



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:02 pm GMT

PDB ID : 4CDK  
Title : Structure of ZNRF3-RSPO1  
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Clevers, H.; Gros, P.  
Deposited on : 2013-11-01  
Resolution : 2.80 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 : trunk28620  
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) : recalc28949

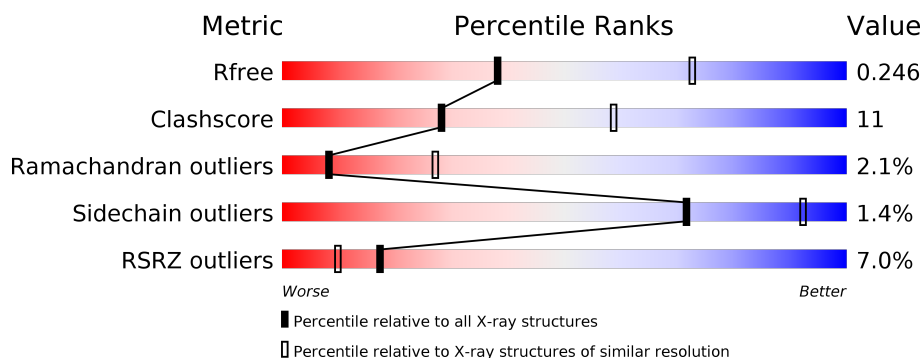
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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. 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	164	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	164	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• 5%</div> </div> </div>
1	C	164	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	D	164	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
2	E	126	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>• 13%</div> </div> </div>
2	F	126	<div> <div>13%</div> <div> <div></div> <div>48%</div> <div>31%</div> <div>• 18%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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 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 E3 UBIQUITIN-PROTEIN LIGASE ZNRF3.

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

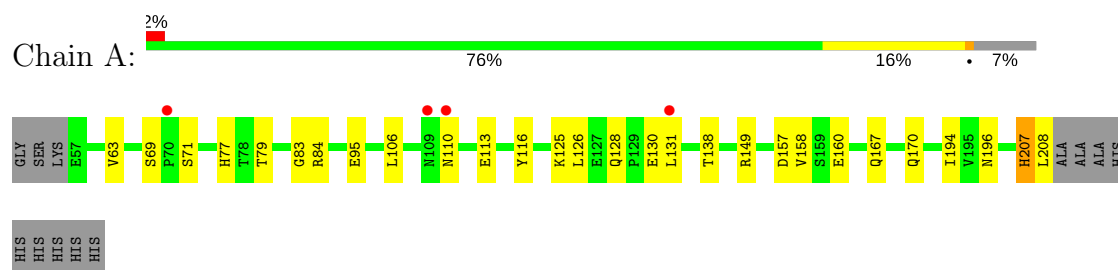
- Molecule 3 is water.

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

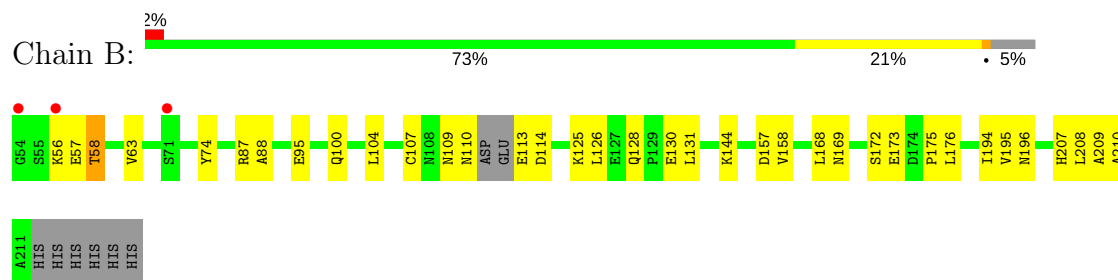
### 3 Residue-property plots [i](#)

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.

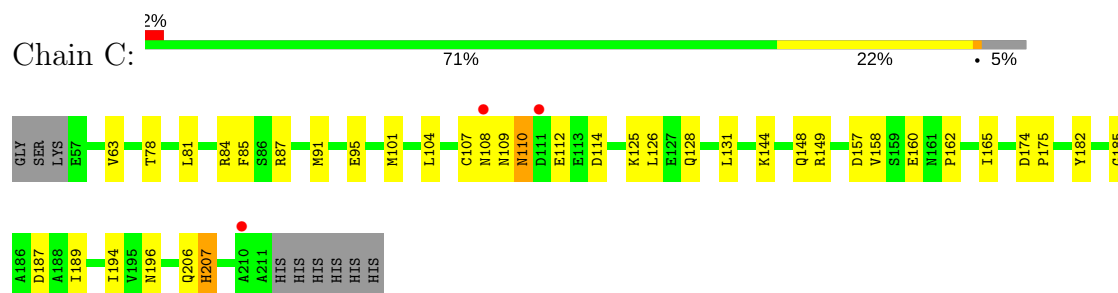
#### • Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



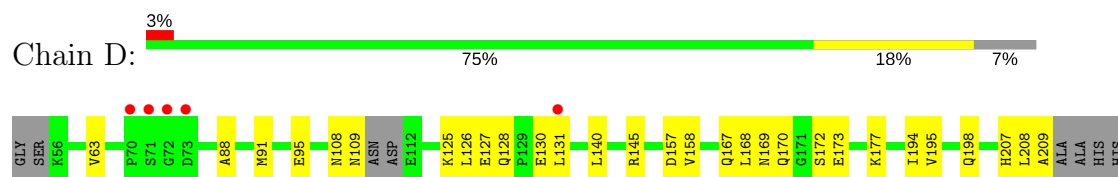
#### • Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



#### • Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



#### • Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3



HIS  
HIS  
HIS

## ● Molecule 2: R-SPONDIN-1



GLY SER ARG ILE SER ALA GLU G36 S37 F61 I62 R70 N88 P89 D90 N91 N92 K93 E103 F106 T112 K113 H121 K122 G123 C129 P130 E131 G132 S133 S134 A135 A136 N137 G138 T139 M140 E141 S144 P145 ALA ALA ALA HIS HIS HIS HIS HIS HIS

## ● Molecule 2: R-SPONDIN-1



GLY SER ARG ILE SER ALA GLU G40 A41 K42 G43 E45 G52 K55 C56 L60 F61 E85 R66 N67 I69 R70 V72 P77 A86 R87 N88 P89 D90 N91 N92 C97 K98 I99 E100 H101 E102 C103 A104 C105 F106 S107 H108 N109 F110

G111 T112 C113 C114 K115 E116 G117 L118 Y119 L120 K122 G123 R124 P127 A128 C129 S133 S134 A135 A136 G138 N137 T139 M140 C142 SER PRO ALA ALA HIS HIS HIS HIS HIS

## ● Molecule 2: R-SPONDIN-1



GLY SER ARG ILE SER ALA GLU G39 C40 L46 G52 F61 R70 Q71 V72 F84 D85 N92 K96 E103 F106 S107 T112 K113 E116 G117 H121 K122 Y126 P127 A128 S133 S134 A135 A136 N137 G138 T139 M140 E141 C142 S144

P145 ALA ALA ALA HIS HIS HIS HIS HIS

## ● Molecule 2: R-SPONDIN-1



GLY SER ARG ILE SER ALA GLU G39 C40 A41 K42 G44 C47 N51 G52 L60 F61 V72 C75 L76 P77 D85 A86 R87 N88 P89 D90 N91 N92 K93 C97 K98 I99 E100 H101 C102 E103 A104 M109 K113 C114 K115 E116 G117 L118 Y119 L120

H121 K122 G123 R124 C125 Y126 P127 A128 C129 P130 E131 G132 S133 S134 A135 A136 N137 G138 T139 M140 E141 C142 S143 SER PRO ALA ALA ALA HIS HIS HIS HIS HIS

## 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) 82.2 (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 0.216 , 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> )	0.31 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.116 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.91	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.

<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	0.28	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 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	1177	0	1178	20	1
1	B	1193	0	1197	26	1
1	C	1184	0	1180	27	0
1	D	1167	0	1172	22	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	827	0	795	18	0
2	F	783	0	752	25	0
2	G	802	0	766	20	1
2	H	794	0	762	31	0
3	A	12	0	0	0	0
3	B	11	0	0	2	0
3	C	14	0	0	3	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	0	0
All	All	7982	0	7802	175	2

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 11.

All (175) 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:57:GLU:HA	1:B:58:THR:HB	1.43	0.97
2:H:101:HIS:HB3	2:H:125:CYS:HB2	1.60	0.82
1:A:63:VAL:HG11	1:A:194:ILE:HG21	1.62	0.80
1:C:101:MET:O	3:C:2007:HOH:O	2.02	0.77
1:A:110:ASN:HD21	2:E:93[A]:LYS:HE2	1.49	0.76
2:F:134:SER:N	2:F:135:ALA:HA	2.02	0.75
1:A:95:GLU:HB3	1:B:95:GLU:HB3	1.72	0.72
2:G:103:GLU:OE2	2:G:113:LYS:HG2	1.91	0.71
2:F:41:ALA:HB3	2:F:44:CYS:HB3	1.72	0.70
2:H:120:LEU:H	2:H:141:GLU:HA	1.56	0.70
1:C:95:GLU:HB3	1:D:95:GLU:HB3	1.74	0.69
2:E:106:PHE:HB2	2:E:112:THR:HG23	1.75	0.69
2:G:52:GLY:HA3	2:G:72:VAL:HG13	1.74	0.68
1:C:112:GLU:HG2	2:G:96:LYS:H	1.57	0.68
1:B:144:LYS:HG2	1:B:176:LEU:HD21	1.74	0.67
1:C:174:ASP:OD1	1:C:175:PRO:HD2	1.96	0.66
1:C:63:VAL:HG11	1:C:194:ILE:HG21	1.78	0.65
2:G:106:PHE:HB2	2:G:112:THR:HG23	1.77	0.65
2:G:121:HIS:CE1	2:G:122:LYS:HD3	2.32	0.65
2:F:91:MET:HE1	2:F:93:LYS:HE3	1.79	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ASN:HB2	2:E:91:MET:O	1.99	0.62
2:E:103:GLU:OE2	2:E:113:LYS:HG2	1.99	0.62
1:C:196:ASN:HA	2:G:70:ARG:HD2	1.82	0.61
2:E:103:GLU:N	2:E:103:GLU:OE1	2.33	0.61
1:B:113:GLU:HG3	1:B:114:ASP:N	2.15	0.61
1:D:126:LEU:HD12	1:D:158:VAL:HG12	1.82	0.61
2:H:114:CYS:SG	2:H:120:LEU:HB2	2.41	0.60
2:F:140:MET:O	2:F:141:GLU:HG3	2.02	0.60
1:A:128:GLN:HG3	1:A:160:GLU:HB3	1.83	0.59
1:A:130:GLU:HG2	1:A:131:LEU:HD12	1.83	0.59
1:A:138:THR:HB	1:A:167:GLN:NE2	2.18	0.59
2:F:133:SER:O	2:F:142:CYS:HA	2.03	0.58
1:D:63:VAL:HG11	1:D:194:ILE:HG21	1.84	0.58
1:A:110:ASN:ND2	2:E:93[A]:LYS:HE2	2.18	0.58
2:H:120:LEU:O	2:H:142:CYS:HB2	2.03	0.58
1:A:207:HIS:CD2	1:A:208:LEU:HG	2.39	0.57
2:F:106:PHE:HB2	2:F:112:THR:OG1	2.03	0.57
2:E:62:ILE:HG23	2:E:93[A]:LYS:HD2	1.86	0.57
2:H:85:ASP:OD1	2:H:86:ALA:N	2.37	0.57
2:H:40:CYS:HB3	2:H:47:CYS:HB3	1.86	0.57
2:G:103:GLU:OE1	2:G:103:GLU:N	2.37	0.57
2:G:139:THR:HG22	2:G:140:MET:H	1.69	0.57
2:H:99:ILE:HG22	2:H:100:GLU:HB3	1.86	0.57
2:F:97:CYS:SG	2:F:99:ILE:HG12	2.45	0.57
1:B:113:GLU:HG3	1:B:114:ASP:H	1.69	0.56
1:C:114:ASP:OD1	1:C:149:ARG:NH2	2.39	0.56
2:H:121:HIS:CE1	2:H:131:GLU:HG3	2.40	0.56
1:B:57:GLU:HA	1:B:58:THR:CB	2.27	0.56
1:A:110:ASN:O	1:A:113:GLU:HB2	2.07	0.55
2:G:133:SER:HB3	2:G:144:SER:HA	1.88	0.55
2:F:134:SER:OG	2:F:137:ASN:O	2.22	0.55
1:A:83:GLY:O	1:A:84:ARG:NH1	2.39	0.55
2:F:114:CYS:HB2	2:F:120:LEU:HB2	1.89	0.55
1:C:125:LYS:HA	1:C:157:ASP:HB3	1.90	0.54
1:C:91:MET:HG2	1:C:207:HIS:CD2	2.42	0.54
1:B:126:LEU:HD12	1:B:158:VAL:HG12	1.87	0.54
1:A:125:LYS:HA	1:A:157:ASP:HB3	1.88	0.54
1:D:127:GLU:OE2	2:H:51:ASN:ND2	2.41	0.54
1:C:87:ARG:O	1:C:175:PRO:HB3	2.08	0.54
2:H:52:GLY:HA3	2:H:72:VAL:HG13	1.90	0.54
1:B:57:GLU:O	3:B:2001:HOH:O	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:MET:HB3	1:D:207:HIS:NE2	2.23	0.53
1:D:91:MET:HB3	1:D:207:HIS:HE2	1.73	0.53
2:H:113:LYS:HG3	2:H:141:GLU:OE2	2.08	0.53
2:H:90:ASP:OD1	2:H:90:ASP:N	2.33	0.53
1:B:209:ALA:HA	1:B:210:ALA:HB3	1.91	0.53
1:B:196:ASN:HA	2:F:70:ARG:HD2	1.91	0.53
2:H:140:MET:O	2:H:141:GLU:HB2	2.09	0.53
2:G:143:SER:OG	2:G:145:PRO:O	2.28	0.52
1:C:104:LEU:HA	1:C:107:CYS:SG	2.50	0.51
2:G:140:MET:O	2:G:141:GLU:HB3	2.10	0.51
1:B:63:VAL:HG11	1:B:194:ILE:HG21	1.92	0.51
2:F:60:LEU:HD22	2:F:77:PRO:HA	1.93	0.51
2:G:136:ALA:HB1	2:G:137:ASN:HA	1.92	0.51
1:D:108:ASN:HB2	1:D:145:ARG:HE	1.76	0.51
1:C:144:LYS:HE3	1:C:148:GLN:NE2	2.25	0.51
2:E:121:HIS:CE1	2:E:122:LYS:HG2	2.46	0.50
2:H:114:CYS:SG	2:H:120:LEU:HD13	2.51	0.50
1:B:109:ASN:OD1	1:B:110:ASN:N	2.44	0.50
1:B:125:LYS:HA	1:B:157:ASP:HB3	1.93	0.50
2:F:52:GLY:HA3	2:F:72:VAL:HG13	1.93	0.50
2:F:103:GLU:N	2:F:103:GLU:OE1	2.41	0.50
2:G:121:HIS:HB3	2:G:126:TYR:CE2	2.46	0.50
2:F:121:HIS:O	2:F:123:GLY:N	2.45	0.50
2:H:44:CYS:HB3	2:H:75:CYS:SG	2.50	0.49
2:H:40:CYS:CB	2:H:47:CYS:HB3	2.42	0.49
1:C:84:ARG:HB2	1:C:182:TYR:CZ	2.47	0.49
1:C:144:LYS:HE3	1:C:148:GLN:HE21	1.77	0.49
2:H:98:LYS:HG3	2:H:109:ASN:OD1	2.13	0.49
2:E:129:CYS:HB3	2:E:134:SER:HB3	1.95	0.49
2:H:104:ALA:HB3	2:H:113:LYS:HB3	1.94	0.49
1:D:170:GLN:C	1:D:172:SER:H	2.16	0.49
2:H:135:ALA:HB2	2:H:142:CYS:SG	2.53	0.49
1:C:128:GLN:HG3	1:C:160:GLU:HB3	1.94	0.48
1:A:126:LEU:HD12	1:A:158:VAL:HG12	1.95	0.48
1:D:125:LYS:HA	1:D:157:ASP:HB3	1.95	0.48
2:G:144:SER:HB2	2:G:145:PRO:HD3	1.95	0.48
2:F:44:CYS:HA	2:F:56:CYS:HA	1.94	0.48
2:H:60:LEU:HD22	2:H:77:PRO:HA	1.95	0.48
2:H:97:CYS:SG	2:H:98:LYS:N	2.86	0.48
2:H:99:ILE:HG22	2:H:100:GLU:CB	2.43	0.48
1:C:126:LEU:HD12	1:C:158:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLN:HB2	1:D:131:LEU:HD13	1.96	0.48
1:B:207:HIS:NE2	1:B:209:ALA:HB3	2.28	0.47
1:D:108:ASN:CB	1:D:145:ARG:HE	2.27	0.47
1:A:128:GLN:HB2	1:A:131:LEU:HD13	1.96	0.47
2:H:42:LYS:HA	2:H:42:LYS:HD2	1.53	0.47
1:B:130:GLU:HG2	1:B:131:LEU:HD12	1.96	0.47
2:F:61:PHE:CD2	2:F:92:ASN:HB3	2.50	0.47
2:H:138:GLY:O	2:H:140:MET:N	2.48	0.47
1:B:87:ARG:NH1	1:B:169:ASN:OD1	2.45	0.46
1:D:130:GLU:HG2	1:D:131:LEU:HD12	1.98	0.46
1:B:209:ALA:HA	1:B:210:ALA:CB	2.46	0.46
1:C:81:LEU:HB2	1:C:187:ASP:HB3	1.97	0.46
1:B:128:GLN:HB2	1:B:131:LEU:HD13	1.98	0.46
2:E:106:PHE:HB2	2:E:112:THR:CG2	2.45	0.46
2:E:135:ALA:HB2	2:E:141:GLU:O	2.15	0.46
1:D:140:LEU:HD21	1:D:168:LEU:HA	1.98	0.45
2:F:121:HIS:O	2:F:124:ARG:N	2.35	0.45
2:G:84:PHE:CZ	2:G:107:SER:HA	2.52	0.45
1:B:104:LEU:HA	1:B:107:CYS:SG	2.57	0.45
2:E:135:ALA:HB1	2:E:138:GLY:HA3	1.98	0.45
1:C:162:PRO:O	1:C:165:ILE:HG13	2.17	0.45
1:B:100:GLN:HG3	1:B:195:VAL:HG11	1.99	0.44
1:A:79:THR:HG22	1:C:78:THR:OG1	2.18	0.44
1:D:91:MET:HB3	1:D:207:HIS:CD2	2.52	0.44
1:A:69:SER:HG	1:A:71:SER:HG	1.65	0.44
1:B:88:ALA:HB2	1:B:168:LEU:O	2.17	0.44
1:C:131:LEU:HD22	2:G:46:LEU:HD22	1.99	0.44
1:C:206:GLN:NE2	3:C:2005:HOH:O	2.50	0.44
2:H:61:PHE:CD2	2:H:92:ASN:HB3	2.52	0.44
2:H:100:GLU:HA	2:H:101:HIS:HA	1.63	0.44
1:C:185:GLY:O	1:C:189:ILE:HD12	2.18	0.44
2:E:144:SER:CB	2:E:145:PRO:HD2	2.47	0.44
2:G:106:PHE:HB2	2:G:112:THR:CG2	2.45	0.43
2:F:65:GLU:HG3	2:F:67[B]:ASN:HD21	1.83	0.43
1:C:110:ASN:O	1:C:112:GLU:N	2.49	0.43
1:C:112:GLU:O	1:C:114:ASP:N	2.51	0.43
2:F:101:HIS:CG	2:F:118:LEU:HD13	2.53	0.43
2:H:86:ALA:HB3	2:H:93:LYS:H	1.84	0.43
2:G:116:GLU:HA	2:G:117:GLY:HA2	1.66	0.43
2:E:138:GLY:O	2:E:140:MET:N	2.52	0.43
2:F:91:MET:HB3	2:F:91:MET:HE2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG23	1:B:208:LEU:HD12	2.00	0.42
1:C:149:ARG:NH2	3:C:2008:HOH:O	2.52	0.42
1:B:125:LYS:N	3:B:2007:HOH:O	2.33	0.42
2:E:121:HIS:O	2:E:123:GLY:N	2.53	0.42
1:A:196:ASN:HA	2:E:70:ARG:HD2	2.01	0.42
2:F:105:CYS:HB2	2:F:110:PHE:O	2.20	0.42
1:A:138:THR:HB	1:A:167:GLN:HE22	1.84	0.42
1:D:88:ALA:HB2	1:D:168:LEU:O	2.20	0.42
1:C:108:ASN:HA	1:C:109:ASN:HA	1.60	0.42
2:H:120:LEU:O	2:H:120:LEU:HG	2.18	0.42
1:B:172:SER:O	1:B:175:PRO:HD3	2.20	0.42
2:G:61:PHE:CD2	2:G:92:ASN:HB3	2.55	0.42
1:D:198:GLN:O	3:D:2005:HOH:O	2.22	0.41
2:E:61:PHE:CD2	2:E:92:ASN:HB3	2.55	0.41
2:F:121:HIS:N	2:F:124:ARG:O	2.50	0.41
2:H:61:PHE:CE2	2:H:92:ASN:HB3	2.55	0.41
1:A:106:LEU:HD23	1:A:149:ARG:HH11	1.84	0.41
1:D:195:VAL:O	3:D:2005:HOH:O	2.21	0.41
1:D:207:HIS:HE1	1:D:209:ALA:HB3	1.85	0.41
1:A:77:HIS:CE1	1:D:177:LYS:HE2	2.56	0.41
1:C:85:PHE:CG	1:C:91:MET:HG3	2.55	0.41
2:G:139:THR:HG22	2:G:140:MET:N	2.35	0.41
1:D:108:ASN:HA	1:D:109:ASN:HA	1.74	0.41
1:D:167:GLN:HA	1:D:170:GLN:HG2	2.03	0.40
2:E:90:ASP:OD1	2:E:90:ASP:N	2.52	0.40
2:F:45:GLU:OE2	2:F:55:LYS:NZ	2.42	0.40
1:B:100:GLN:H	2:F:69:ILE:HG22	1.86	0.40
2:H:88:ASN:HD22	2:H:89:PRO:HD2	1.85	0.40
2:F:88:ASN:HB2	2:F:91:MET:O	2.22	0.40
1:D:167:GLN:O	1:D:170:GLN:HG3	2.21	0.40

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	Interatomic distance (Å)	Clash overlap (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%)	25	59
1	B	153/164 (93%)	149 (97%)	3 (2%)	1 (1%)	25	59
1	C	153/164 (93%)	147 (96%)	5 (3%)	1 (1%)	25	59
1	D	148/164 (90%)	145 (98%)	2 (1%)	1 (1%)	25	59
2	E	109/126 (86%)	96 (88%)	10 (9%)	3 (3%)	6	19
2	F	102/126 (81%)	88 (86%)	10 (10%)	4 (4%)	3	12
2	G	105/126 (83%)	92 (88%)	8 (8%)	5 (5%)	2	8
2	H	104/126 (82%)	94 (90%)	5 (5%)	5 (5%)	2	8
All	All	1025/1160 (88%)	957 (93%)	47 (5%)	21 (2%)	8	28

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

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Mol	Chain	Res	Type
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%)	85	96
1	C	127/135 (94%)	126 (99%)	1 (1%)	85	96
1	D	126/135 (93%)	125 (99%)	1 (1%)	85	96
2	E	95/105 (90%)	92 (97%)	3 (3%)	44	78
2	F	90/105 (86%)	86 (96%)	4 (4%)	33	67
2	G	92/105 (88%)	92 (100%)	0	100	100
2	H	91/105 (87%)	89 (98%)	2 (2%)	57	87
All	All	877/960 (91%)	865 (99%)	12 (1%)	71	92

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

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Mol	Chain	Res	Type
2	H	88	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	167	GLN
1	C	207	HIS
2	E	121	HIS
2	G	121	HIS
2	H	88	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	152/164 (92%)	0.04	4 (2%) 56 45	30, 57, 116, 142	0
1	B	156/164 (95%)	-0.02	3 (1%) 67 58	29, 59, 121, 148	0
1	C	155/164 (94%)	-0.10	3 (1%) 67 58	34, 59, 128, 155	0
1	D	152/164 (92%)	0.05	5 (3%) 47 36	32, 62, 119, 137	0
2	E	110/126 (87%)	0.19	7 (6%) 20 12	39, 76, 151, 179	0
2	F	103/126 (81%)	0.61	16 (15%) 2 1	51, 149, 186, 205	0
2	G	107/126 (84%)	0.09	5 (4%) 32 22	46, 80, 148, 161	0
2	H	105/126 (83%)	1.47	30 (28%) 1 0	48, 147, 215, 246	0
All	All	1040/1160 (89%)	0.23	73 (7%) 17 10	29, 69, 179, 246	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	GLY	10.7
2	H	127	PRO	9.7
2	H	139	THR	9.6
2	E	37	SER	7.2
2	H	137	ASN	6.7
2	H	133	SER	6.3
2	F	136	ALA	5.9
2	F	138	GLY	5.9
2	H	117	GLY	5.5
2	H	128	ALA	5.5
2	H	90	ASP	5.2
1	B	54	GLY	5.1
2	F	40	CYS	4.7
2	H	140	MET	4.7
2	H	129	CYS	4.5
2	G	145	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	H	87	ARG	4.3
2	F	116	GLU	4.2
1	D	70	PRO	4.1
2	H	123	GLY	4.1
1	A	110	ASN	4.0
2	F	137	ASN	3.9
2	F	90	ASP	3.9
2	H	91	MET	3.7
2	H	103	GLU	3.7
2	H	131	GLU	3.6
2	F	139	THR	3.6
2	H	132	GLY	3.6
2	F	108	HIS	3.6
2	F	140	MET	3.3
2	F	101	HIS	3.3
2	H	101	HIS	3.3
1	D	72	GLY	3.2
2	H	126	TYR	3.2
2	H	99	ILE	3.1
1	C	210	ALA	3.1
1	B	71	SER	3.1
2	F	135	ALA	3.0
2	H	109	ASN	3.0
2	H	116	GLU	2.9
2	H	98	LYS	2.9
1	D	73	ASP	2.9
2	F	128	ALA	2.8
2	G	106	PHE	2.8
1	A	131	LEU	2.8
2	E	139	THR	2.8
2	E	138	GLY	2.7
2	H	119	TYR	2.6
2	E	136	ALA	2.6
2	E	137	ASN	2.6
2	H	124	ARG	2.6
2	H	135	ALA	2.6
1	C	111	ASP	2.6
2	H	130	PRO	2.5
2	H	134	SER	2.5
2	E	131	GLU	2.5
1	A	109	ASN	2.4
2	G	140	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	108	ASN	2.3
1	D	131	LEU	2.3
2	G	139	THR	2.3
2	E	36	GLY	2.3
2	F	142	CYS	2.2
2	F	91	MET	2.2
2	H	114	CYS	2.2
1	D	71	SER	2.2
2	F	127	PRO	2.1
2	H	142	CYS	2.1
2	F	122	LYS	2.1
1	B	56	LYS	2.1
1	A	70	PRO	2.0
2	G	85	ASP	2.0
2	H	100	GLU	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 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.