



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:53 pm BST

PDB ID : 2XTQ  
Title : Structure of the P107A Colicin M mutant from E. coli  
Authors : Helbig, S.; Patzer, S.I.; Braun, V.; Zeth, K.  
Deposited on : 2010-10-12  
Resolution : 2.31 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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

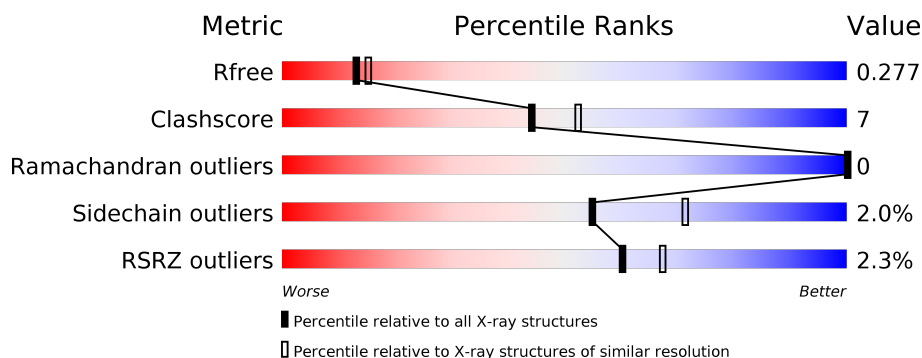
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	271	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	B	271	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	271	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	D	271	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	E	271	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	F	271	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	271	<div><div>%</div><div><div></div><div>86%</div><div>14%</div></div></div>
1	H	271	<div><div>4%</div><div><div></div><div>87%</div><div>11%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17024 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 COLICIN-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	3	0	0
			2067	1317	352	390	8			
1	B	270	Total	C	N	O	S	1	2	0
			2078	1325	354	391	8			
1	C	270	Total	C	N	O	S	1	1	0
			2075	1322	355	390	8			
1	D	270	Total	C	N	O	S	4	1	0
			2073	1322	353	390	8			
1	E	270	Total	C	N	O	S	2	2	0
			2079	1325	355	391	8			
1	F	270	Total	C	N	O	S	1	0	0
			2067	1317	352	390	8			
1	G	270	Total	C	N	O	S	1	0	0
			2067	1317	352	390	8			
1	H	270	Total	C	N	O	S	4	0	0
			2067	1317	352	390	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	PRO	engineered mutation	UNP P05820
B	107	ALA	PRO	engineered mutation	UNP P05820
C	107	ALA	PRO	engineered mutation	UNP P05820
D	107	ALA	PRO	engineered mutation	UNP P05820
E	107	ALA	PRO	engineered mutation	UNP P05820
F	107	ALA	PRO	engineered mutation	UNP P05820
G	107	ALA	PRO	engineered mutation	UNP P05820
H	107	ALA	PRO	engineered mutation	UNP P05820

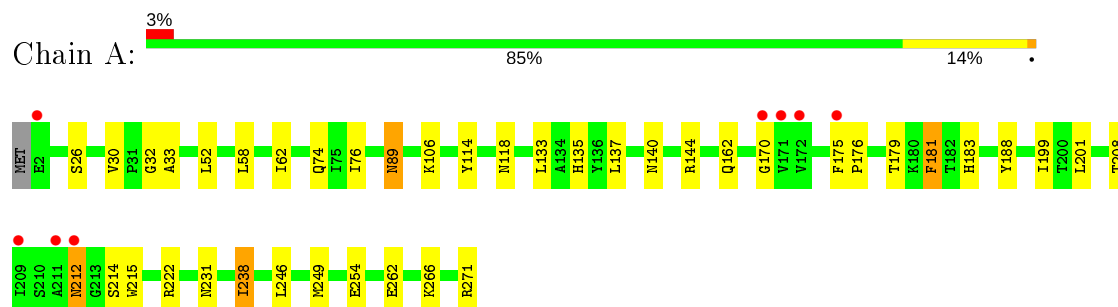
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	67	Total	O	0	0
			67	67		
2	B	59	Total	O	0	0
			59	59		
2	C	61	Total	O	0	0
			61	61		
2	D	60	Total	O	0	0
			60	60		
2	E	50	Total	O	0	0
			50	50		
2	F	52	Total	O	0	0
			52	52		
2	G	49	Total	O	0	0
			49	49		
2	H	53	Total	O	0	0
			53	53		

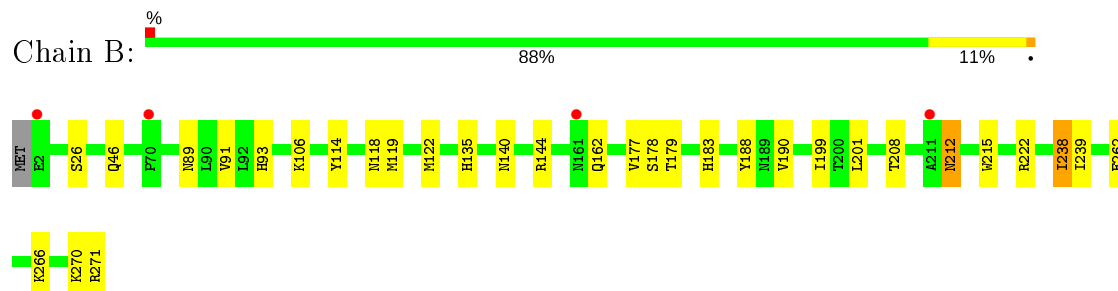
### 3 Residue-property plots [i](#)

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.

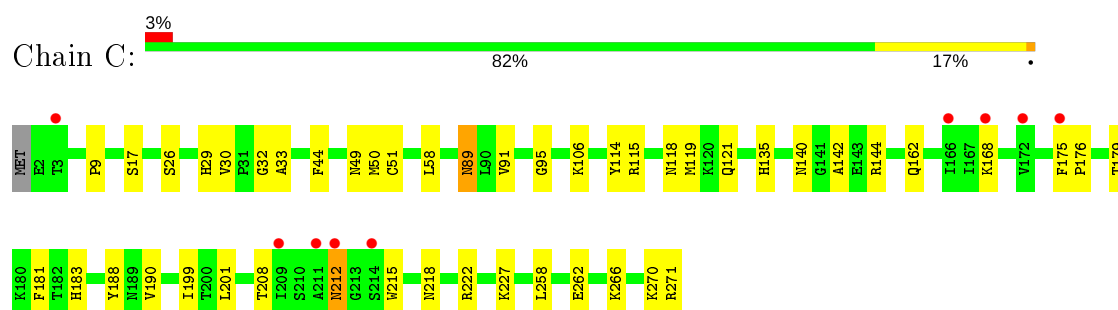
#### • Molecule 1: COLICIN-M



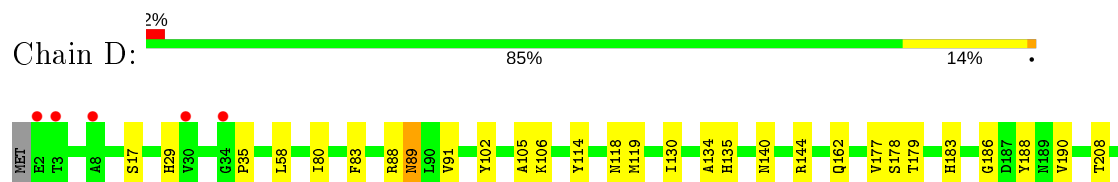
#### • Molecule 1: COLICIN-M



#### • Molecule 1: COLICIN-M

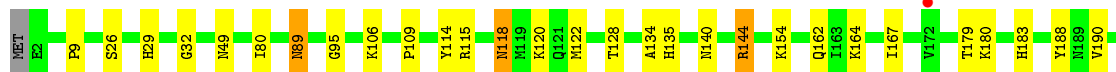
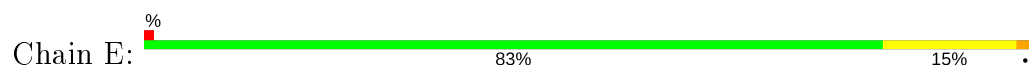


#### • Molecule 1: COLICIN-M

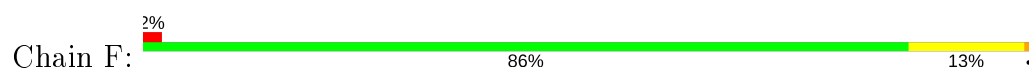




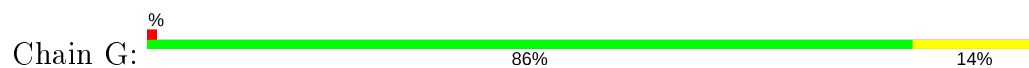
- Molecule 1: COLICIN-M



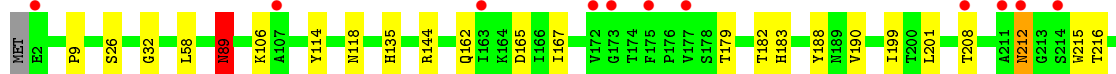
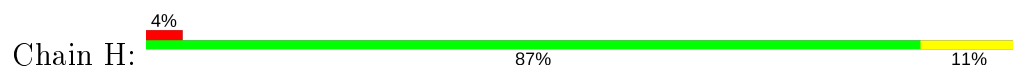
- Molecule 1: COLICIN-M



- Molecule 1: COLICIN-M



- Molecule 1: COLICIN-M



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.85Å 63.11Å 189.34Å 87.59° 82.17° 65.65°	Depositor
Resolution (Å)	48.68 – 2.31 48.68 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.68-2.31) 91.2 (48.68-2.31)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.240 , 0.273 0.242 , 0.277	Depositor DCC
$R_{free}$ test set	4514 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 11.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.419 for h,h-k,h-l 0.167 for -h,-h+k,-l 0.167 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	17024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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	1.63	3/2117 (0.1%)	0.88	4/2879 (0.1%)
1	B	0.97	7/2134 (0.3%)	0.83	2/2901 (0.1%)
1	C	1.25	2/2127 (0.1%)	1.03	2/2890 (0.1%)
1	D	1.85	5/2126 (0.2%)	1.20	6/2890 (0.2%)
1	E	1.24	3/2136 (0.1%)	0.93	7/2905 (0.2%)
1	F	0.94	2/2117 (0.1%)	0.84	2/2879 (0.1%)
1	G	0.81	1/2117 (0.0%)	0.74	2/2879 (0.1%)
1	H	1.02	4/2117 (0.2%)	0.77	3/2879 (0.1%)
All	All	1.26	27/16991 (0.2%)	0.91	28/23102 (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
1	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
All	All	0	5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	ASN	CG-ND2	72.25	3.13	1.32
1	A	266	LYS	CG-CD	62.30	3.64	1.52
1	C	89	ASN	CG-OD1	43.80	2.20	1.24
1	E	89	ASN	CG-OD1	35.46	2.02	1.24
1	H	266	LYS	CG-CD	26.88	2.43	1.52
1	D	140	ASN	CB-CG	23.12	2.04	1.51
1	F	266	LYS	CD-CE	22.11	2.06	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	140[A]	ASN	CG-OD1	-18.55	0.83	1.24
1	E	140[B]	ASN	CG-OD1	-18.55	0.83	1.24
1	B	266	LYS	CD-CE	14.62	1.87	1.51
1	A	89	ASN	CG-OD1	14.52	1.55	1.24
1	G	89	ASN	CG-OD1	-12.44	0.96	1.24
1	B	140[A]	ASN	CG-OD1	-11.46	0.98	1.24
1	B	140[B]	ASN	CG-OD1	-11.46	0.98	1.24
1	D	140	ASN	CG-OD1	-11.03	0.99	1.24
1	A	238	ILE	CG1-CD1	10.14	2.20	1.50
1	H	165	ASP	CG-OD2	9.68	1.47	1.25
1	H	165	ASP	CG-OD1	8.42	1.44	1.25
1	D	266	LYS	CD-CE	8.03	1.71	1.51
1	B	140[A]	ASN	CG-ND2	7.76	1.52	1.32
1	B	140[B]	ASN	CG-ND2	7.76	1.52	1.32
1	F	102	TYR	CD1-CE1	7.13	1.50	1.39
1	B	140[A]	ASN	CB-CG	6.50	1.66	1.51
1	B	140[B]	ASN	CB-CG	6.50	1.66	1.51
1	H	89	ASN	CG-OD1	-6.27	1.10	1.24
1	D	102	TYR	CD1-CE1	5.40	1.47	1.39
1	C	51	CYS	CB-SG	-5.16	1.73	1.81

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	ASN	OD1-CG-ND2	-41.60	26.21	121.90
1	C	89	ASN	OD1-CG-ND2	-37.72	35.13	121.90
1	D	140	ASN	OD1-CG-ND2	-23.32	68.26	121.90
1	E	89	ASN	CB-CG-OD1	-21.57	78.45	121.60
1	F	266	LYS	CD-CE-NZ	-21.14	63.07	111.70
1	A	266	LYS	CG-CD-CE	-20.56	50.22	111.90
1	B	266	LYS	CD-CE-NZ	-20.52	64.50	111.70
1	C	89	ASN	CB-CG-OD1	-17.17	87.26	121.60
1	D	140	ASN	CB-CG-ND2	13.97	150.24	116.70
1	A	89	ASN	OD1-CG-ND2	-12.28	93.65	121.90
1	E	89	ASN	OD1-CG-ND2	12.02	149.54	121.90
1	E	140[A]	ASN	CB-CG-OD1	11.37	144.35	121.60
1	E	140[B]	ASN	CB-CG-OD1	11.37	144.35	121.60
1	F	266	LYS	CG-CD-CE	10.49	143.37	111.90
1	A	266	LYS	CB-CG-CD	-10.19	85.10	111.60
1	E	140[A]	ASN	OD1-CG-ND2	-10.05	98.79	121.90
1	E	140[B]	ASN	OD1-CG-ND2	-10.05	98.79	121.90
1	H	165	ASP	CB-CG-OD1	9.92	127.23	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	ASN	CB-CG-OD1	9.82	141.25	121.60
1	H	266	LYS	CG-CD-CE	-8.83	85.40	111.90
1	G	89	ASN	CB-CG-OD1	8.53	138.65	121.60
1	G	89	ASN	OD1-CG-ND2	-8.18	103.08	121.90
1	D	140	ASN	CA-CB-CG	-8.06	95.67	113.40
1	B	266	LYS	CG-CD-CE	7.46	134.27	111.90
1	H	216	THR	OG1-CB-CG2	-5.89	96.46	110.00
1	D	266	LYS	CD-CE-NZ	5.69	124.78	111.70
1	A	238	ILE	CG1-CB-CG2	5.51	123.52	111.40
1	E	144	ARG	NE-CZ-NH1	-5.20	117.70	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ASN	Sidechain
1	C	89	ASN	Sidechain
1	D	89	ASN	Sidechain
1	E	89	ASN	Sidechain
1	H	89	ASN	Sidechain

## 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	2067	0	2049	29	4
1	B	2078	0	2068	25	0
1	C	2075	0	2062	36	2
1	D	2073	0	2062	28	0
1	E	2079	0	2062	34	1
1	F	2067	0	2049	27	2
1	G	2067	0	2049	24	1
1	H	2067	0	2049	20	1
2	A	67	0	0	6	0
2	B	59	0	0	7	0
2	C	61	0	0	11	0
2	D	60	0	0	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	50	0	0	11	1
2	F	52	0	0	9	0
2	G	49	0	0	3	0
2	H	53	0	0	2	0
All	All	17024	0	16450	219	8

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 7.

All (219) 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:B:89:ASN:ND2	2:B:2015:HOH:O	1.74	1.16
1:A:137:LEU:HG	2:A:2031:HOH:O	1.49	1.09
1:E:250:PHE:CD2	2:E:2046:HOH:O	2.24	0.91
1:E:198:ASN:O	2:E:2040:HOH:O	1.88	0.90
1:C:140:ASN:HB3	2:C:2032:HOH:O	1.71	0.90
1:E:250:PHE:HD2	2:E:2046:HOH:O	1.56	0.87
1:C:118:ASN:HD22	1:C:144:ARG:HH12	1.24	0.84
1:G:118:ASN:HD22	1:G:144:ARG:HH12	1.25	0.83
1:E:118:ASN:HD22	1:E:144:ARG:HH12	1.23	0.82
1:F:234:THR:HB	2:F:2037:HOH:O	1.80	0.82
1:A:118:ASN:HD22	1:A:144:ARG:HH12	1.27	0.79
1:F:212:ASN:OD1	2:F:2040:HOH:O	2.01	0.79
1:C:114:TYR:OH	1:C:135:HIS:HD2	1.66	0.79
1:H:118:ASN:HD22	1:H:144:ARG:HH12	1.27	0.79
1:A:140:ASN:HB3	2:A:2032:HOH:O	1.85	0.77
1:B:190:VAL:HG22	1:B:239:ILE:HD12	1.68	0.76
1:D:118:ASN:HD22	1:D:144:ARG:HH12	1.34	0.76
1:C:115:ARG:CD	2:C:2024:HOH:O	2.34	0.76
1:C:115:ARG:HD3	2:C:2024:HOH:O	1.84	0.75
1:C:142:ALA:HB2	2:C:2030:HOH:O	1.85	0.75
1:E:95:GLY:O	2:E:2014:HOH:O	2.05	0.75
1:G:118:ASN:ND2	1:G:144:ARG:HH12	1.84	0.75
1:F:135:HIS:HE1	2:F:2021:HOH:O	1.69	0.74
1:F:118:ASN:HD22	1:F:144:ARG:HH12	1.34	0.74
1:E:167:ILE:O	1:E:271:ARG:NH2	2.22	0.72
1:C:212:ASN:OD1	1:C:212:ASN:N	2.21	0.72
1:A:114:TYR:OH	1:A:135:HIS:HD2	1.73	0.71
1:A:212:ASN:OD1	1:A:212:ASN:N	2.22	0.71
1:B:118:ASN:HD22	1:B:144:ARG:HH12	1.39	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ASN:OD1	1:D:212:ASN:N	2.24	0.70
1:B:212:ASN:O	1:B:270:LYS:NZ	2.24	0.70
1:C:121:GLN:HB3	2:C:2027:HOH:O	1.90	0.70
1:F:122:MET:HG2	2:F:2021:HOH:O	1.90	0.69
1:F:166:ILE:HG13	2:F:2031:HOH:O	1.92	0.69
1:H:212:ASN:OD1	1:H:212:ASN:N	2.25	0.69
1:B:212:ASN:N	1:B:212:ASN:OD1	2.25	0.69
1:D:218:ASN:OD1	1:D:266:LYS:HG2	1.92	0.69
1:B:135:HIS:HE1	2:B:2026:HOH:O	1.74	0.68
1:H:182:THR:HG23	2:H:2041:HOH:O	1.93	0.67
1:F:118:ASN:ND2	1:F:144:ARG:HH12	1.93	0.66
1:E:212:ASN:N	1:E:212:ASN:OD1	2.28	0.66
1:E:118:ASN:ND2	1:E:144:ARG:HH12	1.93	0.65
1:F:212:ASN:N	1:F:212:ASN:OD1	2.29	0.64
1:A:170:GLY:HA2	1:A:271:ARG:CZ	2.27	0.64
1:H:114:TYR:OH	1:H:135:HIS:HD2	1.81	0.64
1:H:167:ILE:O	1:H:271:ARG:NH2	2.24	0.63
1:A:133:LEU:HG	2:A:2031:HOH:O	1.97	0.63
1:C:17:SER:HB3	1:D:17:SER:HB3	1.79	0.63
1:E:199:ILE:HD12	1:E:201:LEU:HD21	1.80	0.63
1:D:114:TYR:OH	1:D:135:HIS:HD2	1.82	0.63
1:G:212:ASN:N	1:G:212:ASN:OD1	2.30	0.63
1:A:170:GLY:HA2	1:A:271:ARG:NH2	2.15	0.62
1:B:271:ARG:HG3	2:B:2039:HOH:O	1.99	0.62
1:E:162:GLN:NE2	1:E:179:THR:HB	2.15	0.62
1:A:137:LEU:CG	2:A:2031:HOH:O	2.24	0.61
1:H:199:ILE:HD12	1:H:201:LEU:HD21	1.82	0.61
1:B:122:MET:HG2	2:B:2026:HOH:O	2.00	0.61
1:H:162:GLN:NE2	1:H:179:THR:HB	2.16	0.61
1:E:114:TYR:OH	1:E:135:HIS:HD2	1.84	0.61
1:E:114:TYR:O	1:E:118:ASN:HB3	2.01	0.60
1:B:212:ASN:HB2	1:B:270:LYS:HZ3	1.68	0.59
1:G:190:VAL:HG22	1:G:239:ILE:HD12	1.84	0.59
1:C:115:ARG:HD2	2:C:2024:HOH:O	2.01	0.58
1:E:250:PHE:CE2	2:E:2046:HOH:O	2.54	0.58
1:D:190:VAL:HG22	1:D:239:ILE:HD12	1.86	0.57
1:D:35:PRO:HA	2:D:2014:HOH:O	2.03	0.57
1:C:162:GLN:NE2	1:C:179:THR:HB	2.20	0.57
1:H:118:ASN:ND2	1:H:144:ARG:HH12	2.01	0.57
1:A:162:GLN:NE2	1:A:179:THR:HB	2.20	0.57
1:D:135:HIS:HE1	2:D:2030:HOH:O	1.87	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLY:CA	1:A:271:ARG:NH2	2.69	0.56
1:D:88:ARG:HD3	2:D:2022:HOH:O	2.05	0.56
1:D:105:ALA:HB3	2:D:2027:HOH:O	2.06	0.56
1:D:118:ASN:ND2	1:D:144:ARG:HH12	2.03	0.55
1:B:238:ILE:HG12	2:B:2053:HOH:O	2.07	0.55
1:C:95:GLY:HA3	2:C:2019:HOH:O	2.07	0.55
1:F:190:VAL:HG22	1:F:239:ILE:HD12	1.88	0.55
1:B:114:TYR:OH	1:B:135:HIS:HD2	1.90	0.55
1:A:118:ASN:ND2	1:A:144:ARG:HH12	2.01	0.55
1:A:183:HIS:HE1	1:A:188:TYR:OH	1.91	0.54
1:C:118:ASN:ND2	1:C:144:ARG:HH12	2.02	0.54
1:H:9:PRO:HA	2:H:2004:HOH:O	2.08	0.53
1:E:115:ARG:NE	2:E:2020:HOH:O	2.36	0.53
1:A:222:ARG:HG2	1:A:262:GLU:HB3	1.91	0.52
1:E:222:ARG:HG2	1:E:262:GLU:HB3	1.91	0.52
1:E:109:PRO:HG3	2:E:2017:HOH:O	2.10	0.52
1:G:208:THR:O	1:G:215:TRP:HA	2.08	0.52
1:C:114:TYR:OH	1:C:135:HIS:CD2	2.56	0.51
1:E:162:GLN:HE21	1:E:179:THR:HB	1.75	0.51
1:B:118:ASN:ND2	1:B:144:ARG:HH12	2.06	0.51
1:F:114:TYR:O	1:F:118:ASN:HB3	2.11	0.51
1:E:120:LYS:HE3	1:F:116:SER:O	2.10	0.51
1:H:190:VAL:HG21	1:H:238:ILE:HG13	1.93	0.51
1:B:212:ASN:HB2	1:B:270:LYS:NZ	2.25	0.51
1:C:199:ILE:HD12	1:C:201:LEU:HD21	1.92	0.51
1:C:183:HIS:HE1	1:C:188:TYR:OH	1.94	0.50
1:H:162:GLN:HE21	1:H:179:THR:HB	1.76	0.50
1:G:110:SER:HB2	2:G:2019:HOH:O	2.11	0.50
1:C:208:THR:O	1:C:215:TRP:HA	2.12	0.50
1:C:222:ARG:HG2	1:C:262:GLU:HB3	1.94	0.50
1:E:208:THR:O	1:E:215:TRP:HA	2.11	0.50
1:D:222:ARG:HG2	1:D:262:GLU:HB3	1.93	0.50
1:E:218:ASN:OD1	1:E:266:LYS:HE2	2.12	0.49
1:B:208:THR:O	1:B:215:TRP:HA	2.12	0.49
1:G:114:TYR:OH	1:G:135:HIS:HD2	1.95	0.49
1:E:183:HIS:HE1	1:E:188:TYR:OH	1.95	0.49
1:B:89:ASN:CG	2:B:2015:HOH:O	2.30	0.49
1:D:186:GLY:N	2:D:2043:HOH:O	2.36	0.49
1:B:162:GLN:NE2	1:B:179:THR:HB	2.28	0.49
1:G:83:PHE:CE1	1:G:130:ILE:HD12	2.47	0.49
1:F:231:ASN:HB3	1:F:254:GLU:HG2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLY:CA	2:C:2019:HOH:O	2.61	0.49
1:F:83:PHE:CE1	1:F:130:ILE:HD12	2.48	0.49
1:H:222:ARG:HG2	1:H:262:GLU:HB3	1.94	0.49
1:B:93:HIS:CD2	2:B:2015:HOH:O	2.67	0.48
1:E:246:LEU:HB3	2:E:2046:HOH:O	2.14	0.48
1:G:218:ASN:OD1	1:G:266:LYS:HE2	2.13	0.48
1:H:183:HIS:HE1	1:H:188:TYR:OH	1.95	0.48
1:A:208:THR:O	1:A:215:TRP:HA	2.12	0.48
1:F:162:GLN:NE2	1:F:179:THR:HB	2.29	0.48
1:H:208:THR:O	1:H:215:TRP:HA	2.13	0.48
1:F:88:ARG:HD3	2:F:2015:HOH:O	2.14	0.48
1:D:91:VAL:HG11	1:D:119:MET:CE	2.44	0.47
1:D:208:THR:O	1:D:215:TRP:HA	2.14	0.47
1:F:271:ARG:NH2	2:F:2052:HOH:O	2.26	0.47
1:G:162:GLN:NE2	1:G:179:THR:HB	2.30	0.47
1:E:180:LYS:NZ	2:E:2034:HOH:O	2.48	0.47
1:F:271:ARG:NH1	2:F:2052:HOH:O	2.44	0.47
1:B:199:ILE:HD12	1:B:201:LEU:HD21	1.97	0.46
1:C:162:GLN:HE21	1:C:179:THR:HB	1.80	0.46
1:A:199:ILE:HD12	1:A:201:LEU:HD21	1.96	0.46
1:E:154:LYS:HE2	2:E:2029:HOH:O	2.15	0.46
1:E:231:ASN:HB3	1:E:254:GLU:HG2	1.96	0.46
1:D:183:HIS:HE1	1:D:188:TYR:OH	1.98	0.46
1:D:218:ASN:OD1	1:D:266:LYS:HE2	2.15	0.46
1:H:114:TYR:O	1:H:118:ASN:HB3	2.16	0.46
1:G:154:LYS:HE3	2:G:2028:HOH:O	2.16	0.46
1:A:133:LEU:CD1	2:A:2031:HOH:O	2.64	0.45
1:C:181:PHE:N	1:C:181:PHE:CD2	2.84	0.45
1:C:49:ASN:H	1:C:49:ASN:HD22	1.64	0.45
1:D:83:PHE:CE1	1:D:130:ILE:HD12	2.50	0.45
1:F:183:HIS:HE1	1:F:188:TYR:OH	1.98	0.45
1:B:91:VAL:HG11	1:B:119:MET:CE	2.46	0.45
1:A:114:TYR:OH	1:A:135:HIS:CD2	2.62	0.45
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.78	0.45
1:C:218:ASN:OD1	1:C:266:LYS:HE2	2.17	0.45
1:G:199:ILE:HD12	1:G:201:LEU:HD21	1.98	0.45
1:B:46:GLN:HG3	1:E:212:ASN:HA	1.99	0.45
1:G:183:HIS:HE1	1:G:188:TYR:OH	2.00	0.45
1:B:114:TYR:O	1:B:118:ASN:HB3	2.16	0.44
1:F:120:LYS:HE3	2:F:2020:HOH:O	2.18	0.44
1:G:222:ARG:HG2	1:G:262:GLU:HB3	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:SER:OG	1:G:100:ASP:OD2	2.32	0.44
1:F:208:THR:O	1:F:215:TRP:HA	2.17	0.44
1:A:162:GLN:HE21	1:A:179:THR:HB	1.81	0.44
1:G:181:PHE:CD2	1:G:181:PHE:N	2.86	0.43
1:G:162:GLN:HE21	1:G:179:THR:CG2	2.31	0.43
1:E:122:MET:HB3	1:E:128:THR:HG23	2.00	0.43
1:E:190:VAL:HG21	1:E:238:ILE:HG13	1.99	0.43
1:H:227:LYS:HB3	1:H:258:LEU:HD23	2.01	0.43
1:A:175:PHE:HA	1:A:176:PRO:HD3	1.90	0.43
1:F:227:LYS:HB3	1:F:258:LEU:HD23	2.01	0.43
1:H:231:ASN:HB3	1:H:254:GLU:HG2	1.98	0.43
1:B:222:ARG:HG2	1:B:262:GLU:HB3	2.00	0.43
1:C:44:PHE:CZ	1:C:50:MET:HA	2.53	0.43
1:F:222:ARG:HG2	1:F:262:GLU:HB3	2.00	0.43
1:A:30:VAL:HG12	1:A:33:ALA:HB2	2.00	0.43
1:C:168:LYS:NZ	2:C:2040:HOH:O	2.50	0.43
1:C:9:PRO:HD2	1:C:114:TYR:HB2	2.00	0.43
1:E:164:LYS:NZ	2:E:2032:HOH:O	2.29	0.43
1:G:114:TYR:O	1:G:118:ASN:HB3	2.19	0.43
1:D:227:LYS:HB3	1:D:258:LEU:HD23	2.01	0.42
1:F:233:SER:HB3	1:G:64:LYS:HA	2.00	0.42
1:F:162:GLN:HE21	1:F:179:THR:CG2	2.31	0.42
1:D:246:LEU:HA	1:D:249:MET:HE3	2.01	0.42
1:H:114:TYR:OH	1:H:135:HIS:CD2	2.68	0.42
1:H:190:VAL:CG2	1:H:238:ILE:HG13	2.49	0.42
1:A:62:ILE:HD11	1:A:76:ILE:HD11	2.02	0.42
1:F:80:ILE:CG2	1:F:134:ALA:HB2	2.50	0.42
1:A:181:PHE:CD2	1:A:181:PHE:N	2.88	0.42
1:G:231:ASN:HB3	1:G:254:GLU:HG2	2.01	0.42
1:C:190:VAL:HG12	2:C:2046:HOH:O	2.20	0.42
1:D:162:GLN:NE2	1:D:179:THR:HB	2.35	0.42
1:G:164:LYS:NZ	2:G:2029:HOH:O	2.51	0.42
1:G:227:LYS:HB3	1:G:258:LEU:HD23	2.02	0.42
1:A:74:GLN:HA	2:A:2002:HOH:O	2.19	0.41
1:B:162:GLN:HE22	1:B:178:SER:H	1.68	0.41
1:B:183:HIS:HE1	1:B:188:TYR:OH	2.02	0.41
1:F:114:TYR:OH	1:F:135:HIS:HD2	2.03	0.41
1:B:162:GLN:NE2	1:B:177:VAL:HG13	2.35	0.41
1:D:91:VAL:HG11	1:D:119:MET:HE2	2.01	0.41
1:D:162:GLN:HE22	1:D:178:SER:H	1.68	0.41
1:F:196:LEU:HD23	1:F:196:LEU:HA	1.84	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HA	1:A:249:MET:HE3	2.03	0.41
1:G:58:LEU:HD23	1:G:58:LEU:HA	1.84	0.41
1:C:30:VAL:HG12	1:C:33:ALA:HB2	2.01	0.41
1:D:80:ILE:CG2	1:D:134:ALA:HB2	2.50	0.41
1:E:49:ASN:H	1:E:49:ASN:HD22	1.68	0.41
1:C:118:ASN:HA	2:C:2026:HOH:O	2.18	0.41
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.76	0.41
1:C:227:LYS:HB3	1:C:258:LEU:HD23	2.03	0.41
1:A:231:ASN:HB3	1:A:254:GLU:HG2	2.03	0.41
1:D:114:TYR:O	1:D:118:ASN:HB3	2.20	0.41
1:D:162:GLN:NE2	1:D:177:VAL:HG13	2.36	0.41
1:A:52:LEU:HD22	1:A:238:ILE:HD12	2.02	0.41
1:D:58:LEU:HD23	1:D:58:LEU:HA	1.87	0.41
1:E:190:VAL:CG2	1:E:238:ILE:HG13	2.51	0.41
1:C:91:VAL:HG11	1:C:119:MET:CE	2.51	0.40
1:E:29[B]:HIS:H	1:E:29[B]:HIS:CD2	2.39	0.40
1:E:9:PRO:HD2	1:E:114:TYR:HB2	2.03	0.40
1:E:80:ILE:CG2	1:E:134:ALA:HB2	2.51	0.40
1:D:135:HIS:CE1	2:D:2030:HOH:O	2.68	0.40
1:A:222:ARG:HG2	1:A:262:GLU:CB	2.51	0.40
1:C:222:ARG:HG2	1:C:262:GLU:CB	2.51	0.40
1:C:175:PHE:HA	1:C:176:PRO:HD3	1.94	0.40
1:G:58:LEU:O	1:G:62:ILE:HG13	2.20	0.40
1:H:58:LEU:HD23	1:H:58:LEU:HA	1.79	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASN:ND2	1:F:262:GLU:CB[1_565]	1.76	0.44
1:C:212:ASN:ND2	1:G:262:GLU:CB[1_664]	1.89	0.31
1:E:32:GLY:O	1:E:222:ARG:NH1[1_455]	1.91	0.29
1:C:32:GLY:O	1:C:222:ARG:NH1[1_655]	1.97	0.23
1:A:32:GLY:O	1:A:222:ARG:NH1[1_655]	2.01	0.19
1:H:32:GLY:O	1:H:222:ARG:NH1[1_455]	2.10	0.10
1:A:271:ARG:NH1	2:E:2014:HOH:O[1_565]	2.16	0.04
1:A:214:SER:N	1:F:262:GLU:OE2[1_565]	2.19	0.01

## 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	268/271 (99%)	262 (98%)	6 (2%)	0	100	100
1	B	270/271 (100%)	264 (98%)	6 (2%)	0	100	100
1	C	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
1	D	269/271 (99%)	264 (98%)	5 (2%)	0	100	100
1	E	270/271 (100%)	264 (98%)	6 (2%)	0	100	100
1	F	268/271 (99%)	262 (98%)	6 (2%)	0	100	100
1	G	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
1	H	268/271 (99%)	264 (98%)	4 (2%)	0	100	100
All	All	2149/2168 (99%)	2108 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/226 (100%)	221 (98%)	4 (2%)	59	74
1	B	227/226 (100%)	223 (98%)	4 (2%)	59	74
1	C	226/226 (100%)	221 (98%)	5 (2%)	52	68
1	D	226/226 (100%)	222 (98%)	4 (2%)	59	74
1	E	227/226 (100%)	222 (98%)	5 (2%)	52	68
1	F	225/226 (100%)	219 (97%)	6 (3%)	44	60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	225/226 (100%)	221 (98%)	4 (2%)	59	74
1	H	225/226 (100%)	221 (98%)	4 (2%)	59	74
All	All	1806/1808 (100%)	1770 (98%)	36 (2%)	55	71

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	106	LYS
1	A	181	PHE
1	A	212	ASN
1	B	26	SER
1	B	106	LYS
1	B	212	ASN
1	B	238	ILE
1	C	26	SER
1	C	29	HIS
1	C	106	LYS
1	C	212	ASN
1	C	270	LYS
1	D	29	HIS
1	D	106	LYS
1	D	212	ASN
1	D	266	LYS
1	E	26	SER
1	E	106	LYS
1	E	118	ASN
1	E	212	ASN
1	E	271	ARG
1	F	26	SER
1	F	106	LYS
1	F	118	ASN
1	F	174	THR
1	F	212	ASN
1	F	266	LYS
1	G	106	LYS
1	G	159	LYS
1	G	174	THR
1	G	212	ASN
1	H	26	SER
1	H	89	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	106	LYS
1	H	212	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	118	ASN
1	A	135	HIS
1	A	162	GLN
1	A	183	HIS
1	B	49	ASN
1	B	65	HIS
1	B	89	ASN
1	B	93	HIS
1	B	118	ASN
1	B	135	HIS
1	B	162	GLN
1	B	183	HIS
1	C	49	ASN
1	C	118	ASN
1	C	135	HIS
1	C	162	GLN
1	C	183	HIS
1	D	49	ASN
1	D	118	ASN
1	D	135	HIS
1	D	162	GLN
1	D	183	HIS
1	D	198	ASN
1	E	49	ASN
1	E	65	HIS
1	E	118	ASN
1	E	135	HIS
1	E	162	GLN
1	E	183	HIS
1	F	118	ASN
1	F	135	HIS
1	F	162	GLN
1	F	183	HIS
1	G	49	ASN
1	G	103	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	111	GLN
1	G	118	ASN
1	G	135	HIS
1	G	162	GLN
1	G	183	HIS
1	H	39	GLN
1	H	49	ASN
1	H	93	HIS
1	H	118	ASN
1	H	135	HIS
1	H	162	GLN
1	H	183	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	270/271 (99%)	0.17	8 (2%)	50	57	8, 18, 40, 67	7 (2%)
1	B	270/271 (99%)	0.16	4 (1%)	73	79	9, 19, 37, 94	6 (2%)
1	C	270/271 (99%)	0.20	9 (3%)	46	53	9, 19, 42, 72	6 (2%)
1	D	270/271 (99%)	0.12	5 (1%)	66	73	9, 19, 37, 81	6 (2%)
1	E	270/271 (99%)	0.14	3 (1%)	80	85	8, 19, 40, 67	3 (1%)
1	F	270/271 (99%)	0.20	6 (2%)	62	69	8, 19, 39, 90	5 (1%)
1	G	270/271 (99%)	0.16	4 (1%)	73	79	9, 20, 39, 89	5 (1%)
1	H	270/271 (99%)	0.24	11 (4%)	37	44	10, 20, 44, 72	6 (2%)
All	All	2160/2168 (99%)	0.17	50 (2%)	60	67	8, 19, 41, 94	44 (2%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLU	7.9
1	F	30	VAL	7.5
1	A	172	VAL	6.8
1	H	172	VAL	6.4
1	H	107	ALA	4.3
1	D	2	GLU	4.2
1	C	168	LYS	4.1
1	C	172	VAL	4.0
1	A	212	ASN	3.4
1	A	175	PHE	3.1
1	F	2	GLU	3.1
1	C	166	ILE	3.0
1	H	173	GLY	3.0
1	H	177	VAL	2.9
1	A	2	GLU	2.8
1	H	208	THR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	209	ILE	2.7
1	A	171	VAL	2.6
1	C	212	ASN	2.5
1	F	4	LEU	2.5
1	A	170	GLY	2.5
1	G	30	VAL	2.5
1	H	175	PHE	2.5
1	E	213	GLY	2.4
1	E	172	VAL	2.4
1	G	264	HIS	2.3
1	H	163	ILE	2.3
1	A	211	ALA	2.3
1	F	270	LYS	2.3
1	D	3	THR	2.3
1	H	2	GLU	2.3
1	C	175	PHE	2.2
1	F	213	GLY	2.2
1	C	214	SER	2.2
1	C	211	ALA	2.2
1	D	8	ALA	2.2
1	E	254	GLU	2.2
1	G	163	ILE	2.1
1	G	252	GLY	2.1
1	A	209	ILE	2.1
1	B	161	ASN	2.1
1	H	212	ASN	2.1
1	B	211	ALA	2.1
1	D	34	GLY	2.1
1	H	211	ALA	2.1
1	B	70	PRO	2.1
1	F	264	HIS	2.0
1	D	30	VAL	2.0
1	C	3	THR	2.0
1	H	214	SER	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.