



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 08:10 PM EDT

PDB ID : 2HQG
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 : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

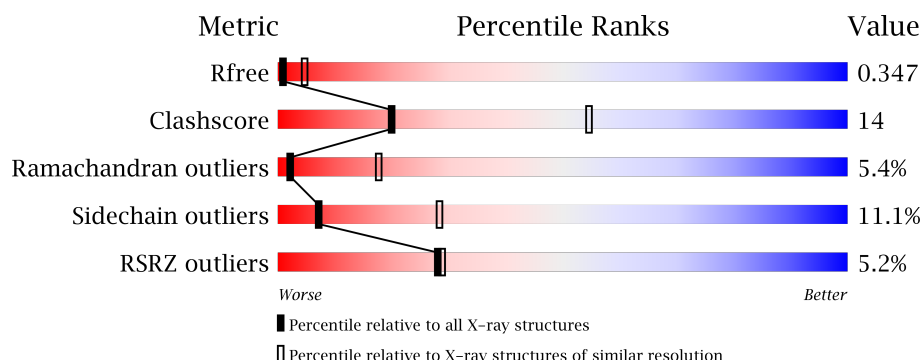
1 Overall quality at a glance

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}	100719	1241 (3.46-3.30)
Clashscore	112137	1319 (3.46-3.30)
Ramachandran outliers	110173	1298 (3.46-3.30)
Sidechain outliers	110143	1297 (3.46-3.30)
RSRZ outliers	101464	1251 (3.46-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7719 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
			7719	4964	1276	1436	43			

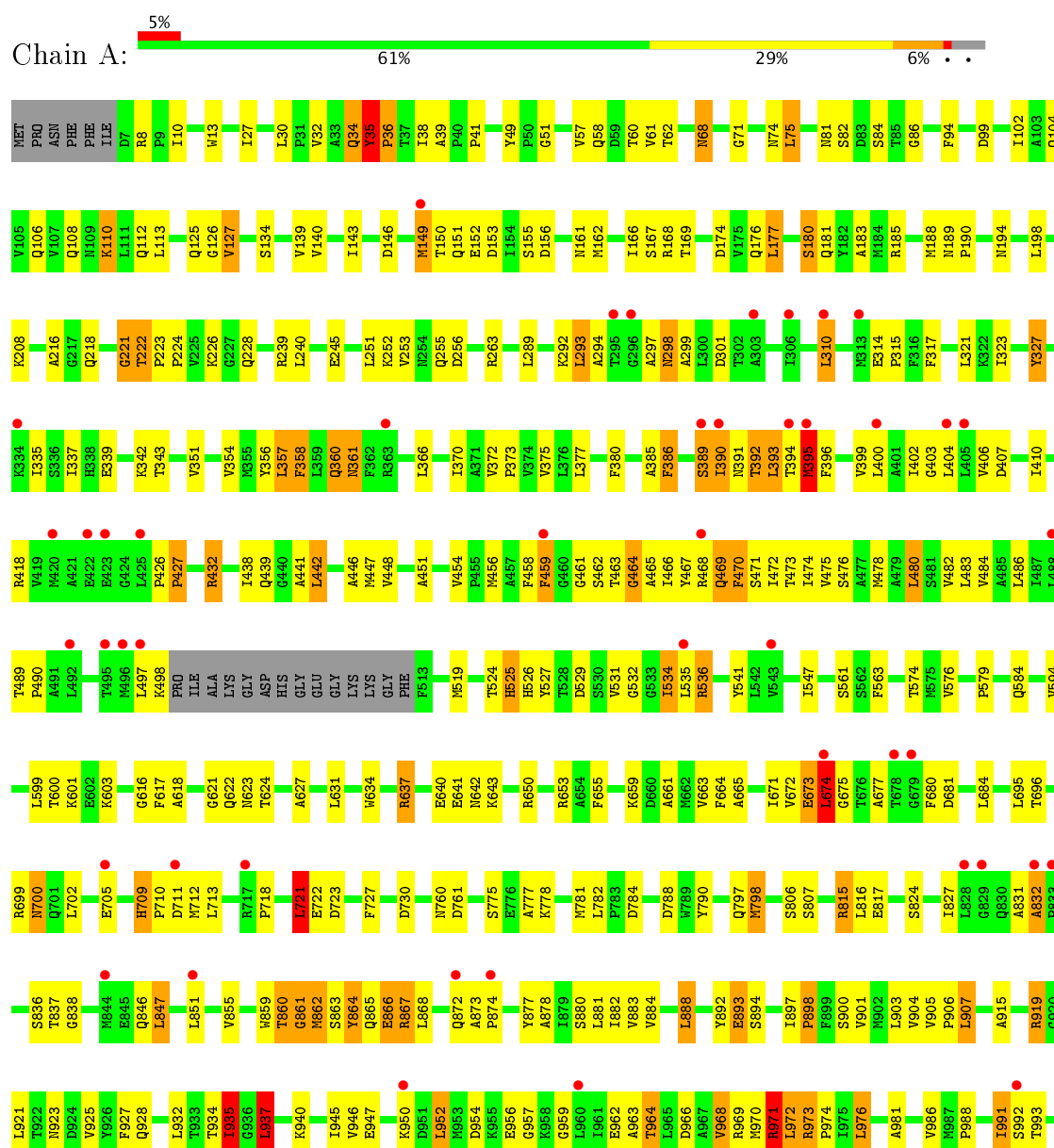
There are 5 discrepancies between the modelled and reference sequences:

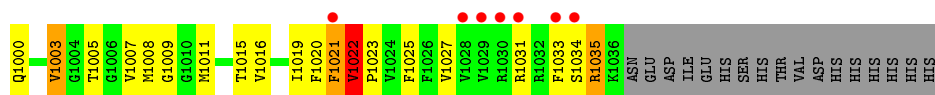
Chain	Residue	Modelled	Actual	Comment	Reference
A	978	ALA	THR	ENGINEERED	UNP P31224
A	1050	HIS	-	CLONING ARTIFACT	UNP P31224
A	1051	HIS	-	CLONING ARTIFACT	UNP P31224
A	1052	HIS	-	CLONING ARTIFACT	UNP P31224
A	1053	HIS	-	CLONING ARTIFACT	UNP P31224

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 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: 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	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
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.254 , 0.275 0.337 , 0.347	Depositor DCC
R_{free} test set	1457 reflections (5.06%)	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 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

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

Continued on next page...

Continued from previous page...

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 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	7719	0	7875	222	10
All	All	7719	0	7875	222	10

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 14.

All (222) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:HB1	1:A:468:ARG:HB3	1.65	0.78
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:637:ARG:HB2	1:A:642:ASN:HB3	1.67	0.75
1:A:861:GLY:HA3	1:A:862:MET:CB	2.16	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:156:ASP:HA	1:A:181:GLN:HA	1.79	0.63
1:A:357:LEU:O	1:A:358:PHE:HB2	1.97	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:1025:PHE:H	1:A:1027:VAL:HG22	1.64	0.62
1:A:861:GLY:H	1:A:862:MET:CE	2.12	0.62
1:A:684:LEU:CD1	1:A:855:VAL:HG13	2.29	0.62
1:A:584:GLN:H	1:A:622:GLN:HE21	1.46	0.61
1:A:681:ASP:N	1:A:862:MET:SD	2.66	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:475:VAL:HA	1:A:478:MET:HB3	1.82	0.61
1:A:915:ALA:O	1:A:919:ARG:HB2	2.00	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:TRP:HB3	1:A:863:SER:HB2	1.82	0.60
1:A:675:GLY:HA3	1:A:867:ARG:NH2	2.17	0.59
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:298:ASN:HB2	1:A:301:ASP:HB2	1.85	0.58
1:A:705:GLU:HG3	1:A:847:LEU:HD13	1.84	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:372:VAL:HG23	1:A:373:PRO:HD3	1.87	0.56
1:A:81:ASN:O	1:A:816:LEU:O	2.23	0.56
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:351:VAL:HG22	1:A:981:ALA:HB1	1.86	0.56
1:A:166:ILE:HG22	1:A:167:SER:N	2.17	0.56
1:A:680:PHE:HA	1:A:862:MET:CG	2.29	0.56
1:A:1023:PRO:O	1:A:1027:VAL:HG13	2.05	0.56
1:A:34:GLN:HG3	1:A:35:TYR:H	1.71	0.56
1:A:74:ASN:O	1:A:75:LEU:HB3	2.06	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:106:GLN:O	1:A:110:LYS:HG2	2.07	0.55
1:A:392:THR:HG22	1:A:393:LEU:H	1.71	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:532:GLY:O	1:A:536:ARG:HB2	2.08	0.54
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.90	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:377:LEU:HA	1:A:380:PHE:CD1	2.44	0.53
1:A:465:ALA:O	1:A:469:GLN:N	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:293:LEU:HD13	1:A:294:ALA:O	2.10	0.52
1:A:721:LEU:O	1:A:723:ASP:N	2.43	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:360:GLN:O	1:A:361:ASN:HB2	2.11	0.51
1:A:634:TRP:HA	1:A:637:ARG:HE	1.75	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:222:THR:O	1:A:224:PRO:HD3	2.13	0.48
1:A:459:PHE:HE1	1:A:468:ARG:HD2	1.78	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:57:VAL:HG11	1:A:86:GLY:HA2	1.95	0.48
1:A:873:ALA:N	1:A:874:PRO:HD2	2.29	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:239:ARG:NE	1:A:761:ASP:O	2.48	0.47
1:A:392:THR:C	1:A:394:THR:N	2.67	0.47
1:A:489:THR:HB	1:A:490:PRO:HD3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:HG21	1:A:594:VAL:HG11	1.95	0.47
1:A:892:TYR:CD2	1:A:897:ILE:HG21	2.49	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
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:817:GLU:HB2	1:A:824:SER:O	2.15	0.47
1:A:877:TYR:O	1:A:881:LEU:HB2	2.14	0.47
1:A:972:LEU:O	1:A:976:LEU:HB2	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:377:LEU:HA	1:A:380:PHE:HD1	1.80	0.45
1:A:393:LEU:HD21	1:A:469:GLN:HG3	1.97	0.45
1:A:860:THR:H	1:A:862:MET:HE1	1.82	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:155:SER:HB3	1:A:180:SER:H	1.81	0.45
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.99	0.45
1:A:859:TRP:HB3	1:A:863:SER:CB	2.46	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:198:LEU:HD13	1:A:251:LEU:HD13	2.00	0.44
1:A:907:LEU:HD21	1:A:1023:PRO:HD2	2.00	0.44
1:A:900:SER:HB3	1:A:1027:VAL:HB	2.00	0.43
1:A:463:THR:HG22	1:A:867:ARG:HB2	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:897:ILE:HG23	1:A:946:VAL:HG11	2.00	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:705:GLU:HG3	1:A:847:LEU:CD1	2.48	0.43
1:A:711:ASP:O	1:A:712:MET:HB2	2.19	0.42
1:A:991:ILE:O	1:A:993:THR:N	2.43	0.42
1:A:905:VAL:HG12	1:A:935:ILE:HG13	2.01	0.42
1:A:1023:PRO:HA	1:A:1031:ARG:NH1	2.35	0.42
1:A:905:VAL:CG2	1:A:906:PRO:HD3	2.49	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:339:GLU:HB3	1:A:1000:GLN:HE22	1.83	0.42
1:A:1016:VAL:O	1:A:1019:ILE:HG22	2.19	0.42
1:A:631:LEU:HD13	1:A:637:ARG:HH12	1.85	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:150:THR:HG22	1:A:151:GLN:N	2.35	0.41
1:A:903:LEU:HD13	1:A:1031:ARG:HE	1.85	0.41
1:A:576:VAL:HG13	1:A:663:VAL:HG22	2.02	0.41
1:A:945:ILE:HG22	1:A:971:ARG:HD2	2.02	0.41
1:A:354:VAL:O	1:A:354:VAL:HG12	2.21	0.41
1:A:1008:MET:HG3	1:A:1009:GLY:N	2.36	0.41
1:A:317:PHE:HE2	1:A:323:ILE:HD11	1.85	0.41
1:A:897:ILE:N	1:A:898:PRO:HD2	2.36	0.41
1:A:403:GLY:O	1:A:406:VAL:N	2.53	0.41
1:A:335:ILE:C	1:A:337:ILE:H	2.24	0.41
1:A:699:ARG:HG2	1:A:827:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLN:HG3	1:A:221:GLY:HA2	2.04	0.40
1:A:372:VAL:CG2	1:A:373:PRO:HD3	2.50	0.40
1:A:375:VAL:HA	1:A:480:LEU:HD12	2.02	0.40
1:A:777:ALA:O	1:A:781:MET:HG2	2.22	0.40
1:A:878:ALA:O	1:A:882:ILE:HG12	2.22	0.40
1:A:964:THR:O	1:A:968:VAL:HG12	2.21	0.40
1:A:897:ILE:H	1:A:897:ILE:HD12	1.86	0.40
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.95	0.40
1:A:476:SER:O	1:A:480:LEU:HB2	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:O	1:A:778:LYS:NZ[6_555]	1.74	0.46
1:A:113:LEU:CD2	1:A:127:VAL:O[3_655]	1.79	0.41
1:A:10:ILE:CG2	1:A:893:GLU:OE1[2_545]	1.79	0.41
1:A:228:GLN:OE1	1:A:781:MET:CE[2_545]	1.88	0.32
1:A:112:GLN:NE2	1:A:112:GLN:NE2[2_545]	1.88	0.32
1:A:51:GLY:O	1:A:216:ALA:O[3_655]	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%)	2 18

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	893	GLU
1	A	898	PRO
1	A	222	THR
1	A	297	ALA
1	A	427	PRO
1	A	832	ALA
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%)	7 28

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 [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 carbohydrates 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 ⓘ

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%)	0.33	53 (5%)	28 29	31, 91, 152, 190	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	LEU	6.7
1	A	1021	PHE	5.8
1	A	425	LEU	5.4
1	A	496	MET	5.2
1	A	303	ALA	4.5
1	A	1030	ARG	4.4
1	A	295	THR	4.3
1	A	400	LEU	4.2
1	A	1031	ARG	3.9
1	A	992	SER	3.9
1	A	543	VAL	3.8
1	A	310	LEU	3.5
1	A	872	GLN	3.5
1	A	1028	VAL	3.2
1	A	363	ARG	3.2
1	A	404	LEU	3.1
1	A	296	GLY	3.1
1	A	833	PRO	2.9
1	A	495	THR	2.9
1	A	711	ASP	2.9
1	A	950	LYS	2.9
1	A	334	LYS	2.8
1	A	497	LEU	2.8
1	A	1034	SER	2.7
1	A	306	ILE	2.7
1	A	717	ARG	2.7
1	A	420	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	468	ARG	2.5
1	A	678	THR	2.5
1	A	829	GLY	2.4
1	A	422	GLU	2.4
1	A	705	GLU	2.4
1	A	535	LEU	2.4
1	A	874	PRO	2.4
1	A	394	THR	2.4
1	A	492	LEU	2.3
1	A	844	MET	2.3
1	A	459	PHE	2.3
1	A	488	LEU	2.3
1	A	390	ILE	2.2
1	A	851	LEU	2.2
1	A	1033	PHE	2.2
1	A	405	LEU	2.2
1	A	1029	VAL	2.2
1	A	674	LEU	2.1
1	A	828	LEU	2.1
1	A	423	GLU	2.1
1	A	313	MET	2.1
1	A	679	GLY	2.1
1	A	389	SER	2.1
1	A	149	MET	2.1
1	A	395	MET	2.0
1	A	832	ALA	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.