Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2025 – 04:23 pm BST

PDB ID	:	9FE3 / pdb_00009fe3
Title	:	Crystallographic structure of AcrB V612W
Authors	:	Lazarova, M.; Pos, K.M.
Deposited on	:	2024-05-17
Resolution	:	2.30 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:

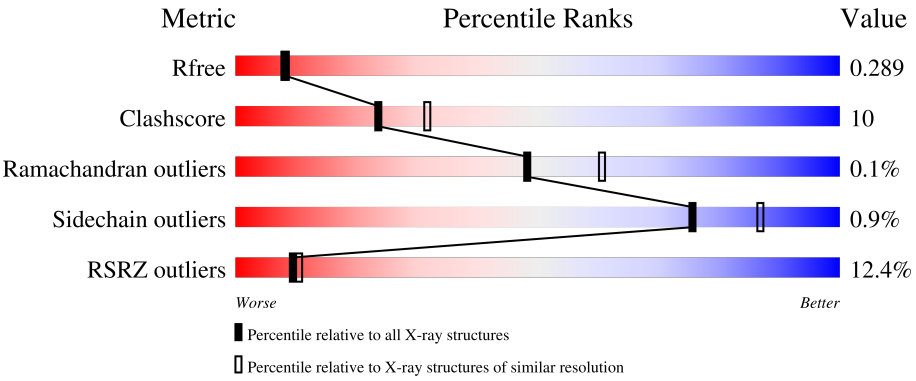
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 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 <=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	D	169	24% 58% 31% 11%
2	A	1057	10% 78% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9079 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 DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	150	Total	C	N	O	S	0	0	0
			1133	714	199	219	1			

- Molecule 2 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1043	Total	C	N	O	S	0	0	0
			7940	5106	1313	1477	44			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	TRP	VAL	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224

- Molecule 3 is water.

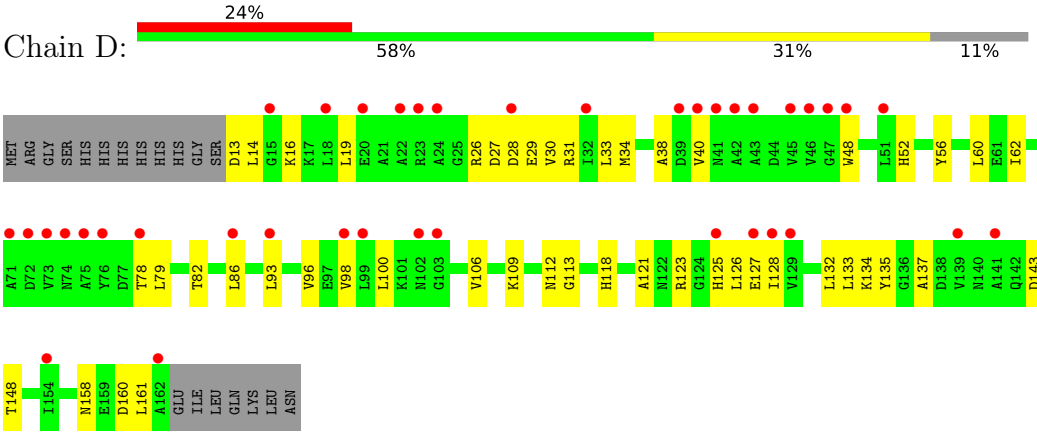
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

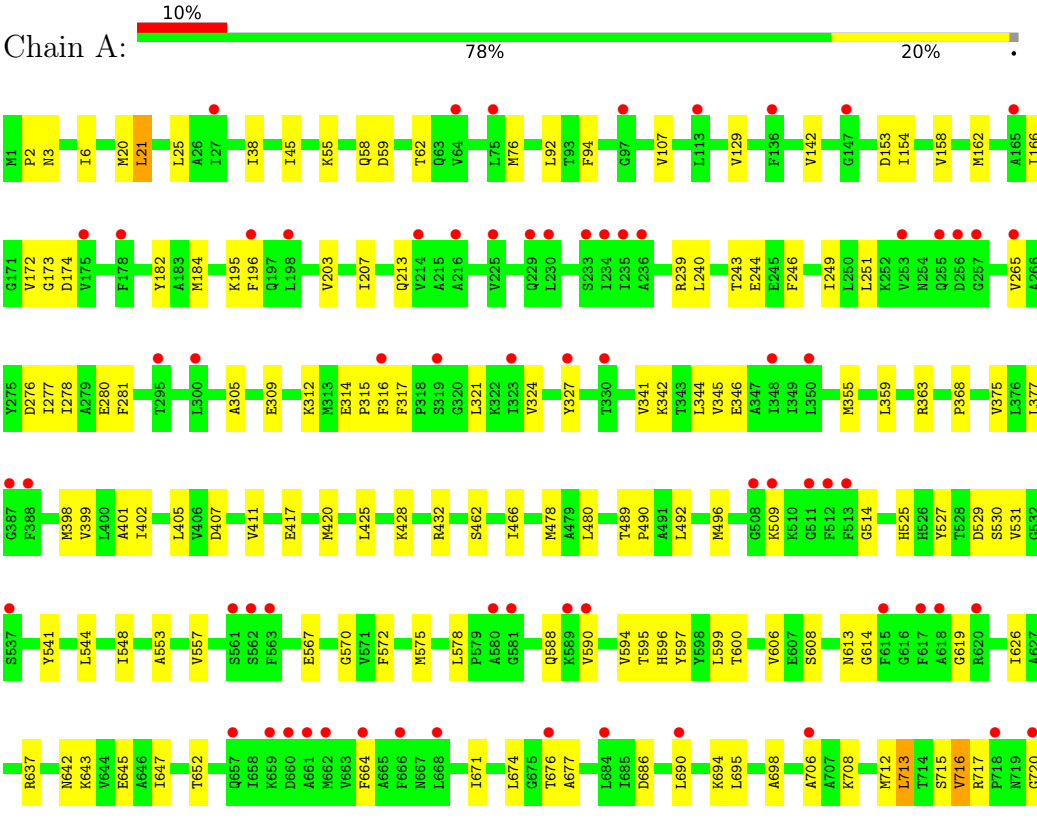
• Molecule 1: DARPIN

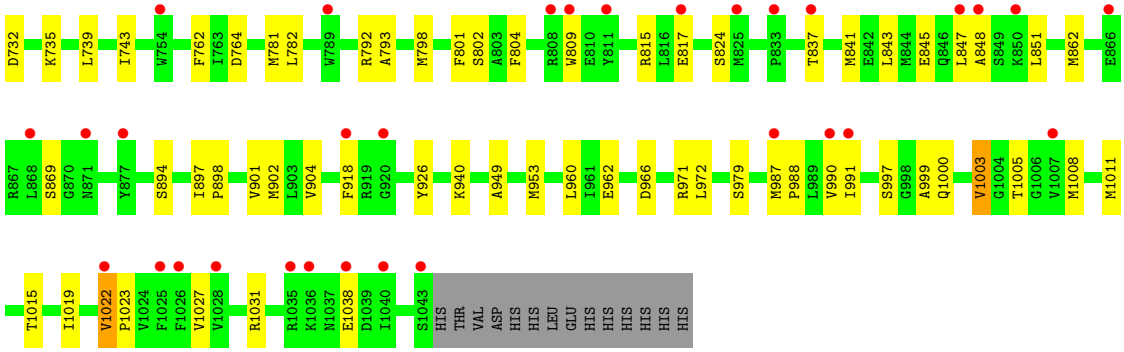
Chain D:



• Molecule 2: Multidrug efflux pump subunit AcrB

Chain A:




D732 K735 L739 I743 W754 F762 I763 D764 M781 L782 W789 R792 A793 M798 F801 S802 A803 F804 R808 W809 E810 Y811 R815 L816 E817 S824 M825 P833 T837 M841 E842 L843 M844 E845 Q846 L847 A848 S849 K850 L851 M862 E866
R867 L868 S869 G870 N871 Y877 S894 I897 P898 V901 M902 L903 V904 F918 R919 G920 Y926 K940 A949 M953 L960 I961 E962 D966 R971 L972 S979 M987 P988 L989 Y990 I991 S997 G998 A999 Q1000 V1003 G1004 T1005 G1006 V1007 M1008 M1011
T1015 I1019 V1022 P1023 V1024 F1025 F1026 V1027 V1028 R1031 R1035 K1036 N1037 E1038 D1039 I1040 S1043 HIS THR VAL ASP HIS HIS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	227.43Å 227.43Å 227.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.30 46.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.42-2.30) 97.7 (46.42-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.253 , 0.290 0.255 , 0.289	Depositor DCC
R_{free} test set	84313 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9079	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	D	0.13	0/1152	0.34	0/1567
2	A	0.15	0/8093	0.36	0/10989
All	All	0.15	0/9245	0.36	0/12556

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1133	0	1115	38	0
2	A	7940	0	8078	149	0
3	A	6	0	0	0	0
All	All	9079	0	9193	182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (182) 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)
2:A:987:MET:HE2	2:A:987:MET:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:158:VAL:HG13	2:A:162:MET:HE2	1.69	0.72
2:A:676:THR:HB	2:A:862:MET:HE3	1.72	0.71
2:A:990:VAL:HG23	2:A:1005:THR:HG22	1.72	0.71
2:A:184:MET:HE1	2:A:243:THR:HG22	1.73	0.71
1:D:100:LEU:HD11	1:D:132:LEU:HD23	1.73	0.70
2:A:715:SER:O	2:A:717:ARG:NH1	2.24	0.70
2:A:274:ASN:ND2	2:A:276:ASP:OD2	2.22	0.69
2:A:572:PHE:HE1	2:A:631:LEU:HD21	1.59	0.66
2:A:344:LEU:HD23	2:A:402:ILE:HD11	1.76	0.66
1:D:126:LEU:HD21	1:D:160:ASP:HB3	1.77	0.66
2:A:280:GLU:OE1	2:A:588:GLN:NE2	2.29	0.66
2:A:637:ARG:HB3	2:A:642:ASN:HB3	1.78	0.65
1:D:106:VAL:HG11	1:D:135:TYR:O	1.97	0.64
2:A:20:MET:HG2	2:A:377:LEU:HD12	1.79	0.64
1:D:112:ASN:HA	1:D:144:LYS:HD2	1.81	0.62
2:A:314:GLU:CG	2:A:315:PRO:HD3	2.28	0.62
2:A:55:LYS:HE2	2:A:59:ASP:OD2	1.99	0.62
2:A:637:ARG:O	2:A:643:LYS:NZ	2.33	0.61
2:A:3:ASN:ND2	2:A:432:ARG:HG2	2.16	0.60
1:D:48:TRP:HA	1:D:52:HIS:HD2	1.65	0.60
2:A:837:THR:O	2:A:841:MET:HG3	2.01	0.60
1:D:158:ASN:OD1	1:D:161:LEU:HB2	2.02	0.60
1:D:27:ASP:N	1:D:27:ASP:OD1	2.34	0.60
1:D:60:LEU:HD11	1:D:98:VAL:HG21	1.83	0.59
1:D:78:THR:HG23	2:A:809:TRP:HE1	1.67	0.59
1:D:29:GLU:OE1	1:D:29:GLU:N	2.21	0.59
2:A:317:PHE:CD2	2:A:321:LEU:HD12	2.38	0.59
2:A:652:THR:CG2	2:A:664:PHE:HD1	2.16	0.59
2:A:732:ASP:OD2	2:A:735:LYS:HG2	2.03	0.58
2:A:3:ASN:HD21	2:A:432:ARG:HG2	1.68	0.58
2:A:195:LYS:HG2	2:A:196:PHE:CD1	2.39	0.58
2:A:960:LEU:HD12	2:A:1038:GLU:OE2	2.04	0.57
2:A:38:ILE:HD12	2:A:466:ILE:HG13	1.87	0.56
2:A:690:LEU:HD12	2:A:694:LYS:HD3	1.86	0.56
2:A:267:LYS:HD2	2:A:268:ILE:H	1.69	0.56
1:D:123:ARG:HD3	1:D:125:HIS:CE1	2.40	0.56
2:A:530:SER:O	2:A:533:GLY:N	2.39	0.56
2:A:203:VAL:O	2:A:207:ILE:HG13	2.06	0.56
1:D:26:ARG:HB3	1:D:29:GLU:CD	2.32	0.55
1:D:48:TRP:HA	1:D:52:HIS:CD2	2.41	0.55
2:A:359:LEU:HD13	2:A:417:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:314:GLU:HG2	2:A:315:PRO:HD3	1.88	0.54
2:A:184:MET:HE3	2:A:184:MET:HA	1.89	0.54
2:A:277:ILE:HD13	2:A:614:GLY:HA3	1.90	0.54
2:A:572:PHE:CE1	2:A:631:LEU:HD21	2.41	0.54
2:A:530:SER:O	2:A:534:ILE:HD12	2.08	0.54
2:A:244:GLU:OE1	2:A:244:GLU:N	2.38	0.54
1:D:56:TYR:HB2	1:D:86:LEU:HD13	1.90	0.54
2:A:901:VAL:O	2:A:904:VAL:HG12	2.09	0.53
2:A:792:ARG:HB2	2:A:798:MET:HE1	1.90	0.53
1:D:96:VAL:HG21	1:D:128:ILE:HD13	1.91	0.53
2:A:527:TYR:OH	2:A:1019:ILE:O	2.21	0.52
2:A:698:ALA:HB1	2:A:851:LEU:HD13	1.92	0.52
2:A:166:ILE:O	2:A:172:VAL:HG11	2.10	0.52
2:A:153:ASP:OD1	2:A:182:TYR:OH	2.28	0.52
2:A:278:ILE:HB	2:A:613:ASN:HB3	1.91	0.52
1:D:79:LEU:HD21	2:A:727:PHE:HE1	1.75	0.52
2:A:92:LEU:HD22	2:A:107:VAL:HG22	1.92	0.51
2:A:407:ASP:OD2	2:A:940:LYS:NZ	2.35	0.51
2:A:346:GLU:OE2	2:A:988:PRO:HG2	2.11	0.51
1:D:34:MET:HE2	1:D:40:VAL:HG12	1.92	0.51
1:D:121:ALA:HA	1:D:161:LEU:HD21	1.92	0.51
2:A:317:PHE:CE2	2:A:321:LEU:HD12	2.46	0.51
1:D:100:LEU:HB3	1:D:135:TYR:CD2	2.46	0.51
1:D:123:ARG:HD3	1:D:125:HIS:NE2	2.26	0.50
2:A:652:THR:CG2	2:A:664:PHE:CD1	2.94	0.50
2:A:712:MET:HG2	2:A:843:LEU:HD22	1.92	0.50
1:D:52:HIS:HE1	1:D:82:THR:HA	1.76	0.50
2:A:990:VAL:HG13	2:A:991:ILE:HG23	1.94	0.50
2:A:652:THR:HG21	2:A:664:PHE:HD1	1.75	0.50
2:A:314:GLU:HG3	2:A:315:PRO:HD3	1.93	0.49
2:A:411:VAL:HG22	2:A:971:ARG:HH12	1.77	0.49
2:A:544:LEU:O	2:A:548:ILE:HG13	2.12	0.49
2:A:652:THR:HG23	2:A:664:PHE:CD1	2.47	0.49
2:A:530:SER:C	2:A:534:ILE:HD12	2.38	0.49
1:D:14:LEU:HD22	1:D:33:LEU:HD11	1.94	0.49
2:A:249:ILE:HG22	2:A:251:LEU:HD23	1.94	0.49
2:A:355:MET:HE2	2:A:368:PRO:HG3	1.95	0.49
1:D:109:LYS:HB2	1:D:113:GLY:HA2	1.95	0.49
2:A:534:ILE:HG23	2:A:541:TYR:CE1	2.47	0.48
1:D:118:HIS:HE2	1:D:148:THR:HA	1.77	0.48
2:A:987:MET:O	2:A:990:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:987:MET:HE1	2:A:1008:MET:SD	2.53	0.48
1:D:30:VAL:HG21	1:D:62:ILE:HD13	1.96	0.48
2:A:960:LEU:CD2	2:A:1027:VAL:HG22	2.44	0.48
2:A:606:VAL:HG13	2:A:629:VAL:HG13	1.95	0.48
2:A:997:SER:HA	2:A:1000:GLN:HB2	1.94	0.48
1:D:16:LYS:HA	1:D:19:LEU:HD12	1.95	0.48
2:A:1011:MET:O	2:A:1015:THR:HG23	2.14	0.47
2:A:848:ALA:HA	2:A:851:LEU:HG	1.96	0.47
2:A:420:MET:HG2	2:A:425:LEU:O	2.15	0.47
2:A:535:LEU:HD22	2:A:1027:VAL:HG21	1.96	0.47
2:A:240:LEU:HB2	2:A:246:PHE:CE1	2.49	0.47
2:A:492:LEU:O	2:A:496:MET:HG3	2.15	0.47
2:A:596:HIS:O	2:A:600:THR:HG23	2.15	0.47
2:A:843:LEU:O	2:A:847:LEU:HG	2.15	0.46
2:A:962:GLU:O	2:A:966:ASP:HB2	2.15	0.46
2:A:643:LYS:HD3	2:A:643:LYS:HA	1.61	0.46
2:A:631:LEU:HD11	2:A:647:ILE:HD13	1.97	0.46
2:A:363:ARG:N	2:A:363:ARG:HD3	2.31	0.46
2:A:595:THR:O	2:A:599:LEU:HD12	2.15	0.46
2:A:706:ALA:HB3	2:A:716:VAL:HG21	1.98	0.46
2:A:21:LEU:O	2:A:25:LEU:HB2	2.16	0.46
2:A:801:PHE:HA	2:A:804:PHE:CZ	2.51	0.46
2:A:169:THR:O	2:A:172:VAL:HG12	2.16	0.46
2:A:898:PRO:O	2:A:902:MET:HG3	2.16	0.46
2:A:478:MET:HE3	2:A:478:MET:HB3	1.84	0.46
2:A:676:THR:OG1	2:A:677:ALA:N	2.27	0.46
2:A:401:ALA:O	2:A:405:LEU:HG	2.16	0.45
2:A:570:GLY:O	2:A:631:LEU:HB2	2.16	0.45
2:A:2:PRO:O	2:A:6:ILE:HD12	2.16	0.45
2:A:926:TYR:HB3	2:A:1003:VAL:HG12	1.98	0.45
2:A:1022:VAL:N	2:A:1023:PRO:HD2	2.32	0.45
2:A:173:GLY:O	2:A:174:ASP:HB2	2.16	0.45
2:A:841:MET:O	2:A:845:GLU:HG3	2.17	0.45
2:A:281:PHE:CZ	2:A:324:VAL:HG21	2.52	0.45
2:A:792:ARG:HG2	2:A:793:ALA:O	2.17	0.45
2:A:960:LEU:HD21	2:A:1027:VAL:HA	1.97	0.45
1:D:79:LEU:HD13	2:A:809:TRP:NE1	2.32	0.45
2:A:597:TYR:C	2:A:597:TYR:CD1	2.95	0.45
2:A:1023:PRO:O	2:A:1027:VAL:HG23	2.16	0.45
2:A:918:PHE:C	2:A:918:PHE:CD1	2.95	0.44
2:A:195:LYS:HE2	2:A:196:PHE:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:375:VAL:HG13	2:A:480:LEU:HB3	1.99	0.44
2:A:553:ALA:O	2:A:557:VAL:HG12	2.17	0.44
2:A:619:GLY:HA3	2:A:815:ARG:HD2	1.99	0.44
1:D:33:LEU:HA	1:D:33:LEU:HD12	1.73	0.44
2:A:489:THR:OG1	2:A:490:PRO:HD3	2.17	0.44
2:A:735:LYS:O	2:A:739:LEU:HD12	2.18	0.44
2:A:305:ALA:O	2:A:309:GLU:HG2	2.16	0.44
2:A:380:PHE:CE2	2:A:398:MET:HE1	2.53	0.44
2:A:979:SER:CB	2:A:1015:THR:HG21	2.48	0.44
2:A:590:VAL:O	2:A:594:VAL:HG23	2.18	0.44
2:A:637:ARG:HA	2:A:642:ASN:HD22	1.83	0.44
2:A:762:PHE:CE2	2:A:764:ASP:HB2	2.52	0.44
2:A:527:TYR:CD2	2:A:972:LEU:HD22	2.53	0.43
1:D:13:ASP:N	1:D:13:ASP:OD1	2.50	0.43
2:A:154:ILE:O	2:A:158:VAL:HG23	2.17	0.43
2:A:327:TYR:HB2	2:A:628:PHE:HE2	1.82	0.43
2:A:781:MET:C	2:A:782:LEU:HD23	2.43	0.43
2:A:686:ASP:HB2	2:A:695:LEU:HD13	1.99	0.43
2:A:316:PHE:CD1	2:A:316:PHE:N	2.87	0.43
1:D:28:ASP:HA	1:D:31:ARG:HD3	2.00	0.43
2:A:708:LYS:HA	2:A:708:LYS:HD2	1.58	0.43
2:A:428:LYS:HE3	2:A:432:ARG:NH2	2.34	0.43
2:A:999:ALA:O	2:A:1003:VAL:HG13	2.18	0.43
1:D:144:LYS:NZ	2:A:802:SER:O	2.50	0.43
2:A:720:GLY:HA3	2:A:817:GLU:OE2	2.19	0.43
2:A:979:SER:HB3	2:A:1015:THR:HG21	2.01	0.43
2:A:341:VAL:HA	2:A:344:LEU:HD12	1.99	0.42
2:A:509:LYS:O	2:A:514:GLY:HA3	2.19	0.42
1:D:134:LYS:O	1:D:134:LYS:HD2	2.20	0.42
2:A:342:LYS:HA	2:A:345:VAL:HG12	2.01	0.42
2:A:58:GLN:HA	2:A:62:THR:OG1	2.20	0.42
2:A:76:MET:HE2	2:A:94:PHE:O	2.19	0.42
2:A:213:GLN:HB2	2:A:239:ARG:HD2	2.02	0.42
2:A:652:THR:HG23	2:A:664:PHE:HD1	1.82	0.42
1:D:33:LEU:HG	1:D:38:ALA:HB2	2.02	0.42
2:A:142:VAL:HG21	2:A:162:MET:HE1	2.02	0.42
1:D:143:ASP:OD1	1:D:147:LYS:N	2.53	0.41
1:D:145:PHE:CD1	2:A:735:LYS:HG3	2.54	0.41
2:A:575:MET:HA	2:A:626:ILE:HG22	2.02	0.41
2:A:527:TYR:O	2:A:531:VAL:HG23	2.21	0.41
2:A:713:LEU:CD2	2:A:843:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD23	1:D:137:ALA:HB3	2.02	0.41
2:A:645:GLU:H	2:A:645:GLU:HG2	1.68	0.41
2:A:1027:VAL:O	2:A:1031:ARG:HG3	2.20	0.41
2:A:316:PHE:N	2:A:316:PHE:HD1	2.19	0.41
2:A:567:GLU:OE2	2:A:999:ALA:N	2.53	0.41
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.88	0.41
2:A:281:PHE:CE1	2:A:608:SER:HB2	2.56	0.41
2:A:45:ILE:HG12	2:A:129:VAL:HG22	2.03	0.41
2:A:312:LYS:HG2	2:A:312:LYS:O	2.21	0.41
2:A:894:SER:OG	2:A:897:ILE:HG13	2.21	0.41
2:A:525:HIS:HD2	2:A:529:ASP:OD2	2.04	0.40
2:A:534:ILE:HG23	2:A:541:TYR:CD1	2.57	0.40
2:A:671:ILE:HG22	2:A:674:LEU:HB2	2.02	0.40
2:A:949:ALA:O	2:A:953:MET:HG3	2.21	0.40
1:D:93:LEU:HD12	1:D:127:GLU:HB3	2.03	0.40
2:A:817:GLU:HB2	2:A:824:SER:O	2.21	0.40
2:A:869:SER:O	2:A:869:SER:OG	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	D	148/169 (88%)	141 (95%)	7 (5%)	0	100	100
2	A	1041/1057 (98%)	998 (96%)	42 (4%)	1 (0%)	48	60
All	All	1189/1226 (97%)	1139 (96%)	49 (4%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	265	VAL

5.3.2 Protein sidechains (i)

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	D	115/132 (87%)	115 (100%)	0	100 100
2	A	849/863 (98%)	840 (99%)	9 (1%)	70 83
All	All	964/995 (97%)	955 (99%)	9 (1%)	75 87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	21	LEU
2	A	399	VAL
2	A	462	SER
2	A	578	LEU
2	A	713	LEU
2	A	716	VAL
2	A	743	ILE
2	A	1003	VAL
2	A	1022	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	52	HIS
1	D	92	HIS
2	A	3	ASN
2	A	58	GLN
2	A	68	ASN
2	A	161	ASN
2	A	237	GLN
2	A	525	HIS
2	A	642	ASN
2	A	657	GLN
2	A	846	GLN
2	A	1001	ASN
2	A	1037	ASN

5.3.3 RNA

There are no RNA molecules 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 oligosaccharides 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, 95^{th} 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	D	150/169 (88%)	1.59	41 (27%) 2 2	104, 135, 166, 178	0
2	A	1043/1057 (98%)	0.88	107 (10%) 13 15	59, 89, 122, 166	0
All	All	1193/1226 (97%)	0.97	148 (12%) 9 10	59, 92, 141, 178	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	617	PHE	5.6
2	A	615	PHE	5.5
1	D	74	ASN	5.2
2	A	113	LEU	4.8
2	A	664	PHE	4.7
2	A	170	SER	4.7
1	D	47	GLY	4.7
2	A	581	GLY	4.7
2	A	508	GLY	4.7
1	D	45	VAL	4.6
2	A	236	ALA	4.5
1	D	72	ASP	4.5
2	A	991	ILE	4.4
1	D	23	ARG	4.3
2	A	64	VAL	4.3
2	A	825	MET	4.2
1	D	43	ALA	4.1
1	D	162	ALA	4.1
1	D	75	ALA	4.0
2	A	561	SER	3.8
1	D	65	VAL	3.8
2	A	230	LEU	3.7
1	D	76	TYR	3.7
2	A	562	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	877	TYR	3.6
2	A	136	PHE	3.6
2	A	837	THR	3.6
2	A	214	VAL	3.5
1	D	128	ILE	3.5
2	A	253	VAL	3.4
2	A	229	GLN	3.4
2	A	628	PHE	3.4
2	A	255	GLN	3.4
2	A	1038	GLU	3.3
2	A	920	GLY	3.3
2	A	169	THR	3.3
1	D	18	LEU	3.3
2	A	809	TRP	3.2
1	D	22	ALA	3.2
1	D	154	ILE	3.2
1	D	42	ALA	3.1
1	D	40	VAL	3.1
2	A	660	ASP	3.1
2	A	27	ILE	3.0
2	A	511	GLY	3.0
2	A	175	VAL	3.0
2	A	848	ALA	3.0
1	D	98	VAL	3.0
2	A	868	LEU	2.9
2	A	620	ARG	2.9
1	D	71	ALA	2.9
1	D	41	ASN	2.9
2	A	833	PRO	2.8
2	A	165	ALA	2.8
2	A	1036	LYS	2.8
2	A	256	ASP	2.8
2	A	661	ALA	2.8
2	A	662	MET	2.8
2	A	987	MET	2.8
2	A	233	SER	2.8
2	A	1025	PHE	2.7
2	A	657	GLN	2.7
1	D	93	LEU	2.7
2	A	1040	ILE	2.7
1	D	46	VAL	2.7
2	A	811	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	257	GLY	2.7
2	A	1026	PHE	2.7
1	D	141	ALA	2.7
1	D	125	HIS	2.6
1	D	73	VAL	2.6
2	A	97	GLY	2.6
1	D	78	THR	2.6
2	A	866	GLU	2.6
2	A	563	PHE	2.6
2	A	1022	VAL	2.6
1	D	32	ILE	2.6
2	A	590	VAL	2.6
2	A	300	LEU	2.6
2	A	319	SER	2.6
2	A	316	PHE	2.5
1	D	99	LEU	2.5
2	A	690	LEU	2.5
1	D	15	GLY	2.5
2	A	668	LEU	2.5
2	A	509	LYS	2.5
2	A	1043	SER	2.5
1	D	103	GLY	2.5
2	A	720	GLY	2.5
1	D	24	ALA	2.5
2	A	589	LYS	2.5
2	A	387	GLY	2.4
2	A	754	TRP	2.4
2	A	666	PHE	2.4
1	D	39	ASP	2.4
2	A	1035	ARG	2.4
2	A	348	ILE	2.4
2	A	727	PHE	2.4
2	A	918	PHE	2.4
2	A	659	LYS	2.4
2	A	216	ALA	2.4
2	A	1028	VAL	2.3
1	D	20	GLU	2.3
1	D	139	VAL	2.3
2	A	718	PRO	2.3
2	A	235	ILE	2.3
2	A	537	SER	2.3
2	A	808	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	67	LEU	2.3
1	D	86	LEU	2.3
2	A	350	LEU	2.3
2	A	684	LEU	2.3
2	A	817	GLU	2.3
2	A	225	VAL	2.3
2	A	513	PHE	2.3
1	D	102	ASN	2.3
2	A	850	LYS	2.2
1	D	51	LEU	2.2
2	A	721	LEU	2.2
2	A	580	ALA	2.2
1	D	48	TRP	2.2
2	A	147	GLY	2.2
2	A	75	LEU	2.2
2	A	871	ASN	2.2
1	D	129	VAL	2.2
2	A	265	VAL	2.2
2	A	990	VAL	2.2
2	A	234	ILE	2.2
2	A	1007	VAL	2.2
2	A	178	PHE	2.2
2	A	386	PHE	2.2
2	A	512	PHE	2.2
2	A	168	ARG	2.2
2	A	706	ALA	2.2
2	A	295	THR	2.2
2	A	676	THR	2.2
2	A	196	PHE	2.2
2	A	323	ILE	2.1
2	A	198	LEU	2.1
2	A	618	ALA	2.1
2	A	330	THR	2.1
1	D	127	GLU	2.1
2	A	388	PHE	2.1
2	A	268	ILE	2.1
2	A	789	TRP	2.1
1	D	28	ASP	2.0
2	A	847	LEU	2.0
2	A	327	TYR	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 monosaccharides 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.