Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 07:32 AM EST

PDB ID	:	3WCK
Title	:	Crystal structure of monomeric photosensitizing fluorescent protein, Supernova
Authors	:	Sakai, N.; Matsuda, T.; Takemoto, K.; Nagai, T.
Deposited on	:	2013-05-27
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

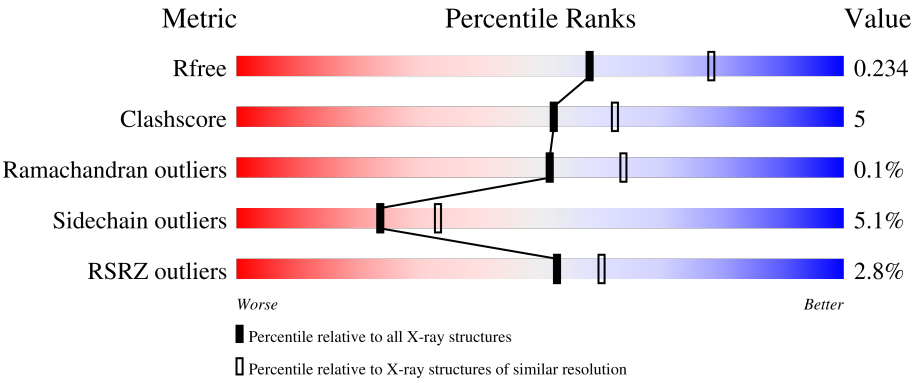
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	271	2% 70% 9% · 20%
1	B	271	4% 63% 16% · 20%
1	C	271	2% 69% 10% · 18%
1	D	271	3% 66% 13% · 20%
1	E	271	% 69% 9% · 20%

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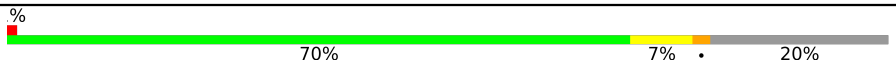
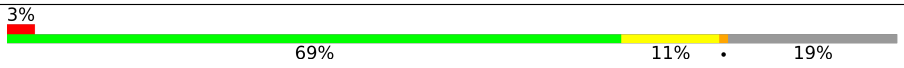
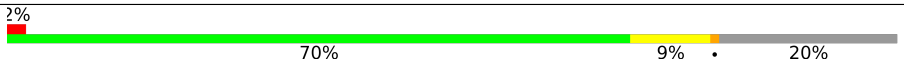
Mol	Chain	Length	Quality of chain
1	F	271	
1	G	271	
1	H	271	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14303 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 Monomeric photosenitizing fluorescent protein supernova.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1718	1087	295	322	14			
1	B	218	Total	C	N	O	S	0	0	0
			1718	1087	295	322	14			
1	C	221	Total	C	N	O	S	0	0	0
			1744	1100	302	328	14			
1	D	218	Total	C	N	O	S	0	0	0
			1718	1087	295	322	14			
1	E	218	Total	C	N	O	S	0	0	0
			1718	1087	295	322	14			
1	F	218	Total	C	N	O	S	0	0	0
			1721	1087	298	322	14			
1	G	220	Total	C	N	O	S	0	0	0
			1740	1099	303	324	14			
1	H	218	Total	C	N	O	S	0	0	0
			1718	1087	295	322	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	CRQ	GLN	chromophore	PDB 3WCK
A	65	CRQ	TYR	chromophore	PDB 3WCK
A	65	CRQ	GLY	chromophore	PDB 3WCK
B	65	CRQ	GLN	chromophore	PDB 3WCK
B	65	CRQ	TYR	chromophore	PDB 3WCK
B	65	CRQ	GLY	chromophore	PDB 3WCK
C	65	CRQ	GLN	chromophore	PDB 3WCK
C	65	CRQ	TYR	chromophore	PDB 3WCK
C	65	CRQ	GLY	chromophore	PDB 3WCK
D	65	CRQ	GLN	chromophore	PDB 3WCK
D	65	CRQ	TYR	chromophore	PDB 3WCK
D	65	CRQ	GLY	chromophore	PDB 3WCK
E	65	CRQ	GLN	chromophore	PDB 3WCK

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Chain	Residue	Modelled	Actual	Comment	Reference
E	65	CRQ	TYR	chromophore	PDB 3WCK
E	65	CRQ	GLY	chromophore	PDB 3WCK
F	65	CRQ	GLN	chromophore	PDB 3WCK
F	65	CRQ	TYR	chromophore	PDB 3WCK
F	65	CRQ	GLY	chromophore	PDB 3WCK
G	65	CRQ	GLN	chromophore	PDB 3WCK
G	65	CRQ	TYR	chromophore	PDB 3WCK
G	65	CRQ	GLY	chromophore	PDB 3WCK
H	65	CRQ	GLN	chromophore	PDB 3WCK
H	65	CRQ	TYR	chromophore	PDB 3WCK
H	65	CRQ	GLY	chromophore	PDB 3WCK

- Molecule 2 is water.

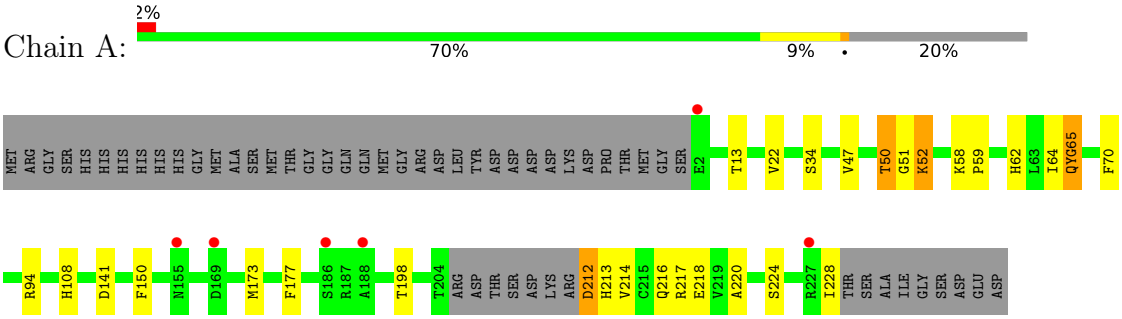
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	58	Total O 58 58	0	0
2	C	66	Total O 66 66	0	0
2	D	69	Total O 69 69	0	0
2	E	60	Total O 60 60	0	0
2	F	75	Total O 75 75	0	0
2	G	61	Total O 61 61	0	0
2	H	61	Total O 61 61	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

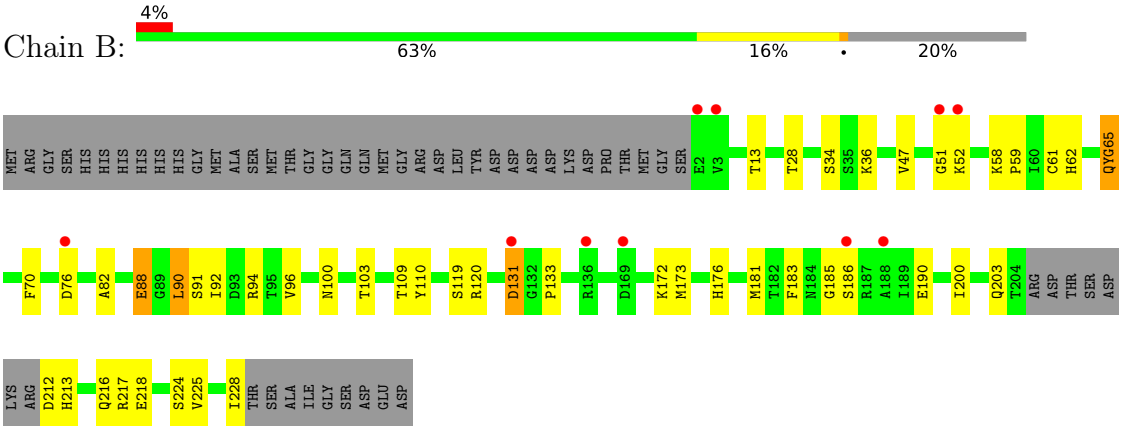
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain A:



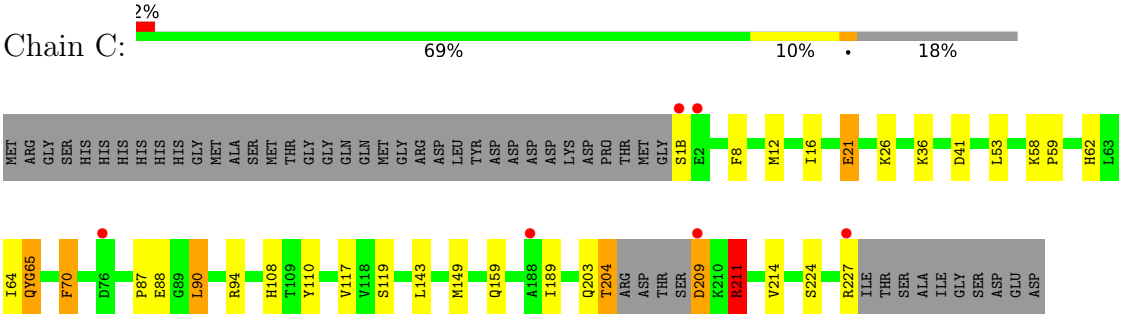
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain B:



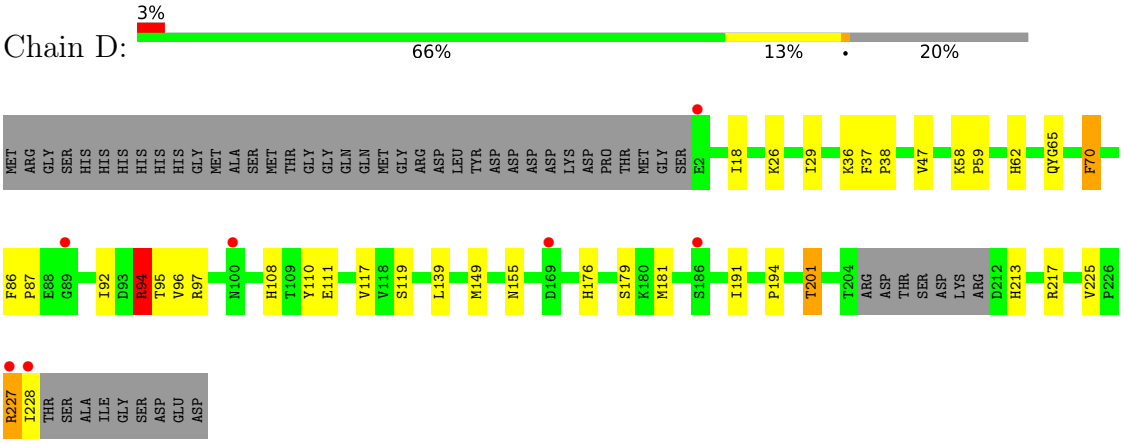
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain C:



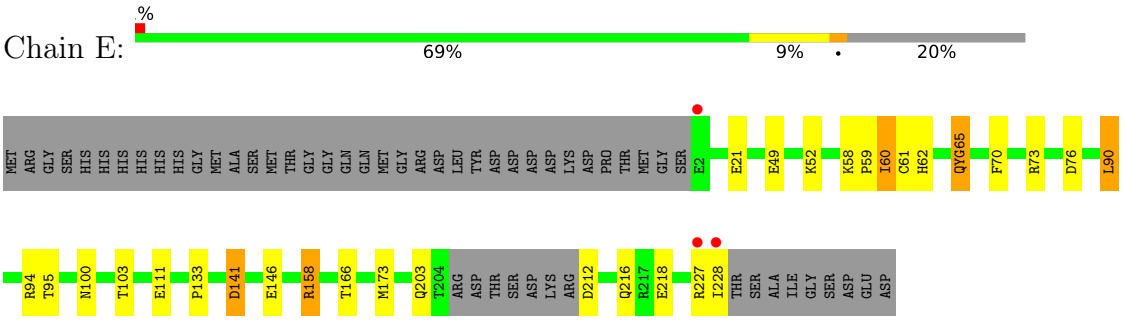
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain D:



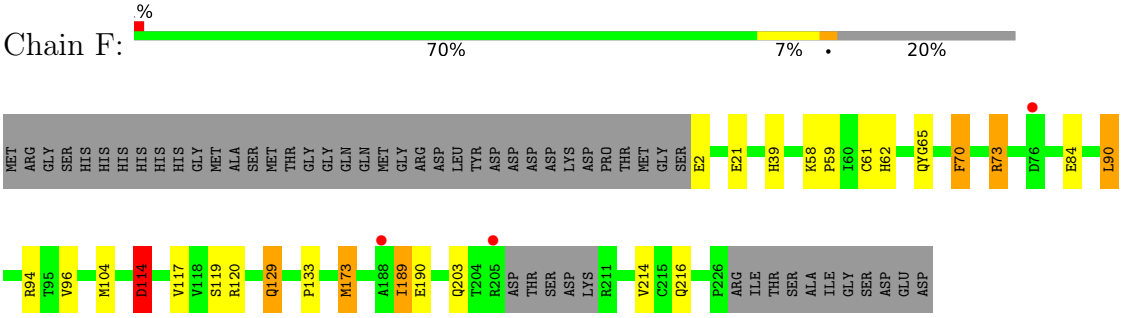
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain E:



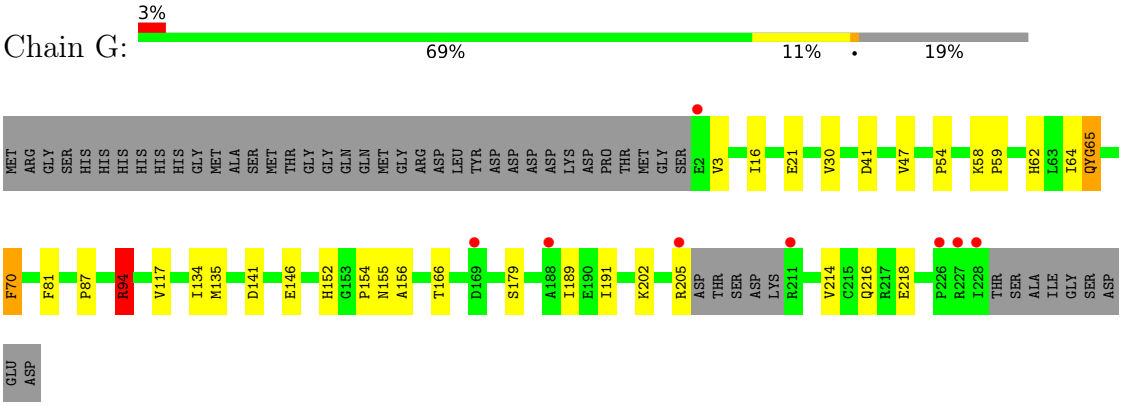
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain F:



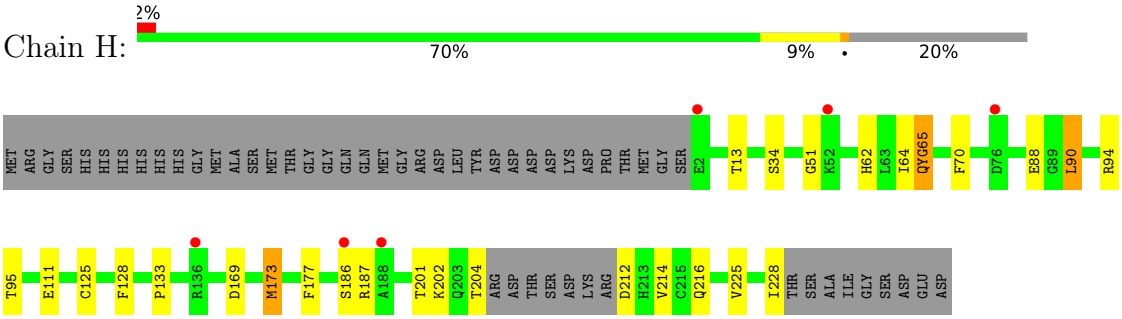
• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain G:



• Molecule 1: Monomeric photosenitizing fluorescent protein supernova

Chain H:


2%
70%
9%
20%
MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP ASP LYS ASP PRO THR MET GLY SER E2 T13 S34 G51 K52 H62 L63 I64 QYG65 F70 D76 E88 G89 L90 R94
T95 E111 C125 F128 P133 R136 D169 M173 F177 S186 R187 A188 T201 K202 Q203 T204 ARG ASP THR SER ASP LYS ARG D212 H213 V214 C215 Q216 V225 I228 THR SER ALA ILE GLY SER ASP GLU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.25Å 89.30Å 109.89Å 70.57° 89.95° 71.62°	Depositor
Resolution (Å)	20.00 – 2.30 36.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.30) 97.6 (36.67-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.181 , 0.234 0.188 , 0.234	Depositor DCC
R_{free} test set	4432 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.167 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14303	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9966e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CRQ

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	0.75	0/1740	0.84	1/2358 (0.0%)
1	B	0.74	0/1740	0.85	2/2358 (0.1%)
1	C	0.79	0/1766	0.93	5/2391 (0.2%)
1	D	0.77	0/1740	0.90	2/2358 (0.1%)
1	E	0.76	0/1740	0.86	3/2358 (0.1%)
1	F	0.76	0/1743	0.88	3/2361 (0.1%)
1	G	0.77	0/1762	0.93	3/2386 (0.1%)
1	H	0.75	0/1740	0.86	1/2358 (0.0%)
All	All	0.76	0/13971	0.88	20/18928 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	94	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	G	94	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	D	94	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	D	94	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	21	GLU	CA-CB-CG	7.20	129.25	113.40
1	C	211	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	E	90	LEU	CA-CB-CG	6.59	130.46	115.30
1	E	141	ASP	CB-CA-C	-6.43	97.53	110.40
1	C	41	ASP	CB-CG-OD1	6.14	123.83	118.30
1	G	41	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	211	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	F	120	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	120	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	120	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	H	90	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	141	ASP	CB-CG-OD1	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	LEU	CA-CB-CG	5.21	127.30	115.30
1	E	158	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	F	90	LEU	CA-CB-CG	5.12	127.09	115.30
1	F	21	GLU	N-CA-CB	-5.06	101.50	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1718	0	1624	17	0
1	B	1718	0	1624	26	0
1	C	1744	0	1651	20	0
1	D	1718	0	1624	27	0
1	E	1718	0	1624	17	0
1	F	1721	0	1626	15	0
1	G	1740	0	1650	22	0
1	H	1718	0	1623	14	0
2	A	58	0	0	0	0
2	B	58	0	0	1	0
2	C	66	0	0	2	0
2	D	69	0	0	1	0
2	E	60	0	0	1	0
2	F	75	0	0	2	0
2	G	61	0	0	1	0
2	H	61	0	0	2	0
All	All	14303	0	13046	147	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 5.

All (147) 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:H:65:CRQ:HE11	1:H:216:GLN:HE21	1.20	0.89
1:E:227:ARG:HB3	1:E:228:ILE:HA	1.64	0.79
1:A:51:GLY:O	1:A:212:ASP:HB3	1.84	0.77
1:F:61:CYS:HA	1:F:216:GLN:HE22	1.53	0.73
1:A:58:LYS:HB2	1:A:59:PRO:HD3	1.73	0.71
1:E:61:CYS:HA	1:E:216:GLN:HE22	1.53	0.71
1:F:203:GLN:HE21	1:F:216:GLN:NE2	1.92	0.68
1:F:62:HIS:HD2	1:F:94:ARG:HH11	1.44	0.66
1:A:50:THR:HG23	1:A:52:LYS:H	1.61	0.65
1:F:2:GLU:OE1	1:F:2:GLU:HA	1.97	0.65
1:G:94:ARG:HD3	1:G:179:SER:OG	1.96	0.65
1:H:51:GLY:O	1:H:212:ASP:HB3	1.97	0.65
1:B:90:LEU:HD13	1:B:110:TYR:HB2	1.80	0.63
1:C:62:HIS:HD2	1:C:94:ARG:HH11	1.47	0.63
1:C:58:LYS:NZ	2:C:361:HOH:O	2.34	0.61
1:A:65:CRQ:HE11	1:A:216:GLN:HE21	1.49	0.61
1:D:201:THR:HG22	2:D:306:HOH:O	2.01	0.60
1:A:62:HIS:HD2	1:A:94:ARG:HH11	1.50	0.60
1:G:65:CRQ:HE11	1:G:216:GLN:HE21	1.49	0.59
1:H:65:CRQ:HE1	1:H:201:THR:HG21	1.85	0.58
1:H:95:THR:HG22	2:H:361:HOH:O	2.03	0.58
1:D:227:ARG:HD3	1:D:227:ARG:H	1.69	0.57
1:B:100:ASN:ND2	1:C:26:LYS:H	2.02	0.57
1:F:39:HIS:O	1:F:73:ARG:HD3	2.05	0.57
1:D:217:ARG:NH1	1:H:228:ILE:HG23	2.20	0.57
1:D:26:LYS:H	1:E:100:ASN:ND2	2.04	0.56
1:E:62:HIS:HD2	1:E:94:ARG:HH11	1.53	0.56
1:B:203:GLN:HE21	1:B:216:GLN:NE2	2.03	0.56
1:C:209:ASP:N	1:C:209:ASP:OD1	2.39	0.56
1:D:58:LYS:HB2	1:D:59:PRO:HD3	1.89	0.55
1:B:88:GLU:HG2	1:B:183:PHE:CE1	2.40	0.55
1:F:203:GLN:HE21	1:F:216:GLN:HE21	1.54	0.55
1:G:30:VAL:HG23	1:G:47:VAL:HG22	1.89	0.55
1:B:62:HIS:HD2	1:B:94:ARG:HH11	1.55	0.54
1:C:16:ILE:HD13	1:C:64:ILE:HA	1.90	0.54
1:E:60:ILE:HD13	1:E:60:ILE:N	2.23	0.54
1:D:86:PHE:HB3	1:D:87:PRO:HA	1.90	0.53
1:D:92:ILE:HG12	1:D:181:MET:HG2	1.90	0.53
1:H:204:THR:HG22	2:H:349:HOH:O	2.08	0.53
1:H:62:HIS:HD2	1:H:94:ARG:HH11	1.55	0.53
1:E:203:GLN:HE21	1:E:216:GLN:NE2	2.06	0.53
1:A:217:ARG:NH1	1:B:228:ILE:HG23	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:VAL:HG12	1:G:87:PRO:HD3	1.91	0.52
1:D:95:THR:HG21	1:D:97:ARG:CZ	2.39	0.52
1:E:146:GLU:CG	1:G:146:GLU:HG2	2.40	0.52
1:G:134:ILE:HG22	1:G:135:MET:CE	2.39	0.52
1:G:64:ILE:O	1:G:65:CRQ:HG11	2.09	0.51
1:A:65:CRQ:NE1	1:A:218:GLU:HB2	2.26	0.51
1:B:58:LYS:HB2	1:B:59:PRO:HD3	1.92	0.51
1:E:146:GLU:HG3	1:G:146:GLU:HG2	1.93	0.51
1:C:58:LYS:HD3	1:C:203:GLN:OE1	2.12	0.50
1:C:58:LYS:HB2	1:C:59:PRO:HD3	1.95	0.49
1:G:16:ILE:HD13	1:G:64:ILE:HA	1.95	0.49
1:B:61:CYS:HA	1:B:216:GLN:HE22	1.77	0.49
1:F:58:LYS:HB2	1:F:59:PRO:HD3	1.94	0.49
1:B:82:ALA:HB2	1:B:181:MET:HE1	1.95	0.48
1:D:155:ASN:HA	1:D:191:ILE:HD11	1.94	0.48
1:E:58:LYS:HB2	1:E:59:PRO:HD3	1.95	0.48
1:G:3:VAL:HG12	1:G:87:PRO:CD	2.44	0.48
1:H:133:PRO:HG2	1:H:173:MET:HE2	1.94	0.48
1:C:70:PHE:CZ	1:C:117:VAL:HG11	2.48	0.48
1:F:70:PHE:CZ	1:F:117:VAL:HG11	2.48	0.48
1:C:53:LEU:O	1:C:211:ARG:NH2	2.47	0.48
1:G:62:HIS:HD2	1:G:94:ARG:HH21	1.61	0.48
1:H:64:ILE:O	1:H:65:CRQ:HG11	2.14	0.48
1:G:154:PRO:O	1:G:191:ILE:HD11	2.14	0.48
1:B:65:CRQ:NE1	1:B:218:GLU:HB2	2.28	0.48
1:D:108:HIS:CD2	1:D:108:HIS:N	2.82	0.48
1:A:228:ILE:HG23	1:B:217:ARG:NH1	2.29	0.47
1:F:133:PRO:HG2	1:F:173:MET:HE2	1.95	0.47
1:H:125:CYS:HB3	1:H:128:PHE:CE1	2.49	0.47
1:H:88:GLU:OE2	1:H:187:ARG:NE	2.46	0.47
1:D:62:HIS:O	1:D:94:ARG:NH2	2.48	0.47
1:G:70:PHE:CZ	1:G:117:VAL:HG11	2.49	0.47
1:A:150:PHE:CD1	1:B:172:LYS:HE2	2.50	0.47
1:C:204:THR:HG22	2:C:334:HOH:O	2.14	0.47
1:D:58:LYS:HG3	1:D:139:LEU:HB2	1.96	0.47
1:C:62:HIS:CD2	1:C:94:ARG:HH11	2.31	0.46
1:D:228:ILE:HG22	1:H:202:LYS:NZ	2.30	0.46
1:D:70:PHE:CZ	1:D:117:VAL:HG11	2.49	0.46
1:G:134:ILE:HG22	1:G:135:MET:HE2	1.97	0.46
1:D:94:ARG:HD2	1:D:179:SER:HB2	1.98	0.45
1:F:114:ASP:HB3	2:F:354:HOH:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:HG12	1:B:181:MET:HG2	1.98	0.45
1:F:119:SER:HB2	2:F:329:HOH:O	2.17	0.45
1:A:13:THR:HA	1:A:34:SER:HA	1.99	0.45
1:G:141:ASP:HB2	1:G:166:THR:OG1	2.16	0.45
1:D:92:ILE:HD12	1:D:110:TYR:HE1	1.82	0.45
1:F:96:VAL:HB	1:F:104:MET:HG2	1.99	0.45
1:A:198:THR:O	1:A:220:ALA:HA	2.17	0.45
1:D:94:ARG:CD	1:D:179:SER:HB2	2.46	0.44
1:C:189:ILE:HD13	1:C:189:ILE:HG21	1.72	0.44
1:E:141:ASP:HB2	1:E:166:THR:HB	1.99	0.44
1:F:129:GLN:HE21	1:F:129:GLN:HA	1.82	0.44
1:G:94:ARG:CD	1:G:179:SER:OG	2.64	0.44
1:C:87:PRO:HD2	1:C:88:GLU:OE2	2.18	0.44
1:A:64:ILE:O	1:A:65:CRQ:HG11	2.17	0.44
1:D:62:HIS:HD2	1:D:94:ARG:HH21	1.64	0.44
1:D:18:ILE:HB	1:D:29:ILE:HB	2.00	0.43
1:D:37:PHE:CD1	1:D:38:PRO:HA	2.52	0.43
1:G:58:LYS:CB	1:G:59:PRO:HD3	2.49	0.43
1:B:51:GLY:O	1:B:212:ASP:HB3	2.19	0.43
1:B:13:THR:HA	1:B:34:SER:HA	2.00	0.43
1:C:149:MET:HG3	1:C:159:GLN:HG3	2.01	0.43
1:A:22:VAL:O	1:A:22:VAL:HG13	2.18	0.43
1:C:110:TYR:CD2	1:C:119:SER:HB3	2.54	0.43
1:D:47:VAL:HG22	1:D:213:HIS:HB2	2.00	0.43
1:B:203:GLN:HE21	1:B:216:GLN:HE21	1.66	0.42
1:E:95:THR:HG23	2:E:307:HOH:O	2.19	0.42
1:C:65:CRQ:HD1	1:C:65:CRQ:N2	2.35	0.42
1:E:203:GLN:HE21	1:E:216:GLN:HE21	1.67	0.42
1:G:81:PHE:CE1	1:G:189:ILE:HD13	2.54	0.42
1:B:109:THR:O	1:B:119:SER:HA	2.19	0.42
1:D:92:ILE:HB	1:D:108:HIS:HB2	2.01	0.42
1:F:62:HIS:CD2	1:F:94:ARG:HH11	2.32	0.42
1:G:65:CRQ:HB11	1:G:218:GLU:OE2	2.19	0.42
1:A:58:LYS:HB2	1:A:59:PRO:CD	2.46	0.42
1:H:13:THR:HA	1:H:34:SER:HA	2.02	0.42
1:E:65:CRQ:N2	1:E:65:CRQ:HD1	2.35	0.42
1:B:131:ASP:OD1	1:B:131:ASP:N	2.47	0.41
1:B:200:ILE:O	1:B:218:GLU:HA	2.20	0.41
1:G:62:HIS:O	1:G:94:ARG:NH2	2.53	0.41
1:H:173:MET:HE2	1:H:173:MET:HB2	1.95	0.41
1:A:47:VAL:HG22	1:A:213:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLU:HG3	1:B:185:GLY:HA3	2.02	0.41
1:B:133:PRO:HG2	1:B:173:MET:HE2	2.02	0.41
1:C:108:HIS:CD2	1:C:108:HIS:N	2.89	0.41
1:E:133:PRO:HG2	1:E:173:MET:CE	2.50	0.41
1:F:84:GLU:HB3	1:F:189:ILE:HG13	2.02	0.41
1:D:26:LYS:H	1:E:100:ASN:HD21	1.67	0.41
1:D:92:ILE:HD12	1:D:110:TYR:CE1	2.55	0.41
1:B:36:LYS:HD2	2:B:354:HOH:O	2.20	0.41
1:E:65:CRQ:NE1	1:E:218:GLU:HB2	2.36	0.41
1:G:152:HIS:O	1:G:156:ALA:HB3	2.21	0.41
1:A:108:HIS:N	1:A:108:HIS:CD2	2.89	0.41
1:B:90:LEU:N	1:B:90:LEU:CD1	2.84	0.41
1:G:54:PRO:C	2:G:354:HOH:O	2.59	0.41
1:D:96:VAL:HA	1:D:176:HIS:O	2.22	0.40
1:D:110:TYR:CD2	1:D:119:SER:HB3	2.56	0.40
1:D:149:MET:O	1:D:194:PRO:HA	2.21	0.40
1:C:64:ILE:O	1:C:65:CRQ:HG11	2.22	0.40
1:B:96:VAL:HA	1:B:176:HIS:O	2.21	0.40
1:C:8:PHE:HA	1:C:12:MET:SD	2.62	0.40
1:E:203:GLN:CG	1:E:216:GLN:HE21	2.35	0.40
1:B:47:VAL:HG22	1:B:213:HIS:HB3	2.02	0.40
1:B:100:ASN:HD22	1:C:26:LYS:H	1.68	0.40
1:A:13:THR:HG22	1:A:34:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/271 (78%)	205 (97%)	6 (3%)	0	100	100
1	B	211/271 (78%)	202 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	214/271 (79%)	204 (95%)	10 (5%)	0	100	100
1	D	211/271 (78%)	201 (95%)	10 (5%)	0	100	100
1	E	211/271 (78%)	203 (96%)	8 (4%)	0	100	100
1	F	211/271 (78%)	203 (96%)	7 (3%)	1 (0%)	29	35
1	G	213/271 (79%)	207 (97%)	6 (3%)	0	100	100
1	H	211/271 (78%)	206 (98%)	5 (2%)	0	100	100
All	All	1693/2168 (78%)	1631 (96%)	61 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	114	ASP

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	188/232 (81%)	180 (96%)	8 (4%)	29	40
1	B	188/232 (81%)	175 (93%)	13 (7%)	15	20
1	C	191/232 (82%)	179 (94%)	12 (6%)	18	24
1	D	188/232 (81%)	181 (96%)	7 (4%)	34	48
1	E	188/232 (81%)	176 (94%)	12 (6%)	17	23
1	F	188/232 (81%)	179 (95%)	9 (5%)	25	36
1	G	190/232 (82%)	183 (96%)	7 (4%)	34	48
1	H	188/232 (81%)	179 (95%)	9 (5%)	25	36
All	All	1509/1856 (81%)	1432 (95%)	77 (5%)	24	33

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR

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Mol	Chain	Res	Type
1	A	52	LYS
1	A	70	PHE
1	A	173	MET
1	A	177	PHE
1	A	212	ASP
1	A	214	VAL
1	A	224	SER
1	B	28	THR
1	B	52	LYS
1	B	70	PHE
1	B	76	ASP
1	B	88	GLU
1	B	90	LEU
1	B	91	SER
1	B	103	THR
1	B	131	ASP
1	B	186	SER
1	B	190	GLU
1	B	224	SER
1	B	225	VAL
1	C	1(B)	SER
1	C	21	GLU
1	C	36	LYS
1	C	70	PHE
1	C	90	LEU
1	C	143	LEU
1	C	204	THR
1	C	209	ASP
1	C	211	ARG
1	C	214	VAL
1	C	224	SER
1	C	227	ARG
1	D	36	LYS
1	D	70	PHE
1	D	94	ARG
1	D	111	GLU
1	D	201	THR
1	D	225	VAL
1	D	227	ARG
1	E	21	GLU
1	E	49	GLU
1	E	52	LYS

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Mol	Chain	Res	Type
1	E	60	ILE
1	E	70	PHE
1	E	73	ARG
1	E	76	ASP
1	E	90	LEU
1	E	103	THR
1	E	111	GLU
1	E	158	ARG
1	E	212	ASP
1	F	70	PHE
1	F	73	ARG
1	F	90	LEU
1	F	114	ASP
1	F	129	GLN
1	F	173	MET
1	F	189	ILE
1	F	190	GLU
1	F	214	VAL
1	G	21	GLU
1	G	70	PHE
1	G	94	ARG
1	G	155	ASN
1	G	202	LYS
1	G	205	ARG
1	G	214	VAL
1	H	70	PHE
1	H	90	LEU
1	H	111	GLU
1	H	169	ASP
1	H	173	MET
1	H	177	PHE
1	H	186	SER
1	H	214	VAL
1	H	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	124	ASN
1	A	129	GLN
1	A	184	ASN

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Mol	Chain	Res	Type
1	B	62	HIS
1	B	100	ASN
1	B	124	ASN
1	B	216	GLN
1	C	62	HIS
1	D	25	GLN
1	D	62	HIS
1	D	176	HIS
1	D	203	GLN
1	D	216	GLN
1	E	62	HIS
1	E	100	ASN
1	E	129	GLN
1	E	184	ASN
1	E	216	GLN
1	F	62	HIS
1	F	100	ASN
1	F	129	GLN
1	F	184	ASN
1	F	216	GLN
1	G	62	HIS
1	G	138	GLN
1	G	155	ASN
1	H	62	HIS
1	H	124	ASN
1	H	184	ASN
1	H	203	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CRQ	F	65	1	24,25,26	3.39	6 (25%)	27,34,36	4.55	8 (29%)
1	CRQ	C	65	1	24,25,26	3.42	4 (16%)	27,34,36	4.54	9 (33%)
1	CRQ	B	65	1	24,25,26	3.81	4 (16%)	27,34,36	4.77	6 (22%)
1	CRQ	E	65	1	24,25,26	3.14	5 (20%)	27,34,36	4.94	9 (33%)
1	CRQ	A	65	1	24,25,26	3.77	4 (16%)	27,34,36	4.34	5 (18%)
1	CRQ	G	65	1	24,25,26	3.48	4 (16%)	27,34,36	4.78	11 (40%)
1	CRQ	H	65	1	24,25,26	3.70	5 (20%)	27,34,36	3.91	6 (22%)
1	CRQ	D	65	1	24,25,26	3.66	6 (25%)	27,34,36	4.61	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRQ	F	65	1	-	2/10/32/33	0/2/2/2
1	CRQ	C	65	1	-	1/10/32/33	0/2/2/2
1	CRQ	B	65	1	-	3/10/32/33	0/2/2/2
1	CRQ	E	65	1	-	3/10/32/33	0/2/2/2
1	CRQ	A	65	1	-	4/10/32/33	0/2/2/2
1	CRQ	G	65	1	-	3/10/32/33	0/2/2/2
1	CRQ	H	65	1	-	3/10/32/33	0/2/2/2
1	CRQ	D	65	1	-	2/10/32/33	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	CRQ	CB2-CA2	17.30	1.49	1.35
1	B	65	CRQ	CB2-CA2	17.03	1.49	1.35
1	H	65	CRQ	CB2-CA2	16.61	1.49	1.35
1	D	65	CRQ	CB2-CA2	16.25	1.48	1.35
1	C	65	CRQ	CB2-CA2	15.03	1.47	1.35
1	G	65	CRQ	CB2-CA2	14.69	1.47	1.35
1	F	65	CRQ	CB2-CA2	14.33	1.47	1.35
1	E	65	CRQ	CB2-CA2	13.02	1.46	1.35
1	G	65	CRQ	CA2-C2	-6.94	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	CRQ	CA2-C2	-5.90	1.42	1.48
1	C	65	CRQ	CA2-C2	-5.33	1.43	1.48
1	E	65	CRQ	CA2-C2	-5.20	1.43	1.48
1	F	65	CRQ	CA2-C2	-4.69	1.44	1.48
1	H	65	CRQ	CA2-C2	-4.62	1.44	1.48
1	D	65	CRQ	CA2-C2	-4.59	1.44	1.48
1	E	65	CRQ	C2-N3	-3.90	1.30	1.39
1	F	65	CRQ	C2-N3	-3.49	1.31	1.39
1	A	65	CRQ	CA2-C2	-3.30	1.45	1.48
1	H	65	CRQ	C2-N3	-3.26	1.32	1.39
1	A	65	CRQ	C2-N3	-3.24	1.32	1.39
1	D	65	CRQ	C2-N3	-3.19	1.32	1.39
1	H	65	CRQ	O2-C2	2.98	1.29	1.23
1	A	65	CRQ	O2-C2	2.98	1.29	1.23
1	C	65	CRQ	C2-N3	-2.86	1.33	1.39
1	F	65	CRQ	CA2-N2	-2.77	1.32	1.38
1	D	65	CRQ	C1-N2	2.61	1.39	1.33
1	B	65	CRQ	O2-C2	2.59	1.28	1.23
1	D	65	CRQ	O2-C2	2.56	1.28	1.23
1	F	65	CRQ	O2-C2	2.54	1.28	1.23
1	C	65	CRQ	O2-C2	2.51	1.28	1.23
1	E	65	CRQ	C1-N2	2.50	1.38	1.33
1	G	65	CRQ	O2-C2	2.46	1.28	1.23
1	B	65	CRQ	C2-N3	-2.22	1.34	1.39
1	F	65	CRQ	C1-N2	2.20	1.38	1.33
1	G	65	CRQ	C2-N3	-2.20	1.34	1.39
1	E	65	CRQ	CA2-N2	-2.19	1.33	1.38
1	D	65	CRQ	CA2-N2	-2.13	1.34	1.38
1	H	65	CRQ	CA2-N2	-2.03	1.34	1.38

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	65	CRQ	O2-C2-CA2	-18.92	120.34	130.96
1	E	65	CRQ	CA2-C2-N3	17.43	111.61	103.37
1	C	65	CRQ	O2-C2-CA2	-17.12	121.35	130.96
1	A	65	CRQ	O2-C2-CA2	-16.21	121.86	130.96
1	D	65	CRQ	CA2-C2-N3	16.14	111.00	103.37
1	B	65	CRQ	O2-C2-CA2	-16.09	121.92	130.96
1	F	65	CRQ	O2-C2-CA2	-15.92	122.02	130.96
1	E	65	CRQ	O2-C2-CA2	-15.90	122.03	130.96
1	D	65	CRQ	O2-C2-CA2	-15.77	122.10	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	65	CRQ	CA2-C2-N3	15.75	110.82	103.37
1	F	65	CRQ	CA2-C2-N3	14.95	110.44	103.37
1	A	65	CRQ	CA2-C2-N3	13.74	109.87	103.37
1	H	65	CRQ	CA2-C2-N3	13.25	109.63	103.37
1	C	65	CRQ	CA2-C2-N3	12.81	109.43	103.37
1	G	65	CRQ	CA2-C2-N3	12.74	109.39	103.37
1	H	65	CRQ	O2-C2-CA2	-12.57	123.90	130.96
1	B	65	CRQ	O3-C3-CA3	-6.67	106.24	126.39
1	H	65	CRQ	O3-C3-CA3	-6.10	107.98	126.39
1	B	65	CRQ	C2-CA2-N2	-5.98	104.74	108.93
1	E	65	CRQ	O3-C3-CA3	-5.85	108.72	126.39
1	F	65	CRQ	O3-C3-CA3	-5.66	109.31	126.39
1	G	65	CRQ	O3-C3-CA3	-5.28	110.46	126.39
1	C	65	CRQ	O3-C3-CA3	-5.18	110.76	126.39
1	A	65	CRQ	O3-C3-CA3	-4.90	111.59	126.39
1	D	65	CRQ	O3-C3-CA3	-4.78	111.96	126.39
1	E	65	CRQ	CA3-N3-C1	4.26	136.58	128.22
1	G	65	CRQ	CG2-CB2-CA2	-3.67	125.45	129.94
1	C	65	CRQ	CB2-CA2-N2	3.60	133.82	128.83
1	C	65	CRQ	CG2-CB2-CA2	-3.40	125.78	129.94
1	C	65	CRQ	CB2-CA2-C2	-3.23	118.42	122.28
1	A	65	CRQ	C2-CA2-N2	-3.17	106.71	108.93
1	E	65	CRQ	CD2-CG2-CD1	3.10	122.23	117.64
1	H	65	CRQ	C2-CA2-N2	-3.07	106.78	108.93
1	H	65	CRQ	CA3-N3-C1	3.04	134.18	128.22
1	F	65	CRQ	C2-CA2-N2	-2.97	106.85	108.93
1	G	65	CRQ	O2-C2-N3	2.85	130.01	124.35
1	D	65	CRQ	CA3-N3-C1	2.78	133.67	128.22
1	C	65	CRQ	CA3-N3-C1	2.78	133.67	128.22
1	D	65	CRQ	C2-CA2-N2	-2.76	107.00	108.93
1	F	65	CRQ	CE2-CD2-CG2	-2.73	117.69	121.25
1	G	65	CRQ	CE2-CD2-CG2	-2.73	117.69	121.25
1	E	65	CRQ	CG2-CB2-CA2	-2.73	126.60	129.94
1	D	65	CRQ	CB2-CA2-N2	2.71	132.58	128.83
1	G	65	CRQ	C2-CA2-N2	-2.69	107.05	108.93
1	G	65	CRQ	CD2-CG2-CD1	2.64	121.55	117.64
1	E	65	CRQ	CE2-CD2-CG2	-2.59	117.87	121.25
1	C	65	CRQ	CE2-CD2-CG2	-2.57	117.90	121.25
1	F	65	CRQ	CA3-N3-C1	2.55	133.22	128.22
1	E	65	CRQ	CB2-CA2-N2	2.49	132.28	128.83
1	H	65	CRQ	CG2-CB2-CA2	-2.48	126.91	129.94
1	C	65	CRQ	O2-C2-N3	2.45	129.22	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	65	CRQ	CD2-CG2-CD1	2.42	121.22	117.64
1	G	65	CRQ	CB2-CA2-N2	2.24	131.94	128.83
1	E	65	CRQ	CB2-CA2-C2	-2.21	119.64	122.28
1	F	65	CRQ	CB2-CA2-N2	2.18	131.85	128.83
1	B	65	CRQ	CA3-N3-C1	2.13	132.39	128.22
1	A	65	CRQ	CG2-CB2-CA2	-2.08	127.40	129.94
1	B	65	CRQ	CA2-N2-C1	2.07	108.12	104.33
1	G	65	CRQ	CA3-N3-C1	2.04	132.22	128.22
1	G	65	CRQ	CD2-CG2-CB2	-2.01	114.37	121.22

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	CRQ	C1-CA1-CB1-CG1
1	B	65	CRQ	C1-CA1-CB1-CG1
1	C	65	CRQ	C1-CA1-CB1-CG1
1	G	65	CRQ	C1-CA1-CB1-CG1
1	H	65	CRQ	C1-CA1-CB1-CG1
1	E	65	CRQ	NE1-CD3-CG1-CB1
1	E	65	CRQ	OE1-CD3-CG1-CB1
1	D	65	CRQ	OE1-CD3-CG1-CB1
1	H	65	CRQ	OE1-CD3-CG1-CB1
1	A	65	CRQ	OE1-CD3-CG1-CB1
1	A	65	CRQ	NE1-CD3-CG1-CB1
1	D	65	CRQ	NE1-CD3-CG1-CB1
1	A	65	CRQ	C3-CA3-N3-C2
1	H	65	CRQ	NE1-CD3-CG1-CB1
1	E	65	CRQ	C1-CA1-CB1-CG1
1	B	65	CRQ	OE1-CD3-CG1-CB1
1	G	65	CRQ	OE1-CD3-CG1-CB1
1	B	65	CRQ	NE1-CD3-CG1-CB1
1	G	65	CRQ	NE1-CD3-CG1-CB1
1	F	65	CRQ	NE1-CD3-CG1-CB1
1	F	65	CRQ	OE1-CD3-CG1-CB1

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	65	CRQ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	65	CRQ	1	0
1	E	65	CRQ	2	0
1	A	65	CRQ	3	0
1	G	65	CRQ	3	0
1	H	65	CRQ	3	0

5.5 Carbohydrates (i)

There are no monosaccharides 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^{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	217/271 (80%)	-0.02	6 (2%)	53	60	16, 26, 46, 76	0
1	B	217/271 (80%)	0.07	10 (4%)	32	39	18, 29, 49, 72	0
1	C	220/271 (81%)	-0.17	6 (2%)	54	62	15, 23, 42, 71	0
1	D	217/271 (80%)	-0.00	7 (3%)	47	54	15, 25, 46, 83	0
1	E	217/271 (80%)	-0.16	3 (1%)	75	80	16, 26, 42, 88	0
1	F	217/271 (80%)	-0.19	3 (1%)	75	80	16, 25, 42, 66	0
1	G	219/271 (80%)	-0.10	8 (3%)	41	48	15, 25, 44, 89	0
1	H	217/271 (80%)	0.00	6 (2%)	53	60	16, 27, 47, 64	0
All	All	1741/2168 (80%)	-0.07	49 (2%)	53	60	15, 26, 46, 89	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	227	ARG	6.5
1	D	227	ARG	5.9
1	A	227	ARG	4.9
1	C	227	ARG	4.1
1	G	211	ARG	3.8
1	E	227	ARG	3.6
1	D	2	GLU	3.3
1	C	1(B)	SER	3.2
1	B	52	LYS	3.1
1	A	169	ASP	3.1
1	D	186	SER	2.9
1	H	188	ALA	2.9
1	H	2	GLU	2.9
1	C	209	ASP	2.8
1	A	186	SER	2.8
1	G	169	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	76	ASP	2.8
1	F	188	ALA	2.7
1	A	2	GLU	2.6
1	B	2	GLU	2.6
1	B	169	ASP	2.6
1	B	76	ASP	2.6
1	D	100	ASN	2.5
1	B	188	ALA	2.4
1	B	51	GLY	2.4
1	B	131	ASP	2.4
1	C	76	ASP	2.3
1	E	2	GLU	2.3
1	H	186	SER	2.3
1	C	2	GLU	2.3
1	D	228	ILE	2.3
1	H	136	ARG	2.3
1	G	226	PRO	2.3
1	E	228	ILE	2.3
1	G	188	ALA	2.3
1	G	228	ILE	2.2
1	B	3	VAL	2.2
1	A	155	ASN	2.2
1	F	205	ARG	2.2
1	G	2	GLU	2.2
1	B	136	ARG	2.2
1	H	76	ASP	2.1
1	H	52	LYS	2.1
1	G	205	ARG	2.1
1	C	188	ALA	2.1
1	D	169	ASP	2.0
1	D	89	GLY	2.0
1	B	186	SER	2.0
1	A	188	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CRQ	E	65	24/25	0.93	0.16	15,21,28,30	0
1	CRQ	B	65	24/25	0.94	0.16	18,21,24,30	0
1	CRQ	F	65	24/25	0.94	0.15	17,21,30,34	0
1	CRQ	A	65	24/25	0.95	0.15	19,24,29,32	0
1	CRQ	C	65	24/25	0.95	0.14	15,19,29,36	0
1	CRQ	G	65	24/25	0.95	0.15	17,21,28,32	0
1	CRQ	H	65	24/25	0.95	0.15	17,20,23,25	0
1	CRQ	D	65	24/25	0.97	0.16	17,20,28,32	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.