Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:30 PM GMT

PDB ID	:	4CDK
Title	:	Structure of ZNRF3-RSPO1
Authors	:	Peng, W.C.; de Lau, W.; Madoori, P.K.; Forneris, F.; Granneman, J.C.M.; 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

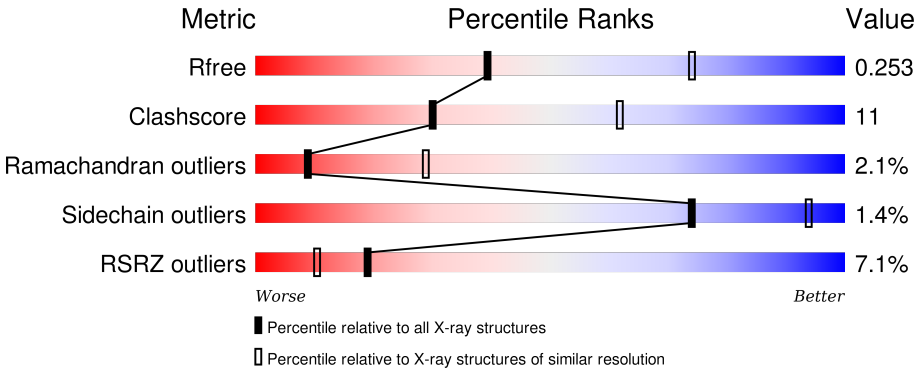
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 >=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 <=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	2% 76% 16% • 7%
1	B	164	2% 73% 21% • 5%
1	C	164	2% 71% 22% • 5%
1	D	164	3% 75% 18% 7%
2	E	126	6% 67% 16% • 13%

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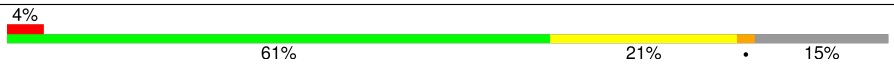
Mol	Chain	Length	Quality of chain
2	F	126	
2	G	126	
2	H	126	

2 Entry composition (i)

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.

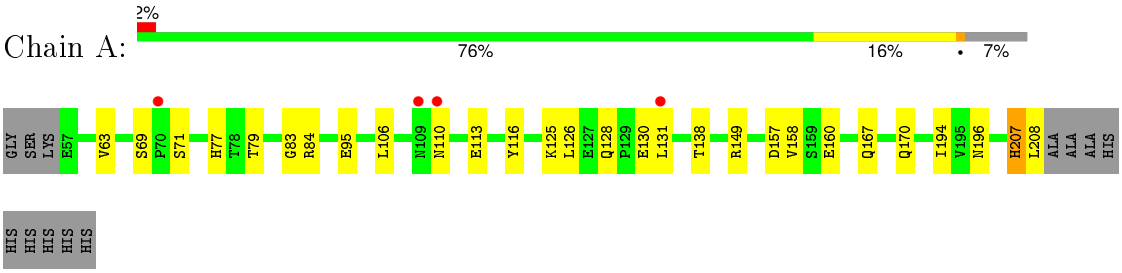
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	12	Total O 12 12	0	0
3	B	11	Total O 11 11	0	0
3	C	14	Total O 14 14	0	0
3	D	5	Total O 5 5	0	0
3	E	6	Total O 6 6	0	0
3	F	1	Total O 1 1	0	0
3	G	6	Total O 6 6	0	0

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 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.

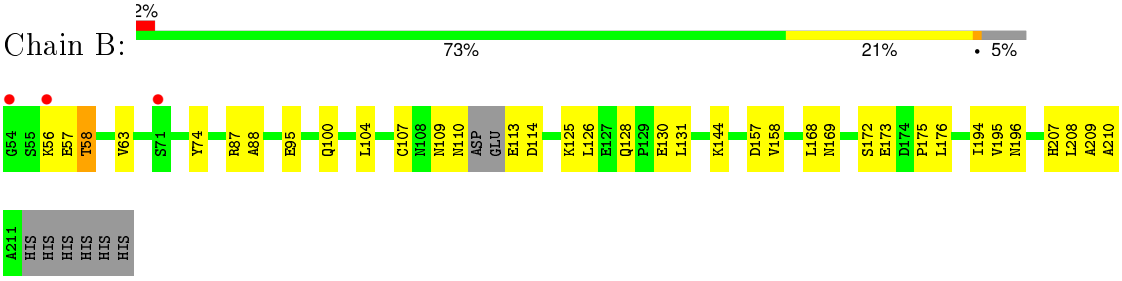
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain A:



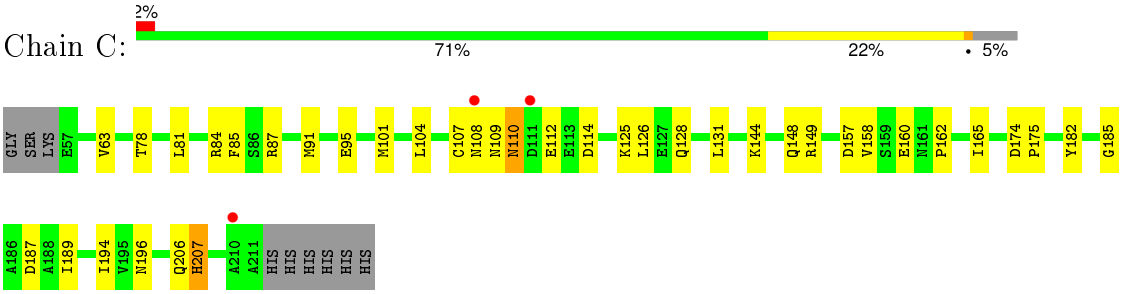
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain B:



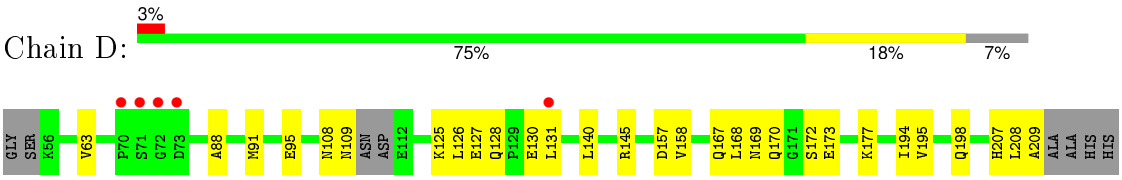
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain C:



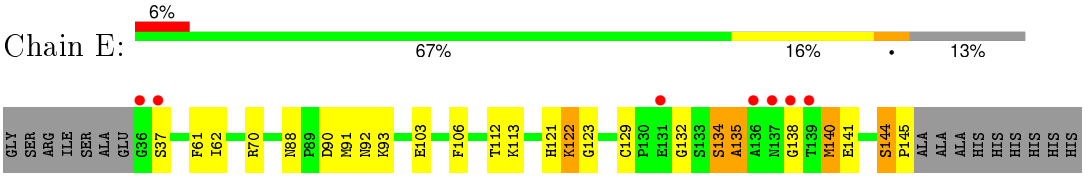
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain D:



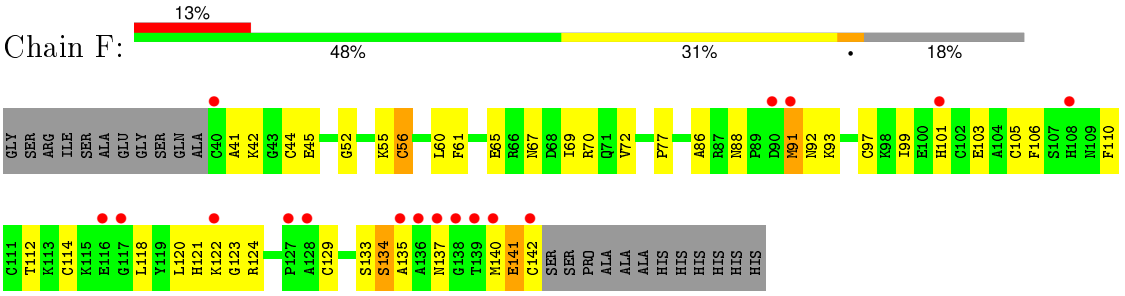
- Molecule 2: R-SPONDIN-1

Chain E:



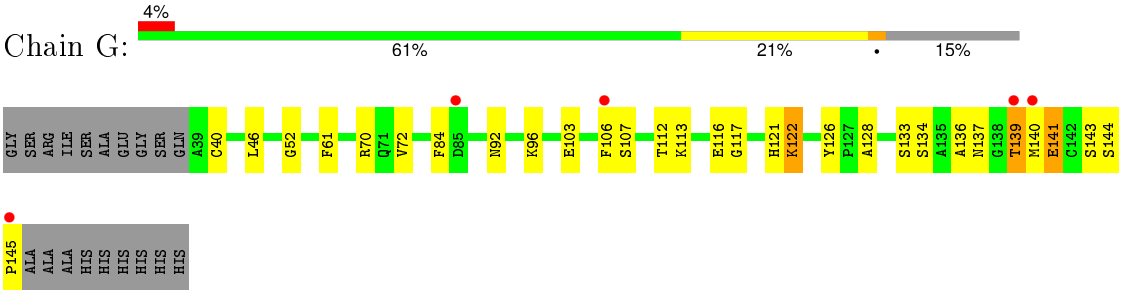
- Molecule 2: R-SPONDIN-1

Chain F:



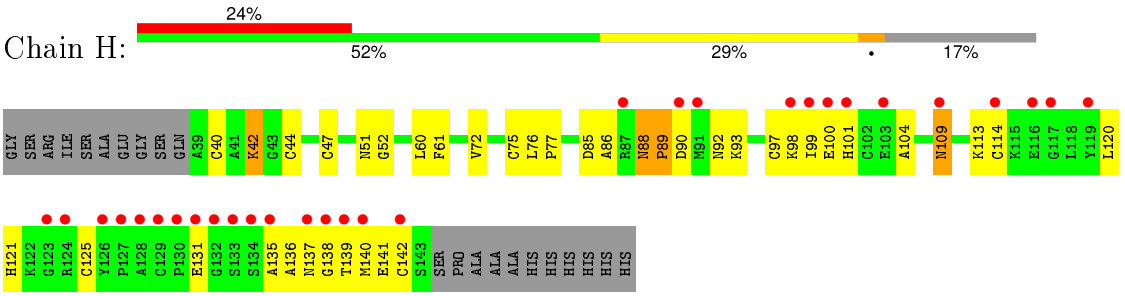
- Molecule 2: R-SPONDIN-1

Chain G:



- Molecule 2: R-SPONDIN-1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.96 (at 2.82Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.246 0.229 , 0.253	Depositor DCC
R_{free} test set	1439 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.1	EDS
Estimated twinning fraction	0.116 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 28148 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7982	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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:130:GLU:HG2	1:A:131:LEU:HD12	1.83	0.59
1:A:128:GLN:HG3	1:A:160:GLU:HB3	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
2:F:106:PHE:HB2	2:F:112:THR:OG1	2.03	0.57
1:A:207:HIS:CD2	1:A:208:LEU:HG	2.39	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:H:99:ILE:HG22	2:H:100:GLU: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: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
2:H:113:LYS:HG3	2:H:141:GLU:OE2	2.08	0.53
1:D:91:MET:HB3	1:D:207:HIS:HE2	1.73	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
2:H:140:MET:O	2:H:141:GLU:HB2	2.09	0.53
1:B:196:ASN:HA	2:F:70:ARG:HD2	1.91	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:G:136:ALA:HB1	2:G:137:ASN:HA	1.92	0.51
2:F:60:LEU:HD22	2:F:77:PRO:HA	1.93	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: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
1:B:109:ASN:OD1	1:B:110:ASN:N	2.44	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
2:H:135:ALA:HB2	2:H:142:CYS:SG	2.53	0.49
1:D:170:GLN:C	1:D:172:SER:H	2.16	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:D:128:GLN:HB2	1:D:131:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD12	1:C:158:VAL:HG12	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
2:E:106:PHE:HB2	2:E:112:THR:CG2	2.45	0.46
1:B:128:GLN:HB2	1:B:131:LEU:HD13	1.98	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
2:E:135:ALA:HB1	2:E:138:GLY:HA3	1.98	0.45
1:B:104:LEU:HA	1:B:107:CYS:SG	2.57	0.45
1:C:162:PRO:O	1:C:165:ILE:HG13	2.17	0.45
1:D:91:MET:HB3	1:D:207:HIS:CD2	2.52	0.44
1:A:79:THR:HG22	1:C:78:THR:OG1	2.18	0.44
1:B:100:GLN:HG3	1:B:195:VAL:HG11	1.99	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
2:E:144:SER:CB	2:E:145:PRO:HD2	2.47	0.44
1:C:185:GLY:O	1:C:189:ILE:HD12	2.18	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:H:86:ALA:HB3	2:H:93:LYS:H	1.84	0.43
2:F:101:HIS:CG	2:F:118:LEU:HD13	2.53	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
2:E:121:HIS:O	2:E:123:GLY:N	2.53	0.42
1:B:125:LYS:N	3:B:2007:HOH:O	2.33	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
2:G:61:PHE:CD2	2:G:92:ASN:HB3	2.55	0.42
1:B:172:SER:O	1:B:175:PRO:HD3	2.20	0.42
2:F:121:HIS:N	2:F:124:ARG:O	2.50	0.41
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:H:61:PHE:CE2	2:H:92:ASN:HB3	2.55	0.41
1:D:207:HIS:HE1	1:D:209:ALA:HB3	1.85	0.41
1:D:195:VAL:O	3:D:2005:HOH:O	2.21	0.41
1:A:106:LEU:HD23	1:A:149:ARG:HH11	1.84	0.41
1:A:77:HIS:CE1	1:D:177:LYS:HE2	2.56	0.41
2:G:139:THR:HG22	2:G:140:MET:N	2.35	0.41
1:C:85:PHE:CG	1:C:91:MET:HG3	2.55	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 (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	151/164 (92%)	146 (97%)	4 (3%)	1 (1%)	26	62
1	B	153/164 (93%)	149 (97%)	3 (2%)	1 (1%)	26	62
1	C	153/164 (93%)	147 (96%)	5 (3%)	1 (1%)	26	62
1	D	148/164 (90%)	145 (98%)	2 (1%)	1 (1%)	26	62
2	E	109/126 (86%)	96 (88%)	10 (9%)	3 (3%)	6	21
2	F	102/126 (81%)	88 (86%)	10 (10%)	4 (4%)	4	12
2	G	105/126 (83%)	92 (88%)	8 (8%)	5 (5%)	3	9
2	H	104/126 (82%)	94 (90%)	5 (5%)	5 (5%)	3	9
All	All	1025/1160 (88%)	957 (93%)	47 (5%)	21 (2%)	9	30

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 (i)

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%)	86	97
1	C	127/135 (94%)	126 (99%)	1 (1%)	86	97
1	D	126/135 (93%)	125 (99%)	1 (1%)	86	97
2	E	95/105 (90%)	92 (97%)	3 (3%)	46	80
2	F	90/105 (86%)	86 (96%)	4 (4%)	35	69
2	G	92/105 (88%)	92 (100%)	0	100	100
2	H	91/105 (87%)	89 (98%)	2 (2%)	60	89
All	All	877/960 (91%)	865 (99%)	12 (1%)	74	94

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

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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	152/164 (92%)	0.06	4 (2%) 59 47	30, 57, 116, 142	0
1	B	156/164 (95%)	-0.01	3 (1%) 70 59	29, 59, 121, 148	0
1	C	155/164 (94%)	-0.08	3 (1%) 70 59	34, 59, 128, 155	0
1	D	152/164 (92%)	0.07	5 (3%) 50 38	32, 62, 119, 137	0
2	E	110/126 (87%)	0.21	7 (6%) 23 14	39, 76, 151, 179	0
2	F	103/126 (81%)	0.64	17 (16%) 2 1	51, 149, 186, 205	0
2	G	107/126 (84%)	0.11	5 (4%) 35 24	46, 80, 148, 161	0
2	H	105/126 (83%)	1.51	30 (28%) 1 0	48, 147, 215, 246	0
All	All	1040/1160 (89%)	0.25	74 (7%) 19 10	29, 69, 179, 246	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	GLY	10.8
2	H	127	PRO	9.9
2	H	139	THR	9.9
2	E	37	SER	7.4
2	H	137	ASN	6.9
2	H	133	SER	6.4
2	F	138	GLY	5.9
2	F	136	ALA	5.9
2	H	117	GLY	5.6
2	H	128	ALA	5.5
2	H	90	ASP	5.4
1	B	54	GLY	5.2
2	F	40	CYS	4.9
2	H	140	MET	4.8
2	H	129	CYS	4.7
2	G	145	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	116	GLU	4.4
1	D	70	PRO	4.3
1	A	110	ASN	4.2
2	H	123	GLY	4.1
2	H	87	ARG	4.1
2	F	137	ASN	4.1
2	F	90	ASP	4.0
2	H	91	MET	3.8
2	H	103	GLU	3.8
2	H	131	GLU	3.7
2	F	139	THR	3.7
2	F	108	HIS	3.6
2	H	132	GLY	3.6
2	F	140	MET	3.4
2	F	101	HIS	3.3
2	H	101	HIS	3.3
2	H	126	TYR	3.2
1	D	72	GLY	3.2
2	H	99	ILE	3.2
1	B	71	SER	3.2
1	C	210	ALA	3.1
2	H	109	ASN	3.1
2	H	116	GLU	3.0
2	F	135	ALA	3.0
2	H	98	LYS	3.0
1	D	73	ASP	3.0
2	E	139	THR	2.9
2	G	106	PHE	2.8
1	A	131	LEU	2.8
2	F	128	ALA	2.8
2	E	138	GLY	2.7
2	E	137	ASN	2.7
2	H	119	TYR	2.7
1	C	111	ASP	2.7
2	H	130	PRO	2.6
2	E	136	ALA	2.6
2	H	134	SER	2.6
2	E	131	GLU	2.5
2	H	135	ALA	2.5
1	A	109	ASN	2.5
2	H	124	ARG	2.5
2	G	140	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	108	ASN	2.4
2	F	142	CYS	2.4
1	D	131	LEU	2.3
2	H	114	CYS	2.3
2	G	139	THR	2.3
2	E	36	GLY	2.3
2	F	91	MET	2.3
1	D	71	SER	2.2
2	F	127	PRO	2.2
2	H	142	CYS	2.2
2	F	122	LYS	2.2
2	G	85	ASP	2.1
1	B	56	LYS	2.1
1	A	70	PRO	2.1
2	H	100	GLU	2.1
2	F	117	GLY	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.