



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:07 PM GMT

PDB ID : 2HQF
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

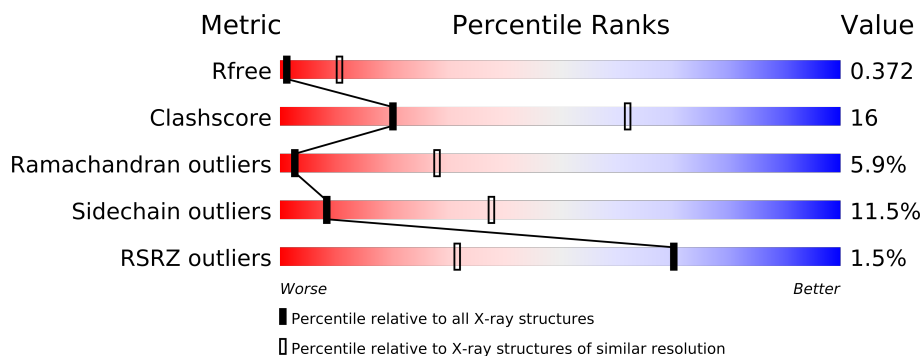
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

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	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 7717 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
			Total	C	N	O	S			
1	A	1016	7717	4962	1275	1437	43	0	0	0

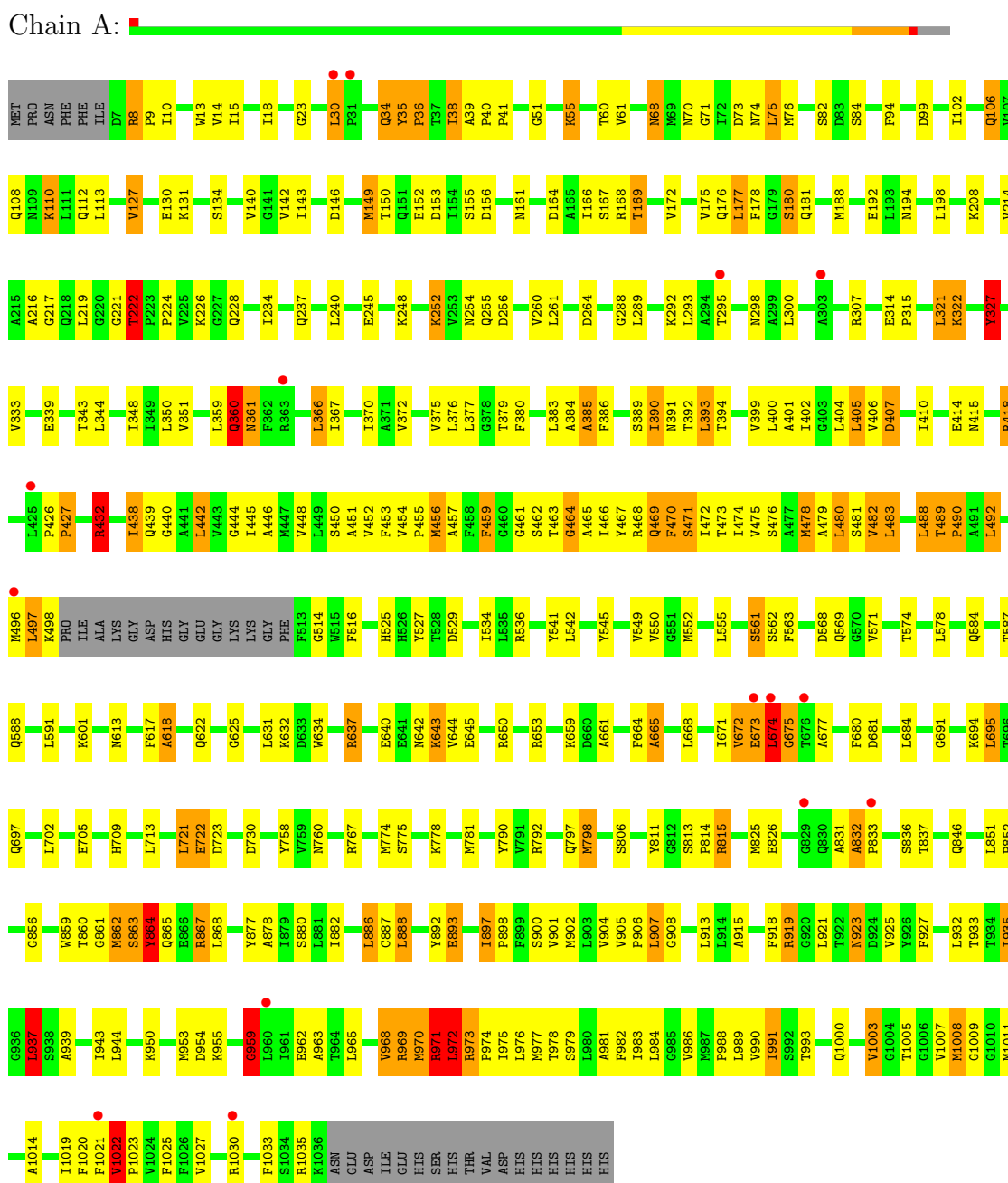
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	940	ALA	LYS	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



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 45.25 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.38) 99.0 (45.25-3.20)	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 5.2.0005	Depositor
R, R_{free}	0.251 , 0.280 0.350 , 0.372	Depositor DCC
R_{free} test set	1769 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 23.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 35254 reflections	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.

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	0.68	15/7860 (0.2%)	0.64	8/10676 (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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	959	GLY	C-O	15.66	1.48	1.23
1	A	322	LYS	CE-NZ	10.86	1.76	1.49
1	A	322	LYS	CD-CE	8.05	1.71	1.51
1	A	826	GLU	CD-OE2	7.64	1.34	1.25
1	A	826	GLU	CD-OE1	6.79	1.33	1.25
1	A	653	ARG	CZ-NH1	6.79	1.41	1.33
1	A	811	TYR	CG-CD1	6.03	1.47	1.39
1	A	811	TYR	CE2-CZ	5.93	1.46	1.38
1	A	811	TYR	CG-CD2	5.71	1.46	1.39
1	A	30	LEU	CG-CD2	5.60	1.72	1.51
1	A	327	TYR	CG-CD2	5.49	1.46	1.39
1	A	55	LYS	CE-NZ	-5.22	1.35	1.49
1	A	432	ARG	CZ-NH1	5.18	1.39	1.33
1	A	327	TYR	CE1-CZ	5.12	1.45	1.38
1	A	106	GLN	CD-OE1	5.11	1.35	1.24

All (8) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	TYR	C-N-CA	9.79	163.11	122.00
1	A	653	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	177	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	432	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	937	LEU	CA-CB-CG	5.51	127.96	115.30
1	A	327	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	A	972	LEU	CA-CB-CG	5.02	126.84	115.30

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 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	7717	0	7869	248	11
All	All	7717	0	7869	248	11

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 16.

All (248) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:545:TYR:HB2	1:A:1022:VAL:HG11	1.64	0.78
1:A:897:ILE:H	1:A:897:ILE:HD13	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: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:863:SER:C	1:A:864:TYR:HD2	1.93	0.71
1:A:864:TYR:HB2	1:A:867:ARG:HG2	1.72	0.70
1:A:149:MET:HB3	1:A:153:ASP:HB3	1.74	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:1023:PRO:O	1:A:1027:VAL:HG13	1.93	0.69
1:A:462:SER:HB2	1:A:867:ARG:HD3	1.73	0.69
1:A:877:TYR:HA	1:A:880:SER:HB2	1.76	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:HE	1:A:8:ARG:H	1.42	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: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:1020:PHE:HA	1:A:1025:PHE:HE1	1.63	0.64
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.79	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:392:THR:C	1:A:394:THR:H	2.02	0.63
1:A:864:TYR:CB	1:A:867:ARG:HG2	2.29	0.63
1:A:462:SER:C	1:A:464:GLY:H	2.03	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:418:ARG:HE	1:A:970:MET:HB2	1.64	0.62
1:A:448:VAL:HG13	1:A:887:CYS:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:862:MET:C	1:A:864:TYR:H	2.02	0.61
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:426:PRO:CD	1:A:427:PRO:HD3	2.33	0.57
1:A:339:GLU:HB3	1:A:1000:GLN:HE22	1.69	0.57
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.86	0.57
1:A:939:ALA:O	1:A:943:ILE:HG22	2.05	0.57
1:A:584:GLN:H	1:A:622:GLN:HE21	1.52	0.57
1:A:900:SER:HA	1:A:1027:VAL:HB	1.86	0.56
1:A:863:SER:C	1:A:864:TYR:CD2	2.78	0.56
1:A:450:SER:HB2	1:A:478:MET:HE2	1.88	0.56
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: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:475:VAL:HG13	1:A:478:MET:HE3	1.89	0.55
1:A:322:LYS:CD	1:A:322:LYS:NZ	2.68	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:H	1:A:367:ILE:HD12	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:407:ASP:HB3	1:A:978:THR:HG23	1.90	0.53
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.91	0.53
1:A:41:PRO:HA	1:A:295:THR:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:LEU:HG	1:A:234:ILE:HD11	1.90	0.53
1:A:1025:PHE:N	1:A:1027:VAL:HG22	2.24	0.52
1:A:479:ALA:O	1:A:483:LEU:HB2	2.09	0.52
1:A:379:THR:CG2	1:A:473:THR:HG23	2.37	0.52
1:A:901:VAL:O	1:A:904:VAL:HG22	2.09	0.52
1:A:390:ILE:HG22	1:A:390:ILE:O	2.07	0.52
1:A:959:GLY:HA3	1:A:963:ALA:CB	2.33	0.52
1:A:1033:PHE:C	1:A:1035:ARG:H	2.12	0.52
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.92	0.52
1:A:445:ILE:HG13	1:A:446:ALA:N	2.24	0.52
1:A:713:LEU:HD23	1:A:833:PRO:HD3	1.91	0.52
1:A:569:GLN:HG3	1:A:668:LEU:HB2	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:695:LEU:HB3	1:A:825:MET:HE3	1.91	0.52
1:A:300:LEU:HD13	1:A:333:VAL:HG11	1.92	0.52
1:A:774:MET:O	1:A:775:SER:HB3	2.09	0.51
1:A:815:ARG:CG	1:A:815:ARG:HH11	2.24	0.51
1:A:986:VAL:HG13	1:A:989:LEU:HD12	1.92	0.51
1:A:973:ARG:CB	1:A:974:PRO:HD3	2.40	0.51
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.91	0.51
1:A:527:TYR:HE1	1:A:1020:PHE:HB3	1.75	0.51
1:A:482:VAL:O	1:A:482:VAL:HG12	2.11	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:459:PHE:CE1	1:A:468:ARG:HD2	2.46	0.51
1:A:214:VAL:HG22	1:A:237:GLN:HB2	1.93	0.51
1:A:831:ALA:O	1:A:832:ALA:HB2	2.10	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:1019:ILE:HG23	1:A:1020:PHE:CD2	2.47	0.50
1:A:248:LYS:HA	1:A:261:LEU:HD23	1.94	0.50
1:A:631:LEU:HD13	1:A:637:ARG:HH12	1.77	0.50
1:A:1023:PRO:C	1:A:1027:VAL:HG13	2.32	0.49
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:456:MET:HB3	1:A:471:SER:OG	2.13	0.49
1:A:407:ASP:O	1:A:410:ILE:HG22	2.11	0.49
1:A:178:PHE:HB2	1:A:288:GLY:H	1.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:VAL:HG11	1:A:175:VAL:HG23	1.94	0.49
1:A:730:ASP:HB3	1:A:806:SER:HB3	1.94	0.49
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:973:ARG:O	1:A:977:MET:HG2	2.14	0.48
1:A:673:GLU:HG3	1:A:674:LEU:H	1.78	0.48
1:A:659:LYS:HG3	1:A:661:ALA:H	1.78	0.48
1:A:867:ARG:CG	1:A:868:LEU:N	2.68	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:392:THR:C	1:A:394:THR:N	2.67	0.47
1:A:380:PHE:HA	1:A:383:LEU:HD12	1.97	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:900:SER:CA	1:A:1027:VAL:HB	2.44	0.47
1:A:675:GLY:HA3	1:A:867:ARG:NH2	2.29	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:366:LEU:O	1:A:370:ILE:HG12	2.14	0.47
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.97	0.47
1:A:991:ILE:C	1:A:993:THR:H	2.17	0.47
1:A:462:SER:C	1:A:464:GLY:N	2.67	0.46
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:466:ILE:HG22	1:A:925:VAL:HG11	1.96	0.46
1:A:134:SER:HA	1:A:292:LYS:HD2	1.98	0.46
1:A:643:LYS:NZ	1:A:645:GLU:HG3	2.30	0.46
1:A:680:PHE:HA	1:A:862:MET:CG	2.31	0.46
1:A:400:LEU:HD13	1:A:1003:VAL:HG22	1.96	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
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:473:THR:HA	1:A:476:SER:CB	2.37	0.45
1:A:188:MET:H	1:A:775:SER:HA	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:897:ILE:H	1:A:897:ILE:CD1	2.23	0.45
1:A:452:VAL:HG12	1:A:880:SER:HB3	1.97	0.45
1:A:445:ILE:HG22	1:A:943:ILE:HG21	1.98	0.45
1:A:937:LEU:HD11	1:A:1011:MET:SD	2.57	0.45
1:A:878:ALA:O	1:A:882:ILE:HG12	2.16	0.45
1:A:343:THR:HG23	1:A:988:PRO:HB2	1.99	0.45
1:A:915:ALA:HB1	1:A:1005:THR:HG22	1.98	0.45
1:A:862:MET:SD	1:A:863:SER:N	2.90	0.45
1:A:568:ASP:OD2	1:A:643:LYS:HB2	2.16	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:470:PHE:HA	1:A:470:PHE:HD1	1.71	0.45
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.99	0.45
1:A:372:VAL:CG1	1:A:406:VAL:HG22	2.47	0.44
1:A:344:LEU:O	1:A:348:ILE:HG12	2.17	0.44
1:A:867:ARG:CG	1:A:868:LEU:H	2.09	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:166:ILE:C	1:A:168:ARG:H	2.21	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: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:456:MET:HG2	1:A:467:TYR:HB3	2.00	0.43
1:A:375:VAL:HG13	1:A:480:LEU: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:617:PHE:O	1:A:618:ALA:CB	2.66	0.43
1:A:142:VAL:HG12	1:A:321:LEU:HD22	2.01	0.43
1:A:953:MET:O	1:A:955:LYS:N	2.51	0.43
1:A:188:MET:HB2	1:A:775:SER:HB2	1.99	0.43
1:A:915:ALA:O	1:A:919:ARG:HB2	2.19	0.43
1:A:542:LEU:HD12	1:A:1030:ARG:NH2	2.34	0.43
1:A:34:GLN:HG3	1:A:35:TYR:H	1.84	0.43
1:A:702:LEU:HB2	1:A:851:LEU:HD11	2.01	0.43
1:A:36:PRO:HD3	1:A:391:ASN:CG	2.39	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:481:SER:C	1:A:483:LEU:H	2.22	0.42
1:A:38:ILE:H	1:A:38:ILE:HG12	1.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:588:GLN:HG2	1:A:613:ASN:ND2	2.34	0.42
1:A:1025:PHE:H	1:A:1027:VAL:HG22	1.84	0.42
1:A:400:LEU:HG	1:A:933:THR:HG21	2.01	0.42
1:A:923:ASN:HA	1:A:927:PHE:HD2	1.83	0.42
1:A:864:TYR:CD2	1:A:865:GLN:HA	2.55	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: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:470:PHE:CE2	1:A:473:THR:HB	2.55	0.42
1:A:451:ALA:O	1:A:880:SER:HA	2.20	0.41
1:A:831:ALA:HB1	1:A:836:SER:HA	2.01	0.41
1:A:723:ASP:HA	1:A:813:SER:HA	2.02	0.41
1:A:472:ILE:O	1:A:476:SER:N	2.45	0.41
1:A:110:LYS:H	1:A:110:LYS:HG2	1.63	0.41
1:A:454:VAL:HA	1:A:471:SER:HB3	2.02	0.41
1:A:367:ILE:HD11	1:A:496:MET:HB3	2.02	0.41
1:A:384:ALA:O	1:A:385:ALA:O	2.38	0.41
1:A:73:ASP:N	1:A:106:GLN:HE22	2.19	0.41
1:A:552:MET:HA	1:A:555:LEU:HD12	2.02	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: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: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:198:LEU:HD11	1:A:260:VAL:HG11	2.03	0.40
1:A:454:VAL:HG23	1:A:455:PRO:HD3	2.04	0.40
1:A:907:LEU:HD21	1:A:1023:PRO:HD2	2.03	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	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	2 28

All (60) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	731 (88%)	95 (12%)	8 38

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	13	TRP
1	A	30	LEU
1	A	34	GLN
1	A	38	ILE
1	A	55	LYS
1	A	68	ASN
1	A	76	MET
1	A	84	SER
1	A	108	GLN
1	A	110	LYS
1	A	130	GLU
1	A	143	ILE
1	A	150	THR
1	A	152	GLU
1	A	161	ASN
1	A	176	GLN
1	A	177	LEU
1	A	180	SER
1	A	194	ASN
1	A	208	LYS
1	A	222	THR
1	A	226	LYS
1	A	252	LYS
1	A	293	LEU
1	A	298	ASN
1	A	307	ARG
1	A	321	LEU
1	A	327	TYR
1	A	359	LEU
1	A	360	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	366	LEU
1	A	376	LEU
1	A	393	LEU
1	A	405	LEU
1	A	407	ASP
1	A	415	ASN
1	A	418	ARG
1	A	432	ARG
1	A	438	ILE
1	A	442	LEU
1	A	456	MET
1	A	478	MET
1	A	480	LEU
1	A	483	LEU
1	A	488	LEU
1	A	489	THR
1	A	492	LEU
1	A	498	LYS
1	A	516	PHE
1	A	534	ILE
1	A	550	VAL
1	A	563	PHE
1	A	601	LYS
1	A	632	LYS
1	A	637	ARG
1	A	640	GLU
1	A	643	LYS
1	A	650	ARG
1	A	672	VAL
1	A	674	LEU
1	A	695	LEU
1	A	697	GLN
1	A	705	GLU
1	A	709	HIS
1	A	758	TYR
1	A	760	ASN
1	A	792	ARG
1	A	797	GLN
1	A	798	MET
1	A	815	ARG
1	A	846	GLN
1	A	862	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	864	TYR
1	A	886	LEU
1	A	888	LEU
1	A	897	ILE
1	A	902	MET
1	A	907	LEU
1	A	913	LEU
1	A	918	PHE
1	A	919	ARG
1	A	932	LEU
1	A	935	ILE
1	A	937	LEU
1	A	950	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	1003	VAL
1	A	1008	MET
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	106	GLN
1	A	108	GLN
1	A	124	GLN
1	A	125	GLN
1	A	176	GLN
1	A	194	ASN
1	A	197	GLN
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	700	ASN
1	A	760	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	0.20	15 (1%)	70 31	17, 76, 136, 175	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	LEU	4.0
1	A	833	PRO	3.8
1	A	1021	PHE	3.4
1	A	496	MET	3.2
1	A	425	LEU	2.9
1	A	31	PRO	2.7
1	A	30	LEU	2.5
1	A	295	THR	2.5
1	A	363	ARG	2.4
1	A	1030	ARG	2.3
1	A	303	ALA	2.2
1	A	673	GLU	2.1
1	A	829	GLY	2.1
1	A	674	LEU	2.1
1	A	676	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.