



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2025 – 03:37 PM JST

PDB ID : 8XZ6 / pdb\_00008xz6  
Title : MERS-CoV S and radixin complex structure  
Authors : Wang, J.M.; Ma, W.F.  
Deposited on : 2024-01-20  
Resolution : 2.12 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 types of validation reports are described at

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

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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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

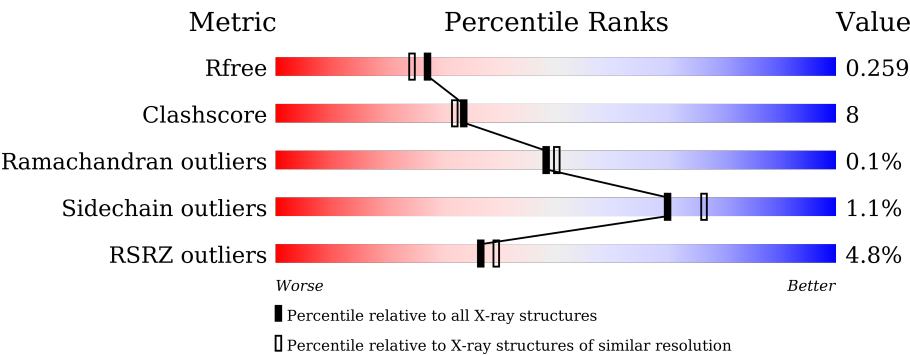
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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))
$R_{free}$	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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  $\geq 3$ , 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	298	<div><div>4%</div><div>83%</div><div>16%</div></div>
1	B	298	<div><div>5%</div><div>78%</div><div>20%</div><div>..</div></div>
1	C	298	<div><div>5%</div><div>82%</div><div>16%</div><div>..</div></div>
1	D	298	<div><div>4%</div><div>83%</div><div>15%</div><div>.</div></div>
2	E	13	<div><div>23%</div><div>54%</div><div>8%</div><div>23%</div><div>15%</div></div>
2	F	13	<div><div>46%</div><div>8%</div><div>46%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	13	 31%23%46%
2	H	13	 8%54%46%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10612 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 Radixin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2476	1600	420	446	10			
1	B	294	Total	C	N	O	S	0	0	0
			2451	1585	416	441	9			
1	C	296	Total	C	N	O	S	0	0	0
			2449	1586	413	440	10			
1	D	296	Total	C	N	O	S	0	0	0
			2453	1585	416	442	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P35241
A	0	SER	-	expression tag	UNP P35241
B	-1	GLY	-	expression tag	UNP P35241
B	0	SER	-	expression tag	UNP P35241
C	-1	GLY	-	expression tag	UNP P35241
C	0	SER	-	expression tag	UNP P35241
D	-1	GLY	-	expression tag	UNP P35241
D	0	SER	-	expression tag	UNP P35241

- Molecule 2 is a protein called Spike protein S2'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	0	0	0
			89	56	14	19			
2	F	7	Total	C	N	O	0	0	0
			63	41	7	15			
2	G	7	Total	C	N	O	0	0	0
			63	41	7	15			
2	H	7	Total	C	N	O	0	0	0
			63	41	7	15			

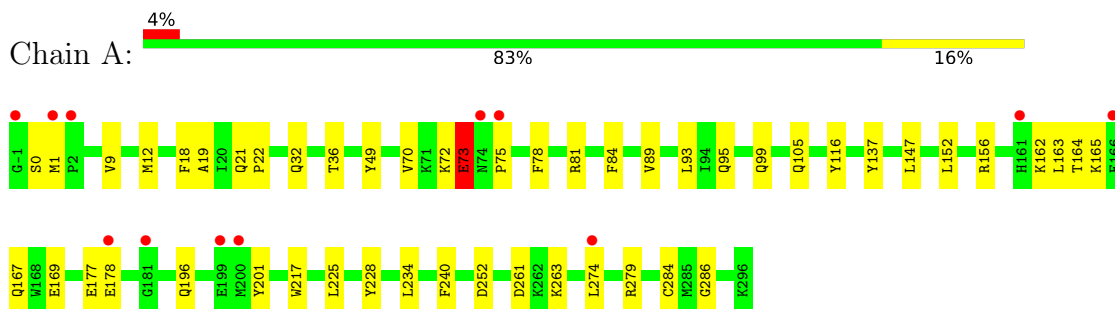
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total 142	O 142	0	0
3	B	111	Total 111	O 111	0	0
3	C	95	Total 95	O 95	0	0
3	D	150	Total 150	O 150	0	0
3	E	1	Total 1	O 1	0	0
3	F	1	Total 1	O 1	0	0
3	G	3	Total 3	O 3	0	0
3	H	2	Total 2	O 2	0	0

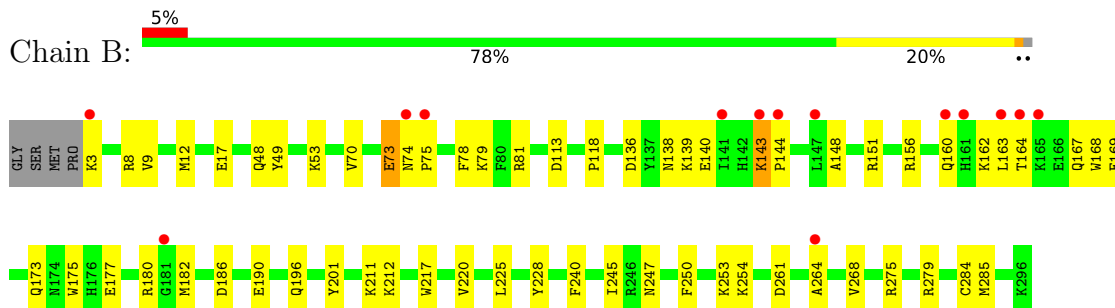
### 3 Residue-property plots

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.

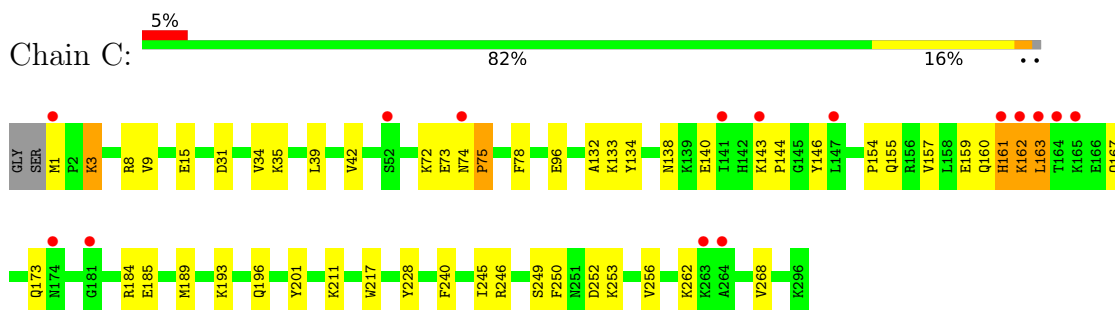
#### • Molecule 1: Radixin



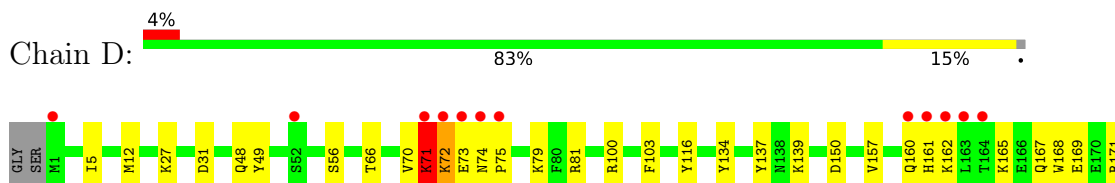
#### • Molecule 1: Radixin



#### • Molecule 1: Radixin

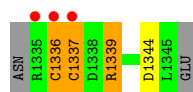


#### • Molecule 1: Radixin

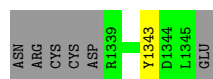




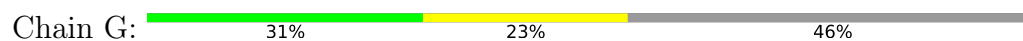
- Molecule 2: Spike protein S2'



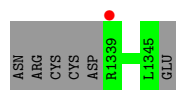
- Molecule 2: Spike protein S2'



- Molecule 2: Spike protein S2'



- Molecule 2: Spike protein S2'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.31Å 94.10Å 134.30Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	32.88 – 2.12 32.88 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.88-2.12) 99.8 (32.88-2.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, $R_{free}$	0.220 , 0.256 0.229 , 0.259	Depositor DCC
$R_{free}$ test set	4940 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6230e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.30	0/2536	0.53	2/3423 (0.1%)
1	B	0.39	1/2510 (0.0%)	0.59	2/3388 (0.1%)
1	C	0.37	0/2509	0.61	2/3390 (0.1%)
1	D	0.34	0/2513	0.57	4/3395 (0.1%)
2	E	0.70	0/90	1.20	1/121 (0.8%)
2	F	0.17	0/64	0.24	0/86
2	G	0.26	0/64	0.30	0/86
2	H	0.62	0/64	0.99	0/86
All	All	0.36	1/10350 (0.0%)	0.59	11/13975 (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
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	PRO	CA-C	-5.19	1.49	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	LYS	N-CA-C	6.50	119.32	110.35
1	A	73	GLU	CA-C-N	-5.46	112.94	120.26
1	A	73	GLU	C-N-CA	-5.46	112.94	120.26
1	B	143	LYS	CB-CA-C	5.45	119.31	109.45
1	C	252	ASP	N-CA-C	-5.38	99.69	108.67
1	D	161	HIS	N-CA-C	-5.22	102.61	110.70
2	E	1336	CYS	CA-C-O	-5.19	115.15	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	LYS	N-CA-C	-5.11	107.10	113.38
1	C	75	PRO	N-CA-C	-5.04	101.95	110.21
1	D	72	LYS	CA-C-N	-5.01	113.11	121.94
1	D	72	LYS	C-N-CA	-5.01	113.11	121.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1339	ARG	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	2476	0	2474	34	0
1	B	2451	0	2447	41	0
1	C	2449	0	2436	37	0
1	D	2453	0	2431	37	0
2	E	89	0	65	2	0
2	F	63	0	46	1	0
2	G	63	0	46	3	0
2	H	63	0	46	0	0
3	A	142	0	0	6	0
3	B	111	0	0	3	0
3	C	95	0	0	2	0
3	D	150	0	0	4	0
3	E	1	0	0	1	0
3	F	1	0	0	0	0
3	G	3	0	0	1	0
3	H	2	0	0	0	0
All	All	10612	0	9991	152	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 (152) 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:74:ASN:HB3	1:C:75:PRO:HD3	1.38	1.04
1:C:256:VAL:HG12	1:C:268:VAL:HG22	1.60	0.83
1:D:160:GLN:O	1:D:160:GLN:NE2	2.11	0.82
1:A:156:ARG:NH2	3:A:301:HOH:O	2.20	0.74
1:D:139:LYS:H	1:D:139:LYS:HE2	1.55	0.72
1:D:72:LYS:HA	3:D:367:HOH:O	1.90	0.71
1:B:136:ASP:OD1	1:B:180:ARG:HA	1.92	0.69
1:D:258:LYS:NZ	3:D:302:HOH:O	2.26	0.67
1:C:211:LYS:HD2	1:C:211:LYS:H	1.60	0.66
1:B:163:LEU:HD12	1:B:167:GLN:HB3	1.76	0.66
1:B:138:ASN:OD1	1:B:140:GLU:HB3	1.96	0.65
1:C:31:ASP:O	1:C:35:LYS:HG2	1.97	0.65
1:C:189:MET:O	1:C:193:LYS:HG3	1.97	0.64
1:D:56:SER:O	1:D:275:ARG:NH2	2.30	0.64
1:C:160:GLN:O	1:C:161:HIS:C	2.41	0.62
1:D:74:ASN:HB3	1:D:75:PRO:HD3	1.82	0.62
1:B:225:LEU:HD21	1:B:284:CYS:SG	2.41	0.61
1:C:74:ASN:HB3	1:C:75:PRO:CD	2.22	0.60
1:D:48:GLN:HG2	1:D:79:LYS:HB2	1.81	0.60
1:B:74:ASN:HB3	1:B:75:PRO:HD3	1.83	0.60
1:A:261:ASP:OD1	1:A:263:LYS:HE2	2.01	0.60
1:B:8:ARG:HG3	1:B:17:GLU:HG2	1.82	0.60
1:B:136:ASP:HB3	1:B:180:ARG:HG3	1.85	0.59
1:B:220:VAL:HG22	1:B:225:LEU:HD22	1.85	0.59
1:A:178:GLU:CD	1:A:178:GLU:O	2.47	0.58
1:B:148:ALA:HA	1:B:169:GLU:OE2	2.04	0.57
1:B:175:TRP:NE1	3:B:302:HOH:O	2.35	0.57
1:A:89:VAL:HG23	1:A:93:LEU:HD12	1.86	0.57
1:D:165:LYS:HG2	1:D:169:GLU:OE2	2.05	0.57
1:D:167:GLN:NE2	3:D:306:HOH:O	2.37	0.57
2:G:1339:ARG:N	3:G:1401:HOH:O	2.38	0.56
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.71	0.56
1:D:207:GLU:HG2	1:D:217:TRP:CZ3	2.41	0.56
1:A:116:TYR:HB3	1:A:234:LEU:HD21	1.88	0.55
1:D:12:MET:HE2	1:D:81:ARG:NE	2.22	0.55
1:A:164:THR:HG23	1:A:167:GLN:H	1.71	0.55
1:B:275:ARG:O	1:B:279:ARG:HG2	2.06	0.55
1:D:72:LYS:CA	3:D:367:HOH:O	2.51	0.55
1:B:163:LEU:CD1	1:B:167:GLN:HB3	2.37	0.55
1:C:96:GLU:HG2	1:C:185:GLU:HG2	1.89	0.54
1:D:116:TYR:HB3	1:D:234:LEU:HD21	1.87	0.54
1:C:146:TYR:CE1	1:C:173:GLN:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LYS:H	1:D:139:LYS:CE	2.19	0.54
1:B:182:MET:HA	3:B:334:HOH:O	2.08	0.53
1:B:240:PHE:HB3	1:B:245:ILE:HD11	1.89	0.53
1:A:21:GLN:HG3	1:A:22:PRO:HD2	1.89	0.53
1:A:73:GLU:HB2	1:A:75:PRO:O	2.09	0.53
1:D:5:ILE:HD13	1:D:66:THR:HG21	1.90	0.53
1:C:154:PRO:HG2	1:C:157:VAL:CG2	2.39	0.52
1:C:253:LYS:NZ	3:C:303:HOH:O	2.40	0.52
1:D:103:PHE:CD2	1:D:188:MET:HE3	2.44	0.52
1:C:34:VAL:HG13	1:C:39:LEU:O	2.10	0.52
1:B:217:TRP:HB2	1:B:228:TYR:HB2	1.92	0.51
1:C:39:LEU:HD23	1:C:42:VAL:HG12	1.92	0.51
1:D:199:GLU:H	1:D:199:GLU:CD	2.19	0.51
1:B:173:GLN:NE2	1:B:177:GLU:OE1	2.44	0.51
1:A:18:PHE:HB2	3:A:305:HOH:O	2.11	0.51
1:D:217:TRP:HB2	1:D:228:TYR:HB2	1.93	0.51
1:D:73:GLU:O	1:D:74:ASN:C	2.53	0.50
1:B:48:GLN:HG3	1:B:79:LYS:HB2	1.94	0.50
1:A:217:TRP:HB2	1:A:228:TYR:HB2	1.93	0.50
1:A:261:ASP:OD1	1:A:263:LYS:CE	2.59	0.50
1:A:0:SER:OG	1:A:1:MET:N	2.45	0.50
1:A:9:VAL:HG22	1:A:78:PHE:HB2	1.93	0.50
1:D:137:TYR:CD2	1:D:177:GLU:HG2	2.46	0.50
1:A:137:TYR:CD2	1:A:177:GLU:HG2	2.47	0.49
2:E:1339:ARG:HB2	3:E:1401:HOH:O	2.12	0.49
1:C:211:LYS:NZ	1:C:268:VAL:O	2.38	0.49
1:C:146:TYR:HE1	1:C:173:GLN:HG3	1.78	0.48
1:C:211:LYS:H	1:C:211:LYS:CD	2.26	0.48
1:B:12:MET:HE2	1:B:81:ARG:NE	2.28	0.48
1:C:249:SER:OG	1:C:256:VAL:HG23	2.14	0.48
1:D:49:TYR:CD2	1:D:70:VAL:HG22	2.49	0.48
1:B:113:ASP:OD1	1:B:156:ARG:HG2	2.14	0.48
1:A:12:MET:HE3	1:A:105:GLN:HA	1.96	0.48
1:C:246:ARG:NH2	1:C:262:LYS:HE2	2.29	0.48
1:B:113:ASP:CG	1:B:156:ARG:HG2	2.39	0.47
1:C:72:LYS:HG2	3:C:350:HOH:O	2.13	0.47
1:B:225:LEU:HB2	1:B:240:PHE:HB2	1.95	0.47
1:B:247:ASN:ND2	3:B:307:HOH:O	2.47	0.47
1:C:9:VAL:HG22	1:C:78:PHE:HB2	1.96	0.47
1:A:72:LYS:CB	3:A:361:HOH:O	2.63	0.47
1:C:250:PHE:C	1:C:250:PHE:CD1	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:HG3	1:D:188:MET:HE1	1.96	0.47
1:A:164:THR:HG22	1:A:167:GLN:OE1	2.14	0.47
1:A:165:LYS:HG2	1:A:169:GLU:OE2	2.14	0.47
1:A:32:GLN:O	1:A:36:THR:HG23	2.15	0.47
1:D:160:GLN:O	1:D:162:LYS:N	2.41	0.47
1:A:72:LYS:C	1:A:73:GLU:HG2	2.39	0.47
1:B:9:VAL:HG22	1:B:78:PHE:HB2	1.97	0.46
1:C:3:LYS:HB2	1:C:3:LYS:HE2	1.68	0.46
1:B:139:LYS:HE2	1:B:139:LYS:HB3	1.85	0.46
1:A:225:LEU:HD21	1:A:284:CYS:SG	2.55	0.46
1:C:217:TRP:HB2	1:C:228:TYR:HB2	1.97	0.46
1:A:49:TYR:CD2	1:A:70:VAL:HG22	2.51	0.46
1:D:167:GLN:OE1	1:D:171:ARG:HD2	2.16	0.46
1:C:74:ASN:CB	1:C:75:PRO:HD3	2.26	0.45
1:A:84:PHE:CZ	1:A:286:GLY:HA3	2.51	0.45
1:C:138:ASN:OD1	1:C:140:GLU:HB2	2.16	0.45
1:A:225:LEU:HB2	1:A:240:PHE:HB2	1.98	0.45
1:D:157:VAL:O	1:D:160:GLN:HG3	2.16	0.45
1:A:72:LYS:CA	3:A:361:HOH:O	2.65	0.45
1:A:19:ALA:N	3:A:305:HOH:O	2.41	0.44
2:E:1336:CYS:O	2:E:1337:CYS:CB	2.65	0.44
1:B:164:THR:H	1:B:167:GLN:HB2	1.81	0.44
1:B:285:MET:HG2	2:G:1343:TYR:CG	2.52	0.44
1:D:71:LYS:HG2	1:D:72:LYS:H	1.83	0.44
1:D:196:GLN:HA	1:D:201:TYR:CG	2.52	0.44
1:B:73:GLU:O	1:B:74:ASN:C	2.60	0.44
1:A:252:ASP:HA	1:A:274:LEU:HD23	1.99	0.44
1:D:27:LYS:HE3	1:D:31:ASP:OD2	2.18	0.43
1:B:212:LYS:HD3	1:B:212:LYS:HA	1.89	0.43
1:B:143:LYS:HD3	1:B:144:PRO:HD2	2.00	0.43
1:A:147:LEU:HB3	1:A:152:LEU:HD11	2.01	0.43
1:D:182:MET:HG2	1:D:187:SER:HB2	2.00	0.43
1:C:143:LYS:HB2	1:C:144:PRO:HD2	2.00	0.43
1:D:134:TYR:OH	1:D:150:ASP:OD2	2.24	0.43
1:A:12:MET:HE2	1:A:81:ARG:NE	2.33	0.43
1:C:133:LYS:HE3	1:C:134:TYR:CE2	2.54	0.43
1:A:162:LYS:O	1:A:163:LEU:HD23	2.19	0.43
1:B:49:TYR:CD2	1:B:70:VAL:HG22	2.54	0.43
1:B:254:LYS:HE3	1:B:268:VAL:HG21	2.00	0.43
1:B:186:ASP:O	1:B:190:GLU:HG2	2.19	0.42
1:C:196:GLN:HA	1:C:201:TYR:CG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLN:HA	1:C:201:TYR:CD1	2.54	0.42
1:A:196:GLN:HA	1:A:201:TYR:CG	2.54	0.42
1:D:137:TYR:HB2	1:D:176:HIS:CE1	2.54	0.42
1:B:160:GLN:OE1	1:B:162:LYS:HB2	2.19	0.42
1:D:262:LYS:HE3	1:D:262:LYS:HB2	1.91	0.42
1:C:163:LEU:HG	1:C:167:GLN:OE1	2.20	0.42
1:C:240:PHE:HB3	1:C:245:ILE:HD11	2.02	0.42
1:A:95:GLN:O	1:A:99:GLN:HG3	2.20	0.41
1:C:8:ARG:HH11	1:C:15:GLU:CD	2.28	0.41
1:B:74:ASN:HB3	1:B:75:PRO:CD	2.47	0.41
1:C:211:LYS:CE	1:C:268:VAL:O	2.68	0.41
1:B:163:LEU:HB2	1:B:168:TRP:CE2	2.56	0.41
1:B:261:ASP:O	1:B:264:ALA:HB3	2.20	0.41
1:C:211:LYS:HE3	1:C:268:VAL:O	2.20	0.41
1:C:162:LYS:O	1:C:163:LEU:HB2	2.21	0.41
1:D:182:MET:HB2	1:D:182:MET:HE3	1.78	0.41
1:A:261:ASP:OD1	1:A:263:LYS:NZ	2.50	0.41
1:C:132:ALA:O	1:C:184:ARG:NE	2.54	0.41
1:B:196:GLN:HA	1:B:201:TYR:CG	2.56	0.41
1:D:74:ASN:HB3	1:D:75:PRO:CD	2.49	0.41
1:D:285:MET:HG2	2:F:1343:TYR:CG	2.55	0.41
1:D:160:GLN:NE2	1:D:168:TRP:HZ2	2.19	0.41
1:B:250:PHE:CZ	2:G:1341:GLU:HB2	2.56	0.40
1:C:155:GLN:O	1:C:159:GLU:N	2.48	0.40
1:D:137:TYR:CE2	1:D:139:LYS:HD3	2.57	0.40
1:A:279:ARG:HD2	3:A:396:HOH:O	2.20	0.40
1:B:156:ARG:N	1:B:156:ARG:HD2	2.35	0.40
1:B:211:LYS:HE2	1:B:211:LYS:HB2	1.90	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	296/298 (99%)	290 (98%)	6 (2%)	0	100	100
1	B	292/298 (98%)	285 (98%)	7 (2%)	0	100	100
1	C	294/298 (99%)	285 (97%)	9 (3%)	0	100	100
1	D	294/298 (99%)	289 (98%)	5 (2%)	0	100	100
2	E	9/13 (69%)	7 (78%)	1 (11%)	1 (11%)	0	0
2	F	5/13 (38%)	5 (100%)	0	0	100	100
2	G	5/13 (38%)	5 (100%)	0	0	100	100
2	H	5/13 (38%)	5 (100%)	0	0	100	100
All	All	1200/1244 (96%)	1171 (98%)	28 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1337	CYS

### 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	267/270 (99%)	266 (100%)	1 (0%)	89	93
1	B	264/270 (98%)	261 (99%)	3 (1%)	70	76
1	C	262/270 (97%)	256 (98%)	6 (2%)	45	50
1	D	262/270 (97%)	261 (100%)	1 (0%)	89	93
2	E	7/13 (54%)	6 (86%)	1 (14%)	2	1
2	F	6/13 (46%)	6 (100%)	0	100	100
2	G	6/13 (46%)	6 (100%)	0	100	100
2	H	6/13 (46%)	6 (100%)	0	100	100
All	All	1080/1132 (95%)	1068 (99%)	12 (1%)	70	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	3	LYS
1	B	53	LYS
1	B	73	GLU
1	C	1	MET
1	C	3	LYS
1	C	73	GLU
1	C	161	HIS
1	C	162	LYS
1	C	163	LEU
1	D	71	LYS
2	E	1344	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	161	HIS
1	A	226	ASN
1	A	230	HIS
1	B	67	GLN
1	B	155	GLN
1	C	6	ASN
1	C	112	ASN
1	C	155	GLN
1	C	204	ASN
1	C	226	ASN
1	C	247	ASN
1	D	160	GLN
1	D	179	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	298/298 (100%)	0.39	12 (4%) 43 45	31, 49, 67, 79	0
1	B	294/298 (98%)	0.47	14 (4%) 36 39	33, 50, 85, 103	0
1	C	296/298 (99%)	0.53	15 (5%) 34 37	35, 52, 85, 104	0
1	D	296/298 (99%)	0.25	13 (4%) 39 42	30, 44, 70, 91	0
2	E	11/13 (84%)	1.45	3 (27%) 2 2	53, 65, 92, 93	0
2	F	7/13 (53%)	0.72	0 100 100	47, 53, 61, 62	0
2	G	7/13 (53%)	0.94	0 100 100	44, 53, 60, 63	0
2	H	7/13 (53%)	1.29	1 (14%) 7 8	56, 65, 69, 74	0
All	All	1216/1244 (97%)	0.43	58 (4%) 36 39	30, 49, 79, 104	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.3
1	B	163	LEU	4.2
1	A	74	ASN	4.1
1	C	163	LEU	4.0
2	E	1337	CYS	3.9
1	B	74	ASN	3.7
1	C	74	ASN	3.6
1	D	161	HIS	3.6
1	D	75	PRO	3.5
1	C	1	MET	3.3
1	C	264	ALA	3.1
1	B	144	PRO	3.1
2	E	1335	ARG	3.1
1	D	52	SER	3.1
1	B	141	ILE	3.0
1	C	141	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	181	GLY	3.0
1	D	181	GLY	2.9
1	B	75	PRO	2.8
1	B	3	LYS	2.8
2	E	1336	CYS	2.8
1	C	147	LEU	2.8
1	B	264	ALA	2.8
1	D	74	ASN	2.8
1	A	161	HIS	2.7
1	C	181	GLY	2.7
1	D	162	LYS	2.7
1	A	181	GLY	2.7
1	C	52	SER	2.7
1	A	178	GLU	2.6
1	D	72	LYS	2.6
1	A	166	GLU	2.6
1	B	160	GLN	2.6
1	A	75	PRO	2.5
1	B	161	HIS	2.5
1	C	161	HIS	2.5
1	C	164	THR	2.5
1	C	174	ASN	2.4
1	A	274	LEU	2.3
1	D	163	LEU	2.3
1	A	2	PRO	2.3
1	C	143	LYS	2.3
1	B	165	LYS	2.2
1	B	143	LYS	2.2
1	C	165	LYS	2.2
1	D	71	LYS	2.2
1	A	-1	GLY	2.2
1	D	73	GLU	2.1
1	B	147	LEU	2.1
1	B	164	THR	2.1
1	C	263	LYS	2.0
2	H	1339	ARG	2.0
1	D	160	GLN	2.0
1	D	164	THR	2.0
1	A	199	GLU	2.0
1	C	162	LYS	2.0
1	A	1	MET	2.0
1	A	200	MET	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 oligosaccharides 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.