



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2022 – 05:17 PM JST

PDB ID : 5ZQ2  
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](mailto: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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

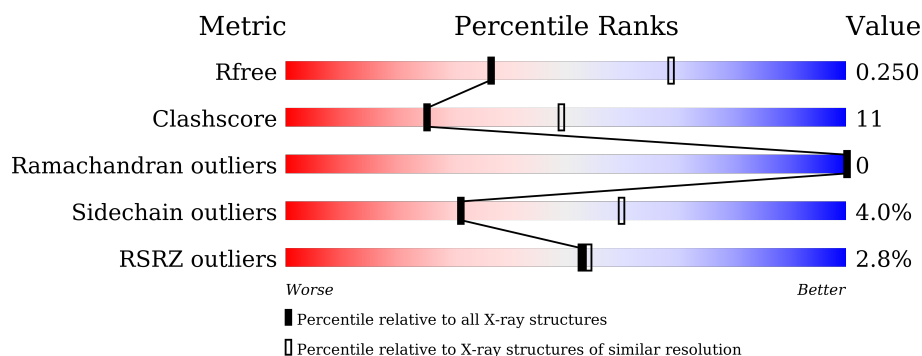
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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  $\geq 3$ , 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	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	845	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>

## 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...*

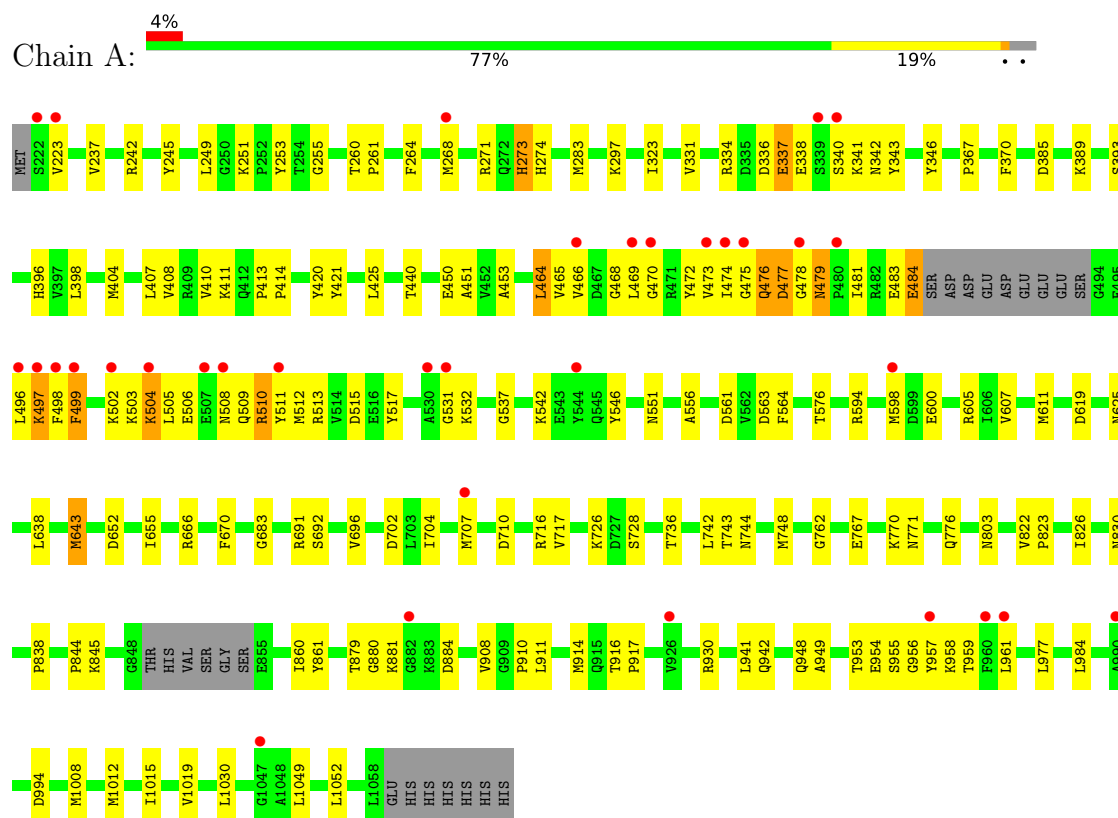
*Continued from previous page...*

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

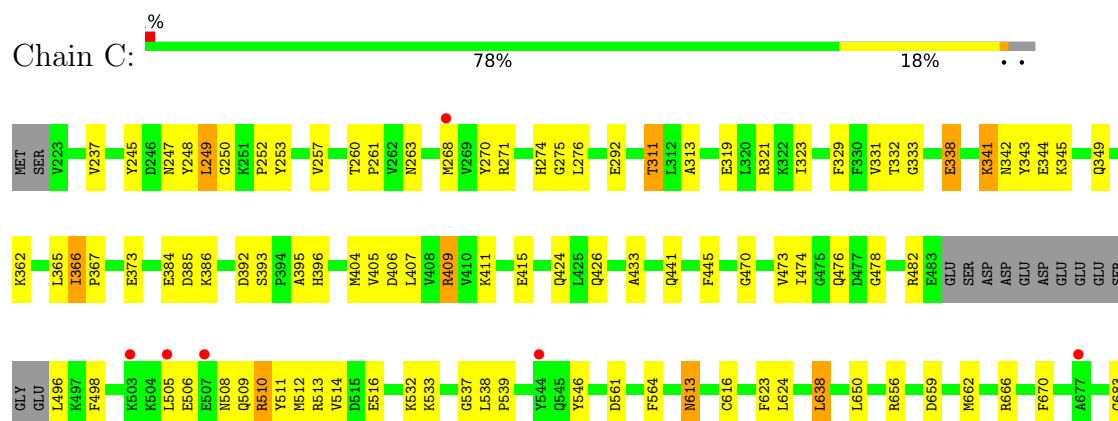
### 3 Residue-property plots [i](#)

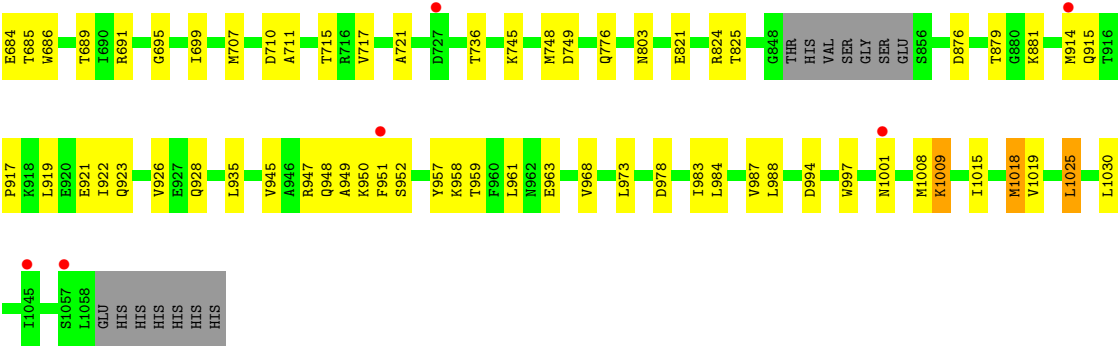
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SidE



#### • Molecule 1: SidE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.203 , 0.247 0.213 , 0.250	Depositor DCC
$R_{free}$ test set	3223 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.30	0/6690	0.44	0/9037
1	C	0.33	0/6657	0.44	0/8993
All	All	0.31	0/13347	0.44	0/18030

There are no bond length outliers.

There are no bond angle outliers.

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	163	0
1	C	6529	0	6479	120	0
2	A	71	0	0	3	0
2	C	79	0	0	1	0
All	All	13241	0	12980	279	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 (279) 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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:468:GLY:HA3	1:A:498:PHE:CZ	2.00	0.95
1:C:476:GLN:HE21	1:C:508:ASN:CG	1.70	0.94
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: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:A:338:GLU:CD	1:A:342:ASN:H	1.81	0.84
1:A:338:GLU:OE1	1:A:342:ASN:HB2	1.79	0.82
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: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:C:476:GLN:CD	1:C:508:ASN:HB3	2.03	0.79
1:A:470:GLY:HA3	1:A:498:PHE:CE1	2.18	0.78
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: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:A:512:MET:HE2	1:A:517:TYR:CA	2.18	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:512:MET:HE2	1:A:517:TYR:HA	1.72	0.70
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:C:476:GLN:CD	1:C:508:ASN:CB	2.60	0.67
1:A:261:PRO:HB2	1:A:268:MET:HE3	1.75	0.67
1:A:474:ILE:HD11	1:A:510:ARG:CD	2.25	0.66
1:C:948:GLN:O	1:C:949:ALA:C	2.33	0.66
1:C:476:GLN:HA	1:C:476:GLN:OE1	1.95	0.66
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
1:C:505:LEU:HB3	1:C:509:GLN:HB2	1.80	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:512:MET:HE1	1:A:517:TYR: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: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:474:ILE:HD13	1:A:510:ARG:NH1	2.15	0.60
1:A:512:MET:CE	1:A:517:TYR:CA	2.72	0.60
1:A:408:VAL:HG12	1:A:408:VAL:O	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:PRO:HB2	1:A:268:MET:CE	2.34	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:1012:MET:HA	1:A:1012:MET:HE2	1.87	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:A:953:THR:OG1	1:A:954:GLU:N	2.38	0.56
1:A:468:GLY:C	1:A:498:PHE:CZ	2.79	0.56
1:A:264:PHE:HB2	1:A:556:ALA:HB2	1.89	0.55
1:A:404:MET:HG2	1:A:421:TYR:CE1	2.42	0.55
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
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:366:ILE:HG12	1:C:367:PRO:HA	1.88	0.54
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:C:945:VAL:CG2	1:C:1008:MET:HE2	2.38	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LYS:CG	1:A:504:LYS:N	2.73	0.51
1:A:879:THR:OG1	1:A:880:GLY:N	2.43	0.51
1:C:404:MET:HE3	1:C:424:GLN:HG3	1.93	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:512:MET:HE2	1:A:517:TYR:N	2.24	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:C:945:VAL:HG22	1:C:1008:MET:HE2	1.92	0.50
1:A:245:TYR:HA	1:A:249:LEU:HB2	1.92	0.50
1:C:948:GLN:C	1:C:950:LYS:N	2.62	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:249:LEU:HD21	1:C:275:GLY:C	2.32	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
1:A:911:LEU:HD12	1:A:914:MET:HE2	1.95	0.49
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:1008:MET:HA	1:A:1008:MET:CE	2.44	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:344:GLU:H	1:C:344:GLU:CD	2.18	0.47
1:A:748:MET:HG2	1:A:845:LYS:HE3	1.96	0.46
1:A:941:LEU:HD11	1:A:1008:MET:HE1	1.97	0.46
1:C:406:ASP:O	1:C:409:ARG:HD2	2.16	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
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:510:ARG:HG2	1:A:511:TYR:N	2.32	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:404:MET:CE	1:C:424:GLN:HG3	2.47	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: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: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: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: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:C:624:LEU:HB3	1:C:914:MET:HE2	2.01	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:464:LEU:CD2	1:A:464:LEU:C	2.88	0.42
1:A:531:GLY:C	1:A:532:LYS:HG2	2.40	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:948:GLN:C	1:C:950:LYS:H	2.22	0.41
1:A:261:PRO:HG2	1:A:268:MET:HE2	2.01	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: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:C:476:GLN:C	1:C:478:GLY:N	2.72	0.41
1:C:506:GLU:HG2	1:C:509:GLN:CD	2.41	0.41
1:A:954:GLU:O	1:A:957:TYR:N	2.54	0.41
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:393:SER:OG	1:A:396:HIS:ND1	2.35	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:C:247:ASN:C	1:C:248:TYR:CG	2.95	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

### 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	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 ⓘ

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%)	683 (96%)	30 (4%)	30	58
1	C	710/736 (96%)	683 (96%)	27 (4%)	33	62
All	All	1423/1472 (97%)	1366 (96%)	57 (4%)	31	60

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	THR
1	A	273	HIS
1	A	337	GLU
1	A	340	SER
1	A	341	LYS
1	A	389	LYS
1	A	411	LYS
1	A	425	LEU
1	A	464	LEU
1	A	476	GLN
1	A	477	ASP
1	A	479	ASN
1	A	484	GLU
1	A	497	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	710	ASP
1	A	726	LYS
1	A	948	GLN
1	A	994	ASP
1	A	1049	LEU
1	A	1052	LEU
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	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	710	ASP
1	C	923	GLN
1	C	928	GLN
1	C	952	SER
1	C	983	ILE
1	C	988	LEU
1	C	1001	ASN
1	C	1009	LYS
1	C	1018	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	1025	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	C	247	ASN
1	C	342	ASN
1	C	424	GLN
1	C	476	GLN
1	C	509	GLN
1	C	915	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	822/845 (97%)	0.07	34 (4%) 37 36	23, 46, 92, 134	0
1	C	817/845 (96%)	0.00	12 (1%) 73 76	21, 51, 88, 119	0
All	All	1639/1690 (96%)	0.04	46 (2%) 53 54	21, 49, 89, 134	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	PHE	9.4
1	A	478	GLY	6.2
1	A	497	LYS	5.3
1	A	498	PHE	4.8
1	A	339	SER	4.0
1	A	222	SER	3.9
1	A	502	LYS	3.6
1	A	469	LEU	3.6
1	A	268	MET	3.5
1	C	951	PHE	3.5
1	A	504	LYS	3.4
1	A	223	VAL	3.3
1	A	496	LEU	3.3
1	A	531	GLY	3.3
1	A	470	GLY	3.3
1	A	957	TYR	3.2
1	C	544	TYR	3.1
1	C	268	MET	3.1
1	C	507	GLU	3.0
1	A	340	SER	2.9
1	A	926	VAL	2.8
1	C	1001	ASN	2.7
1	A	508	ASN	2.7
1	A	511	TYR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	473	VAL	2.7
1	A	474	ILE	2.6
1	A	507	GLU	2.6
1	C	505	LEU	2.6
1	C	914	MET	2.6
1	A	1047	GLY	2.5
1	A	960	PHE	2.4
1	A	466	VAL	2.4
1	A	475	GLY	2.3
1	A	480	PRO	2.3
1	A	882	GLY	2.2
1	A	990	ALA	2.2
1	A	961	LEU	2.2
1	A	530	ALA	2.1
1	C	727	ASP	2.1
1	C	677	ALA	2.1
1	C	1045	ILE	2.1
1	A	598	MET	2.1
1	A	544	TYR	2.1
1	C	1057	SER	2.0
1	C	503	LYS	2.0
1	A	707	MET	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 monosaccharides 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.