



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:40 PM GMT

PDB ID : 3FPP
Title : Crystal structure of E.coli MacA
Authors : Yum, S.; Xu, Y.; Piao, S.; Ha, N.-C.
Deposited on : 2009-01-06
Resolution : 2.99 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>

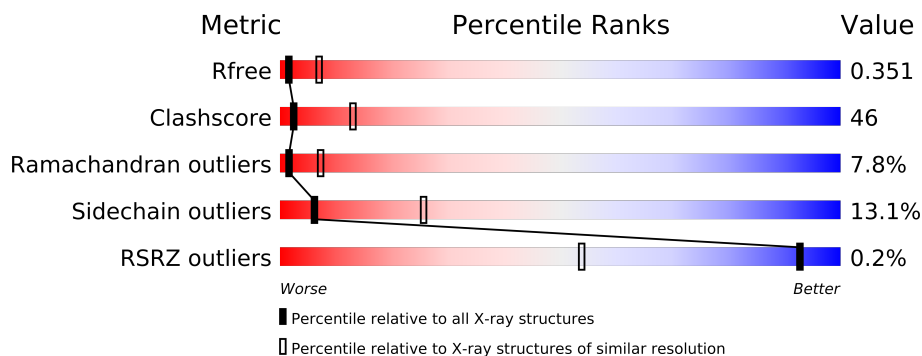
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.99 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	341	
1	B	341	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4097 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 Macrolide-specific efflux protein macA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2043	1274	361	402	6			
1	B	267	Total	C	N	O	S	0	0	0
			2054	1280	365	403	6			

There are 6 discrepancies between the modelled and reference sequences:

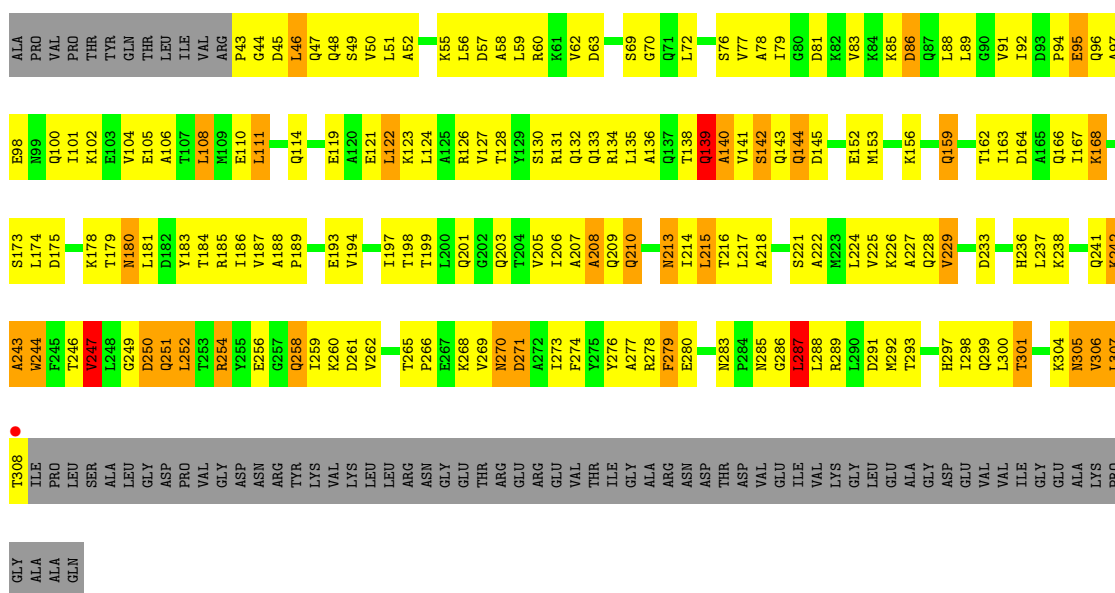
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	GLN	LYS	SEE REMARK 999	UNP P75830
A	148	ASN	THR	SEE REMARK 999	UNP P75830
A	251	GLN	PRO	SEE REMARK 999	UNP P75830
B	139	GLN	LYS	SEE REMARK 999	UNP P75830
B	148	ASN	THR	SEE REMARK 999	UNP P75830
B	251	GLN	PRO	SEE REMARK 999	UNP P75830

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.

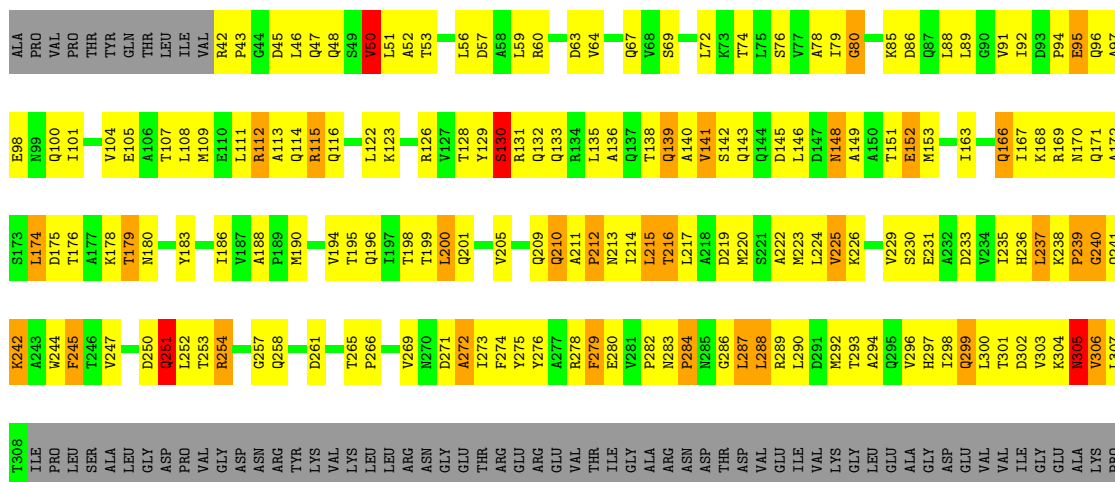
- Molecule 1: Macrolide-specific efflux protein macA

Chain A:



- Molecule 1: Macrolide-specific efflux protein macA

Chain B:



GLY
ALA
ALA
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.52Å 128.52Å 110.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.69 – 2.99 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (49.69-2.99) 92.1 (49.69-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.283 , 0.349 0.284 , 0.351	Depositor DCC
R_{free} test set	1950 reflections (9.83%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 4.3	EDS
Estimated twinning fraction	0.447 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 19873 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4097	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.45	0/2063	0.74	0/2797
1	B	0.44	0/2074	0.75	1/2812 (0.0%)
All	All	0.44	0/4137	0.74	1/5609 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	SER	N-CA-C	5.29	125.30	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2043	0	2104	199	0
1	B	2054	0	2116	195	0
All	All	4097	0	4220	380	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 46.

All (380) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:GLN:HE21	1:A:159:GLN:HA	1.15	1.10
1:B:135:LEU:HD22	1:B:140:ALA:HB2	1.35	1.06
1:B:205:VAL:HG21	1:B:212:PRO:HG3	1.32	1.05
1:B:226:LYS:HZ2	1:B:278:ARG:HD3	1.23	1.04
1:A:285:ASN:ND2	1:A:286:GLY:H	1.55	1.03
1:A:242:LYS:HD2	1:A:242:LYS:H	1.20	1.02
1:B:226:LYS:NZ	1:B:278:ARG:HD3	1.74	1.00
1:A:164:ASP:O	1:A:168:LYS:HD3	1.62	0.99
1:A:124:LEU:HD21	1:B:148:ASN:ND2	1.79	0.98
1:B:109:MET:HA	1:B:112:ARG:HB2	1.50	0.93
1:B:237:LEU:HA	1:B:241:GLN:HE22	1.28	0.93
1:A:44:GLY:H	1:A:307:LEU:HA	1.30	0.93
1:A:50:VAL:HB	1:A:298:ILE:HD11	1.50	0.92
1:A:261:ASP:HB3	1:A:278:ARG:HB2	1.49	0.92
1:B:136:ALA:HB2	1:B:146:LEU:HD21	1.52	0.92
1:A:258:GLN:H	1:A:258:GLN:NE2	1.68	0.92
1:A:243:ALA:HA	1:A:297:HIS:O	1.70	0.91
1:B:224:LEU:HD13	1:B:278:ARG:HD2	1.51	0.91
1:A:285:ASN:CG	1:A:286:GLY:H	1.76	0.88
1:B:215:LEU:O	1:B:215:LEU:HD22	1.75	0.86
1:A:242:LYS:HD3	1:A:299:GLN:HB2	1.58	0.85
1:A:268:LYS:HE2	1:A:271:ASP:HA	1.56	0.85
1:B:251:GLN:HE21	1:B:251:GLN:HA	1.41	0.84
1:A:48:GLN:H	1:A:301:THR:HG23	1.42	0.84
1:B:198:THR:HB	1:B:213:ASN:HD22	1.42	0.83
1:A:242:LYS:CD	1:A:242:LYS:H	1.86	0.83
1:A:124:LEU:HD21	1:B:148:ASN:HD22	1.42	0.82
1:B:205:VAL:HG21	1:B:212:PRO:CG	2.09	0.81
1:A:285:ASN:ND2	1:A:286:GLY:N	2.29	0.81
1:A:159:GLN:NE2	1:A:159:GLN:HA	1.95	0.79
1:B:56:LEU:HD13	1:B:225:VAL:HG12	1.67	0.77
1:B:136:ALA:HB1	1:B:146:LEU:HD11	1.68	0.76
1:B:224:LEU:CD1	1:B:278:ARG:HD2	2.16	0.76
1:A:70:GLY:HA2	1:B:67:GLN:CD	2.06	0.76
1:B:269:VAL:O	1:B:269:VAL:HG23	1.85	0.75
1:B:74:THR:HA	1:B:201:GLN:NE2	2.02	0.75
1:B:59:LEU:HD22	1:B:222:ALA:HB3	1.67	0.75
1:A:105:GLU:HG2	1:A:174:LEU:HD11	1.68	0.74
1:A:159:GLN:HE21	1:A:159:GLN:CA	1.96	0.74
1:B:46:LEU:HD13	1:B:47:GLN:N	2.02	0.74
1:A:288:LEU:HA	1:A:292:MET:SD	2.28	0.74
1:A:43:PRO:HB3	1:A:305:ASN:HD21	1.52	0.74
1:B:46:LEU:HD22	1:B:47:GLN:H	1.51	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:92:ILE:O	1:B:94:PRO:HD3	1.88	0.73
1:A:135:LEU:HB3	1:A:140:ALA:HB3	1.68	0.73
1:A:44:GLY:H	1:A:307:LEU:CA	2.00	0.72
1:A:199:THR:HB	1:A:214:ILE:HA	1.70	0.72
1:B:47:GLN:HB2	1:B:301:THR:O	1.88	0.72
1:A:43:PRO:HB3	1:A:305:ASN:ND2	2.05	0.71
1:A:89:LEU:HD21	1:A:188:ALA:HB2	1.72	0.71
1:B:225:VAL:HG22	1:B:279:PHE:HB2	1.71	0.71
1:B:132:GLN:O	1:B:136:ALA:HB2	1.90	0.71
1:A:111:LEU:HA	1:A:114:GLN:HG3	1.72	0.70
1:A:47:GLN:HB2	1:A:301:THR:O	1.92	0.70
1:B:238:LYS:HG3	1:B:239:PRO:HD2	1.72	0.70
1:A:162:THR:HG22	1:A:166:GLN:NE2	2.07	0.69
1:B:74:THR:CG2	1:B:91:VAL:HB	2.22	0.69
1:A:270:ASN:O	1:A:271:ASP:HB2	1.92	0.68
1:B:48:GLN:HG3	1:B:300:LEU:HD12	1.76	0.67
1:B:100:GLN:O	1:B:104:VAL:HG23	1.93	0.67
1:B:56:LEU:HD21	1:B:288:LEU:HB3	1.76	0.67
1:B:141:VAL:HB	1:B:145:ASP:OD2	1.95	0.67
1:B:237:LEU:HD11	1:B:298:ILE:HG21	1.77	0.67
1:A:285:ASN:CG	1:A:286:GLY:N	2.44	0.67
1:A:229:VAL:HG21	1:A:237:LEU:HD22	1.77	0.67
1:B:198:THR:CB	1:B:213:ASN:HD22	2.08	0.67
1:B:48:GLN:O	1:B:300:LEU:HB2	1.95	0.66
1:A:249:GLY:O	1:A:250:ASP:HB3	1.96	0.66
1:B:247:VAL:CG2	1:B:250:ASP:HB2	2.26	0.66
1:A:238:LYS:O	1:A:241:GLN:HG3	1.96	0.66
1:B:226:LYS:HB3	1:B:276:TYR:CD2	2.31	0.65
1:A:305:ASN:HD22	1:A:305:ASN:C	2.00	0.65
1:A:69:SER:OG	1:A:206:ILE:HA	1.96	0.65
1:B:138:THR:O	1:B:139:GLN:HB2	1.94	0.65
1:A:268:LYS:CE	1:A:271:ASP:HA	2.26	0.65
1:B:56:LEU:CD1	1:B:225:VAL:HG12	2.26	0.65
1:A:134:ARG:C	1:A:136:ALA:H	2.00	0.64
1:A:131:ARG:O	1:A:135:LEU:HG	1.96	0.64
1:A:110:GLU:O	1:A:114:GLN:HG2	1.98	0.64
1:B:286:GLY:O	1:B:287:LEU:O	2.16	0.64
1:A:43:PRO:HA	1:A:307:LEU:HB2	1.80	0.64
1:A:259:ILE:HA	1:A:279:PHE:HB3	1.79	0.63
1:A:236:HIS:HB3	1:A:300:LEU:HD13	1.80	0.63
1:A:260:LYS:NZ	1:A:280:GLU:HB2	2.13	0.63
1:B:251:GLN:HE21	1:B:251:GLN:CA	2.08	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50:VAL:O	1:A:298:ILE:HG12	1.99	0.63
1:B:97:ALA:HA	1:B:100:GLN:NE2	2.13	0.63
1:B:205:VAL:CG2	1:B:212:PRO:HG3	2.20	0.63
1:B:63:ASP:OD1	1:B:216:THR:HB	1.99	0.63
1:B:283:ASN:OD1	1:B:287:LEU:O	2.17	0.62
1:A:287:LEU:H	1:A:287:LEU:HD13	1.65	0.62
1:A:242:LYS:CD	1:A:299:GLN:HB2	2.27	0.62
1:B:226:LYS:HZ3	1:B:278:ARG:HD3	1.64	0.62
1:A:122:LEU:O	1:A:126:ARG:HG2	1.99	0.62
1:B:180:ASN:HA	1:B:183:TYR:HD2	1.64	0.62
1:A:48:GLN:N	1:A:301:THR:HG23	2.13	0.61
1:B:51:LEU:HD22	1:B:297:HIS:CD2	2.36	0.60
1:A:62:VAL:HG11	1:A:189:PRO:HG3	1.82	0.60
1:A:69:SER:HA	1:A:205:VAL:O	2.01	0.60
1:B:107:THR:HG21	1:B:170:ASN:ND2	2.16	0.60
1:B:251:GLN:NE2	1:B:251:GLN:HA	2.15	0.60
1:B:142:SER:OG	1:B:143:GLN:N	2.34	0.60
1:B:168:LYS:C	1:B:168:LYS:HD3	2.21	0.60
1:A:88:LEU:HA	1:A:187:VAL:HG12	1.84	0.60
1:B:74:THR:HG22	1:B:91:VAL:HB	1.83	0.60
1:A:130:SER:O	1:A:133:GLN:HG2	2.00	0.60
1:A:57:ASP:OD1	1:A:58:ALA:N	2.35	0.60
1:B:53:THR:O	1:B:53:THR:HG22	2.01	0.60
1:A:287:LEU:O	1:A:288:LEU:HB2	2.02	0.59
1:A:214:ILE:HD12	1:A:214:ILE:N	2.17	0.59
1:B:78:ALA:O	1:B:80:GLY:N	2.31	0.59
1:A:246:THR:O	1:A:247:VAL:HG13	2.02	0.59
1:B:136:ALA:CB	1:B:146:LEU:HD21	2.30	0.59
1:A:242:LYS:O	1:A:243:ALA:HB3	2.02	0.59
1:A:258:GLN:N	1:A:258:GLN:NE2	2.45	0.59
1:A:59:LEU:HB2	1:A:222:ALA:O	2.03	0.59
1:B:266:PRO:HB3	1:B:275:TYR:CE1	2.38	0.58
1:A:164:ASP:HA	1:A:167:ILE:HD12	1.85	0.58
1:B:45:ASP:CB	1:B:304:LYS:HG3	2.33	0.58
1:A:229:VAL:HG22	1:A:229:VAL:O	2.01	0.58
1:B:95:GLU:HA	1:B:98:GLU:OE1	2.04	0.58
1:B:122:LEU:O	1:B:126:ARG:HB2	2.04	0.58
1:B:238:LYS:H	1:B:241:GLN:NE2	2.01	0.58
1:B:237:LEU:CD1	1:B:298:ILE:HG21	2.32	0.58
1:B:72:LEU:HD12	1:B:199:THR:HG22	1.86	0.58
1:B:190:MET:HE1	1:B:219:ASP:H	1.68	0.57
1:A:85:LYS:O	1:A:86:ASP:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:VAL:HG12	1:B:298:ILE:HD12	1.87	0.57
1:B:167:ILE:HG22	1:B:171:GLN:HG3	1.87	0.57
1:B:96:GLN:NE2	1:B:96:GLN:HA	2.18	0.56
1:B:132:GLN:O	1:B:146:LEU:HD21	2.05	0.56
1:B:190:MET:HE1	1:B:219:ASP:N	2.19	0.56
1:A:286:GLY:O	1:A:287:LEU:O	2.22	0.56
1:B:244:TRP:HZ3	1:B:299:GLN:HG2	1.70	0.56
1:A:122:LEU:HG	1:A:156:LYS:HB3	1.86	0.56
1:A:237:LEU:HD21	1:A:277:ALA:HB2	1.87	0.56
1:A:138:THR:O	1:A:138:THR:HG22	2.05	0.56
1:B:235:ILE:HD12	1:B:235:ILE:H	1.69	0.56
1:B:266:PRO:HB3	1:B:275:TYR:CD1	2.41	0.56
1:A:180:ASN:O	1:A:183:TYR:HB2	2.05	0.56
1:B:89:LEU:HD11	1:B:188:ALA:HB2	1.88	0.56
1:B:283:ASN:N	1:B:284:PRO:HD3	2.20	0.55
1:B:109:MET:CA	1:B:112:ARG:HB2	2.30	0.55
1:B:85:LYS:HG2	1:B:86:ASP:N	2.21	0.55
1:B:245:PHE:CD1	1:B:245:PHE:C	2.78	0.55
1:B:215:LEU:CD2	1:B:215:LEU:O	2.53	0.55
1:B:122:LEU:HD23	1:B:123:LYS:HE2	1.88	0.55
1:A:251:GLN:O	1:A:252:LEU:HD13	2.07	0.55
1:A:130:SER:O	1:A:133:GLN:N	2.39	0.55
1:A:108:LEU:O	1:A:108:LEU:HD13	2.07	0.55
1:B:168:LYS:O	1:B:168:LYS:HD3	2.07	0.55
1:A:83:VAL:HG21	1:A:217:LEU:HD21	1.89	0.55
1:A:46:LEU:HB2	1:A:308:THR:CG2	2.37	0.55
1:A:46:LEU:HB2	1:A:308:THR:HG22	1.89	0.54
1:A:163:ILE:HG22	1:A:167:ILE:HD11	1.89	0.54
1:A:227:ALA:O	1:A:276:TYR:HA	2.07	0.54
1:B:224:LEU:HA	1:B:279:PHE:O	2.08	0.54
1:A:270:ASN:O	1:A:271:ASP:CB	2.55	0.54
1:A:260:LYS:HZ2	1:A:280:GLU:HB2	1.73	0.54
1:A:51:LEU:HD21	1:A:297:HIS:ND1	2.23	0.53
1:A:43:PRO:CB	1:A:305:ASN:HD21	2.21	0.53
1:B:230:SER:HB3	1:B:233:ASP:OD2	2.09	0.53
1:A:79:ILE:HA	1:A:194:VAL:HG12	1.89	0.53
1:B:175:ASP:O	1:B:179:THR:HB	2.07	0.53
1:B:46:LEU:HD22	1:B:47:GLN:N	2.23	0.53
1:B:186:ILE:HD12	1:B:186:ILE:N	2.23	0.53
1:A:305:ASN:C	1:A:305:ASN:ND2	2.60	0.53
1:A:229:VAL:HG11	1:A:237:LEU:CD2	2.38	0.53
1:B:235:ILE:N	1:B:235:ILE:HD12	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:ALA:CA	1:A:297:HIS:O	2.52	0.53
1:B:198:THR:HB	1:B:213:ASN:ND2	2.20	0.53
1:B:205:VAL:HG23	1:B:212:PRO:HB3	1.92	0.52
1:A:279:PHE:N	1:A:279:PHE:CD1	2.78	0.52
1:B:69:SER:O	1:B:92:ILE:HG21	2.10	0.52
1:A:94:PRO:HA	1:A:184:THR:HG21	1.91	0.52
1:A:52:ALA:HB1	1:A:228:GLN:O	2.10	0.52
1:B:50:VAL:O	1:B:50:VAL:HG12	2.10	0.52
1:A:62:VAL:HG12	1:A:63:ASP:N	2.25	0.52
1:B:225:VAL:HG11	1:B:245:PHE:CE2	2.44	0.52
1:A:92:ILE:HD11	1:A:186:ILE:HD11	1.91	0.52
1:A:186:ILE:HD13	1:A:214:ILE:HG12	1.90	0.52
1:B:72:LEU:HD13	1:B:200:LEU:O	2.10	0.52
1:B:163:ILE:O	1:B:166:GLN:N	2.43	0.52
1:A:95:GLU:HA	1:A:98:GLU:HG3	1.92	0.51
1:A:258:GLN:H	1:A:258:GLN:HE21	1.55	0.51
1:A:79:ILE:HG23	1:A:194:VAL:O	2.11	0.51
1:B:235:ILE:CD1	1:B:235:ILE:H	2.23	0.51
1:A:246:THR:C	1:A:247:VAL:HG22	2.31	0.51
1:A:105:GLU:CG	1:A:174:LEU:HD11	2.40	0.50
1:B:128:THR:O	1:B:129:TYR:C	2.49	0.50
1:A:62:VAL:HG11	1:A:189:PRO:CG	2.41	0.50
1:B:56:LEU:HD12	1:B:224:LEU:O	2.11	0.50
1:A:134:ARG:C	1:A:136:ALA:N	2.64	0.50
1:B:283:ASN:CG	1:B:283:ASN:O	2.49	0.50
1:B:130:SER:O	1:B:132:GLN:N	2.45	0.50
1:A:214:ILE:HD12	1:A:214:ILE:H	1.77	0.50
1:A:203:GLN:HE21	1:B:63:ASP:H	1.60	0.50
1:B:306:VAL:HG22	1:B:307:LEU:N	2.27	0.50
1:B:282:PRO:C	1:B:284:PRO:HD3	2.32	0.50
1:A:241:GLN:O	1:A:242:LYS:O	2.31	0.49
1:B:252:LEU:HD12	1:B:254:ARG:HG3	1.93	0.49
1:A:57:ASP:O	1:A:224:LEU:N	2.45	0.49
1:A:55:LYS:HD2	1:A:291:ASP:OD1	2.12	0.49
1:A:56:LEU:HD12	1:A:292:MET:O	2.11	0.49
1:A:108:LEU:CD1	1:A:108:LEU:O	2.60	0.49
1:B:290:LEU:HD12	1:B:290:LEU:N	2.26	0.49
1:A:51:LEU:CD2	1:A:297:HIS:ND1	2.76	0.49
1:A:45:ASP:OD2	1:A:305:ASN:N	2.43	0.49
1:B:96:GLN:C	1:B:100:GLN:HE22	2.16	0.49
1:A:94:PRO:HB2	1:A:181:LEU:HD11	1.93	0.49
1:A:175:ASP:O	1:A:179:THR:HG23	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:GLN:O	1:A:210:GLN:HB2	2.12	0.49
1:B:224:LEU:HD22	1:B:279:PHE:O	2.13	0.49
1:B:231:GLU:CD	1:B:273:ILE:HB	2.33	0.49
1:B:135:LEU:CD2	1:B:140:ALA:HB2	2.25	0.49
1:B:74:THR:HA	1:B:201:GLN:HE21	1.74	0.49
1:B:226:LYS:HD3	1:B:278:ARG:HG2	1.95	0.49
1:B:196:GLN:HB3	1:B:216:THR:CG2	2.43	0.49
1:B:250:ASP:OD1	1:B:250:ASP:O	2.30	0.48
1:A:88:LEU:CD1	1:A:185:ARG:HB3	2.43	0.48
1:B:94:PRO:O	1:B:96:GLN:N	2.45	0.48
1:A:47:GLN:HA	1:A:301:THR:HG23	1.94	0.48
1:B:46:LEU:C	1:B:46:LEU:HD13	2.33	0.48
1:B:293:THR:HG22	1:B:294:ALA:N	2.28	0.48
1:B:293:THR:CG2	1:B:294:ALA:N	2.77	0.48
1:A:78:ALA:HA	1:A:197:ILE:HD11	1.95	0.48
1:A:306:VAL:HG12	1:A:306:VAL:O	2.14	0.48
1:A:233:ASP:OD2	1:A:233:ASP:N	2.46	0.48
1:A:206:ILE:HG22	1:B:211:ALA:HB2	1.95	0.48
1:A:279:PHE:N	1:A:279:PHE:HD1	2.12	0.48
1:A:121:GLU:HB3	1:A:156:LYS:HE2	1.96	0.48
1:A:251:GLN:H	1:A:251:GLN:CD	2.14	0.48
1:A:238:LYS:H	1:A:241:GLN:CD	2.16	0.48
1:B:141:VAL:HG23	1:B:145:ASP:HB2	1.96	0.48
1:B:115:ARG:HA	1:B:163:ILE:CD1	2.43	0.48
1:B:198:THR:CB	1:B:213:ASN:ND2	2.74	0.48
1:A:69:SER:CB	1:A:206:ILE:HA	2.43	0.47
1:A:237:LEU:HD13	1:A:298:ILE:HD12	1.95	0.47
1:B:289:ARG:HG3	1:B:292:MET:CE	2.44	0.47
1:B:89:LEU:HD11	1:B:188:ALA:CA	2.45	0.47
1:A:142:SER:OG	1:A:143:GLN:N	2.46	0.47
1:A:244:TRP:CE3	1:A:254:ARG:HD3	2.50	0.47
1:B:180:ASN:HA	1:B:183:TYR:CD2	2.46	0.47
1:B:205:VAL:HG21	1:B:212:PRO:CB	2.45	0.47
1:B:108:LEU:HD11	1:B:170:ASN:HB3	1.97	0.47
1:B:209:GLN:HB3	1:B:210:GLN:OE1	2.15	0.47
1:A:72:LEU:HD22	1:A:201:GLN:HA	1.97	0.47
1:A:203:GLN:HG2	1:B:63:ASP:O	2.14	0.47
1:A:106:ALA:HB2	1:B:168:LYS:HD2	1.96	0.46
1:B:229:VAL:HG22	1:B:230:SER:N	2.30	0.46
1:B:186:ILE:CD1	1:B:186:ILE:N	2.79	0.46
1:B:205:VAL:CG2	1:B:212:PRO:HB3	2.45	0.46
1:A:304:LYS:O	1:A:305:ASN:HB3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:LEU:CD1	1:A:199:THR:HG22	2.45	0.46
1:A:162:THR:HG22	1:A:166:GLN:HE22	1.79	0.46
1:A:133:GLN:O	1:A:136:ALA:HB3	2.14	0.46
1:A:251:GLN:OE1	1:A:251:GLN:N	2.43	0.46
1:A:207:ALA:O	1:A:208:ALA:C	2.54	0.46
1:A:242:LYS:N	1:A:242:LYS:CD	2.65	0.46
1:A:124:LEU:HD22	1:B:151:THR:OG1	2.15	0.46
1:B:52:ALA:N	1:B:296:VAL:O	2.47	0.46
1:B:240:GLY:HA2	1:B:258:GLN:HB3	1.97	0.46
1:B:135:LEU:HD22	1:B:140:ALA:CB	2.25	0.46
1:A:47:GLN:OE1	1:A:47:GLN:N	2.48	0.46
1:A:163:ILE:O	1:A:167:ILE:HG13	2.16	0.46
1:A:269:VAL:O	1:A:270:ASN:ND2	2.49	0.46
1:A:121:GLU:HB3	1:A:156:LYS:CE	2.46	0.46
1:B:149:ALA:O	1:B:152:GLU:HB3	2.15	0.46
1:A:215:LEU:C	1:A:215:LEU:HD23	2.36	0.46
1:B:174:LEU:O	1:B:178:LYS:HG3	2.16	0.46
1:B:128:THR:HG23	1:B:132:GLN:HG2	1.98	0.45
1:B:108:LEU:CD1	1:B:170:ASN:HB3	2.46	0.45
1:B:237:LEU:CA	1:B:241:GLN:HE22	2.14	0.45
1:A:72:LEU:HD13	1:A:199:THR:HG22	1.98	0.45
1:A:143:GLN:O	1:A:144:GLN:C	2.54	0.45
1:A:76:SER:O	1:A:77:VAL:HG13	2.16	0.45
1:A:43:PRO:CB	1:A:305:ASN:ND2	2.77	0.45
1:B:242:LYS:HG3	1:B:258:GLN:OE1	2.16	0.45
1:A:119:GLU:O	1:A:123:LYS:HG3	2.16	0.45
1:A:163:ILE:O	1:A:166:GLN:HB2	2.17	0.45
1:A:225:VAL:HB	1:A:279:PHE:CE1	2.52	0.45
1:B:242:LYS:HA	1:B:257:GLY:O	2.15	0.45
1:B:290:LEU:CD1	1:B:290:LEU:N	2.80	0.45
1:A:229:VAL:HG11	1:A:237:LEU:HD22	1.99	0.45
1:B:51:LEU:HA	1:B:297:HIS:HA	1.99	0.45
1:A:47:GLN:HA	1:A:301:THR:CG2	2.47	0.45
1:B:115:ARG:HB2	1:B:163:ILE:HG21	1.97	0.45
1:B:253:THR:HG22	1:B:253:THR:O	2.17	0.45
1:B:88:LEU:C	1:B:88:LEU:HD23	2.37	0.45
1:B:136:ALA:HA	1:B:140:ALA:H	1.82	0.45
1:B:244:TRP:CZ3	1:B:299:GLN:HG2	2.52	0.45
1:A:70:GLY:HA2	1:B:67:GLN:OE1	2.16	0.45
1:A:261:ASP:O	1:A:262:VAL:HG23	2.17	0.45
1:A:249:GLY:O	1:A:250:ASP:CB	2.65	0.45
1:A:69:SER:OG	1:A:206:ILE:HD12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:85:LYS:HG2	1:B:86:ASP:H	1.82	0.44
1:A:287:LEU:O	1:A:288:LEU:CB	2.66	0.44
1:B:107:THR:HG21	1:B:170:ASN:HD22	1.79	0.44
1:A:60:ARG:O	1:A:218:ALA:HA	2.16	0.44
1:A:213:ASN:HD22	1:A:213:ASN:C	2.21	0.44
1:B:305:ASN:O	1:B:306:VAL:HB	2.17	0.44
1:A:128:THR:O	1:A:132:GLN:HG3	2.18	0.44
1:A:46:LEU:HD23	1:A:308:THR:HG21	1.99	0.44
1:A:138:THR:O	1:A:139:GLN:O	2.36	0.44
1:B:111:LEU:HD13	1:B:166:GLN:HB3	1.99	0.44
1:B:126:ARG:HG3	1:B:153:MET:SD	2.58	0.43
1:A:141:VAL:CG2	1:A:145:ASP:HB2	2.48	0.43
1:A:178:LYS:C	1:A:180:ASN:H	2.21	0.43
1:B:269:VAL:CG2	1:B:269:VAL:O	2.59	0.43
1:A:241:GLN:NE2	1:A:300:LEU:HA	2.33	0.43
1:A:242:LYS:O	1:A:243:ALA:CB	2.66	0.43
1:B:74:THR:HG23	1:B:91:VAL:HB	1.96	0.43
1:A:101:ILE:O	1:A:102:LYS:C	2.56	0.43
1:A:100:GLN:O	1:A:104:VAL:HG23	2.19	0.43
1:A:236:HIS:CB	1:A:300:LEU:HD13	2.47	0.43
1:A:229:VAL:CG2	1:A:229:VAL:O	2.66	0.43
1:B:169:ARG:O	1:B:172:ALA:HB3	2.18	0.43
1:B:105:GLU:O	1:B:108:LEU:HB2	2.19	0.43
1:B:56:LEU:HD11	1:B:223:MET:HB3	1.99	0.43
1:B:225:VAL:HG13	1:B:279:PHE:HB3	2.00	0.43
1:B:266:PRO:HB2	1:B:274:PHE:O	2.18	0.43
1:B:302:ASP:OD1	1:B:302:ASP:O	2.37	0.43
1:A:56:LEU:HA	1:A:224:LEU:O	2.19	0.43
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.74	0.43
1:B:199:THR:HB	1:B:214:ILE:HA	1.99	0.43
1:B:85:LYS:O	1:B:86:ASP:HB2	2.18	0.43
1:A:110:GLU:O	1:A:114:GLN:CG	2.67	0.42
1:B:108:LEU:O	1:B:112:ARG:N	2.52	0.42
1:A:43:PRO:N	1:A:307:LEU:HG	2.35	0.42
1:A:193:GLU:O	1:A:217:LEU:HA	2.19	0.42
1:B:114:GLN:HB2	1:B:114:GLN:HE21	1.66	0.42
1:B:133:GLN:O	1:B:136:ALA:HB3	2.19	0.42
1:A:164:ASP:OD2	1:A:167:ILE:HD12	2.19	0.42
1:B:296:VAL:HG12	1:B:298:ILE:CD1	2.48	0.42
1:A:130:SER:O	1:A:131:ARG:C	2.57	0.42
1:A:94:PRO:O	1:A:97:ALA:N	2.51	0.42
1:A:266:PRO:HB2	1:A:273:ILE:HG13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:GLN:HB2	1:A:301:THR:C	2.39	0.42
1:A:141:VAL:O	1:A:142:SER:OG	2.25	0.42
1:B:101:ILE:O	1:B:105:GLU:HG3	2.20	0.42
1:A:269:VAL:O	1:A:270:ASN:CG	2.58	0.42
1:B:188:ALA:HB1	1:B:217:LEU:HD11	2.01	0.42
1:A:79:ILE:H	1:A:79:ILE:HG13	1.65	0.42
1:A:96:GLN:HE21	1:B:176:THR:HG23	1.85	0.42
1:B:226:LYS:NZ	1:B:278:ARG:CD	2.65	0.42
1:B:288:LEU:HA	1:B:292:MET:SD	2.60	0.42
1:B:225:VAL:O	1:B:225:VAL:CG2	2.68	0.42
1:B:238:LYS:O	1:B:239:PRO:C	2.58	0.42
1:A:258:GLN:N	1:A:258:GLN:CD	2.72	0.42
1:A:203:GLN:CG	1:B:63:ASP:O	2.68	0.42
1:B:60:ARG:HH12	1:B:219:ASP:CG	2.23	0.41
1:B:92:ILE:O	1:B:94:PRO:CD	2.62	0.41
1:A:92:ILE:O	1:A:94:PRO:HD3	2.20	0.41
1:A:289:ARG:HB2	1:B:275:TYR:OH	2.21	0.41
1:A:242:LYS:HD3	1:A:299:GLN:CB	2.39	0.41
1:A:50:VAL:HB	1:A:298:ILE:CD1	2.37	0.41
1:A:249:GLY:O	1:B:235:ILE:HG12	2.20	0.41
1:A:269:VAL:HB	1:A:274:PHE:CE2	2.56	0.41
1:B:129:TYR:O	1:B:130:SER:C	2.59	0.41
1:B:299:GLN:O	1:B:300:LEU:C	2.59	0.41
1:B:296:VAL:HG12	1:B:297:HIS:N	2.36	0.41
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.84	0.41
1:A:79:ILE:HA	1:A:194:VAL:CG1	2.51	0.41
1:A:49:SER:HA	1:A:298:ILE:O	2.21	0.41
1:A:139:GLN:O	1:A:140:ALA:HB2	2.21	0.41
1:A:62:VAL:CG1	1:A:63:ASP:N	2.84	0.41
1:A:96:GLN:NE2	1:B:176:THR:HG23	2.36	0.41
1:B:42:ARG:HA	1:B:43:PRO:HD3	1.91	0.41
1:B:72:LEU:HD12	1:B:199:THR:CG2	2.51	0.41
1:B:289:ARG:HG3	1:B:292:MET:HE3	2.03	0.40
1:A:286:GLY:O	1:A:287:LEU:C	2.59	0.40
1:A:229:VAL:HG11	1:A:237:LEU:HD21	2.01	0.40
1:A:226:LYS:HG2	1:A:278:ARG:HD3	2.02	0.40
1:B:271:ASP:O	1:B:272:ALA:O	2.40	0.40
1:B:236:HIS:O	1:B:237:LEU:CB	2.69	0.40
1:B:238:LYS:HA	1:B:238:LYS:HD2	1.96	0.40
1:B:59:LEU:HD23	1:B:219:ASP:OD2	2.21	0.40
1:B:298:ILE:HG22	1:B:299:GLN:N	2.36	0.40
1:A:127:VAL:O	1:A:128:THR:C	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:113:ALA:O	1:B:116:GLN:N	2.55	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	264/341 (77%)	207 (78%)	39 (15%)	18 (7%)	2	10
1	B	265/341 (78%)	203 (77%)	39 (15%)	23 (9%)	1	5
All	All	529/682 (78%)	410 (78%)	78 (15%)	41 (8%)	1	7

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ALA
1	A	221	SER
1	A	242	LYS
1	A	247	VAL
1	A	252	LEU
1	A	254	ARG
1	A	271	ASP
1	A	287	LEU
1	B	79	ILE
1	B	139	GLN
1	B	254	ARG
1	B	287	LEU
1	A	95	GLU
1	A	144	GLN
1	A	208	ALA
1	A	250	ASP
1	A	306	VAL
1	B	50	VAL
1	B	95	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	130	SER
1	B	131	ARG
1	B	242	LYS
1	B	272	ALA
1	A	139	GLN
1	A	210	GLN
1	B	80	GLY
1	B	194	VAL
1	B	251	GLN
1	B	305	ASN
1	B	306	VAL
1	A	86	ASP
1	A	142	SER
1	A	243	ALA
1	B	239	PRO
1	B	261	ASP
1	B	288	LEU
1	B	212	PRO
1	B	237	LEU
1	B	240	GLY
1	B	284	PRO
1	B	141	VAL

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	221/281 (79%)	189 (86%)	32 (14%)	5	22
1	B	222/281 (79%)	196 (88%)	26 (12%)	8	31
All	All	443/562 (79%)	385 (87%)	58 (13%)	6	25

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	81	ASP
1	A	91	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	LEU
1	A	111	LEU
1	A	122	LEU
1	A	139	GLN
1	A	152	GLU
1	A	153	MET
1	A	159	GLN
1	A	168	LYS
1	A	173	SER
1	A	180	ASN
1	A	198	THR
1	A	213	ASN
1	A	215	LEU
1	A	216	THR
1	A	229	VAL
1	A	244	TRP
1	A	247	VAL
1	A	251	GLN
1	A	256	GLU
1	A	258	GLN
1	A	265	THR
1	A	270	ASN
1	A	279	PHE
1	A	283	ASN
1	A	287	LEU
1	A	293	THR
1	A	301	THR
1	A	305	ASN
1	A	307	LEU
1	B	50	VAL
1	B	57	ASP
1	B	64	VAL
1	B	112	ARG
1	B	115	ARG
1	B	130	SER
1	B	148	ASN
1	B	152	GLU
1	B	166	GLN
1	B	174	LEU
1	B	179	THR
1	B	195	THR
1	B	200	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	210	GLN
1	B	215	LEU
1	B	216	THR
1	B	220	MET
1	B	225	VAL
1	B	245	PHE
1	B	251	GLN
1	B	265	THR
1	B	279	PHE
1	B	280	GLU
1	B	299	GLN
1	B	303	VAL
1	B	305	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	96	GLN
1	A	99	ASN
1	A	116	GLN
1	A	133	GLN
1	A	148	ASN
1	A	159	GLN
1	A	166	GLN
1	A	180	ASN
1	A	203	GLN
1	A	213	ASN
1	A	258	GLN
1	A	283	ASN
1	A	299	GLN
1	A	305	ASN
1	B	96	GLN
1	B	100	GLN
1	B	114	GLN
1	B	116	GLN
1	B	133	GLN
1	B	144	GLN
1	B	148	ASN
1	B	170	ASN
1	B	201	GLN
1	B	209	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	213	ASN
1	B	241	GLN
1	B	251	GLN
1	B	299	GLN
1	B	305	ASN

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 ⓘ

There are no ligands in this entry.

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	266/341 (78%)	-0.20	1 (0%) 90 41	10, 28, 60, 75	0
1	B	267/341 (78%)	-0.20	0 100 100	9, 28, 51, 69	0
All	All	533/682 (78%)	-0.20	1 (0%) 93 54	9, 28, 57, 75	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	THR	2.1

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.