



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:47 PM EDT

PDB ID : 2FY8
Title : Crystal structure of MthK rck domain in its ligand-free gating-ring form
Authors : Ye, S.; Jiang, Y.
Deposited on : 2006-02-07
Resolution : 2.79 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	:	2.23.2
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)	:	2.23.2

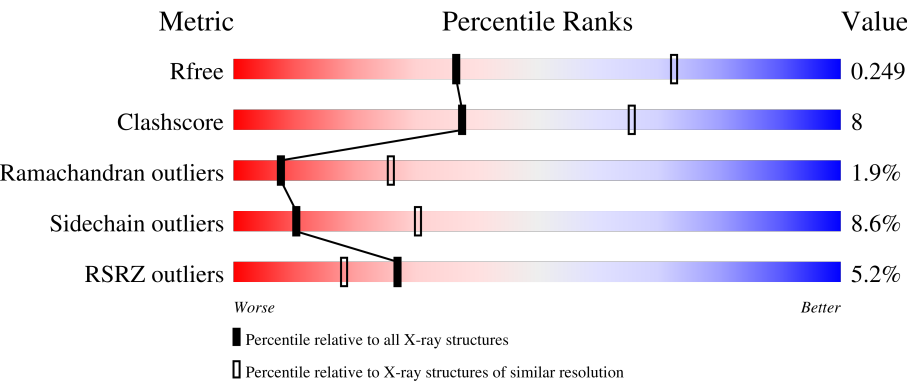
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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 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	230	<div><div>3%</div><div><div></div><div>75%</div><div>18%</div><div></div></div><div></div></div>
1	B	230	<div><div>2%</div><div><div></div><div>74%</div><div>17%</div><div>5%</div></div><div></div></div>
1	C	230	<div><div>4%</div><div><div></div><div>79%</div><div>16%</div><div></div></div><div></div></div>
1	D	230	<div><div>5%</div><div><div></div><div>74%</div><div>19%</div><div></div></div><div></div></div>
1	E	230	<div><div>7%</div><div><div></div><div>73%</div><div>20%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	230	<div> <div>9%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>
1	G	230	<div> <div>3%</div> <div>74%</div> <div>20%</div> <div>• •</div> </div>
1	H	230	<div> <div>7%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13851 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 Calcium-gated potassium channel mthK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1724	1072	307	338	7			
1	B	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			
1	C	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			
1	D	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			
1	E	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			
1	F	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			
1	G	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			
1	H	222	Total	C	N	O	S	0	0	0
			1725	1072	307	339	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	ASN	ASP	engineered mutation	UNP O27564
B	184	ASN	ASP	engineered mutation	UNP O27564
C	184	ASN	ASP	engineered mutation	UNP O27564
D	184	ASN	ASP	engineered mutation	UNP O27564
E	184	ASN	ASP	engineered mutation	UNP O27564
F	184	ASN	ASP	engineered mutation	UNP O27564
G	184	ASN	ASP	engineered mutation	UNP O27564
H	184	ASN	ASP	engineered mutation	UNP O27564

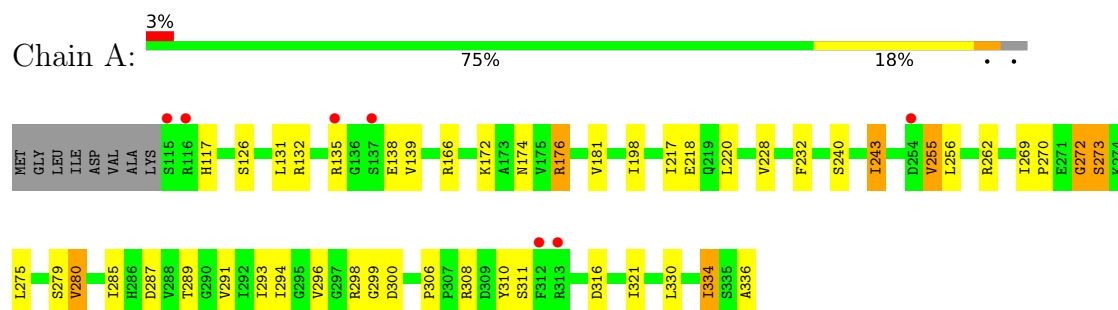
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	10	Total 10	O 10	0	0
2	C	5	Total 5	O 5	0	0
2	D	7	Total 7	O 7	0	0
2	E	5	Total 5	O 5	0	0
2	F	5	Total 5	O 5	0	0
2	G	9	Total 9	O 9	0	0
2	H	4	Total 4	O 4	0	0

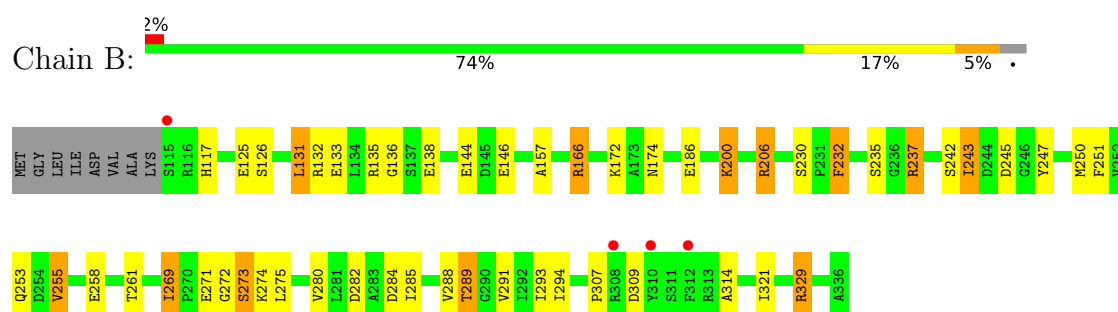
3 Residue-property plots [i](#)

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.

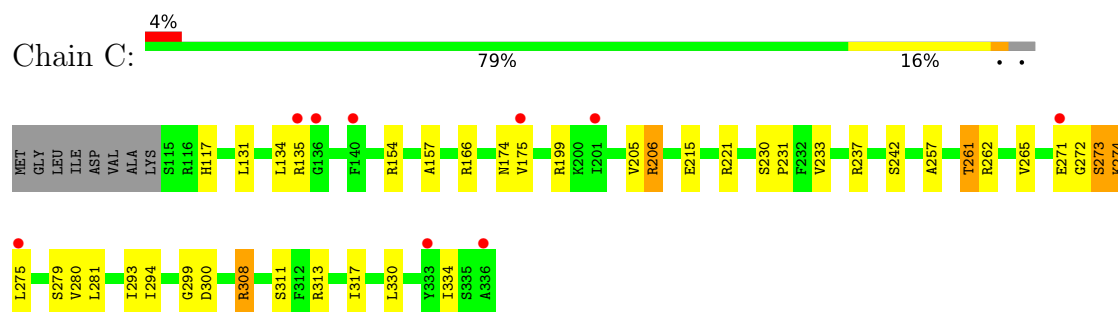
- Molecule 1: Calcium-gated potassium channel mthK



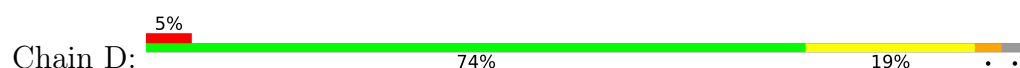
- Molecule 1: Calcium-gated potassium channel mthK

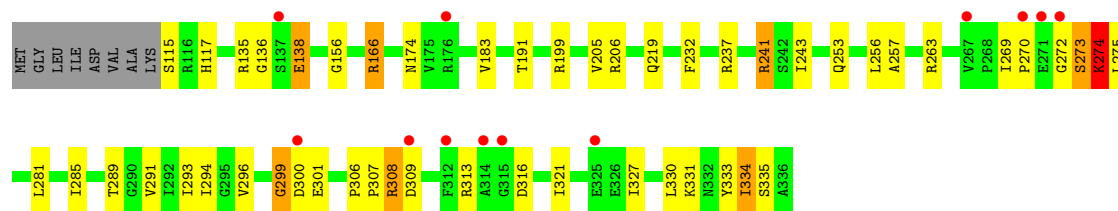


- Molecule 1: Calcium-gated potassium channel mthK

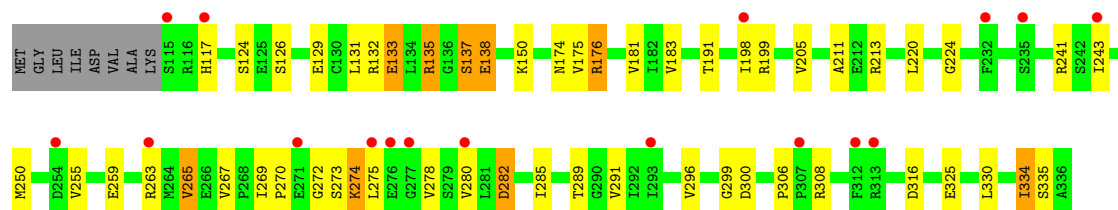
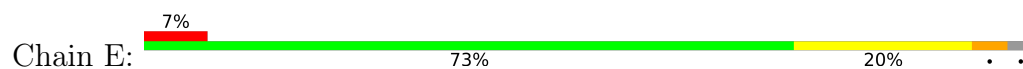


- Molecule 1: Calcium-gated potassium channel mthK

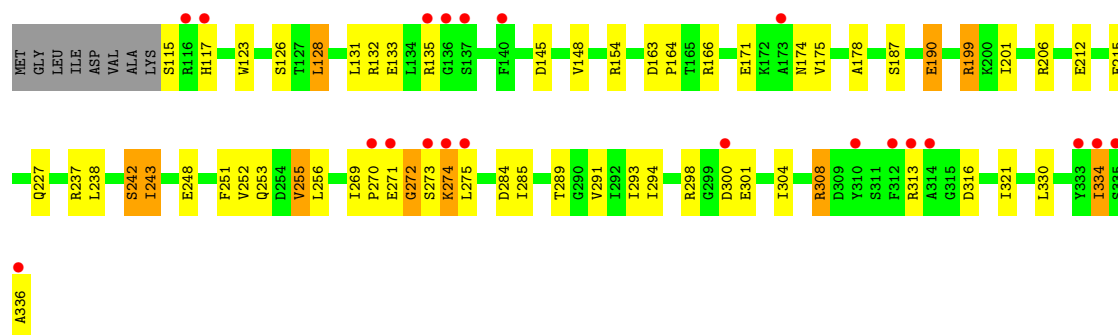




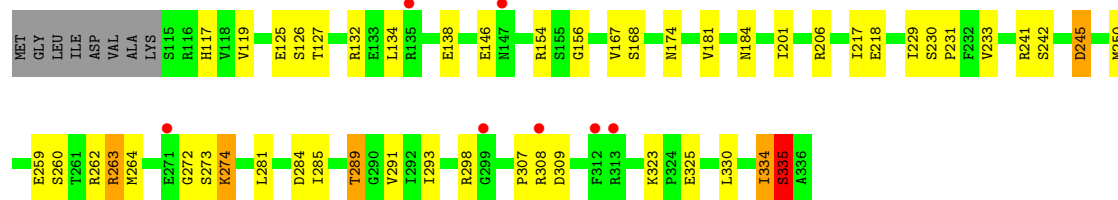
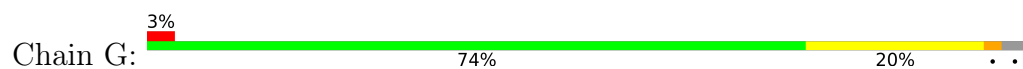
• Molecule 1: Calcium-gated potassium channel mthK



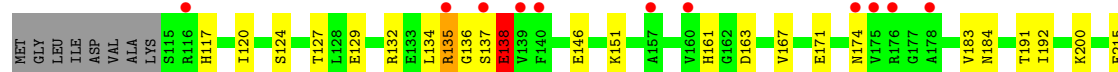
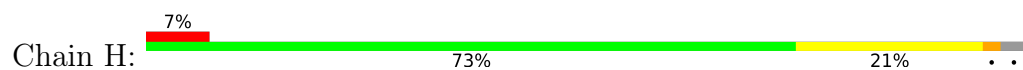
• Molecule 1: Calcium-gated potassium channel mthK



• Molecule 1: Calcium-gated potassium channel mthK



• Molecule 1: Calcium-gated potassium channel mthK





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.14Å 180.97Å 252.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.79 47.21 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.19-2.79) 97.3 (47.21-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005, XTALVIEW	Depositor
R, R_{free}	0.212 , 0.254 0.209 , 0.249	Depositor DCC
R_{free} test set	1923 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13851	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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](#)

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	0.51	0/1745	0.64	0/2355
1	B	0.51	0/1746	0.65	0/2355
1	C	0.53	0/1746	0.63	0/2355
1	D	0.56	0/1746	0.69	0/2355
1	E	0.47	0/1746	0.61	0/2355
1	F	0.52	2/1746 (0.1%)	0.61	0/2355
1	G	0.52	0/1746	0.68	0/2355
1	H	0.52	0/1746	0.67	1/2355 (0.0%)
All	All	0.52	2/13967 (0.0%)	0.65	1/18840 (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
1	G	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	336	ALA	C-OXT	5.73	1.34	1.23
1	F	336	ALA	C-O	5.56	1.33	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	163	ASP	CB-CG-OD1	5.19	122.97	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	SER	Peptide
1	G	273	SER	Peptide
1	G	335	SER	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	1724	0	1733	26	0
1	B	1725	0	1733	34	0
1	C	1725	0	1733	22	0
1	D	1725	0	1733	30	0
1	E	1725	0	1733	30	0
1	F	1725	0	1733	37	0
1	G	1725	0	1733	29	0
1	H	1725	0	1733	27	0
2	A	7	0	0	0	0
2	B	10	0	0	2	0
2	C	5	0	0	0	0
2	D	7	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	9	0	0	0	0
2	H	4	0	0	0	0
All	All	13851	0	13864	214	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 8.

All (214) 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:329:ARG:HH11	1:B:329:ARG:HG2	1.17	1.00
1:E:274:LYS:HB2	1:E:335:SER:HA	1.52	0.90
1:D:135:ARG:O	1:D:138:GLU:HB2	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:GLU:HG3	1:G:264:MET:HE2	1.57	0.86
1:B:186:GLU:HG3	2:B:21:HOH:O	1.76	0.84
1:B:329:ARG:HG2	1:B:329:ARG:NH1	1.94	0.82
1:F:269:ILE:HG12	1:F:334:ILE:HD11	1.63	0.80
1:H:219:GLN:H	1:H:219:GLN:HE21	1.28	0.80
1:F:285:ILE:O	1:F:289:THR:HG22	1.81	0.79
1:B:206:ARG:NH1	1:C:242:SER:O	2.18	0.76
1:F:285:ILE:HB	1:F:293:ILE:HD11	1.67	0.76
1:A:299:GLY:O	1:A:300:ASP:HB2	1.84	0.76
1:B:242:SER:O	1:C:206:ARG:NH2	2.19	0.75
1:E:273:SER:O	1:E:275:LEU:N	2.21	0.74
1:H:138:GLU:O	1:H:138:GLU:HG3	1.86	0.74
1:F:285:ILE:HB	1:F:293:ILE:CD1	2.19	0.73
1:G:281:LEU:HB2	1:G:308:ARG:HB2	1.71	0.70
1:C:280:VAL:HG22	1:C:308:ARG:HA	1.74	0.69
1:D:275:LEU:HD12	1:D:334:ILE:HG22	1.73	0.68
1:E:285:ILE:O	1:E:289:THR:HG22	1.94	0.68
1:E:199:ARG:NH2	1:E:205:VAL:O	2.25	0.67
1:A:289:THR:HG23	1:A:291:VAL:H	1.60	0.67
1:D:289:THR:HG21	1:D:330:LEU:HB2	1.77	0.67
1:A:294:ILE:HD11	1:A:321:ILE:HD11	1.75	0.66
1:H:117:HIS:HE1	1:H:174:ASN:O	1.79	0.66
1:D:117:HIS:HE1	1:D:174:ASN:O	1.79	0.66
1:A:294:ILE:HD11	1:A:321:ILE:CD1	2.27	0.65
1:H:219:GLN:HE21	1:H:219:GLN:N	1.95	0.65
1:G:127:THR:HG23	1:G:184:ASN:HD22	1.62	0.65
1:F:187:SER:OG	1:F:190:GLU:HG3	1.97	0.64
1:G:325:GLU:CD	1:G:325:GLU:H	2.01	0.64
1:B:273:SER:O	1:B:275:LEU:N	2.32	0.63
1:D:237:ARG:O	1:D:241:ARG:HG2	1.99	0.63
1:D:274:LYS:NZ	1:D:333:TYR:HA	2.13	0.63
1:A:285:ILE:O	1:A:289:THR:HG22	1.98	0.62
1:A:117:HIS:HE1	1:A:174:ASN:O	1.82	0.62
1:B:251:PHE:O	1:B:255:VAL:HG12	1.99	0.62
1:E:269:ILE:HD13	1:E:316:ASP:HB2	1.82	0.62
1:D:270:PRO:HG2	1:D:335:SER:HB3	1.81	0.61
1:F:242:SER:O	1:G:206:ARG:NH1	2.33	0.61
1:E:274:LYS:CB	1:E:335:SER:HA	2.29	0.61
1:F:251:PHE:O	1:F:255:VAL:HG13	2.01	0.60
1:G:117:HIS:H	1:G:117:HIS:CD2	2.17	0.60
1:F:117:HIS:HE1	1:F:174:ASN:O	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:269:ILE:HD12	1:H:316:ASP:HB2	1.83	0.59
1:D:333:TYR:O	1:D:334:ILE:HG23	2.02	0.59
1:B:166:ARG:HD2	2:B:5:HOH:O	2.02	0.59
1:A:135:ARG:HD2	1:A:138:GLU:HG3	1.85	0.58
1:F:304:ILE:HG21	1:G:262:ARG:HD2	1.84	0.58
1:H:124:SER:OG	1:H:184:ASN:ND2	2.37	0.58
1:C:280:VAL:CG2	1:C:308:ARG:HA	2.34	0.58
1:G:285:ILE:HD12	1:G:293:ILE:HD11	1.87	0.57
1:B:132:ARG:NH2	1:C:237:ARG:HH22	2.04	0.56
1:B:235:SER:HB2	1:C:231:PRO:HG3	1.88	0.56
1:B:269:ILE:HG22	1:B:314:ALA:HA	1.87	0.56
1:F:251:PHE:HZ	1:F:321:ILE:HD13	1.70	0.55
1:H:129:GLU:O	1:H:132:ARG:HB2	2.06	0.55
1:A:131:LEU:HD21	1:A:139:VAL:HG11	1.89	0.55
1:F:273:SER:O	1:F:275:LEU:N	2.40	0.55
1:A:285:ILE:HG21	1:A:293:ILE:HD11	1.88	0.54
1:H:192:ILE:HG13	1:H:220:LEU:HD23	1.89	0.54
1:E:259:GLU:CD	1:E:263:ARG:HG3	2.28	0.53
1:H:146:GLU:HG2	1:H:161:HIS:CE1	2.44	0.53
1:C:261:THR:HG23	1:C:262:ARG:H	1.74	0.53
1:D:269:ILE:HD12	1:D:316:ASP:HB2	1.89	0.53
1:H:167:VAL:O	1:H:171:GLU:HG3	2.08	0.53
1:E:124:SER:OG	1:E:126:SER:HB2	2.07	0.53
1:B:237:ARG:NH1	1:C:257:ALA:O	2.41	0.53
1:D:199:ARG:NH2	1:D:205:VAL:O	2.38	0.52
1:F:269:ILE:HG12	1:F:334:ILE:CD1	2.36	0.52
1:E:289:THR:HG23	1:E:291:VAL:H	1.74	0.52
1:F:330:LEU:O	1:F:334:ILE:HB	2.08	0.52
1:E:199:ARG:NH1	1:E:224:GLY:O	2.42	0.52
1:B:284:ASP:O	1:B:288:VAL:HG23	2.10	0.52
1:B:232:PHE:N	1:B:232:PHE:CD2	2.78	0.52
1:A:285:ILE:HG21	1:A:293:ILE:CD1	2.40	0.51
1:D:273:SER:O	1:D:275:LEU:N	2.43	0.51
1:E:265:VAL:HB	1:E:267:VAL:HG23	1.92	0.51
1:B:329:ARG:NH1	1:B:329:ARG:CG	2.69	0.51
1:C:334:ILE:HG22	1:C:334:ILE:O	2.11	0.51
1:D:289:THR:CG2	1:D:330:LEU:HB2	2.41	0.51
1:F:294:ILE:HD11	1:F:321:ILE:HD12	1.93	0.51
1:G:285:ILE:O	1:G:289:THR:HG22	2.11	0.51
1:F:285:ILE:CB	1:F:293:ILE:HD11	2.40	0.51
1:F:171:GLU:HG3	1:F:201:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:HB	1:D:293:ILE:HD11	1.92	0.51
1:F:313:ARG:O	1:F:316:ASP:HB2	2.10	0.50
1:F:206:ARG:NH1	1:G:242:SER:O	2.45	0.50
1:E:135:ARG:NH1	1:E:137:SER:HB2	2.26	0.50
1:H:262:ARG:HD3	1:H:323:LYS:HG3	1.92	0.50
1:G:285:ILE:HB	1:G:293:ILE:HD11	1.93	0.50
1:D:183:VAL:HG12	1:D:191:THR:HG23	1.94	0.50
1:H:262:ARG:NH2	1:H:323:LYS:HE3	2.27	0.49
1:H:288:VAL:HG11	1:H:333:TYR:CE1	2.47	0.49
1:B:253:GLN:HA	1:B:253:GLN:NE2	2.27	0.49
1:A:298:ARG:HD3	1:A:316:ASP:OD1	2.13	0.49
1:E:175:VAL:HG13	1:E:181:VAL:HG21	1.93	0.49
1:G:117:HIS:HE1	1:G:174:ASN:O	1.96	0.49
1:F:212:GLU:HG2	1:G:125:GLU:HG3	1.95	0.49
1:G:230:SER:HB3	1:G:233:VAL:HB	1.95	0.49
1:D:299:GLY:O	1:D:300:ASP:HB2	2.12	0.49
1:G:229:ILE:HG22	1:G:231:PRO:HD3	1.95	0.49
1:E:211:ALA:HB2	1:E:220:LEU:HD22	1.94	0.48
1:H:270:PRO:HD3	1:H:334:ILE:HG22	1.95	0.48
1:E:133:GLU:O	1:E:133:GLU:HG2	2.12	0.48
1:B:285:ILE:HD12	1:B:293:ILE:HD11	1.95	0.48
1:C:273:SER:O	1:C:275:LEU:N	2.44	0.48
1:H:273:SER:O	1:H:276:GLU:HB2	2.14	0.48
1:H:296:VAL:HG23	1:H:306:PRO:HG3	1.96	0.48
1:B:232:PHE:N	1:B:232:PHE:HD2	2.11	0.48
1:E:129:GLU:OE2	1:E:132:ARG:HD3	2.13	0.48
1:E:117:HIS:HE1	1:E:174:ASN:O	1.96	0.48
1:A:280:VAL:HG12	1:A:310:TYR:HB3	1.95	0.48
1:C:334:ILE:O	1:C:334:ILE:CG2	2.61	0.48
1:E:213:ARG:HG2	1:F:166:ARG:NH1	2.29	0.48
1:E:299:GLY:O	1:E:300:ASP:HB2	2.14	0.48
1:H:318:ILE:HD12	1:H:334:ILE:HD11	1.95	0.48
1:F:199:ARG:HA	1:F:199:ARG:HD3	1.71	0.47
1:G:334:ILE:HG22	1:G:334:ILE:O	2.14	0.47
1:G:307:PRO:HB2	1:G:309:ASP:OD2	2.14	0.47
1:H:270:PRO:CD	1:H:334:ILE:HG22	2.43	0.47
1:A:240:SER:HA	1:A:243:ILE:HD12	1.95	0.47
1:C:117:HIS:HE1	1:C:174:ASN:O	1.96	0.47
1:B:251:PHE:O	1:B:255:VAL:CG1	2.62	0.47
1:H:280:VAL:HG22	1:H:308:ARG:HA	1.96	0.47
1:A:217:ILE:HG23	1:A:228:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PRO:HB2	1:B:309:ASP:OD1	2.15	0.47
1:H:120:ILE:HG21	1:H:127:THR:HG23	1.96	0.47
1:C:281:LEU:HB2	1:C:308:ARG:HB3	1.97	0.46
1:F:298:ARG:O	1:F:301:GLU:HB2	2.15	0.46
1:B:243:ILE:HD13	1:C:134:LEU:HD21	1.96	0.46
1:F:270:PRO:C	1:F:272:GLY:N	2.68	0.46
1:A:273:SER:CB	1:A:336:ALA:HA	2.45	0.46
1:A:296:VAL:HG23	1:A:306:PRO:HG3	1.98	0.46
1:C:279:SER:HA	1:C:311:SER:HA	1.97	0.46
1:G:119:VAL:HB	1:G:181:VAL:HG13	1.97	0.46
1:C:154:ARG:NH1	1:E:282:ASP:OD2	2.48	0.46
1:G:259:GLU:HG2	1:G:263:ARG:HB2	1.97	0.46
1:H:167:VAL:HG21	1:H:200:LYS:HD3	1.97	0.46
1:B:289:THR:CG2	1:B:291:VAL:H	2.29	0.46
1:B:294:ILE:HD11	1:B:321:ILE:HG13	1.98	0.46
1:B:136:GLY:O	1:B:157:ALA:HA	2.16	0.46
1:E:296:VAL:HG23	1:E:306:PRO:HG3	1.96	0.46
1:F:115:SER:OG	1:F:117:HIS:HD2	1.99	0.46
1:A:270:PRO:C	1:A:272:GLY:H	2.20	0.45
1:F:298:ARG:HH12	1:F:313:ARG:HB2	1.81	0.45
1:D:232:PHE:HD1	1:D:232:PHE:N	2.14	0.45
1:D:274:LYS:HZ3	1:D:333:TYR:HA	1.81	0.45
1:D:294:ILE:HD11	1:D:321:ILE:HG13	1.98	0.45
1:F:270:PRO:C	1:F:272:GLY:H	2.19	0.45
1:B:289:THR:HG23	1:B:291:VAL:H	1.81	0.45
1:A:270:PRO:C	1:A:272:GLY:N	2.70	0.45
1:B:285:ILE:O	1:B:289:THR:HG22	2.17	0.45
1:D:232:PHE:N	1:D:232:PHE:CD1	2.83	0.45
1:E:183:VAL:HG12	1:E:191:THR:HG23	1.99	0.45
1:H:270:PRO:C	1:H:272:GLY:N	2.71	0.44
1:D:253:GLN:O	1:D:257:ALA:HB3	2.17	0.44
1:A:255:VAL:HG23	1:A:256:LEU:HD12	2.00	0.44
1:D:274:LYS:HZ2	1:D:333:TYR:HA	1.82	0.44
1:D:289:THR:HG22	1:D:291:VAL:HG23	1.98	0.44
1:F:253:GLN:HE22	1:G:230:SER:H	1.66	0.44
1:H:134:LEU:O	1:H:136:GLY:N	2.51	0.44
1:A:273:SER:HB3	1:A:336:ALA:HA	2.00	0.44
1:A:181:VAL:HG11	1:A:198:ILE:CD1	2.48	0.44
1:B:258:GLU:CD	1:C:221:ARG:HH22	2.21	0.44
1:C:131:LEU:HD21	1:C:157:ALA:HB2	2.00	0.44
1:E:334:ILE:O	1:E:335:SER:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HB3	1:B:138:GLU:HG2	2.00	0.43
1:H:219:GLN:H	1:H:219:GLN:NE2	2.07	0.43
1:B:125:GLU:CD	1:D:166:ARG:HH22	2.21	0.43
1:D:296:VAL:HG23	1:D:306:PRO:HG3	2.00	0.43
1:A:280:VAL:CG1	1:A:310:TYR:HB3	2.48	0.43
1:C:199:ARG:NH2	1:C:205:VAL:O	2.41	0.43
1:A:269:ILE:HD12	1:A:316:ASP:HB2	2.00	0.43
1:A:275:LEU:HD12	1:A:334:ILE:HG13	2.00	0.43
1:G:167:VAL:HG13	1:G:201:ILE:HD11	2.01	0.43
1:D:306:PRO:HA	1:D:307:PRO:HD3	1.93	0.42
1:B:247:TYR:HE1	1:C:317:ILE:HD12	1.83	0.42
1:F:243:ILE:HD13	1:G:134:LEU:HD21	2.00	0.42
1:D:136:GLY:HA3	1:D:156:GLY:O	2.18	0.42
1:H:183:VAL:HG12	1:H:191:THR:HG23	2.01	0.42
1:E:270:PRO:C	1:E:272:GLY:N	2.73	0.42
1:G:217:ILE:HD11	1:G:230:SER:OG	2.19	0.42
1:B:117:HIS:CE1	1:B:174:ASN:HB3	2.55	0.42
1:D:294:ILE:HD12	1:D:294:ILE:N	2.35	0.42
1:E:129:GLU:OE2	1:E:132:ARG:NH1	2.51	0.42
1:B:131:LEU:HD21	1:B:157:ALA:HB2	2.02	0.42
1:G:241:ARG:O	1:G:245:ASP:HB2	2.20	0.42
1:E:138:GLU:H	1:E:138:GLU:HG3	1.48	0.42
1:E:275:LEU:HD23	1:E:278:VAL:HB	2.02	0.42
1:F:227:GLN:OE1	1:G:250:MET:HG2	2.20	0.42
1:F:252:VAL:HG13	1:F:256:LEU:HD12	2.01	0.42
1:H:270:PRO:C	1:H:272:GLY:H	2.23	0.42
1:F:145:ASP:O	1:F:148:VAL:HG22	2.19	0.42
1:C:273:SER:HB3	1:C:274:LYS:H	1.62	0.41
1:F:163:ASP:HA	1:F:164:PRO:HD3	1.92	0.41
1:D:219:GLN:NE2	1:D:219:GLN:HA	2.35	0.41
1:E:175:VAL:HG11	1:E:198:ILE:HG23	2.02	0.41
1:G:154:ARG:C	1:G:156:GLY:H	2.23	0.41
1:G:289:THR:HG23	1:G:291:VAL:H	1.86	0.41
1:E:280:VAL:HG13	1:E:308:ARG:HA	2.03	0.41
1:F:304:ILE:CG2	1:G:262:ARG:HD2	2.51	0.41
1:A:218:GLU:OE1	1:B:200:LYS:HE3	2.20	0.41
1:B:251:PHE:CE1	1:B:255:VAL:HG11	2.56	0.41
1:D:281:LEU:HD13	1:D:308:ARG:HG2	2.03	0.41
1:E:135:ARG:HH12	1:E:137:SER:HB2	1.85	0.41
1:H:270:PRO:HG2	1:H:335:SER:HA	2.03	0.41
1:C:230:SER:HB3	1:C:233:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:SER:OG	1:D:117:HIS:HD2	2.04	0.40
1:G:323:LYS:HB3	1:G:325:GLU:OE2	2.22	0.40
1:A:279:SER:HA	1:A:310:TYR:O	2.22	0.40
1:F:238:LEU:HD11	1:F:252:VAL:HG11	2.02	0.40
1:F:123:TRP:CZ2	1:F:128:LEU:HG	2.57	0.40
1:F:289:THR:HG23	1:F:291:VAL:H	1.86	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	220/230 (96%)	205 (93%)	13 (6%)	2 (1%)	17	46
1	B	220/230 (96%)	208 (94%)	9 (4%)	3 (1%)	11	34
1	C	220/230 (96%)	198 (90%)	17 (8%)	5 (2%)	6	21
1	D	220/230 (96%)	202 (92%)	12 (6%)	6 (3%)	5	17
1	E	220/230 (96%)	201 (91%)	17 (8%)	2 (1%)	17	46
1	F	220/230 (96%)	201 (91%)	13 (6%)	6 (3%)	5	17
1	G	220/230 (96%)	202 (92%)	13 (6%)	5 (2%)	6	21
1	H	220/230 (96%)	205 (93%)	11 (5%)	4 (2%)	8	28
All	All	1760/1840 (96%)	1622 (92%)	105 (6%)	33 (2%)	8	26

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	B	274	LYS
1	C	274	LYS
1	D	274	LYS

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Mol	Chain	Res	Type
1	E	176	ARG
1	F	178	ALA
1	F	274	LYS
1	G	335	SER
1	A	272	GLY
1	B	272	GLY
1	B	273	SER
1	C	272	GLY
1	C	299	GLY
1	D	138	GLU
1	D	272	GLY
1	D	299	GLY
1	D	334	ILE
1	E	274	LYS
1	F	272	GLY
1	F	308	ARG
1	G	245	ASP
1	G	272	GLY
1	H	272	GLY
1	C	215	GLU
1	D	273	SER
1	F	215	GLU
1	F	242	SER
1	G	274	LYS
1	G	284	ASP
1	H	135	ARG
1	H	138	GLU
1	C	271	GLU
1	H	215	GLU

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	190/196 (97%)	174 (92%)	16 (8%)	11	31
1	B	190/196 (97%)	167 (88%)	23 (12%)	5	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	190/196 (97%)	177 (93%)	13 (7%)	16	42
1	D	190/196 (97%)	177 (93%)	13 (7%)	16	42
1	E	190/196 (97%)	174 (92%)	16 (8%)	11	31
1	F	190/196 (97%)	171 (90%)	19 (10%)	7	22
1	G	190/196 (97%)	176 (93%)	14 (7%)	13	37
1	H	190/196 (97%)	174 (92%)	16 (8%)	11	31
All	All	1520/1568 (97%)	1390 (91%)	130 (9%)	10	30

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	132	ARG
1	A	166	ARG
1	A	172	LYS
1	A	176	ARG
1	A	220	LEU
1	A	232	PHE
1	A	243	ILE
1	A	255	VAL
1	A	262	ARG
1	A	280	VAL
1	A	287	ASP
1	A	308	ARG
1	A	311	SER
1	A	330	LEU
1	A	334	ILE
1	B	126	SER
1	B	131	LEU
1	B	133	GLU
1	B	144	GLU
1	B	146	GLU
1	B	166	ARG
1	B	172	LYS
1	B	200	LYS
1	B	206	ARG
1	B	230	SER
1	B	232	PHE
1	B	237	ARG
1	B	243	ILE

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Mol	Chain	Res	Type
1	B	245	ASP
1	B	250	MET
1	B	255	VAL
1	B	261	THR
1	B	269	ILE
1	B	271	GLU
1	B	280	VAL
1	B	282	ASP
1	B	289	THR
1	B	329	ARG
1	C	135	ARG
1	C	166	ARG
1	C	175	VAL
1	C	206	ARG
1	C	261	THR
1	C	265	VAL
1	C	273	SER
1	C	293	ILE
1	C	294	ILE
1	C	300	ASP
1	C	308	ARG
1	C	313	ARG
1	C	330	LEU
1	D	166	ARG
1	D	206	ARG
1	D	241	ARG
1	D	243	ILE
1	D	256	LEU
1	D	263	ARG
1	D	274	LYS
1	D	301	GLU
1	D	308	ARG
1	D	309	ASP
1	D	313	ARG
1	D	327	ILE
1	D	331	LYS
1	E	131	LEU
1	E	133	GLU
1	E	135	ARG
1	E	137	SER
1	E	138	GLU
1	E	150	LYS

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Mol	Chain	Res	Type
1	E	176	ARG
1	E	241	ARG
1	E	243	ILE
1	E	250	MET
1	E	255	VAL
1	E	265	VAL
1	E	282	ASP
1	E	325	GLU
1	E	330	LEU
1	E	334	ILE
1	F	126	SER
1	F	128	LEU
1	F	131	LEU
1	F	132	ARG
1	F	133	GLU
1	F	135	ARG
1	F	154	ARG
1	F	175	VAL
1	F	190	GLU
1	F	199	ARG
1	F	237	ARG
1	F	243	ILE
1	F	255	VAL
1	F	271	GLU
1	F	274	LYS
1	F	284	ASP
1	F	300	ASP
1	F	308	ARG
1	F	334	ILE
1	G	126	SER
1	G	132	ARG
1	G	138	GLU
1	G	146	GLU
1	G	168	SER
1	G	218	GLU
1	G	260	SER
1	G	263	ARG
1	G	274	LYS
1	G	289	THR
1	G	298	ARG
1	G	330	LEU
1	G	334	ILE

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Mol	Chain	Res	Type
1	G	335	SER
1	H	135	ARG
1	H	137	SER
1	H	138	GLU
1	H	151	LYS
1	H	219	GLN
1	H	237	ARG
1	H	243	ILE
1	H	261	THR
1	H	262	ARG
1	H	271	GLU
1	H	289	THR
1	H	293	ILE
1	H	300	ASP
1	H	301	GLU
1	H	319	LEU
1	H	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	184	ASN
1	A	286	HIS
1	B	117	HIS
1	B	184	ASN
1	B	253	GLN
1	C	117	HIS
1	C	184	ASN
1	D	117	HIS
1	D	184	ASN
1	D	219	GLN
1	D	253	GLN
1	E	117	HIS
1	E	219	GLN
1	E	253	GLN
1	F	117	HIS
1	F	184	ASN
1	F	253	GLN
1	G	117	HIS
1	G	184	ASN
1	H	117	HIS

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Mol	Chain	Res	Type
1	H	147	ASN
1	H	184	ASN
1	H	219	GLN

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 monosaccharides 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, 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	222/230 (96%)	0.45	7 (3%) 47 37	49, 72, 84, 89	0
1	B	222/230 (96%)	0.51	4 (1%) 68 61	48, 65, 83, 90	0
1	C	222/230 (96%)	0.54	9 (4%) 37 27	51, 71, 86, 88	0
1	D	222/230 (96%)	0.58	12 (5%) 25 17	49, 69, 91, 98	0
1	E	222/230 (96%)	0.67	17 (7%) 13 7	59, 80, 100, 105	0
1	F	222/230 (96%)	0.76	21 (9%) 8 4	57, 76, 96, 102	0
1	G	222/230 (96%)	0.48	7 (3%) 47 37	50, 70, 79, 88	0
1	H	222/230 (96%)	0.61	15 (6%) 17 10	47, 64, 81, 87	0
All	All	1776/1840 (96%)	0.57	92 (5%) 27 18	47, 71, 94, 105	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	271	GLU	8.2
1	F	271	GLU	6.1
1	C	336	ALA	5.8
1	A	137	SER	5.5
1	F	274	LYS	5.3
1	H	271	GLU	5.3
1	H	137	SER	5.1
1	A	115	SER	5.0
1	G	271	GLU	4.2
1	H	135	ARG	4.1
1	E	312	PHE	4.0
1	D	271	GLU	4.0
1	C	271	GLU	3.9
1	F	336	ALA	3.8
1	E	115	SER	3.7
1	F	137	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	277	GLY	3.6
1	E	307	PRO	3.5
1	F	312	PHE	3.5
1	F	135	ARG	3.4
1	F	310	TYR	3.3
1	F	140	PHE	3.3
1	C	140	PHE	3.2
1	C	175	VAL	3.1
1	F	136	GLY	3.1
1	F	334	ILE	3.0
1	H	273	SER	3.0
1	G	312	PHE	3.0
1	E	263	ARG	3.0
1	D	312	PHE	2.9
1	H	140	PHE	2.9
1	F	300	ASP	2.9
1	E	275	LEU	2.9
1	H	176	ARG	2.9
1	F	173	ALA	2.8
1	E	243	ILE	2.8
1	F	335	SER	2.8
1	H	174	ASN	2.8
1	E	280	VAL	2.7
1	H	175	VAL	2.7
1	E	293	ILE	2.6
1	F	270	PRO	2.6
1	F	273	SER	2.6
1	B	308	ARG	2.6
1	H	116	ARG	2.6
1	D	314	ALA	2.6
1	D	315	GLY	2.5
1	H	272	GLY	2.5
1	D	137	SER	2.5
1	B	115	SER	2.5
1	C	136	GLY	2.5
1	H	157	ALA	2.5
1	G	308	ARG	2.5
1	B	312	PHE	2.4
1	G	147	ASN	2.4
1	E	117	HIS	2.4
1	B	310	TYR	2.4
1	F	116	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	139	VAL	2.4
1	D	267	VAL	2.4
1	F	333	TYR	2.4
1	G	299	GLY	2.4
1	F	313	ARG	2.4
1	E	313	ARG	2.3
1	E	276	GLU	2.3
1	E	198	ILE	2.3
1	H	300	ASP	2.3
1	D	176	ARG	2.2
1	D	270	PRO	2.2
1	F	117	HIS	2.2
1	D	309	ASP	2.2
1	A	135	ARG	2.2
1	C	135	ARG	2.2
1	H	178	ALA	2.2
1	G	313	ARG	2.1
1	D	272	GLY	2.1
1	D	325	GLU	2.1
1	C	201	ILE	2.1
1	H	160	VAL	2.1
1	G	135	ARG	2.1
1	D	300	ASP	2.1
1	C	333	TYR	2.1
1	F	314	ALA	2.1
1	A	116	ARG	2.1
1	A	313	ARG	2.1
1	A	254	ASP	2.1
1	E	254	ASP	2.1
1	C	275	LEU	2.1
1	F	275	LEU	2.1
1	A	312	PHE	2.1
1	E	235	SER	2.0
1	E	232	PHE	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 monosaccharides 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.