



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:36 PM GMT

PDB ID : 3QT1
Title : RNA polymerase II variant containing A Chimeric RPB9-C11 subunit
Authors : Ruan, W.; Lehmann, E.; Thomm, M.; Kostrewa, D.; Cramer, P.
Deposited on : 2011-02-22
Resolution : 4.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

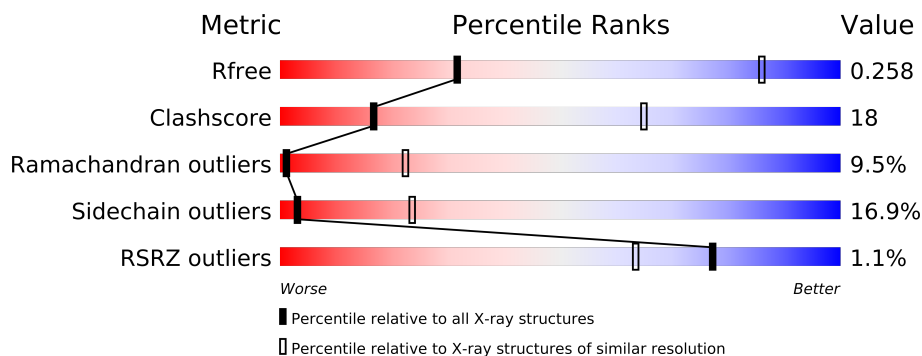
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.30 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}	66092	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
Sidechain outliers	78261	1192 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	219	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	133	
10	J	70	
11	K	120	
12	L	70	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
14	MG	A	3009	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30535 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1103	Total	C	N	O	S	0	0	0
			8770	5554	1535	1626	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9, DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	47	Total	C	N	O	S	0	0	0
			398	246	72	75	5			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	1	Total 1	Zn 1	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

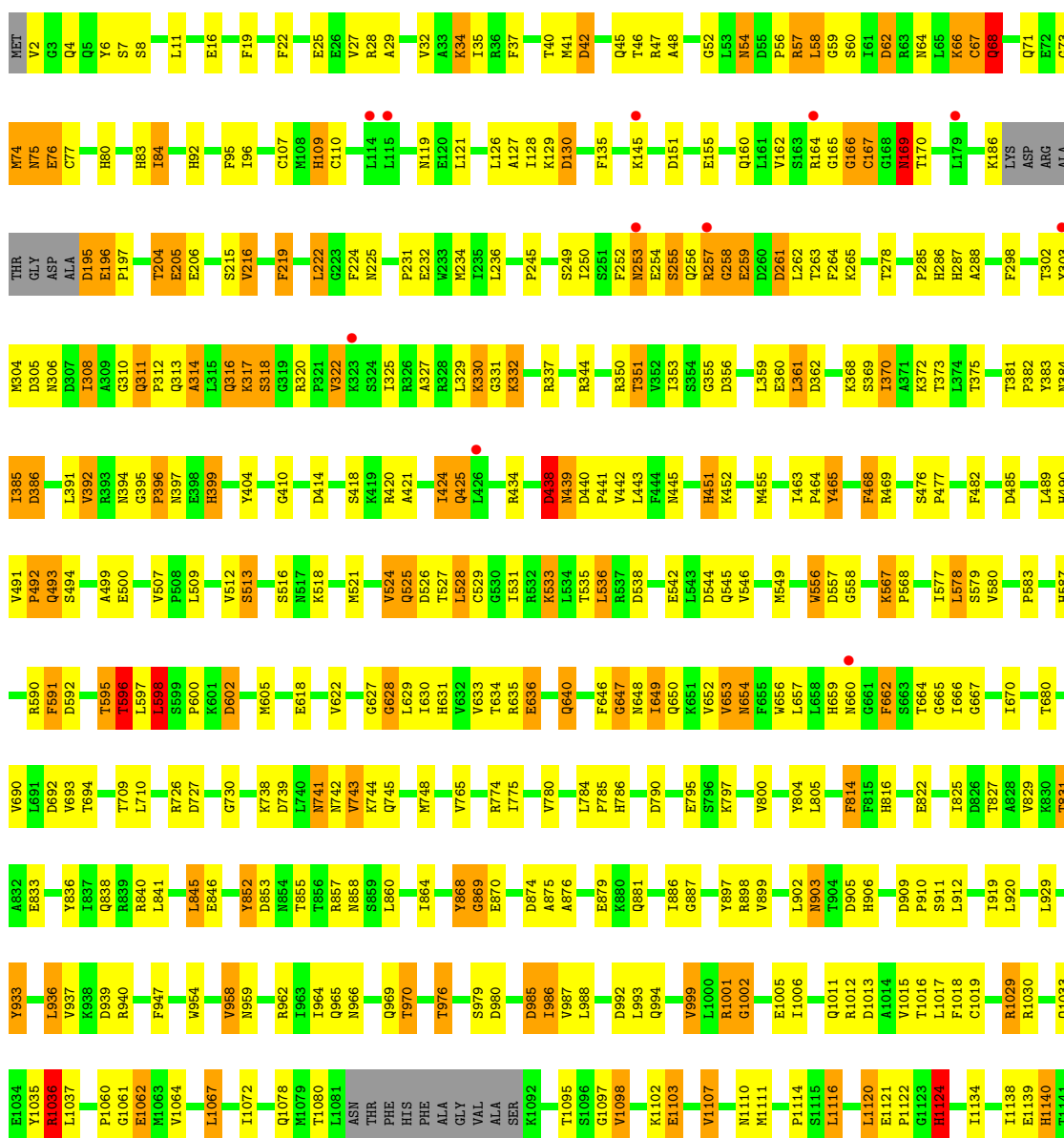
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0

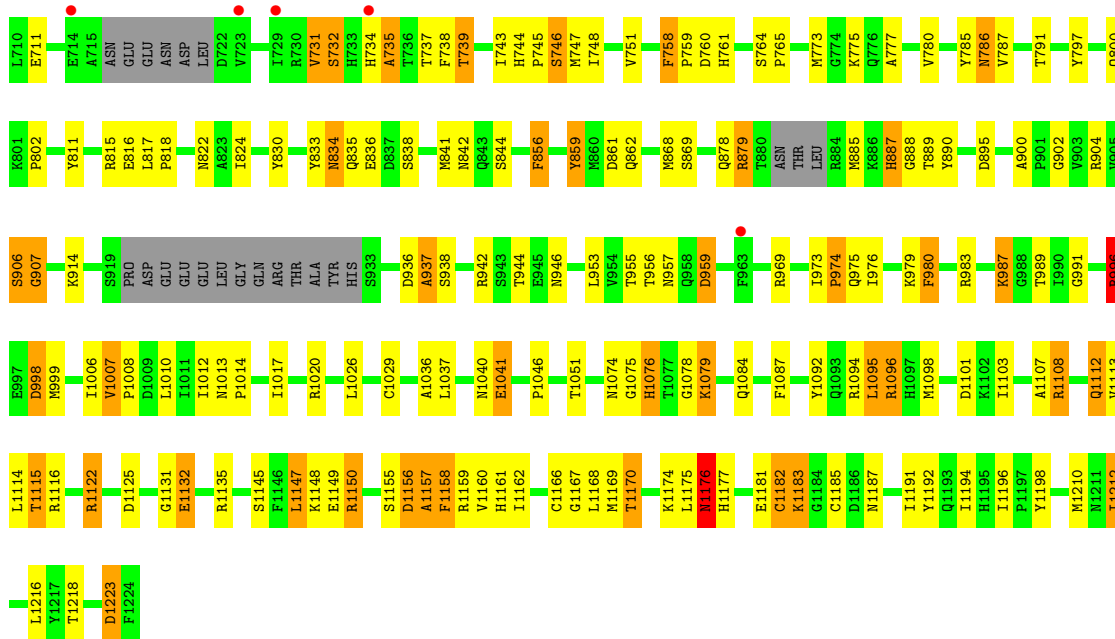
3 Residue-property plots

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: DNA-directed RNA polymerase II subunit RPB1

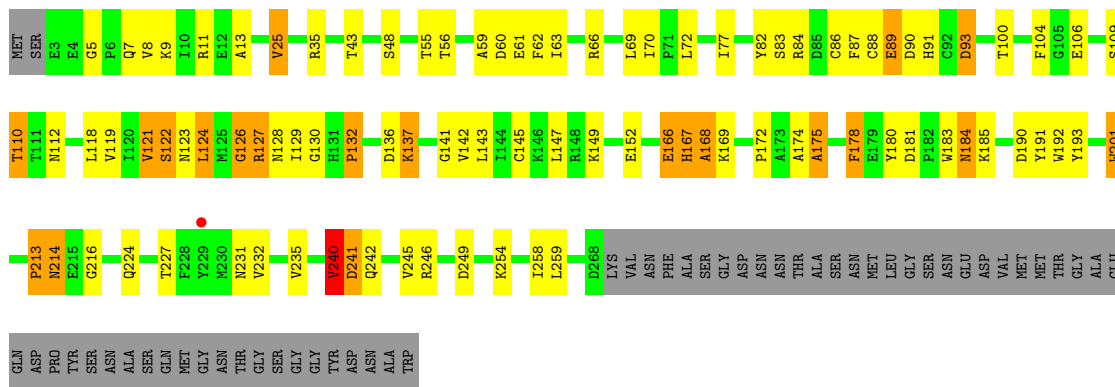
Chain A: 





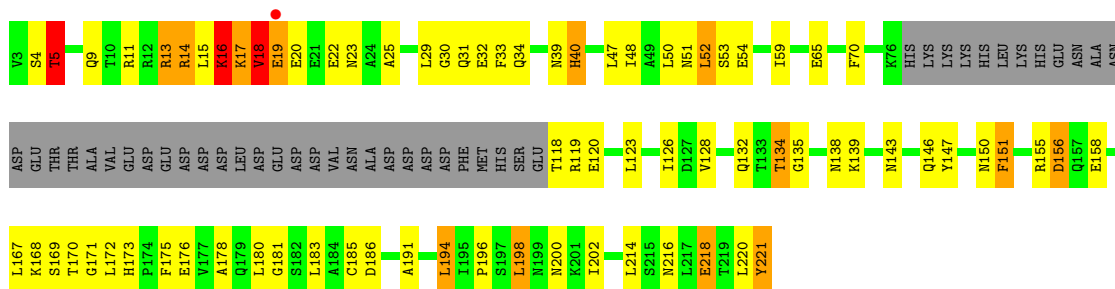
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

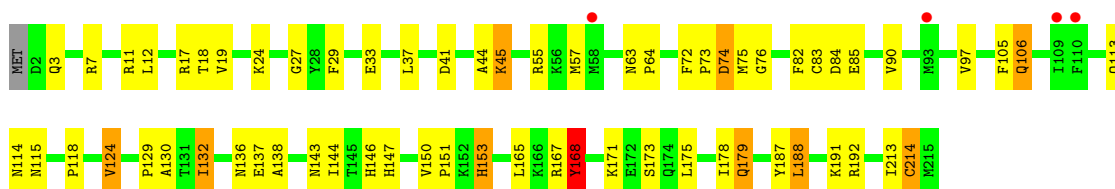
Chain D:



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

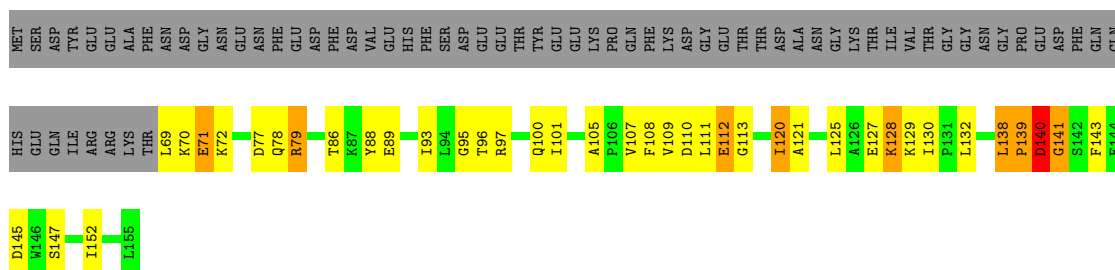
Chain E:





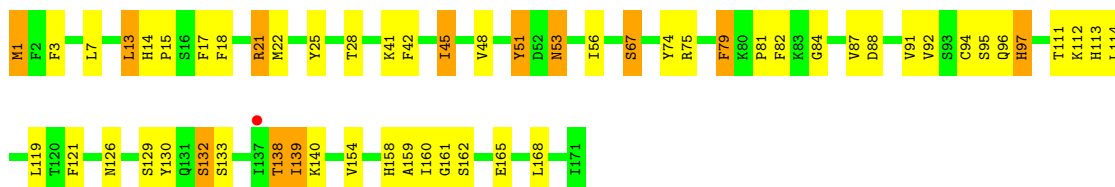
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



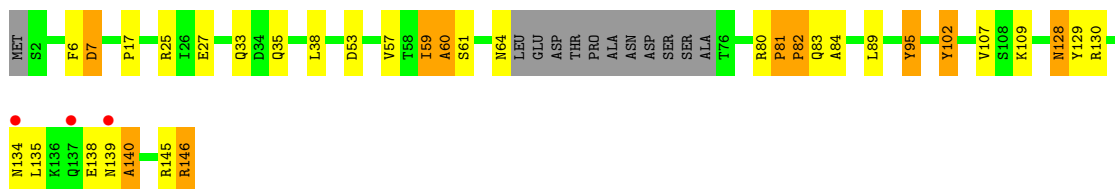
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



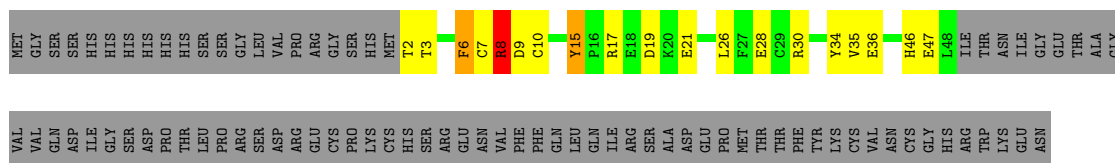
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9, DNA-directed RNA polymerase III subunit RPC10

Chain I:



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.38Å 393.38Å 281.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 4.30 48.66 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.60-4.30) 98.5 (48.66-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1.357)	Depositor
R, R_{free}	0.235 , 0.281 0.209 , 0.258	Depositor DCC
R_{free} test set	2021 reflections (2.45%)	DCC
Wilson B-factor (Å ²)	172.3	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 92.7	EDS
Estimated twinning fraction	0.057 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.067 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 82532 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30535	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.35	0/11342	0.58	0/15337
2	B	0.34	0/8939	0.56	0/12051
3	C	0.33	0/2133	0.56	0/2891
4	D	0.32	0/1444	0.52	0/1935
5	E	0.32	0/1788	0.54	0/2406
6	F	0.40	0/717	0.63	0/967
7	G	0.33	0/1368	0.55	0/1844
8	H	0.29	0/1094	0.50	0/1481
9	I	0.36	0/406	0.57	0/546
10	J	0.33	0/541	0.57	0/727
11	K	0.38	0/937	0.56	0/1265
12	L	0.36	0/365	0.64	0/485
All	All	0.34	0/31074	0.56	0/41935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11143	0	0	227	0
2	B	8770	0	0	138	0
3	C	2095	0	0	37	0
4	D	1434	0	8	34	0
5	E	1752	0	0	21	0
6	F	705	0	29	23	0
7	G	1340	0	0	23	0
8	H	1076	0	0	9	0
9	I	398	0	0	7	0
10	J	532	0	0	19	0
11	K	919	0	0	22	0
12	L	363	0	0	15	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30535	0	37	547	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (547) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:775:ILE:CB	1:A:797:LYS:O	2.26	0.84
11:K:65:HIS:CD2	11:K:67:PHE:N	2.55	0.74
11:K:5:ASP:N	11:K:5:ASP:OD2	2.21	0.71
10:J:8:PHE:N	10:J:8:PHE:CD2	2.56	0.71
1:A:947:PHE:CE1	1:A:954:TRP:CE2	2.79	0.70
1:A:933:TYR:O	1:A:933:TYR:CD2	2.44	0.70
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.51	0.69
1:A:492:PRO:O	1:A:493:GLN:NE2	2.26	0.67
1:A:1138:ILE:O	1:A:1140:HIS:N	2.29	0.66
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.44	0.66
1:A:567:LYS:CB	1:A:568:PRO:CD	2.74	0.66
1:A:1434:ALA:O	1:A:1436:ILE:N	2.29	0.65
4:D:134:THR:CG2	4:D:135:GLY:N	2.59	0.65
3:C:55:THR:OG1	3:C:152:GLU:N	2.30	0.65
1:A:814:PHE:CD1	2:B:519:TRP:CE3	2.84	0.64
2:B:955:THR:CG2	2:B:956:THR:N	2.61	0.64
1:A:482:PHE:CB	2:B:836:GLU:O	2.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.87	0.63
12:L:66:GLN:C	12:L:67:PHE:CD1	2.72	0.63
1:A:256:GLN:O	1:A:257:ARG:CB	2.47	0.63
2:B:202:TYR:N	2:B:202:TYR:CD2	2.65	0.62
6:F:100:GLN:O	6:F:105:ALA:CB	2.47	0.62
4:D:147:TYR:O	4:D:151:PHE:CD1	2.51	0.62
11:K:63:VAL:O	11:K:65:HIS:N	2.33	0.61
2:B:486:TYR:CD1	2:B:1096:ARG:NH2	2.68	0.61
2:B:430:ARG:CG	2:B:430:ARG:NH1	2.63	0.61
12:L:62:LYS:O	12:L:64:LEU:N	2.32	0.61
6:F:111:LEU:O	6:F:113:GLY:N	2.33	0.61
1:A:741:ASN:ND2	1:A:743:VAL:N	2.49	0.60
1:A:75:ASN:O	1:A:76:GLU:CB	2.48	0.60
7:G:158:HIS:CD2	7:G:159:ALA:N	2.69	0.60
7:G:51:TYR:O	7:G:51:TYR:CD2	2.55	0.60
1:A:1349:TYR:O	1:A:1350:LYS:C	2.40	0.60
12:L:38:LEU:O	12:L:39:SER:CB	2.49	0.60
2:B:1076:HIS:CD2	11:K:40:HIS:CE1	2.90	0.59
2:B:879:ARG:NE	2:B:879:ARG:N	2.49	0.59
6:F:140:ASP:CG	6:F:141:GLY:N	2.56	0.59
9:I:6:PHE:CD1	9:I:6:PHE:N	2.69	0.59
11:K:65:HIS:CD2	11:K:65:HIS:C	2.76	0.59
1:A:979:SER:OG	1:A:980:ASP:N	2.35	0.59
1:A:1354:ASN:O	1:A:1358:SER:CB	2.51	0.59
2:B:734:HIS:O	2:B:735:ALA:CB	2.51	0.59
1:A:71:GLN:O	1:A:73:GLY:N	2.35	0.59
8:H:102:TYR:N	8:H:102:TYR:CD2	2.69	0.58
2:B:975:GLN:CG	2:B:976:ILE:N	2.67	0.58
2:B:1116:ARG:CG	2:B:1198:TYR:CD2	2.87	0.58
1:A:1012:ARG:O	1:A:1013:ASP:C	2.42	0.58
10:J:37:SER:OG	10:J:47:ARG:NH2	2.36	0.58
7:G:79:PHE:C	7:G:79:PHE:CD1	2.72	0.58
2:B:326:ASP:O	2:B:330:ALA:CB	2.50	0.58
6:F:130:ILE:O	6:F:132:LEU:N	2.36	0.57
2:B:1166:CYS:O	2:B:1168:LEU:N	2.36	0.57
1:A:6:TYR:CG	1:A:7:SER:N	2.72	0.57
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.58	0.57
2:B:859:TYR:N	2:B:859:TYR:CD1	2.71	0.57
12:L:58:LYS:O	12:L:59:ALA:O	2.22	0.57
11:K:63:VAL:O	11:K:64:GLU:C	2.42	0.57
1:A:355:GLY:N	1:A:482:PHE:CZ	2.72	0.57
9:I:15:TYR:CD1	9:I:15:TYR:N	2.73	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1315:GLU:O	1:A:1317:MET:N	2.37	0.57
4:D:170:THR:O	4:D:172:LEU:N	2.38	0.57
3:C:88:CYS:SG	3:C:91:HIS:CA	2.93	0.56
2:B:363:HIS:O	2:B:364:ILE:CB	2.52	0.56
6:F:100:GLN:NE2	7:G:18:PHE:CE2	2.73	0.56
2:B:1157:ALA:O	2:B:1158:PHE:CB	2.52	0.56
1:A:490:HIS:ND1	2:B:1150:ARG:NH1	2.53	0.56
11:K:68:PHE:CD2	11:K:68:PHE:N	2.71	0.56
1:A:640:GLN:N	1:A:640:GLN:CD	2.57	0.56
1:A:962:ARG:O	1:A:965:GLN:N	2.38	0.56
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.74	0.56
1:A:399:HIS:C	1:A:399:HIS:ND1	2.58	0.56
4:D:151:PHE:N	4:D:151:PHE:CD1	2.74	0.56
2:B:1131:GLY:O	2:B:1132:GLU:C	2.44	0.56
1:A:386:ASP:OD1	1:A:386:ASP:N	2.38	0.56
6:F:139:PRO:O	6:F:140:ASP:C	2.44	0.56
6:F:111:LEU:C	6:F:113:GLY:N	2.59	0.56
8:H:82:PRO:O	8:H:84:ALA:N	2.40	0.55
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.40	0.55
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.53	0.55
1:A:425:GLN:NE2	1:A:425:GLN:N	2.54	0.55
2:B:785:TYR:CE2	10:J:60:PHE:CE1	2.95	0.55
2:B:459:TYR:C	2:B:459:TYR:CD2	2.80	0.55
5:E:143:ASN:ND2	5:E:146:HIS:ND1	2.55	0.55
1:A:556:TRP:O	1:A:558:GLY:N	2.40	0.55
1:A:909:ASP:O	1:A:911:SER:N	2.40	0.55
2:B:57:TYR:N	2:B:57:TYR:CD1	2.72	0.54
4:D:39:ASN:CG	4:D:40:HIS:N	2.60	0.54
1:A:1344:GLY:O	1:A:1345:ARG:C	2.46	0.54
2:B:856:PHE:CD1	2:B:856:PHE:N	2.74	0.54
1:A:1313:LEU:O	1:A:1315:GLU:N	2.41	0.54
1:A:665:GLY:O	1:A:667:GLY:N	2.40	0.54
2:B:936:ASP:CG	2:B:937:ALA:N	2.61	0.54
10:J:64:ASN:CB	10:J:65:PRO:CD	2.86	0.54
3:C:167:HIS:O	3:C:168:ALA:C	2.45	0.54
4:D:167:LEU:O	4:D:169:SER:N	2.41	0.54
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.41	0.54
1:A:1427:ASN:O	1:A:1430:LEU:N	2.40	0.54
3:C:70:ILE:O	3:C:72:LEU:CD1	2.56	0.54
10:J:44:TYR:N	10:J:44:TYR:CD2	2.76	0.54
2:B:522:VAL:CG1	2:B:523:CYS:N	2.70	0.53
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.82	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:508:LEU:O	2:B:509:ALA:CB	2.57	0.53
2:B:515:HIS:CD2	2:B:517:THR:N	2.76	0.53
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.71	0.53
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.91	0.53
1:A:19:PHE:CZ	1:A:1397:LEU:CD2	2.92	0.53
2:B:744:HIS:CD2	2:B:746:SER:OG	2.60	0.53
3:C:62:PHE:O	3:C:66:ARG:CG	2.57	0.53
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.53
9:I:7:CYS:SG	9:I:8:ARG:O	2.66	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.55	0.53
1:A:535:THR:O	1:A:536:LEU:O	2.27	0.53
12:L:39:SER:O	12:L:40:LEU:CG	2.57	0.53
6:F:109:VAL:CG1	6:F:110:ASP:N	2.71	0.53
1:A:381:THR:O	1:A:384:ASN:OD1	2.27	0.53
6:F:69:LEU:HB3	6:F:71:GLU:OE1	2.09	0.53
2:B:124:TYR:CD2	2:B:124:TYR:O	2.61	0.53
1:A:396:PRO:O	1:A:397:ASN:OD1	2.27	0.53
1:A:1376:THR:O	1:A:1377:THR:C	2.48	0.53
8:H:145:ARG:O	8:H:146:ARG:CB	2.56	0.52
1:A:903:ASN:ND2	1:A:905:ASP:N	2.57	0.52
1:A:285:PRO:O	1:A:287:HIS:N	2.42	0.52
1:A:590:ARG:O	1:A:591:PHE:CB	2.57	0.52
2:B:996:ARG:NH2	3:C:175:ALA:N	2.58	0.52
1:A:129:LYS:O	1:A:130:ASP:CB	2.56	0.52
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.72	0.52
1:A:438:ASP:O	1:A:439:ASN:C	2.47	0.52
1:A:596:THR:O	1:A:598:LEU:N	2.42	0.52
1:A:1219:THR:CG2	1:A:1220:PHE:N	2.72	0.52
2:B:702:LEU:O	2:B:739:THR:N	2.42	0.52
1:A:469:ARG:NH2	2:B:991:GLY:O	2.42	0.52
1:A:463:ILE:CB	1:A:464:PRO:CD	2.87	0.52
5:E:55:ARG:C	5:E:57:MET:N	2.61	0.52
5:E:153:HIS:N	5:E:153:HIS:ND1	2.58	0.52
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.78	0.52
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.73	0.52
1:A:1035:TYR:O	1:A:1036:ARG:CB	2.58	0.51
4:D:14:ARG:O	4:D:16:LYS:N	2.43	0.51
1:A:68:GLN:O	1:A:68:GLN:NE2	2.43	0.51
4:D:18:VAL:O	4:D:19:GLU:CB	2.57	0.51
12:L:34:CYS:O	12:L:35:SER:C	2.48	0.51
1:A:370:ILE:C	1:A:372:LYS:N	2.64	0.51
2:B:211:VAL:O	2:B:480:SER:CA	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1437:GLY:O	1:A:1441:PHE:CE2	2.64	0.51
2:B:1174:LYS:O	2:B:1176:ASN:N	2.44	0.51
8:H:59:ILE:O	8:H:60:ALA:CB	2.59	0.51
10:J:8:PHE:CE2	10:J:49:MET:SD	3.04	0.51
1:A:490:HIS:CD2	1:A:490:HIS:N	2.79	0.50
4:D:52:LEU:O	4:D:54:GLU:N	2.44	0.50
1:A:331:GLY:O	1:A:332:LYS:O	2.29	0.50
3:C:66:ARG:NH2	10:J:3:VAL:O	2.45	0.50
2:B:390:LEU:O	2:B:391:ASP:C	2.49	0.50
11:K:83:PRO:O	11:K:84:LYS:C	2.49	0.50
3:C:121:VAL:CG1	3:C:122:SER:N	2.73	0.50
7:G:81:PRO:O	7:G:82:PHE:CD2	2.65	0.50
1:A:966:ASN:O	1:A:970:THR:CB	2.60	0.50
1:A:464:PRO:O	1:A:465:TYR:O	2.30	0.50
1:A:633:VAL:O	1:A:634:THR:C	2.48	0.50
2:B:429:PHE:CD2	2:B:433:GLN:NE2	2.79	0.50
4:D:30:GLY:C	4:D:32:GLU:N	2.64	0.50
7:G:13:LEU:CD2	7:G:17:PHE:CD2	2.95	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.75	0.50
8:H:139:ASN:O	8:H:140:ALA:CB	2.59	0.50
1:A:947:PHE:CD2	1:A:947:PHE:N	2.80	0.50
3:C:127:ARG:O	3:C:129:ILE:N	2.45	0.50
1:A:476:SER:N	1:A:477:PRO:CD	2.75	0.50
11:K:35:PHE:N	11:K:35:PHE:CD1	2.78	0.50
2:B:188:ASP:N	2:B:188:ASP:OD2	2.44	0.49
1:A:74:MET:O	1:A:77:CYS:N	2.46	0.49
1:A:525:GLN:O	1:A:526:ASP:C	2.50	0.49
4:D:155:ARG:NH2	4:D:221:TYR:CD1	2.81	0.49
10:J:57:ILE:CG2	10:J:58:GLU:N	2.75	0.49
6:F:139:PRO:O	6:F:141:GLY:N	2.45	0.49
1:A:1124:HIS:N	1:A:1124:HIS:CD2	2.80	0.49
1:A:1227:ILE:C	1:A:1228:TRP:CE3	2.86	0.49
2:B:458:LYS:O	2:B:459:TYR:C	2.51	0.49
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.75	0.49
3:C:86:CYS:SG	3:C:87:PHE:N	2.86	0.49
2:B:900:ALA:CB	12:L:61:THR:OG1	2.61	0.49
4:D:156:ASP:C	4:D:158:GLU:N	2.64	0.49
10:J:17:LYS:O	10:J:20:SER:N	2.45	0.49
1:A:56:PRO:O	1:A:57:ARG:CG	2.60	0.49
9:I:17:ARG:NH2	9:I:30:ARG:NH2	2.61	0.49
1:A:600:PRO:CA	8:H:25:ARG:NH1	2.75	0.49
1:A:1325:THR:O	5:E:147:HIS:CD2	2.66	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:5:ASP:CB	11:K:7:PHE:CZ	2.96	0.49
6:F:88:TYR:O	6:F:89:GLU:C	2.50	0.49
2:B:226:PHE:CE2	2:B:398:ARG:NH2	2.80	0.49
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.61	0.49
12:L:55:ILE:O	12:L:56:LEU:CB	2.60	0.49
4:D:138:ASN:O	4:D:139:LYS:C	2.51	0.49
1:A:1332:PHE:CD2	1:A:1332:PHE:N	2.80	0.49
1:A:224:PHE:CD2	1:A:231:PRO:CD	2.95	0.49
6:F:79:ARG:NH2	6:F:145:ASP:O	2.46	0.49
1:A:58:LEU:CB	1:A:80:HIS:O	2.61	0.49
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.48
3:C:61:GLU:O	3:C:62:PHE:C	2.50	0.48
1:A:1362:TYR:C	1:A:1362:TYR:CD1	2.85	0.48
1:A:360:GLU:O	1:A:361:LEU:C	2.51	0.48
2:B:360:PHE:O	2:B:361:LEU:C	2.52	0.48
1:A:874:ASP:O	1:A:876:ALA:N	2.46	0.48
11:K:109:TRP:C	11:K:109:TRP:CD1	2.87	0.48
3:C:167:HIS:O	3:C:169:LYS:N	2.47	0.48
2:B:516:ASN:ND2	2:B:516:ASN:N	2.62	0.48
2:B:287:ARG:NE	2:B:292:ILE:O	2.46	0.48
1:A:1393:ASN:O	1:A:1394:THR:O	2.30	0.48
1:A:298:PHE:CD2	1:A:298:PHE:C	2.87	0.48
1:A:1005:GLU:O	1:A:1006:ILE:C	2.51	0.48
6:F:138:LEU:O	6:F:139:PRO:C	2.52	0.48
12:L:59:ALA:O	12:L:60:ARG:O	2.31	0.48
1:A:67:CYS:O	1:A:68:GLN:C	2.52	0.48
6:F:72:LYS:O	6:F:143:PHE:CD2	2.67	0.48
3:C:183:TRP:O	3:C:185:LYS:N	2.47	0.48
9:I:34:TYR:OH	9:I:36:GLU:OE1	2.30	0.48
1:A:1227:ILE:CA	1:A:1228:TRP:CE3	2.96	0.48
1:A:245:PRO:O	2:B:1114:LEU:CD1	2.61	0.48
1:A:741:ASN:C	1:A:741:ASN:ND2	2.67	0.48
4:D:4:SER:O	4:D:5:THR:CB	2.62	0.48
1:A:1001:ARG:O	1:A:1002:GLY:O	2.32	0.47
2:B:785:TYR:C	2:B:787:VAL:N	2.67	0.47
4:D:139:LYS:O	4:D:143:ASN:ND2	2.47	0.47
1:A:1346:ALA:O	1:A:1347:ALA:C	2.52	0.47
3:C:82:TYR:CD2	3:C:84:ARG:NH2	2.82	0.47
2:B:27:ALA:O	2:B:29:ASP:N	2.47	0.47
10:J:36:LEU:CB	10:J:47:ARG:NH1	2.77	0.47
2:B:1101:ASP:O	2:B:1122:ARG:CZ	2.63	0.47
1:A:513:SER:N	1:A:518:LYS:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1364:ASN:O	1:A:1365:TYR:C	2.53	0.47
1:A:1364:ASN:O	1:A:1366:ARG:N	2.47	0.47
1:A:1391:ARG:O	1:A:1392:SER:O	2.33	0.47
1:A:356:ASP:OD2	2:B:833:TYR:CE2	2.67	0.47
11:K:63:VAL:O	11:K:63:VAL:CG2	2.61	0.47
9:I:7:CYS:C	9:I:8:ARG:O	2.51	0.47
2:B:310:MET:O	2:B:311:LEU:C	2.52	0.47
1:A:451:HIS:N	1:A:451:HIS:ND1	2.62	0.47
1:A:864:ILE:CD1	1:A:864:ILE:N	2.78	0.47
11:K:61:TYR:CD1	11:K:61:TYR:C	2.88	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
1:A:1313:LEU:C	1:A:1315:GLU:N	2.68	0.47
8:H:82:PRO:C	8:H:84:ALA:N	2.68	0.47
1:A:164:ARG:CG	1:A:165:GLY:N	2.78	0.47
3:C:213:PRO:O	3:C:214:ASN:CB	2.63	0.47
1:A:1446:ASP:O	1:A:1447:GLU:C	2.52	0.47
1:A:649:ILE:O	1:A:650:GLN:C	2.53	0.47
3:C:178:PHE:C	3:C:178:PHE:CD2	2.88	0.47
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.63	0.47
1:A:653:VAL:O	1:A:654:ASN:C	2.53	0.47
1:A:933:TYR:C	1:A:933:TYR:CD2	2.88	0.47
1:A:656:TRP:CH2	1:A:660:ASN:CG	2.88	0.47
6:F:125:LEU:O	6:F:128:LYS:N	2.48	0.47
4:D:15:LEU:O	4:D:17:LYS:N	2.48	0.47
2:B:702:LEU:N	2:B:739:THR:OG1	2.48	0.47
1:A:135:PHE:CD1	1:A:222:LEU:CD2	2.98	0.47
2:B:311:LEU:O	2:B:312:GLU:C	2.54	0.46
1:A:166:GLY:O	1:A:167:CYS:O	2.33	0.46
1:A:659:HIS:ND1	2:B:1074:ASN:ND2	2.63	0.46
5:E:136:ASN:OD1	5:E:137:GLU:N	2.48	0.46
7:G:94:CYS:SG	7:G:130:TYR:CE1	3.08	0.46
1:A:1436:ILE:O	1:A:1438:THR:N	2.47	0.46
1:A:350:ARG:C	1:A:351:THR:CG2	2.84	0.46
2:B:1158:PHE:CE2	2:B:1160:VAL:CG2	2.99	0.46
2:B:515:HIS:CD2	2:B:516:ASN:N	2.83	0.46
2:B:800:GLN:OE1	2:B:822:ASN:N	2.48	0.46
10:J:1:MET:N	10:J:56:LEU:N	2.63	0.46
1:A:216:VAL:O	1:A:219:PHE:CB	2.62	0.46
2:B:405:ARG:NH1	2:B:632:ARG:CG	2.79	0.46
1:A:66:LYS:O	1:A:67:CYS:CB	2.63	0.46
2:B:906:SER:O	2:B:907:GLY:C	2.54	0.46
2:B:824:ILE:CG1	10:J:48:ARG:NH1	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:95:GLY:O	6:F:96:THR:C	2.54	0.46
2:B:834:ASN:O	2:B:1013:ASN:CB	2.63	0.46
1:A:204:THR:O	1:A:205:GLU:C	2.54	0.46
1:A:964:ILE:O	1:A:964:ILE:CG2	2.64	0.46
7:G:97:HIS:N	7:G:97:HIS:CD2	2.84	0.46
10:J:1:MET:O	10:J:2:ILE:CG2	2.64	0.46
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.78	0.46
11:K:113:THR:CG2	11:K:114:LEU:N	2.78	0.46
6:F:120:ILE:CG2	6:F:121:ALA:N	2.78	0.46
1:A:692:ASP:O	1:A:694:THR:N	2.49	0.46
1:A:95:PHE:CE2	1:A:1410:PHE:CD2	3.03	0.46
1:A:881:GLN:NE2	1:A:958:VAL:O	2.49	0.46
11:K:65:HIS:CD2	11:K:66:PRO:N	2.84	0.46
2:B:887:HIS:CD2	2:B:888:GLY:N	2.84	0.46
1:A:521:MET:O	1:A:646:PHE:CE2	2.68	0.46
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.49	0.46
2:B:811:TYR:N	2:B:811:TYR:CD1	2.83	0.46
6:F:70:LYS:HA	6:F:70:LYS:HD3	1.42	0.46
7:G:17:PHE:CE2	7:G:25:TYR:CE2	3.04	0.46
1:A:1215:ARG:O	1:A:1218:GLN:N	2.49	0.46
10:J:12:LYS:O	10:J:13:VAL:C	2.54	0.46
7:G:95:SER:O	7:G:121:PHE:CE1	2.68	0.46
2:B:1095:LEU:O	2:B:1096:ARG:O	2.34	0.46
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.84	0.46
5:E:44:ALA:O	5:E:45:LYS:CB	2.63	0.46
2:B:446:LEU:O	2:B:447:ALA:CB	2.64	0.46
2:B:1181:GLU:CA	2:B:1187:ASN:O	2.64	0.46
1:A:664:THR:CG2	1:A:664:THR:O	2.64	0.46
11:K:61:TYR:CG	11:K:61:TYR:O	2.69	0.45
1:A:709:THR:CG2	1:A:710:LEU:N	2.79	0.45
1:A:529:CYS:SG	1:A:662:PHE:CZ	3.10	0.45
1:A:46:THR:O	1:A:47:ARG:C	2.55	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.80	0.45
1:A:855:THR:CG2	1:A:857:ARG:NE	2.79	0.45
1:A:549:MET:CE	1:A:656:TRP:CD1	3.00	0.45
6:F:127:GLU:O	6:F:129:LYS:N	2.49	0.45
1:A:261:ASP:OD2	1:A:261:ASP:N	2.48	0.45
10:J:48:ARG:NH1	10:J:48:ARG:CG	2.78	0.45
2:B:1147:LEU:O	2:B:1148:LYS:C	2.53	0.45
2:B:259:TYR:N	2:B:259:TYR:CD1	2.85	0.45
1:A:1107:VAL:O	1:A:1107:VAL:CG1	2.64	0.45
2:B:510:LYS:O	2:B:511:PRO:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:544:ASP:OD1	1:A:545:GLN:N	2.49	0.45
4:D:146:GLN:O	4:D:150:ASN:ND2	2.49	0.45
1:A:929:LEU:CD2	1:A:929:LEU:N	2.79	0.45
7:G:1:MET:SD	7:G:79:PHE:CE1	3.10	0.45
1:A:489:LEU:C	1:A:490:HIS:CD2	2.90	0.45
10:J:56:LEU:O	10:J:60:PHE:CD2	2.70	0.45
4:D:39:ASN:ND2	4:D:40:HIS:N	2.64	0.45
1:A:362:ASP:OD2	1:A:362:ASP:N	2.50	0.45
12:L:49:LYS:O	12:L:50:ASP:CB	2.64	0.45
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.45
1:A:73:GLY:O	1:A:74:MET:C	2.55	0.45
1:A:252:PHE:O	1:A:253:ASN:CB	2.65	0.45
4:D:126:ILE:C	4:D:128:VAL:N	2.70	0.45
2:B:1078:GLY:O	2:B:1079:LYS:C	2.55	0.45
1:A:351:THR:CG2	1:A:468:PHE:CE1	3.00	0.45
1:A:726:ARG:CD	1:A:765:VAL:O	2.65	0.45
2:B:398:ARG:CB	2:B:398:ARG:NH1	2.80	0.45
3:C:183:TRP:O	3:C:184:ASN:C	2.55	0.45
1:A:84:ILE:CG2	1:A:84:ILE:O	2.65	0.45
11:K:56:VAL:CG1	11:K:56:VAL:O	2.64	0.45
7:G:129:SER:OG	7:G:130:TYR:N	2.49	0.45
1:A:814:PHE:CD2	1:A:814:PHE:C	2.90	0.44
1:A:1116:LEU:CB	1:A:1308:THR:CG2	2.95	0.44
1:A:500:GLU:OE2	2:B:1145:SER:OG	2.34	0.44
1:A:1370:LEU:O	1:A:1371:LEU:C	2.55	0.44
2:B:179:CYS:O	2:B:181:LEU:N	2.50	0.44
3:C:166:GLU:O	11:K:6:ARG:CG	2.65	0.44
1:A:425:GLN:CD	1:A:425:GLN:N	2.71	0.44
4:D:167:LEU:C	4:D:169:SER:N	2.70	0.44
1:A:1424:VAL:O	1:A:1425:SER:C	2.56	0.44
2:B:1076:HIS:CD2	11:K:40:HIS:CD2	3.05	0.44
1:A:868:TYR:O	1:A:870:GLU:N	2.50	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.54	0.44
1:A:27:VAL:O	1:A:29:ALA:N	2.50	0.44
3:C:109:SER:O	3:C:110:THR:C	2.55	0.44
2:B:759:PRO:O	2:B:761:HIS:N	2.50	0.44
2:B:980:PHE:CD1	2:B:980:PHE:N	2.86	0.44
1:A:822:GLU:O	1:A:825:ILE:N	2.50	0.44
4:D:185:CYS:SG	4:D:186:ASP:N	2.90	0.44
2:B:651:LEU:O	2:B:654:ARG:NE	2.50	0.44
1:A:795:GLU:CD	1:A:795:GLU:N	2.71	0.44
1:A:744:LYS:O	1:A:748:MET:CB	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:192:TRP:CE3	3:C:192:TRP:O	2.71	0.44
1:A:313:GLN:O	1:A:314:ALA:C	2.56	0.44
5:E:187:TYR:CD2	5:E:188:LEU:CD2	3.00	0.44
1:A:92:HIS:CE1	1:A:1410:PHE:CE2	3.06	0.44
8:H:81:PRO:O	8:H:82:PRO:O	2.36	0.44
2:B:619:ILE:CG2	2:B:620:ARG:N	2.80	0.44
1:A:329:LEU:O	1:A:330:LYS:O	2.36	0.44
1:A:897:TYR:CD2	1:A:936:LEU:CD1	3.01	0.44
4:D:178:ALA:O	4:D:181:GLY:N	2.50	0.44
4:D:173:HIS:C	4:D:175:PHE:N	2.71	0.44
1:A:633:VAL:O	1:A:636:GLU:N	2.51	0.44
1:A:360:GLU:O	1:A:362:ASP:N	2.51	0.44
7:G:14:HIS:CD2	7:G:15:PRO:CD	3.01	0.44
1:A:254:GLU:O	1:A:255:SER:C	2.56	0.44
1:A:195:ASP:O	1:A:196:GLU:O	2.36	0.44
4:D:33:PHE:CE2	7:G:3:PHE:CD1	3.06	0.44
5:E:90:VAL:CG2	5:E:90:VAL:O	2.66	0.44
1:A:1018:PHE:O	1:A:1019:CYS:C	2.57	0.43
2:B:1212:ILE:O	2:B:1212:ILE:CG2	2.66	0.43
1:A:1402:PHE:O	1:A:1404:GLU:N	2.51	0.43
2:B:205:ILE:O	2:B:207:GLY:N	2.51	0.43
4:D:48:ILE:CG2	4:D:48:ILE:O	2.66	0.43
3:C:130:GLY:O	3:C:132:PRO:CD	2.67	0.43
7:G:112:LYS:NZ	7:G:119:LEU:O	2.51	0.43
1:A:95:PHE:CD1	1:A:234:MET:CG	3.02	0.43
2:B:979:LYS:C	2:B:980:PHE:CD1	2.91	0.43
5:E:213:ILE:CG1	5:E:214:CYS:N	2.81	0.43
2:B:1191:ILE:CG2	2:B:1192:TYR:N	2.82	0.43
7:G:1:MET:SD	7:G:79:PHE:CD1	3.12	0.43
1:A:993:LEU:O	1:A:994:GLN:C	2.56	0.43
3:C:240:VAL:O	3:C:241:ASP:C	2.56	0.43
1:A:37:PHE:CD1	1:A:37:PHE:N	2.87	0.43
5:E:82:PHE:CD1	5:E:82:PHE:N	2.87	0.43
1:A:490:HIS:CB	2:B:1150:ARG:NH1	2.81	0.43
1:A:531:ILE:O	1:A:535:THR:OG1	2.36	0.43
2:B:640:VAL:O	2:B:641:GLU:C	2.57	0.43
1:A:528:LEU:CG	1:A:529:CYS:N	2.81	0.43
1:A:499:ALA:O	1:A:500:GLU:C	2.56	0.43
2:B:181:LEU:O	2:B:182:SER:C	2.57	0.43
5:E:63:ASN:CB	5:E:64:PRO:CD	2.96	0.43
2:B:533:CYS:C	2:B:535:LEU:N	2.72	0.43
1:A:578:LEU:O	1:A:580:VAL:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:6:PHE:CD2	8:H:7:ASP:N	2.87	0.43
5:E:74:ASP:OD1	5:E:74:ASP:N	2.51	0.43
11:K:31:VAL:CG1	11:K:32:VAL:N	2.82	0.43
12:L:63:ARG:O	12:L:64:LEU:C	2.57	0.43
1:A:27:VAL:C	1:A:29:ALA:N	2.71	0.43
4:D:175:PHE:O	4:D:176:GLU:C	2.57	0.43
1:A:985:ASP:O	1:A:986:ILE:C	2.57	0.43
2:B:351:TYR:CE1	2:B:355:ILE:CD1	3.01	0.43
2:B:333:PHE:CD2	2:B:333:PHE:O	2.72	0.43
2:B:764:SER:N	2:B:765:PRO:CD	2.81	0.43
7:G:138:THR:O	7:G:140:LYS:N	2.51	0.43
2:B:998:ASP:N	2:B:998:ASP:OD1	2.51	0.43
2:B:650:GLU:CG	2:B:651:LEU:N	2.82	0.43
2:B:352:ALA:O	2:B:353:LYS:C	2.58	0.43
1:A:853:ASP:OD1	1:A:855:THR:CB	2.67	0.42
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.67	0.42
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.52	0.42
3:C:242:GLN:NE2	3:C:246:ARG:NE	2.67	0.42
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.87	0.42
7:G:160:ILE:CG2	7:G:161:GLY:N	2.81	0.42
2:B:459:TYR:O	2:B:463:THR:OG1	2.38	0.42
10:J:17:LYS:O	10:J:18:TRP:C	2.56	0.42
1:A:1362:TYR:CE1	1:A:1363:VAL:O	2.72	0.42
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.93	0.42
5:E:167:ARG:O	5:E:168:TYR:CG	2.72	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.42
2:B:281:PRO:O	2:B:283:VAL:N	2.53	0.42
4:D:173:HIS:O	4:D:175:PHE:N	2.53	0.42
1:A:41:MET:O	1:A:42:ASP:O	2.37	0.42
1:A:109:HIS:NE2	1:A:169:ASN:ND2	2.67	0.42
3:C:69:LEU:O	10:J:6:ARG:NH1	2.52	0.42
2:B:1168:LEU:O	2:B:1170:THR:N	2.52	0.42
6:F:88:TYR:CD1	6:F:88:TYR:N	2.86	0.42
2:B:973:ILE:CG2	2:B:974:PRO:CD	2.97	0.42
2:B:345:LYS:O	2:B:347:LYS:N	2.53	0.42
1:A:784:LEU:O	1:A:786:HIS:N	2.53	0.42
2:B:1040:ASN:O	2:B:1041:GLU:C	2.57	0.42
2:B:205:ILE:O	2:B:206:ASN:C	2.57	0.42
1:A:369:SER:O	1:A:373:THR:OG1	2.38	0.42
1:A:647:GLY:O	1:A:648:ASN:C	2.57	0.42
2:B:817:LEU:N	2:B:818:PRO:CD	2.81	0.42
2:B:731:VAL:O	2:B:732:SER:CB	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:167:HIS:CD2	12:L:70:ARG:CG	3.03	0.42
4:D:53:SER:O	4:D:54:GLU:C	2.57	0.42
1:A:524:VAL:CG1	1:A:525:GLN:N	2.82	0.42
2:B:745:PRO:O	2:B:747:MET:N	2.53	0.42
2:B:1166:CYS:C	2:B:1168:LEU:N	2.73	0.42
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.52	0.42
2:B:1115:THR:O	2:B:1116:ARG:CB	2.68	0.42
2:B:1122:ARG:O	2:B:1125:ASP:N	2.53	0.42
1:A:881:GLN:NE2	1:A:959:ASN:CA	2.83	0.42
3:C:136:ASP:OD2	3:C:137:LYS:N	2.53	0.42
2:B:515:HIS:CG	2:B:516:ASN:N	2.88	0.42
1:A:396:PRO:O	1:A:397:ASN:CG	2.58	0.42
6:F:127:GLU:O	6:F:128:LYS:C	2.57	0.42
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.53	0.42
1:A:316:GLN:O	1:A:317:LYS:C	2.58	0.41
1:A:451:HIS:O	1:A:452:LYS:C	2.57	0.41
1:A:1242:VAL:O	1:A:1243:VAL:CG1	2.67	0.41
1:A:1215:ARG:O	1:A:1216:ILE:C	2.58	0.41
3:C:245:VAL:O	3:C:246:ARG:C	2.58	0.41
1:A:1102:LYS:O	1:A:1103:GLU:C	2.57	0.41
1:A:887:GLY:O	1:A:940:ARG:NH2	2.53	0.41
11:K:5:ASP:O	11:K:6:ARG:C	2.59	0.41
3:C:93:ASP:O	3:C:127:ARG:NH2	2.52	0.41
1:A:205:GLU:CD	1:A:205:GLU:N	2.74	0.41
2:B:565:PRO:C	2:B:567:GLU:N	2.73	0.41
1:A:591:PHE:CD2	1:A:595:THR:CB	3.03	0.41
4:D:216:ASN:C	4:D:218:GLU:N	2.73	0.41
2:B:487:THR:O	2:B:490:SER:N	2.53	0.41
4:D:25:ALA:CB	4:D:196:PRO:CG	2.98	0.41
1:A:258:GLY:O	1:A:259:GLU:O	2.39	0.41
2:B:248:SER:O	2:B:249:ARG:C	2.59	0.41
12:L:47:ARG:O	12:L:48:CYS:CB	2.68	0.41
1:A:1097:GLY:O	1:A:1098:VAL:C	2.59	0.41
5:E:33:GLU:OE1	5:E:33:GLU:N	2.54	0.41
9:I:35:VAL:CG1	9:I:36:GLU:N	2.83	0.41
2:B:179:CYS:C	2:B:181:LEU:N	2.74	0.41
3:C:124:LEU:C	3:C:126:GLY:N	2.73	0.41
2:B:230:ALA:CB	2:B:231:PRO:CD	2.99	0.41
1:A:1280:GLU:O	1:A:1281:ARG:C	2.58	0.41
4:D:194:LEU:CD2	4:D:194:LEU:N	2.82	0.41
5:E:24:LYS:O	5:E:27:GLY:N	2.53	0.41
12:L:67:PHE:CD1	12:L:67:PHE:N	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:198:ASP:OD2	2:B:202:TYR:OH	2.39	0.41
1:A:578:LEU:C	1:A:580:VAL:N	2.74	0.41
6:F:77:ASP:O	6:F:78:GLN:CB	2.67	0.41
1:A:285:PRO:O	1:A:288:ALA:N	2.53	0.41
7:G:21:ARG:O	7:G:22:MET:C	2.59	0.41
1:A:1265:ASN:C	1:A:1267:MET:N	2.73	0.41
1:A:1269:GLU:O	1:A:1270:ASN:CB	2.68	0.41
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.41
1:A:1318:THR:OG1	5:E:11:ARG:NH1	2.54	0.41
3:C:167:HIS:ND1	3:C:167:HIS:C	2.74	0.41
5:E:136:ASN:OD1	5:E:138:ALA:N	2.54	0.41
1:A:1304:TRP:O	1:A:1305:VAL:CG2	2.69	0.41
5:E:124:VAL:O	5:E:132:ILE:CD1	2.69	0.41
2:B:1007:VAL:CG2	2:B:1008:PRO:N	2.83	0.41
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.78	0.41
1:A:224:PHE:CD2	1:A:231:PRO:CG	3.03	0.41
2:B:822:ASN:N	2:B:822:ASN:ND2	2.69	0.41
1:A:545:GLN:O	1:A:546:VAL:C	2.59	0.41
1:A:1061:GLY:O	1:A:1062:GLU:C	2.59	0.41
2:B:512:ARG:O	2:B:513:GLN:O	2.39	0.41
3:C:180:TYR:O	3:C:181:ASP:C	2.59	0.41
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.54	0.41
7:G:45:ILE:O	7:G:45:ILE:CG2	2.68	0.41
3:C:88:CYS:O	3:C:89:GLU:C	2.58	0.41
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.54	0.41
4:D:13:ARG:O	4:D:15:LEU:N	2.54	0.41
1:A:204:THR:O	1:A:206:GLU:N	2.54	0.41
1:A:311:GLN:O	1:A:313:GLN:N	2.53	0.41
1:A:627:GLY:O	1:A:628:GLY:C	2.60	0.41
1:A:836:TYR:CE2	1:A:840:ARG:CD	3.04	0.41
1:A:391:LEU:O	1:A:392:VAL:C	2.60	0.41
2:B:294:ASP:C	2:B:296:GLU:N	2.74	0.41
5:E:178:ILE:O	5:E:179:GLN:O	2.39	0.41
1:A:1315:GLU:C	1:A:1317:MET:N	2.75	0.40
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.84	0.40
2:B:27:ALA:O	2:B:28:GLU:C	2.59	0.40
2:B:640:VAL:CG1	2:B:640:VAL:O	2.69	0.40
12:L:36:SER:O	12:L:37:LYS:C	2.60	0.40
2:B:243:ALA:O	2:B:244:LEU:C	2.59	0.40
1:A:25:GLU:OE2	1:A:25:GLU:N	2.54	0.40
7:G:53:ASN:ND2	7:G:53:ASN:N	2.70	0.40
1:A:441:PRO:O	1:A:492:PRO:CG	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1313:LEU:O	1:A:1314:SER:C	2.59	0.40
1:A:395:GLY:O	1:A:397:ASN:N	2.54	0.40
3:C:121:VAL:O	3:C:122:SER:C	2.59	0.40
2:B:398:ARG:CB	2:B:398:ARG:CZ	3.00	0.40
2:B:833:TYR:C	2:B:835:GLN:N	2.73	0.40
1:A:195:ASP:OD1	1:A:195:ASP:N	2.54	0.40
1:A:391:LEU:O	1:A:394:ASN:N	2.55	0.40
3:C:8:VAL:CG1	3:C:9:LYS:N	2.85	0.40
1:A:325:ILE:C	1:A:327:ALA:N	2.75	0.40
10:J:8:PHE:CD2	10:J:49:MET:SD	3.15	0.40
2:B:312:GLU:O	2:B:313:MET:C	2.60	0.40
1:A:305:ASP:OD1	1:A:306:ASN:N	2.55	0.40
1:A:829:VAL:C	1:A:831:THR:N	2.74	0.40
2:B:38:PHE:CD2	2:B:43:LEU:CD2	3.05	0.40
2:B:276:ILE:CG2	2:B:276:ILE:O	2.68	0.40
7:G:91:VAL:CG1	7:G:92:VAL:N	2.85	0.40
1:A:868:TYR:O	1:A:869:GLY:C	2.59	0.40
1:A:68:GLN:O	1:A:68:GLN:CD	2.59	0.40
5:E:83:CYS:O	5:E:113:GLN:NE2	2.54	0.40
2:B:549:THR:CG2	2:B:550:ASP:N	2.84	0.40
5:E:18:THR:O	5:E:19:VAL:C	2.59	0.40
7:G:132:SER:O	7:G:133:SER:C	2.58	0.40
1:A:127:ALA:O	1:A:129:LYS:N	2.55	0.40
4:D:52:LEU:O	4:D:53:SER:OG	2.40	0.40
1:A:1351:GLU:C	1:A:1353:TYR:N	2.75	0.40
3:C:59:ALA:O	3:C:60:ASP:C	2.59	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	1406/1733 (81%)	974 (69%)	284 (20%)	148 (10%)	1	18
2	B	1081/1224 (88%)	754 (70%)	232 (22%)	95 (9%)	1	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/318 (83%)	187 (71%)	48 (18%)	29 (11%)	1	17
4	D	174/219 (80%)	116 (67%)	43 (25%)	15 (9%)	1	25
5	E	212/215 (99%)	156 (74%)	41 (19%)	15 (7%)	2	32
6	F	85/155 (55%)	61 (72%)	19 (22%)	5 (6%)	2	38
7	G	169/171 (99%)	120 (71%)	43 (25%)	6 (4%)	5	53
8	H	130/146 (89%)	90 (69%)	29 (22%)	11 (8%)	1	26
9	I	45/133 (34%)	31 (69%)	10 (22%)	4 (9%)	1	25
10	J	63/70 (90%)	43 (68%)	14 (22%)	6 (10%)	1	22
11	K	112/120 (93%)	79 (70%)	24 (21%)	9 (8%)	1	28
12	L	44/70 (63%)	21 (48%)	8 (18%)	15 (34%)	0	0
All	All	3785/4574 (83%)	2632 (70%)	795 (21%)	358 (10%)	1	22

All (358) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	42	ASP
1	A	48	ALA
1	A	54	ASN
1	A	57	ARG
1	A	67	CYS
1	A	68	GLN
1	A	74	MET
1	A	119	ASN
1	A	128	ILE
1	A	130	ASP
1	A	167	CYS
1	A	257	ARG
1	A	259	GLU
1	A	286	HIS
1	A	318	SER
1	A	330	LYS
1	A	332	LYS
1	A	361	LEU
1	A	424	ILE
1	A	439	ASN
1	A	465	TYR
1	A	525	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	527	THR
1	A	536	LEU
1	A	557	ASP
1	A	567	LYS
1	A	591	PHE
1	A	597	LEU
1	A	598	LEU
1	A	666	ILE
1	A	790	ASP
1	A	868	TYR
1	A	986	ILE
1	A	1002	GLY
1	A	1036	ARG
1	A	1098	VAL
1	A	1139	GLU
1	A	1223	ASP
1	A	1229	SER
1	A	1232	ASN
1	A	1255	GLU
1	A	1270	ASN
1	A	1339	LEU
1	A	1365	TYR
1	A	1392	SER
1	A	1394	THR
1	A	1405	THR
1	A	1424	VAL
2	B	108	VAL
2	B	184	ALA
2	B	206	ASN
2	B	258	LEU
2	B	364	ILE
2	B	367	LEU
2	B	509	ALA
2	B	732	SER
2	B	735	ALA
2	B	738	PHE
2	B	1036	ALA
2	B	1046	PRO
2	B	1096	ARG
2	B	1103	ILE
2	B	1132	GLU
2	B	1155	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1156	ASP
2	B	1183	LYS
3	C	110	THR
3	C	121	VAL
3	C	128	ASN
3	C	137	LYS
3	C	184	ASN
3	C	227	THR
4	D	19	GLU
4	D	119	ARG
5	E	45	LYS
5	E	105	PHE
5	E	168	TYR
5	E	179	GLN
6	F	128	LYS
6	F	139	PRO
6	F	140	ASP
7	G	41	LYS
7	G	139	ILE
8	H	82	PRO
8	H	128	ASN
8	H	140	ALA
10	J	2	ILE
10	J	42	LYS
10	J	64	ASN
11	K	28	PRO
11	K	64	GLU
12	L	35	SER
12	L	39	SER
12	L	46	VAL
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
12	L	63	ARG
1	A	52	GLY
1	A	66	LYS
1	A	76	GLU
1	A	166	GLY
1	A	204	THR
1	A	253	ASN
1	A	308	ILE
1	A	310	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	314	ALA
1	A	322	VAL
1	A	418	SER
1	A	421	ALA
1	A	438	ASP
1	A	592	ASP
1	A	605	MET
1	A	628	GLY
1	A	636	GLU
1	A	653	VAL
1	A	693	VAL
1	A	780	VAL
1	A	875	ALA
1	A	912	LEU
1	A	985	ASP
1	A	999	VAL
1	A	1067	LEU
1	A	1120	LEU
1	A	1140	HIS
1	A	1188	GLN
1	A	1206	ASP
1	A	1221	LYS
1	A	1233	ASP
1	A	1242	VAL
1	A	1314	SER
1	A	1316	VAL
1	A	1367	HIS
1	A	1437	GLY
2	B	28	GLU
2	B	65	GLU
2	B	68	THR
2	B	369	GLY
2	B	435	THR
2	B	447	ALA
2	B	449	ASN
2	B	483	LEU
2	B	513	GLN
2	B	591	ARG
2	B	731	VAL
2	B	751	VAL
2	B	777	ALA
2	B	786	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	838	SER
2	B	887	HIS
2	B	937	ALA
2	B	938	SER
2	B	1041	GLU
2	B	1079	LYS
2	B	1108	ARG
2	B	1112	GLN
2	B	1157	ALA
2	B	1158	PHE
2	B	1167	GLY
3	C	5	GLY
3	C	11	ARG
3	C	126	GLY
3	C	141	GLY
3	C	149	LYS
3	C	168	ALA
3	C	213	PRO
3	C	240	VAL
4	D	5	THR
4	D	14	ARG
4	D	16	LYS
4	D	168	LYS
4	D	171	GLY
5	E	3	GLN
5	E	75	MET
5	E	106	GLN
6	F	112	GLU
7	G	154	VAL
8	H	95	TYR
8	H	109	LYS
9	I	3	THR
9	I	8	ARG
10	J	6	ARG
11	K	68	PHE
12	L	26	THR
12	L	47	ARG
12	L	48	CYS
12	L	55	ILE
12	L	56	LEU
1	A	28	ARG
1	A	59	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	169	ASN
1	A	219	PHE
1	A	255	SER
1	A	312	PRO
1	A	317	LYS
1	A	382	PRO
1	A	556	TRP
1	A	596	THR
1	A	785	PRO
1	A	869	GLY
1	A	910	PRO
1	A	1062	GLU
1	A	1114	PRO
1	A	1388	GLY
1	A	1403	GLU
1	A	1422	ARG
1	A	1448	GLU
2	B	27	ALA
2	B	45	SER
2	B	171	PRO
2	B	180	TYR
2	B	249	ARG
2	B	250	PHE
2	B	291	ILE
2	B	409	ALA
2	B	468	GLU
2	B	562	GLY
2	B	575	PRO
2	B	746	SER
2	B	760	ASP
2	B	775	LYS
2	B	802	PRO
2	B	834	ASN
2	B	907	GLY
2	B	959	ASP
2	B	1175	LEU
2	B	1176	ASN
2	B	1223	ASP
3	C	90	ASP
3	C	122	SER
3	C	142	VAL
3	C	167	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	214	ASN
3	C	241	ASP
4	D	31	GLN
4	D	134	THR
4	D	191	ALA
4	D	198	LEU
5	E	73	PRO
5	E	76	GLY
5	E	130	ALA
5	E	151	PRO
7	G	28	THR
7	G	67	SER
8	H	59	ILE
8	H	60	ALA
8	H	81	PRO
9	I	47	GLU
11	K	8	GLU
12	L	45	ALA
12	L	64	LEU
1	A	170	THR
1	A	196	GLU
1	A	420	ARG
1	A	649	ILE
1	A	654	ASN
1	A	958	VAL
1	A	1016	THR
1	A	1124	HIS
1	A	1266	THR
1	A	1377	THR
1	A	1435	PRO
2	B	106	ASP
2	B	186	GLU
2	B	459	TYR
2	B	510	LYS
2	B	524	PRO
2	B	566	LEU
2	B	711	GLU
2	B	906	SER
2	B	1017	ILE
2	B	1169	MET
3	C	13	ALA
3	C	25	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	174	ALA
3	C	224	GLN
5	E	97	VAL
6	F	141	GLY
8	H	83	GLN
10	J	13	VAL
11	K	54	ARG
12	L	40	LEU
1	A	45	GLN
1	A	62	ASP
1	A	75	ASN
1	A	155	GLU
1	A	205	GLU
1	A	396	PRO
1	A	579	SER
1	A	583	PRO
1	A	602	ASP
1	A	647	GLY
1	A	920	LEU
1	A	1080	THR
1	A	1345	ARG
2	B	46	GLN
2	B	124	TYR
2	B	304	ASP
2	B	636	PRO
2	B	707	PRO
2	B	758	PHE
2	B	889	THR
2	B	974	PRO
2	B	987	LYS
2	B	996	ARG
3	C	127	ARG
3	C	132	PRO
4	D	218	GLU
8	H	107	VAL
9	I	9	ASP
10	J	14	VAL
11	K	7	PHE
11	K	10	PHE
11	K	83	PRO
1	A	4	GLN
1	A	492	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	533	LYS
1	A	662	PHE
1	A	976	THR
1	A	1302	PRO
1	A	1428	VAL
2	B	218	SER
2	B	219	ALA
2	B	463	THR
2	B	902	GLY
3	C	175	ALA
4	D	9	GLN
4	D	52	LEU
5	E	118	PRO
5	E	124	VAL
7	G	84	GLY
1	A	311	GLN
1	A	410	GLY
1	A	730	GLY
2	B	323	VAL
2	B	478	GLY
3	C	216	GLY
4	D	18	VAL
8	H	17	PRO
1	A	258	GLY
1	A	385	ILE
1	A	1107	VAL
2	B	24	PRO
1	A	197	PRO
1	A	392	VAL
2	B	100	PRO
2	B	260	GLY
1	A	250	ILE
1	A	800	VAL
1	A	937	VAL
1	A	1122	PRO
3	C	172	PRO
1	A	1190	PRO
2	B	114	PRO
2	B	1014	PRO
11	K	66	PRO
5	E	129	PRO

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	1239/1520 (82%)	1031 (83%)	208 (17%)	3	24
2	B	957/1061 (90%)	800 (84%)	157 (16%)	3	25
3	C	234/274 (85%)	200 (86%)	34 (14%)	5	31
4	D	160/198 (81%)	127 (79%)	33 (21%)	2	13
5	E	196/197 (100%)	170 (87%)	26 (13%)	6	36
6	F	77/137 (56%)	65 (84%)	12 (16%)	4	28
7	G	152/152 (100%)	124 (82%)	28 (18%)	2	18
8	H	118/128 (92%)	98 (83%)	20 (17%)	3	23
9	I	45/122 (37%)	35 (78%)	10 (22%)	1	11
10	J	60/65 (92%)	50 (83%)	10 (17%)	3	24
11	K	99/102 (97%)	76 (77%)	23 (23%)	1	9
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	6
All	All	3377/4013 (84%)	2805 (83%)	572 (17%)	3	23

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	8	SER
1	A	11	LEU
1	A	22	PHE
1	A	32	VAL
1	A	34	LYS
1	A	40	THR
1	A	54	ASN
1	A	58	LEU
1	A	60	SER
1	A	62	ASP
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	84	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	ILE
1	A	107	CYS
1	A	109	HIS
1	A	110	CYS
1	A	121	LEU
1	A	126	LEU
1	A	145	LYS
1	A	151	ASP
1	A	160	GLN
1	A	162	VAL
1	A	169	ASN
1	A	186	LYS
1	A	195	ASP
1	A	215	SER
1	A	216	VAL
1	A	222	LEU
1	A	225	ASN
1	A	232	GLU
1	A	236	LEU
1	A	249	SER
1	A	261	ASP
1	A	262	LEU
1	A	263	THR
1	A	264	PHE
1	A	265	LYS
1	A	278	THR
1	A	302	THR
1	A	303	TYR
1	A	304	MET
1	A	308	ILE
1	A	316	GLN
1	A	320	ARG
1	A	322	VAL
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	368	LYS
1	A	370	ILE
1	A	375	THR
1	A	383	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	386	ASP
1	A	399	HIS
1	A	404	TYR
1	A	414	ASP
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	438	ASP
1	A	440	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	455	MET
1	A	468	PHE
1	A	485	ASP
1	A	491	VAL
1	A	493	GLN
1	A	494	SER
1	A	507	VAL
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	516	SER
1	A	524	VAL
1	A	528	LEU
1	A	533	LYS
1	A	538	ASP
1	A	542	GLU
1	A	577	ILE
1	A	578	LEU
1	A	587	HIS
1	A	595	THR
1	A	596	THR
1	A	598	LEU
1	A	602	ASP
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	630	ILE
1	A	631	HIS
1	A	635	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	640	GLN
1	A	652	VAL
1	A	657	LEU
1	A	670	ILE
1	A	680	THR
1	A	690	VAL
1	A	727	ASP
1	A	738	LYS
1	A	739	ASP
1	A	741	ASN
1	A	742	ASN
1	A	743	VAL
1	A	745	GLN
1	A	774	ARG
1	A	805	LEU
1	A	814	PHE
1	A	827	THR
1	A	831	THR
1	A	833	GLU
1	A	838	GLN
1	A	841	LEU
1	A	845	LEU
1	A	852	TYR
1	A	858	ASN
1	A	860	LEU
1	A	886	ILE
1	A	899	VAL
1	A	902	LEU
1	A	903	ASN
1	A	906	HIS
1	A	919	ILE
1	A	933	TYR
1	A	936	LEU
1	A	939	ASP
1	A	969	GLN
1	A	970	THR
1	A	976	THR
1	A	987	VAL
1	A	988	LEU
1	A	992	ASP
1	A	999	VAL
1	A	1001	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1017	LEU
1	A	1029	ARG
1	A	1033	GLN
1	A	1036	ARG
1	A	1037	LEU
1	A	1067	LEU
1	A	1072	ILE
1	A	1078	GLN
1	A	1095	THR
1	A	1103	GLU
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1134	ILE
1	A	1142	THR
1	A	1159	ARG
1	A	1171	GLN
1	A	1217	LYS
1	A	1219	THR
1	A	1223	ASP
1	A	1228	TRP
1	A	1229	SER
1	A	1241	ARG
1	A	1255	GLU
1	A	1259	MET
1	A	1263	ILE
1	A	1264	GLU
1	A	1271	ILE
1	A	1272	THR
1	A	1274	ARG
1	A	1280	GLU
1	A	1284	MET
1	A	1289	ARG
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1308	THR
1	A	1309	ASP
1	A	1325	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1329	THR
1	A	1331	SER
1	A	1333	ILE
1	A	1336	MET
1	A	1349	TYR
1	A	1362	TYR
1	A	1368	MET
1	A	1370	LEU
1	A	1373	ASP
1	A	1377	THR
1	A	1378	GLN
1	A	1382	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1397	LEU
1	A	1401	SER
1	A	1402	PHE
1	A	1403	GLU
1	A	1405	THR
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1429	ILE
1	A	1442	ASP
1	A	1451	VAL
2	B	29	ASP
2	B	44	VAL
2	B	46	GLN
2	B	47	GLN
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	90	ILE
2	B	95	ILE
2	B	102	VAL
2	B	115	GLN
2	B	165	VAL
2	B	181	LEU
2	B	185	THR
2	B	188	ASP
2	B	194	GLU
2	B	202	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	217	ARG
2	B	218	SER
2	B	225	VAL
2	B	249	ARG
2	B	259	TYR
2	B	261	ARG
2	B	276	ILE
2	B	283	VAL
2	B	286	PHE
2	B	289	LEU
2	B	294	ASP
2	B	324	ILE
2	B	328	GLU
2	B	329	THR
2	B	363	HIS
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	387	LEU
2	B	401	PHE
2	B	413	LEU
2	B	416	LEU
2	B	427	ASP
2	B	429	PHE
2	B	430	ARG
2	B	463	THR
2	B	466	TRP
2	B	473	MET
2	B	476	ARG
2	B	479	VAL
2	B	482	VAL
2	B	485	ARG
2	B	489	SER
2	B	496	ARG
2	B	516	ASN
2	B	531	GLN
2	B	538	ASN
2	B	539	LEU
2	B	552	MET
2	B	557	PHE
2	B	558	LEU
2	B	559	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	563	MET
2	B	568	ASP
2	B	570	VAL
2	B	576	ASP
2	B	580	VAL
2	B	597	MET
2	B	602	THR
2	B	615	MET
2	B	616	ILE
2	B	619	ILE
2	B	626	ILE
2	B	628	THR
2	B	635	ARG
2	B	641	GLU
2	B	646	LEU
2	B	648	HIS
2	B	678	GLU
2	B	684	LEU
2	B	708	GLU
2	B	709	ASP
2	B	737	THR
2	B	739	THR
2	B	743	ILE
2	B	748	ILE
2	B	773	MET
2	B	780	VAL
2	B	786	ASN
2	B	791	THR
2	B	797	TYR
2	B	815	ARG
2	B	816	GLU
2	B	830	TYR
2	B	841	MET
2	B	842	ASN
2	B	844	SER
2	B	856	PHE
2	B	859	TYR
2	B	868	MET
2	B	869	SER
2	B	878	GLN
2	B	879	ARG
2	B	885	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	890	TYR
2	B	895	ASP
2	B	904	ARG
2	B	914	LYS
2	B	942	ARG
2	B	944	THR
2	B	946	ASN
2	B	953	LEU
2	B	957	ASN
2	B	959	ASP
2	B	969	ARG
2	B	980	PHE
2	B	983	ARG
2	B	987	LYS
2	B	989	THR
2	B	996	ARG
2	B	998	ASP
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1020	ARG
2	B	1026	LEU
2	B	1029	CYS
2	B	1037	LEU
2	B	1051	THR
2	B	1076	HIS
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU
2	B	1112	GLN
2	B	1113	VAL
2	B	1115	THR
2	B	1122	ARG
2	B	1135	ARG
2	B	1147	LEU
2	B	1149	GLU
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1162	ILE
2	B	1170	THR
2	B	1176	ASN
2	B	1177	HIS
2	B	1182	CYS
2	B	1183	LYS
2	B	1185	CYS
2	B	1194	ILE
2	B	1196	ILE
2	B	1210	MET
2	B	1212	ILE
2	B	1216	LEU
2	B	1218	THR
2	B	1223	ASP
3	C	7	GLN
3	C	25	VAL
3	C	43	THR
3	C	48	SER
3	C	56	THR
3	C	63	ILE
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	93	ASP
3	C	100	THR
3	C	104	PHE
3	C	106	GLU
3	C	112	ASN
3	C	118	LEU
3	C	119	VAL
3	C	123	ASN
3	C	124	LEU
3	C	143	LEU
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	178	PHE
3	C	190	ASP
3	C	193	TYR
3	C	201	TRP
3	C	231	ASN
3	C	232	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	235	VAL
3	C	240	VAL
3	C	249	ASP
3	C	254	LYS
3	C	258	ILE
3	C	259	LEU
4	D	5	THR
4	D	11	ARG
4	D	13	ARG
4	D	16	LYS
4	D	17	LYS
4	D	18	VAL
4	D	20	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	34	GLN
4	D	40	HIS
4	D	47	LEU
4	D	50	LEU
4	D	51	ASN
4	D	59	ILE
4	D	65	GLU
4	D	70	PHE
4	D	118	THR
4	D	120	GLU
4	D	123	LEU
4	D	132	GLN
4	D	151	PHE
4	D	156	ASP
4	D	180	LEU
4	D	183	LEU
4	D	194	LEU
4	D	198	LEU
4	D	200	ASN
4	D	202	ILE
4	D	214	LEU
4	D	220	LEU
4	D	221	TYR
5	E	7	ARG
5	E	12	LEU
5	E	17	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	29	PHE
5	E	37	LEU
5	E	41	ASP
5	E	72	PHE
5	E	74	ASP
5	E	84	ASP
5	E	85	GLU
5	E	106	GLN
5	E	114	ASN
5	E	115	ASN
5	E	132	ILE
5	E	144	ILE
5	E	150	VAL
5	E	153	HIS
5	E	165	LEU
5	E	168	TYR
5	E	171	LYS
5	E	173	SER
5	E	175	LEU
5	E	188	LEU
5	E	191	LYS
5	E	192	ARG
5	E	214	CYS
6	F	71	GLU
6	F	79	ARG
6	F	86	THR
6	F	93	ILE
6	F	101	ILE
6	F	107	VAL
6	F	112	GLU
6	F	120	ILE
6	F	138	LEU
6	F	140	ASP
6	F	147	SER
6	F	152	ILE
7	G	1	MET
7	G	7	LEU
7	G	13	LEU
7	G	21	ARG
7	G	42	PHE
7	G	45	ILE
7	G	48	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	51	TYR
7	G	53	ASN
7	G	56	ILE
7	G	67	SER
7	G	74	TYR
7	G	75	ARG
7	G	79	PHE
7	G	87	VAL
7	G	88	ASP
7	G	96	GLN
7	G	97	HIS
7	G	111	THR
7	G	113	HIS
7	G	114	LEU
7	G	126	ASN
7	G	132	SER
7	G	138	THR
7	G	139	ILE
7	G	162	SER
7	G	165	GLU
7	G	168	LEU
8	H	7	ASP
8	H	27	GLU
8	H	33	GLN
8	H	35	GLN
8	H	38	LEU
8	H	53	ASP
8	H	57	VAL
8	H	61	SER
8	H	64	ASN
8	H	80	ARG
8	H	89	LEU
8	H	95	TYR
8	H	102	TYR
8	H	128	ASN
8	H	129	TYR
8	H	130	ARG
8	H	134	ASN
8	H	135	LEU
8	H	138	GLU
8	H	146	ARG
9	I	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	6	PHE
9	I	8	ARG
9	I	10	CYS
9	I	15	TYR
9	I	19	ASP
9	I	21	GLU
9	I	26	LEU
9	I	28	GLU
9	I	46	HIS
10	J	7	CYS
10	J	8	PHE
10	J	26	GLN
10	J	28	ASP
10	J	41	LEU
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
10	J	55	ASP
10	J	64	ASN
11	K	2	ASN
11	K	5	ASP
11	K	11	LEU
11	K	32	VAL
11	K	34	THR
11	K	35	PHE
11	K	41	THR
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	53	ASP
11	K	54	ARG
11	K	56	VAL
11	K	57	LEU
11	K	61	TYR
11	K	65	HIS
11	K	68	PHE
11	K	74	ARG
11	K	75	ILE
11	K	81	TYR
11	K	111	LEU
11	K	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	27	LEU
12	L	38	LEU
12	L	46	VAL
12	L	47	ARG
12	L	48	CYS
12	L	54	ARG
12	L	55	ILE
12	L	61	THR
12	L	64	LEU
12	L	65	VAL
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1416/1733 (81%)	0.12	18 (1%) 74 60	31, 133, 223, 314	0
2	B	1103/1224 (90%)	0.18	11 (0%) 79 66	23, 141, 230, 357	0
3	C	266/318 (83%)	0.11	1 (0%) 90 83	58, 139, 209, 281	0
4	D	178/219 (81%)	-0.09	1 (0%) 86 76	64, 146, 212, 263	0
5	E	214/215 (99%)	0.03	4 (1%) 64 50	71, 165, 246, 367	0
6	F	87/155 (56%)	0.03	0 100 100	48, 95, 156, 221	0
7	G	171/171 (100%)	0.19	1 (0%) 86 76	43, 121, 199, 230	0
8	H	134/146 (91%)	0.33	3 (2%) 59 46	115, 185, 250, 406	0
9	I	47/133 (35%)	0.16	0 100 100	93, 163, 204, 221	0
10	J	65/70 (92%)	0.11	0 100 100	80, 147, 210, 261	0
11	K	114/120 (95%)	0.05	0 100 100	63, 128, 194, 254	0
12	L	46/70 (65%)	0.38	1 (2%) 59 46	93, 159, 240, 306	0
All	All	3841/4574 (83%)	0.13	40 (1%) 77 66	23, 140, 227, 406	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1209	MET	3.1
1	A	257	ARG	2.9
5	E	58	MET	2.8
8	H	139	ASN	2.8
5	E	93	MET	2.8
2	B	729	ILE	2.7
1	A	179	LEU	2.7
1	A	114	LEU	2.7
5	E	110	PHE	2.6
2	B	714	GLU	2.6
1	A	1317	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	426	LEU	2.6
8	H	134	ASN	2.5
4	D	19	GLU	2.5
3	C	229	TYR	2.5
1	A	253	ASN	2.4
2	B	92	PHE	2.4
2	B	963	PHE	2.4
5	E	109	ILE	2.4
2	B	723	VAL	2.4
12	L	27	LEU	2.4
2	B	134	LYS	2.4
2	B	267	ARG	2.4
1	A	115	LEU	2.3
2	B	734	HIS	2.3
2	B	130	VAL	2.3
1	A	145	LYS	2.2
7	G	137	ILE	2.2
2	B	259	TYR	2.2
2	B	245	GLU	2.2
1	A	164	ARG	2.1
1	A	1455	PRO	2.1
1	A	660	ASN	2.1
1	A	1445	ILE	2.1
1	A	1204	ASP	2.1
8	H	137	GLN	2.1
1	A	303	TYR	2.0
1	A	1327	ILE	2.0
1	A	1381	LEU	2.0
1	A	323	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	MG	A	3009	1/1	0.85	7.24	89,89,89,89	0
13	ZN	J	3001	1/1	0.33	0.98	153,153,153,153	0
13	ZN	B	3007	1/1	0.22	-0.08	116,116,116,116	0
13	ZN	A	3008	1/1	0.16	-0.29	97,97,97,97	0
13	ZN	I	3003	1/1	0.13	-0.44	133,133,133,133	0
13	ZN	C	3002	1/1	0.12	-0.77	129,129,129,129	0
13	ZN	L	3005	1/1	0.09	-1.10	229,229,229,229	0
13	ZN	A	3006	1/1	0.05	-1.44	274,274,274,274	0

6.5 Other polymers

There are no such residues in this entry.