



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2016 – 05:55 PM EDT

PDB ID : 4ZLJ
Title : Crystal structure of transporter AcrB
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-05-01
Resolution : 3.26 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

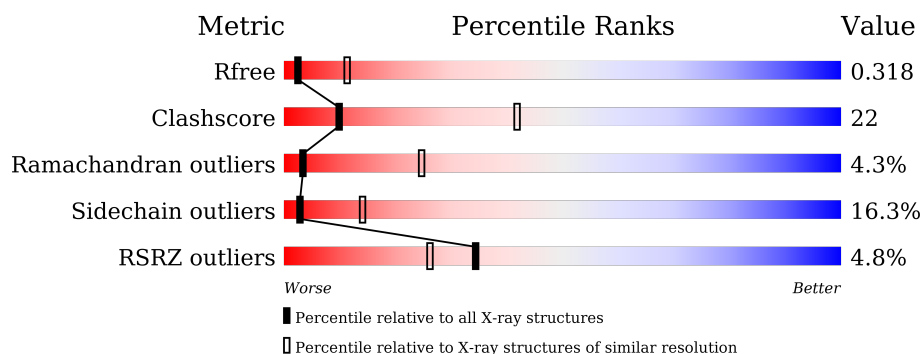
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	<div> <div>5%</div> <div>47%</div> <div>43%</div> <div>8%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7855 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.

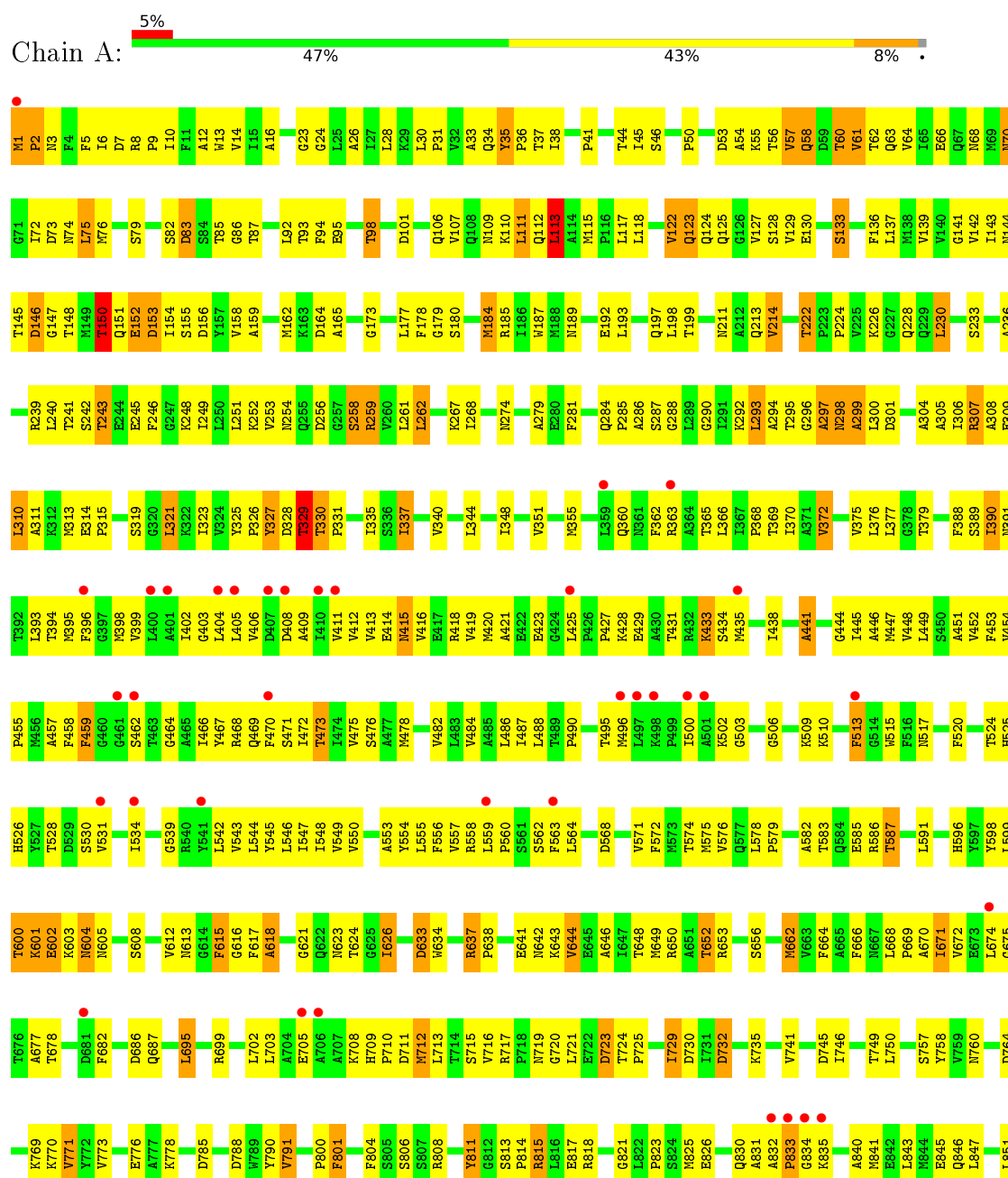
- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1034	7855	5055	1296	1460	44	0	0	0

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	144.99Å 144.99Å 521.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 3.26 80.20 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.97-3.26) 97.3 (80.20-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.248 , 0.318 0.252 , 0.318	Depositor DCC
R_{free} test set	1637 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7855	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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	0.54	0/8005	0.74	3/10871 (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	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	113	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	576	VAL	CB-CA-C	-5.59	100.78	111.40
1	A	867	ARG	N-CA-C	5.26	125.21	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ALA	Peptide
1	A	459	PHE	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	7855	0	8006	350	0
All	All	7855	0	8006	350	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 (350) 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:242:SER:HB3	1:A:245:GLU:HG3	1.55	0.86
1:A:254:ASN:HB2	1:A:258:SER:HB2	1.57	0.84
1:A:653:ARG:O	1:A:656:SER:OG	1.95	0.82
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.60	0.81
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.61	0.81
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.64	0.80
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.63	0.80
1:A:469:GLN:O	1:A:473:THR:OG1	2.00	0.78
1:A:75:LEU:HD12	1:A:92:LEU:HD23	1.67	0.77
1:A:445:ILE:HG21	1:A:940:LYS:HZ3	1.49	0.77
1:A:403:GLY:HA3	1:A:982:PHE:HE1	1.50	0.77
1:A:419:VAL:HG21	1:A:434:SER:HB2	1.67	0.76
1:A:713:LEU:HD13	1:A:843:LEU:HD23	1.67	0.76
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.66	0.76
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.52	0.75
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.20	0.74
1:A:678:THR:O	1:A:830:GLN:NE2	2.21	0.73
1:A:41:PRO:HG2	1:A:98:THR:HG22	1.70	0.73
1:A:907:LEU:HD22	1:A:1017:LEU:HB3	1.71	0.73
1:A:945:ILE:HD13	1:A:968:VAL:HG22	1.70	0.73
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.25	0.71
1:A:35:TYR:HD2	1:A:671:ILE:HD12	1.56	0.71
1:A:859:TRP:HE3	1:A:863:SER:HG	1.39	0.71
1:A:712:MET:SD	1:A:835:LYS:NZ	2.57	0.70
1:A:420:MET:HB3	1:A:500:ILE:HB	1.73	0.70
1:A:571:VAL:HG23	1:A:668:LEU:HD11	1.73	0.70
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.75	0.69
1:A:421:ALA:O	1:A:503:GLY:N	2.21	0.68
1:A:466:ILE:H	1:A:466:ILE:HD12	1.58	0.68
1:A:187:TRP:HB2	1:A:267:LYS:HB2	1.75	0.67
1:A:307:ARG:HH21	1:A:311:ALA:HA	1.60	0.66
1:A:189:ASN:HD22	1:A:192:GLU:H	1.41	0.66
1:A:26:ALA:O	1:A:30:LEU:HB2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.29	0.66
1:A:329:THR:O	1:A:329:THR:OG1	2.12	0.65
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.78	0.65
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.77	0.65
1:A:612:VAL:HG23	1:A:626:ILE:HG23	1.79	0.65
1:A:404:LEU:HD23	1:A:940:LYS:HD2	1.79	0.65
1:A:604:ASN:N	1:A:604:ASN:OD1	2.23	0.65
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.80	0.64
1:A:524:THR:HG22	1:A:972:LEU:HD12	1.80	0.64
1:A:539:GLY:HA2	1:A:542:LEU:HD22	1.78	0.63
1:A:877:TYR:O	1:A:880:SER:N	2.31	0.63
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.79	0.63
1:A:1022:VAL:HA	1:A:1025:PHE:HB2	1.79	0.63
1:A:431:THR:HA	1:A:434:SER:HB3	1.80	0.63
1:A:112:GLN:HA	1:A:115:MET:HB2	1.79	0.63
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.79	0.63
1:A:894:SER:HB3	1:A:897:ILE:HB	1.80	0.63
1:A:960:LEU:HD11	1:A:1031:ARG:HG3	1.81	0.63
1:A:429:GLU:O	1:A:433:LYS:HG2	1.99	0.62
1:A:363:ARG:NE	1:A:496:MET:O	2.28	0.62
1:A:960:LEU:HD13	1:A:1030:ARG:HB3	1.82	0.62
1:A:372:VAL:HG22	1:A:405:LEU:HD13	1.81	0.62
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.81	0.62
1:A:228:GLN:NE2	1:A:230:LEU:HD23	2.14	0.62
1:A:563:PHE:HB2	1:A:867:ARG:NH2	2.15	0.62
1:A:668:LEU:O	1:A:670:ALA:N	2.32	0.62
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.81	0.61
1:A:402:ILE:O	1:A:406:VAL:HG13	2.00	0.61
1:A:662:MET:HG3	1:A:664:PHE:CE1	2.35	0.61
1:A:641:GLU:O	1:A:650:ARG:NH2	2.34	0.60
1:A:111:LEU:HD22	1:A:115:MET:HG2	1.83	0.60
1:A:638:PRO:O	1:A:642:ASN:ND2	2.33	0.60
1:A:845:GLU:OE2	1:A:859:TRP:NE1	2.32	0.60
1:A:58:GLN:O	1:A:63:GLN:HG3	2.03	0.59
1:A:293:LEU:HG	1:A:297:ALA:HB3	1.85	0.59
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.35	0.59
1:A:281:PHE:HE1	1:A:608:SER:HB2	1.67	0.59
1:A:677:ALA:HB2	1:A:867:ARG:NH1	2.18	0.59
1:A:246:PHE:O	1:A:249:ILE:HG13	2.03	0.58
1:A:709:HIS:O	1:A:711:ASP:N	2.35	0.58
1:A:395:MET:O	1:A:399:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.86	0.58
1:A:758:TYR:CE1	1:A:770:LYS:HD3	2.38	0.58
1:A:150:THR:OG1	1:A:151:GLN:N	2.33	0.58
1:A:473:THR:O	1:A:476:SER:OG	2.22	0.58
1:A:695:LEU:HB3	1:A:825:MET:HE3	1.84	0.58
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.86	0.58
1:A:719:ASN:ND2	1:A:826:GLU:OE1	2.37	0.57
1:A:297:ALA:HA	1:A:298:ASN:HB2	1.85	0.57
1:A:83:ASP:OD2	1:A:83:ASP:N	2.37	0.57
1:A:841:MET:O	1:A:845:GLU:HG3	2.03	0.57
1:A:1:MET:H2	1:A:2:PRO:HD3	1.70	0.56
1:A:467:TYR:HE2	1:A:868:LEU:HD21	1.70	0.56
1:A:305:ALA:O	1:A:308:ALA:HB3	2.06	0.56
1:A:602:GLU:OE2	1:A:605:ASN:ND2	2.36	0.56
1:A:366:LEU:O	1:A:370:ILE:HG13	2.05	0.56
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.88	0.56
1:A:455:PRO:HB3	1:A:879:ILE:HD11	1.87	0.56
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.87	0.55
1:A:919:ARG:HD2	1:A:921:LEU:HD13	1.89	0.55
1:A:393:LEU:HD22	1:A:470:PHE:HE2	1.71	0.55
1:A:249:ILE:HD12	1:A:262:LEU:HD12	1.88	0.55
1:A:615:PHE:H	1:A:624:THR:HG23	1.71	0.55
1:A:897:ILE:O	1:A:900:SER:OG	2.22	0.55
1:A:375:VAL:HG22	1:A:484:VAL:HG21	1.89	0.55
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.42	0.55
1:A:61:VAL:HG13	1:A:118:LEU:HD22	1.88	0.55
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.89	0.55
1:A:897:ILE:HD13	1:A:950:LYS:HD2	1.88	0.55
1:A:259:ARG:HD2	1:A:261:LEU:HD21	1.89	0.54
1:A:467:TYR:CE2	1:A:868:LEU:HD21	2.42	0.54
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.88	0.54
1:A:600:THR:OG1	1:A:601:LYS:N	2.41	0.54
1:A:35:TYR:CD2	1:A:671:ILE:HD12	2.39	0.54
1:A:53:ASP:O	1:A:55:LYS:N	2.40	0.54
1:A:458:PHE:O	1:A:876:LEU:HD13	2.07	0.54
1:A:637:ARG:CB	1:A:642:ASN:HB3	2.37	0.54
1:A:712:MET:HA	1:A:835:LYS:HD2	1.90	0.54
1:A:454:VAL:HG23	1:A:475:VAL:HG21	1.89	0.54
1:A:572:PHE:HZ	1:A:598:TYR:HE1	1.56	0.54
1:A:144:ASN:OD1	1:A:147:GLY:N	2.41	0.53
1:A:393:LEU:HD22	1:A:470:PHE:CE2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:HD2	1:A:703:LEU:HG	1.91	0.53
1:A:118:LEU:HB3	1:A:122:VAL:CG1	2.39	0.53
1:A:556:PHE:CD1	1:A:913:LEU:HD21	2.44	0.53
1:A:56:THR:O	1:A:60:THR:HB	2.08	0.53
1:A:596:HIS:CE1	1:A:600:THR:HG21	2.43	0.53
1:A:677:ALA:HB2	1:A:867:ARG:HH12	1.73	0.53
1:A:582:ALA:HB3	1:A:623:ASN:HD22	1.74	0.53
1:A:396:PHE:HE1	1:A:999:ALA:HB1	1.74	0.53
1:A:214:VAL:HG13	1:A:236:ALA:HB3	1.91	0.53
1:A:418:ARG:HD3	1:A:970:MET:CG	2.36	0.52
1:A:869:SER:HB2	1:A:928:GLN:HE22	1.73	0.52
1:A:466:ILE:HG21	1:A:925:VAL:HG11	1.92	0.52
1:A:328:ASP:C	1:A:330:THR:H	2.12	0.52
1:A:38:ILE:HG21	1:A:674:LEU:HD22	1.90	0.52
1:A:582:ALA:HA	1:A:586:ARG:CZ	2.39	0.52
1:A:633:ASP:O	1:A:637:ARG:HD3	2.09	0.52
1:A:5:PHE:CE2	1:A:487:ILE:HG23	2.45	0.52
1:A:979:SER:O	1:A:983:ILE:HG13	2.10	0.52
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.92	0.52
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.91	0.52
1:A:110:LYS:O	1:A:113:LEU:HB3	2.10	0.51
1:A:530:SER:O	1:A:534:ILE:HG23	2.10	0.51
1:A:475:VAL:O	1:A:478:MET:HB2	2.11	0.51
1:A:173:GLY:HA3	1:A:294:ALA:HB2	1.90	0.51
1:A:729:ILE:HD12	1:A:750:LEU:HD21	1.93	0.51
1:A:448:VAL:HG12	1:A:887:CYS:HB2	1.91	0.51
1:A:72:ILE:HG23	1:A:106:GLN:HB2	1.93	0.51
1:A:10:ILE:HA	1:A:13:TRP:HD1	1.76	0.51
1:A:213:GLN:OE1	1:A:239:ARG:N	2.43	0.51
1:A:874:PRO:O	1:A:877:TYR:HB2	2.11	0.51
1:A:899:PHE:HA	1:A:902:MET:HB2	1.93	0.51
1:A:506:GLY:HA3	1:A:517:ASN:HD22	1.76	0.51
1:A:403:GLY:HA2	1:A:406:VAL:HG22	1.92	0.50
1:A:23:GLY:HA3	1:A:377:LEU:O	2.11	0.50
1:A:241:THR:OG1	1:A:245:GLU:OE1	2.27	0.50
1:A:438:ILE:O	1:A:441:ALA:HB3	2.10	0.50
1:A:458:PHE:HA	1:A:459:PHE:HB3	1.94	0.50
1:A:60:THR:HG22	1:A:61:VAL:CG2	2.42	0.50
1:A:64:VAL:HG21	1:A:117:LEU:HB3	1.94	0.50
1:A:252:LYS:NZ	1:A:254:ASN:OD1	2.44	0.50
1:A:732:ASP:OD2	1:A:735:LYS:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:O	1:A:471:SER:OG	2.26	0.50
1:A:553:ALA:O	1:A:557:VAL:HG22	2.12	0.50
1:A:675:GLY:C	1:A:677:ALA:H	2.15	0.50
1:A:151:GLN:HB3	1:A:285:PRO:HB3	1.94	0.50
1:A:388:PHE:HE2	1:A:472:ILE:HB	1.76	0.50
1:A:150:THR:O	1:A:154:ILE:HG13	2.12	0.49
1:A:394:THR:O	1:A:398:MET:HG2	2.12	0.49
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.94	0.49
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.47	0.49
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.94	0.49
1:A:445:ILE:HD13	1:A:940:LYS:HG2	1.93	0.49
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.94	0.49
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.47	0.49
1:A:907:LEU:HD11	1:A:1025:PHE:HE2	1.76	0.49
1:A:142:VAL:HG21	1:A:158:VAL:HG11	1.94	0.49
1:A:177:LEU:HG	1:A:178:PHE:N	2.27	0.49
1:A:419:VAL:O	1:A:423:GLU:HB2	2.11	0.49
1:A:544:LEU:O	1:A:547:ILE:HB	2.13	0.49
1:A:562:SER:O	1:A:924:ASP:HA	2.12	0.49
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.94	0.49
1:A:524:THR:O	1:A:528:THR:HG23	2.13	0.49
1:A:832:ALA:O	1:A:834:GLY:N	2.46	0.49
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.95	0.49
1:A:50:PRO:HG3	1:A:125:GLN:NE2	2.28	0.49
1:A:531:VAL:O	1:A:534:ILE:HG12	2.13	0.49
1:A:545:TYR:O	1:A:549:VAL:HG23	2.13	0.49
1:A:960:LEU:H	1:A:960:LEU:HD23	1.78	0.48
1:A:987:MET:O	1:A:991:ILE:HD13	2.12	0.48
1:A:137:LEU:HD12	1:A:293:LEU:HB2	1.96	0.48
1:A:35:TYR:HB3	1:A:36:PRO:HD2	1.95	0.48
1:A:616:GLY:O	1:A:618:ALA:N	2.46	0.48
1:A:466:ILE:O	1:A:469:GLN:HB2	2.13	0.48
1:A:578:LEU:HD13	1:A:587:THR:HG23	1.94	0.48
1:A:184:MET:HB3	1:A:771:VAL:HG22	1.95	0.48
1:A:10:ILE:O	1:A:14:VAL:HG23	2.13	0.48
1:A:403:GLY:O	1:A:406:VAL:HG22	2.14	0.48
1:A:412:VAL:O	1:A:416:VAL:HG23	2.12	0.48
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.68	0.48
1:A:677:ALA:HB2	1:A:867:ARG:NH2	2.28	0.48
1:A:118:LEU:HB3	1:A:122:VAL:HG11	1.95	0.48
1:A:723:ASP:N	1:A:723:ASP:OD1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.48	0.48
1:A:441:ALA:HB1	1:A:944:LEU:HD21	1.96	0.47
1:A:575:MET:HG2	1:A:666:PHE:HE1	1.79	0.47
1:A:831:ALA:HA	1:A:840:ALA:HB2	1.96	0.47
1:A:76:MET:HG3	1:A:95:GLU:OE2	2.14	0.47
1:A:709:HIS:C	1:A:711:ASP:H	2.16	0.47
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.78	0.47
1:A:956:GLU:HB3	1:A:958:LYS:HG3	1.96	0.47
1:A:568:ASP:OD1	1:A:644:VAL:HG13	2.13	0.47
1:A:418:ARG:NH1	1:A:970:MET:HA	2.30	0.47
1:A:677:ALA:HB2	1:A:867:ARG:CZ	2.44	0.47
1:A:189:ASN:ND2	1:A:192:GLU:H	2.11	0.47
1:A:360:GLN:HB3	1:A:513:PHE:CE2	2.49	0.47
1:A:708:LYS:O	1:A:709:HIS:ND1	2.48	0.47
1:A:459:PHE:O	1:A:464:GLY:HA3	2.14	0.47
1:A:58:GLN:OE1	1:A:818:ARG:HD2	2.14	0.47
1:A:444:GLY:HA3	1:A:891:LEU:HD22	1.95	0.47
1:A:391:ASN:O	1:A:395:MET:HG2	2.15	0.47
1:A:145:THR:OG1	1:A:146:ASP:N	2.47	0.46
1:A:662:MET:HG3	1:A:664:PHE:HE1	1.77	0.46
1:A:458:PHE:HB3	1:A:459:PHE:HD1	1.81	0.46
1:A:60:THR:HG22	1:A:61:VAL:HG22	1.97	0.46
1:A:34:GLN:O	1:A:391:ASN:HB2	2.16	0.46
1:A:448:VAL:O	1:A:451:ALA:HB3	2.16	0.46
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.98	0.46
1:A:587:THR:HB	1:A:613:ASN:HD21	1.80	0.46
1:A:1:MET:N	1:A:2:PRO:HD3	2.31	0.46
1:A:35:TYR:HE2	1:A:671:ILE:HB	1.80	0.46
1:A:10:ILE:HA	1:A:13:TRP:CD1	2.50	0.46
1:A:555:LEU:HB3	1:A:913:LEU:HB3	1.97	0.46
1:A:599:LEU:O	1:A:603:LYS:HG2	2.16	0.46
1:A:142:VAL:HG12	1:A:321:LEU:HD22	1.97	0.45
1:A:513:PHE:HA	1:A:513:PHE:HD1	1.69	0.45
1:A:38:ILE:HG23	1:A:462:SER:HB2	1.98	0.45
1:A:546:LEU:O	1:A:550:VAL:HG23	2.17	0.45
1:A:695:LEU:O	1:A:699:ARG:HB2	2.16	0.45
1:A:58:GLN:O	1:A:62:THR:HB	2.16	0.45
1:A:985:GLY:O	1:A:988:PRO:HD2	2.16	0.45
1:A:73:ASP:O	1:A:74:ASN:HB2	2.15	0.45
1:A:254:ASN:HD22	1:A:258:SER:HB3	1.81	0.45
1:A:300:LEU:HD23	1:A:304:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:LEU:HA	1:A:968:VAL:HB	1.98	0.45
1:A:199:THR:HG22	1:A:791:VAL:HA	1.99	0.45
1:A:94:PHE:CB	1:A:98:THR:HG21	2.47	0.45
1:A:33:ALA:HB2	1:A:299:ALA:HB2	1.99	0.44
1:A:445:ILE:O	1:A:449:LEU:HD13	2.17	0.44
1:A:637:ARG:O	1:A:643:LYS:NZ	2.38	0.44
1:A:885:PHE:HA	1:A:888:LEU:HD12	1.99	0.44
1:A:972:LEU:HD23	1:A:1019:ILE:HD11	1.99	0.44
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.99	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	2.00	0.44
1:A:328:ASP:C	1:A:330:THR:N	2.70	0.44
1:A:574:THR:O	1:A:626:ILE:HA	2.18	0.44
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.80	0.44
1:A:702:LEU:HA	1:A:702:LEU:HD12	1.68	0.44
1:A:165:ALA:HB1	1:A:309:GLU:OE1	2.18	0.44
1:A:314:GLU:N	1:A:315:PRO:HD2	2.33	0.44
1:A:520:PHE:O	1:A:524:THR:HG23	2.17	0.44
1:A:582:ALA:HB3	1:A:623:ASN:HB3	2.00	0.44
1:A:649:MET:O	1:A:652:THR:HG22	2.17	0.44
1:A:674:LEU:HA	1:A:674:LEU:HD12	1.86	0.44
1:A:1021:PHE:HB3	1:A:1025:PHE:CE2	2.53	0.44
1:A:162:MET:HG2	1:A:313:MET:SD	2.58	0.44
1:A:987:MET:N	1:A:988:PRO:HD2	2.33	0.44
1:A:70:ASN:O	1:A:110:LYS:HE2	2.18	0.43
1:A:924:ASP:OD2	1:A:926:TYR:HB2	2.17	0.43
1:A:997:SER:O	1:A:1000:GLN:N	2.52	0.43
1:A:544:LEU:O	1:A:548:ILE:HG13	2.18	0.43
1:A:62:THR:O	1:A:66:GLU:HG3	2.18	0.43
1:A:297:ALA:CA	1:A:298:ASN:HB2	2.47	0.43
1:A:448:VAL:HG23	1:A:449:LEU:HD13	1.99	0.43
1:A:892:TYR:CD1	1:A:897:ILE:HG22	2.53	0.43
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.74	0.43
1:A:411:VAL:O	1:A:415:ASN:HB2	2.18	0.43
1:A:868:LEU:HB3	1:A:869:SER:H	1.60	0.43
1:A:415:ASN:OD1	1:A:971:ARG:NH2	2.52	0.43
1:A:1024:VAL:HA	1:A:1027:VAL:HG22	2.00	0.43
1:A:162:MET:HA	1:A:313:MET:SD	2.58	0.43
1:A:287:SER:OG	1:A:288:GLY:N	2.50	0.43
1:A:389:SER:O	1:A:391:ASN:N	2.49	0.43
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.99	0.43
1:A:866:GLU:O	1:A:867:ARG:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:O	1:A:13:TRP:HB2	2.19	0.43
1:A:111:LEU:HD12	1:A:129:VAL:CG2	2.49	0.43
1:A:262:LEU:HB3	1:A:268:ILE:HD11	1.99	0.43
1:A:310:LEU:HD21	1:A:323:ILE:HD12	2.01	0.43
1:A:877:TYR:OH	1:A:928:GLN:HG2	2.19	0.43
1:A:572:PHE:HB2	1:A:666:PHE:O	2.18	0.43
1:A:633:ASP:OD2	1:A:634:TRP:N	2.52	0.43
1:A:641:GLU:HA	1:A:646:ALA:HB3	2.00	0.43
1:A:445:ILE:HD13	1:A:940:LYS:HZ3	1.83	0.43
1:A:355:MET:SD	1:A:368:PRO:HG3	2.59	0.43
1:A:559:LEU:HD12	1:A:560:PRO:HD2	2.00	0.43
1:A:575:MET:HG2	1:A:666:PHE:CE1	2.53	0.43
1:A:144:ASN:O	1:A:284:GLN:NE2	2.52	0.42
1:A:152:GLU:H	1:A:152:GLU:HG2	1.44	0.42
1:A:409:ALA:O	1:A:413:VAL:HG23	2.18	0.42
1:A:712:MET:O	1:A:713:LEU:HD12	2.19	0.42
1:A:922:THR:OG1	1:A:923:ASN:N	2.52	0.42
1:A:150:THR:HG23	1:A:153:ASP:OD2	2.20	0.42
1:A:300:LEU:O	1:A:300:LEU:HD23	2.19	0.42
1:A:325:TYR:O	1:A:327:TYR:N	2.47	0.42
1:A:141:GLY:HA2	1:A:288:GLY:HA3	2.01	0.42
1:A:211:ASN:O	1:A:760:ASN:ND2	2.53	0.42
1:A:785:ASP:O	1:A:788:ASP:HB2	2.19	0.42
1:A:1020:PHE:O	1:A:1023:PRO:HD2	2.18	0.42
1:A:5:PHE:HD2	1:A:12:ALA:HB2	1.85	0.42
1:A:1001:ASN:O	1:A:1005:THR:HG23	2.20	0.42
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.86	0.42
1:A:337:ILE:HA	1:A:337:ILE:HD12	1.91	0.42
1:A:6:ILE:O	1:A:428:LYS:HE3	2.20	0.42
1:A:720:GLY:O	1:A:721:LEU:HD23	2.20	0.42
1:A:110:LYS:HA	1:A:110:LYS:HD2	1.89	0.42
1:A:297:ALA:HA	1:A:298:ASN:CB	2.50	0.42
1:A:813:SER:HA	1:A:814:PRO:HD3	1.76	0.42
1:A:68:ASN:O	1:A:110:LYS:HB3	2.20	0.42
1:A:1019:ILE:HD12	1:A:1019:ILE:HA	1.89	0.41
1:A:971:ARG:HG2	1:A:975:ILE:HD11	2.02	0.41
1:A:725:PRO:HG3	1:A:811:TYR:CE1	2.55	0.41
1:A:931:LEU:O	1:A:935:ILE:HG23	2.20	0.41
1:A:177:LEU:HD23	1:A:179:GLY:O	2.20	0.41
1:A:24:GLY:O	1:A:28:LEU:HG	2.21	0.41
1:A:133:SER:O	1:A:292:LYS:HD3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLN:HG2	1:A:513:PHE:CE1	2.55	0.41
1:A:621:GLY:O	1:A:624:THR:HG22	2.20	0.41
1:A:279:ALA:HB3	1:A:286:ALA:O	2.20	0.41
1:A:423:GLU:N	1:A:502:LYS:HG3	2.36	0.41
1:A:155:SER:OG	1:A:179:GLY:HA3	2.21	0.41
1:A:449:LEU:HA	1:A:452:VAL:HG13	2.01	0.41
1:A:10:ILE:HA	1:A:13:TRP:HB2	2.02	0.41
1:A:222:THR:HA	1:A:224:PRO:HD3	2.02	0.41
1:A:366:LEU:O	1:A:369:THR:HB	2.20	0.41
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.56	0.41
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.20	0.41
1:A:123:GLN:HG3	1:A:123:GLN:H	1.69	0.41
1:A:294:ALA:O	1:A:296:GLY:N	2.53	0.41
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.78	0.41
1:A:818:ARG:NH2	1:A:821:GLY:O	2.43	0.41
1:A:644:VAL:O	1:A:648:THR:HG23	2.21	0.41
1:A:111:LEU:HD11	1:A:127:VAL:HG21	2.03	0.41
1:A:156:ASP:O	1:A:159:ALA:N	2.54	0.41
1:A:251:LEU:HA	1:A:251:LEU:HD23	1.64	0.41
1:A:745:ASP:O	1:A:749:THR:HG23	2.20	0.41
1:A:896:SER:O	1:A:899:PHE:N	2.54	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.82	0.40
1:A:331:PRO:O	1:A:335:ILE:HG13	2.22	0.40
1:A:408:ASP:O	1:A:412:VAL:HG23	2.21	0.40
1:A:933:THR:O	1:A:937:LEU:HB2	2.21	0.40
1:A:242:SER:OG	1:A:243:THR:N	2.54	0.40
1:A:677:ALA:HB2	1:A:867:ARG:HH22	1.86	0.40
1:A:72:ILE:HG23	1:A:106:GLN:CB	2.51	0.40
1:A:45:ILE:HD11	1:A:107:VAL:HG12	2.04	0.40
1:A:543:VAL:O	1:A:547:ILE:HG13	2.21	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%)	865 (84%)	123 (12%)	44 (4%)	3	25

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	113	LEU
1	A	146	ASP
1	A	295	THR
1	A	299	ALA
1	A	510	LYS
1	A	579	PRO
1	A	617	PHE
1	A	833	PRO
1	A	866	GLU
1	A	867	ARG
1	A	919	ARG
1	A	921	LEU
1	A	150	THR
1	A	298	ASN
1	A	319	SER
1	A	327	TYR
1	A	390	ILE
1	A	601	LYS
1	A	618	ALA
1	A	672	VAL
1	A	865	GLN
1	A	136	PHE
1	A	301	ASP
1	A	330	THR
1	A	600	THR
1	A	615	PHE
1	A	633	ASP
1	A	669	PRO
1	A	9	PRO
1	A	54	ALA
1	A	877	TYR
1	A	329	THR
1	A	441	ALA
1	A	602	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	710	PRO
1	A	862	MET
1	A	997	SER
1	A	326	PRO
1	A	427	PRO
1	A	776	GLU
1	A	815	ARG
1	A	35	TYR
1	A	746	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	840/855 (98%)	703 (84%)	137 (16%)	3 14

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ASN
1	A	7	ASP
1	A	8	ARG
1	A	37	THR
1	A	44	THR
1	A	46	SER
1	A	57	VAL
1	A	58	GLN
1	A	60	THR
1	A	61	VAL
1	A	70	ASN
1	A	75	LEU
1	A	79	SER
1	A	82	SER
1	A	83	ASP
1	A	85	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	THR
1	A	93	THR
1	A	98	THR
1	A	101	ASP
1	A	109	ASN
1	A	111	LEU
1	A	113	LEU
1	A	122	VAL
1	A	123	GLN
1	A	124	GLN
1	A	128	SER
1	A	130	GLU
1	A	133	SER
1	A	150	THR
1	A	152	GLU
1	A	153	ASP
1	A	164	ASP
1	A	180	SER
1	A	184	MET
1	A	185	ARG
1	A	197	GLN
1	A	198	LEU
1	A	214	VAL
1	A	222	THR
1	A	226	LYS
1	A	230	LEU
1	A	233	SER
1	A	243	THR
1	A	248	LYS
1	A	253	VAL
1	A	256	ASP
1	A	258	SER
1	A	259	ARG
1	A	262	LEU
1	A	274	ASN
1	A	293	LEU
1	A	306	ILE
1	A	307	ARG
1	A	310	LEU
1	A	321	LEU
1	A	329	THR
1	A	337	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	ILE
1	A	362	PHE
1	A	365	THR
1	A	372	VAL
1	A	376	LEU
1	A	379	THR
1	A	414	GLU
1	A	415	ASN
1	A	433	LYS
1	A	447	MET
1	A	473	THR
1	A	486	LEU
1	A	495	THR
1	A	509	LYS
1	A	513	PHE
1	A	515	TRP
1	A	525	HIS
1	A	526	HIS
1	A	564	LEU
1	A	583	THR
1	A	585	GLU
1	A	587	THR
1	A	591	LEU
1	A	604	ASN
1	A	626	ILE
1	A	637	ARG
1	A	644	VAL
1	A	652	THR
1	A	662	MET
1	A	671	ILE
1	A	687	GLN
1	A	695	LEU
1	A	712	MET
1	A	715	SER
1	A	716	VAL
1	A	717	ARG
1	A	723	ASP
1	A	724	THR
1	A	729	ILE
1	A	730	ASP
1	A	732	ASP
1	A	741	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	757	SER
1	A	771	VAL
1	A	773	VAL
1	A	778	LYS
1	A	791	VAL
1	A	801	PHE
1	A	806	SER
1	A	808	ARG
1	A	811	TYR
1	A	815	ARG
1	A	817	GLU
1	A	833	PRO
1	A	846	GLN
1	A	851	LEU
1	A	858	ASP
1	A	865	GLN
1	A	868	LEU
1	A	879	ILE
1	A	881	LEU
1	A	886	LEU
1	A	902	MET
1	A	904	VAL
1	A	919	ARG
1	A	922	THR
1	A	937	LEU
1	A	938	SER
1	A	956	GLU
1	A	960	LEU
1	A	969	ARG
1	A	971	ARG
1	A	973	ARG
1	A	976	LEU
1	A	987	MET
1	A	1007	VAL
1	A	1015	THR
1	A	1022	VAL

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	120	GLN
1	A	189	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	588	GLN
1	A	623	ASN
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%)	0.27	50 (4%) 34 26	14, 69, 128, 143	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	961	ILE	6.0
1	A	833	PRO	5.8
1	A	497	LEU	4.5
1	A	496	MET	4.4
1	A	461	GLY	4.3
1	A	501	ALA	4.1
1	A	995	ALA	3.9
1	A	1	MET	3.7
1	A	359	LEU	3.6
1	A	1026	PHE	3.6
1	A	832	ALA	3.4
1	A	408	ASP	3.3
1	A	425	LEU	3.0
1	A	396	PHE	3.0
1	A	462	SER	3.0
1	A	944	LEU	3.0
1	A	401	ALA	2.9
1	A	705	GLU	2.8
1	A	498	LYS	2.8
1	A	945	ILE	2.7
1	A	500	ILE	2.7
1	A	1031	ARG	2.7
1	A	706	ALA	2.7
1	A	563	PHE	2.7
1	A	967	ALA	2.6
1	A	407	ASP	2.5
1	A	964	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	400	LEU	2.5
1	A	1027	VAL	2.4
1	A	531	VAL	2.4
1	A	513	PHE	2.4
1	A	541	TYR	2.4
1	A	559	LEU	2.3
1	A	834	GLY	2.3
1	A	960	LEU	2.3
1	A	404	LEU	2.2
1	A	410	ILE	2.2
1	A	411	VAL	2.2
1	A	681	ASP	2.2
1	A	949	ALA	2.2
1	A	470	PHE	2.1
1	A	534	ILE	2.1
1	A	965	LEU	2.1
1	A	435	MET	2.1
1	A	405	LEU	2.1
1	A	674	LEU	2.1
1	A	835	LYS	2.0
1	A	966	ASP	2.0
1	A	1003	VAL	2.0
1	A	363	ARG	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.