Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2025 – 04:35 pm BST

PDB ID	:	9FE4 / pdb_00009fe4
Title	:	Crystallographic structure of AcrB V612F
Authors	:	Lazarova, M.; Diederichs, K.; Pos, K.M.
Deposited on	:	2024-05-17
Resolution	:	2.80 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:

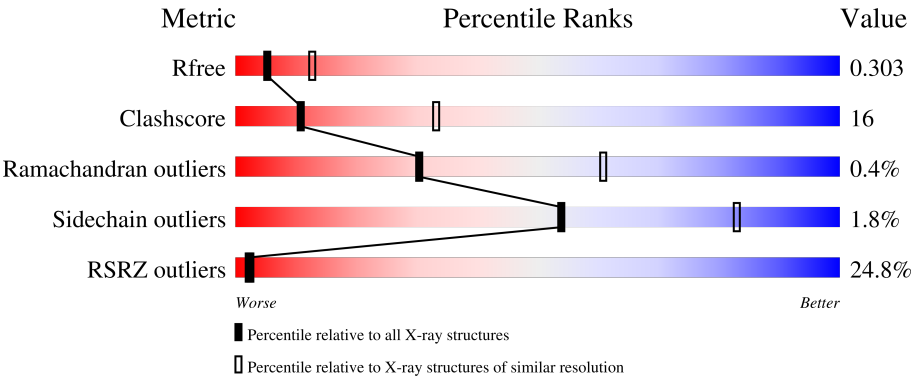
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	B	1057	24% 67% 29% ..

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7842 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1032	Total	C	N	O	S	0	0	0
			7842	5047	1294	1457	44			

There are 9 discrepancies between the modelled and reference sequences:

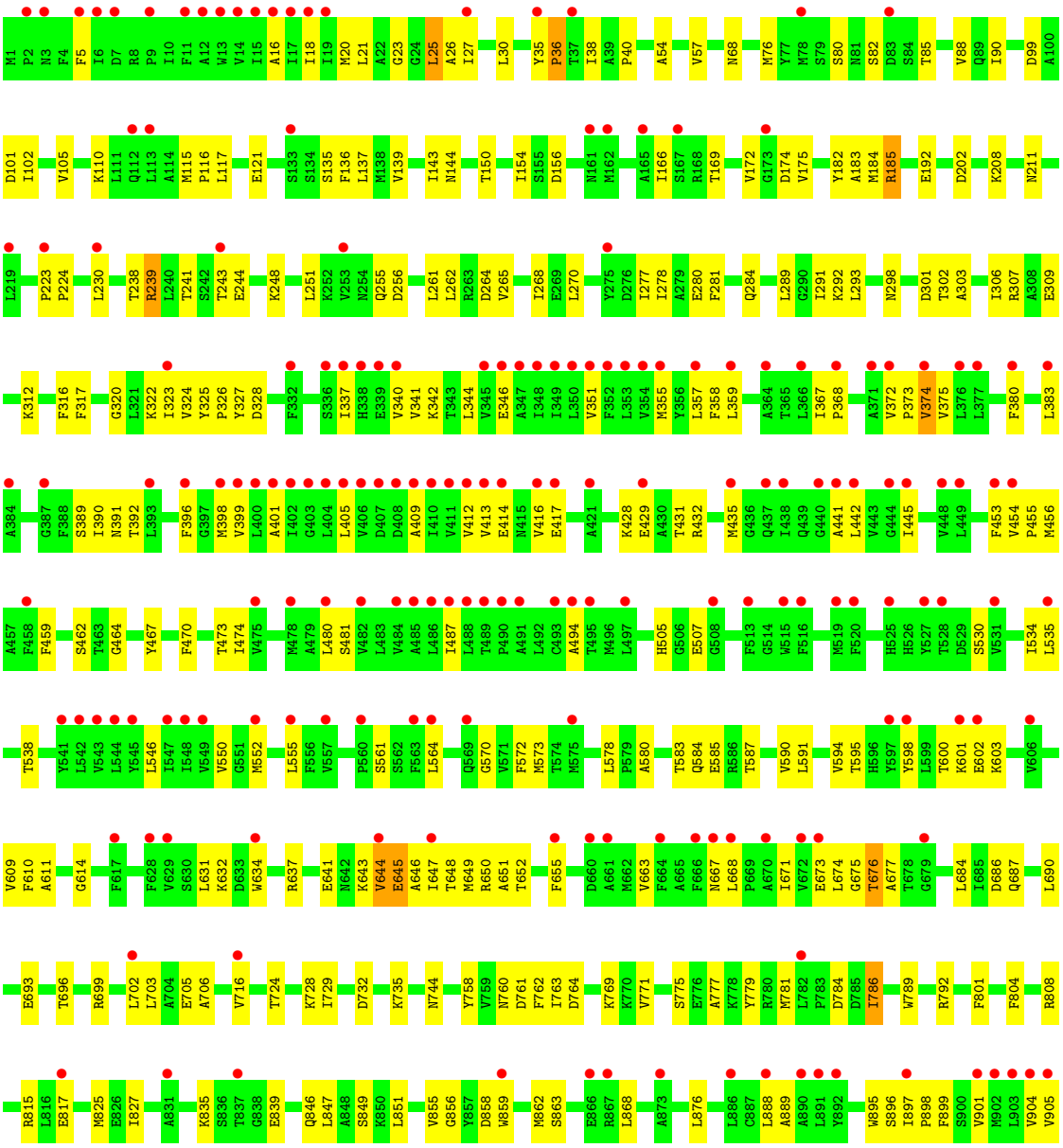
Chain	Residue	Modelled	Actual	Comment	Reference
B	612	PHE	VAL	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-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

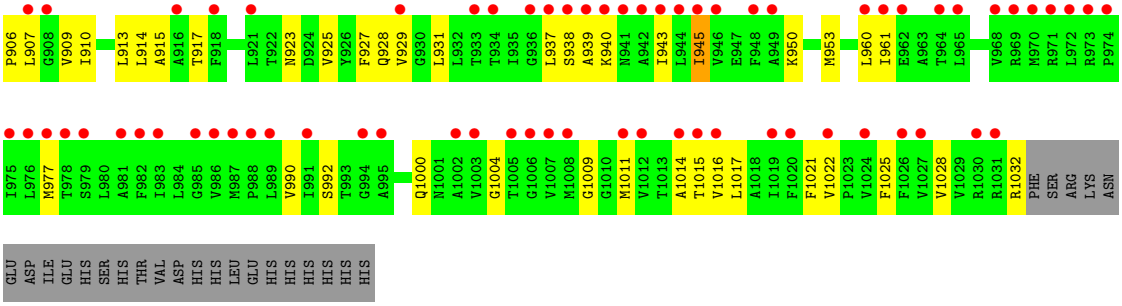
3 Residue-property plots (i)

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: Multidrug efflux pump subunit AcrB

Chain B:




P906 L907 G908 V909 I910 L913 L914 A915 A916 T917 F918 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932 T933 T934 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 M953 L960 I961 E962 A963 T964 L965 V968 R969 M970 R971 L972 R973 P974
I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 S992 T993 G994 A995 Q1000 N1001 A1002 V1003 G1004 T1005 G1006 V1007 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 V1028 V1029 R1030 R1031 R1032 PHE SER ARG LYS ASN
GLU ASP ILE GLU HIS SER 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	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.41Å 134.41Å 190.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.70 – 2.80 49.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.70-2.80) 99.7 (49.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.259 , 0.300 0.270 , 0.303	Depositor DCC
R_{free} test set	2594 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	83.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 73.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7842	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	B	0.49	0/7992	0.77	4/10853 (0.0%)

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	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	THR	N-CA-C	-5.88	105.88	113.16
1	B	645	GLU	N-CA-C	-5.73	104.72	110.97
1	B	76	MET	N-CA-C	5.70	117.36	111.03
1	B	644	VAL	N-CA-C	5.00	119.75	109.34

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1032	ARG	Sidechain
1	B	185	ARG	Sidechain
1	B	239	ARG	Sidechain

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	B	7842	0	7992	259	0
All	All	7842	0	7992	259	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 16.

All (259) 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:B:57:VAL:CG2	1:B:88:VAL:HG23	1.69	1.22
1:B:535:LEU:CD1	1:B:961:ILE:HD12	1.74	1.18
1:B:57:VAL:HG22	1:B:88:VAL:CG2	1.75	1.15
1:B:535:LEU:HD11	1:B:961:ILE:CD1	1.78	1.13
1:B:953:MET:HE1	1:B:960:LEU:HD23	1.32	1.06
1:B:57:VAL:HG13	1:B:82:SER:HB3	1.36	1.01
1:B:644:VAL:O	1:B:648:THR:HG23	1.60	1.01
1:B:302:THR:O	1:B:306:ILE:HD12	1.63	0.97
1:B:355:MET:SD	1:B:368:PRO:HG2	2.04	0.97
1:B:905:VAL:CG2	1:B:906:PRO:HD3	1.96	0.95
1:B:355:MET:HE1	1:B:368:PRO:CD	1.97	0.94
1:B:57:VAL:HG22	1:B:88:VAL:HG23	1.40	0.92
1:B:57:VAL:HG21	1:B:88:VAL:HG23	1.49	0.92
1:B:57:VAL:CG2	1:B:88:VAL:CG2	2.41	0.89
1:B:535:LEU:HD13	1:B:961:ILE:HG23	1.51	0.89
1:B:909:VAL:O	1:B:913:LEU:HD13	1.74	0.88
1:B:905:VAL:HG23	1:B:906:PRO:HD3	1.56	0.86
1:B:459:PHE:HD2	1:B:467:TYR:CD2	1.94	0.85
1:B:412:VAL:HG22	1:B:435:MET:HE1	1.61	0.83
1:B:324:VAL:HG12	1:B:326:PRO:HD3	1.60	0.82
1:B:355:MET:HE1	1:B:368:PRO:HD2	1.60	0.82
1:B:535:LEU:HD11	1:B:961:ILE:HD12	0.86	0.81
1:B:355:MET:CE	1:B:368:PRO:HG2	2.13	0.79
1:B:429:GLU:HA	1:B:432:ARG:HG3	1.69	0.75
1:B:953:MET:HE1	1:B:960:LEU:CD2	2.12	0.74
1:B:729:ILE:HD11	1:B:786:ILE:HD12	1.68	0.74
1:B:57:VAL:CG1	1:B:82:SER:HB3	2.16	0.73
1:B:953:MET:CE	1:B:960:LEU:HD23	2.14	0.73
1:B:905:VAL:HG22	1:B:906:PRO:HD3	1.69	0.72
1:B:535:LEU:CD1	1:B:961:ILE:HG23	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:MET:HG3	1:B:459:PHE:CE2	2.26	0.71
1:B:243:THR:HG23	1:B:268:ILE:HB	1.72	0.70
1:B:728:LYS:HD3	1:B:808:ARG:CZ	2.22	0.70
1:B:909:VAL:O	1:B:913:LEU:CD1	2.41	0.68
1:B:905:VAL:HG23	1:B:906:PRO:CD	2.24	0.68
1:B:243:THR:CG2	1:B:268:ILE:HB	2.24	0.68
1:B:590:VAL:O	1:B:594:VAL:HG23	1.94	0.68
1:B:815:ARG:NH1	1:B:817:GLU:OE2	2.22	0.68
1:B:298:ASN:ND2	1:B:301:ASP:HB2	2.09	0.67
1:B:530:SER:O	1:B:534:ILE:HG12	1.95	0.67
1:B:57:VAL:HG22	1:B:88:VAL:HG21	1.72	0.67
1:B:535:LEU:HD13	1:B:961:ILE:CG2	2.22	0.66
1:B:166:ILE:HD12	1:B:306:ILE:HG23	1.78	0.66
1:B:243:THR:HG23	1:B:268:ILE:CG2	2.26	0.66
1:B:667:ASN:OD1	1:B:668:LEU:N	2.29	0.66
1:B:340:VAL:O	1:B:344:LEU:HD12	1.96	0.65
1:B:555:LEU:HB3	1:B:913:LEU:HD23	1.77	0.65
1:B:244:GLU:N	1:B:244:GLU:OE2	2.29	0.64
1:B:30:LEU:HD22	1:B:390:ILE:HG13	1.78	0.64
1:B:591:LEU:HD13	1:B:611:ALA:HB1	1.79	0.63
1:B:445:ILE:HG21	1:B:940:LYS:HE2	1.80	0.62
1:B:243:THR:HG23	1:B:268:ILE:CB	2.30	0.62
1:B:909:VAL:HG12	1:B:913:LEU:HD11	1.81	0.62
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.35	0.62
1:B:729:ILE:HD11	1:B:786:ILE:CD1	2.29	0.62
1:B:375:VAL:HA	1:B:480:LEU:HD23	1.83	0.61
1:B:938:SER:HB3	1:B:1014:ALA:HB1	1.81	0.61
1:B:36:PRO:O	1:B:38:ILE:HD12	2.01	0.60
1:B:342:LYS:O	1:B:346:GLU:HG3	2.01	0.60
1:B:355:MET:SD	1:B:368:PRO:CG	2.84	0.60
1:B:696:THR:OG1	1:B:825:MET:HE1	2.02	0.60
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.82	0.60
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.35	0.60
1:B:135:SER:HB2	1:B:673:GLU:HB3	1.83	0.59
1:B:901:VAL:O	1:B:904:VAL:HG12	2.01	0.59
1:B:459:PHE:CD2	1:B:467:TYR:CD2	2.84	0.59
1:B:30:LEU:HD21	1:B:389:SER:HA	1.83	0.59
1:B:729:ILE:CD1	1:B:786:ILE:HD12	2.33	0.59
1:B:777:ALA:O	1:B:781:MET:HG2	2.02	0.59
1:B:20:MET:HE3	1:B:374:VAL:HG22	1.83	0.59
1:B:101:ASP:O	1:B:105:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TYR:CD2	1:B:671:ILE:HD13	2.38	0.58
1:B:555:LEU:HD21	1:B:917:THR:HG21	1.84	0.58
1:B:355:MET:CE	1:B:368:PRO:CG	2.80	0.58
1:B:646:ALA:HA	1:B:649:MET:HE2	1.86	0.58
1:B:337:ILE:O	1:B:341:VAL:HG22	2.04	0.57
1:B:456:MET:CG	1:B:459:PHE:CE2	2.86	0.57
1:B:925:VAL:HA	1:B:928:GLN:OE1	2.04	0.57
1:B:302:THR:OG1	1:B:303:ALA:N	2.38	0.57
1:B:355:MET:CE	1:B:368:PRO:CD	2.79	0.57
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.86	0.57
1:B:16:ALA:O	1:B:20:MET:HG3	2.06	0.56
1:B:243:THR:HG23	1:B:268:ILE:HG22	1.88	0.55
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.41	0.55
1:B:412:VAL:HG22	1:B:435:MET:CE	2.35	0.55
1:B:192:GLU:HG2	1:B:264:ASP:O	2.06	0.55
1:B:953:MET:HE2	1:B:960:LEU:HA	1.88	0.55
1:B:351:VAL:O	1:B:355:MET:HG3	2.07	0.54
1:B:862:MET:HG3	1:B:863:SER:N	2.23	0.54
1:B:416:VAL:HG22	1:B:431:THR:HA	1.89	0.54
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.89	0.54
1:B:583:THR:HG22	1:B:585:GLU:H	1.72	0.54
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.42	0.54
1:B:923:ASN:HA	1:B:927:PHE:CD2	2.43	0.54
1:B:241:THR:HA	1:B:763:ILE:O	2.09	0.53
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.91	0.53
1:B:909:VAL:HG12	1:B:913:LEU:CD1	2.39	0.53
1:B:573:MET:HG2	1:B:668:LEU:HD21	1.90	0.53
1:B:686:ASP:OD1	1:B:690:LEU:HB2	2.09	0.53
1:B:192:GLU:HB3	1:B:265:VAL:HG12	1.91	0.52
1:B:441:ALA:O	1:B:445:ILE:N	2.41	0.52
1:B:762:PHE:CE1	1:B:769:LYS:HB2	2.45	0.52
1:B:459:PHE:HB2	1:B:464:GLY:HA2	1.92	0.52
1:B:909:VAL:HG13	1:B:931:LEU:HD22	1.91	0.52
1:B:298:ASN:O	1:B:302:THR:HG23	2.09	0.52
1:B:699:ARG:HG2	1:B:703:LEU:HD23	1.92	0.51
1:B:396:PHE:HA	1:B:399:VAL:HG12	1.92	0.51
1:B:650:ARG:HG3	1:B:650:ARG:HH11	1.75	0.51
1:B:383:LEU:HD21	1:B:473:THR:HA	1.93	0.51
1:B:54:ALA:O	1:B:57:VAL:HG12	2.11	0.51
1:B:674:LEU:O	1:B:676:THR:N	2.44	0.51
1:B:602:GLU:CD	1:B:647:ILE:HG23	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ALA:O	1:B:30:LEU:HB2	2.11	0.50
1:B:634:TRP:CD1	1:B:637:ARG:HH22	2.29	0.50
1:B:307:ARG:NH1	1:B:328:ASP:OD2	2.45	0.50
1:B:602:GLU:OE2	1:B:647:ILE:HG23	2.11	0.50
1:B:1017:LEU:HB3	1:B:1021:PHE:CE2	2.46	0.50
1:B:641:GLU:H	1:B:641:GLU:CD	2.19	0.50
1:B:990:VAL:HG22	1:B:1004:GLY:C	2.36	0.50
1:B:732:ASP:HB3	1:B:735:LYS:HB2	1.94	0.50
1:B:535:LEU:O	1:B:538:THR:HG23	2.12	0.50
1:B:277:ILE:HD13	1:B:614:GLY:HA3	1.93	0.50
1:B:357:LEU:HD23	1:B:358:PHE:CE1	2.47	0.50
1:B:591:LEU:O	1:B:595:THR:HG23	2.13	0.49
1:B:705:GLU:HB3	1:B:847:LEU:CD2	2.43	0.49
1:B:27:ILE:HG12	1:B:380:PHE:CD2	2.47	0.49
1:B:211:ASN:ND2	1:B:761:ASP:O	2.45	0.49
1:B:895:TRP:O	1:B:899:PHE:HE1	1.95	0.49
1:B:303:ALA:O	1:B:307:ARG:HG3	2.13	0.49
1:B:905:VAL:CG2	1:B:906:PRO:CD	2.80	0.49
1:B:676:THR:HA	1:B:862:MET:HE3	1.95	0.49
1:B:239:ARG:NH1	1:B:761:ASP:HB2	2.28	0.48
1:B:312:LYS:O	1:B:316:PHE:HE1	1.96	0.48
1:B:572:PHE:CE1	1:B:631:LEU:HD21	2.47	0.48
1:B:702:LEU:HB2	1:B:851:LEU:HD11	1.95	0.48
1:B:38:ILE:HD13	1:B:671:ILE:HD12	1.96	0.48
1:B:570:GLY:HA2	1:B:631:LEU:HD12	1.94	0.48
1:B:572:PHE:HE1	1:B:631:LEU:HD21	1.78	0.48
1:B:899:PHE:H	1:B:899:PHE:HD1	1.62	0.48
1:B:401:ALA:O	1:B:405:LEU:HG	2.14	0.48
1:B:355:MET:HE1	1:B:368:PRO:CG	2.42	0.48
1:B:561:SER:HA	1:B:923:ASN:HB3	1.94	0.48
1:B:68:ASN:O	1:B:110:LYS:HB3	2.14	0.48
1:B:156:ASP:CG	1:B:182:TYR:CD2	2.91	0.48
1:B:302:THR:C	1:B:306:ILE:HD12	2.36	0.48
1:B:456:MET:HG3	1:B:459:PHE:HE2	1.78	0.48
1:B:169:THR:O	1:B:172:VAL:HG12	2.14	0.47
1:B:835:LYS:HE3	1:B:839:GLU:OE2	2.14	0.47
1:B:901:VAL:HG11	1:B:943:ILE:HG13	1.97	0.47
1:B:359:LEU:HD12	1:B:417:GLU:OE2	2.14	0.47
1:B:5:PHE:CD2	1:B:487:ILE:HG23	2.48	0.47
1:B:30:LEU:CD2	1:B:389:SER:HA	2.45	0.47
1:B:693:GLU:O	1:B:696:THR:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ALA:N	1:B:898:PRO:HG3	2.30	0.47
1:B:306:ILE:O	1:B:309:GLU:N	2.47	0.47
1:B:454:VAL:N	1:B:455:PRO:HD2	2.30	0.47
1:B:655:PHE:HB3	1:B:663:VAL:HB	1.96	0.47
1:B:992:SER:OG	1:B:1000:GLN:OE1	2.31	0.47
1:B:375:VAL:HG11	1:B:481:SER:HA	1.97	0.46
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.96	0.46
1:B:858:ASP:OD1	1:B:859:TRP:N	2.36	0.46
1:B:603:LYS:O	1:B:632:LYS:NZ	2.48	0.46
1:B:248:LYS:HB2	1:B:248:LYS:HE2	1.70	0.46
1:B:409:ALA:O	1:B:413:VAL:HG22	2.15	0.46
1:B:913:LEU:O	1:B:917:THR:HG22	2.15	0.46
1:B:641:GLU:OE1	1:B:641:GLU:N	2.37	0.46
1:B:927:PHE:CZ	1:B:931:LEU:HD11	2.51	0.46
1:B:564:LEU:HD13	1:B:925:VAL:HG22	1.98	0.46
1:B:375:VAL:HG23	1:B:405:LEU:HD13	1.97	0.45
1:B:1017:LEU:O	1:B:1021:PHE:HD2	1.99	0.45
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.98	0.45
1:B:137:LEU:HD13	1:B:293:LEU:HB2	1.98	0.45
1:B:897:ILE:HD13	1:B:950:LYS:HD2	1.97	0.45
1:B:846:GLN:O	1:B:849:SER:OG	2.31	0.45
1:B:23:GLY:O	1:B:27:ILE:HG13	2.17	0.45
1:B:572:PHE:HZ	1:B:598:TYR:CE1	2.35	0.45
1:B:910:ILE:HG13	1:B:914:LEU:HD13	1.98	0.45
1:B:645:GLU:O	1:B:649:MET:HG3	2.17	0.45
1:B:359:LEU:HA	1:B:359:LEU:HD13	1.75	0.45
1:B:391:ASN:O	1:B:392:THR:C	2.59	0.45
1:B:591:LEU:HD23	1:B:591:LEU:HA	1.79	0.45
1:B:862:MET:HG3	1:B:863:SER:H	1.81	0.45
1:B:255:GLN:NE2	1:B:256:ASP:OD1	2.50	0.44
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.67	0.44
1:B:530:SER:O	1:B:534:ILE:N	2.46	0.44
1:B:470:PHE:CD2	1:B:929:VAL:HG21	2.52	0.44
1:B:40:PRO:HD3	1:B:462:SER:OG	2.18	0.44
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.52	0.44
1:B:572:PHE:HZ	1:B:598:TYR:HE1	1.65	0.44
1:B:896:SER:HA	1:B:899:PHE:CE1	2.53	0.44
1:B:578:LEU:HD23	1:B:587:THR:HG23	1.98	0.44
1:B:905:VAL:O	1:B:909:VAL:HG23	2.18	0.44
1:B:634:TRP:CD1	1:B:637:ARG:NH2	2.86	0.44
1:B:690:LEU:HD23	1:B:690:LEU:HA	1.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.99	0.44
1:B:595:THR:HG22	1:B:609:VAL:HG11	2.00	0.44
1:B:121:GLU:H	1:B:121:GLU:CD	2.26	0.43
1:B:372:VAL:O	1:B:373:PRO:C	2.58	0.43
1:B:775:SER:HB2	1:B:789:TRP:HZ2	1.83	0.43
1:B:442:LEU:HA	1:B:445:ILE:HD12	1.99	0.43
1:B:945:ILE:HG21	1:B:1022:VAL:HG13	1.99	0.43
1:B:355:MET:CE	1:B:368:PRO:HD2	2.41	0.43
1:B:687:GLN:NE2	1:B:856:GLY:HA3	2.34	0.43
1:B:762:PHE:CE2	1:B:764:ASP:HB2	2.53	0.43
1:B:953:MET:CE	1:B:960:LEU:HA	2.47	0.43
1:B:456:MET:HE2	1:B:456:MET:HB3	1.82	0.43
1:B:904:VAL:HG11	1:B:939:ALA:HA	2.00	0.43
1:B:453:PHE:CE2	1:B:474:ILE:HG21	2.54	0.43
1:B:414:GLU:HG3	1:B:977:MET:HE1	2.00	0.43
1:B:594:VAL:O	1:B:598:TYR:HD2	2.02	0.43
1:B:208:LYS:HA	1:B:760:ASN:ND2	2.34	0.42
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.95	0.42
1:B:552:MET:HG3	1:B:913:LEU:HD22	2.00	0.42
1:B:1025:PHE:HA	1:B:1028:VAL:HG22	2.01	0.42
1:B:115:MET:HB2	1:B:116:PRO:HD3	2.00	0.42
1:B:278:ILE:HG13	1:B:584:GLN:NE2	2.34	0.42
1:B:505:HIS:HB2	1:B:507:GLU:HG3	2.02	0.42
1:B:643:LYS:O	1:B:647:ILE:HG13	2.20	0.42
1:B:183:ALA:O	1:B:185:ARG:HG2	2.19	0.42
1:B:389:SER:OG	1:B:391:ASN:OD1	2.31	0.42
1:B:428:LYS:HD2	1:B:494:ALA:O	2.19	0.42
1:B:888:LEU:HD13	1:B:901:VAL:HB	2.02	0.42
1:B:699:ARG:O	1:B:703:LEU:HD23	2.20	0.42
1:B:702:LEU:HD12	1:B:702:LEU:O	2.20	0.42
1:B:1011:MET:O	1:B:1015:THR:HG22	2.20	0.42
1:B:913:LEU:N	1:B:913:LEU:HD12	2.35	0.42
1:B:175:VAL:HG11	1:B:289:LEU:HD13	2.02	0.42
1:B:80:SER:HB2	1:B:90:ILE:HG12	2.02	0.41
1:B:139:VAL:HB	1:B:327:TYR:HB3	2.01	0.41
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.88	0.41
1:B:631:LEU:HD11	1:B:644:VAL:HG22	2.02	0.41
1:B:184:MET:HB3	1:B:771:VAL:HG22	2.01	0.41
1:B:398:MET:HE2	1:B:398:MET:HB3	1.88	0.41
1:B:923:ASN:HA	1:B:927:PHE:HD2	1.85	0.41
1:B:143:ILE:HG13	1:B:322:LYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:GLU:HA	1:B:284:GLN:O	2.20	0.41
1:B:907:LEU:HD12	1:B:907:LEU:H	1.86	0.41
1:B:244:GLU:H	1:B:244:GLU:CD	2.29	0.41
1:B:298:ASN:CG	1:B:301:ASP:H	2.28	0.41
1:B:904:VAL:HA	1:B:907:LEU:HD13	2.02	0.41
1:B:323:ILE:HG22	1:B:325:TYR:CE1	2.55	0.41
1:B:546:LEU:O	1:B:550:VAL:HG13	2.21	0.41
1:B:699:ARG:HG2	1:B:699:ARG:O	2.19	0.41
1:B:459:PHE:HD1	1:B:876:LEU:CD1	2.34	0.41
1:B:136:PHE:HD1	1:B:291:ILE:O	2.04	0.41
1:B:144:ASN:HA	1:B:320:GLY:O	2.21	0.41
1:B:459:PHE:CD1	1:B:876:LEU:CD1	3.03	0.41
1:B:684:LEU:HD11	1:B:855:VAL:CG1	2.51	0.41
1:B:456:MET:HG2	1:B:467:TYR:HB3	2.03	0.40
1:B:573:MET:HG2	1:B:668:LEU:CD2	2.50	0.40
1:B:937:LEU:HD13	1:B:1011:MET:CE	2.51	0.40
1:B:651:ALA:O	1:B:652:THR:C	2.63	0.40
1:B:21:LEU:O	1:B:25:LEU:HB3	2.22	0.40
1:B:600:THR:OG1	1:B:601:LYS:N	2.53	0.40
1:B:699:ARG:HG3	1:B:827:ILE:HD11	2.04	0.40
1:B:706:ALA:HB3	1:B:716:VAL:HG11	2.04	0.40
1:B:758:TYR:OH	1:B:761:ASP:OD1	2.36	0.40
1:B:1017:LEU:O	1:B:1021:PHE:CD2	2.75	0.40
1:B:150:THR:O	1:B:154:ILE:HD12	2.22	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	B	1030/1057 (97%)	952 (92%)	74 (7%)	4 (0%)	30 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	675	GLY
1	B	36	PRO
1	B	676	THR
1	B	677	ALA

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	B	838/863 (97%)	823 (98%)	15 (2%)	54 83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	ILE
1	B	25	LEU
1	B	117	LEU
1	B	230	LEU
1	B	238	THR
1	B	261	LEU
1	B	374	VAL
1	B	610	PHE
1	B	744	ASN
1	B	779	TYR
1	B	784	ASP
1	B	786	ILE
1	B	868	LEU
1	B	945	ILE
1	B	1016	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	74	ASN
1	B	191	ASN
1	B	255	GLN
1	B	391	ASN
1	B	415	ASN
1	B	469	GLN
1	B	687	GLN
1	B	726	GLN
1	B	744	ASN
1	B	797	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	1032/1057 (97%)	1.35	256 (24%)	2 2	40, 119, 158, 190	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	438	ILE	5.9
1	B	7	ASP	5.8
1	B	944	LEU	5.7
1	B	938	SER	5.6
1	B	960	LEU	5.4
1	B	937	LEU	5.3
1	B	12	ALA	5.3
1	B	945	ILE	5.2
1	B	964	THR	5.2
1	B	399	VAL	5.1
1	B	961	ILE	5.1
1	B	866	GLU	5.1
1	B	542	LEU	5.1
1	B	13	TRP	5.0
1	B	409	ALA	5.0
1	B	941	ASN	4.9
1	B	949	ALA	4.8
1	B	946	VAL	4.7
1	B	435	MET	4.6
1	B	411	VAL	4.6
1	B	3	ASN	4.6
1	B	357	LEU	4.5
1	B	527	TYR	4.4
1	B	1022	VAL	4.4
1	B	408	ASP	4.3
1	B	1007	VAL	4.3
1	B	520	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	962	GLU	4.2
1	B	113	LEU	4.2
1	B	133	SER	4.2
1	B	664	PHE	4.1
1	B	1019	ILE	4.1
1	B	37	THR	4.1
1	B	973	ARG	4.1
1	B	535	LEU	4.0
1	B	982	PHE	4.0
1	B	972	LEU	4.0
1	B	965	LEU	3.9
1	B	410	ILE	3.9
1	B	934	THR	3.9
1	B	485	ALA	3.9
1	B	1002	ALA	3.9
1	B	907	LEU	3.8
1	B	969	ARG	3.8
1	B	908	GLY	3.8
1	B	1027	VAL	3.8
1	B	441	ALA	3.8
1	B	355	MET	3.7
1	B	886	LEU	3.7
1	B	490	PRO	3.7
1	B	939	ALA	3.7
1	B	11	PHE	3.6
1	B	402	ILE	3.6
1	B	413	VAL	3.6
1	B	661	ALA	3.6
1	B	831	ALA	3.6
1	B	940	LYS	3.6
1	B	406	VAL	3.5
1	B	936	GLY	3.5
1	B	1005	THR	3.5
1	B	401	ALA	3.5
1	B	983	ILE	3.5
1	B	1014	ALA	3.5
1	B	1003	VAL	3.5
1	B	1024	VAL	3.5
1	B	442	LEU	3.4
1	B	549	VAL	3.4
1	B	349	ILE	3.4
1	B	548	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	647	ILE	3.4
1	B	351	VAL	3.4
1	B	544	LEU	3.3
1	B	981	ALA	3.3
1	B	19	ILE	3.3
1	B	353	LEU	3.3
1	B	17	ILE	3.3
1	B	985	GLY	3.3
1	B	976	LEU	3.3
1	B	9	PRO	3.2
1	B	416	VAL	3.2
1	B	1011	MET	3.2
1	B	897	ILE	3.2
1	B	489	THR	3.2
1	B	569	GLN	3.2
1	B	904	VAL	3.2
1	B	405	LEU	3.2
1	B	655	PHE	3.2
1	B	18	ILE	3.2
1	B	437	GLN	3.2
1	B	979	SER	3.2
1	B	1016	VAL	3.2
1	B	891	LEU	3.2
1	B	417	GLU	3.1
1	B	974	PRO	3.1
1	B	112	GLN	3.1
1	B	890	ALA	3.1
1	B	531	VAL	3.1
1	B	516	PHE	3.1
1	B	374	VAL	3.1
1	B	384	ALA	3.1
1	B	445	ILE	3.1
1	B	859	TRP	3.1
1	B	873	ALA	3.1
1	B	888	LEU	3.0
1	B	458	PHE	3.0
1	B	902	MET	3.0
1	B	977	MET	3.0
1	B	494	ALA	3.0
1	B	488	LEU	3.0
1	B	230	LEU	3.0
1	B	545	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	348	ILE	3.0
1	B	948	PHE	3.0
1	B	449	LEU	2.9
1	B	14	VAL	2.9
1	B	515	TRP	2.9
1	B	484	VAL	2.9
1	B	486	LEU	2.9
1	B	541	TYR	2.9
1	B	491	ALA	2.9
1	B	1031	ARG	2.9
1	B	6	ILE	2.8
1	B	359	LEU	2.8
1	B	412	VAL	2.8
1	B	346	GLU	2.8
1	B	161	ASN	2.8
1	B	15	ILE	2.8
1	B	354	VAL	2.8
1	B	372	VAL	2.8
1	B	918	PHE	2.8
1	B	564	LEU	2.8
1	B	396	PHE	2.8
1	B	2	PRO	2.7
1	B	478	MET	2.7
1	B	345	VAL	2.7
1	B	921	LEU	2.7
1	B	978	THR	2.7
1	B	162	MET	2.7
1	B	16	ALA	2.7
1	B	347	ALA	2.7
1	B	448	VAL	2.7
1	B	601	LYS	2.7
1	B	453	PHE	2.7
1	B	989	LEU	2.7
1	B	995	ALA	2.7
1	B	480	LEU	2.7
1	B	167	SER	2.7
1	B	35	TYR	2.7
1	B	519	MET	2.7
1	B	1006	GLY	2.7
1	B	916	ALA	2.6
1	B	377	LEU	2.6
1	B	400	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	243	THR	2.6
1	B	598	TYR	2.6
1	B	986	VAL	2.6
1	B	942	ALA	2.6
1	B	275	TYR	2.6
1	B	629	VAL	2.6
1	B	219	LEU	2.6
1	B	376	LEU	2.6
1	B	393	LEU	2.6
1	B	337	ILE	2.6
1	B	673	GLU	2.6
1	B	667	ASN	2.6
1	B	602	GLU	2.6
1	B	253	VAL	2.6
1	B	933	THR	2.5
1	B	975	ILE	2.5
1	B	668	LEU	2.5
1	B	165	ALA	2.5
1	B	332	PHE	2.5
1	B	440	GLY	2.5
1	B	444	GLY	2.5
1	B	903	LEU	2.5
1	B	495	THR	2.5
1	B	991	ILE	2.5
1	B	644	VAL	2.4
1	B	929	VAL	2.4
1	B	1012	VAL	2.4
1	B	223	PRO	2.4
1	B	560	PRO	2.4
1	B	366	LEU	2.4
1	B	987	MET	2.4
1	B	547	ILE	2.4
1	B	837	THR	2.4
1	B	597	TYR	2.4
1	B	336	SER	2.4
1	B	528	THR	2.4
1	B	782	LEU	2.4
1	B	679	GLY	2.4
1	B	994	GLY	2.4
1	B	487	ILE	2.4
1	B	670	ALA	2.4
1	B	404	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	968	VAL	2.3
1	B	666	PHE	2.3
1	B	1015	THR	2.3
1	B	575	MET	2.3
1	B	508	GLY	2.3
1	B	5	PHE	2.3
1	B	364	ALA	2.3
1	B	1026	PHE	2.3
1	B	971	ARG	2.3
1	B	970	MET	2.3
1	B	1008	MET	2.3
1	B	482	VAL	2.3
1	B	943	ILE	2.3
1	B	368	PRO	2.3
1	B	454	VAL	2.3
1	B	525	HIS	2.3
1	B	339	GLU	2.3
1	B	628	PHE	2.3
1	B	716	VAL	2.2
1	B	352	PHE	2.2
1	B	421	ALA	2.2
1	B	892	TYR	2.2
1	B	817	GLU	2.2
1	B	557	VAL	2.2
1	B	606	VAL	2.2
1	B	513	PHE	2.2
1	B	1030	ARG	2.2
1	B	988	PRO	2.2
1	B	173	GLY	2.2
1	B	350	LEU	2.2
1	B	429	GLU	2.2
1	B	555	LEU	2.2
1	B	901	VAL	2.2
1	B	905	VAL	2.2
1	B	867	ARG	2.1
1	B	414	GLU	2.1
1	B	387	GLY	2.1
1	B	403	GLY	2.1
1	B	338	HIS	2.1
1	B	340	VAL	2.1
1	B	83	ASP	2.1
1	B	407	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	398	MET	2.1
1	B	617	PHE	2.1
1	B	660	ASP	2.1
1	B	497	LEU	2.1
1	B	27	ILE	2.1
1	B	323	ILE	2.1
1	B	493	CYS	2.1
1	B	552	MET	2.1
1	B	475	VAL	2.0
1	B	634	TRP	2.0
1	B	380	PHE	2.0
1	B	702	LEU	2.0
1	B	371	ALA	2.0
1	B	78	MET	2.0
1	B	543	VAL	2.0
1	B	672	VAL	2.0
1	B	383	LEU	2.0
1	B	563	PHE	2.0
1	B	1020	PHE	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.