



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:19 PM UTC

PDB ID : 2HQD / pdb_00002hqd
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

<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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

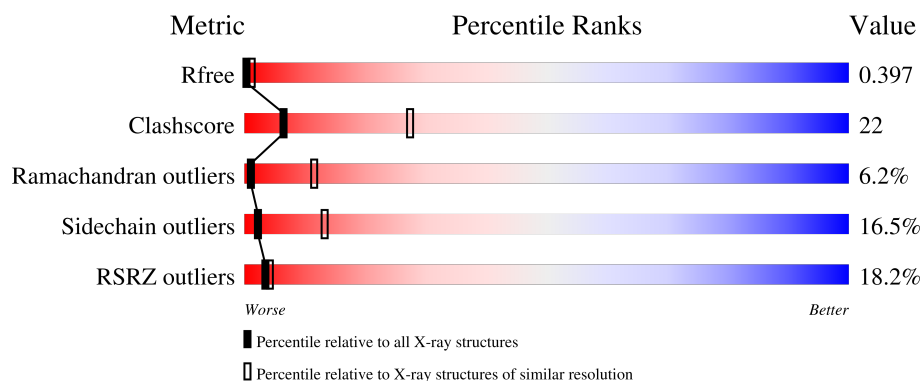
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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 $\leq 5\%$. 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 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
			Total	C	N	O	S			
1	A	1016	7718	4964	1276	1435	43	0	0	0

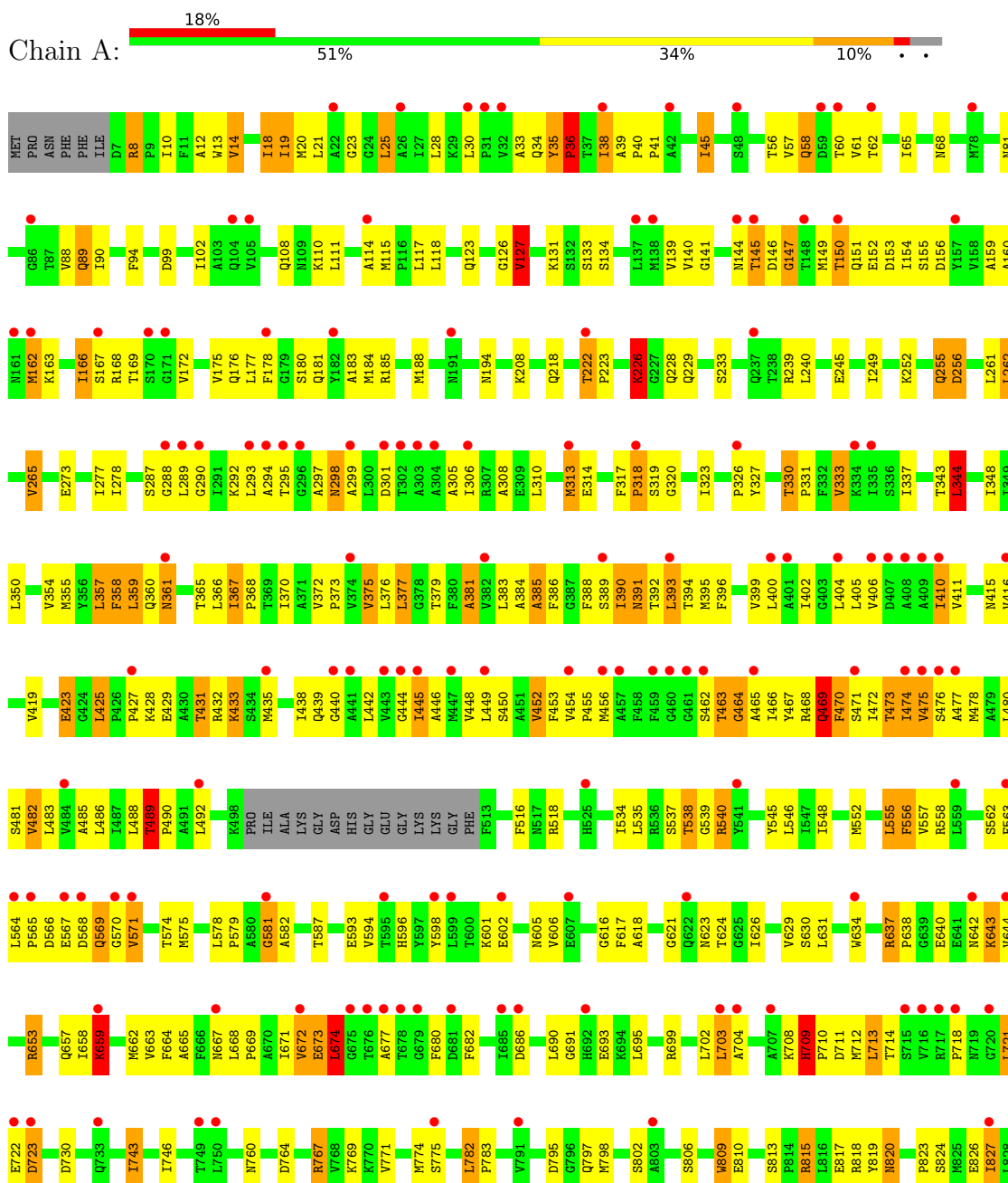
There are 5 discrepancies between the modelled and reference sequences:

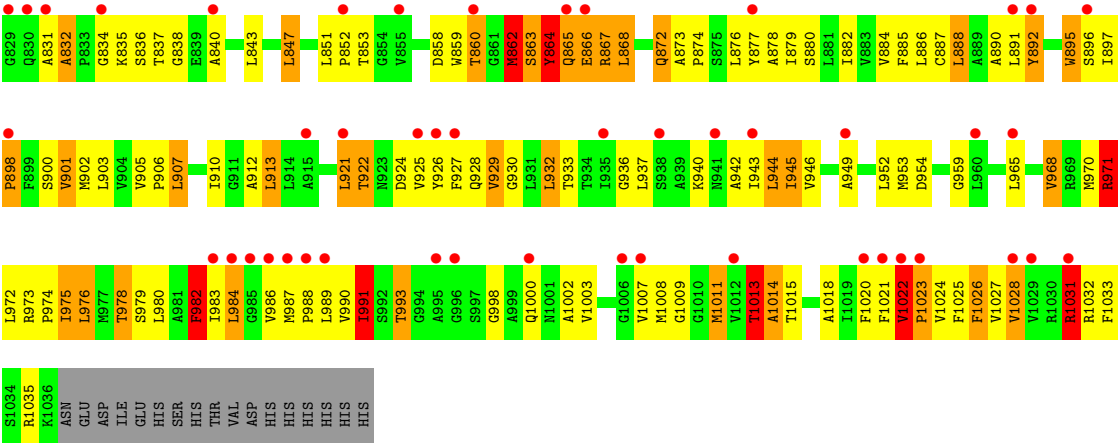
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	ALA	ASP	engineered mutation	UNP P31224
A	1050	HIS	-	cloning artifact	UNP P31224
A	1051	HIS	-	cloning artifact	UNP P31224
A	1052	HIS	-	cloning artifact	UNP P31224
A	1053	HIS	-	cloning artifact	UNP P31224

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	145.03Å 145.03Å 513.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.65 20.00 – 3.65	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-3.65) 89.2 (20.00-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.76 (at 3.66Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.261 , 0.303 0.369 , 0.397	Depositor DCC
R_{free} test set	1101 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	101.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	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.*

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	0.91	19/7861 (0.2%)	0.98	25/10676 (0.2%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	ASP	C-O	18.26	1.47	1.24
1	A	1031	ARG	NE-CZ	18.10	1.52	1.33
1	A	1035	ARG	CZ-NH1	13.83	1.52	1.32
1	A	433	LYS	CD-CE	12.59	1.90	1.52
1	A	1031	ARG	CZ-NH1	12.41	1.50	1.32
1	A	444	GLY	N-CA	10.25	1.60	1.45
1	A	892	TYR	C-O	9.70	1.37	1.24
1	A	1035	ARG	NE-CZ	7.34	1.41	1.33
1	A	255	GLN	C-N	7.24	1.43	1.33
1	A	81	ASN	C-O	7.15	1.30	1.24
1	A	662	MET	SD-CE	6.37	1.95	1.79
1	A	89	GLN	CD-NE2	6.25	1.46	1.33
1	A	145	THR	C-O	6.11	1.32	1.23
1	A	998	GLY	C-O	5.59	1.30	1.23
1	A	89	GLN	CD-OE1	5.40	1.33	1.23
1	A	256	ASP	C-N	5.25	1.41	1.33
1	A	593	GLU	CB-CG	5.21	1.68	1.52
1	A	255	GLN	C-O	5.20	1.30	1.23
1	A	653	ARG	CZ-NH1	5.18	1.40	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	TYR	C-N-CD	-16.10	85.18	120.60
1	A	35	TYR	CA-C-N	15.48	164.15	127.00
1	A	35	TYR	C-N-CA	15.48	164.15	127.00
1	A	1031	ARG	NE-CZ-NH2	-12.18	108.24	119.20
1	A	89	GLN	OE1-CD-NE2	8.09	130.69	122.60
1	A	929	VAL	N-CA-C	-7.66	106.03	113.53
1	A	425	LEU	CA-C-N	6.56	127.13	120.38
1	A	425	LEU	C-N-CA	6.56	127.13	120.38
1	A	1035	ARG	NE-CZ-NH2	-6.46	113.38	119.20
1	A	945	ILE	N-CA-C	-6.45	107.58	113.71
1	A	1031	ARG	CD-NE-CZ	-6.19	115.73	124.40
1	A	463	THR	N-CA-C	-6.03	105.00	113.20
1	A	864	TYR	N-CA-C	5.77	123.10	110.80
1	A	255	GLN	O-C-N	5.57	129.09	122.46
1	A	1026	PHE	N-CA-C	-5.56	106.28	112.57
1	A	1035	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	445	ILE	N-CA-C	-5.38	107.18	111.81
1	A	110	LYS	N-CA-C	-5.29	107.48	114.31
1	A	782	LEU	CA-C-N	5.22	126.37	119.84
1	A	782	LEU	C-N-CA	5.22	126.37	119.84
1	A	888	LEU	N-CA-C	-5.16	106.83	113.02
1	A	36	PRO	CA-N-CD	-5.12	104.33	111.50
1	A	1028	VAL	N-CA-C	-5.10	107.78	112.83
1	A	333	VAL	CA-CB-CG2	-5.09	101.74	110.40
1	A	393	LEU	N-CA-C	-5.01	107.52	113.38

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 ⓘ

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	342	0
All	All	7718	0	7878	342	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 22.

All (342) 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:CE	1:A:433:LYS:CD	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:58:GLN:HE22	1:A:818:ARG:HD2	1.27	0.98
1:A:680:PHE:HA	1:A:862:MET:HG3	1.45	0.98
1:A:355:MET:HE3	1:A:359:LEU:HD11	1.44	0.97
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:HG3	1:A:815:ARG:HH11	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:863:SER:C	1:A:864:TYR:CD2	2.69	0.70
1:A:901:VAL:C	1:A:903:LEU:H	1.99	0.70
1:A:39:ALA:HB2	1:A:672:VAL:HG11	1.72	0.70
1:A:416:VAL:HG22	1:A:431:THR:HG21	1.72	0.70
1:A:699:ARG:HG2	1:A:827:ILE:HD11	1.73	0.70
1:A:188:MET:H	1:A:775:SER:HA	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1:A:433:LYS:CG	2.71	0.68
1:A:867:ARG:HG3	1:A:868:LEU:H	1.59	0.68
1:A:162:MET:HB3	1:A:313:MET:HG2	1.75	0.67
1:A:188:MET:N	1:A:775:SER:HA	2.09	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
1:A:454:VAL:HG23	1:A:455:PRO:HD3	1.77	0.66
1:A:56:THR:O	1:A:60:THR:HG22	1.97	0.65
1:A:470:PHE:CG	1:A:473:THR:HB	2.31	0.65
1:A:709:HIS:N	1:A:710:PRO:CD	2.59	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: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:926:TYR:HB3	1:A:1003:VAL:CG2	2.20	0.63
1:A:900:SER:HB3	1:A:946:VAL:HG21	1.79	0.63
1:A:134:SER:H	1:A:292:LYS:HE3	1.62	0.63
1:A:965:LEU:HA	1:A:968:VAL:HG12	1.79	0.63
1:A:470:PHE:C	1:A:472:ILE:H	2.06	0.62
1:A:34:GLN:HB3	1:A:333:VAL:CG2	2.29	0.62
1:A:885:PHE:HA	1:A:888:LEU:HD22	1.81	0.62
1:A:481:SER:O	1:A:485:ALA:HB3	2.01	0.61
1:A:556:PHE:C	1:A:558:ARG:H	2.09	0.61
1:A:389:SER:HB3	1:A:391:ASN:HD21	1.65	0.61
1:A:907:LEU:O	1:A:910:ILE:HG22	2.01	0.61
1:A:982:PHE:O	1:A:984:LEU:N	2.34	0.61
1:A:184:MET:HE3	1:A:184:MET:HA	1.83	0.60
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:991:ILE:C	1:A:993:THR:H	2.09	0.60
1:A:433:LYS:HE2	1:A:433:LYS:HB3	1.84	0.60
1:A:863:SER:O	1:A:864:TYR:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:HB3	1:A:333:VAL:HG21	1.84	0.60
1:A:978:THR:C	1:A:980:LEU:H	2.09	0.60
1:A:640:GLU:HA	1:A:643:LYS:HZ2	1.68	0.59
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.84	0.59
1:A:180:SER:OG	1:A:273:GLU:HG2	2.03	0.59
1:A:463:THR:H	1:A:867:ARG:HD2	1.67	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:355:MET:HE2	1:A:368:PRO:HG3	1.84	0.58
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:159:ALA:HA	1:A:163:LYS:HB2	1.84	0.58
1:A:682:PHE:HB3	1:A:827:ILE:CG2	2.34	0.58
1:A:710:PRO:HA	1:A:713:LEU:HA	1.85	0.58
1:A:864:TYR:CB	1:A:867:ARG:HG2	2.33	0.58
1:A:159:ALA:HA	1:A:163:LYS:CB	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:862:MET:C	1:A:864:TYR:H	2.11	0.57
1:A:156:ASP:HA	1:A:181:GLN:HA	1.86	0.56
1:A:8:ARG:H	1:A:8:ARG:HE	1.53	0.56
1:A:449:LEU:HD13	1:A:936:GLY:HA3	1.88	0.56
1:A:482:VAL:O	1:A:486:LEU:HB2	2.05	0.56
1:A:400:LEU:HD21	1:A:1003:VAL:HG21	1.87	0.56
1:A:545:TYR:HB2	1:A:1022:VAL:HG11	1.87	0.56
1:A:971:ARG:O	1:A:974:PRO:HD2	2.05	0.56
1:A:446:ALA:HB1	1:A:478:MET:HE3	1.87	0.56
1:A:262:LEU:HA	1:A:265:VAL:HG12	1.86	0.56
1:A:569:GLN:HG3	1:A:668:LEU:HB2	1.88	0.56
1:A:1013:THR:HG23	1:A:1014:ALA:H	1.71	0.56
1:A:115:MET:HE2	1:A:123:GLN:HG3	1.87	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:974:PRO:C	1:A:976:LEU:H	2.15	0.55
1:A:367:ILE:HG12	1:A:492:LEU:O	2.06	0.55
1:A:384:ALA:HB2	1:A:390:ILE:HD11	1.89	0.55
1:A:888:LEU:HD23	1:A:898:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:GLU:O	1:A:723:ASP:HB2	2.05	0.54
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.90	0.54
1:A:367:ILE:H	1:A:368:PRO:HD2	1.72	0.54
1:A:350:LEU:HD11	1:A:984:LEU:HB2	1.88	0.54
1:A:864:TYR:CD2	1:A:865:GLN:HA	2.43	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:831:ALA:HA	1:A:840:ALA:HB1	1.89	0.54
1:A:890:ALA:O	1:A:891:LEU:HB2	2.08	0.54
1:A:45:ILE:HD12	1:A:90:ILE:HB	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: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
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:594:VAL:C	1:A:596:HIS:H	2.15	0.53
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:901:VAL:O	1:A:903:LEU:N	2.39	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:836:SER:O	1:A:838:GLY:N	2.43	0.52
1:A:979:SER:OG	1:A:1015:THR:HG23	2.10	0.52
1:A:820:ASN:N	1:A:820:ASN:HD22	2.07	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:146:ASP:O	1:A:147:GLY:C	2.53	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:154:ILE:HG22	1:A:287:SER:HB3	1.92	0.52
1:A:831:ALA:O	1:A:832:ALA:HB2	2.09	0.51
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:375:VAL:HG21	1:A:405:LEU:HB2	1.92	0.51
1:A:682:PHE:HB3	1:A:827:ILE:HG22	1.93	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:435:MET:HE2	1:A:486:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLY:O	1:A:127:VAL:HG22	2.11	0.50
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.92	0.50
1:A:640:GLU:HA	1:A:643:LYS:NZ	2.25	0.50
1:A:897:ILE:N	1:A:898:PRO:CD	2.73	0.50
1:A:462:SER:C	1:A:464:GLY:H	2.20	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: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:722:GLU:O	1:A:723:ASP:CB	2.59	0.50
1:A:99:ASP:HB3	1:A:102:ILE:HG22	1.93	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:21:LEU:O	1:A:25:LEU:HB2	2.11	0.49
1:A:454:VAL:HG13	1:A:475:VAL:HG21	1.94	0.49
1:A:392:THR:C	1:A:394:THR:H	2.20	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
1:A:468:ARG:HG3	1:A:472:ILE:HD13	1.93	0.49
1:A:712:MET:HG3	1:A:835:LYS:HD3	1.94	0.49
1:A:990:VAL:HG23	1:A:991:ILE:HG13	1.93	0.49
1:A:172:VAL:HG11	1:A:175:VAL:HG23	1.94	0.49
1:A:686:ASP:HB3	1:A:823:PRO:HG2	1.94	0.49
1:A:36:PRO:HG3	1:A:469:GLN:CD	2.38	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:38:ILE:HD13	1:A:38:ILE:H	1.79	0.48
1:A:166:ILE:O	1:A:169:THR:N	2.37	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:392:THR:C	1:A:394:THR:N	2.71	0.48
1:A:465:ALA:O	1:A:469:GLN:N	2.46	0.48
1:A:472:ILE:O	1:A:476:SER:N	2.40	0.48
1:A:973:ARG:CB	1:A:974:PRO:CD	2.91	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:896:SER:HB2	1:A:1032:ARG:HG3	1.95	0.48
1:A:924:ASP:O	1:A:928:GLN:HB2	2.14	0.48
1:A:383:LEU:HB3	1:A:390:ILE:HG13	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:TRP:O	1:A:810:GLU:HB3	2.13	0.47
1:A:222:THR:OG1	1:A:223:PRO:HD3	2.15	0.47
1:A:456:MET:HG2	1:A:467:TYR:HB3	1.95	0.47
1:A:537:SER:O	1:A:538:THR:C	2.57	0.47
1:A:925:VAL:HG12	1:A:925:VAL:O	2.14	0.47
1:A:149:MET:O	1:A:150:THR:CB	2.61	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:23:GLY:HA3	1:A:377:LEU:O	2.15	0.47
1:A:864:TYR:HD1	1:A:868:LEU:HD11	1.79	0.47
1:A:470:PHE:C	1:A:472:ILE:N	2.72	0.46
1:A:682:PHE:HB3	1:A:827:ILE:HG21	1.97	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:975:ILE:HD12	1:A:975:ILE:H	1.81	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
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.98	0.46
1:A:463:THR:HA	1:A:466:ILE:HD12	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:453:PHE:C	1:A:471:SER:HB3	2.41	0.46
1:A:1013:THR:O	1:A:1015:THR:N	2.49	0.46
1:A:131:LYS:HD2	1:A:295:THR:HB	1.98	0.45
1:A:488:LEU:HG	1:A:489:THR:H	1.80	0.45
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.45	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:570:GLY:HA2	1:A:637:ARG:HH22	1.81	0.45
1:A:621:GLY:C	1:A:623:ASN:H	2.24	0.45
1:A:831:ALA:HA	1:A:840:ALA:CB	2.46	0.45
1:A:831:ALA:O	1:A:832:ALA:CB	2.65	0.45
1:A:354:VAL:O	1:A:354:VAL:HG12	2.17	0.45
1:A:442:LEU:O	1:A:482:VAL:HG21	2.16	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:372:VAL:HG11	1:A:406:VAL:HG22	1.98	0.45
1:A:419:VAL:HA	1:A:423:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:GLY:CA	1:A:582:ALA:HB3	2.47	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:28:LEU:C	1:A:30:LEU:H	2.25	0.45
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.17	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: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:379:THR:HG21	1:A:473:THR:HG23	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:228:GLN:HE21	1:A:229:GLN:H	1.64	0.44
1:A:668:LEU:HA	1:A:669:PRO:HD3	1.87	0.44
1:A:570:GLY:C	1:A:631:LEU:HD12	2.43	0.44
1:A:1020:PHE:HE1	1:A:1021:PHE:CE1	2.35	0.44
1:A:702:LEU:HD11	1:A:847:LEU:HB3	2.00	0.44
1:A:438:ILE:HG22	1:A:944:LEU:HD21	2.00	0.44
1:A:819:TYR:HE1	1:A:860:THR:CG2	2.30	0.44
1:A:897:ILE:N	1:A:898:PRO:HD2	2.33	0.44
1:A:149:MET:O	1:A:150:THR:HB	2.18	0.44
1:A:556:PHE:C	1:A:558:ARG:N	2.74	0.44
1:A:489:THR:OG1	1:A:490:PRO:HD2	2.18	0.43
1:A:723:ASP:HA	1:A:813:SER:HA	2.00	0.43
1:A:905:VAL:CG2	1:A:906:PRO:HD3	2.48	0.43
1:A:1014:ALA:O	1:A:1018:ALA:HB3	2.18	0.43
1:A:149:MET:HE3	1:A:154:ILE:HG13	2.00	0.43
1:A:575:MET:HA	1:A:626:ILE:HG22	2.00	0.43
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:360:GLN:O	1:A:361:ASN:CB	2.65	0.43
1:A:826:GLU:HB3	1:A:827:ILE:O	2.18	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:721:LEU:HD23	1:A:722:GLU:N	2.33	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:462:SER:C	1:A:464:GLY:N	2.77	0.43
1:A:556:PHE:CD1	1:A:913:LEU:HD23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:TYR:CD1	1:A:868:LEU:HD11	2.54	0.43
1:A:953:MET:HE1	1:A:959:GLY:O	2.19	0.43
1:A:372:VAL:N	1:A:373:PRO:HD2	2.34	0.43
1:A:394:THR:HB	1:A:470:PHE:HE2	1.83	0.43
1:A:468:ARG:C	1:A:470:PHE:N	2.76	0.43
1:A:240:LEU:HD22	1:A:245:GLU:HB3	2.01	0.42
1:A:317:PHE:HE2	1:A:323:ILE:HD11	1.84	0.42
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: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:39:ALA:HA	1:A:40:PRO:HD2	1.91	0.42
1:A:62:THR:HG23	1:A:88:VAL:HG21	2.00	0.42
1:A:862:MET:C	1:A:864:TYR:N	2.77	0.42
1:A:912:ALA:HB1	1:A:927:PHE:CE1	2.54	0.42
1:A:12:ALA:C	1:A:14:VAL:H	2.27	0.42
1:A:318:PRO:HB2	1:A:319:SER:H	1.66	0.42
1:A:987:MET:N	1:A:988:PRO:CD	2.82	0.42
1:A:139:VAL:HB	1:A:327:TYR:HB3	2.01	0.42
1:A:310:LEU:HD21	1:A:323:ILE:HD13	2.02	0.42
1:A:819:TYR:CE1	1:A:860:THR:HG23	2.54	0.42
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: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:978:THR:C	1:A:980:LEU:N	2.77	0.42
1:A:1008:MET:HG3	1:A:1009:GLY:N	2.35	0.42
1:A:473:THR:HA	1:A:476:SER:HB2	2.00	0.41
1:A:709:HIS:C	1:A:711:ASP:H	2.28	0.41
1:A:764:ASP:HB3	1:A:769:LYS:HD3	2.02	0.41
1:A:815:ARG:NH1	1:A:815:ARG:CG	2.83	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:991:ILE:C	1:A:993:THR:N	2.76	0.41
1:A:606:VAL:HG13	1:A:629:VAL:HG13	2.02	0.41
1:A:634:TRP:HA	1:A:637:ARG:HE	1.85	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:133:SER:H	1:A:292:LYS:HE3	1.85	0.41
1:A:144:ASN:HA	1:A:320:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:LEU:CB	1:A:783:PRO:HD2	2.49	0.41
1:A:832:ALA:C	1:A:834:GLY:H	2.29	0.41
1:A:863:SER:O	1:A:864:TYR:CD2	2.67	0.41
1:A:867:ARG:CG	1:A:868:LEU:N	2.82	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: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:439:GLN:HG3	1:A:440:GLY:N	2.36	0.41
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:886:LEU:O	1:A:887:CYS:CB	2.68	0.40
1:A:218:GLN:HB3	1:A:233:SER:HA	2.03	0.40
1:A:570:GLY:O	1:A:631:LEU:HB2	2.19	0.40
1:A:862:MET:SD	1:A:863:SER:N	2.94	0.40
1:A:901:VAL:C	1:A:903:LEU:N	2.68	0.40
1:A:979:SER:HA	1:A:1011:MET:HE1	2.02	0.40
1:A:305:ALA:HA	1:A:308:ALA:HB3	2.04	0.40
1:A:1021:PHE:O	1:A:1022:VAL:O	2.40	0.40
1:A:384:ALA:O	1:A:385:ALA:HB2	2.21	0.40
1:A:185:ARG:HH22	1:A:774:MET:HE2	1.87	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%)	1 11

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	690 (84%)	136 (16%)	2 13

All (136) 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	14	VAL
1	A	18	ILE
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	45	ILE
1	A	58	GLN
1	A	68	ASN
1	A	108	GLN
1	A	127	VAL
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	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	306	ILE
1	A	313	MET
1	A	314	GLU
1	A	330	THR
1	A	337	ILE
1	A	344	LEU
1	A	348	ILE
1	A	357	LEU
1	A	359	LEU
1	A	366	LEU
1	A	370	ILE
1	A	375	VAL
1	A	376	LEU
1	A	377	LEU
1	A	388	PHE
1	A	391	ASN
1	A	404	LEU
1	A	410	ILE

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Mol	Chain	Res	Type
1	A	415	ASN
1	A	423	GLU
1	A	425	LEU
1	A	429	GLU
1	A	431	THR
1	A	432	ARG
1	A	452	VAL
1	A	469	GLN
1	A	473	THR
1	A	474	ILE
1	A	475	VAL
1	A	480	LEU
1	A	482	VAL
1	A	483	LEU
1	A	489	THR
1	A	516	PHE
1	A	518	ARG
1	A	534	ILE
1	A	535	LEU
1	A	540	ARG
1	A	546	LEU
1	A	548	ILE
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	571	VAL
1	A	601	LYS
1	A	637	ARG
1	A	643	LYS
1	A	644	VAL
1	A	659	LYS
1	A	663	VAL
1	A	667	ASN
1	A	671	ILE
1	A	672	VAL
1	A	674	LEU
1	A	693	GLU
1	A	703	LEU

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Mol	Chain	Res	Type
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	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	932	LEU
1	A	937	LEU
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	993	THR
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	68	ASN
1	A	104	GLN
1	A	108	GLN
1	A	123	GLN
1	A	151	GLN
1	A	176	GLN
1	A	194	ASN
1	A	211	ASN
1	A	228	GLN
1	A	254	ASN
1	A	284	GLN
1	A	298	ASN
1	A	391	ASN
1	A	437	GLN
1	A	526	HIS
1	A	588	GLN
1	A	604	ASN
1	A	605	ASN
1	A	622	GLN
1	A	657	GLN
1	A	687	GLN
1	A	701	GLN
1	A	744	ASN
1	A	760	ASN
1	A	820	ASN
1	A	871	ASN
1	A	872	GLN
1	A	1000	GLN
1	A	1001	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 [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, 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%)	1.16	185 (18%) 3 4	20, 93, 179, 203	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	GLY	6.8
1	A	474	ILE	5.6
1	A	401	ALA	5.6
1	A	454	VAL	5.3
1	A	896	SER	5.2
1	A	865	GLN	5.1
1	A	461	GLY	4.9
1	A	829	GLY	4.8
1	A	941	ASN	4.8
1	A	830	GLN	4.7
1	A	31	PRO	4.7
1	A	676	THR	4.6
1	A	1028	VAL	4.3
1	A	303	ALA	4.2
1	A	984	LEU	4.2
1	A	996	GLY	4.1
1	A	445	ILE	4.1
1	A	987	MET	4.0
1	A	622	GLN	4.0
1	A	960	LEU	4.0
1	A	393	LEU	4.0
1	A	59	ASP	4.0
1	A	150	THR	3.9
1	A	568	ASP	3.9
1	A	803	ALA	3.9
1	A	299	ALA	3.8
1	A	677	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1021	PHE	3.8
1	A	460	GLY	3.8
1	A	986	VAL	3.8
1	A	667	ASN	3.7
1	A	1022	VAL	3.7
1	A	570	GLY	3.6
1	A	866	GLU	3.5
1	A	290	GLY	3.5
1	A	484	VAL	3.4
1	A	295	THR	3.3
1	A	138	MET	3.3
1	A	178	PHE	3.3
1	A	443	VAL	3.3
1	A	1031	ARG	3.2
1	A	170	SER	3.2
1	A	459	PHE	3.2
1	A	22	ALA	3.2
1	A	1006	GLY	3.2
1	A	296	GLY	3.2
1	A	162	MET	3.1
1	A	171	GLY	3.1
1	A	148	THR	3.1
1	A	634	TRP	3.1
1	A	891	LEU	3.1
1	A	995	ALA	3.1
1	A	564	LEU	3.1
1	A	301	ASP	3.1
1	A	427	PRO	3.1
1	A	898	PRO	3.1
1	A	145	THR	3.1
1	A	722	GLU	3.0
1	A	32	VAL	3.0
1	A	457	ALA	3.0
1	A	718	PRO	3.0
1	A	581	GLY	3.0
1	A	60	THR	3.0
1	A	302	THR	3.0
1	A	1020	PHE	3.0
1	A	477	ALA	3.0
1	A	389	SER	2.9
1	A	892	TYR	2.9
1	A	78	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	565	PRO	2.9
1	A	288	GLY	2.8
1	A	925	VAL	2.8
1	A	926	TYR	2.8
1	A	1023	PRO	2.8
1	A	720	GLY	2.8
1	A	678	THR	2.8
1	A	723	ASP	2.8
1	A	989	LEU	2.8
1	A	716	VAL	2.8
1	A	1029	VAL	2.8
1	A	525	HIS	2.8
1	A	435	MET	2.8
1	A	167	SER	2.7
1	A	440	GLY	2.7
1	A	294	ALA	2.7
1	A	456	MET	2.7
1	A	599	LEU	2.7
1	A	105	VAL	2.6
1	A	104	GLN	2.6
1	A	943	ILE	2.6
1	A	707	ALA	2.6
1	A	335	ILE	2.6
1	A	834	GLY	2.6
1	A	595	THR	2.5
1	A	717	ARG	2.5
1	A	571	VAL	2.5
1	A	114	ALA	2.5
1	A	465	ALA	2.5
1	A	949	ALA	2.5
1	A	852	PRO	2.5
1	A	985	GLY	2.5
1	A	775	SER	2.5
1	A	877	TYR	2.5
1	A	441	ALA	2.4
1	A	293	LEU	2.4
1	A	1000	GLN	2.4
1	A	447	MET	2.4
1	A	692	HIS	2.4
1	A	406	VAL	2.4
1	A	559	LEU	2.4
1	A	1007	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	642	ASN	2.4
1	A	476	SER	2.4
1	A	222	THR	2.4
1	A	672	VAL	2.4
1	A	400	LEU	2.4
1	A	404	LEU	2.4
1	A	831	ALA	2.4
1	A	361	ASN	2.4
1	A	855	VAL	2.4
1	A	749	THR	2.3
1	A	840	ALA	2.3
1	A	86	GLY	2.3
1	A	137	LEU	2.3
1	A	462	SER	2.3
1	A	304	ALA	2.3
1	A	318	PRO	2.3
1	A	409	ALA	2.3
1	A	410	ILE	2.3
1	A	598	TYR	2.3
1	A	938	SER	2.3
1	A	675	GLY	2.3
1	A	988	PRO	2.3
1	A	449	LEU	2.3
1	A	541	TYR	2.3
1	A	567	GLU	2.3
1	A	602	GLU	2.3
1	A	62	THR	2.2
1	A	30	LEU	2.2
1	A	471	SER	2.2
1	A	374	VAL	2.2
1	A	334	LYS	2.2
1	A	326	PRO	2.2
1	A	827	ILE	2.2
1	A	681	ASP	2.2
1	A	408	ALA	2.2
1	A	983	ILE	2.2
1	A	407	ASP	2.2
1	A	313	MET	2.2
1	A	48	SER	2.2
1	A	182	TYR	2.2
1	A	416	VAL	2.2
1	A	42	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	492	LEU	2.2
1	A	644	VAL	2.1
1	A	289	LEU	2.1
1	A	750	LEU	2.1
1	A	38	ILE	2.1
1	A	382	VAL	2.1
1	A	1012	VAL	2.1
1	A	161	ASN	2.1
1	A	935	ILE	2.1
1	A	306	ILE	2.1
1	A	685	ILE	2.1
1	A	733	GLN	2.1
1	A	921	LEU	2.1
1	A	860	THR	2.1
1	A	659	LYS	2.1
1	A	237	GLN	2.1
1	A	157	TYR	2.0
1	A	686	ASP	2.0
1	A	703	LEU	2.0
1	A	475	VAL	2.0
1	A	791	VAL	2.0
1	A	144	ASN	2.0
1	A	191	ASN	2.0
1	A	679	GLY	2.0
1	A	715	SER	2.0
1	A	915	ALA	2.0
1	A	965	LEU	2.0
1	A	563	PHE	2.0
1	A	607	GLU	2.0
1	A	927	PHE	2.0
1	A	26	ALA	2.0
1	A	704	ALA	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 oligosaccharides 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.