



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:39 AM UTC

PDB ID : 3H5A / pdb_00003h5a
Title : Crystal structure of E. coli MccB
Authors : Regni, C.A.; Roush, R.F.; Miller, D.; Nourse, A.; Walsh, C.T.; Schulman, B.A.
Deposited on : 2009-04-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

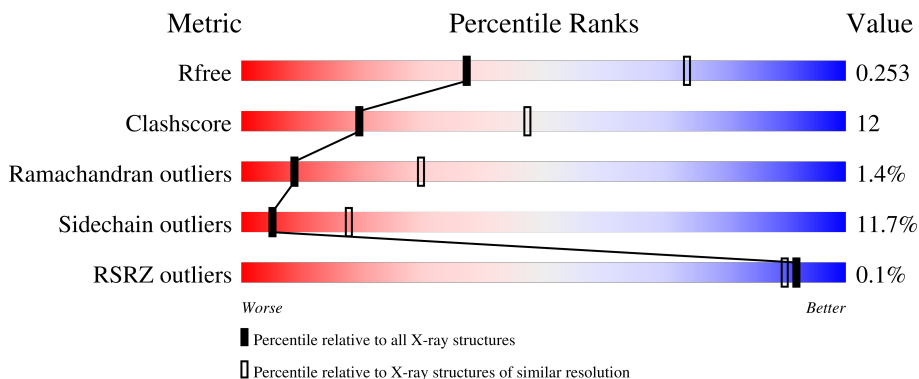
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	 72% 21% 6%
1	B	358	 68% 27% 5%
1	C	358	 74% 21%
1	D	358	 67% 27%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11064 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 MccB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2770	1766	478	515	11			
1	B	357	Total	C	N	O	S	0	0	0
			2768	1761	477	518	12			
1	C	358	Total	C	N	O	S	0	0	0
			2786	1775	480	520	11			
1	D	350	Total	C	N	O	S	0	0	0
			2736	1744	474	506	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	351	LEU	-	expression tag	UNP Q47506
A	352	GLU	-	expression tag	UNP Q47506
A	353	HIS	-	expression tag	UNP Q47506
A	354	HIS	-	expression tag	UNP Q47506
A	355	HIS	-	expression tag	UNP Q47506
A	356	HIS	-	expression tag	UNP Q47506
A	357	HIS	-	expression tag	UNP Q47506
A	358	HIS	-	expression tag	UNP Q47506
B	351	LEU	-	expression tag	UNP Q47506
B	352	GLU	-	expression tag	UNP Q47506
B	353	HIS	-	expression tag	UNP Q47506
B	354	HIS	-	expression tag	UNP Q47506
B	355	HIS	-	expression tag	UNP Q47506
B	356	HIS	-	expression tag	UNP Q47506
B	357	HIS	-	expression tag	UNP Q47506
B	358	HIS	-	expression tag	UNP Q47506
C	351	LEU	-	expression tag	UNP Q47506
C	352	GLU	-	expression tag	UNP Q47506
C	353	HIS	-	expression tag	UNP Q47506
C	354	HIS	-	expression tag	UNP Q47506
C	355	HIS	-	expression tag	UNP Q47506

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	356	HIS	-	expression tag	UNP Q47506
C	357	HIS	-	expression tag	UNP Q47506
C	358	HIS	-	expression tag	UNP Q47506
D	351	LEU	-	expression tag	UNP Q47506
D	352	GLU	-	expression tag	UNP Q47506
D	353	HIS	-	expression tag	UNP Q47506
D	354	HIS	-	expression tag	UNP Q47506
D	355	HIS	-	expression tag	UNP Q47506
D	356	HIS	-	expression tag	UNP Q47506
D	357	HIS	-	expression tag	UNP Q47506
D	358	HIS	-	expression tag	UNP Q47506

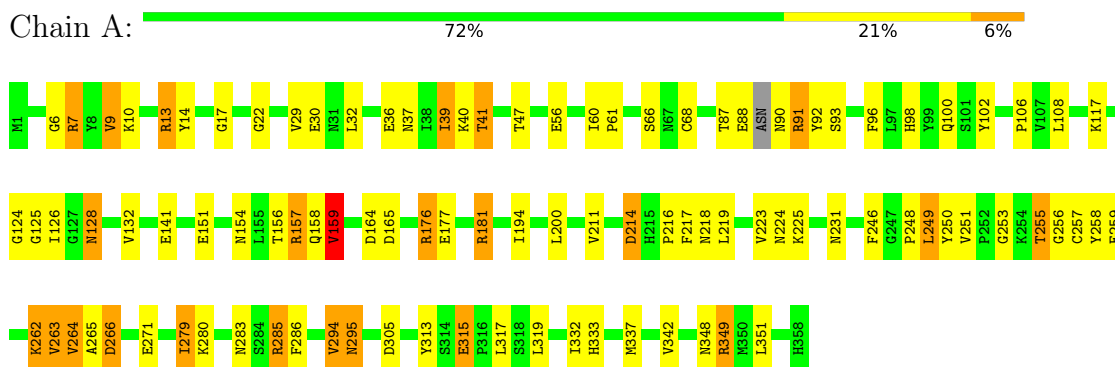
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0

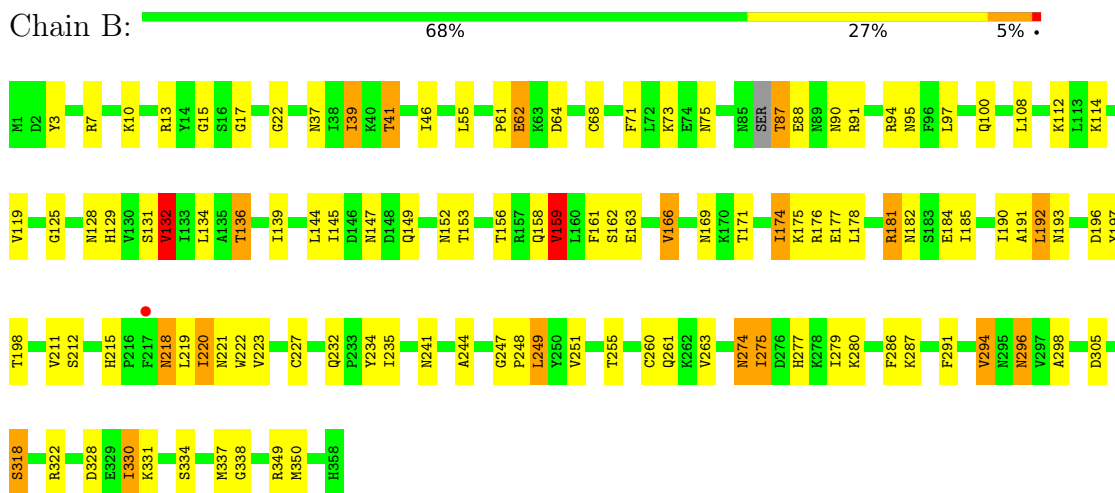
3 Residue-property plots

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.

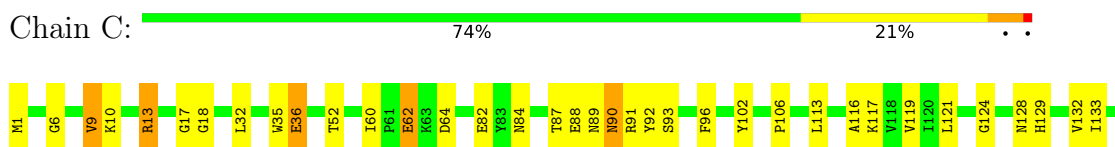
• Molecule 1: MccB protein

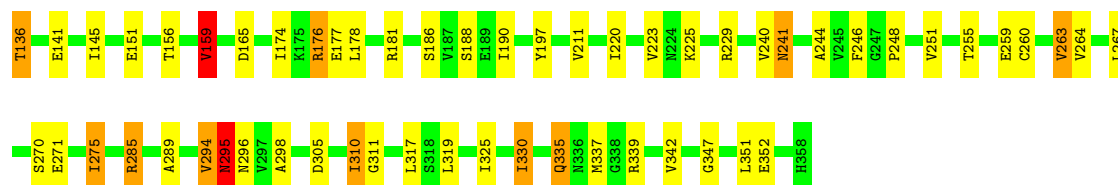


• Molecule 1: MccB protein



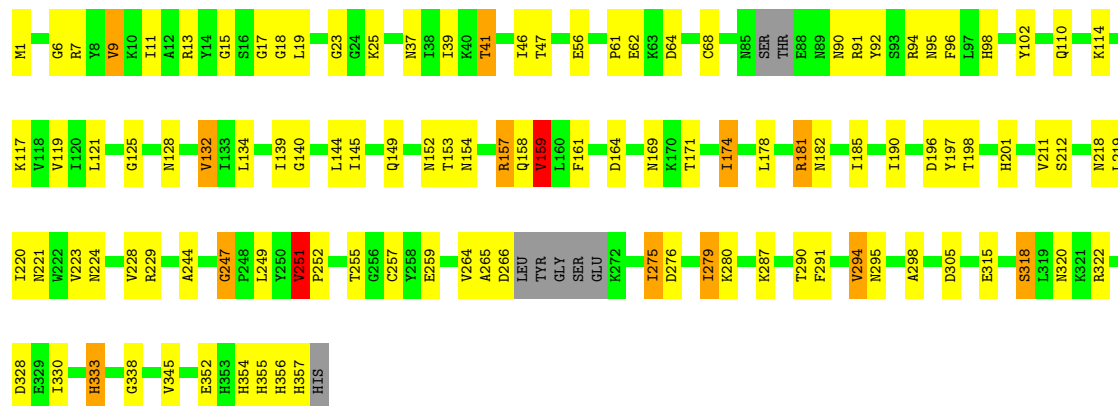
• Molecule 1: MccB protein





• Molecule 1: MccB protein

Chain D: 67% 27% ...



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	144.65Å 145.03Å 158.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.80 49.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.69-2.80) 98.2 (49.69-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.255 0.222 , 0.253	Depositor DCC
R_{free} test set	4120 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.460 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11064	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.78	0/2831	0.99	3/3845 (0.1%)
1	B	0.74	0/2828	1.00	5/3839 (0.1%)
1	C	0.78	0/2848	0.98	1/3868 (0.0%)
1	D	0.77	0/2795	1.00	8/3791 (0.2%)
All	All	0.77	0/11302	0.99	17/15343 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	VAL	CA-C-N	6.92	128.50	119.84
1	D	251	VAL	C-N-CA	6.92	128.50	119.84
1	B	132	VAL	CB-CA-C	-6.29	103.92	111.97
1	B	159	VAL	N-CA-C	6.10	122.03	109.34
1	D	132	VAL	CB-CA-C	-5.55	104.86	111.97
1	D	159	VAL	N-CA-C	5.40	120.57	109.34
1	D	18	GLY	N-CA-C	5.37	118.59	110.75
1	A	315	GLU	CA-C-N	-5.36	114.24	119.76
1	A	315	GLU	C-N-CA	-5.36	114.24	119.76
1	C	159	VAL	N-CA-C	5.24	120.24	109.34
1	D	247	GLY	N-CA-C	-5.16	101.81	112.34
1	B	241	ASN	CA-C-N	5.14	127.68	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	ASN	C-N-CA	5.14	127.68	120.28
1	D	356	HIS	CA-C-N	5.05	130.79	121.70
1	D	356	HIS	C-N-CA	5.05	130.79	121.70
1	A	262	LYS	N-CA-C	5.05	117.97	109.95
1	B	90	ASN	N-CA-C	5.01	116.89	108.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	253	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2770	0	2694	74	0
1	B	2768	0	2685	73	0
1	C	2786	0	2714	63	0
1	D	2736	0	2679	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	11064	0	10772	253	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 12.

All (253) 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:248:PRO:HD3	1:C:337:MET:HE1	1.13	1.13
1:C:156:THR:HG21	1:D:95:ASN:HD21	1.19	1.04
1:C:248:PRO:CD	1:C:337:MET:HE1	1.88	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:HG3	1:A:337:MET:HE1	1.39	1.01
1:D:305:ASP:OD2	1:D:318:SER:HB2	1.73	0.89
1:A:248:PRO:CG	1:A:337:MET:HE1	2.05	0.87
1:A:157:ARG:HD3	1:B:94:ARG:HH11	1.39	0.86
1:C:263:VAL:HG11	1:C:335:GLN:HG2	1.58	0.84
1:B:149:GLN:NE2	1:B:169:ASN:OD1	2.12	0.82
1:B:128:ASN:ND2	1:B:158:GLN:HB3	1.94	0.82
1:A:156:THR:HG21	1:B:95:ASN:OD1	1.81	0.81
1:B:128:ASN:HD22	1:B:158:GLN:HB3	1.45	0.81
1:C:113:LEU:HA	1:C:310:ILE:HD11	1.63	0.80
1:B:349:ARG:H	1:B:350:MET:HB2	1.49	0.78
1:A:181:ARG:NH1	1:B:159:VAL:O	2.17	0.78
1:D:244:ALA:HB1	1:D:298:ALA:HB2	1.65	0.78
1:C:263:VAL:CG1	1:C:335:GLN:HG2	2.15	0.77
1:D:218:ASN:HB2	1:D:221:ASN:HD22	1.51	0.75
1:D:37:ASN:O	1:D:41:THR:HG23	1.87	0.73
1:C:248:PRO:HD3	1:C:337:MET:CE	2.07	0.73
1:A:90:ASN:O	1:A:91:ARG:HB3	1.89	0.72
1:C:90:ASN:O	1:C:92:TYR:N	2.21	0.72
1:D:224:ASN:HD21	1:D:257:CYS:HB2	1.55	0.71
1:D:218:ASN:HB2	1:D:221:ASN:ND2	2.06	0.71
1:D:61:PRO:HG2	1:D:64:ASP:OD2	1.92	0.69
1:D:13:ARG:HD3	1:D:17:GLY:O	1.93	0.69
1:D:90:ASN:ND2	1:D:92:TYR:H	1.91	0.69
1:A:102:TYR:OH	1:B:328:ASP:HB3	1.93	0.68
1:D:320:ASN:HD22	1:D:338:GLY:HA2	1.57	0.68
1:D:247:GLY:HA2	1:D:322:ARG:HG3	1.75	0.68
1:A:248:PRO:HG3	1:A:337:MET:CE	2.22	0.68
1:A:87:THR:HG22	1:A:88:GLU:H	1.59	0.68
1:A:17:GLY:HA3	1:A:29:VAL:O	1.94	0.67
1:A:279:ILE:HD12	1:A:283:ASN:ND2	2.09	0.67
1:C:156:THR:HG21	1:D:95:ASN:ND2	2.01	0.66
1:A:251:VAL:H	1:A:255:THR:HG21	1.61	0.65
1:A:255:THR:HG23	1:A:256:GLY:O	1.95	0.65
1:B:244:ALA:HB1	1:B:298:ALA:HB2	1.75	0.65
1:B:349:ARG:N	1:B:350:MET:HB2	2.10	0.65
1:C:102:TYR:OH	1:D:328:ASP:HB3	1.96	0.64
1:C:330:ILE:HG13	1:C:330:ILE:O	1.97	0.64
1:A:96:PHE:O	1:A:100:GLN:HG3	1.97	0.64
1:A:36:GLU:HG2	1:B:275:ILE:HD13	1.79	0.63
1:A:194:ILE:HD13	1:A:200:LEU:CD2	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:O	1:B:166:VAL:HG12	1.98	0.63
1:D:251:VAL:HG13	1:D:255:THR:HG23	1.81	0.63
1:D:333:HIS:C	1:D:333:HIS:CD2	2.77	0.63
1:C:248:PRO:CG	1:C:337:MET:HE1	2.29	0.62
1:A:211:VAL:HG21	1:A:223:VAL:HG11	1.81	0.62
1:A:248:PRO:HB3	1:A:337:MET:HE2	1.81	0.62
1:C:211:VAL:HG21	1:C:223:VAL:HG11	1.81	0.62
1:D:196:ASP:HB2	1:D:198:THR:HG22	1.82	0.62
1:A:7:ARG:HG3	1:A:7:ARG:HH11	1.64	0.62
1:B:13:ARG:HD3	1:B:17:GLY:O	2.00	0.61
1:D:144:LEU:HD22	1:D:174:ILE:HD11	1.80	0.61
1:A:214:ASP:OD1	1:A:214:ASP:N	2.32	0.61
1:C:36:GLU:HG3	1:D:275:ILE:HD13	1.80	0.61
1:C:342:VAL:HG12	1:C:342:VAL:O	2.01	0.60
1:D:149:GLN:NE2	1:D:169:ASN:OD1	2.26	0.60
1:C:248:PRO:HB3	1:C:337:MET:HE3	1.83	0.60
1:D:128:ASN:HD22	1:D:128:ASN:C	2.09	0.60
1:A:224:ASN:HD21	1:A:257:CYS:HB2	1.68	0.59
1:A:248:PRO:CG	1:A:337:MET:CE	2.80	0.59
1:A:251:VAL:H	1:A:255:THR:CG2	2.15	0.59
1:D:90:ASN:HD22	1:D:92:TYR:H	1.48	0.59
1:B:182:ASN:OD1	1:B:184:GLU:HB2	2.02	0.59
1:D:228:VAL:HG21	1:D:345:VAL:HG12	1.85	0.58
1:C:13:ARG:NH2	1:C:32:LEU:HD13	2.18	0.58
1:B:218:ASN:HB2	1:B:221:ASN:ND2	2.18	0.58
1:D:219:LEU:O	1:D:223:VAL:HG23	2.04	0.58
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.17	0.57
1:A:96:PHE:CD2	1:A:106:PRO:HB2	2.38	0.57
1:B:61:PRO:HG2	1:B:64:ASP:OD2	2.04	0.57
1:C:116:ALA:CB	1:C:310:ILE:HD13	2.34	0.57
1:C:241:ASN:ND2	1:C:289:ALA:H	2.02	0.57
1:A:250:TYR:HA	1:A:255:THR:HG21	1.86	0.57
1:A:10:LYS:HG3	1:B:286:PHE:CD1	2.40	0.57
1:C:92:TYR:O	1:C:96:PHE:CD1	2.58	0.57
1:B:174:ILE:O	1:B:178:LEU:HG	2.05	0.56
1:D:159:VAL:HG13	1:D:159:VAL:O	2.04	0.56
1:D:279:ILE:HG13	1:D:280:LYS:N	2.19	0.56
1:C:244:ALA:HB1	1:C:298:ALA:HB2	1.87	0.56
1:D:255:THR:O	1:D:320:ASN:ND2	2.39	0.56
1:D:37:ASN:O	1:D:41:THR:CG2	2.53	0.56
1:A:194:ILE:HD13	1:A:200:LEU:HD23	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TYR:O	1:A:96:PHE:CD1	2.59	0.55
1:D:211:VAL:HG21	1:D:223:VAL:HG11	1.88	0.55
1:B:132:VAL:O	1:B:136:THR:HB	2.06	0.55
1:B:261:GLN:NE2	1:B:338:GLY:O	2.39	0.54
1:A:271:GLU:HG3	1:D:201:HIS:HB2	1.89	0.54
1:B:3:TYR:OH	1:B:73:LYS:HE3	2.07	0.54
1:A:125:GLY:H	1:A:157:ARG:HH21	1.55	0.54
1:A:224:ASN:ND2	1:A:258:TYR:H	2.04	0.54
1:C:156:THR:CG2	1:D:95:ASN:HD21	2.07	0.54
1:B:37:ASN:O	1:B:41:THR:HG22	2.08	0.54
1:A:264:VAL:HG12	1:A:266:ASP:H	1.71	0.53
1:C:248:PRO:HB3	1:C:337:MET:CE	2.38	0.53
1:D:23:GLY:C	1:D:25:LYS:H	2.16	0.53
1:A:249:LEU:HD12	1:A:249:LEU:C	2.34	0.53
1:C:96:PHE:CD2	1:C:106:PRO:HB2	2.43	0.53
1:D:174:ILE:O	1:D:178:LEU:HG	2.08	0.53
1:C:225:LYS:O	1:C:229:ARG:HG2	2.09	0.53
1:B:87:THR:HA	1:B:88:GLU:C	2.32	0.52
1:B:144:LEU:HD22	1:B:174:ILE:HD11	1.92	0.52
1:C:124:GLY:O	1:C:128:ASN:HB2	2.09	0.52
1:A:248:PRO:CD	1:A:337:MET:HE1	2.40	0.52
1:A:279:ILE:CD1	1:A:283:ASN:ND2	2.73	0.52
1:A:6:GLY:O	1:A:9:VAL:HG13	2.10	0.52
1:A:248:PRO:HB3	1:A:337:MET:CE	2.40	0.52
1:B:248:PRO:HD3	1:B:337:MET:HE2	1.90	0.52
1:A:7:ARG:CG	1:A:7:ARG:NH1	2.72	0.51
1:A:159:VAL:O	1:A:159:VAL:HG13	2.11	0.51
1:B:125:GLY:O	1:B:128:ASN:HB3	2.10	0.51
1:B:331:LYS:NZ	1:D:355:HIS:CE1	2.79	0.51
1:D:159:VAL:O	1:D:159:VAL:CG1	2.58	0.51
1:B:71:PHE:O	1:B:75:ASN:ND2	2.37	0.51
1:C:263:VAL:HG12	1:C:264:VAL:N	2.25	0.51
1:D:119:VAL:HG13	1:D:145:ILE:HD12	1.92	0.51
1:B:13:ARG:NH1	1:B:15:GLY:O	2.44	0.51
1:C:132:VAL:O	1:C:136:THR:HB	2.11	0.51
1:A:124:GLY:O	1:A:128:ASN:HB2	2.10	0.51
1:B:211:VAL:HG21	1:B:223:VAL:HG11	1.92	0.51
1:B:218:ASN:HB2	1:B:221:ASN:HD22	1.76	0.51
1:A:98:HIS:HE1	1:A:313:TYR:OH	1.94	0.51
1:B:41:THR:HG21	1:B:68:CYS:CB	2.41	0.51
1:D:251:VAL:HG13	1:D:255:THR:CG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HD3	1:B:46:ILE:HG23	1.93	0.50
1:B:91:ARG:NH2	1:B:181:ARG:O	2.43	0.50
1:B:331:LYS:NZ	1:D:355:HIS:HE1	2.09	0.50
1:A:41:THR:HG21	1:A:68:CYS:CB	2.42	0.50
1:D:13:ARG:NH1	1:D:15:GLY:O	2.44	0.50
1:A:246:PHE:HE2	1:A:305:ASP:OD2	1.95	0.49
1:B:219:LEU:O	1:B:223:VAL:HG23	2.12	0.49
1:A:41:THR:HG21	1:A:68:CYS:HB2	1.93	0.49
1:C:82:GLU:C	1:C:84:ASN:H	2.20	0.49
1:C:6:GLY:O	1:C:9:VAL:HG13	2.12	0.49
1:A:349:ARG:HH22	1:D:266:ASP:C	2.21	0.49
1:A:177:GLU:OE1	1:A:181:ARG:NH2	2.46	0.49
1:A:342:VAL:HG11	1:A:351:LEU:HG	1.95	0.49
1:D:333:HIS:C	1:D:333:HIS:HD2	2.21	0.48
1:B:196:ASP:HA	1:B:222:TRP:CZ3	2.48	0.48
1:A:96:PHE:CE2	1:A:106:PRO:HB2	2.48	0.48
1:C:88:GLU:C	1:C:90:ASN:H	2.21	0.48
1:C:241:ASN:HB2	1:D:23:GLY:HA3	1.94	0.48
1:C:246:PHE:HE2	1:C:305:ASP:OD2	1.95	0.48
1:C:116:ALA:HB2	1:C:310:ILE:HD13	1.94	0.48
1:B:161:PHE:HE2	1:B:174:ILE:HG22	1.79	0.48
1:D:196:ASP:O	1:D:197:TYR:C	2.56	0.48
1:B:196:ASP:HA	1:B:222:TRP:CH2	2.49	0.48
1:C:176:ARG:NH1	1:C:177:GLU:OE2	2.44	0.48
1:B:37:ASN:O	1:B:41:THR:CG2	2.61	0.48
1:C:113:LEU:HD23	1:C:310:ILE:HD11	1.95	0.48
1:C:342:VAL:O	1:C:342:VAL:CG1	2.61	0.48
1:B:279:ILE:HG13	1:B:280:LYS:N	2.29	0.48
1:D:182:ASN:ND2	1:D:185:ILE:HG23	2.29	0.48
1:C:92:TYR:O	1:C:96:PHE:HD1	1.96	0.47
1:C:133:ILE:O	1:C:136:THR:HG22	2.14	0.47
1:B:305:ASP:OD2	1:B:318:SER:HB2	2.14	0.47
1:D:125:GLY:O	1:D:128:ASN:HB3	2.13	0.47
1:A:159:VAL:O	1:B:181:ARG:NH1	2.47	0.47
1:A:194:ILE:CD1	1:A:200:LEU:HD23	2.45	0.47
1:C:6:GLY:O	1:C:9:VAL:CG1	2.63	0.47
1:A:165:ASP:OD1	1:A:176:ARG:NH2	2.48	0.47
1:C:285:ARG:HD3	1:D:46:ILE:HG23	1.96	0.47
1:D:154:ASN:O	1:D:158:GLN:HG3	2.15	0.47
1:A:96:PHE:CD2	1:A:106:PRO:CB	2.98	0.47
1:A:92:TYR:O	1:A:96:PHE:HD1	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HB3	1:B:139:ILE:HG13	1.96	0.47
1:B:192:LEU:HD22	1:B:193:ASN:O	2.14	0.47
1:B:196:ASP:O	1:B:197:TYR:C	2.58	0.47
1:C:87:THR:HB	1:C:90:ASN:HB2	1.96	0.47
1:B:296:ASN:N	1:B:296:ASN:HD22	2.13	0.47
1:D:161:PHE:HE2	1:D:174:ILE:HG22	1.80	0.46
1:D:134:LEU:HB3	1:D:139:ILE:HG13	1.97	0.46
1:C:251:VAL:HB	1:C:255:THR:HG23	1.98	0.46
1:B:234:TYR:CD2	1:B:234:TYR:C	2.94	0.46
1:D:333:HIS:HD2	1:D:333:HIS:O	1.98	0.46
1:A:332:ILE:CG2	1:B:330:ILE:HD11	2.46	0.46
1:B:182:ASN:ND2	1:B:185:ILE:HG23	2.31	0.46
1:D:294:VAL:HG12	1:D:295:ASN:N	2.31	0.46
1:C:159:VAL:O	1:D:181:ARG:NH1	2.49	0.46
1:C:310:ILE:HG13	1:C:311:GLY:N	2.31	0.46
1:C:330:ILE:O	1:C:330:ILE:CG1	2.64	0.46
1:A:60:ILE:HB	1:A:61:PRO:HD2	1.98	0.46
1:B:87:THR:HA	1:B:88:GLU:O	2.15	0.45
1:B:235:ILE:HD12	1:B:249:LEU:HB2	1.99	0.45
1:C:145:ILE:HG12	1:C:190:ILE:HB	1.98	0.45
1:A:39:ILE:HG13	1:A:40:LYS:N	2.31	0.45
1:D:291:PHE:O	1:D:294:VAL:HB	2.16	0.45
1:B:41:THR:HG21	1:B:68:CYS:HB2	1.98	0.45
1:B:55:LEU:HD21	1:B:62:GLU:HG2	1.99	0.45
1:C:13:ARG:NH1	1:C:17:GLY:O	2.50	0.45
1:C:117:LYS:HE2	1:C:141:GLU:OE2	2.16	0.45
1:C:119:VAL:HG13	1:C:145:ILE:HD12	1.99	0.45
1:D:6:GLY:O	1:D:9:VAL:HG13	2.17	0.45
1:D:98:HIS:CE1	1:D:102:TYR:CE1	3.05	0.45
1:C:294:VAL:HG12	1:C:295:ASN:N	2.32	0.45
1:A:37:ASN:O	1:A:41:THR:CG2	2.65	0.44
1:D:11:ILE:HD13	1:D:39:ILE:HG12	1.99	0.44
1:D:275:ILE:HG13	1:D:276:ASP:N	2.31	0.44
1:B:119:VAL:HG13	1:B:145:ILE:HD12	2.00	0.44
1:C:129:HIS:HE1	1:C:296:ASN:OD1	2.00	0.44
1:D:41:THR:HG21	1:D:68:CYS:HB2	1.99	0.44
1:A:265:ALA:O	1:A:266:ASP:CB	2.65	0.44
1:A:286:PHE:CD1	1:B:10:LYS:HG3	2.53	0.44
1:B:128:ASN:O	1:B:131:SER:OG	2.34	0.43
1:C:270:SER:HB2	1:C:275:ILE:HD11	1.99	0.43
1:B:39:ILE:HD12	1:B:39:ILE:HG21	1.68	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASN:OD1	1:B:191:ALA:HB1	2.19	0.43
1:B:87:THR:CA	1:B:88:GLU:C	2.91	0.43
1:D:354:HIS:H	1:D:354:HIS:CD2	2.36	0.43
1:A:125:GLY:HA2	1:A:158:GLN:HG2	2.01	0.43
1:C:197:TYR:CD2	1:C:197:TYR:C	2.97	0.43
1:C:342:VAL:HG21	1:C:351:LEU:HG	2.01	0.43
1:D:264:VAL:O	1:D:265:ALA:HB3	2.18	0.43
1:A:13:ARG:NH1	1:A:32:LEU:CD1	2.82	0.43
1:A:333:HIS:CD2	1:D:352:GLU:HG2	2.54	0.43
1:B:220:ILE:H	1:B:220:ILE:HG13	1.38	0.43
1:B:291:PHE:O	1:B:294:VAL:HB	2.19	0.42
1:D:145:ILE:HG12	1:D:190:ILE:HB	2.00	0.42
1:A:176:ARG:NH1	1:A:177:GLU:OE2	2.52	0.42
1:A:294:VAL:HG12	1:A:295:ASN:N	2.34	0.42
1:A:348:ASN:C	1:A:349:ARG:HG2	2.44	0.42
1:A:263:VAL:O	1:A:265:ALA:N	2.40	0.42
1:C:18:GLY:HA3	1:C:35:TRP:CE2	2.54	0.42
1:C:129:HIS:CE1	1:C:296:ASN:OD1	2.73	0.42
1:B:227:CYS:HB3	1:B:232:GLN:O	2.20	0.42
1:A:248:PRO:HD3	1:A:337:MET:HE1	2.01	0.42
1:C:174:ILE:O	1:C:178:LEU:HG	2.20	0.42
1:C:294:VAL:O	1:C:295:ASN:C	2.62	0.42
1:A:262:LYS:O	1:A:263:VAL:HG23	2.20	0.41
1:B:108:LEU:O	1:B:112:LYS:HG3	2.20	0.41
1:B:251:VAL:HB	1:B:255:THR:HG23	2.02	0.41
1:B:274:ASN:HD22	1:B:274:ASN:H	1.66	0.41
1:A:216:PRO:C	1:A:218:ASN:N	2.78	0.41
1:B:129:HIS:HE1	1:B:296:ASN:OD1	2.04	0.41
1:B:247:GLY:O	1:B:322:ARG:HG3	2.20	0.41
1:D:114:LYS:O	1:D:140:GLY:HA3	2.20	0.41
1:A:117:LYS:HE2	1:A:141:GLU:OE2	2.21	0.41
1:A:151:GLU:H	1:A:154:ASN:ND2	2.19	0.41
1:D:96:PHE:HE1	1:D:110:GLN:HG2	1.86	0.41
1:B:97:LEU:HA	1:B:100:GLN:HE21	1.85	0.41
1:B:176:ARG:NH1	1:B:177:GLU:OE2	2.49	0.41
1:C:165:ASP:CG	1:C:176:ARG:HH22	2.29	0.41
1:A:265:ALA:HB2	1:D:229:ARG:HH22	1.85	0.41
1:B:334:SER:O	1:D:357:HIS:N	2.54	0.41
1:C:159:VAL:O	1:C:159:VAL:HG13	2.21	0.41
1:D:157:ARG:H	1:D:157:ARG:HG2	1.63	0.41
1:B:7:ARG:HE	1:B:7:ARG:HB3	1.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:O	1:C:241:ASN:C	2.64	0.41
1:B:190:ILE:HG22	1:B:192:LEU:HB2	2.03	0.40
1:D:7:ARG:HE	1:D:7:ARG:HB3	1.72	0.40
1:C:60:ILE:HD12	1:C:64:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/358 (99%)	325 (92%)	22 (6%)	6 (2%)	7	25
1	B	353/358 (99%)	316 (90%)	34 (10%)	3 (1%)	16	44
1	C	356/358 (99%)	324 (91%)	24 (7%)	8 (2%)	5	19
1	D	344/358 (96%)	310 (90%)	32 (9%)	2 (1%)	21	51
All	All	1406/1432 (98%)	1275 (91%)	112 (8%)	19 (1%)	9	30

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ASP
1	B	159	VAL
1	C	90	ASN
1	C	347	GLY
1	D	159	VAL
1	A	22	GLY
1	C	159	VAL
1	A	91	ARG
1	A	217	PHE
1	B	260	CYS
1	C	62	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	91	ARG
1	A	159	VAL
1	C	89	ASN
1	D	252	PRO
1	C	241	ASN
1	C	295	ASN
1	B	22	GLY
1	A	264	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	295/310 (95%)	258 (88%)	37 (12%)	4	15
1	B	295/310 (95%)	262 (89%)	33 (11%)	6	19
1	C	298/310 (96%)	264 (89%)	34 (11%)	5	19
1	D	294/310 (95%)	260 (88%)	34 (12%)	5	18
All	All	1182/1240 (95%)	1044 (88%)	138 (12%)	5	18

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	9	VAL
1	A	13	ARG
1	A	14	TYR
1	A	30	GLU
1	A	39	ILE
1	A	41	THR
1	A	47	THR
1	A	56	GLU
1	A	66	SER
1	A	93	SER
1	A	108	LEU
1	A	126	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	128	ASN
1	A	132	VAL
1	A	157	ARG
1	A	159	VAL
1	A	164	ASP
1	A	176	ARG
1	A	181	ARG
1	A	214	ASP
1	A	219	LEU
1	A	225	LYS
1	A	231	ASN
1	A	249	LEU
1	A	255	THR
1	A	259	GLU
1	A	263	VAL
1	A	279	ILE
1	A	280	LYS
1	A	285	ARG
1	A	294	VAL
1	A	295	ASN
1	A	315	GLU
1	A	317	LEU
1	A	319	LEU
1	A	349	ARG
1	B	39	ILE
1	B	41	THR
1	B	62	GLU
1	B	87	THR
1	B	114	LYS
1	B	132	VAL
1	B	136	THR
1	B	152	ASN
1	B	153	THR
1	B	156	THR
1	B	159	VAL
1	B	162	SER
1	B	166	VAL
1	B	171	THR
1	B	174	ILE
1	B	175	LYS
1	B	181	ARG
1	B	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	198	THR
1	B	212	SER
1	B	215	HIS
1	B	218	ASN
1	B	220	ILE
1	B	249	LEU
1	B	263	VAL
1	B	274	ASN
1	B	275	ILE
1	B	277	HIS
1	B	287	LYS
1	B	294	VAL
1	B	296	ASN
1	B	318	SER
1	B	330	ILE
1	C	1	MET
1	C	9	VAL
1	C	10	LYS
1	C	13	ARG
1	C	36	GLU
1	C	52	THR
1	C	62	GLU
1	C	93	SER
1	C	121	LEU
1	C	136	THR
1	C	151	GLU
1	C	159	VAL
1	C	176	ARG
1	C	181	ARG
1	C	186	SER
1	C	188	SER
1	C	220	ILE
1	C	259	GLU
1	C	260	CYS
1	C	263	VAL
1	C	267	LEU
1	C	271	GLU
1	C	275	ILE
1	C	285	ARG
1	C	294	VAL
1	C	295	ASN
1	C	310	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	317	LEU
1	C	319	LEU
1	C	325	ILE
1	C	330	ILE
1	C	335	GLN
1	C	339	ARG
1	C	352	GLU
1	D	1	MET
1	D	9	VAL
1	D	19	LEU
1	D	41	THR
1	D	47	THR
1	D	56	GLU
1	D	62	GLU
1	D	91	ARG
1	D	94	ARG
1	D	117	LYS
1	D	121	LEU
1	D	132	VAL
1	D	152	ASN
1	D	153	THR
1	D	157	ARG
1	D	159	VAL
1	D	164	ASP
1	D	171	THR
1	D	174	ILE
1	D	181	ARG
1	D	212	SER
1	D	220	ILE
1	D	249	LEU
1	D	251	VAL
1	D	259	GLU
1	D	275	ILE
1	D	279	ILE
1	D	287	LYS
1	D	290	THR
1	D	294	VAL
1	D	315	GLU
1	D	318	SER
1	D	330	ILE
1	D	333	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	98	HIS
1	A	128	ASN
1	A	158	GLN
1	A	221	ASN
1	A	224	ASN
1	A	232	GLN
1	A	274	ASN
1	A	336	ASN
1	B	84	ASN
1	B	85	ASN
1	B	98	HIS
1	B	100	GLN
1	B	115	ASN
1	B	129	HIS
1	B	218	ASN
1	B	221	ASN
1	B	224	ASN
1	B	231	ASN
1	B	236	ASN
1	B	274	ASN
1	B	354	HIS
1	B	355	HIS
1	C	31	ASN
1	C	85	ASN
1	C	128	ASN
1	C	129	HIS
1	C	149	GLN
1	C	152	ASN
1	C	158	GLN
1	C	169	ASN
1	C	221	ASN
1	C	236	ASN
1	C	241	ASN
1	C	274	ASN
1	C	295	ASN
1	C	336	ASN
1	C	356	HIS
1	C	357	HIS
1	D	27	GLN
1	D	84	ASN
1	D	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	95	ASN
1	D	98	HIS
1	D	128	ASN
1	D	221	ASN
1	D	224	ASN
1	D	274	ASN
1	D	320	ASN
1	D	333	HIS
1	D	354	HIS
1	D	355	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	357/358 (99%)	-1.29	0 100 100	33, 49, 76, 85	0
1	B	357/358 (99%)	-1.19	1 (0%) 90 86	34, 53, 82, 97	0
1	C	358/358 (100%)	-1.27	0 100 100	33, 50, 76, 85	0
1	D	350/358 (97%)	-1.24	0 100 100	34, 54, 73, 87	0
All	All	1422/1432 (99%)	-1.25	1 (0%) 92 90	33, 52, 77, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	PHE	2.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	360	1/1	1.00	0.02	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	360	1/1	1.00	0.02	81,81,81,81	0
2	ZN	C	360	1/1	1.00	0.01	68,68,68,68	0
2	ZN	D	360	1/1	1.00	0.02	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.