WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 03:07 PM GMT

PDB ID : 2HQG

Title : Conformation of the AcrB Multidrug Efflux Pump in Mutants of the Putative Proton Relay Pathway

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Deposited on : 2006-07-18

Resolution : 3.38 Å(reported)

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.358
Clashscore		14
Ramachandran outliers		5.4%
Sidechain outliers		11.1%
RSRZ outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
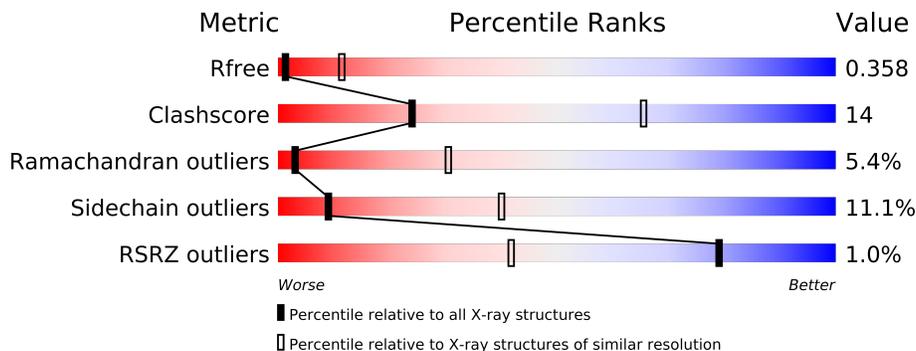
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1059 (3.50-3.26)
Clashscore	79885	1340 (3.50-3.26)
Ramachandran outliers	78287	1300 (3.50-3.26)
Sidechain outliers	78261	1300 (3.50-3.26)
RSRZ outliers	66119	1059 (3.50-3.26)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1053	

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 7719 atoms, of which 0 are hydrogen and 0 are deuterium.

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 7719	C 4964	N 1276	O 1436	S 43	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	978	ALA	THR	ENGINEERED	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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Acriflavine resistance protein B

Chain A:
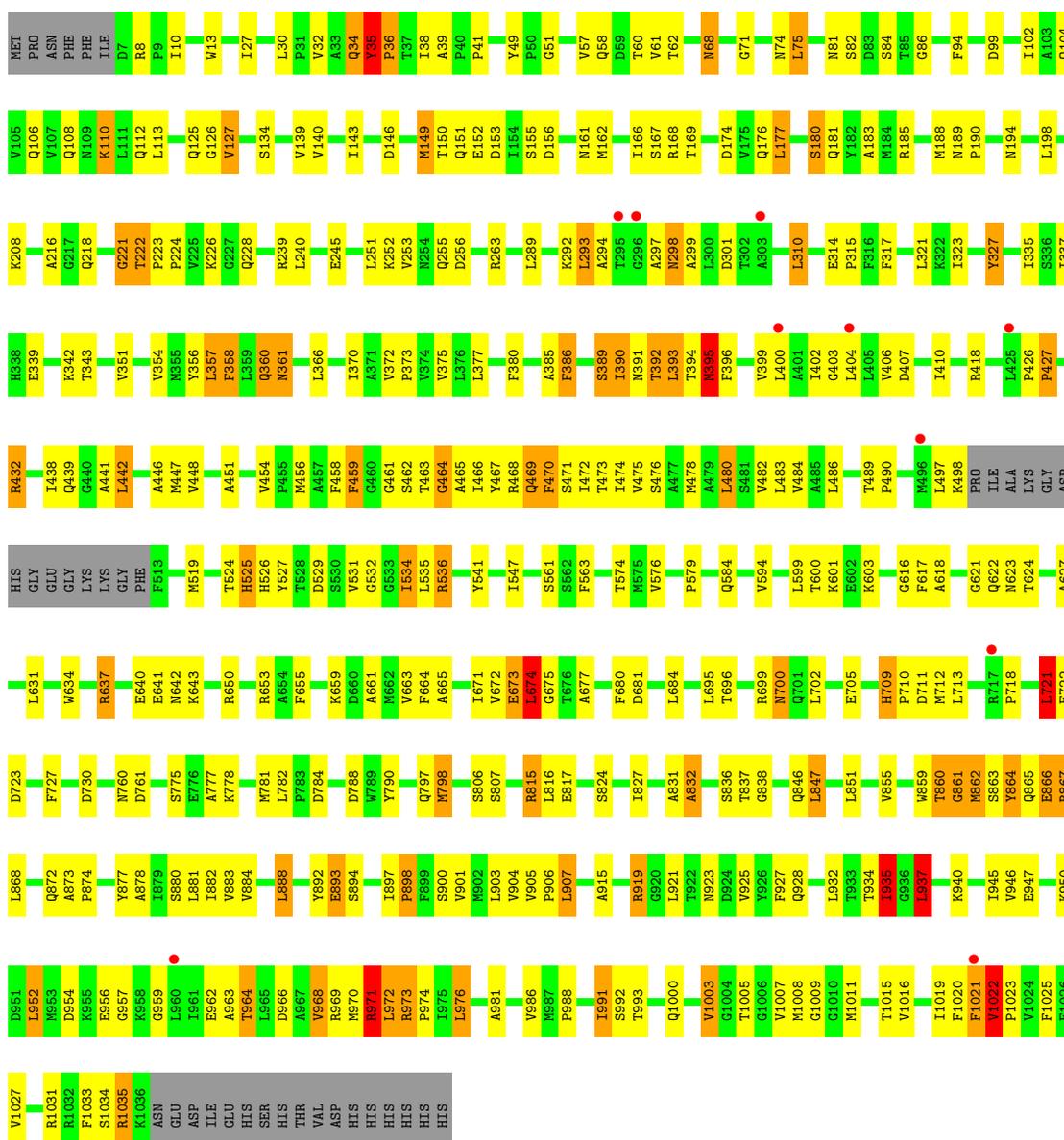
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.90Å 144.90Å 518.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.38 46.66 – 3.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-3.38) 92.6 (46.66-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.254 , 0.275 0.352 , 0.358	Depositor DCC
R_{free} test set	1965 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	101.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.54, < L^2 > = 0.38$	Xtriage
Outliers	0 of 39083 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7719	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.67	9/7862 (0.1%)	0.64	13/10677 (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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1035	ARG	CZ-NH1	18.96	1.57	1.33
1	A	815	ARG	CZ-NH1	9.16	1.45	1.33
1	A	536	ARG	CZ-NH1	7.96	1.43	1.33
1	A	964	THR	CB-OG1	6.79	1.56	1.43
1	A	1035	ARG	NE-CZ	5.76	1.40	1.33
1	A	653	ARG	CZ-NH1	5.75	1.40	1.33
1	A	110	LYS	CE-NZ	5.37	1.62	1.49
1	A	395	MET	C-O	-5.35	1.13	1.23
1	A	536	ARG	CZ-NH2	5.15	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1035	ARG	NE-CZ-NH2	-14.89	112.85	120.30
1	A	815	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	35	TYR	C-N-CD	-6.52	106.26	120.60
1	A	536	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	815	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	966	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	177	LEU	CA-CB-CG	6.00	129.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	310	LEU	CA-CB-CG	5.78	128.60	115.30
1	A	674	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	1035	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	35	TYR	C-N-CA	5.31	144.31	122.00
1	A	937	LEU	CA-CB-CG	5.20	127.27	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	TYR	Peptide
1	A	469	GLN	Peptide

5.2　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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7719	0	7875	222	10
All	All	7719	0	7875	222	10

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (222) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:680:PHE:HA	1:A:862:MET:HG3	1.44	1.00
1:A:864:TYR:HB3	1:A:867:ARG:HG2	1.47	0.96
1:A:861:GLY:HA3	1:A:862:MET:HB3	1.44	0.96
1:A:867:ARG:HG3	1:A:868:LEU:H	1.37	0.89
1:A:861:GLY:H	1:A:862:MET:HE2	1.41	0.82
1:A:934:THR:O	1:A:935:ILE:HB	1.81	0.80
1:A:525:HIS:HA	1:A:529:ASP:HB2	1.63	0.79
1:A:166:ILE:HG22	1:A:167:SER:H	1.48	0.79
1:A:465:ALA:HB1	1:A:468:ARG:HB3	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ARG:HG3	1:A:868:LEU:N	2.00	0.76
1:A:426:PRO:HD2	1:A:427:PRO:HD3	1.65	0.76
1:A:864:TYR:HB2	1:A:865:GLN:C	2.06	0.75
1:A:861:GLY:HA3	1:A:862:MET:CB	2.16	0.75
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.67	0.75
1:A:472:ILE:O	1:A:476:SER:N	2.17	0.75
1:A:861:GLY:CA	1:A:862:MET:HB3	2.17	0.74
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.69	0.72
1:A:968:VAL:HG21	1:A:1025:PHE:CZ	2.24	0.72
1:A:462:SER:HB2	1:A:867:ARG:HD3	1.73	0.71
1:A:864:TYR:HB2	1:A:866:GLU:N	2.05	0.71
1:A:466:ILE:HA	1:A:469:GLN:HG2	1.74	0.70
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.75	0.67
1:A:372:VAL:HG12	1:A:406:VAL:HG22	1.76	0.67
1:A:790:TYR:HB3	1:A:798:MET:HG3	1.78	0.65
1:A:923:ASN:HD22	1:A:927:PHE:HD2	1.45	0.65
1:A:188:MET:N	1:A:775:SER:HA	2.11	0.65
1:A:1022:VAL:HG23	1:A:1023:PRO:HD3	1.79	0.65
1:A:451:ALA:HB1	1:A:883:VAL:HG13	1.77	0.65
1:A:426:PRO:CD	1:A:427:PRO:HD3	2.27	0.64
1:A:357:LEU:O	1:A:358:PHE:HB2	1.97	0.63
1:A:156:ASP:HA	1:A:181:GLN:HA	1.79	0.63
1:A:407:ASP:HA	1:A:410:ILE:HD12	1.81	0.63
1:A:462:SER:C	1:A:464:GLY:H	2.00	0.62
1:A:959:GLY:HA3	1:A:963:ALA:HB2	1.80	0.62
1:A:861:GLY:H	1:A:862:MET:CE	2.12	0.62
1:A:1025:PHE:H	1:A:1027:VAL:HG22	1.64	0.62
1:A:684:LEU:CD1	1:A:855:VAL:HG13	2.29	0.62
1:A:681:ASP:N	1:A:862:MET:SD	2.66	0.61
1:A:584:GLN:H	1:A:622:GLN:HE21	1.46	0.61
1:A:574:THR:HA	1:A:665:ALA:HA	1.81	0.61
1:A:392:THR:C	1:A:394:THR:H	2.04	0.61
1:A:39:ALA:HB2	1:A:672:VAL:HG21	1.82	0.61
1:A:915:ALA:O	1:A:919:ARG:HB2	2.00	0.61
1:A:475:VAL:HA	1:A:478:MET:HB3	1.82	0.61
1:A:393:LEU:HA	1:A:396:PHE:HB3	1.83	0.61
1:A:860:THR:H	1:A:862:MET:CE	2.14	0.61
1:A:884:VAL:O	1:A:888:LEU:HB2	2.02	0.60
1:A:859:TRP:HB3	1:A:863:SER:HB2	1.82	0.60
1:A:1025:PHE:N	1:A:1027:VAL:HG22	2.17	0.60
1:A:673:GLU:HG3	1:A:674:LEU:H	1.65	0.60
1:A:675:GLY:HA3	1:A:867:ARG:NH2	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:473:THR:HA	1:A:476:SER:HB2	1.83	0.59
1:A:343:THR:HG23	1:A:988:PRO:HB2	1.85	0.58
1:A:864:TYR:HB2	1:A:865:GLN:CA	2.33	0.58
1:A:705:GLU:HG3	1:A:847:LEU:HD13	1.84	0.58
1:A:298:ASN:HB2	1:A:301:ASP:HB2	1.85	0.58
1:A:448:VAL:HA	1:A:451:ALA:HB3	1.86	0.57
1:A:462:SER:HB2	1:A:867:ARG:CD	2.34	0.57
1:A:1015:THR:O	1:A:1019:ILE:HB	2.05	0.57
1:A:718:PRO:HG2	1:A:721:LEU:HD13	1.86	0.57
1:A:864:TYR:HD2	1:A:865:GLN:HA	1.69	0.56
1:A:867:ARG:CG	1:A:868:LEU:N	2.65	0.56
1:A:372:VAL:HG23	1:A:373:PRO:HD3	1.87	0.56
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.86	0.56
1:A:81:ASN:O	1:A:816:LEU:O	2.23	0.56
1:A:680:PHE:HA	1:A:862:MET:CG	2.29	0.56
1:A:166:ILE:HG22	1:A:167:SER:N	2.17	0.56
1:A:1023:PRO:O	1:A:1027:VAL:HG13	2.05	0.56
1:A:74:ASN:O	1:A:75:LEU:HB3	2.06	0.56
1:A:34:GLN:HG3	1:A:35:TYR:H	1.71	0.56
1:A:134:SER:H	1:A:292:LYS:HZ2	1.54	0.56
1:A:466:ILE:HG22	1:A:925:VAL:HG11	1.88	0.55
1:A:968:VAL:O	1:A:968:VAL:HG22	2.07	0.55
1:A:392:THR:HG22	1:A:393:LEU:H	1.71	0.55
1:A:106:GLN:O	1:A:110:LYS:HG2	2.07	0.55
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.89	0.55
1:A:188:MET:H	1:A:775:SER:HA	1.72	0.55
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.89	0.55
1:A:149:MET:HB3	1:A:153:ASP:HB3	1.88	0.55
1:A:641:GLU:O	1:A:650:ARG:NH2	2.39	0.54
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.90	0.54
1:A:532:GLY:O	1:A:536:ARG:HB2	2.08	0.54
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.36	0.54
1:A:438:ILE:HG22	1:A:442:LEU:HD23	1.89	0.54
1:A:901:VAL:O	1:A:904:VAL:HG22	2.08	0.54
1:A:470:PHE:CD1	1:A:473:THR:N	2.69	0.53
1:A:465:ALA:O	1:A:469:GLN:N	2.42	0.53
1:A:377:LEU:HA	1:A:380:PHE:CD1	2.44	0.53
1:A:390:ILE:HG22	1:A:390:ILE:O	2.09	0.53
1:A:659:LYS:HG3	1:A:661:ALA:H	1.74	0.52
1:A:240:LEU:HD22	1:A:245:GLU:HB3	1.91	0.52
1:A:134:SER:H	1:A:292:LYS:NZ	2.07	0.52
1:A:721:LEU:O	1:A:723:ASP:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:293:LEU:HD13	1:A:294:ALA:O	2.10	0.52
1:A:864:TYR:CD2	1:A:865:GLN:HA	2.45	0.51
1:A:986:VAL:HG11	1:A:1007:VAL:HG23	1.92	0.51
1:A:474:ILE:O	1:A:478:MET:HB2	2.10	0.51
1:A:634:TRP:HA	1:A:637:ARG:HE	1.75	0.51
1:A:360:GLN:O	1:A:361:ASN:HB2	2.11	0.51
1:A:389:SER:O	1:A:390:ILE:HB	2.11	0.51
1:A:1020:PHE:HA	1:A:1025:PHE:CE1	2.46	0.51
1:A:372:VAL:CG1	1:A:406:VAL:HG22	2.41	0.51
1:A:454:VAL:HA	1:A:471:SER:HB3	1.92	0.51
1:A:194:ASN:HD22	1:A:798:MET:HG2	1.75	0.50
1:A:991:ILE:C	1:A:993:THR:H	2.14	0.50
1:A:541:TYR:HB3	1:A:1022:VAL:HG12	1.93	0.50
1:A:456:MET:HG2	1:A:467:TYR:HB3	1.94	0.50
1:A:139:VAL:HB	1:A:327:TYR:HB3	1.94	0.50
1:A:438:ILE:HA	1:A:441:ALA:HB3	1.93	0.50
1:A:919:ARG:HD2	1:A:921:LEU:HD13	1.94	0.49
1:A:937:LEU:HD11	1:A:1011:MET:SD	2.52	0.49
1:A:1020:PHE:HA	1:A:1025:PHE:HE1	1.75	0.49
1:A:709:HIS:N	1:A:710:PRO:HD3	2.28	0.49
1:A:674:LEU:HD22	1:A:674:LEU:O	2.12	0.49
1:A:140:VAL:HG23	1:A:289:LEU:HB2	1.94	0.49
1:A:1022:VAL:CG2	1:A:1023:PRO:HD3	2.42	0.49
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.95	0.49
1:A:459:PHE:HE1	1:A:468:ARG:HD2	1.78	0.48
1:A:222:THR:O	1:A:224:PRO:HD3	2.13	0.48
1:A:1033:PHE:C	1:A:1035:ARG:H	2.14	0.48
1:A:126:GLY:O	1:A:127:VAL:HG22	2.13	0.48
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.94	0.48
1:A:617:PHE:O	1:A:618:ALA:HB3	2.14	0.48
1:A:873:ALA:N	1:A:874:PRO:HD2	2.29	0.48
1:A:57:VAL:HG11	1:A:86:GLY:HA2	1.95	0.48
1:A:637:ARG:O	1:A:637:ARG:HG2	2.13	0.47
1:A:727:PHE:CZ	1:A:807:SER:HB3	2.49	0.47
1:A:730:ASP:HB3	1:A:806:SER:HB3	1.96	0.47
1:A:392:THR:C	1:A:394:THR:N	2.67	0.47
1:A:574:THR:HG21	1:A:594:VAL:HG11	1.95	0.47
1:A:239:ARG:NE	1:A:761:ASP:O	2.48	0.47
1:A:892:TYR:CD2	1:A:897:ILE:HG21	2.49	0.47
1:A:489:THR:HB	1:A:490:PRO:HD3	1.95	0.47
1:A:441:ALA:HB2	1:A:947:GLU:HG2	1.95	0.47
1:A:68:ASN:HD21	1:A:113:LEU:HB2	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:462:SER:C	1:A:464:GLY:N	2.68	0.47
1:A:675:GLY:HA3	1:A:867:ARG:HH22	1.78	0.47
1:A:531:VAL:HA	1:A:534:ILE:HD13	1.96	0.47
1:A:470:PHE:CD1	1:A:472:ILE:HB	2.50	0.47
1:A:972:LEU:O	1:A:976:LEU:HB2	2.15	0.47
1:A:877:TYR:O	1:A:881:LEU:HB2	2.14	0.47
1:A:817:GLU:HB2	1:A:824:SER:O	2.15	0.47
1:A:35:TYR:HB3	1:A:36:PRO:O	2.15	0.46
1:A:971:ARG:HH22	1:A:972:LEU:HB3	1.80	0.46
1:A:380:PHE:HE2	1:A:395:MET:SD	2.38	0.46
1:A:527:TYR:HE1	1:A:1020:PHE:HB3	1.79	0.46
1:A:166:ILE:C	1:A:168:ARG:H	2.19	0.46
1:A:314:GLU:N	1:A:315:PRO:CD	2.79	0.46
1:A:621:GLY:C	1:A:623:ASN:H	2.19	0.46
1:A:426:PRO:N	1:A:427:PRO:HD3	2.31	0.46
1:A:915:ALA:HB1	1:A:1005:THR:HG22	1.97	0.46
1:A:862:MET:HG2	1:A:863:SER:H	1.80	0.46
1:A:36:PRO:CD	1:A:391:ASN:HB3	2.46	0.45
1:A:860:THR:H	1:A:862:MET:HE1	1.82	0.45
1:A:393:LEU:HD21	1:A:469:GLN:HG3	1.97	0.45
1:A:377:LEU:HA	1:A:380:PHE:HD1	1.80	0.45
1:A:166:ILE:CG2	1:A:167:SER:H	2.23	0.45
1:A:366:LEU:O	1:A:370:ILE:HG12	2.16	0.45
1:A:859:TRP:HB3	1:A:863:SER:CB	2.46	0.45
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.99	0.45
1:A:155:SER:HB3	1:A:180:SER:H	1.81	0.45
1:A:524:THR:O	1:A:526:HIS:N	2.47	0.45
1:A:877:TYR:HA	1:A:880:SER:HB2	1.99	0.45
1:A:664:PHE:O	1:A:665:ALA:HB3	2.17	0.44
1:A:58:GLN:HA	1:A:62:THR:HB	1.99	0.44
1:A:458:PHE:O	1:A:459:PHE:O	2.36	0.44
1:A:907:LEU:HD21	1:A:1023:PRO:HD2	2.00	0.44
1:A:198:LEU:HD13	1:A:251:LEU:HD13	2.00	0.44
1:A:463:THR:HG22	1:A:867:ARG:HB2	2.01	0.43
1:A:900:SER:HB3	1:A:1027:VAL:HB	2.00	0.43
1:A:952:LEU:O	1:A:956:GLU:HB3	2.18	0.43
1:A:862:MET:HG2	1:A:863:SER:N	2.33	0.43
1:A:959:GLY:HA3	1:A:963:ALA:CB	2.47	0.43
1:A:174:ASP:O	1:A:292:LYS:HB3	2.18	0.43
1:A:859:TRP:HE3	1:A:862:MET:SD	2.42	0.43
1:A:956:GLU:HG2	1:A:957:GLY:H	1.83	0.43
1:A:470:PHE:CE1	1:A:472:ILE:HB	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:897:ILE:HG23	1:A:946:VAL:HG11	2.00	0.43
1:A:705:GLU:HG3	1:A:847:LEU:CD1	2.48	0.43
1:A:399:VAL:HA	1:A:402:ILE:HB	2.00	0.43
1:A:699:ARG:HH21	1:A:700:ASN:HD21	1.65	0.43
1:A:991:ILE:O	1:A:993:THR:N	2.43	0.42
1:A:711:ASP:O	1:A:712:MET:HB2	2.19	0.42
1:A:905:VAL:HG12	1:A:935:ILE:HG13	2.01	0.42
1:A:905:VAL:CG2	1:A:906:PRO:HD3	2.49	0.42
1:A:1023:PRO:HA	1:A:1031:ARG:NH1	2.35	0.42
1:A:574:THR:HG22	1:A:627:ALA:HB3	2.00	0.42
1:A:616:GLY:HA3	1:A:624:THR:HB	2.01	0.42
1:A:631:LEU:HD13	1:A:637:ARG:HH12	1.85	0.42
1:A:1016:VAL:O	1:A:1019:ILE:HG22	2.19	0.42
1:A:339:GLU:HB3	1:A:1000:GLN:HE22	1.83	0.42
1:A:183:ALA:HB3	1:A:185:ARG:HD3	2.00	0.42
1:A:314:GLU:N	1:A:315:PRO:HD3	2.34	0.42
1:A:655:PHE:O	1:A:659:LYS:HB2	2.20	0.42
1:A:699:ARG:HH21	1:A:700:ASN:ND2	2.17	0.42
1:A:831:ALA:O	1:A:832:ALA:HB2	2.20	0.42
1:A:484:VAL:C	1:A:486:LEU:H	2.24	0.42
1:A:392:THR:O	1:A:394:THR:HG23	2.20	0.41
1:A:897:ILE:N	1:A:898:PRO:CD	2.83	0.41
1:A:1022:VAL:CB	1:A:1023:PRO:HD3	2.50	0.41
1:A:836:SER:O	1:A:838:GLY:N	2.54	0.41
1:A:1019:ILE:HG23	1:A:1020:PHE:CD2	2.55	0.41
1:A:903:LEU:HD13	1:A:1031:ARG:HE	1.85	0.41
1:A:150:THR:HG22	1:A:151:GLN:N	2.35	0.41
1:A:945:ILE:HG22	1:A:971:ARG:HD2	2.02	0.41
1:A:576:VAL:HG13	1:A:663:VAL:HG22	2.02	0.41
1:A:354:VAL:O	1:A:354:VAL:HG12	2.21	0.41
1:A:897:ILE:N	1:A:898:PRO:HD2	2.36	0.41
1:A:317:PHE:HE2	1:A:323:ILE:HD11	1.85	0.41
1:A:1008:MET:HG3	1:A:1009:GLY:N	2.36	0.41
1:A:403:GLY:O	1:A:406:VAL:N	2.53	0.41
1:A:699:ARG:HG2	1:A:827:ILE:HD11	2.03	0.41
1:A:335:ILE:C	1:A:337:ILE:H	2.24	0.41
1:A:375:VAL:HA	1:A:480:LEU:HD12	2.02	0.40
1:A:372:VAL:CG2	1:A:373:PRO:HD3	2.50	0.40
1:A:218:GLN:HG3	1:A:221:GLY:HA2	2.04	0.40
1:A:964:THR:O	1:A:968:VAL:HG12	2.21	0.40
1:A:878:ALA:O	1:A:882:ILE:HG12	2.22	0.40
1:A:777:ALA:O	1:A:781:MET:HG2	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:897:ILE:H	1:A:897:ILE:HD12	1.86	0.40
1:A:476:SER:O	1:A:480:LEU:HB2	2.21	0.40
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.95	0.40

All (10) 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	Distance(Å)	Clash(Å)
1:A:599:LEU:O	1:A:778:LYS:NZ[6_555]	1.74	0.46
1:A:10:ILE:CG2	1:A:893:GLU:OE1[2_545]	1.79	0.41
1:A:113:LEU:CD2	1:A:127:VAL:O[3_655]	1.79	0.41
1:A:51:GLY:O	1:A:216:ALA:O[3_655]	1.88	0.32
1:A:112:GLN:NE2	1:A:112:GLN:NE2[2_545]	1.88	0.32
1:A:228:GLN:OE1	1:A:781:MET:CE[2_545]	1.88	0.32
1:A:536:ARG:NE	1:A:962:GLU:OE2[16_544]	1.89	0.31
1:A:600:THR:CG2	1:A:782:LEU:CD1[6_555]	1.98	0.22
1:A:71:GLY:N	1:A:167:SER:O[3_655]	2.05	0.15
1:A:603:LYS:NZ	1:A:778:LYS:O[6_555]	2.15	0.05

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%)	838 (83%)	119 (12%)	55 (5%)	3	30

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	36	PRO
1	A	221	GLY
1	A	385	ALA
1	A	404	LEU
1	A	432	ARG
1	A	459	PHE

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Mol	Chain	Res	Type
1	A	470	PHE
1	A	722	GLU
1	A	894	SER
1	A	935	ILE
1	A	82	SER
1	A	127	VAL
1	A	146	ASP
1	A	255	GLN
1	A	256	ASP
1	A	361	ASN
1	A	390	ILE
1	A	461	GLY
1	A	464	GLY
1	A	525	HIS
1	A	671	ILE
1	A	673	GLU
1	A	674	LEU
1	A	954	ASP
1	A	971	ARG
1	A	991	ILE
1	A	1021	PHE
1	A	75	LEU
1	A	169	THR
1	A	299	ALA
1	A	358	PHE
1	A	389	SER
1	A	677	ALA
1	A	721	LEU
1	A	837	THR
1	A	149	MET
1	A	386	PHE
1	A	497	LEU
1	A	561	SER
1	A	579	PRO
1	A	861	GLY
1	A	867	ARG
1	A	893	GLU
1	A	898	PRO
1	A	222	THR
1	A	297	ALA
1	A	427	PRO
1	A	832	ALA

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Mol	Chain	Res	Type
1	A	866	GLU
1	A	1022	VAL
1	A	1034	SER
1	A	992	SER
1	A	968	VAL
1	A	223	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	826/858 (96%)	734 (89%)	92 (11%)	9 40

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	13	TRP
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	49	TYR
1	A	68	ASN
1	A	84	SER
1	A	104	GLN
1	A	108	GLN
1	A	125	GLN
1	A	143	ILE
1	A	152	GLU
1	A	161	ASN
1	A	162	MET
1	A	176	GLN
1	A	177	LEU
1	A	180	SER
1	A	208	LYS
1	A	226	LYS
1	A	252	LYS

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Mol	Chain	Res	Type
1	A	253	VAL
1	A	263	ARG
1	A	293	LEU
1	A	298	ASN
1	A	310	LEU
1	A	321	LEU
1	A	327	TYR
1	A	342	LYS
1	A	356	TYR
1	A	357	LEU
1	A	360	GLN
1	A	386	PHE
1	A	392	THR
1	A	393	LEU
1	A	395	MET
1	A	418	ARG
1	A	432	ARG
1	A	439	GLN
1	A	442	LEU
1	A	447	MET
1	A	480	LEU
1	A	483	LEU
1	A	498	LYS
1	A	519	MET
1	A	534	ILE
1	A	535	LEU
1	A	547	ILE
1	A	563	PHE
1	A	601	LYS
1	A	637	ARG
1	A	640	GLU
1	A	643	LYS
1	A	674	LEU
1	A	695	LEU
1	A	696	THR
1	A	700	ASN
1	A	709	HIS
1	A	713	LEU
1	A	721	LEU
1	A	760	ASN
1	A	784	ASP
1	A	788	ASP

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Mol	Chain	Res	Type
1	A	797	GLN
1	A	798	MET
1	A	815	ARG
1	A	846	GLN
1	A	847	LEU
1	A	860	THR
1	A	862	MET
1	A	864	TYR
1	A	872	GLN
1	A	888	LEU
1	A	907	LEU
1	A	919	ARG
1	A	928	GLN
1	A	932	LEU
1	A	935	ILE
1	A	937	LEU
1	A	940	LYS
1	A	950	LYS
1	A	952	LEU
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	1003	VAL
1	A	1021	PHE
1	A	1022	VAL

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

Mol	Chain	Res	Type
1	A	34	GLN
1	A	108	GLN
1	A	112	GLN
1	A	124	GLN
1	A	176	GLN
1	A	194	ASN
1	A	298	ASN
1	A	361	ASN
1	A	437	GLN
1	A	517	ASN

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Mol	Chain	Res	Type
1	A	604	ASN
1	A	605	ASN
1	A	622	GLN
1	A	687	GLN
1	A	700	ASN
1	A	760	ASN
1	A	820	ASN
1	A	923	ASN
1	A	1000	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1016/1053 (96%)	0.11	10 (0%)	79	42	31, 91, 152, 190	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	LEU	5.1
1	A	496	MET	3.3
1	A	425	LEU	3.1
1	A	1021	PHE	3.1
1	A	400	LEU	2.6
1	A	404	LEU	2.4
1	A	296	GLY	2.3
1	A	295	THR	2.3
1	A	303	ALA	2.3
1	A	717	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.