



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:46 AM UTC

PDB ID : 5ZQ2 / pdb_00005zq2
Title : SidE apo form
Authors : Wang, Y.; Gao, A.; Gao, P.
Deposited on : 2018-04-17
Resolution : 2.70 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

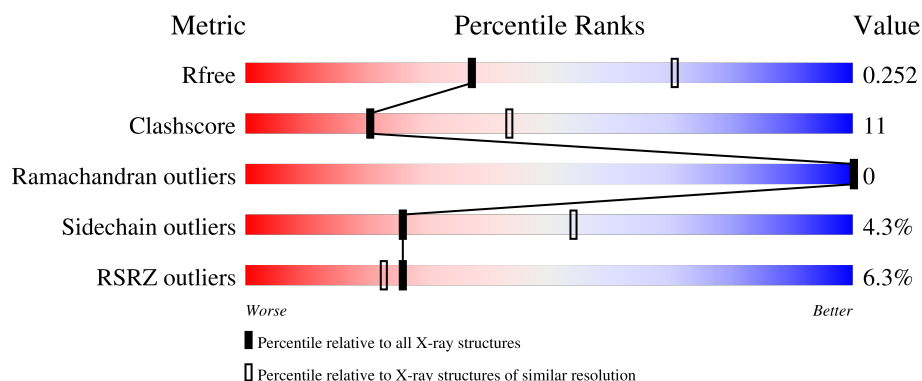
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	845	7% 76% 19% ..
1	C	845	5% 77% 17% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13241 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 SidE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6562	4139	1145	1256	22			
1	C	817	Total	C	N	O	S	0	0	0
			6529	4121	1140	1246	22			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	initiating methionine	UNP Q6RCR1
A	1058	LEU	-	expression tag	UNP Q6RCR1
A	1059	GLU	-	expression tag	UNP Q6RCR1
A	1060	HIS	-	expression tag	UNP Q6RCR1
A	1061	HIS	-	expression tag	UNP Q6RCR1
A	1062	HIS	-	expression tag	UNP Q6RCR1
A	1063	HIS	-	expression tag	UNP Q6RCR1
A	1064	HIS	-	expression tag	UNP Q6RCR1
A	1065	HIS	-	expression tag	UNP Q6RCR1
C	221	MET	-	initiating methionine	UNP Q6RCR1
C	1058	LEU	-	expression tag	UNP Q6RCR1
C	1059	GLU	-	expression tag	UNP Q6RCR1
C	1060	HIS	-	expression tag	UNP Q6RCR1
C	1061	HIS	-	expression tag	UNP Q6RCR1
C	1062	HIS	-	expression tag	UNP Q6RCR1
C	1063	HIS	-	expression tag	UNP Q6RCR1
C	1064	HIS	-	expression tag	UNP Q6RCR1
C	1065	HIS	-	expression tag	UNP Q6RCR1

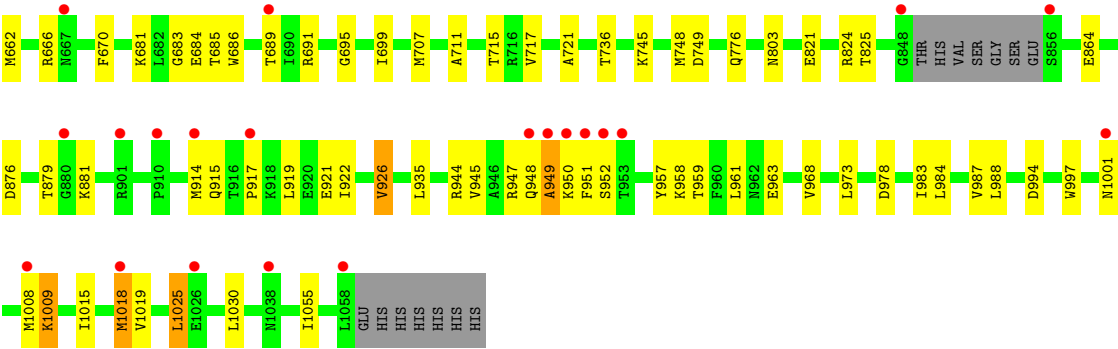
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	79	Total	O	0	0
			79	79		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.30Å 129.36Å 192.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 2.70 48.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.82-2.70) 99.2 (48.82-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.203 , 0.247 0.217 , 0.252	Depositor DCC
R_{free} test set	3223 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13241	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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	0.42	0/6690	0.72	1/9037 (0.0%)
1	C	0.46	2/6657 (0.0%)	0.75	2/8993 (0.0%)
All	All	0.44	2/13347 (0.0%)	0.73	3/18030 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	274	HIS	CG-ND1	-6.33	1.31	1.38
1	C	274	HIS	CD2-NE2	-5.55	1.31	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	248	TYR	N-CA-C	-7.58	98.23	108.24
1	C	949	ALA	N-CA-C	-5.82	104.31	111.75
1	A	505	LEU	N-CA-C	5.58	117.72	109.69

There are no chirality outliers.

There are no planarity outliers.

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	6562	0	6501	173	0
1	C	6529	0	6479	122	0
2	A	71	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	79	0	0	1	0
All	All	13241	0	12980	291	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 11.

All (291) 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:C:476:GLN:CG	1:C:508:ASN:HB2	1.63	1.28
1:C:476:GLN:NE2	1:C:508:ASN:HB3	1.50	1.24
1:C:476:GLN:HG2	1:C:508:ASN:HB2	1.27	1.12
1:C:476:GLN:HE21	1:C:508:ASN:CB	1.64	1.08
1:A:499:PHE:CZ	1:A:503:LYS:NZ	2.23	1.06
1:A:483:GLU:O	1:A:484:GLU:HB3	1.46	1.05
1:C:476:GLN:CG	1:C:508:ASN:CB	2.36	1.04
1:C:476:GLN:NE2	1:C:508:ASN:CB	2.21	1.01
1:A:464:LEU:CD2	1:A:465:VAL:O	2.09	1.01
1:C:476:GLN:HE21	1:C:508:ASN:CG	1.70	0.99
1:A:468:GLY:HA3	1:A:498:PHE:CZ	2.00	0.95
1:A:512:MET:CE	1:A:517:TYR:HA	1.96	0.94
1:C:476:GLN:HG3	1:C:508:ASN:HB2	1.46	0.93
1:A:598:MET:HG3	1:A:908:VAL:HG21	1.50	0.93
1:A:273:HIS:HB3	1:A:337:GLU:OE2	1.70	0.91
1:A:338:GLU:CD	1:A:342:ASN:H	1.81	0.88
1:C:476:GLN:HE21	1:C:508:ASN:HB3	1.22	0.86
1:A:474:ILE:HD13	1:A:510:ARG:HH11	1.40	0.85
1:A:475:GLY:HA2	1:A:509:GLN:HG2	1.58	0.84
1:A:468:GLY:CA	1:A:498:PHE:CZ	2.60	0.84
1:A:472:TYR:HE1	1:A:497:LYS:O	1.61	0.84
1:C:476:GLN:CD	1:C:508:ASN:HB3	2.03	0.84
1:A:261:PRO:HB2	1:A:268:MET:HE2	1.61	0.82
1:A:338:GLU:OE1	1:A:342:ASN:HB2	1.79	0.82
1:A:1008:MET:HA	1:A:1008:MET:HE3	1.63	0.81
1:A:472:TYR:CE1	1:A:497:LYS:O	2.33	0.81
1:A:474:ILE:CG1	1:A:510:ARG:HD3	2.10	0.80
1:A:420:TYR:CG	1:A:466:VAL:HG11	2.16	0.80
1:A:512:MET:HE2	1:A:517:TYR:HA	1.63	0.80
1:A:464:LEU:HD23	1:A:465:VAL:O	1.81	0.80
1:A:483:GLU:O	1:A:484:GLU:CB	2.26	0.79
1:A:470:GLY:HA3	1:A:498:PHE:CE1	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:HD21	1:C:276:LEU:N	1.98	0.78
1:C:476:GLN:HG2	1:C:508:ASN:CB	2.08	0.77
1:C:473:VAL:HG12	1:C:511:TYR:HD1	1.50	0.76
1:C:473:VAL:HG12	1:C:511:TYR:CD1	2.21	0.76
1:A:512:MET:HE2	1:A:517:TYR:CA	2.15	0.75
1:A:474:ILE:CD1	1:A:510:ARG:HH11	2.00	0.75
1:A:477:ASP:N	1:A:478:GLY:HA2	2.00	0.75
1:A:474:ILE:HG12	1:A:510:ARG:HD3	1.68	0.74
1:A:499:PHE:CE1	1:A:503:LYS:NZ	2.49	0.73
1:C:659:ASP:OD2	1:C:691:ARG:NH1	2.22	0.73
1:A:338:GLU:OE1	1:A:342:ASN:N	2.22	0.73
1:C:249:LEU:HD21	1:C:276:LEU:CA	2.19	0.72
1:A:470:GLY:N	1:A:498:PHE:HE1	1.87	0.72
1:A:1012:MET:HA	1:A:1012:MET:HE2	1.72	0.72
1:A:503:LYS:HE2	1:A:505:LEU:HD21	1.72	0.72
1:A:472:TYR:CE1	1:A:496:LEU:HB3	2.24	0.72
1:C:476:GLN:CD	1:C:508:ASN:CB	2.60	0.72
1:A:464:LEU:HD22	1:A:465:VAL:O	1.90	0.71
1:C:945:VAL:O	1:C:949:ALA:N	2.23	0.71
1:C:948:GLN:O	1:C:949:ALA:C	2.33	0.71
1:C:257:VAL:HG21	1:C:338:GLU:HG2	1.73	0.71
1:A:338:GLU:HG2	1:A:346:TYR:HE2	1.56	0.71
1:C:311:THR:HG22	1:C:313:ALA:H	1.57	0.70
1:A:474:ILE:HD11	1:A:510:ARG:HD3	1.72	0.70
1:A:474:ILE:CD1	1:A:510:ARG:HD3	2.21	0.69
1:A:956:GLY:O	1:A:959:THR:HG22	1.92	0.69
1:A:942:GLN:HG2	2:A:1112:HOH:O	1.92	0.69
1:C:824:ARG:NH1	1:C:876:ASP:OD2	2.25	0.69
1:A:475:GLY:O	1:A:478:GLY:HA3	1.92	0.68
1:A:468:GLY:HA3	1:A:498:PHE:CE1	2.28	0.68
1:C:476:GLN:HG3	1:C:508:ASN:CB	2.15	0.68
1:A:503:LYS:HG3	1:A:504:LYS:H	1.59	0.67
1:A:504:LYS:O	1:A:505:LEU:HD22	1.94	0.67
1:A:251:LYS:O	1:A:271:ARG:NH1	2.28	0.67
1:A:474:ILE:HD11	1:A:510:ARG:CD	2.25	0.66
1:C:476:GLN:HA	1:C:476:GLN:OE1	1.95	0.66
1:A:261:PRO:CB	1:A:268:MET:HE2	2.24	0.66
1:A:512:MET:HE2	1:A:517:TYR:CB	2.27	0.65
1:A:910:PRO:O	1:A:914:MET:HG3	1.97	0.65
1:A:464:LEU:HD21	1:A:469:LEU:HA	1.79	0.64
1:C:253:TYR:CZ	1:C:271:ARG:HG2	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:MET:CE	1:A:517:TYR:CA	2.72	0.64
1:C:505:LEU:HB3	1:C:509:GLN:HB2	1.80	0.63
1:A:512:MET:HE2	1:A:517:TYR:HB2	1.79	0.63
1:C:947:ARG:O	1:C:951:PHE:HD2	1.80	0.63
1:A:707:MET:SD	1:A:743:THR:HG21	2.39	0.62
1:C:482:ARG:HD2	1:C:496:LEU:HA	1.81	0.62
1:A:977:LEU:O	1:C:915:GLN:NE2	2.32	0.62
1:C:345:LYS:NZ	1:C:349:GLN:OE1	2.32	0.62
1:A:476:GLN:HB3	1:A:508:ASN:HB2	1.82	0.61
1:C:944:ARG:HG2	1:C:1008:MET:HE3	1.83	0.61
1:A:503:LYS:HE2	1:A:505:LEU:CD2	2.30	0.60
1:C:341:LYS:O	1:C:342:ASN:HB2	2.00	0.60
1:A:253:TYR:HE2	1:A:337:GLU:OE1	1.84	0.60
1:A:468:GLY:C	1:A:498:PHE:CZ	2.79	0.60
1:A:474:ILE:HD13	1:A:510:ARG:NH1	2.15	0.60
1:A:408:VAL:HG12	1:A:408:VAL:O	2.02	0.60
1:A:691:ARG:NH1	1:A:702:ASP:OD2	2.35	0.59
1:A:473:VAL:O	1:A:481:ILE:HG13	2.03	0.59
1:A:503:LYS:CE	1:A:505:LEU:HD21	2.32	0.59
1:C:745:LYS:NZ	1:C:749:ASP:OD2	2.35	0.59
1:A:468:GLY:O	1:A:498:PHE:HZ	1.85	0.59
1:C:249:LEU:HD21	1:C:276:LEU:HA	1.84	0.59
1:A:911:LEU:HD12	1:A:914:MET:HE2	1.85	0.58
1:A:941:LEU:HD11	1:A:1008:MET:HE1	1.86	0.58
1:A:338:GLU:HG2	1:A:346:TYR:CE2	2.36	0.58
1:C:994:ASP:OD1	1:C:1009:LYS:NZ	2.37	0.57
1:A:420:TYR:CG	1:A:466:VAL:CG1	2.88	0.57
1:A:470:GLY:CA	1:A:498:PHE:CE1	2.87	0.57
1:C:341:LYS:HG2	1:C:342:ASN:N	2.20	0.57
1:C:245:TYR:HA	1:C:249:LEU:HB3	1.87	0.56
1:A:479:ASN:OD1	1:A:479:ASN:N	2.38	0.56
1:A:474:ILE:HG13	1:A:510:ARG:O	2.04	0.56
1:A:499:PHE:CE2	1:A:503:LYS:HE2	2.41	0.56
1:C:948:GLN:C	1:C:950:LYS:N	2.62	0.55
1:A:264:PHE:HB2	1:A:556:ALA:HB2	1.89	0.55
1:A:261:PRO:HB2	1:A:268:MET:CE	2.34	0.55
1:A:404:MET:HG2	1:A:421:TYR:CE1	2.42	0.55
1:C:624:LEU:HB3	1:C:914:MET:HE2	1.89	0.55
1:C:249:LEU:HD21	1:C:275:GLY:C	2.32	0.54
1:A:410:VAL:HG11	1:A:451:ALA:HB1	1.89	0.54
1:A:767:GLU:O	1:A:771:ASN:ND2	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:GLU:N	1:A:954:GLU:OE2	2.40	0.54
1:C:505:LEU:HD11	1:C:511:TYR:CE1	2.41	0.54
1:C:945:VAL:HA	1:C:1008:MET:HE1	1.88	0.54
1:C:366:ILE:HG12	1:C:367:PRO:HA	1.88	0.54
1:A:953:THR:OG1	1:A:954:GLU:N	2.38	0.53
1:A:611:MET:HE1	1:A:661:LEU:HD22	1.90	0.53
1:A:502:LYS:HZ2	1:A:504:LYS:HE3	1.73	0.53
1:C:776:GLN:HB3	1:C:803:ASN:HB3	1.89	0.53
1:A:334:ARG:NH1	1:A:336:ASP:O	2.42	0.53
1:A:440:THR:HG23	1:A:576:THR:HG21	1.90	0.53
1:C:263:ASN:HD22	1:C:268:MET:HG2	1.73	0.52
1:C:249:LEU:CD2	1:C:276:LEU:N	2.71	0.52
1:A:338:GLU:OE1	1:A:342:ASN:CB	2.56	0.52
1:A:410:VAL:HG11	1:A:451:ALA:CB	2.39	0.52
1:C:406:ASP:O	1:C:409:ARG:NH1	2.36	0.52
1:A:274:HIS:HB3	1:A:331:VAL:HG11	1.90	0.52
1:A:502:LYS:NZ	1:A:504:LYS:HE3	2.25	0.52
1:C:393:SER:OG	1:C:396:HIS:ND1	2.36	0.52
1:A:605:ARG:NH1	1:C:978:ASP:OD2	2.42	0.52
1:A:242:ARG:NH1	1:A:563:ASP:OD2	2.42	0.52
1:C:344:GLU:H	1:C:344:GLU:CD	2.18	0.51
1:A:879:THR:OG1	1:A:880:GLY:N	2.43	0.51
1:A:420:TYR:CB	1:A:466:VAL:HG11	2.40	0.51
1:C:474:ILE:N	1:C:510:ARG:O	2.25	0.51
1:A:762:GLY:HA3	1:A:823:PRO:HB3	1.93	0.51
1:C:248:TYR:O	1:C:250:GLY:N	2.41	0.51
1:A:483:GLU:OE2	1:A:497:LYS:HG3	2.11	0.51
1:A:776:GLN:NE2	1:A:803:ASN:O	2.41	0.51
1:A:503:LYS:CG	1:A:504:LYS:N	2.73	0.50
1:A:245:TYR:HA	1:A:249:LEU:HB2	1.92	0.50
1:C:681:LYS:O	1:C:685:THR:OG1	2.22	0.50
1:A:537:GLY:HA2	1:A:546:TYR:CZ	2.47	0.50
1:A:477:ASP:N	1:A:478:GLY:CA	2.73	0.50
1:A:237:VAL:CG1	1:A:283:MET:CE	2.89	0.50
1:C:717:VAL:HG13	1:C:736:THR:HG23	1.93	0.50
1:C:476:GLN:HG2	1:C:508:ASN:O	2.11	0.50
1:C:949:ALA:O	1:C:958:LYS:HG2	2.11	0.50
1:C:274:HIS:HB3	1:C:331:VAL:HG21	1.94	0.49
1:A:503:LYS:HG3	1:A:504:LYS:N	2.25	0.49
1:A:468:GLY:O	1:A:498:PHE:CZ	2.65	0.49
1:C:656:ARG:HH12	1:C:695:GLY:HA2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LYS:HB2	2:C:1138:HOH:O	2.11	0.49
1:A:652:ASP:HB3	1:A:696:VAL:HG11	1.94	0.49
1:C:638:LEU:HG	1:C:721:ALA:HA	1.95	0.49
1:A:484:GLU:O	1:A:484:GLU:HG2	2.12	0.49
1:C:921:GLU:OE1	1:C:921:GLU:N	2.42	0.49
1:C:1015:ILE:O	1:C:1018:MET:HB2	2.13	0.49
1:A:393:SER:OG	1:A:396:HIS:ND1	2.35	0.48
1:C:691:ARG:NH1	1:C:699:ILE:HG12	2.29	0.48
1:A:475:GLY:O	1:A:478:GLY:CA	2.62	0.48
1:A:343:TYR:OH	1:A:385:ASP:OD2	2.23	0.48
1:A:470:GLY:CA	1:A:498:PHE:HE1	2.23	0.48
1:C:748:MET:O	1:C:748:MET:HG3	2.13	0.48
1:C:513:ARG:NE	1:C:516:GLU:OE2	2.45	0.48
1:A:844:PRO:HB3	1:A:860:ILE:HG22	1.95	0.47
1:A:499:PHE:CZ	1:A:503:LYS:CE	2.96	0.47
1:A:594:ARG:NH2	1:A:600:GLU:OE2	2.43	0.47
1:C:685:THR:O	1:C:689:THR:HG22	2.13	0.47
1:A:607:VAL:O	1:A:611:MET:HB2	2.15	0.47
1:C:1025:LEU:HD22	1:C:1030:LEU:HG	1.96	0.47
1:A:464:LEU:CD2	1:A:464:LEU:C	2.88	0.47
1:A:531:GLY:C	1:A:532:LYS:HG2	2.40	0.47
1:A:822:VAL:HA	1:A:826:ILE:HD13	1.96	0.47
1:C:237:VAL:HG23	1:C:321:ARG:HG3	1.97	0.47
1:C:662:MET:O	1:C:683:GLY:HA3	2.14	0.47
1:A:323:ILE:HD13	1:A:398:LEU:HD12	1.97	0.47
1:C:474:ILE:HD11	1:C:512:MET:HB2	1.97	0.47
1:C:613:ASN:OD1	1:C:613:ASN:N	2.48	0.47
1:C:662:MET:HG3	1:C:686:TRP:CD1	2.50	0.47
1:C:968:VAL:HG13	1:C:987:VAL:HG22	1.96	0.47
1:A:930:ARG:NH2	1:C:917:PRO:O	2.48	0.47
1:A:949:ALA:O	1:A:958:LYS:HG3	2.14	0.47
1:A:748:MET:HG2	1:A:845:LYS:HE3	1.96	0.46
1:C:406:ASP:O	1:C:409:ARG:HD2	2.16	0.46
1:C:948:GLN:C	1:C:950:LYS:H	2.22	0.46
1:A:822:VAL:HB	1:A:823:PRO:HD3	1.98	0.46
1:A:957:TYR:CE2	1:A:961:LEU:HD11	2.50	0.46
1:C:879:THR:HG23	1:C:881:LYS:H	1.81	0.46
1:C:984:LEU:HD22	1:C:1019:VAL:HG13	1.98	0.46
1:A:367:PRO:HA	1:A:370:PHE:O	2.15	0.46
1:A:504:LYS:HE2	1:A:504:LYS:HB3	1.77	0.46
1:A:770:LYS:NZ	1:A:830:ASN:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:GLU:HG2	1:C:509:GLN:CD	2.41	0.46
1:C:476:GLN:C	1:C:478:GLY:N	2.72	0.45
1:A:643:MET:HB2	1:A:861:TYR:CZ	2.51	0.45
1:C:319:GLU:O	1:C:323:ILE:HG12	2.17	0.45
1:A:879:THR:HG23	1:A:881:LYS:H	1.81	0.45
1:C:409:ARG:HG3	1:C:445:PHE:CE2	2.52	0.45
1:C:949:ALA:O	1:C:958:LYS:CG	2.65	0.45
1:C:666:ARG:NH2	1:C:684:GLU:OE2	2.49	0.45
1:C:247:ASN:C	1:C:248:TYR:CG	2.95	0.45
1:C:957:TYR:CZ	1:C:961:LEU:HD11	2.52	0.45
1:A:498:PHE:O	1:A:498:PHE:CG	2.70	0.44
1:A:953:THR:CB	1:A:954:GLU:OE2	2.65	0.44
1:C:329:PHE:HA	1:C:332:THR:HG23	1.99	0.44
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.77	0.44
1:A:474:ILE:HD11	1:A:510:ARG:HD2	1.97	0.44
1:A:561:ASP:HB3	1:A:564:PHE:HB3	1.99	0.44
1:A:691:ARG:HG2	1:A:691:ARG:HH11	1.82	0.44
1:A:955:SER:HA	1:A:956:GLY:HA2	1.50	0.44
1:C:245:TYR:HB2	1:C:276:LEU:HD13	1.98	0.44
1:A:506:GLU:OE1	1:A:508:ASN:ND2	2.46	0.44
1:A:770:LYS:NZ	1:A:884:ASP:O	2.42	0.44
1:C:711:ALA:O	1:C:715:THR:OG1	2.29	0.44
1:C:323:ILE:HD12	1:C:395:ALA:HA	1.98	0.44
1:C:343:TYR:OH	1:C:385:ASP:OD2	2.34	0.44
1:C:404:MET:CE	1:C:424:GLN:HG3	2.47	0.44
1:C:247:ASN:O	1:C:248:TYR:CG	2.70	0.44
1:C:405:VAL:HG12	1:C:441:GLN:HG3	1.98	0.44
1:C:538:LEU:HD23	1:C:539:PRO:HD2	2.00	0.44
1:A:984:LEU:HD22	1:A:1019:VAL:HG13	1.99	0.44
1:C:616:CYS:HB2	1:C:623:PHE:O	2.18	0.44
1:A:717:VAL:HG13	1:A:736:THR:HG23	1.99	0.43
1:C:245:TYR:O	1:C:248:TYR:O	2.35	0.43
1:A:625:ASN:HB2	1:A:914:MET:HB3	1.99	0.43
1:A:1015:ILE:HA	1:A:1018:MET:HE3	2.01	0.43
1:C:474:ILE:HB	1:C:510:ARG:HG3	2.00	0.43
1:C:537:GLY:HA2	1:C:546:TYR:CE2	2.53	0.43
1:C:821:GLU:OE1	1:C:825:THR:OG1	2.36	0.43
1:A:470:GLY:H	1:A:498:PHE:HE1	1.61	0.43
1:A:1030:LEU:HD13	1:C:919:LEU:HD21	1.99	0.43
1:A:404:MET:O	1:A:407:LEU:HB2	2.19	0.43
1:A:921:GLU:CD	1:A:921:GLU:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:CD2	1:C:276:LEU:HB2	2.48	0.43
1:C:252:PRO:HG3	1:C:270:TYR:CE1	2.53	0.43
1:C:594:ARG:HE	1:C:864:GLU:CD	2.27	0.43
1:C:959:THR:O	1:C:963:GLU:HG3	2.19	0.43
1:A:473:VAL:HB	1:A:481:ILE:HD12	1.99	0.43
1:A:513:ARG:NH2	1:A:515:ASP:OD1	2.45	0.43
1:A:510:ARG:HG2	1:A:511:TYR:N	2.32	0.43
1:A:707:MET:SD	1:A:743:THR:CG2	3.07	0.43
1:C:384:GLU:OE2	1:C:386:LYS:HE3	2.19	0.43
1:A:279:THR:O	1:A:282:THR:OG1	2.37	0.43
1:C:935:LEU:HD22	1:C:973:LEU:HD12	2.01	0.43
1:A:223:VAL:HG22	1:A:297:LYS:HD3	1.99	0.42
1:A:235:GLU:H	1:A:235:GLU:CD	2.25	0.42
1:A:704:ILE:HA	1:A:707:MET:HG2	2.02	0.42
1:C:292:GLU:HB3	1:C:433:ALA:HB1	2.01	0.42
1:A:744:ASN:O	1:A:748:MET:HG3	2.19	0.42
1:C:333:GLY:O	1:C:349:GLN:NE2	2.46	0.42
1:A:410:VAL:HA	1:A:453:ALA:HB2	2.02	0.42
1:A:506:GLU:H	1:A:506:GLU:HG3	1.57	0.42
1:C:997:TRP:CG	1:C:1009:LYS:HG2	2.55	0.42
1:C:917:PRO:HB2	1:C:919:LEU:HG	2.02	0.42
1:C:1025:LEU:HD23	1:C:1025:LEU:HA	1.85	0.42
1:A:479:ASN:O	1:A:480:PRO:C	2.63	0.42
1:A:504:LYS:C	1:A:505:LEU:HD22	2.45	0.42
1:A:953:THR:HB	1:A:954:GLU:OE2	2.20	0.42
1:A:420:TYR:CD2	1:A:466:VAL:HG11	2.53	0.41
1:A:941:LEU:HD22	1:A:1015:ILE:HD13	2.02	0.41
1:C:409:ARG:HG3	1:C:445:PHE:HE2	1.85	0.41
1:C:260:THR:HA	1:C:261:PRO:HD3	1.90	0.41
1:A:413:PRO:HA	1:A:414:PRO:HD3	1.86	0.41
1:A:474:ILE:CD1	1:A:510:ARG:CD	2.92	0.41
1:A:953:THR:OG1	1:A:954:GLU:OE2	2.35	0.41
1:A:499:PHE:CE2	1:A:503:LYS:CE	3.03	0.41
1:A:655:ILE:HD13	1:A:742:LEU:HD22	2.02	0.41
1:A:838:PRO:HD2	2:A:1129:HOH:O	2.20	0.41
1:C:479:ASN:O	1:C:480:PRO:C	2.63	0.41
1:A:464:LEU:HD23	1:A:464:LEU:C	2.45	0.41
1:A:716:ARG:NH1	1:A:728:SER:OG	2.53	0.41
1:A:255:GLY:HA3	1:A:336:ASP:HB3	2.03	0.41
1:A:468:GLY:C	1:A:498:PHE:CE1	2.99	0.41
1:A:954:GLU:O	1:A:957:TYR:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLY:HA3	1:C:498:PHE:CZ	2.56	0.41
1:C:561:ASP:HB3	1:C:564:PHE:HB3	2.03	0.41
1:C:922:ILE:O	1:C:926:VAL:HG13	2.21	0.41
1:A:499:PHE:HE2	1:A:505:LEU:HG	1.86	0.41
1:A:916:THR:HA	1:A:917:PRO:HD3	1.84	0.41
1:C:362:LYS:O	1:C:366:ILE:HG22	2.21	0.41
1:A:450:GLU:OE2	2:A:1101:HOH:O	2.21	0.40
1:C:650:LEU:O	1:C:745:LYS:HE2	2.22	0.40
1:A:464:LEU:HD23	1:A:465:VAL:N	2.36	0.40
1:A:666:ARG:HA	1:A:683:GLY:HA3	2.04	0.40
1:A:608:GLN:HG2	1:A:654:ASP:CG	2.46	0.40
1:A:704:ILE:O	1:A:707:MET:HG2	2.22	0.40
1:C:415:GLU:HB2	1:C:514:VAL:HG21	2.02	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	816/845 (97%)	775 (95%)	41 (5%)	0	100	100
1	C	811/845 (96%)	782 (96%)	29 (4%)	0	100	100
All	All	1627/1690 (96%)	1557 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	713/736 (97%)	680 (95%)	33 (5%)	24	51
1	C	710/736 (96%)	682 (96%)	28 (4%)	28	57
All	All	1423/1472 (97%)	1362 (96%)	61 (4%)	26	54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	THR
1	A	337	GLU
1	A	338	GLU
1	A	340	SER
1	A	341	LYS
1	A	389	LYS
1	A	411	LYS
1	A	412	GLN
1	A	425	LEU
1	A	464	LEU
1	A	466	VAL
1	A	476	GLN
1	A	477	ASP
1	A	479	ASN
1	A	484	GLU
1	A	496	LEU
1	A	497	LYS
1	A	499	PHE
1	A	504	LYS
1	A	510	ARG
1	A	542	LYS
1	A	551	ASN
1	A	619	ASP
1	A	638	LEU
1	A	643	MET
1	A	670	PHE
1	A	692	SER
1	A	726	LYS
1	A	914	MET
1	A	1004	GLU
1	A	1012	MET
1	A	1049	LEU
1	A	1052	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	249	LEU
1	C	311	THR
1	C	338	GLU
1	C	341	LYS
1	C	365	LEU
1	C	366	ILE
1	C	373	GLU
1	C	392	ASP
1	C	409	ARG
1	C	426	GLN
1	C	506	GLU
1	C	508	ASN
1	C	510	ARG
1	C	532	LYS
1	C	533	LYS
1	C	613	ASN
1	C	638	LEU
1	C	670	PHE
1	C	707	MET
1	C	926	VAL
1	C	952	SER
1	C	983	ILE
1	C	988	LEU
1	C	1001	ASN
1	C	1009	LYS
1	C	1018	MET
1	C	1025	LEU
1	C	1055	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	HIS
1	A	361	ASN
1	A	412	GLN
1	A	476	GLN
1	A	509	GLN
1	A	609	GLN
1	A	902	HIS
1	A	915	GLN
1	A	979	ASN
1	C	247	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	342	ASN
1	C	361	ASN
1	C	401	GLN
1	C	424	GLN
1	C	426	GLN
1	C	476	GLN
1	C	509	GLN
1	C	609	GLN
1	C	618	HIS
1	C	625	ASN
1	C	701	HIS
1	C	787	HIS

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	822/845 (97%)	0.36	61 (7%)	20	18	23, 46, 92, 134	0
1	C	817/845 (96%)	0.31	43 (5%)	32	28	21, 51, 88, 119	0
All	All	1639/1690 (96%)	0.33	104 (6%)	26	23	21, 49, 89, 134	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	PHE	9.7
1	A	497	LYS	6.9
1	A	531	GLY	6.5
1	A	530	ALA	6.2
1	A	498	PHE	6.1
1	C	951	PHE	5.6
1	C	952	SER	5.3
1	C	268	MET	4.6
1	A	957	TYR	4.4
1	A	470	GLY	4.4
1	A	268	MET	4.3
1	A	478	GLY	4.2
1	A	502	LYS	4.2
1	A	496	LEU	4.1
1	A	473	VAL	4.1
1	A	480	PRO	4.0
1	C	948	GLN	4.0
1	A	511	TYR	4.0
1	A	466	VAL	4.0
1	A	494	GLY	3.9
1	A	474	ILE	3.7
1	C	914	MET	3.7
1	C	660	THR	3.7
1	A	953	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	3.5
1	A	505	LEU	3.4
1	A	707	MET	3.3
1	C	848	GLY	3.3
1	A	540	GLY	3.3
1	A	479	ASN	3.3
1	A	981	VAL	3.3
1	A	477	ASP	3.2
1	C	544	TYR	3.2
1	A	337	GLU	3.2
1	A	1058	LEU	3.1
1	A	339	SER	3.1
1	C	482	ARG	3.1
1	C	511	TYR	3.0
1	C	949	ALA	3.0
1	A	338	GLU	2.9
1	A	951	PHE	2.9
1	A	961	LEU	2.9
1	A	475	GLY	2.9
1	C	496	LEU	2.9
1	C	475	GLY	2.8
1	A	1045	ILE	2.8
1	A	481	ILE	2.7
1	A	508	ASN	2.7
1	A	955	SER	2.7
1	C	339	SER	2.7
1	C	1026	GLU	2.7
1	C	1001	ASN	2.6
1	A	222	SER	2.6
1	C	910	PRO	2.6
1	A	529	GLY	2.5
1	A	954	GLU	2.5
1	A	926	VAL	2.5
1	C	950	LYS	2.5
1	A	544	TYR	2.5
1	A	482	ARG	2.4
1	C	505	LEU	2.4
1	C	689	THR	2.4
1	C	856	SER	2.4
1	C	506	GLU	2.4
1	C	1038	ASN	2.4
1	C	410	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	624	LEU	2.3
1	C	460	LYS	2.3
1	A	848	GLY	2.3
1	C	510	ARG	2.3
1	C	366	ILE	2.3
1	A	476	GLN	2.3
1	A	258	GLU	2.3
1	C	390	TRP	2.3
1	C	901	ARG	2.3
1	A	504	LYS	2.3
1	C	479	ASN	2.3
1	C	667	ASN	2.3
1	C	917	PRO	2.3
1	A	472	TYR	2.2
1	A	263	ASN	2.2
1	A	880	GLY	2.2
1	A	417	TYR	2.2
1	C	224	PRO	2.2
1	A	542	LYS	2.2
1	C	341	LYS	2.2
1	A	411	LYS	2.2
1	C	1058	LEU	2.2
1	C	473	VAL	2.2
1	A	273	HIS	2.2
1	A	464	LEU	2.2
1	A	404	MET	2.1
1	C	249	LEU	2.1
1	A	468	GLY	2.1
1	C	1008	MET	2.1
1	A	510	ARG	2.1
1	A	598	MET	2.1
1	C	481	ILE	2.1
1	A	620	ASP	2.1
1	C	953	THR	2.1
1	C	1018	MET	2.0
1	A	265	GLY	2.0
1	A	539	PRO	2.0
1	C	880	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.