



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:09 AM GMT

PDB ID : 4CDK  
Title : Structure of ZNRF3-RSPO1  
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Deposited on : 2013-11-01  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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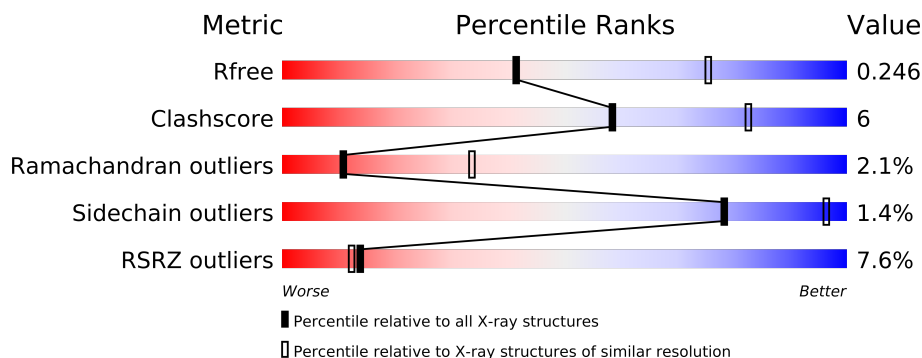
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	164	
1	B	164	
1	C	164	
1	D	164	
2	E	126	
2	F	126	
2	G	126	
2	H	126	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7982 atoms, of which 0 are hydrogen and 0 are deuterium.

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 E3 UBIQUITIN-PROTEIN LIGASE ZNR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	1	0
			1177	739	206	227	5			
1	B	156	Total	C	N	O	S	0	1	0
			1193	750	210	228	5			
1	C	155	Total	C	N	O	S	0	0	0
			1184	743	206	230	5			
1	D	152	Total	C	N	O	S	0	0	0
			1167	735	203	224	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
A	55	SER	-	EXPRESSION TAG	UNP Q5SSZ7
A	209	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
A	210	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
A	211	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
A	212	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	213	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	214	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	215	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	216	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
A	217	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
B	54	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
B	55	SER	-	EXPRESSION TAG	UNP Q5SSZ7
B	209	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
B	210	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
B	211	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
B	212	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
B	213	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
B	214	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
B	215	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
B	216	HIS	-	EXPRESSION TAG	UNP Q5SSZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	217	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	54	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
C	55	SER	-	EXPRESSION TAG	UNP Q5SSZ7
C	209	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
C	210	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
C	211	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
C	212	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	213	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	214	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	215	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	216	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
C	217	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
D	54	GLY	-	EXPRESSION TAG	UNP Q5SSZ7
D	55	SER	-	EXPRESSION TAG	UNP Q5SSZ7
D	209	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
D	210	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
D	211	ALA	-	EXPRESSION TAG	UNP Q5SSZ7
D	212	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
D	213	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
D	214	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
D	215	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
D	216	HIS	-	EXPRESSION TAG	UNP Q5SSZ7
D	217	HIS	-	EXPRESSION TAG	UNP Q5SSZ7

- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	110	Total	C	N	O	S	0	1	0
			827	509	146	154	18			
2	F	103	Total	C	N	O	S	0	1	0
			783	483	138	144	18			
2	G	107	Total	C	N	O	S	0	0	0
			802	494	141	149	18			
2	H	105	Total	C	N	O	S	0	1	0
			794	489	140	147	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
E	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
E	146	ALA	-	EXPRESSION TAG	UNP Q2MKA7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
E	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
E	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
E	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
E	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
E	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
E	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
E	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7
F	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
F	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
F	146	ALA	-	EXPRESSION TAG	UNP Q2MKA7
F	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
F	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
F	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
F	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
F	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
F	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
F	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
F	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
G	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
G	146	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
H	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
H	146	ALA	-	EXPRESSION TAG	UNP Q2MKA7
H	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
H	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
H	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	11	Total 11	O 11	0	0
3	C	14	Total 14	O 14	0	0
3	D	5	Total 5	O 5	0	0
3	E	6	Total 6	O 6	0	0
3	F	1	Total 1	O 1	0	0
3	G	6	Total 6	O 6	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

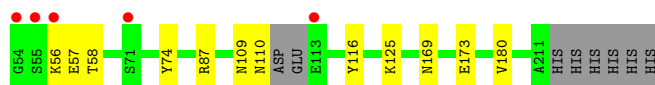
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain A: 



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain B: 



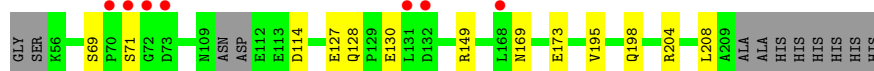
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain C: 



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain D: 



- Molecule 2: R-SPONDIN-1

Chain E: 



- Molecule 2: R-SPONDIN-1

Chain F: 



HIS

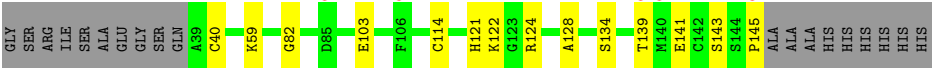
HIS

HIS

HIS

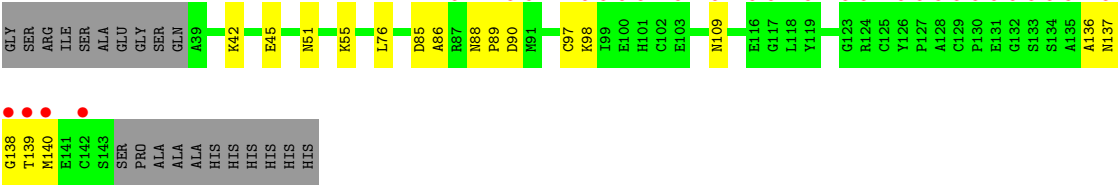
• Molecule 2: R-SPONDIN-1

Chain G: 



• Molecule 2: R-SPONDIN-1

Chain H: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.70Å 80.16Å 82.98Å 66.27° 81.36° 80.66°	Depositor
Resolution (Å)	44.71 – 2.80 75.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (44.71-2.80) 95.3 (75.63-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.82Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.218 , 0.246 0.217 , 0.246	Depositor DCC
$R_{free}$ test set	1437 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.6	EDS
Estimated twinning fraction	0.116 for -h,-l,-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28148 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.28	0/1200	0.52	0/1626
1	B	0.32	0/1216	0.58	0/1646
1	C	0.29	0/1204	0.56	0/1633
1	D	0.27	0/1186	0.48	0/1605
2	E	0.32	0/847	0.64	1/1137 (0.1%)
2	F	0.34	0/802	0.68	0/1077
2	G	0.33	0/819	0.64	0/1101
2	H	0.31	0/813	0.68	0/1092
All	All	0.30	0/8087	0.59	1/10917 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	132	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1177	0	0	6	1
1	B	1193	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1184	0	0	8	0
1	D	1167	0	0	7	1
2	E	827	0	0	6	0
2	F	783	0	0	6	0
2	G	802	0	0	6	1
2	H	794	0	0	7	0
3	A	12	0	0	1	0
3	B	11	0	0	3	0
3	C	14	0	0	5	0
3	D	5	0	0	2	0
3	E	6	0	0	0	0
3	F	1	0	0	0	0
3	G	6	0	0	3	0
All	All	7982	0	0	49	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (49) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:180:VAL:N	3:B:2003:HOH:O	2.08	0.85
1:C:101:MET:O	3:C:2007:HOH:O	2.02	0.77
1:A:116:TYR:O	1:B:74:TYR:OH	2.16	0.64
2:H:136:ALA:O	2:H:138:GLY:N	2.31	0.63
2:E:103:GLU:N	2:E:103:GLU:OE1	2.33	0.61
1:B:125:LYS:N	3:B:2007:HOH:O	2.33	0.61
2:F:121:HIS:O	2:F:124:ARG:N	2.35	0.60
2:H:90:ASP:OD1	2:H:90:ASP:N	2.33	0.59
1:A:80:GLY:O	1:A:190:LYS:NZ	2.36	0.59
2:F:134:SER:OG	2:F:137:ASN:O	2.22	0.58
2:H:85:ASP:OD1	2:H:86:ALA:N	2.37	0.57
2:E:121:HIS:O	2:E:124:ARG:N	2.38	0.57
2:G:103:GLU:OE1	2:G:103:GLU:N	2.37	0.57
1:C:114:ASP:OD1	1:C:149:ARG:NH2	2.39	0.56
1:A:83:GLY:O	1:A:84:ARG:NH1	2.39	0.55
1:D:127:GLU:OE2	2:H:51:ASN:ND2	2.41	0.54
3:A:2005:HOH:O	2:E:93[A]:LYS:NZ	2.40	0.54
2:F:103:GLU:N	2:F:103:GLU:OE1	2.41	0.54
1:B:57:GLU:O	3:B:2001:HOH:O	2.19	0.54
2:F:45:GLU:OE2	2:F:55:LYS:NZ	2.42	0.53
2:G:143:SER:OG	2:G:145:PRO:O	2.28	0.52
1:B:109:ASN:OD1	1:B:110:ASN:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:87:ARG:NH1	1:B:169:ASN:OD1	2.45	0.50
2:F:121:HIS:O	2:F:123:GLY:N	2.45	0.50
2:G:82:GLY:N	3:G:2003:HOH:O	2.44	0.49
2:H:97:CYS:SG	2:H:98:LYS:N	2.86	0.49
2:H:45:GLU:OE2	2:H:55:LYS:NZ	2.46	0.47
1:C:177:LYS:N	3:C:2013:HOH:O	2.48	0.47
2:H:138:GLY:O	2:H:140:MET:N	2.48	0.47
1:D:128:GLN:NE2	1:D:130:GLU:OE2	2.48	0.46
2:G:121:HIS:O	2:G:124:ARG:N	2.49	0.46
1:C:110:ASN:O	1:C:112:GLU:N	2.49	0.45
2:F:121:HIS:N	2:F:124:ARG:O	2.50	0.45
1:A:87:ARG:NH1	1:A:169:ASN:O	2.50	0.44
1:D:69:SER:OG	1:D:71:SER:OG	2.35	0.44
1:C:206:GLN:NE2	3:C:2005:HOH:O	2.50	0.44
2:E:90:ASP:N	2:E:90:ASP:OD1	2.52	0.43
1:C:112:GLU:O	1:C:114:ASP:N	2.51	0.43
2:E:138:GLY:O	2:E:140:MET:N	2.52	0.43
1:A:74:TYR:OH	1:B:116:TYR:O	2.37	0.43
1:C:149:ARG:NH2	3:C:2008:HOH:O	2.52	0.42
2:E:121:HIS:O	2:E:123:GLY:N	2.53	0.42
2:G:114:CYS:N	3:G:2005:HOH:O	2.53	0.42
2:G:59:LYS:N	3:G:2001:HOH:O	2.52	0.42
1:D:198:GLN:O	3:D:2005:HOH:O	2.22	0.41
1:D:195:VAL:O	3:D:2005:HOH:O	2.21	0.41
3:C:2009:HOH:O	1:D:204:ARG:NH1	2.53	0.41
1:D:114:ASP:O	1:D:149:ARG:NH2	2.54	0.41
1:A:77:HIS:ND1	1:C:76:THR:OG1	2.54	0.41

All (2) 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	Distance(Å)	Clash(Å)
1:B:173:GLU:OE2	1:D:169:ASN:ND2[1_655]	2.16	0.04
1:A:170:GLN:NE2	2:G:128:ALA:O[1_545]	2.18	0.02

## 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	151/164 (92%)	146 (97%)	4 (3%)	1 (1%)	30	69
1	B	153/164 (93%)	149 (97%)	3 (2%)	1 (1%)	30	69
1	C	153/164 (93%)	147 (96%)	5 (3%)	1 (1%)	30	69
1	D	148/164 (90%)	145 (98%)	2 (1%)	1 (1%)	30	69
2	E	109/126 (86%)	96 (88%)	10 (9%)	3 (3%)	8	24
2	F	102/126 (81%)	88 (86%)	10 (10%)	4 (4%)	5	15
2	G	105/126 (83%)	92 (88%)	8 (8%)	5 (5%)	4	10
2	H	104/126 (82%)	94 (90%)	5 (5%)	5 (5%)	4	10
All	All	1025/1160 (88%)	957 (93%)	47 (5%)	21 (2%)	11	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	58	THR
1	D	173	GLU
2	E	122	LYS
2	E	140	MET
2	F	42	LYS
2	F	86	ALA
2	F	122	LYS
2	F	141	GLU
2	G	122	LYS
2	H	42	LYS
2	H	89	PRO
1	A	207	HIS
1	C	110	ASN
2	G	139	THR
2	G	141	GLU
2	H	109	ASN
2	H	137	ASN
2	H	139	THR
2	G	134	SER
2	E	135	ALA
2	G	40	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	128/135 (95%)	128 (100%)	0	100	100
1	B	128/135 (95%)	127 (99%)	1 (1%)	89	98
1	C	127/135 (94%)	126 (99%)	1 (1%)	89	98
1	D	126/135 (93%)	125 (99%)	1 (1%)	89	98
2	E	95/105 (90%)	92 (97%)	3 (3%)	51	85
2	F	90/105 (86%)	86 (96%)	4 (4%)	39	75
2	G	92/105 (88%)	92 (100%)	0	100	100
2	H	91/105 (87%)	89 (98%)	2 (2%)	64	92
All	All	877/960 (91%)	865 (99%)	12 (1%)	78	96

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

Mol	Chain	Res	Type
1	B	56	LYS
1	C	207	HIS
1	D	208	LEU
2	E	37	SER
2	E	134	SER
2	E	144	SER
2	F	56	CYS
2	F	91	MET
2	F	129	CYS
2	F	134	SER
2	H	76	LEU
2	H	88	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	152/164 (92%)	0.13	4 (2%)	53	54	30, 57, 116, 142	0
1	B	156/164 (95%)	0.17	5 (3%)	45	46	29, 59, 121, 148	0
1	C	155/164 (94%)	0.09	5 (3%)	45	46	34, 59, 128, 155	0
1	D	152/164 (92%)	0.23	7 (4%)	31	31	32, 62, 119, 137	0
2	E	110/126 (87%)	0.29	7 (6%)	19	17	39, 76, 151, 179	0
2	F	103/126 (81%)	0.87	17 (16%)	2	2	51, 149, 186, 205	0
2	G	107/126 (84%)	0.24	5 (4%)	30	30	46, 80, 148, 161	0
2	H	105/126 (83%)	1.43	29 (27%)	1	1	48, 147, 215, 246	0
All	All	1040/1160 (89%)	0.38	79 (7%)	14	12	29, 69, 179, 246	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	GLY	9.8
2	H	127	PRO	9.2
2	H	139	THR	9.0
2	E	37	SER	8.0
2	F	136	ALA	6.8
2	F	138	GLY	6.8
1	B	54	GLY	6.3
2	F	40	CYS	6.3
2	H	137	ASN	6.1
2	H	128	ALA	5.5
2	H	117	GLY	5.5
2	H	90	ASP	5.4
2	H	133	SER	5.4
2	F	116	GLU	5.2
2	F	139	THR	4.8
2	H	129	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
2	H	87	ARG	4.5
2	F	101	HIS	4.4
1	A	110	ASN	4.4
1	D	70	PRO	4.3
2	F	90	ASP	4.2
2	H	140	MET	4.0
2	F	140	MET	4.0
2	H	123	GLY	3.9
2	F	137	ASN	3.9
2	F	108	HIS	3.9
2	F	128	ALA	3.8
1	C	210	ALA	3.8
2	H	103	GLU	3.7
2	G	145	PRO	3.7
2	H	99	ILE	3.7
2	H	132	GLY	3.6
1	D	72	GLY	3.6
1	D	73	ASP	3.6
2	H	91	MET	3.5
2	H	101	HIS	3.4
2	H	131	GLU	3.3
2	E	36	GLY	3.3
2	F	135	ALA	3.3
1	C	111	ASP	3.3
2	G	106	PHE	3.1
2	E	136	ALA	3.1
2	E	139	THR	3.0
1	C	108	ASN	3.0
2	H	98	LYS	3.0
2	H	109	ASN	3.0
2	F	127	PRO	2.9
2	H	116	GLU	2.9
2	E	138	GLY	2.9
2	H	126	TYR	2.8
2	E	137	ASN	2.8
2	H	130	PRO	2.8
2	F	91	MET	2.7
2	E	131	GLU	2.6
1	B	71	SER	2.6
1	D	71	SER	2.6
2	G	85	ASP	2.6
2	H	124	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	70	PRO	2.5
1	A	131	LEU	2.5
2	H	135	ALA	2.4
2	F	117	GLY	2.3
1	C	211	ALA	2.3
1	B	55	SER	2.3
2	H	119	TYR	2.3
2	F	122	LYS	2.3
2	G	140	MET	2.3
1	D	131	LEU	2.2
2	F	142	CYS	2.2
1	B	56	LYS	2.2
1	C	173	GLU	2.2
2	H	100	GLU	2.2
2	H	142	CYS	2.1
2	H	134	SER	2.1
1	D	168	LEU	2.1
1	A	109	ASN	2.0
1	B	113	GLU	2.0
2	G	139	THR	2.0
1	D	132	ASP	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.