



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2016 – 02:20 AM EDT

PDB ID : 4ZLL
Title : Crystal structure of transporter AcrB triple mutant
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-05-01
Resolution : 3.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

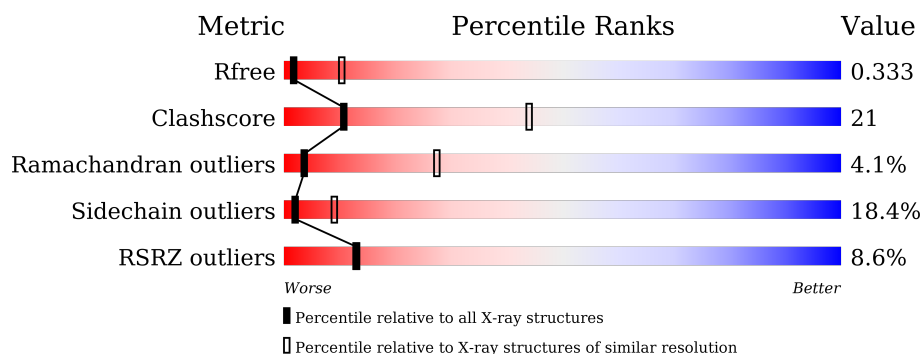
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.36 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7837 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	A	1034	Total	C	N	O	S	0	0	0
			7837	5040	1293	1460	44			

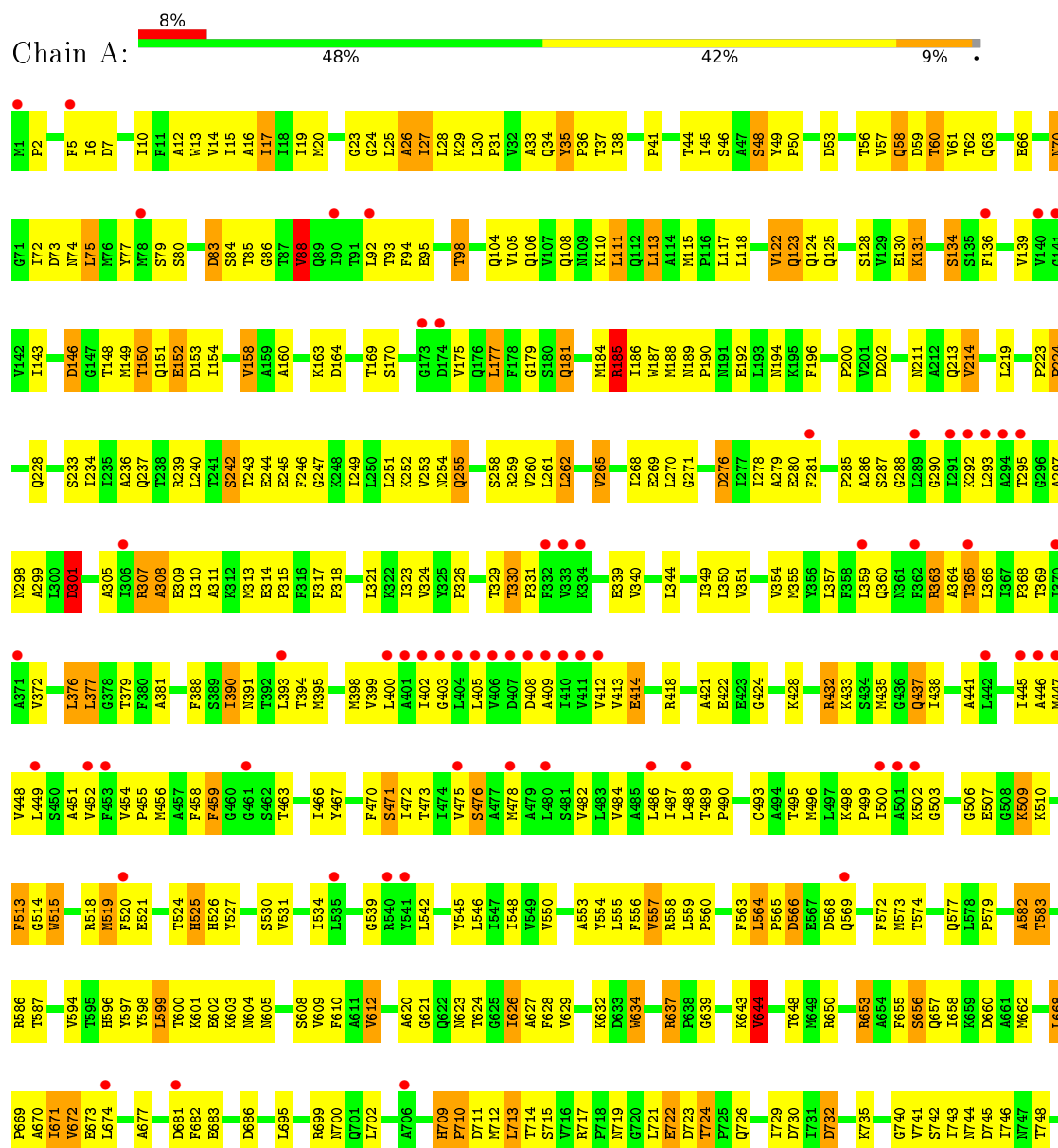
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	146.71Å 146.71Å 523.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.90 – 3.36 123.47 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.90-3.36) 99.0 (123.47-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.245 , 0.312 0.254 , 0.333	Depositor DCC
R_{free} test set	1567 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	107.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	7837	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.54	0/7985	0.74	2/10846 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	88	VAL	CB-CA-C	-7.37	97.39	111.40
1	A	185	ARG	NE-CZ-NH2	-5.98	117.31	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ALA	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	7837	0	7990	336	0
All	All	7837	0	7990	336	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 (336) 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:445:ILE:HG21	1:A:940:LYS:HZ3	1.39	0.87
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.59	0.85
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.61	0.83
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.61	0.82
1:A:860:THR:OG1	1:A:861:GLY:N	2.11	0.78
1:A:252:LYS:NZ	1:A:254:ASN:OD1	2.16	0.77
1:A:983:ILE:HD13	1:A:1012:VAL:HG22	1.65	0.77
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.70	0.74
1:A:740:GLY:O	1:A:794:ALA:N	2.20	0.72
1:A:722:GLU:O	1:A:724:THR:N	2.22	0.71
1:A:146:ASP:OD1	1:A:146:ASP:N	2.23	0.71
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.73	0.70
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.73	0.70
1:A:467:TYR:OH	1:A:928:GLN:NE2	2.24	0.70
1:A:609:VAL:HG22	1:A:629:VAL:HG22	1.73	0.70
1:A:458:PHE:HA	1:A:459:PHE:HB3	1.74	0.70
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.25	0.70
1:A:59:ASP:HA	1:A:63:GLN:HG3	1.72	0.69
1:A:719:ASN:HB2	1:A:828:LEU:HD13	1.74	0.69
1:A:187:TRP:HA	1:A:774:MET:O	1.93	0.69
1:A:721:LEU:HG	1:A:815:ARG:HD3	1.75	0.69
1:A:475:VAL:O	1:A:478:MET:HB2	1.94	0.67
1:A:448:VAL:HG12	1:A:887:CYS:HB2	1.77	0.67
1:A:276:ASP:N	1:A:276:ASP:OD1	2.26	0.67
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.77	0.67
1:A:574:THR:HB	1:A:627:ALA:HB3	1.76	0.67
1:A:24:GLY:O	1:A:27:ILE:HG22	1.95	0.66
1:A:632:LYS:O	1:A:637:ARG:HD2	1.95	0.66
1:A:682:PHE:HB3	1:A:827:ILE:HG22	1.78	0.66
1:A:832:ALA:O	1:A:834:GLY:N	2.25	0.66
1:A:626:ILE:HD11	1:A:628:PHE:CE1	2.31	0.66
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.78	0.65
1:A:329:THR:O	1:A:329:THR:OG1	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HG2	1:A:769:LYS:HE2	1.78	0.64
1:A:80:SER:HB3	1:A:818:ARG:HB2	1.77	0.64
1:A:35:TYR:HB3	1:A:36:PRO:HD2	1.78	0.64
1:A:539:GLY:HA2	1:A:542:LEU:HD22	1.78	0.64
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.79	0.63
1:A:150:THR:OG1	1:A:152:GLU:HG2	1.99	0.63
1:A:50:PRO:HG3	1:A:125:GLN:HE21	1.64	0.63
1:A:527:TYR:OH	1:A:1019:ILE:O	2.18	0.62
1:A:376:LEU:O	1:A:379:THR:N	2.32	0.62
1:A:612:VAL:HG23	1:A:626:ILE:HG23	1.81	0.62
1:A:743:ILE:HD12	1:A:743:ILE:H	1.63	0.62
1:A:421:ALA:HA	1:A:500:ILE:HG21	1.81	0.62
1:A:644:VAL:O	1:A:648:THR:HG23	2.00	0.62
1:A:38:ILE:HG21	1:A:674:LEU:HD22	1.82	0.61
1:A:35:TYR:HD2	1:A:671:ILE:HD12	1.65	0.61
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.82	0.61
1:A:105:VAL:O	1:A:108:GLN:N	2.33	0.60
1:A:463:THR:HG21	1:A:868:LEU:HG	1.83	0.60
1:A:531:VAL:HG13	1:A:534:ILE:HD11	1.81	0.60
1:A:455:PRO:HB3	1:A:879:ILE:HD11	1.83	0.60
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.82	0.60
1:A:484:VAL:HG12	1:A:489:THR:HG23	1.84	0.60
1:A:653:ARG:O	1:A:656:SER:OG	2.12	0.59
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.85	0.59
1:A:987:MET:HA	1:A:990:VAL:HG12	1.85	0.59
1:A:813:SER:HB3	1:A:816:LEU:HD12	1.85	0.59
1:A:677:ALA:HB2	1:A:867:ARG:HH12	1.68	0.58
1:A:1024:VAL:HA	1:A:1027:VAL:HG22	1.84	0.58
1:A:104:GLN:HB2	1:A:131:LYS:HD3	1.84	0.58
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.38	0.57
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.86	0.57
1:A:650:ARG:HA	1:A:653:ARG:HD2	1.86	0.57
1:A:702:LEU:HD13	1:A:851:LEU:HD11	1.86	0.57
1:A:287:SER:OG	1:A:288:GLY:N	2.38	0.57
1:A:709:HIS:O	1:A:711:ASP:N	2.37	0.57
1:A:732:ASP:OD2	1:A:735:LYS:HB2	2.04	0.57
1:A:202:ASP:OD1	1:A:792:ARG:NH2	2.38	0.57
1:A:846:GLN:O	1:A:849:SER:OG	2.16	0.57
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.69	0.57
1:A:712:MET:HA	1:A:832:ALA:HB3	1.86	0.56
1:A:110:LYS:HD3	1:A:113:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:HB3	1:A:252:LYS:HE2	1.86	0.56
1:A:35:TYR:CD2	1:A:671:ILE:HD12	2.40	0.56
1:A:596:HIS:CE1	1:A:600:THR:HG21	2.41	0.56
1:A:15:ILE:O	1:A:19:ILE:HG13	2.05	0.56
1:A:709:HIS:N	1:A:710:PRO:HD3	2.20	0.56
1:A:53:ASP:O	1:A:57:VAL:HG23	2.06	0.56
1:A:421:ALA:O	1:A:503:GLY:N	2.30	0.56
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.88	0.55
1:A:246:PHE:O	1:A:249:ILE:HG13	2.06	0.55
1:A:572:PHE:HE1	1:A:598:TYR:HH	1.54	0.55
1:A:399:VAL:HG11	1:A:989:LEU:HD21	1.89	0.55
1:A:150:THR:N	1:A:153:ASP:OD2	2.39	0.55
1:A:409:ALA:O	1:A:413:VAL:HG23	2.06	0.55
1:A:605:ASN:OD1	1:A:637:ARG:HB3	2.07	0.55
1:A:160:ALA:HA	1:A:767:ARG:NH1	2.22	0.54
1:A:909:VAL:HG13	1:A:931:LEU:HD21	1.90	0.54
1:A:262:LEU:HD13	1:A:268:ILE:HD11	1.89	0.54
1:A:577:GLN:HB2	1:A:662:MET:HE2	1.89	0.54
1:A:894:SER:OG	1:A:895:TRP:N	2.39	0.54
1:A:907:LEU:HD22	1:A:1017:LEU:HB3	1.88	0.54
1:A:58:GLN:OE1	1:A:818:ARG:NH1	2.34	0.54
1:A:744:ASN:O	1:A:748:THR:OG1	2.15	0.54
1:A:682:PHE:O	1:A:827:ILE:N	2.37	0.53
1:A:305:ALA:O	1:A:308:ALA:HB3	2.08	0.53
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.91	0.53
1:A:150:THR:HG23	1:A:153:ASP:OD2	2.08	0.53
1:A:214:VAL:HG13	1:A:237:GLN:HB3	1.90	0.52
1:A:422:GLU:O	1:A:502:LYS:HE3	2.09	0.52
1:A:372:VAL:HG22	1:A:405:LEU:HD13	1.92	0.52
1:A:896:SER:OG	1:A:897:ILE:N	2.43	0.52
1:A:472:ILE:O	1:A:476:SER:OG	2.23	0.52
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.90	0.52
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.92	0.52
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.92	0.52
1:A:154:ILE:O	1:A:158:VAL:HG13	2.10	0.51
1:A:25:LEU:O	1:A:28:LEU:N	2.44	0.51
1:A:455:PRO:O	1:A:876:LEU:HB3	2.11	0.51
1:A:566:ASP:OD1	1:A:566:ASP:N	2.44	0.51
1:A:979:SER:O	1:A:983:ILE:HG13	2.10	0.51
1:A:620:ALA:HA	1:A:624:THR:HG21	1.93	0.51
1:A:726:GLN:NE2	1:A:812:GLY:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG22	1:A:236:ALA:HB3	1.93	0.51
1:A:5:PHE:CD2	1:A:12:ALA:HB2	2.46	0.51
1:A:350:LEU:O	1:A:354:VAL:HG23	2.11	0.51
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.46	0.51
1:A:668:LEU:O	1:A:670:ALA:N	2.43	0.51
1:A:979:SER:OG	1:A:1015:THR:HG21	2.10	0.51
1:A:582:ALA:HB3	1:A:623:ASN:HB3	1.92	0.51
1:A:33:ALA:HB2	1:A:299:ALA:HB2	1.93	0.50
1:A:506:GLY:HA2	1:A:509:LYS:HD2	1.92	0.50
1:A:742:SER:HB3	1:A:745:ASP:CG	2.31	0.50
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.46	0.50
1:A:17:ILE:HA	1:A:20:MET:HE2	1.92	0.50
1:A:942:ALA:O	1:A:946:VAL:HG13	2.11	0.50
1:A:259:ARG:HD2	1:A:261:LEU:HD21	1.93	0.50
1:A:394:THR:O	1:A:398:MET:HG2	2.11	0.50
1:A:621:GLY:O	1:A:624:THR:HG22	2.12	0.50
1:A:470:PHE:HA	1:A:473:THR:OG1	2.11	0.50
1:A:134:SER:HA	1:A:292:LYS:HE2	1.94	0.50
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.94	0.50
1:A:879:ILE:O	1:A:883:VAL:HG23	2.12	0.50
1:A:899:PHE:HD1	1:A:902:MET:HG3	1.75	0.50
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.94	0.50
1:A:555:LEU:HB3	1:A:913:LEU:HB3	1.94	0.50
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.93	0.50
1:A:841:MET:O	1:A:845:GLU:HG3	2.10	0.50
1:A:424:GLY:HA3	1:A:502:LYS:HB2	1.94	0.50
1:A:521:GLU:O	1:A:525:HIS:HB2	2.12	0.50
1:A:58:GLN:OE1	1:A:818:ARG:HD2	2.11	0.50
1:A:243:THR:OG1	1:A:244:GLU:N	2.45	0.49
1:A:414:GLU:HG2	1:A:974:PRO:HB3	1.93	0.49
1:A:526:HIS:O	1:A:530:SER:OG	2.28	0.49
1:A:35:TYR:HB3	1:A:36:PRO:CD	2.42	0.49
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.93	0.49
1:A:520:PHE:O	1:A:524:THR:HG23	2.13	0.49
1:A:418:ARG:HD3	1:A:970:MET:SD	2.53	0.49
1:A:990:VAL:HG23	1:A:1005:THR:HG22	1.93	0.49
1:A:448:VAL:O	1:A:451:ALA:HB3	2.13	0.48
1:A:896:SER:O	1:A:899:PHE:N	2.37	0.48
1:A:671:ILE:HG12	1:A:672:VAL:HG23	1.96	0.48
1:A:964:THR:O	1:A:968:VAL:HG23	2.13	0.48
1:A:876:LEU:O	1:A:880:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ALA:C	1:A:301:ASP:N	2.67	0.48
1:A:610:PHE:HB3	1:A:628:PHE:HB2	1.95	0.48
1:A:997:SER:O	1:A:1000:GLN:N	2.47	0.48
1:A:839:GLU:HG3	1:A:839:GLU:H	1.43	0.48
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.94	0.48
1:A:363:ARG:HH21	1:A:496:MET:HA	1.79	0.48
1:A:699:ARG:NH2	1:A:700:ASN:OD1	2.36	0.47
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.43	0.47
1:A:62:THR:O	1:A:66:GLU:HG3	2.14	0.47
1:A:931:LEU:O	1:A:934:THR:HB	2.15	0.47
1:A:6:ILE:HG22	1:A:428:LYS:HE3	1.95	0.47
1:A:564:LEU:HD22	1:A:565:PRO:HD2	1.95	0.47
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.49	0.47
1:A:330:THR:HB	1:A:331:PRO:HD3	1.97	0.47
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.97	0.47
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.79	0.47
1:A:363:ARG:NH2	1:A:496:MET:HA	2.30	0.47
1:A:989:LEU:HB3	1:A:1000:GLN:O	2.15	0.47
1:A:104:GLN:HG3	1:A:131:LYS:HG2	1.97	0.47
1:A:25:LEU:O	1:A:27:ILE:N	2.48	0.47
1:A:655:PHE:O	1:A:657:GLN:N	2.48	0.47
1:A:865:GLN:HG3	1:A:866:GLU:H	1.80	0.47
1:A:969:ARG:HG3	1:A:970:MET:N	2.29	0.47
1:A:1015:THR:O	1:A:1019:ILE:HB	2.14	0.46
1:A:150:THR:O	1:A:154:ILE:HG13	2.16	0.46
1:A:152:GLU:HG2	1:A:152:GLU:H	1.54	0.46
1:A:360:GLN:HB3	1:A:513:PHE:CE2	2.51	0.46
1:A:38:ILE:HD13	1:A:674:LEU:HD22	1.97	0.46
1:A:952:LEU:O	1:A:956:GLU:HB2	2.15	0.46
1:A:177:LEU:HD23	1:A:179:GLY:O	2.15	0.46
1:A:108:GLN:HA	1:A:111:LEU:HB2	1.97	0.46
1:A:355:MET:HE2	1:A:365:THR:HA	1.96	0.46
1:A:498:LYS:HG2	1:A:499:PRO:HD2	1.98	0.46
1:A:185:ARG:HG2	1:A:271:GLY:HA3	1.98	0.46
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.97	0.46
1:A:59:ASP:O	1:A:63:GLN:HB2	2.15	0.46
1:A:72:ILE:HG23	1:A:106:GLN:HB3	1.98	0.46
1:A:366:LEU:O	1:A:369:THR:HB	2.16	0.46
1:A:456:MET:HG3	1:A:467:TYR:CD1	2.51	0.46
1:A:907:LEU:HD13	1:A:1018:ALA:HB2	1.97	0.46
1:A:1001:ASN:O	1:A:1005:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:O	1:A:391:ASN:HB2	2.16	0.46
1:A:75:LEU:CD1	1:A:92:LEU:HD23	2.46	0.46
1:A:455:PRO:HG2	1:A:880:SER:HA	1.97	0.46
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.78	0.46
1:A:307:ARG:HA	1:A:307:ARG:HD2	1.48	0.46
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.71	0.45
1:A:376:LEU:O	1:A:377:LEU:C	2.55	0.45
1:A:281:PHE:HE1	1:A:608:SER:HB2	1.82	0.45
1:A:27:ILE:HG12	1:A:390:ILE:CD1	2.46	0.45
1:A:671:ILE:HG12	1:A:672:VAL:N	2.32	0.45
1:A:41:PRO:HD2	1:A:94:PHE:O	2.16	0.45
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.50	0.45
1:A:110:LYS:HA	1:A:113:LEU:HD13	1.98	0.45
1:A:323:ILE:HG22	1:A:324:VAL:N	2.32	0.45
1:A:58:GLN:HA	1:A:62:THR:OG1	2.17	0.45
1:A:20:MET:HB3	1:A:377:LEU:HD13	1.98	0.45
1:A:524:THR:HA	1:A:527:TYR:HB3	1.99	0.45
1:A:169:THR:OG1	1:A:309:GLU:OE2	2.35	0.44
1:A:467:TYR:O	1:A:471:SER:OG	2.33	0.44
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.52	0.44
1:A:931:LEU:O	1:A:935:ILE:HG23	2.17	0.44
1:A:5:PHE:HD2	1:A:12:ALA:HB2	1.82	0.44
1:A:48:SER:O	1:A:50:PRO:HD3	2.17	0.44
1:A:181:GLN:CG	1:A:769:LYS:HE2	2.44	0.44
1:A:36:PRO:HD3	1:A:393:LEU:HD12	1.99	0.44
1:A:515:TRP:O	1:A:519:MET:HB3	2.17	0.44
1:A:983:ILE:HG23	1:A:1008:MET:HG3	2.00	0.44
1:A:151:GLN:NE2	1:A:152:GLU:OE2	2.47	0.44
1:A:445:ILE:O	1:A:449:LEU:HD13	2.17	0.44
1:A:463:THR:HG23	1:A:563:PHE:CE2	2.52	0.44
1:A:118:LEU:HB3	1:A:122:VAL:CG1	2.47	0.44
1:A:10:ILE:HA	1:A:13:TRP:HB2	1.99	0.44
1:A:151:GLN:HB3	1:A:285:PRO:HB3	2.00	0.44
1:A:563:PHE:O	1:A:564:LEU:HD23	2.17	0.44
1:A:211:ASN:O	1:A:760:ASN:ND2	2.51	0.44
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.99	0.44
1:A:530:SER:O	1:A:534:ILE:HG23	2.18	0.44
1:A:672:VAL:HG12	1:A:673:GLU:H	1.83	0.44
1:A:16:ALA:HA	1:A:19:ILE:HD12	2.00	0.44
1:A:219:LEU:HG	1:A:234:ILE:HD11	2.00	0.44
1:A:242:SER:OG	1:A:245:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ASP:CB	1:A:823:PRO:HB2	2.48	0.43
1:A:681:ASP:OD1	1:A:860:THR:HG23	2.18	0.43
1:A:1019:ILE:HD12	1:A:1019:ILE:HA	1.84	0.43
1:A:26:ALA:O	1:A:30:LEU:HB2	2.19	0.43
1:A:553:ALA:O	1:A:557:VAL:HG22	2.18	0.43
1:A:671:ILE:CD1	1:A:672:VAL:HG23	2.48	0.43
1:A:254:ASN:HB2	1:A:258:SER:HB2	2.00	0.43
1:A:569:GLN:NE2	1:A:670:ALA:O	2.51	0.43
1:A:899:PHE:CD1	1:A:902:MET:HG3	2.54	0.43
1:A:414:GLU:CD	1:A:974:PRO:HD3	2.38	0.43
1:A:413:VAL:HG22	1:A:493:CYS:SG	2.58	0.43
1:A:56:THR:O	1:A:60:THR:HB	2.18	0.43
1:A:882:ILE:HA	1:A:882:ILE:HD13	1.81	0.43
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.93	0.42
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.54	0.42
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.84	0.42
1:A:484:VAL:O	1:A:488:LEU:N	2.50	0.42
1:A:742:SER:O	1:A:745:ASP:N	2.51	0.42
1:A:41:PRO:HG2	1:A:98:THR:HG22	2.00	0.42
1:A:897:ILE:HD13	1:A:950:LYS:HD2	2.02	0.42
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.42
1:A:424:GLY:CA	1:A:502:LYS:HB2	2.49	0.42
1:A:813:SER:HA	1:A:814:PRO:HD3	1.73	0.42
1:A:388:PHE:CZ	1:A:472:ILE:HG13	2.55	0.42
1:A:597:TYR:O	1:A:599:LEU:N	2.52	0.42
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.20	0.42
1:A:786:ILE:HG12	1:A:786:ILE:H	1.65	0.42
1:A:438:ILE:O	1:A:441:ALA:HB3	2.20	0.42
1:A:456:MET:O	1:A:467:TYR:HB3	2.19	0.42
1:A:987:MET:N	1:A:988:PRO:HD2	2.33	0.42
1:A:713:LEU:HD11	1:A:844:MET:HG2	2.01	0.42
1:A:935:ILE:HG13	1:A:936:GLY:N	2.33	0.42
1:A:408:ASP:O	1:A:412:VAL:HG23	2.20	0.42
1:A:433:LYS:HD3	1:A:433:LYS:HA	1.86	0.42
1:A:471:SER:O	1:A:475:VAL:HG23	2.20	0.42
1:A:5:PHE:CE2	1:A:487:ILE:HG23	2.55	0.42
1:A:50:PRO:HG3	1:A:125:GLN:NE2	2.33	0.42
1:A:639:GLY:O	1:A:643:LYS:HD3	2.19	0.42
1:A:70:ASN:OD1	1:A:70:ASN:N	2.53	0.42
1:A:73:ASP:O	1:A:75:LEU:N	2.53	0.42
1:A:843:LEU:HA	1:A:846:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:HG3	1:A:123:GLN:H	1.56	0.42
1:A:192:GLU:HB3	1:A:265:VAL:HG12	2.02	0.42
1:A:251:LEU:HB2	1:A:260:VAL:O	2.20	0.42
1:A:307:ARG:HH21	1:A:311:ALA:HA	1.84	0.42
1:A:572:PHE:HA	1:A:668:LEU:HD21	2.02	0.42
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.83	0.41
1:A:324:VAL:HG23	1:A:326:PRO:HD3	2.02	0.41
1:A:782:LEU:HA	1:A:783:PRO:HD3	1.94	0.41
1:A:950:LYS:NZ	1:A:954:ASP:OD1	2.45	0.41
1:A:163:LYS:HG3	1:A:175:VAL:HG11	2.02	0.41
1:A:281:PHE:CE2	1:A:324:VAL:HG11	2.56	0.41
1:A:594:VAL:HG13	1:A:655:PHE:CZ	2.56	0.41
1:A:1030:ARG:HA	1:A:1030:ARG:HE	1.85	0.41
1:A:403:GLY:HA3	1:A:982:PHE:CZ	2.55	0.41
1:A:838:GLY:O	1:A:842:GLU:HG3	2.21	0.41
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	2.02	0.41
1:A:1030:ARG:HA	1:A:1030:ARG:NE	2.35	0.41
1:A:10:ILE:O	1:A:14:VAL:HG23	2.20	0.41
1:A:395:MET:O	1:A:399:VAL:HG23	2.21	0.41
1:A:709:HIS:C	1:A:711:ASP:H	2.22	0.41
1:A:14:VAL:HA	1:A:17:ILE:HD12	2.02	0.41
1:A:240:LEU:HD23	1:A:245:GLU:HB3	2.03	0.41
1:A:254:ASN:HD22	1:A:258:SER:HB2	1.85	0.41
1:A:313:MET:HB3	1:A:317:PHE:CE1	2.56	0.41
1:A:359:LEU:HD13	1:A:364:ALA:HB1	2.02	0.41
1:A:568:ASP:OD1	1:A:634:TRP:HZ3	2.03	0.41
1:A:973:ARG:N	1:A:974:PRO:HD2	2.34	0.41
1:A:23:GLY:HA3	1:A:377:LEU:O	2.19	0.41
1:A:514:GLY:O	1:A:518:ARG:HG3	2.21	0.41
1:A:27:ILE:HG12	1:A:390:ILE:HD13	2.03	0.41
1:A:355:MET:SD	1:A:368:PRO:HG3	2.61	0.41
1:A:83:ASP:OD2	1:A:83:ASP:N	2.54	0.41
1:A:860:THR:HG1	1:A:861:GLY:N	2.15	0.41
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.84	0.41
1:A:546:LEU:O	1:A:550:VAL:HG23	2.20	0.41
1:A:907:LEU:HD11	1:A:1025:PHE:CE2	2.55	0.41
1:A:118:LEU:HB3	1:A:122:VAL:HG11	2.03	0.41
1:A:699:ARG:HG2	1:A:699:ARG:O	2.21	0.41
1:A:904:VAL:HG21	1:A:942:ALA:HB2	2.01	0.41
1:A:169:THR:HG21	1:A:305:ALA:HB1	2.02	0.41
1:A:255:GLN:H	1:A:255:GLN:HG2	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LYS:O	1:A:432:ARG:HB2	2.21	0.41
1:A:972:LEU:HD22	1:A:972:LEU:HA	1.86	0.41
1:A:1018:ALA:HB1	1:A:1022:VAL:HG23	2.02	0.40
1:A:10:ILE:HG22	1:A:14:VAL:HG23	2.02	0.40
1:A:244:GLU:O	1:A:247:GLY:N	2.54	0.40
1:A:279:ALA:O	1:A:280:GLU:HG3	2.20	0.40
1:A:545:TYR:O	1:A:548:ILE:HB	2.20	0.40
1:A:583:THR:OG1	1:A:586:ARG:HG3	2.21	0.40
1:A:150:THR:OG1	1:A:151:GLN:N	2.54	0.40
1:A:185:ARG:HA	1:A:185:ARG:HD2	1.68	0.40
1:A:454:VAL:C	1:A:456:MET:H	2.25	0.40
1:A:903:LEU:O	1:A:906:PRO:HD2	2.21	0.40
1:A:456:MET:HE3	1:A:932:LEU:HD11	2.04	0.40
1:A:30:LEU:HA	1:A:30:LEU:HD12	1.78	0.40
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.50	0.40
1:A:354:VAL:HG21	1:A:981:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1032/1049 (98%)	849 (82%)	141 (14%)	42 (4%)	3 27

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	35	TYR
1	A	579	PRO
1	A	656	SER
1	A	723	ASP

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Mol	Chain	Res	Type
1	A	833	PRO
1	A	921	LEU
1	A	26	ALA
1	A	136	PHE
1	A	377	LEU
1	A	390	ILE
1	A	437	GLN
1	A	582	ALA
1	A	602	GLU
1	A	644	VAL
1	A	672	VAL
1	A	746	ILE
1	A	776	GLU
1	A	865	GLN
1	A	866	GLU
1	A	867	ARG
1	A	919	ARG
1	A	74	ASN
1	A	170	SER
1	A	295	THR
1	A	301	ASP
1	A	330	THR
1	A	713	LEU
1	A	916	ALA
1	A	318	PRO
1	A	459	PHE
1	A	669	PRO
1	A	710	PRO
1	A	814	PRO
1	A	923	ASN
1	A	181	GLN
1	A	298	ASN
1	A	308	ALA
1	A	510	LYS
1	A	994	GLY
1	A	224	PRO
1	A	17	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	837/852 (98%)	683 (82%)	154 (18%)	2 9

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	27	ILE
1	A	29	LYS
1	A	37	THR
1	A	44	THR
1	A	45	ILE
1	A	46	SER
1	A	48	SER
1	A	49	TYR
1	A	58	GLN
1	A	60	THR
1	A	70	ASN
1	A	75	LEU
1	A	77	TYR
1	A	79	SER
1	A	83	ASP
1	A	84	SER
1	A	85	THR
1	A	88	VAL
1	A	93	THR
1	A	95	GLU
1	A	98	THR
1	A	111	LEU
1	A	113	LEU
1	A	115	MET
1	A	122	VAL
1	A	123	GLN
1	A	124	GLN
1	A	128	SER
1	A	130	GLU
1	A	131	LYS
1	A	134	SER
1	A	146	ASP
1	A	149	MET

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Mol	Chain	Res	Type
1	A	150	THR
1	A	152	GLU
1	A	158	VAL
1	A	164	ASP
1	A	177	LEU
1	A	185	ARG
1	A	188	MET
1	A	194	ASN
1	A	200	PRO
1	A	213	GLN
1	A	214	VAL
1	A	228	GLN
1	A	233	SER
1	A	239	ARG
1	A	242	SER
1	A	253	VAL
1	A	255	GLN
1	A	262	LEU
1	A	265	VAL
1	A	269	GLU
1	A	276	ASP
1	A	278	ILE
1	A	293	LEU
1	A	301	ASP
1	A	307	ARG
1	A	310	LEU
1	A	314	GLU
1	A	315	PRO
1	A	321	LEU
1	A	339	GLU
1	A	349	ILE
1	A	357	LEU
1	A	363	ARG
1	A	365	THR
1	A	376	LEU
1	A	400	LEU
1	A	414	GLU
1	A	432	ARG
1	A	437	GLN
1	A	447	MET
1	A	452	VAL
1	A	471	SER

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Mol	Chain	Res	Type
1	A	476	SER
1	A	486	LEU
1	A	495	THR
1	A	507	GLU
1	A	509	LYS
1	A	513	PHE
1	A	515	TRP
1	A	519	MET
1	A	525	HIS
1	A	557	VAL
1	A	564	LEU
1	A	566	ASP
1	A	573	MET
1	A	583	THR
1	A	587	THR
1	A	599	LEU
1	A	601	LYS
1	A	603	LYS
1	A	604	ASN
1	A	612	VAL
1	A	626	ILE
1	A	634	TRP
1	A	637	ARG
1	A	644	VAL
1	A	653	ARG
1	A	658	ILE
1	A	660	ASP
1	A	668	LEU
1	A	671	ILE
1	A	683	GLU
1	A	695	LEU
1	A	709	HIS
1	A	714	THR
1	A	715	SER
1	A	717	ARG
1	A	722	GLU
1	A	724	THR
1	A	729	ILE
1	A	730	ASP
1	A	732	ASP
1	A	741	VAL
1	A	758	TYR

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Mol	Chain	Res	Type
1	A	765	ARG
1	A	784	ASP
1	A	788	ASP
1	A	806	SER
1	A	816	LEU
1	A	822	LEU
1	A	824	SER
1	A	826	GLU
1	A	827	ILE
1	A	839	GLU
1	A	846	GLN
1	A	847	LEU
1	A	858	ASP
1	A	860	THR
1	A	868	LEU
1	A	880	SER
1	A	882	ILE
1	A	886	LEU
1	A	900	SER
1	A	901	VAL
1	A	917	THR
1	A	919	ARG
1	A	921	LEU
1	A	931	LEU
1	A	946	VAL
1	A	948	PHE
1	A	960	LEU
1	A	969	ARG
1	A	970	MET
1	A	971	ARG
1	A	972	LEU
1	A	978	THR
1	A	982	PHE
1	A	993	THR
1	A	1005	THR
1	A	1030	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	709	HIS
1	A	846	GLN
1	A	928	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	1034/1049 (98%)	0.55	89 (8%) 13 13	22, 81, 139, 161	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TYR	7.7
1	A	405	LEU	6.9
1	A	404	LEU	6.9
1	A	982	PHE	6.1
1	A	408	ASP	6.1
1	A	409	ALA	5.5
1	A	136	PHE	5.2
1	A	407	ASP	5.0
1	A	406	VAL	4.9
1	A	403	GLY	4.6
1	A	291	ILE	4.5
1	A	461	GLY	4.4
1	A	488	LEU	4.2
1	A	411	VAL	4.1
1	A	400	LEU	4.0
1	A	828	LEU	3.9
1	A	306	ILE	3.9
1	A	410	ILE	3.9
1	A	292	LYS	3.8
1	A	833	PRO	3.7
1	A	362	PHE	3.5
1	A	442	LEU	3.5
1	A	1028	VAL	3.3
1	A	371	ALA	3.2
1	A	981	ALA	3.2
1	A	1027	VAL	3.2
1	A	295	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	569	GLN	3.2
1	A	332	PHE	3.1
1	A	904	VAL	3.0
1	A	501	ALA	3.0
1	A	1026	PHE	3.0
1	A	502	LYS	3.0
1	A	334	LYS	2.9
1	A	980	LEU	2.9
1	A	402	ILE	2.9
1	A	359	LEU	2.9
1	A	706	ALA	2.8
1	A	500	ILE	2.7
1	A	5	PHE	2.7
1	A	965	LEU	2.7
1	A	173	GLY	2.7
1	A	681	ASP	2.7
1	A	535	LEU	2.6
1	A	294	ALA	2.6
1	A	958	LYS	2.6
1	A	401	ALA	2.6
1	A	365	THR	2.6
1	A	1031	ARG	2.6
1	A	1	MET	2.6
1	A	289	LEU	2.6
1	A	333	VAL	2.5
1	A	940	LYS	2.5
1	A	486	LEU	2.5
1	A	964	THR	2.5
1	A	984	LEU	2.5
1	A	540	ARG	2.5
1	A	174	ASP	2.5
1	A	393	LEU	2.5
1	A	78	MET	2.4
1	A	961	ILE	2.4
1	A	447	MET	2.4
1	A	777	ALA	2.4
1	A	452	VAL	2.3
1	A	956	GLU	2.3
1	A	674	LEU	2.3
1	A	983	ILE	2.3
1	A	412	VAL	2.3
1	A	445	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	281	PHE	2.3
1	A	370	ILE	2.2
1	A	92	LEU	2.2
1	A	453	PHE	2.2
1	A	141	GLY	2.2
1	A	937	LEU	2.2
1	A	90	ILE	2.2
1	A	977	MET	2.2
1	A	446	ALA	2.1
1	A	945	ILE	2.1
1	A	478	MET	2.1
1	A	933	THR	2.1
1	A	475	VAL	2.1
1	A	520	PHE	2.0
1	A	942	ALA	2.0
1	A	943	ILE	2.0
1	A	293	LEU	2.0
1	A	140	VAL	2.0
1	A	480	LEU	2.0
1	A	449	LEU	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.