



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 08:44 AM EDT

PDB ID : 1RJ7  
Title : Crystal structure of EDA-A1  
Authors : Hymowitz, S.G.; Compaan, D.M.; Yan, M.; Ackerly, H.; Dixit, V.M.; Starovastnik, M.A.; de Vos, A.M.  
Deposited on : unknown  
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

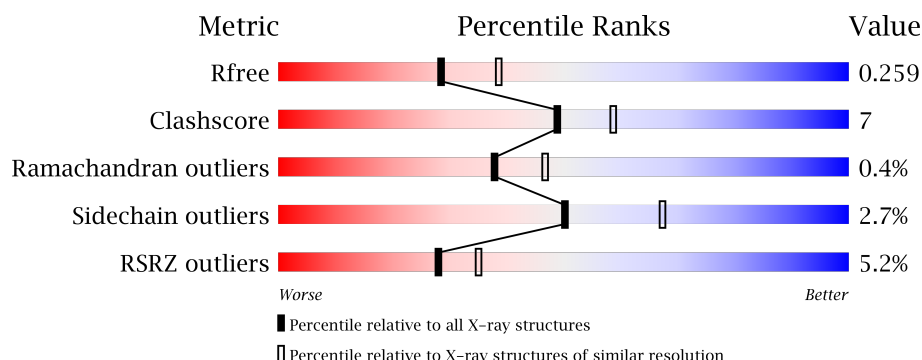
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.






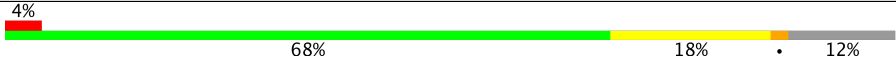
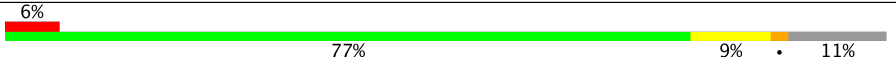
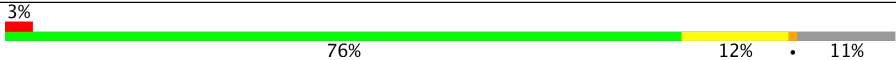
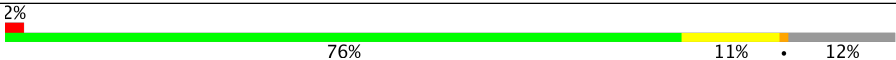
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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. 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	163	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	163	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	163	<div> <div>13%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	163	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	163	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div></div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	163	
1	H	163	
1	I	163	
1	J	163	
1	K	163	
1	L	163	
1	M	163	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13887 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 Ectodysplasin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	B	144	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	D	144	Total	C	N	O	S	0	0	0
			1125	720	190	209	6			
1	E	149	Total	C	N	O	S	0	0	0
			1168	743	200	219	6			
1	F	144	Total	C	N	O	S	0	0	0
			1129	722	191	210	6			
1	G	144	Total	C	N	O	S	0	0	0
			1125	720	190	209	6			
1	H	142	Total	C	N	O	S	0	0	0
			1113	712	188	207	6			
1	I	143	Total	C	N	O	S	0	0	0
			1124	719	190	209	6			
1	J	143	Total	C	N	O	S	0	0	0
			1118	715	189	208	6			
1	K	145	Total	C	N	O	S	0	0	0
			1136	725	192	213	6			
1	L	145	Total	C	N	O	S	0	0	0
			1133	724	192	211	6			
1	M	144	Total	C	N	O	S	0	0	0
			1129	722	191	210	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	GLY	-	CLONING ARTIFACT	UNP Q92838
A	230	SER	-	CLONING ARTIFACT	UNP Q92838
A	231	HIS	-	CLONING ARTIFACT	UNP Q92838
A	232	MET	-	CLONING ARTIFACT	UNP Q92838
B	229	GLY	-	CLONING ARTIFACT	UNP Q92838

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	SER	-	CLONING ARTIFACT	UNP Q92838
B	231	HIS	-	CLONING ARTIFACT	UNP Q92838
B	232	MET	-	CLONING ARTIFACT	UNP Q92838
D	229	GLY	-	CLONING ARTIFACT	UNP Q92838
D	230	SER	-	CLONING ARTIFACT	UNP Q92838
D	231	HIS	-	CLONING ARTIFACT	UNP Q92838
D	232	MET	-	CLONING ARTIFACT	UNP Q92838
E	229	GLY	-	CLONING ARTIFACT	UNP Q92838
E	230	SER	-	CLONING ARTIFACT	UNP Q92838
E	231	HIS	-	CLONING ARTIFACT	UNP Q92838
E	232	MET	-	CLONING ARTIFACT	UNP Q92838
F	229	GLY	-	CLONING ARTIFACT	UNP Q92838
F	230	SER	-	CLONING ARTIFACT	UNP Q92838
F	231	HIS	-	CLONING ARTIFACT	UNP Q92838
F	232	MET	-	CLONING ARTIFACT	UNP Q92838
G	229	GLY	-	CLONING ARTIFACT	UNP Q92838
G	230	SER	-	CLONING ARTIFACT	UNP Q92838
G	231	HIS	-	CLONING ARTIFACT	UNP Q92838
G	232	MET	-	CLONING ARTIFACT	UNP Q92838
H	229	GLY	-	CLONING ARTIFACT	UNP Q92838
H	230	SER	-	CLONING ARTIFACT	UNP Q92838
H	231	HIS	-	CLONING ARTIFACT	UNP Q92838
H	232	MET	-	CLONING ARTIFACT	UNP Q92838
I	229	GLY	-	CLONING ARTIFACT	UNP Q92838
I	230	SER	-	CLONING ARTIFACT	UNP Q92838
I	231	HIS	-	CLONING ARTIFACT	UNP Q92838
I	232	MET	-	CLONING ARTIFACT	UNP Q92838
J	229	GLY	-	CLONING ARTIFACT	UNP Q92838
J	230	SER	-	CLONING ARTIFACT	UNP Q92838
J	231	HIS	-	CLONING ARTIFACT	UNP Q92838
J	232	MET	-	CLONING ARTIFACT	UNP Q92838
K	229	GLY	-	CLONING ARTIFACT	UNP Q92838
K	230	SER	-	CLONING ARTIFACT	UNP Q92838
K	231	HIS	-	CLONING ARTIFACT	UNP Q92838
K	232	MET	-	CLONING ARTIFACT	UNP Q92838
L	229	GLY	-	CLONING ARTIFACT	UNP Q92838
L	230	SER	-	CLONING ARTIFACT	UNP Q92838
L	231	HIS	-	CLONING ARTIFACT	UNP Q92838
L	232	MET	-	CLONING ARTIFACT	UNP Q92838
M	229	GLY	-	CLONING ARTIFACT	UNP Q92838
M	230	SER	-	CLONING ARTIFACT	UNP Q92838
M	231	HIS	-	CLONING ARTIFACT	UNP Q92838

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Chain	Residue	Modelled	Actual	Comment	Reference
M	232	MET	-	CLONING ARTIFACT	UNP Q92838

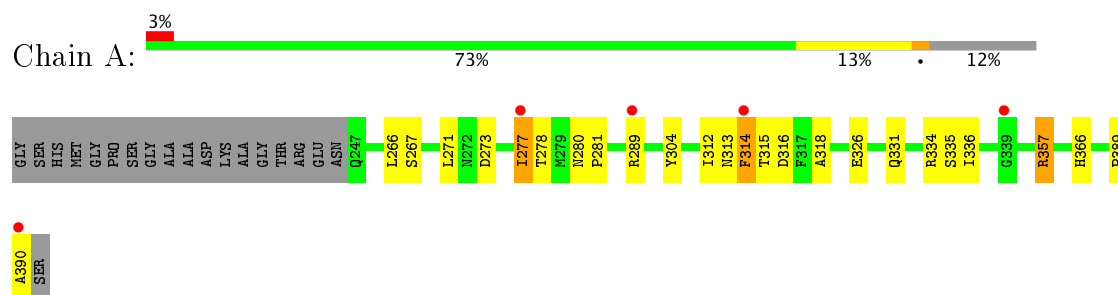
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	35	Total O 35 35	0	0
2	B	17	Total O 17 17	0	0
2	D	19	Total O 19 19	0	0
2	E	37	Total O 37 37	0	0
2	F	41	Total O 41 41	0	0
2	G	43	Total O 43 43	0	0
2	H	22	Total O 22 22	0	0
2	I	22	Total O 22 22	0	0
2	J	19	Total O 19 19	0	0
2	K	32	Total O 32 32	0	0
2	L	29	Total O 29 29	0	0
2	M	23	Total O 23 23	0	0

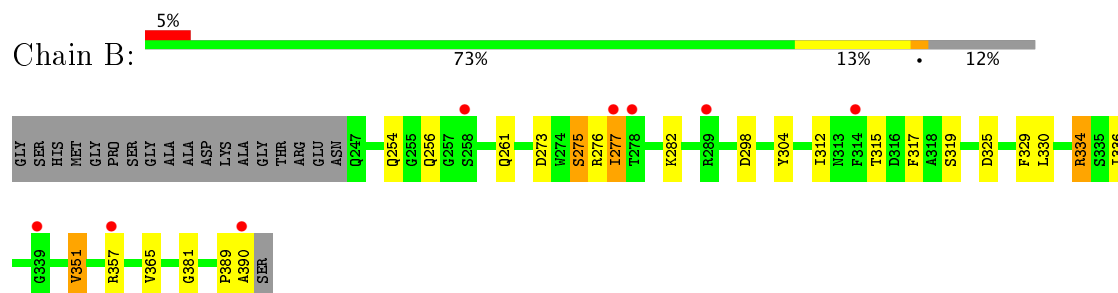
### 3 Residue-property plots [i](#)

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.

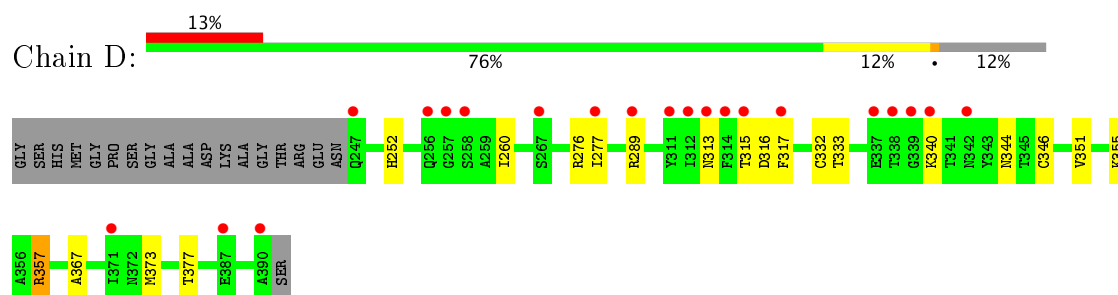
#### • Molecule 1: Ectodysplasin A



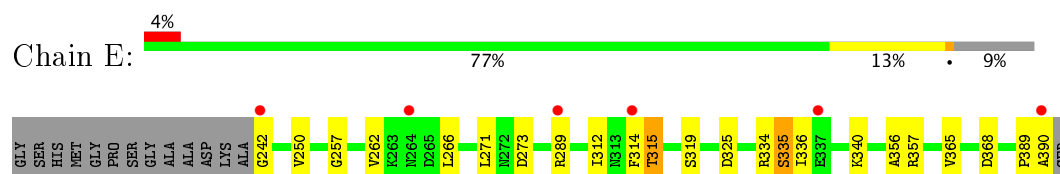
#### • Molecule 1: Ectodysplasin A



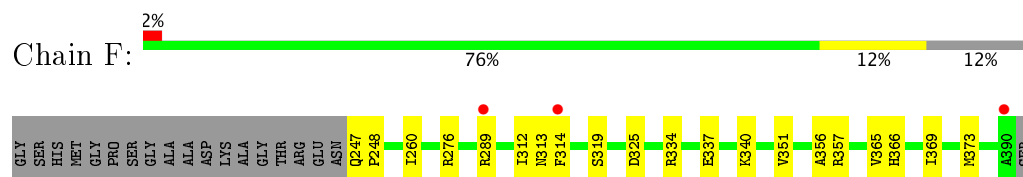
#### • Molecule 1: Ectodysplasin A



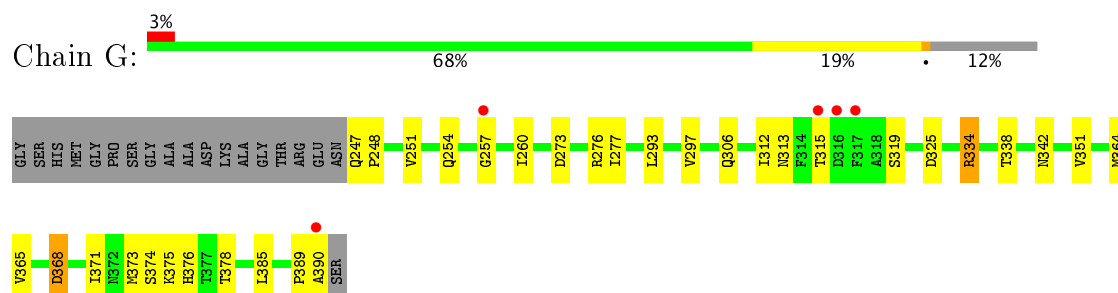
#### • Molecule 1: Ectodysplasin A



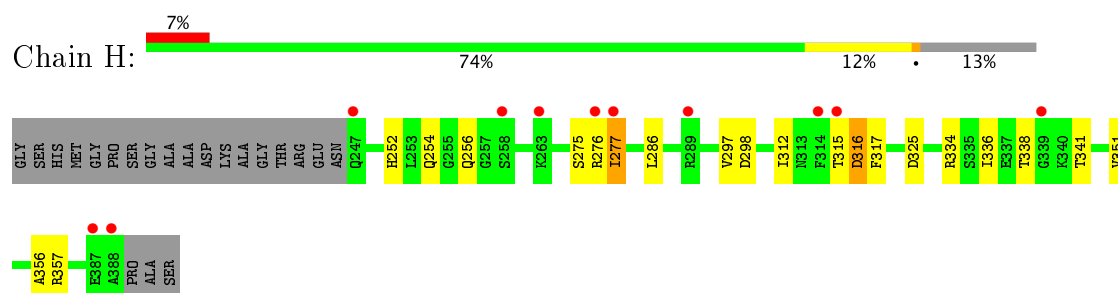
- Molecule 1: Ectodysplasin A



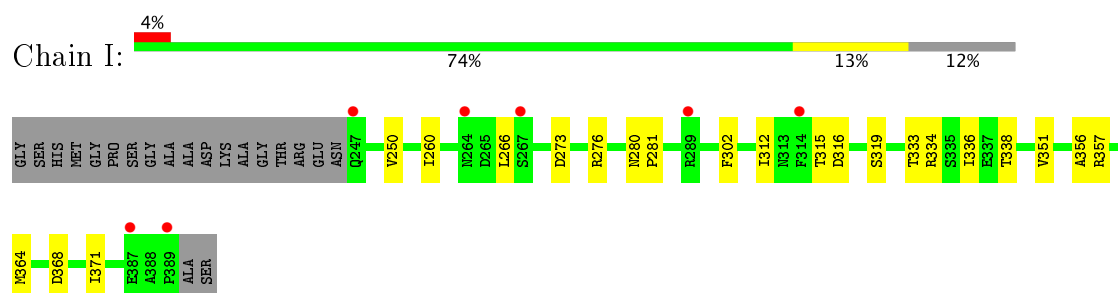
- Molecule 1: Ectodysplasin A



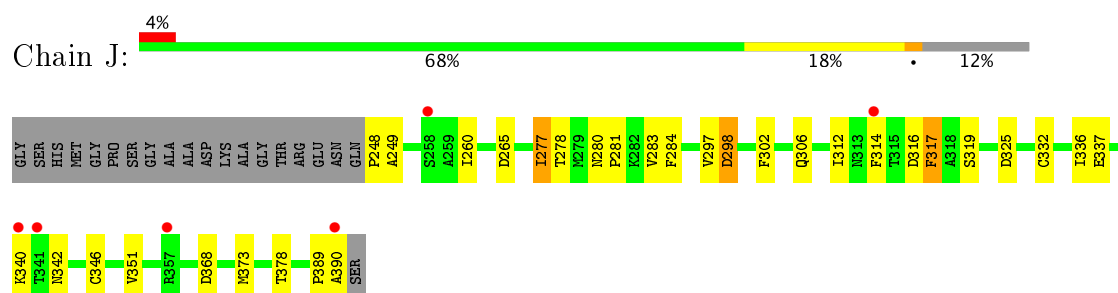
- Molecule 1: Ectodysplasin A



- Molecule 1: Ectodysplasin A

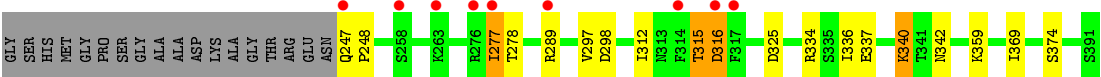
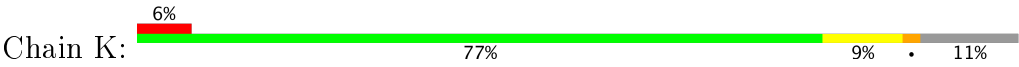


- Molecule 1: Ectodysplasin A

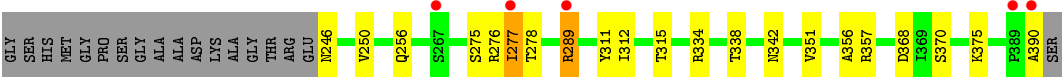
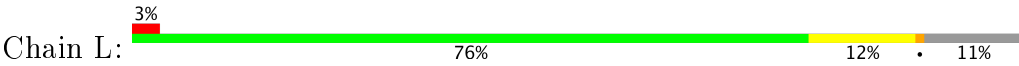


- Molecule 1: Ectodysplasin A

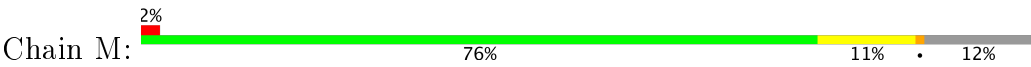




• Molecule 1: Ectodysplasin A



• Molecule 1: Ectodysplasin A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.66Å 279.69Å 54.17Å 90.00° 91.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.30) 94.4 (19.99-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.07	Depositor
R, $R_{free}$	0.194 , 0.260 0.197 , 0.259	Depositor DCC
$R_{free}$ test set	7099 reflections (12.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.046 for h,-k,-l 0.031 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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	0.50	0/1148	0.77	2/1556 (0.1%)
1	B	0.50	0/1148	0.78	3/1556 (0.2%)
1	D	0.49	0/1149	0.74	1/1558 (0.1%)
1	E	0.54	0/1192	0.79	3/1615 (0.2%)
1	F	0.53	0/1153	0.76	1/1563 (0.1%)
1	G	0.53	0/1149	0.78	3/1558 (0.2%)
1	H	0.47	0/1136	0.74	2/1539 (0.1%)
1	I	0.46	0/1148	0.75	2/1556 (0.1%)
1	J	0.48	0/1141	0.76	6/1546 (0.4%)
1	K	0.52	0/1160	0.77	1/1571 (0.1%)
1	L	0.52	0/1157	0.76	1/1569 (0.1%)
1	M	0.50	0/1153	0.75	1/1563 (0.1%)
All	All	0.50	0/13834	0.76	26/18750 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	325	ASP	CB-CG-OD2	7.22	124.80	118.30
1	B	273	ASP	CB-CG-OD2	6.67	124.30	118.30
1	E	273	ASP	CB-CG-OD2	6.43	124.08	118.30
1	M	325	ASP	CB-CG-OD2	6.40	124.06	118.30
1	F	325	ASP	CB-CG-OD2	6.21	123.89	118.30
1	I	273	ASP	CB-CG-OD2	6.10	123.79	118.30
1	J	248	PRO	N-CA-CB	6.07	110.59	103.30
1	A	273	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	316	ASP	CB-CG-OD2	5.75	123.48	118.30
1	H	325	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	357	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	E	325	ASP	CB-CG-OD2	5.38	123.14	118.30
1	G	273	ASP	CB-CG-OD2	5.38	123.14	118.30
1	G	368	ASP	CB-CG-OD2	5.33	123.09	118.30
1	L	368	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	368	ASP	CB-CG-OD2	5.28	123.05	118.30
1	J	325	ASP	CB-CG-OD2	5.27	123.04	118.30
1	G	325	ASP	CB-CG-OD2	5.26	123.04	118.30
1	J	316	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	368	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	298	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	298	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	325	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	368	ASP	CB-CG-OD2	5.13	122.92	118.30
1	J	265	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	316	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1124	0	1118	23	0
1	B	1124	0	1118	17	0
1	D	1125	0	1119	14	0
1	E	1168	0	1160	19	0
1	F	1129	0	1125	16	0
1	G	1125	0	1119	26	0
1	H	1113	0	1107	14	0
1	I	1124	0	1120	13	0
1	J	1118	0	1112	16	0
1	K	1136	0	1130	14	0
1	L	1133	0	1125	16	0
1	M	1129	0	1125	18	0
2	A	35	0	0	1	0
2	B	17	0	0	4	0
2	D	19	0	0	1	0
2	E	37	0	0	2	0
2	F	41	0	0	2	0
2	G	43	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	22	0	0	0	0
2	I	22	0	0	0	0
2	J	19	0	0	0	0
2	K	32	0	0	3	0
2	L	29	0	0	4	0
2	M	23	0	0	2	0
All	All	13887	0	13478	184	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 7.

All (184) 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:G:334:ARG:NH2	2:G:392:HOH:O	2.00	0.94
1:G:297:VAL:HB	2:G:426:HOH:O	1.69	0.92
1:F:260:ILE:HD12	1:F:373:MET:HG3	1.61	0.83
1:F:247:GLN:N	2:F:426:HOH:O	2.15	0.80
1:E:242:GLY:HA2	2:E:422:HOH:O	1.84	0.76
1:H:256:GLN:HG3	1:H:275:SER:HB2	1.67	0.75
1:E:314:PHE:O	1:E:315:THR:OG1	2.05	0.74
1:A:314:PHE:HB2	1:E:314:PHE:CD1	2.23	0.73
1:F:312:ILE:HG13	1:F:369:ILE:HG22	1.72	0.72
1:A:334:ARG:HH12	1:B:334:ARG:HE	1.38	0.70
1:H:312:ILE:HD12	1:H:336:ILE:HB	1.75	0.68
1:K:337:GLU:HB3	1:K:340:LYS:HE3	1.76	0.68
1:F:247:GLN:N	2:F:427:HOH:O	2.26	0.68
1:G:254:GLN:NE2	1:G:375:LYS:HG2	2.09	0.67
1:G:364:MET:SD	1:G:371:ILE:HD11	2.37	0.66
1:L:276:ARG:HD2	2:L:405:HOH:O	1.97	0.65
1:A:277:ILE:HG13	1:A:278:THR:H	1.62	0.65
1:B:365:VAL:HG13	2:B:7:HOH:O	1.97	0.65
1:A:312:ILE:HD12	1:A:336:ILE:HB	1.78	0.65
1:D:260:ILE:HD12	1:D:373:MET:HG3	1.78	0.64
1:L:277:ILE:HG23	1:L:278:THR:H	1.63	0.63
1:E:389:PRO:O	1:E:390:ALA:CB	2.46	0.62
1:L:256:GLN:NE2	2:L:407:HOH:O	2.33	0.62
1:K:247:GLN:HB3	1:K:248:PRO:HD3	1.82	0.61
1:H:315:THR:HG22	1:H:317:PHE:HB3	1.83	0.61
1:D:355:LYS:HE2	2:D:120:HOH:O	2.02	0.60
1:A:314:PHE:CD1	1:E:314:PHE:HB3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:337:GLU:HB2	1:F:340:LYS:HE2	1.84	0.59
1:K:312:ILE:CG2	1:K:315:THR:HG23	2.33	0.59
1:L:312:ILE:O	1:L:338:THR:O	2.21	0.59
1:M:254:GLN:NE2	1:M:277:ILE:HD11	2.19	0.58
1:B:256:GLN:HG3	1:B:275:SER:HB2	1.86	0.57
1:F:312:ILE:CG1	1:F:369:ILE:HG22	2.34	0.57
1:J:340:LYS:HE3	1:J:342:ASN:HD21	1.68	0.57
1:E:312:ILE:HD12	1:E:336:ILE:HB	1.87	0.57
1:M:312:ILE:HD11	1:M:336:ILE:HB	1.86	0.57
1:A:334:ARG:NH1	1:B:334:ARG:HE	2.03	0.57
1:E:266:LEU:HD11	1:E:271:LEU:HD23	1.86	0.56
1:M:260:ILE:HD12	1:M:373:MET:HG3	1.88	0.55
1:M:260:ILE:HD12	1:M:373:MET:CG	2.37	0.55
1:H:252:HIS:HD2	1:H:277:ILE:HD11	1.71	0.55
1:B:312:ILE:HD12	1:B:336:ILE:HB	1.89	0.55
1:D:315:THR:HG21	1:D:367:ALA:HB1	1.88	0.54
1:G:312:ILE:O	1:G:312:ILE:HG13	2.07	0.54
1:M:312:ILE:HG23	1:M:369:ILE:HG12	1.89	0.54
1:H:254:GLN:HG3	1:H:277:ILE:HD11	1.90	0.54
1:I:302:PHE:HD1	1:I:351:VAL:HG22	1.73	0.54
1:M:312:ILE:CD1	1:M:336:ILE:HB	2.37	0.54
1:D:357:ARG:HH11	1:D:357:ARG:CG	2.21	0.53
1:B:365:VAL:CG1	2:B:7:HOH:O	2.54	0.53
1:A:314:PHE:CB	1:E:314:PHE:CD1	2.90	0.53
1:I:260:ILE:HD13	1:I:266:LEU:HD21	1.90	0.53
1:G:254:GLN:NE2	1:G:277:ILE:CD1	2.72	0.53
1:B:282:LYS:HA	2:B:125:HOH:O	2.08	0.53
1:K:312:ILE:CD1	1:K:336:ILE:HB	2.39	0.53
1:A:335:SER:HB2	1:D:344:ASN:HD21	1.73	0.53
1:K:312:ILE:HD12	1:K:336:ILE:HB	1.90	0.53
1:H:276:ARG:HH11	1:H:286:LEU:HD23	1.74	0.52
1:J:317:PHE:CE1	1:J:319:SER:HB2	2.43	0.52
1:D:357:ARG:HG3	1:D:357:ARG:NH1	2.23	0.52
1:G:389:PRO:O	1:G:390:ALA:CB	2.58	0.52
1:E:389:PRO:O	1:E:390:ALA:HB2	2.11	0.51
1:A:304:TYR:OH	1:B:351:VAL:HG23	2.11	0.51
1:B:389:PRO:O	1:B:390:ALA:HB3	2.10	0.51
1:K:337:GLU:HB3	1:K:340:LYS:CE	2.41	0.51
1:A:313:ASN:O	1:A:314:PHE:CD1	2.63	0.51
1:G:247:GLN:N	2:G:422:HOH:O	2.44	0.51
1:A:331:GLN:HB3	1:D:377:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:VAL:HG11	1:G:293:LEU:HD21	1.93	0.50
1:I:364:MET:SD	1:I:371:ILE:HD11	2.52	0.50
1:M:248:PRO:HD2	2:M:169:HOH:O	2.09	0.50
1:M:254:GLN:NE2	1:M:375:LYS:O	2.44	0.50
1:A:314:PHE:CE1	1:E:314:PHE:O	2.65	0.50
1:E:334:ARG:HH12	1:F:334:ARG:NH1	2.09	0.50
1:L:356:ALA:O	1:L:357:ARG:HB2	2.12	0.50
1:I:312:ILE:HD12	1:I:336:ILE:HB	1.94	0.49
1:M:364:MET:CE	1:M:371:ILE:HD11	2.42	0.49
1:I:250:VAL:HG11	1:J:351:VAL:HG11	1.95	0.49
1:J:249:ALA:CB	1:J:283:VAL:HG21	2.42	0.49
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.24	0.49
1:D:357:ARG:HG3	1:D:357:ARG:HH11	1.76	0.49
1:G:247:GLN:N	1:G:248:PRO:CD	2.76	0.49
1:L:390:ALA:HA	2:L:403:HOH:O	2.13	0.49
1:J:260:ILE:HD12	1:J:373:MET:HG3	1.95	0.48
1:M:357:ARG:HH11	1:M:357:ARG:HG3	1.78	0.48
1:M:357:ARG:NH1	1:M:357:ARG:HG3	2.28	0.48
1:L:250:VAL:HG11	1:M:351:VAL:HG21	1.96	0.48
1:A:366:HIS:ND1	1:A:366:HIS:C	2.67	0.48
1:A:314:PHE:HB2	1:E:314:PHE:CG	2.49	0.48
1:J:302:PHE:HD1	1:J:351:VAL:HG22	1.79	0.48
1:F:313:ASN:HB3	1:F:314:PHE:CD2	2.48	0.48
1:H:312:ILE:CD1	1:H:336:ILE:HB	2.44	0.47
1:B:317:PHE:CE1	1:B:319:SER:HB2	2.49	0.47
1:A:267:SER:HA	2:A:60:HOH:O	2.14	0.47
1:G:334:ARG:HH11	1:G:334:ARG:HG3	1.79	0.47
1:L:375:LYS:HG2	2:L:408:HOH:O	2.14	0.47
1:D:317:PHE:HE1	1:D:333:THR:HB	1.80	0.47
1:H:356:ALA:O	1:H:357:ARG:HB2	2.14	0.47
1:L:289:ARG:HH11	1:L:289:ARG:HB3	1.80	0.47
1:E:356:ALA:O	1:E:357:ARG:HB2	2.15	0.47
1:K:315:THR:HB	2:K:410:HOH:O	2.15	0.47
1:J:337:GLU:HB3	1:J:340:LYS:HE2	1.97	0.47
1:D:276:ARG:HG3	1:D:276:ARG:O	2.15	0.47
1:J:332:CYS:SG	1:J:346:CYS:HB3	2.54	0.47
1:M:357:ARG:HH11	1:M:357:ARG:CG	2.28	0.47
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.28	0.47
1:L:256:GLN:HG2	1:L:275:SER:HB2	1.96	0.47
1:H:315:THR:O	1:H:316:ASP:HB2	2.15	0.46
1:I:315:THR:O	1:I:338:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLN:HG3	1:B:277:ILE:HD11	1.98	0.46
1:F:356:ALA:O	1:F:357:ARG:HB2	2.15	0.46
1:G:254:GLN:NE2	1:G:277:ILE:HD11	2.30	0.46
1:I:312:ILE:CD1	1:I:336:ILE:HB	2.46	0.46
1:E:334:ARG:HH12	1:F:334:ARG:CZ	2.28	0.46
1:D:332:CYS:SG	1:D:346:CYS:HB3	2.56	0.46
1:I:319:SER:OG	1:I:333:THR:HG22	2.14	0.46
1:A:326:GLU:OE1	1:G:376:HIS:NE2	2.47	0.46
1:D:317:PHE:CE1	1:D:333:THR:HB	2.51	0.46
1:H:256:GLN:CG	1:H:275:SER:HB2	2.42	0.46
1:J:297:VAL:HG12	1:J:298:ASP:O	2.16	0.46
1:M:258:SER:HB2	2:M:141:HOH:O	2.15	0.46
1:K:316:ASP:C	1:K:316:ASP:OD1	2.55	0.45
1:D:252:HIS:O	1:D:277:ILE:HG22	2.16	0.45
1:K:369:ILE:HD12	2:K:411:HOH:O	2.17	0.45
1:G:368:ASP:HB2	2:G:413:HOH:O	2.16	0.45
1:J:283:VAL:HG23	1:J:284:PHE:CD2	2.52	0.45
1:L:334:ARG:HH12	1:M:334:ARG:CZ	2.30	0.45
1:G:260:ILE:HD12	1:G:373:MET:HG3	1.98	0.45
1:L:342:ASN:HD22	1:L:342:ASN:HA	1.59	0.45
1:E:340:LYS:HG3	2:E:392:HOH:O	2.17	0.44
1:H:334:ARG:HH12	1:I:334:ARG:CZ	2.30	0.44
1:J:280:ASN:HB3	1:J:283:VAL:HG22	1.98	0.44
1:B:261:GLN:HB3	2:B:3:HOH:O	2.16	0.44
1:G:247:GLN:N	1:G:248:PRO:HD2	2.33	0.44
1:H:357:ARG:HH11	1:H:357:ARG:HG3	1.82	0.44
1:J:280:ASN:HA	1:J:281:PRO:HD3	1.85	0.44
1:L:250:VAL:HB	1:M:351:VAL:HG11	1.99	0.44
1:D:252:HIS:O	1:D:277:ILE:CG2	2.66	0.44
1:G:276:ARG:HG2	2:G:408:HOH:O	2.18	0.44
1:J:312:ILE:HD11	1:J:336:ILE:O	2.18	0.44
1:G:315:THR:O	1:G:315:THR:HG23	2.17	0.43
1:K:334:ARG:HH12	1:L:334:ARG:CZ	2.32	0.43
1:A:312:ILE:HD11	1:A:318:ALA:HB2	2.00	0.43
1:B:312:ILE:HG22	1:B:315:THR:O	2.18	0.43
1:B:389:PRO:O	1:B:390:ALA:CB	2.66	0.43
1:A:315:THR:O	1:A:316:ASP:OD1	2.37	0.43
1:E:319:SER:O	1:E:365:VAL:HG22	2.19	0.43
1:G:319:SER:O	1:G:365:VAL:HG22	2.19	0.43
1:I:280:ASN:HA	1:I:281:PRO:HD3	1.88	0.43
1:G:313:ASN:HB3	1:G:368:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:HIS:O	1:F:366:HIS:CD2	2.72	0.42
1:J:306:GLN:O	1:J:378:THR:HA	2.19	0.42
1:G:306:GLN:O	1:G:378:THR:HA	2.20	0.42
1:K:337:GLU:HB2	1:K:342:ASN:ND2	2.34	0.42
1:A:389:PRO:O	1:A:390:ALA:HB3	2.19	0.42
1:E:250:VAL:HG11	1:F:351:VAL:HG21	2.02	0.42
1:J:389:PRO:O	1:J:390:ALA:CB	2.67	0.42
1:B:329:PHE:CD2	1:B:330:LEU:HG	2.55	0.42
1:I:316:ASP:HB2	1:I:336:ILE:O	2.20	0.42
1:K:297:VAL:HG12	1:K:298:ASP:O	2.19	0.42
1:L:315:THR:O	1:L:338:THR:HG22	2.20	0.42
1:M:247:GLN:OE1	1:M:247:GLN:HA	2.19	0.42
1:A:357:ARG:NH1	1:A:357:ARG:CG	2.83	0.41
1:E:312:ILE:HD11	1:E:336:ILE:HD12	2.02	0.41
1:M:254:GLN:HB2	1:M:375:LYS:O	2.20	0.41
1:G:312:ILE:O	1:G:338:THR:O	2.38	0.41
1:F:312:ILE:HG13	1:F:369:ILE:CG2	2.47	0.41
1:I:356:ALA:O	1:I:357:ARG:HB2	2.21	0.41
1:K:277:ILE:HG13	1:K:278:THR:N	2.34	0.41
1:F:319:SER:O	1:F:365:VAL:HG22	2.21	0.41
1:B:304:TYR:CZ	1:B:381:GLY:HA3	2.55	0.41
1:G:368:ASP:CB	2:G:413:HOH:O	2.68	0.41
1:L:311:TYR:HB3	1:L:370:SER:HB2	2.02	0.41
1:J:277:ILE:HG23	1:J:278:THR:O	2.20	0.41
1:F:276:ARG:HG2	1:F:276:ARG:H	1.76	0.41
1:A:280:ASN:HA	1:A:281:PRO:HD3	1.90	0.41
1:K:359:LYS:HE3	2:K:414:HOH:O	2.21	0.40
1:E:335:SER:OG	1:G:342:ASN:HB2	2.21	0.40
1:H:297:VAL:HG12	1:H:298:ASP:O	2.21	0.40
1:H:357:ARG:HG3	1:H:357:ARG:NH1	2.37	0.40
1:A:266:LEU:HD11	1:A:271:LEU:HD23	2.04	0.40
1:G:254:GLN:CD	1:G:277:ILE:HD12	2.40	0.40
1:F:248:PRO:HG2	1:G:385:LEU:HB3	2.02	0.40
1:I:357:ARG:CG	1:I:357:ARG:HH11	2.35	0.40

There are no symmetry-related clashes.

## 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	142/163 (87%)	132 (93%)	9 (6%)	1 (1%)	25	30
1	B	142/163 (87%)	132 (93%)	10 (7%)	0	100	100
1	D	142/163 (87%)	137 (96%)	5 (4%)	0	100	100
1	E	147/163 (90%)	138 (94%)	6 (4%)	3 (2%)	9	7
1	F	142/163 (87%)	132 (93%)	10 (7%)	0	100	100
1	G	142/163 (87%)	134 (94%)	7 (5%)	1 (1%)	25	30
1	H	140/163 (86%)	133 (95%)	7 (5%)	0	100	100
1	I	141/163 (86%)	136 (96%)	5 (4%)	0	100	100
1	J	141/163 (86%)	133 (94%)	8 (6%)	0	100	100
1	K	143/163 (88%)	137 (96%)	6 (4%)	0	100	100
1	L	143/163 (88%)	132 (92%)	10 (7%)	1 (1%)	25	30
1	M	142/163 (87%)	137 (96%)	5 (4%)	0	100	100
All	All	1707/1956 (87%)	1613 (94%)	88 (5%)	6 (0%)	38	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	257	GLY
1	E	262	VAL
1	E	315	THR
1	G	257	GLY
1	A	277	ILE
1	L	277	ILE

### 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	123/136 (90%)	121 (98%)	2 (2%)	68	82
1	B	123/136 (90%)	118 (96%)	5 (4%)	35	48
1	D	123/136 (90%)	118 (96%)	5 (4%)	35	48
1	E	128/136 (94%)	126 (98%)	2 (2%)	68	82
1	F	124/136 (91%)	123 (99%)	1 (1%)	85	93
1	G	123/136 (90%)	120 (98%)	3 (2%)	54	72
1	H	122/136 (90%)	118 (97%)	4 (3%)	43	59
1	I	124/136 (91%)	123 (99%)	1 (1%)	85	93
1	J	122/136 (90%)	119 (98%)	3 (2%)	53	70
1	K	125/136 (92%)	119 (95%)	6 (5%)	30	40
1	L	124/136 (91%)	121 (98%)	3 (2%)	54	72
1	M	124/136 (91%)	119 (96%)	5 (4%)	36	50
All	All	1485/1632 (91%)	1445 (97%)	40 (3%)	50	67

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	ARG
1	A	314	PHE
1	B	275	SER
1	B	276	ARG
1	B	277	ILE
1	B	334	ARG
1	B	351	VAL
1	D	289	ARG
1	D	313	ASN
1	D	340	LYS
1	D	351	VAL
1	D	357	ARG
1	E	289	ARG
1	E	335	SER
1	F	289	ARG
1	G	334	ARG
1	G	351	VAL
1	G	374	SER

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Mol	Chain	Res	Type
1	H	277	ILE
1	H	338	THR
1	H	341	THR
1	H	351	VAL
1	I	276	ARG
1	J	277	ILE
1	J	314	PHE
1	J	317	PHE
1	K	277	ILE
1	K	289	ARG
1	K	315	THR
1	K	316	ASP
1	K	340	LYS
1	K	374	SER
1	L	246	ASN
1	L	289	ARG
1	L	351	VAL
1	M	258	SER
1	M	267	SER
1	M	342	ASN
1	M	357	ARG
1	M	374	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	GLN
1	B	342	ASN
1	D	313	ASN
1	F	366	HIS
1	F	376	HIS
1	G	254	GLN
1	H	376	HIS
1	I	254	GLN
1	J	342	ASN
1	K	254	GLN
1	L	342	ASN
1	M	254	GLN
1	M	342	ASN

### 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	144/163 (88%)	-0.08	5 (3%)	44	51	2, 5, 15, 21	0
1	B	144/163 (88%)	0.25	8 (5%)	25	32	2, 5, 14, 19	0
1	D	144/163 (88%)	0.56	21 (14%)	3	4	2, 5, 12, 16	0
1	E	149/163 (91%)	-0.14	6 (4%)	39	46	2, 5, 16, 27	0
1	F	144/163 (88%)	-0.28	3 (2%)	64	70	2, 5, 13, 24	0
1	G	144/163 (88%)	-0.11	5 (3%)	44	51	2, 5, 15, 23	0
1	H	142/163 (87%)	0.31	11 (7%)	14	19	2, 5, 13, 18	0
1	I	143/163 (87%)	-0.01	7 (4%)	30	37	2, 5, 14, 20	0
1	J	143/163 (87%)	0.20	6 (4%)	37	44	2, 5, 11, 16	0
1	K	145/163 (88%)	0.02	9 (6%)	21	28	2, 5, 14, 24	0
1	L	145/163 (88%)	-0.13	5 (3%)	46	53	2, 5, 14, 22	0
1	M	144/163 (88%)	-0.08	4 (2%)	53	61	2, 5, 14, 21	0
All	All	1731/1956 (88%)	0.04	90 (5%)	28	35	2, 5, 14, 27	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	390	ALA	9.6
1	B	390	ALA	9.1
1	A	390	ALA	7.6
1	G	390	ALA	7.0
1	F	390	ALA	6.8
1	D	390	ALA	6.7
1	B	277	ILE	6.4
1	H	258	SER	6.4
1	L	390	ALA	6.1
1	D	314	PHE	5.7
1	M	258	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	M	390	ALA	5.6
1	D	315	THR	5.4
1	I	314	PHE	5.3
1	H	387	GLU	5.0
1	B	278	THR	4.4
1	H	314	PHE	4.4
1	J	258	SER	4.4
1	K	317	PHE	4.1
1	E	314	PHE	4.0
1	L	277	ILE	3.9
1	A	277	ILE	3.9
1	H	388	ALA	3.9
1	B	258	SER	3.8
1	D	258	SER	3.7
1	G	316	ASP	3.7
1	H	315	THR	3.7
1	F	289	ARG	3.5
1	D	257	GLY	3.5
1	H	247	GLN	3.5
1	B	314	PHE	3.4
1	D	312	ILE	3.4
1	D	247	GLN	3.3
1	F	314	PHE	3.3
1	A	289	ARG	3.3
1	I	389	PRO	3.2
1	D	289	ARG	3.2
1	G	257	GLY	3.2
1	D	277	ILE	3.2
1	H	263	LYS	3.0
1	D	311	TYR	3.0
1	I	267	SER	3.0
1	B	289	ARG	3.0
1	I	264	ASN	3.0
1	D	339	GLY	2.9
1	I	289	ARG	2.9
1	E	242	GLY	2.9
1	B	339	GLY	2.8
1	K	316	ASP	2.8
1	H	277	ILE	2.8
1	D	387	GLU	2.8
1	K	276	ARG	2.7
1	K	247	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	314	PHE	2.7
1	E	264	ASN	2.7
1	K	277	ILE	2.6
1	H	289	ARG	2.6
1	J	341	THR	2.6
1	K	314	PHE	2.6
1	L	389	PRO	2.6
1	K	289	ARG	2.5
1	D	340	LYS	2.5
1	L	289	ARG	2.5
1	G	317	PHE	2.5
1	M	264	ASN	2.5
1	J	357	ARG	2.5
1	K	263	LYS	2.5
1	A	314	PHE	2.5
1	E	289	ARG	2.4
1	G	315	THR	2.3
1	L	267	SER	2.3
1	I	247	GLN	2.3
1	D	338	THR	2.3
1	D	267	SER	2.2
1	D	337	GLU	2.2
1	J	340	LYS	2.2
1	J	314	PHE	2.2
1	B	357	ARG	2.2
1	E	337	GLU	2.1
1	D	317	PHE	2.1
1	A	339	GLY	2.1
1	H	339	GLY	2.1
1	I	387	GLU	2.1
1	D	342	ASN	2.1
1	K	258	SER	2.1
1	D	313	ASN	2.0
1	J	390	ALA	2.0
1	D	256	GLN	2.0
1	H	276	ARG	2.0
1	D	371	ILE	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.