



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:45 am BST

PDB ID : 3H5A
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

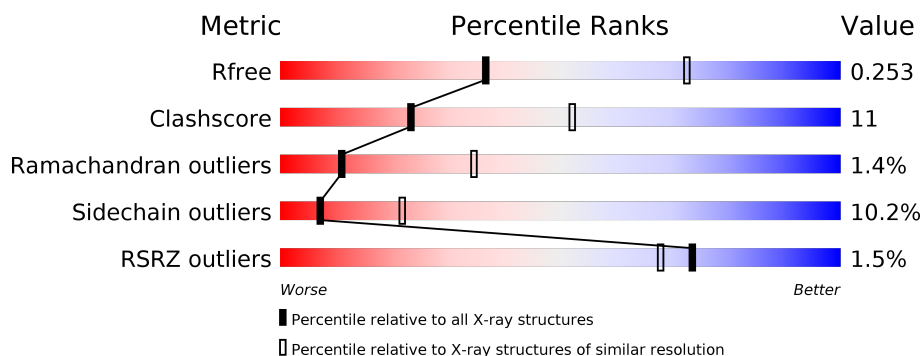
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>5%</div> </div> </div>
1	B	358	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>5%</div> </div> </div>
1	C	358	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>.</div> </div> </div>
1	D	358	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>.</div> </div> </div>

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

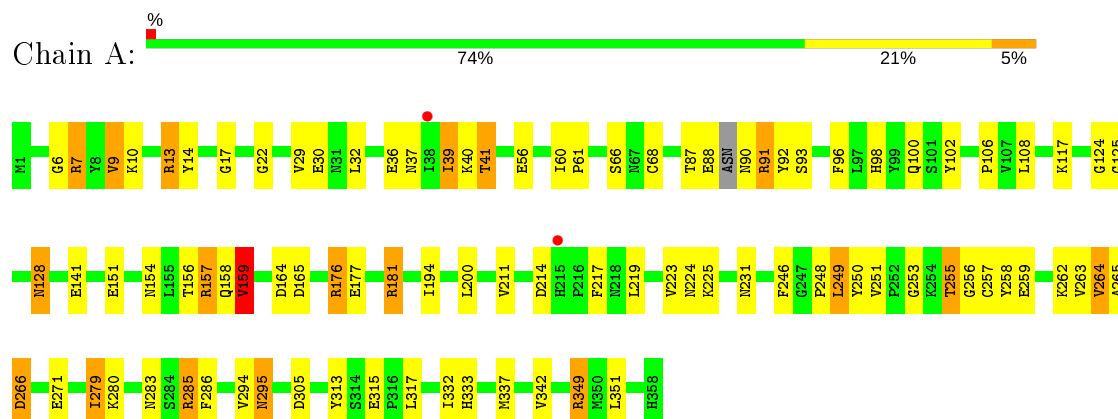
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

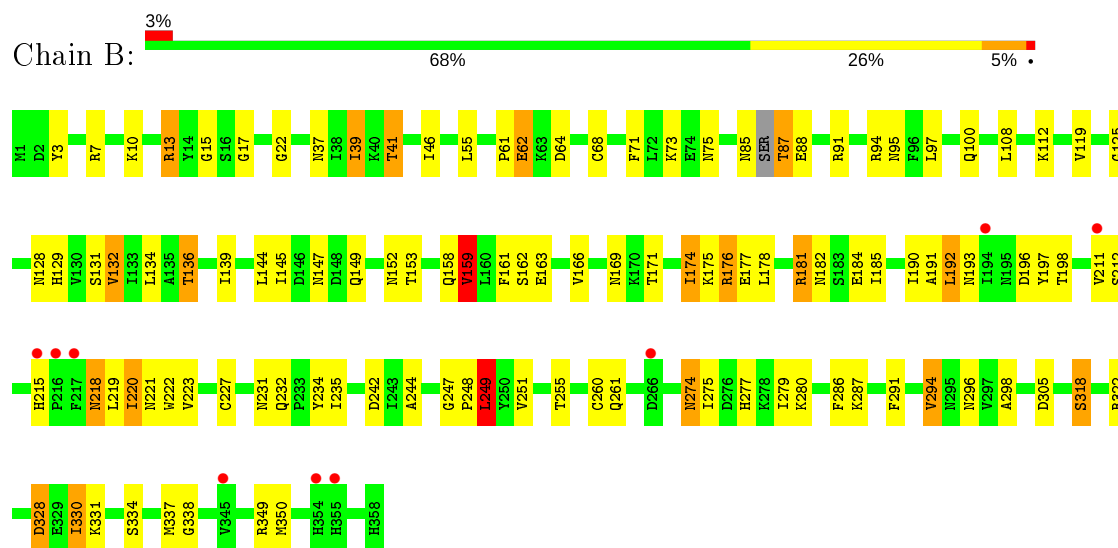
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

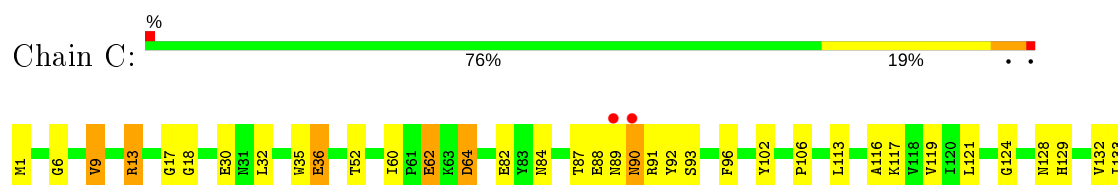
• Molecule 1: MccB protein

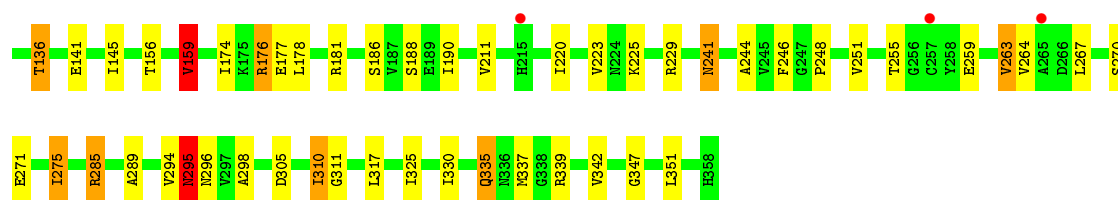


• Molecule 1: MccB protein

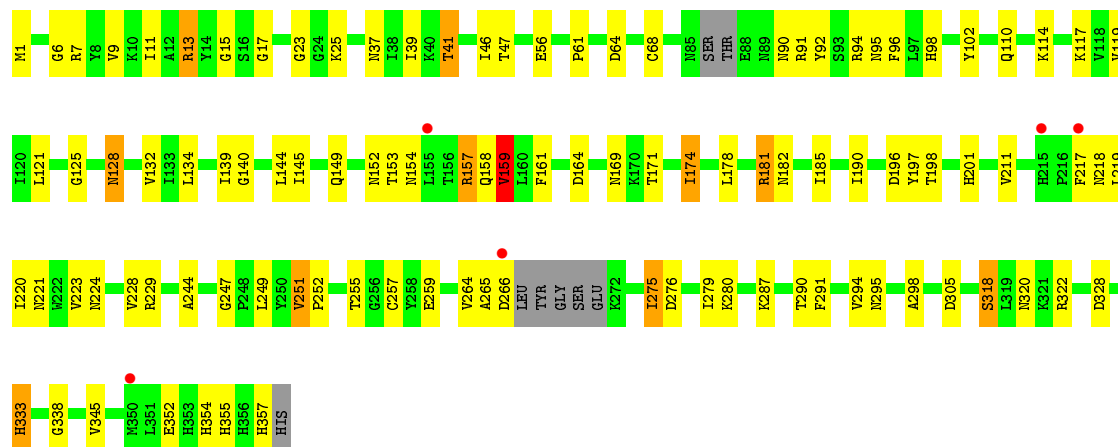


• Molecule 1: MccB protein





• Molecule 1: MccB protein



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) 98.0 (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 , 16.1	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	0.94	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 [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/2831	0.71	0/3845
1	B	0.60	0/2828	0.71	1/3839 (0.0%)
1	C	0.61	0/2848	0.68	0/3868
1	D	0.62	0/2795	0.72	0/3791
All	All	0.61	0/11302	0.71	1/15343 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	249	LEU	CA-CB-CG	5.19	127.24	115.30

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	71	0
1	B	2768	0	2685	73	0
1	C	2786	0	2714	60	0
1	D	2736	0	2679	69	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	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (247) 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	1.17	1.14
1:C:156:THR:HG21	1:D:95:ASN:HD21	1.19	1.04
1:A:248:PRO:HG3	1:A:337:MET:HE1	1.39	1.04
1:C:248:PRO:CD	1:C:337:MET:HE1	2.02	0.89
1:D:305:ASP:OD2	1:D:318:SER:HB2	1.73	0.89
1:A:157:ARG:HD3	1:B:94:ARG:HH11	1.39	0.86
1:A:248:PRO:CG	1:A:337:MET:HE1	2.08	0.84
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:C:248:PRO:HD3	1:C:337:MET:CE	2.07	0.81
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ASN:O	1:D:41:THR:HG23	1.87	0.73
1:A:90:ASN:O	1:A:91:ARG:HB3	1.89	0.73
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:C:248:PRO:HB3	1:C:337:MET:HE3	1.74	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:A:248:PRO:HB3	1:A:337:MET:HE2	1.79	0.64
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:194:ILE:HD13	1:A:200:LEU:CD2	2.29	0.63
1:A:36:GLU:HG2	1:B:275:ILE:HD13	1.79	0.63
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:A:211:VAL:HG21	1:A:223:VAL:HG11	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:HH11	1:A:7:ARG:HG3	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:N	1:A:214:ASP:OD1	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:333:HIS:C	1:D:333:HIS:CD2	2.77	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:96:PHE:CD2	1:A:106:PRO:HB2	2.38	0.57
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.17	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:D:279:ILE:HG13	1:D:280:LYS:N	2.19	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:O	1:D:159:VAL:HG13	2.04	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:D:128:ASN:C	1:D:128:ASN:HD22	2.09	0.55
1:A:194:ILE:HD13	1:A:200:LEU:HD23	1.87	0.55
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:B:3:TYR:OH	1:B:73:LYS:HE3	2.07	0.54
1:A:271:GLU:HG3	1:D:201:HIS:HB2	1.89	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:CD1	1:A:283:ASN:ND2	2.73	0.52
1:A:248:PRO:HB3	1:A:337:MET:CE	2.40	0.52
1:A:6:GLY:O	1:A:9:VAL:HG13	2.10	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:C:263:VAL:HG12	1:C:264:VAL:N	2.25	0.51
1:D:159:VAL:CG1	1:D:159:VAL:O	2.58	0.51
1:B:71:PHE:O	1:B:75:ASN:ND2	2.37	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:218:ASN:HB2	1:B:221:ASN:HD22	1.76	0.51
1:B:211:VAL:HG21	1:B:223:VAL:HG11	1.92	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
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:6:GLY:O	1:C:9:VAL:HG13	2.12	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:23:GLY:C	1:D:25:LYS:H	2.16	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:A:249:LEU:C	1:A:249:LEU:HD12	2.34	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:HA	1:B:88:GLU:C	2.32	0.48
1:C:113:LEU:HD23	1:C:310:ILE:HD11	1.95	0.48
1:C:342:VAL:CG1	1:C:342:VAL:O	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:133:ILE:O	1:C:136:THR:HG22	2.14	0.47
1:C:92:TYR:O	1:C:96:PHE:HD1	1.96	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:C:248:PRO:CB	1:C:337:MET:HE3	2.44	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
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:C:87:THR:HB	1:C:90:ASN:HB2	1.96	0.47
1:A:248:PRO:CD	1:A:337:MET:HE1	2.45	0.47
1:B:296:ASN:HD22	1:B:296:ASN:N	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:D:333:HIS:O	1:D:333:HIS:HD2	1.98	0.46
1:B:182:ASN:ND2	1:B:185:ILE:HG23	2.31	0.46
1:A:332:ILE:CG2	1:B:330:ILE:HD11	2.46	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:CG1	1:C:330:ILE:O	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:55:LEU:HD21	1:B:62:GLU:HG2	1.99	0.45
1:B:41:THR:HG21	1:B:68:CYS:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:82:GLU:C	1:C:84:ASN:H	2.20	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:A:349:ARG:HH22	1:D:266:ASP:C	2.21	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:B:331:LYS:HZ1	1:D:355:HIS:HE1	1.63	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:C:248:PRO:CD	1:C:337:MET:CE	2.82	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:D:196:ASP:O	1:D:197:TYR:C	2.56	0.43
1:B:147:ASN:OD1	1:B:191:ALA:HB1	2.19	0.43
1:B:39:ILE:HD12	1:B:39:ILE:HG21	1.68	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:342:VAL:HG21	1:C:351:LEU:HG	2.01	0.43
1:C:88:GLU:C	1:C:90:ASN:H	2.21	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:263:VAL:O	1:A:265:ALA:N	2.40	0.42
1:C:129:HIS:CE1	1:C:296:ASN:OD1	2.73	0.42
1:C:18:GLY:HA3	1:C:35:TRP:CE2	2.54	0.42
1:B:196:ASP:O	1:B:197:TYR:C	2.58	0.42
1:B:227:CYS:HB3	1:B:232:GLN:O	2.20	0.42
1:C:174:ILE:O	1:C:178:LEU:HG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:234:TYR:C	1:B:234:TYR:CD2	2.94	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: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:B:334:SER:O	1:D:357:HIS:N	2.54	0.41
1:A:265:ALA:HB2	1:D:229:ARG:HH22	1.85	0.41
1:D:333:HIS:C	1:D:333:HIS:HD2	2.21	0.41
1:C:159:VAL:HG13	1:C:159:VAL:O	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
1:B:190:ILE:HG22	1:B:192:LEU:HB2	2.03	0.40
1:D:7:ARG:HB3	1:D:7:ARG:HE	1.72	0.40
1:C:60:ILE:HD12	1:C:64:ASP:HB2	2.04	0.40
1:B:248:PRO:HG3	1:B:337:MET:HE3	2.03	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%)	9	29
1	B	353/358 (99%)	316 (90%)	34 (10%)	3 (1%)	19	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	356/358 (99%)	324 (91%)	24 (7%)	8 (2%)	6	22
1	D	344/358 (96%)	310 (90%)	32 (9%)	2 (1%)	25	56
All	All	1406/1432 (98%)	1275 (91%)	112 (8%)	19 (1%)	11	34

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
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%)	265 (90%)	30 (10%)	7	22
1	B	295/310 (95%)	262 (89%)	33 (11%)	6	18
1	C	298/310 (96%)	269 (90%)	29 (10%)	8	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	294/310 (95%)	265 (90%)	29 (10%)	8	23
All	All	1182/1240 (95%)	1061 (90%)	121 (10%)	7	22

All (121) 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	56	GLU
1	A	66	SER
1	A	93	SER
1	A	108	LEU
1	A	128	ASN
1	A	157	ARG
1	A	159	VAL
1	A	164	ASP
1	A	176	ARG
1	A	181	ARG
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	279	ILE
1	A	280	LYS
1	A	285	ARG
1	A	295	ASN
1	A	315	GLU
1	A	317	LEU
1	A	349	ARG
1	B	13	ARG
1	B	39	ILE
1	B	41	THR
1	B	62	GLU
1	B	85	ASN
1	B	87	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	VAL
1	B	136	THR
1	B	152	ASN
1	B	153	THR
1	B	159	VAL
1	B	162	SER
1	B	171	THR
1	B	174	ILE
1	B	175	LYS
1	B	176	ARG
1	B	181	ARG
1	B	192	LEU
1	B	198	THR
1	B	212	SER
1	B	215	HIS
1	B	218	ASN
1	B	220	ILE
1	B	231	ASN
1	B	242	ASP
1	B	249	LEU
1	B	274	ASN
1	B	277	HIS
1	B	287	LYS
1	B	294	VAL
1	B	318	SER
1	B	328	ASP
1	B	330	ILE
1	C	1	MET
1	C	9	VAL
1	C	13	ARG
1	C	30	GLU
1	C	36	GLU
1	C	52	THR
1	C	62	GLU
1	C	64	ASP
1	C	93	SER
1	C	121	LEU
1	C	136	THR
1	C	159	VAL
1	C	176	ARG
1	C	181	ARG
1	C	186	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	188	SER
1	C	220	ILE
1	C	259	GLU
1	C	263	VAL
1	C	267	LEU
1	C	271	GLU
1	C	275	ILE
1	C	285	ARG
1	C	295	ASN
1	C	310	ILE
1	C	317	LEU
1	C	325	ILE
1	C	335	GLN
1	C	339	ARG
1	D	1	MET
1	D	13	ARG
1	D	41	THR
1	D	47	THR
1	D	56	GLU
1	D	91	ARG
1	D	94	ARG
1	D	117	LYS
1	D	121	LEU
1	D	128	ASN
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	217	PHE
1	D	220	ILE
1	D	249	LEU
1	D	251	VAL
1	D	259	GLU
1	D	275	ILE
1	D	287	LYS
1	D	290	THR
1	D	318	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	333	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	85	ASN
1	A	98	HIS
1	A	100	GLN
1	A	221	ASN
1	A	224	ASN
1	B	84	ASN
1	B	98	HIS
1	B	100	GLN
1	B	129	HIS
1	B	221	ASN
1	B	224	ASN
1	B	231	ASN
1	B	274	ASN
1	B	354	HIS
1	B	355	HIS
1	C	128	ASN
1	C	129	HIS
1	C	152	ASN
1	C	158	GLN
1	C	221	ASN
1	C	236	ASN
1	C	241	ASN
1	C	295	ASN
1	D	27	GLN
1	D	84	ASN
1	D	90	ASN
1	D	95	ASN
1	D	110	GLN
1	D	128	ASN
1	D	147	ASN
1	D	221	ASN
1	D	224	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 carbohydrates 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	357/358 (99%)	0.45	2 (0%) 89 86	33, 49, 76, 85	0
1	B	357/358 (99%)	0.50	9 (2%) 57 47	34, 53, 82, 97	0
1	C	358/358 (100%)	0.51	5 (1%) 75 70	33, 50, 76, 85	0
1	D	350/358 (97%)	0.51	5 (1%) 75 70	34, 54, 73, 87	0
All	All	1422/1432 (99%)	0.49	21 (1%) 73 68	33, 52, 77, 97	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	PHE	4.3
1	A	215	HIS	3.3
1	D	155	LEU	3.2
1	D	215	HIS	3.1
1	C	265	ALA	3.0
1	B	215	HIS	2.8
1	D	217	PHE	2.7
1	D	350	MET	2.4
1	B	345	VAL	2.4
1	B	194	ILE	2.3
1	B	355	HIS	2.3
1	B	216	PRO	2.3
1	C	257	CYS	2.3
1	B	354	HIS	2.2
1	C	90	ASN	2.2
1	A	38	ILE	2.2
1	B	266	ASP	2.2
1	C	215	HIS	2.1
1	B	211	VAL	2.1
1	D	266	ASP	2.1
1	C	89	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
2	ZN	D	360	1/1	0.88	0.17	76,76,76,76	0
2	ZN	B	360	1/1	0.93	0.14	81,81,81,81	0
2	ZN	C	360	1/1	0.97	0.16	68,68,68,68	0
2	ZN	A	360	1/1	0.98	0.15	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.