	2.2
1	A	457	ALA	2.2
1	A	498	LYS	2.2
1	A	380	PHE	2.2
1	A	556	PHE	2.2
1	A	615	PHE	2.2
1	A	948	PHE	2.2
1	A	1025	PHE	2.2
1	A	888	LEU	2.1
1	A	1026	PHE	2.1
1	A	901	VAL	2.1
1	A	22	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1023	PRO	2.1
1	A	459	PHE	2.1
1	A	526	HIS	2.1
1	A	148	THR	2.1
1	A	883	VAL	2.1
1	A	961	ILE	2.1
1	A	304	ALA	2.1
1	A	567	GLU	2.1
1	A	826	GLU	2.1
1	A	894	SER	2.1
1	A	420	MET	2.1
1	A	890	ALA	2.1
1	A	41	PRO	2.1
1	A	454	VAL	2.0
1	A	828	LEU	2.0
1	A	161	ASN	2.0
1	A	439	GLN	2.0
1	A	673	GLU	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.