Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:34 AM GMT

PDB ID	:	2HQD
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	:	3.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

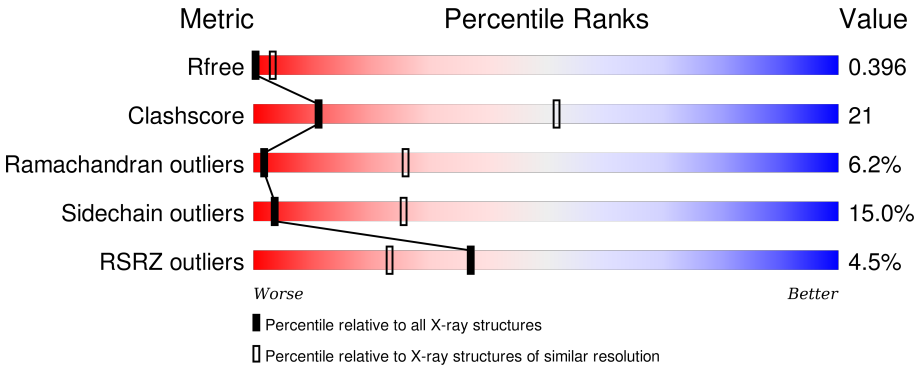
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.65 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}	91344	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)

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 <=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	4% 52% 34% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7718 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
			7718	4964	1276	1435	43			

There are 5 discrepancies between the modelled and reference sequences:

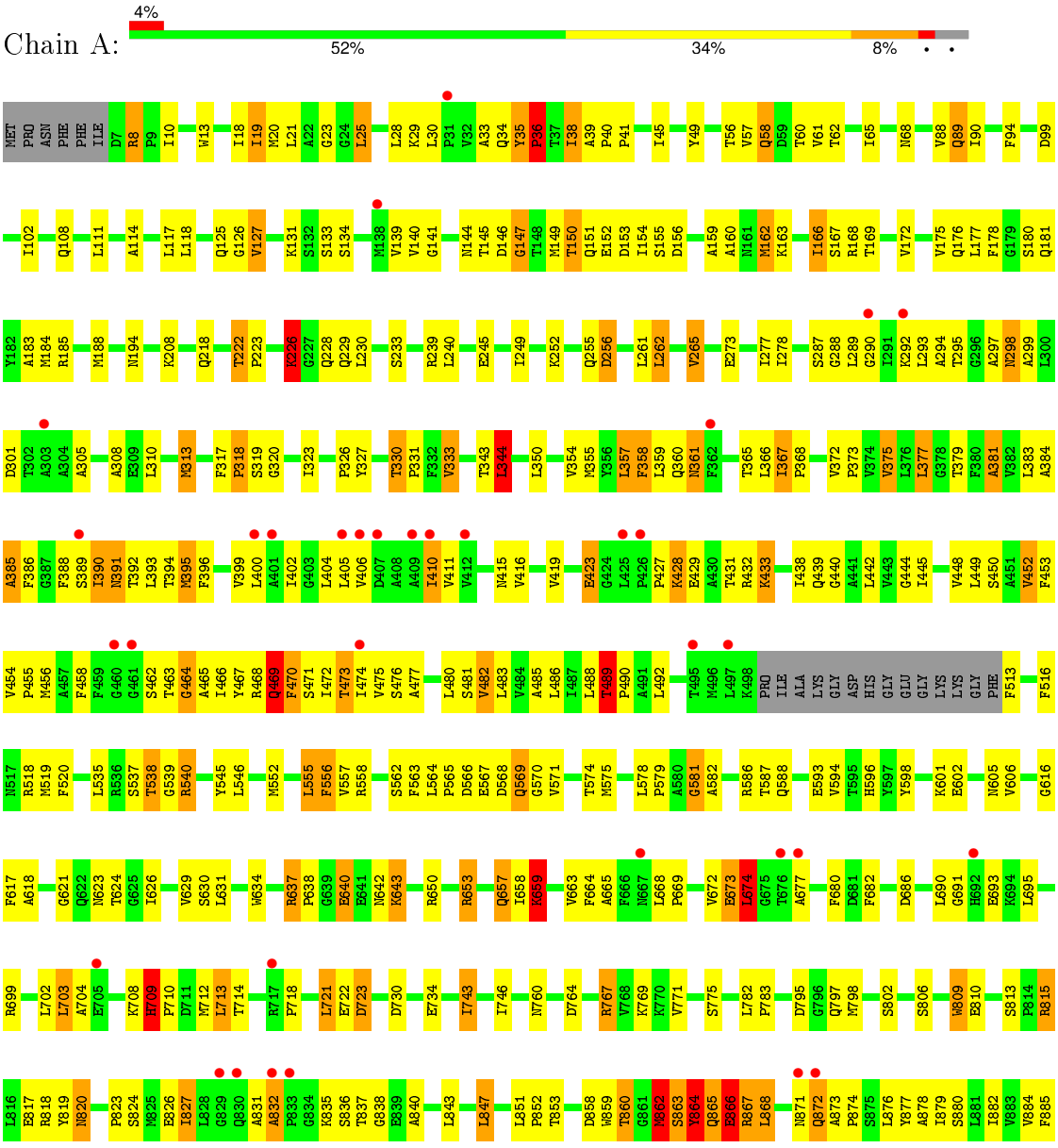
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	ALA	ASP	ENGINEERED	UNP P31224
A	1050	HIS	-	CLONING ARTIFACT	UNP P31224
A	1051	HIS	-	CLONING ARTIFACT	UNP P31224
A	1052	HIS	-	CLONING ARTIFACT	UNP P31224
A	1053	HIS	-	CLONING ARTIFACT	UNP P31224

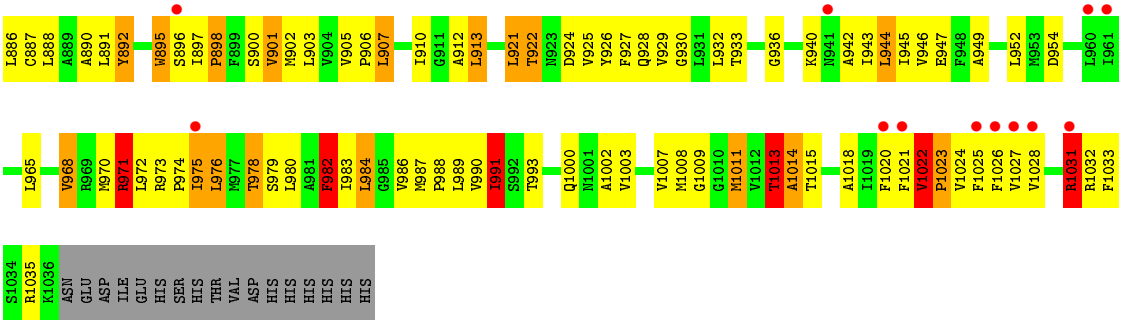
3 Residue-property plots (i)

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

- Molecule 1: Acriflavine resistance protein B

Chain A:




L886 C887 L888 A889 A890 L891 Y892 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 I910 G911 A912 L913 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932 T933 G936 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 L952 M953 D954 L960 I961
L965 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 I980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 S992 T993 Q1000 N1001 A1002 V1003 V1007 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 V1028 R1031 R1032 F1033
S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	145.03Å 145.03Å 513.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.65 46.68 – 3.65	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-3.65) 89.7 (46.68-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.76 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.261 , 0.303 0.377 , 0.396	Depositor DCC
R_{free} test set	1093 reflections (5.46%)	DCC
Wilson B-factor (Å^2)	101.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Outliers	0 of 21219 reflections	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	7718	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	23/7861 (0.3%)	0.74	10/10676 (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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	LYS	CD-CE	15.58	1.90	1.51
1	A	1031	ARG	NE-CZ	15.31	1.52	1.33
1	A	1035	ARG	CZ-NH1	14.66	1.52	1.33
1	A	1031	ARG	CZ-NH1	13.14	1.50	1.33
1	A	256	ASP	C-O	12.44	1.47	1.23
1	A	444	GLY	N-CA	9.46	1.60	1.46
1	A	593	GLU	CB-CG	8.38	1.68	1.52
1	A	640	GLU	CD-OE2	8.33	1.34	1.25
1	A	35	TYR	CG-CD2	8.22	1.49	1.39
1	A	734	GLU	CD-OE2	7.40	1.33	1.25
1	A	892	TYR	C-O	7.39	1.37	1.23
1	A	35	TYR	CE2-CZ	6.85	1.47	1.38
1	A	333	VAL	CB-CG1	6.24	1.66	1.52
1	A	1035	ARG	NE-CZ	6.21	1.41	1.33
1	A	29	LYS	CE-NZ	6.11	1.64	1.49
1	A	35	TYR	CE1-CZ	5.96	1.46	1.38
1	A	866	GLU	CG-CD	5.66	1.60	1.51
1	A	89	GLN	CD-NE2	5.41	1.46	1.32
1	A	653	ARG	CZ-NH1	5.35	1.40	1.33
1	A	593	GLU	CD-OE1	5.19	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	947	GLU	CD-OE1	5.10	1.31	1.25
1	A	428	LYS	CE-NZ	5.08	1.61	1.49
1	A	433	LYS	CB-CG	5.07	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1031	ARG	NE-CZ-NH2	-24.13	108.24	120.30
1	A	35	TYR	C-N-CD	-16.10	85.18	120.60
1	A	1035	ARG	NE-CZ-NH2	-13.84	113.38	120.30
1	A	35	TYR	C-N-CA	10.04	164.15	122.00
1	A	1031	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	1035	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	A	333	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	A	1031	ARG	CD-NE-CZ	-5.62	115.73	123.60
1	A	653	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	36	PRO	CA-N-CD	-5.12	104.33	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1031	ARG	Sidechain
1	A	469	GLN	Peptide

5.2 Too-close contacts (i)

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	7718	0	7878	325	0
All	All	7718	0	7878	325	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 21.

All (325) 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:433:LYS:CD	1:A:433:LYS:CE	1.90	1.46
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.11	1.08
1:A:926:TYR:HB3	1:A:1003:VAL:HG23	1.31	1.07
1:A:1022:VAL:HB	1:A:1023:PRO:CD	1.83	1.07
1:A:653:ARG:O	1:A:657:GLN:HB2	1.61	0.99
1:A:680:PHE:HA	1:A:862:MET:HG3	1.45	0.98
1:A:58:GLN:HE22	1:A:818:ARG:HD2	1.27	0.98
1:A:709:HIS:H	1:A:710:PRO:HD3	1.30	0.92
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.55	0.88
1:A:709:HIS:N	1:A:710:PRO:HD3	1.91	0.85
1:A:888:LEU:HD21	1:A:901:VAL:HG23	1.57	0.85
1:A:815:ARG:HH11	1:A:815:ARG:HG3	1.43	0.82
1:A:298:ASN:HB2	1:A:301:ASP:HB3	1.60	0.82
1:A:942:ALA:O	1:A:945:ILE:HG13	1.80	0.82
1:A:456:MET:CG	1:A:467:TYR:HB3	2.10	0.81
1:A:20:MET:HA	1:A:377:LEU:HD13	1.60	0.81
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.63	0.80
1:A:929:VAL:HA	1:A:932:LEU:HG	1.65	0.79
1:A:877:TYR:HA	1:A:880:SER:HB2	1.67	0.77
1:A:343:THR:O	1:A:344:LEU:HB3	1.85	0.77
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.69	0.74
1:A:1022:VAL:CB	1:A:1023:PRO:CD	2.65	0.74
1:A:901:VAL:HG22	1:A:943:ILE:HD13	1.71	0.72
1:A:450:SER:HA	1:A:453:PHE:HB2	1.72	0.72
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.72	0.71
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.71	0.71
1:A:39:ALA:HB2	1:A:672:VAL:HG11	1.72	0.70
1:A:699:ARG:HG2	1:A:827:ILE:HD11	1.73	0.70
1:A:416:VAL:HG22	1:A:431:THR:HG21	1.72	0.70
1:A:188:MET:H	1:A:775:SER:HA	1.57	0.69
1:A:864:TYR:HB3	1:A:867:ARG:HG2	1.75	0.69
1:A:574:THR:HA	1:A:665:ALA:HA	1.73	0.68
1:A:357:LEU:O	1:A:358:PHE:HB2	1.91	0.68
1:A:730:ASP:HB3	1:A:806:SER:HB3	1.75	0.68
1:A:433:LYS:CG	1:A:433:LYS:CE	2.71	0.68
1:A:867:ARG:HG3	1:A:868:LEU:H	1.59	0.68
1:A:188:MET:N	1:A:775:SER:HA	2.09	0.67
1:A:162:MET:HB3	1:A:313:MET:HG2	1.75	0.67
1:A:470:PHE:CD2	1:A:473:THR:HB	2.29	0.67
1:A:58:GLN:NE2	1:A:818:ARG:HD2	2.06	0.66
1:A:392:THR:HG22	1:A:393:LEU:H	1.58	0.66
1:A:864:TYR:HA	1:A:867:ARG:HE	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:SER:C	1:A:864:TYR:CD2	2.69	0.66
1:A:454:VAL:HG23	1:A:455:PRO:HD3	1.77	0.66
1:A:901:VAL:C	1:A:903:LEU:H	1.99	0.66
1:A:709:HIS:N	1:A:710:PRO:CD	2.59	0.65
1:A:470:PHE:CG	1:A:473:THR:HB	2.31	0.65
1:A:56:THR:O	1:A:60:THR:HG22	1.97	0.65
1:A:672:VAL:HG22	1:A:673:GLU:HG2	1.78	0.64
1:A:166:ILE:O	1:A:168:ARG:N	2.30	0.64
1:A:888:LEU:HD21	1:A:901:VAL:CG2	2.27	0.64
1:A:578:LEU:HG	1:A:587:THR:HG22	1.80	0.63
1:A:886:LEU:O	1:A:887:CYS:HB2	1.97	0.63
1:A:926:TYR:HB3	1:A:1003:VAL:CG2	2.20	0.63
1:A:470:PHE:O	1:A:471:SER:HB2	1.97	0.63
1:A:673:GLU:HG3	1:A:674:LEU:HD13	1.78	0.63
1:A:900:SER:HB3	1:A:946:VAL:HG21	1.79	0.63
1:A:965:LEU:HA	1:A:968:VAL:HG12	1.79	0.63
1:A:134:SER:H	1:A:292:LYS:HE3	1.62	0.63
1:A:885:PHE:HA	1:A:888:LEU:HD22	1.81	0.62
1:A:34:GLN:HB3	1:A:333:VAL:CG2	2.29	0.62
1:A:481:SER:O	1:A:485:ALA:HB3	2.01	0.61
1:A:389:SER:HB3	1:A:391:ASN:HD21	1.65	0.61
1:A:982:PHE:O	1:A:984:LEU:N	2.34	0.61
1:A:907:LEU:O	1:A:910:ILE:HG22	2.01	0.61
1:A:968:VAL:HG21	1:A:1025:PHE:CZ	2.36	0.60
1:A:815:ARG:HG3	1:A:815:ARG:NH1	2.15	0.60
1:A:433:LYS:HB3	1:A:433:LYS:HE2	1.84	0.60
1:A:863:SER:O	1:A:864:TYR:HD2	1.84	0.60
1:A:34:GLN:HB3	1:A:333:VAL:HG21	1.84	0.60
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.84	0.59
1:A:463:THR:H	1:A:867:ARG:HD2	1.67	0.59
1:A:180:SER:OG	1:A:273:GLU:HG2	2.03	0.59
1:A:477:ALA:O	1:A:481:SER:HB2	2.02	0.59
1:A:155:SER:HB3	1:A:180:SER:H	1.68	0.59
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.33	0.59
1:A:456:MET:SD	1:A:876:LEU:HG	2.42	0.58
1:A:471:SER:H	1:A:474:ILE:HD12	1.67	0.58
1:A:658:ILE:O	1:A:659:LYS:HB3	2.03	0.58
1:A:682:PHE:HB3	1:A:827:ILE:CG2	2.34	0.58
1:A:159:ALA:HA	1:A:163:LYS:HB2	1.84	0.58
1:A:470:PHE:C	1:A:472:ILE:H	2.06	0.58
1:A:710:PRO:HA	1:A:713:LEU:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:TYR:CB	1:A:867:ARG:HG2	2.33	0.58
1:A:640:GLU:HA	1:A:643:LYS:HZ2	1.68	0.58
1:A:159:ALA:HA	1:A:163:LYS:CB	2.34	0.58
1:A:355:MET:CE	1:A:359:LEU:HD11	2.34	0.58
1:A:140:VAL:HG23	1:A:289:LEU:HB2	1.85	0.57
1:A:394:THR:HB	1:A:470:PHE:CE2	2.39	0.57
1:A:867:ARG:HG3	1:A:868:LEU:N	2.20	0.57
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.87	0.57
1:A:556:PHE:C	1:A:558:ARG:H	2.09	0.57
1:A:156:ASP:HA	1:A:181:GLN:HA	1.86	0.56
1:A:482:VAL:O	1:A:486:LEU:HB2	2.05	0.56
1:A:8:ARG:HE	1:A:8:ARG:H	1.53	0.56
1:A:449:LEU:HD13	1:A:936:GLY:HA3	1.88	0.56
1:A:545:TYR:HB2	1:A:1022:VAL:HG11	1.87	0.56
1:A:400:LEU:HD21	1:A:1003:VAL:HG21	1.87	0.56
1:A:971:ARG:O	1:A:974:PRO:HD2	2.05	0.56
1:A:569:GLN:HG3	1:A:668:LEU:HB2	1.88	0.56
1:A:262:LEU:HA	1:A:265:VAL:HG12	1.86	0.56
1:A:1013:THR:HG23	1:A:1014:ALA:H	1.71	0.56
1:A:991:ILE:C	1:A:993:THR:H	2.09	0.55
1:A:389:SER:HB3	1:A:391:ASN:ND2	2.21	0.55
1:A:571:VAL:HG22	1:A:630:SER:HA	1.88	0.55
1:A:367:ILE:HG12	1:A:492:LEU:O	2.06	0.55
1:A:888:LEU:HD23	1:A:898:PRO:HA	1.89	0.55
1:A:384:ALA:HB2	1:A:390:ILE:HD11	1.89	0.55
1:A:722:GLU:O	1:A:723:ASP:HB2	2.05	0.54
1:A:978:THR:C	1:A:980:LEU:H	2.09	0.54
1:A:367:ILE:H	1:A:368:PRO:HD2	1.72	0.54
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.90	0.54
1:A:864:TYR:CD2	1:A:865:GLN:HA	2.43	0.54
1:A:350:LEU:HD11	1:A:984:LEU:HB2	1.88	0.54
1:A:392:THR:HG23	1:A:395:MET:HB2	1.90	0.54
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.90	0.54
1:A:488:LEU:O	1:A:490:PRO:HD2	2.07	0.54
1:A:890:ALA:O	1:A:891:LEU:HB2	2.08	0.54
1:A:831:ALA:HA	1:A:840:ALA:HB1	1.89	0.54
1:A:864:TYR:HD2	1:A:865:GLN:HA	1.73	0.54
1:A:872:GLN:O	1:A:876:LEU:HB2	2.08	0.54
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.89	0.54
1:A:555:LEU:HB3	1:A:913:LEU:HD22	1.90	0.53
1:A:396:PHE:O	1:A:399:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:O	1:A:540:ARG:HG2	2.07	0.53
1:A:400:LEU:HD11	1:A:1003:VAL:HG22	1.91	0.53
1:A:563:PHE:HE1	1:A:868:LEU:HD23	1.74	0.53
1:A:901:VAL:O	1:A:903:LEU:N	2.39	0.52
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.90	0.52
1:A:445:ILE:O	1:A:449:LEU:HD23	2.10	0.52
1:A:986:VAL:HG11	1:A:1007:VAL:HB	1.90	0.52
1:A:34:GLN:HG3	1:A:35:TYR:H	1.75	0.52
1:A:979:SER:OG	1:A:1015:THR:HG23	2.10	0.52
1:A:836:SER:O	1:A:838:GLY:N	2.43	0.52
1:A:820:ASN:HD22	1:A:820:ASN:N	2.07	0.52
1:A:862:MET:C	1:A:864:TYR:H	2.11	0.52
1:A:149:MET:HB3	1:A:153:ASP:HB3	1.92	0.52
1:A:45:ILE:O	1:A:89:GLN:HA	2.09	0.52
1:A:390:ILE:HG22	1:A:390:ILE:O	2.10	0.52
1:A:40:PRO:HD2	1:A:674:LEU:HD21	1.92	0.52
1:A:831:ALA:O	1:A:832:ALA:HB2	2.09	0.52
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.92	0.52
1:A:452:VAL:HG12	1:A:932:LEU:HD22	1.92	0.51
1:A:1000:GLN:HA	1:A:1003:VAL:HG12	1.93	0.51
1:A:682:PHE:HB3	1:A:827:ILE:HG22	1.93	0.51
1:A:375:VAL:HG21	1:A:405:LEU:HB2	1.92	0.51
1:A:450:SER:HB3	1:A:454:VAL:HG22	1.92	0.51
1:A:782:LEU:HB2	1:A:783:PRO:HD2	1.93	0.51
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.92	0.50
1:A:126:GLY:O	1:A:127:VAL:HG22	2.11	0.50
1:A:897:ILE:N	1:A:898:PRO:CD	2.73	0.50
1:A:984:LEU:HA	1:A:987:MET:HB2	1.92	0.50
1:A:1027:VAL:HG23	1:A:1028:VAL:HG23	1.93	0.50
1:A:974:PRO:C	1:A:976:LEU:H	2.15	0.50
1:A:1008:MET:HA	1:A:1011:MET:HB2	1.93	0.50
1:A:562:SER:HB2	1:A:922:THR:HG23	1.93	0.50
1:A:640:GLU:HA	1:A:643:LYS:NZ	2.25	0.50
1:A:722:GLU:O	1:A:723:ASP:CB	2.59	0.50
1:A:463:THR:OG1	1:A:867:ARG:HB2	2.12	0.50
1:A:973:ARG:CB	1:A:974:PRO:HD3	2.36	0.50
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.93	0.50
1:A:454:VAL:HG13	1:A:475:VAL:HG21	1.94	0.49
1:A:21:LEU:O	1:A:25:LEU:HB2	2.11	0.49
1:A:1022:VAL:O	1:A:1024:VAL:N	2.41	0.49
1:A:718:PRO:HA	1:A:827:ILE:H	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:HG3	1:A:472:ILE:HD13	1.93	0.49
1:A:990:VAL:HG23	1:A:991:ILE:HG13	1.93	0.49
1:A:712:MET:HG3	1:A:835:LYS:HD3	1.94	0.49
1:A:686:ASP:HB3	1:A:823:PRO:HG2	1.94	0.49
1:A:594:VAL:C	1:A:596:HIS:H	2.15	0.49
1:A:172:VAL:HG11	1:A:175:VAL:HG23	1.94	0.49
1:A:355:MET:HB3	1:A:365:THR:HG22	1.94	0.49
1:A:410:ILE:HG13	1:A:411:VAL:N	2.27	0.48
1:A:166:ILE:O	1:A:169:THR:N	2.37	0.48
1:A:38:ILE:H	1:A:38:ILE:HD13	1.79	0.48
1:A:465:ALA:O	1:A:469:GLN:N	2.46	0.48
1:A:144:ASN:OD1	1:A:146:ASP:O	2.31	0.48
1:A:360:GLN:O	1:A:361:ASN:HB2	2.12	0.48
1:A:973:ARG:CB	1:A:974:PRO:CD	2.91	0.48
1:A:472:ILE:O	1:A:476:SER:N	2.40	0.48
1:A:617:PHE:O	1:A:618:ALA:HB3	2.13	0.48
1:A:885:PHE:HD1	1:A:898:PRO:HB3	1.78	0.48
1:A:924:ASP:O	1:A:928:GLN:HB2	2.14	0.48
1:A:896:SER:HB2	1:A:1032:ARG:HG3	1.95	0.48
1:A:383:LEU:HB3	1:A:390:ILE:HG13	1.96	0.48
1:A:149:MET:O	1:A:150:THR:CB	2.61	0.48
1:A:970:MET:O	1:A:971:ARG:HB3	2.13	0.47
1:A:249:ILE:HB	1:A:262:LEU:CD2	2.44	0.47
1:A:809:TRP:O	1:A:810:GLU:HB3	2.13	0.47
1:A:456:MET:HG2	1:A:467:TYR:HB3	1.95	0.47
1:A:925:VAL:O	1:A:925:VAL:HG12	2.14	0.47
1:A:222:THR:OG1	1:A:223:PRO:HD3	2.15	0.47
1:A:146:ASP:O	1:A:147:GLY:C	2.53	0.47
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.33	0.47
1:A:912:ALA:HB1	1:A:927:PHE:HE1	1.80	0.47
1:A:160:ALA:HA	1:A:767:ARG:NH1	2.30	0.47
1:A:864:TYR:HD1	1:A:868:LEU:HD11	1.79	0.47
1:A:23:GLY:HA3	1:A:377:LEU:O	2.15	0.47
1:A:682:PHE:HB3	1:A:827:ILE:HG21	1.97	0.46
1:A:355:MET:HE1	1:A:359:LEU:HD11	1.98	0.46
1:A:975:ILE:HD12	1:A:975:ILE:H	1.81	0.46
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.96	0.46
1:A:921:LEU:HD11	1:A:1002:ALA:HA	1.96	0.46
1:A:249:ILE:HB	1:A:262:LEU:HD23	1.97	0.46
1:A:975:ILE:O	1:A:975:ILE:HG22	2.14	0.46
1:A:18:ILE:HG22	1:A:19:ILE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:HA	1:A:466:ILE:HD12	1.98	0.46
1:A:901:VAL:C	1:A:903:LEU:N	2.68	0.46
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.98	0.46
1:A:456:MET:HG3	1:A:467:TYR:CB	2.36	0.46
1:A:873:ALA:N	1:A:874:PRO:CD	2.79	0.46
1:A:330:THR:N	1:A:331:PRO:CD	2.79	0.46
1:A:1013:THR:O	1:A:1015:THR:N	2.49	0.46
1:A:462:SER:C	1:A:464:GLY:H	2.20	0.46
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.45	0.45
1:A:488:LEU:HG	1:A:489:THR:H	1.80	0.45
1:A:131:LYS:HD2	1:A:295:THR:HB	1.98	0.45
1:A:570:GLY:HA2	1:A:637:ARG:HH22	1.81	0.45
1:A:831:ALA:O	1:A:832:ALA:CB	2.65	0.45
1:A:831:ALA:HA	1:A:840:ALA:CB	2.46	0.45
1:A:139:VAL:O	1:A:326:PRO:HD2	2.16	0.45
1:A:151:GLN:HG2	1:A:278:ILE:HG22	1.98	0.45
1:A:895:TRP:HA	1:A:898:PRO:HG2	1.98	0.45
1:A:968:VAL:HA	1:A:971:ARG:NH2	2.32	0.45
1:A:442:LEU:O	1:A:482:VAL:HG21	2.16	0.45
1:A:354:VAL:O	1:A:354:VAL:HG12	2.17	0.45
1:A:581:GLY:CA	1:A:582:ALA:HB3	2.47	0.45
1:A:419:VAL:HA	1:A:423:GLU:HG2	1.99	0.45
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.98	0.45
1:A:859:TRP:HB2	1:A:863:SER:OG	2.17	0.45
1:A:616:GLY:HA3	1:A:624:THR:HB	1.98	0.45
1:A:392:THR:C	1:A:394:THR:H	2.20	0.45
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.17	0.45
1:A:355:MET:HE3	1:A:359:LEU:HD11	1.98	0.45
1:A:704:ALA:O	1:A:708:LYS:HG2	2.17	0.45
1:A:65:ILE:HD12	1:A:111:LEU:HD12	1.99	0.45
1:A:819:TYR:HE1	1:A:860:THR:HG23	1.81	0.45
1:A:379:THR:HG21	1:A:473:THR:HG23	1.99	0.45
1:A:34:GLN:HB3	1:A:333:VAL:HG22	1.98	0.45
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.99	0.45
1:A:878:ALA:O	1:A:882:ILE:HG12	2.17	0.44
1:A:448:VAL:HG11	1:A:888:LEU:HD13	1.99	0.44
1:A:452:VAL:CG1	1:A:932:LEU:HD22	2.47	0.44
1:A:664:PHE:O	1:A:665:ALA:HB3	2.17	0.44
1:A:668:LEU:HA	1:A:669:PRO:HD3	1.87	0.44
1:A:228:GLN:HE21	1:A:229:GLN:H	1.64	0.44
1:A:1020:PHE:HE1	1:A:1021:PHE:CE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:PRO:HG3	1:A:469:GLN:CD	2.38	0.44
1:A:702:LEU:HD11	1:A:847:LEU:HB3	2.00	0.44
1:A:897:ILE:N	1:A:898:PRO:HD2	2.33	0.44
1:A:819:TYR:HE1	1:A:860:THR:CG2	2.30	0.44
1:A:438:ILE:HG22	1:A:944:LEU:HD21	2.00	0.44
1:A:149:MET:O	1:A:150:THR:HB	2.18	0.44
1:A:392:THR:C	1:A:394:THR:N	2.71	0.44
1:A:723:ASP:HA	1:A:813:SER:HA	2.00	0.43
1:A:489:THR:OG1	1:A:490:PRO:HD2	2.18	0.43
1:A:1014:ALA:O	1:A:1018:ALA:HB3	2.18	0.43
1:A:905:VAL:CG2	1:A:906:PRO:HD3	2.48	0.43
1:A:575:MET:HA	1:A:626:ILE:HG22	2.00	0.43
1:A:826:GLU:HB3	1:A:827:ILE:O	2.18	0.43
1:A:360:GLN:O	1:A:361:ASN:CB	2.65	0.43
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:721:LEU:HD23	1:A:722:GLU:N	2.33	0.43
1:A:33:ALA:HB1	1:A:299:ALA:HB3	2.00	0.43
1:A:598:TYR:HB3	1:A:606:VAL:HG21	2.00	0.43
1:A:162:MET:O	1:A:166:ILE:HG12	2.19	0.43
1:A:949:ALA:HB3	1:A:1028:VAL:HG21	2.01	0.43
1:A:864:TYR:CD1	1:A:868:LEU:HD11	2.54	0.43
1:A:556:PHE:CD1	1:A:913:LEU:HD23	2.54	0.43
1:A:394:THR:HB	1:A:470:PHE:HE2	1.83	0.43
1:A:372:VAL:N	1:A:373:PRO:HD2	2.34	0.43
1:A:466:ILE:HA	1:A:469:GLN:HB2	2.00	0.42
1:A:892:TYR:O	1:A:897:ILE:HD13	2.19	0.42
1:A:897:ILE:HG23	1:A:943:ILE:HD11	2.00	0.42
1:A:317:PHE:HE2	1:A:323:ILE:HD11	1.84	0.42
1:A:240:LEU:HD22	1:A:245:GLU:HB3	2.01	0.42
1:A:926:TYR:O	1:A:930:GLY:N	2.53	0.42
1:A:114:ALA:HA	1:A:117:LEU:HD13	2.01	0.42
1:A:537:SER:O	1:A:538:THR:C	2.57	0.42
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.91	0.42
1:A:912:ALA:HB1	1:A:927:PHE:CE1	2.54	0.42
1:A:62:THR:HG23	1:A:88:VAL:HG21	2.00	0.42
1:A:470:PHE:C	1:A:472:ILE:N	2.72	0.42
1:A:987:MET:N	1:A:988:PRO:CD	2.82	0.42
1:A:318:PRO:HB2	1:A:319:SER:H	1.66	0.42
1:A:139:VAL:HB	1:A:327:TYR:HB3	2.01	0.42
1:A:819:TYR:CE1	1:A:860:THR:HG23	2.54	0.42
1:A:310:LEU:HD21	1:A:323:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:O	1:A:879:ILE:HG22	2.20	0.42
1:A:56:THR:HG23	1:A:57:VAL:N	2.35	0.42
1:A:1008:MET:HG3	1:A:1009:GLY:N	2.35	0.42
1:A:65:ILE:HD11	1:A:118:LEU:HD11	2.02	0.42
1:A:690:LEU:HB3	1:A:691:GLY:H	1.75	0.42
1:A:815:ARG:CG	1:A:815:ARG:NH1	2.83	0.41
1:A:473:THR:HA	1:A:476:SER:HB2	2.00	0.41
1:A:764:ASP:HB3	1:A:769:LYS:HD3	2.02	0.41
1:A:178:PHE:HB2	1:A:288:GLY:H	1.85	0.41
1:A:183:ALA:HB3	1:A:185:ARG:HD3	2.02	0.41
1:A:634:TRP:HA	1:A:637:ARG:HE	1.85	0.41
1:A:606:VAL:HG13	1:A:629:VAL:HG13	2.02	0.41
1:A:817:GLU:HB2	1:A:824:SER:O	2.21	0.41
1:A:602:GLU:HG2	1:A:605:ASN:HB2	2.03	0.41
1:A:863:SER:O	1:A:864:TYR:CD2	2.67	0.41
1:A:133:SER:H	1:A:292:LYS:HE3	1.85	0.41
1:A:782:LEU:CB	1:A:783:PRO:HD2	2.49	0.41
1:A:144:ASN:HA	1:A:320:GLY:O	2.21	0.41
1:A:867:ARG:CG	1:A:868:LEU:N	2.82	0.41
1:A:864:TYR:CG	1:A:866:GLU:N	2.89	0.41
1:A:991:ILE:O	1:A:993:THR:N	2.49	0.41
1:A:330:THR:N	1:A:331:PRO:HD2	2.36	0.41
1:A:743:ILE:HA	1:A:746:ILE:HD12	2.03	0.41
1:A:439:GLN:HG3	1:A:440:GLY:N	2.36	0.41
1:A:886:LEU:O	1:A:887:CYS:CB	2.68	0.40
1:A:226:LYS:H	1:A:226:LYS:HG3	1.62	0.40
1:A:564:LEU:HA	1:A:565:PRO:HD3	1.92	0.40
1:A:862:MET:SD	1:A:863:SER:N	2.94	0.40
1:A:570:GLY:O	1:A:631:LEU:HB2	2.19	0.40
1:A:218:GLN:HB3	1:A:233:SER:HA	2.03	0.40
1:A:621:GLY:C	1:A:623:ASN:H	2.24	0.40
1:A:1021:PHE:O	1:A:1022:VAL:O	2.40	0.40
1:A:453:PHE:C	1:A:471:SER:HB3	2.41	0.40
1:A:305:ALA:HA	1:A:308:ALA:HB3	2.04	0.40
1:A:384:ALA:O	1:A:385:ALA:HB2	2.21	0.40
1:A:28:LEU:C	1:A:30:LEU:H	2.25	0.40
1:A:930:GLY:HA2	1:A:933:THR:OG1	2.21	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	A	1012/1053 (96%)	770 (76%)	179 (18%)	63 (6%)	2 26

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	150	THR
1	A	166	ILE
1	A	167	SER
1	A	358	PHE
1	A	361	ASN
1	A	386	PHE
1	A	390	ILE
1	A	470	PHE
1	A	489	THR
1	A	703	LEU
1	A	723	ASP
1	A	802	SER
1	A	832	ALA
1	A	837	THR
1	A	971	ARG
1	A	982	PHE
1	A	983	ILE
1	A	1014	ALA
1	A	1022	VAL
1	A	127	VAL
1	A	147	GLY
1	A	256	ASP
1	A	318	PRO
1	A	539	GLY
1	A	557	VAL
1	A	581	GLY
1	A	673	GLU

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Mol	Chain	Res	Type
1	A	674	LEU
1	A	677	ALA
1	A	862	MET
1	A	975	ILE
1	A	991	ILE
1	A	294	ALA
1	A	297	ALA
1	A	344	LEU
1	A	381	ALA
1	A	427	PRO
1	A	538	THR
1	A	638	PRO
1	A	864	TYR
1	A	866	GLU
1	A	867	ARG
1	A	898	PRO
1	A	901	VAL
1	A	954	ASP
1	A	367	ILE
1	A	428	LYS
1	A	579	PRO
1	A	659	LYS
1	A	709	HIS
1	A	713	LEU
1	A	721	LEU
1	A	902	MET
1	A	1013	THR
1	A	226	LYS
1	A	385	ALA
1	A	464	GLY
1	A	809	TRP
1	A	827	ILE
1	A	968	VAL
1	A	1023	PRO
1	A	19	ILE

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	A	826/858 (96%)	702 (85%)	124 (15%)	3 26

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	10	ILE
1	A	13	TRP
1	A	25	LEU
1	A	38	ILE
1	A	49	TYR
1	A	58	GLN
1	A	68	ASN
1	A	108	GLN
1	A	125	GLN
1	A	145	THR
1	A	152	GLU
1	A	162	MET
1	A	176	GLN
1	A	177	LEU
1	A	194	ASN
1	A	208	LYS
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	239	ARG
1	A	252	LYS
1	A	255	GLN
1	A	261	LEU
1	A	262	LEU
1	A	265	VAL
1	A	277	ILE
1	A	293	LEU
1	A	298	ASN
1	A	313	MET
1	A	330	THR
1	A	344	LEU
1	A	357	LEU
1	A	366	LEU
1	A	375	VAL
1	A	377	LEU

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Mol	Chain	Res	Type
1	A	388	PHE
1	A	391	ASN
1	A	395	MET
1	A	404	LEU
1	A	410	ILE
1	A	415	ASN
1	A	423	GLU
1	A	429	GLU
1	A	432	ARG
1	A	452	VAL
1	A	458	PHE
1	A	469	GLN
1	A	473	THR
1	A	480	LEU
1	A	482	VAL
1	A	483	LEU
1	A	489	THR
1	A	513	PHE
1	A	516	PHE
1	A	518	ARG
1	A	519	MET
1	A	520	PHE
1	A	535	LEU
1	A	540	ARG
1	A	546	LEU
1	A	552	MET
1	A	555	LEU
1	A	556	PHE
1	A	566	ASP
1	A	567	GLU
1	A	568	ASP
1	A	569	GLN
1	A	586	ARG
1	A	588	GLN
1	A	601	LYS
1	A	637	ARG
1	A	643	LYS
1	A	650	ARG
1	A	657	GLN
1	A	659	LYS
1	A	663	VAL
1	A	674	LEU

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Mol	Chain	Res	Type
1	A	693	GLU
1	A	703	LEU
1	A	709	HIS
1	A	714	THR
1	A	743	ILE
1	A	760	ASN
1	A	767	ARG
1	A	795	ASP
1	A	797	GLN
1	A	798	MET
1	A	815	ARG
1	A	820	ASN
1	A	843	LEU
1	A	847	LEU
1	A	853	THR
1	A	858	ASP
1	A	860	THR
1	A	862	MET
1	A	863	SER
1	A	864	TYR
1	A	865	GLN
1	A	868	LEU
1	A	871	ASN
1	A	872	GLN
1	A	884	VAL
1	A	895	TRP
1	A	907	LEU
1	A	913	LEU
1	A	921	LEU
1	A	922	THR
1	A	940	LYS
1	A	944	LEU
1	A	952	LEU
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	978	THR
1	A	982	PHE
1	A	984	LEU
1	A	989	LEU
1	A	991	ILE
1	A	1011	MET

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Mol	Chain	Res	Type
1	A	1013	THR
1	A	1022	VAL
1	A	1031	ARG
1	A	1033	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	58	GLN
1	A	104	GLN
1	A	108	GLN
1	A	112	GLN
1	A	123	GLN
1	A	151	GLN
1	A	176	GLN
1	A	211	ASN
1	A	228	GLN
1	A	254	ASN
1	A	298	ASN
1	A	360	GLN
1	A	391	ASN
1	A	604	ASN
1	A	605	ASN
1	A	622	GLN
1	A	657	GLN
1	A	687	GLN
1	A	744	ASN
1	A	760	ASN
1	A	820	ASN
1	A	871	ASN

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

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, 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	A	1016/1053 (96%)	0.23	46 (4%) 37 23	20, 93, 179, 203	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	GLY	6.7
1	A	960	LEU	5.9
1	A	1021	PHE	5.2
1	A	460	GLY	5.0
1	A	425	LEU	5.0
1	A	407	ASP	4.3
1	A	833	PRO	4.2
1	A	1020	PHE	3.8
1	A	1031	ARG	3.5
1	A	667	ASN	3.5
1	A	426	PRO	3.4
1	A	31	PRO	3.3
1	A	410	ILE	3.3
1	A	409	ALA	3.2
1	A	961	ILE	3.2
1	A	941	ASN	3.2
1	A	497	LEU	3.1
1	A	495	THR	3.1
1	A	871	ASN	3.0
1	A	401	ALA	2.9
1	A	406	VAL	2.8
1	A	1027	VAL	2.7
1	A	829	GLY	2.7
1	A	677	ALA	2.7
1	A	830	GLN	2.7
1	A	290	GLY	2.7
1	A	405	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	389	SER	2.5
1	A	705	GLU	2.5
1	A	1025	PHE	2.5
1	A	872	GLN	2.5
1	A	896	SER	2.5
1	A	138	MET	2.4
1	A	303	ALA	2.4
1	A	975	ILE	2.4
1	A	676	THR	2.4
1	A	474	ILE	2.4
1	A	412	VAL	2.3
1	A	362	PHE	2.2
1	A	1026	PHE	2.2
1	A	400	LEU	2.2
1	A	717	ARG	2.2
1	A	1028	VAL	2.2
1	A	832	ALA	2.1
1	A	692	HIS	2.1
1	A	292	LYS	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 carbohydrates 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.