Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 AM GMT

PDB ID	:	2IB5
Title	:	Structural characterization of a blue chromoprotein and its yellow mutant from the sea anemone cnidopus japonicus
Authors	:	Chan, M.C.Y.; Bosanac, I.; Ikura, M.
Deposited on	:	2006-09-10
Resolution	:	1.80 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 ⓘ symbol.

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

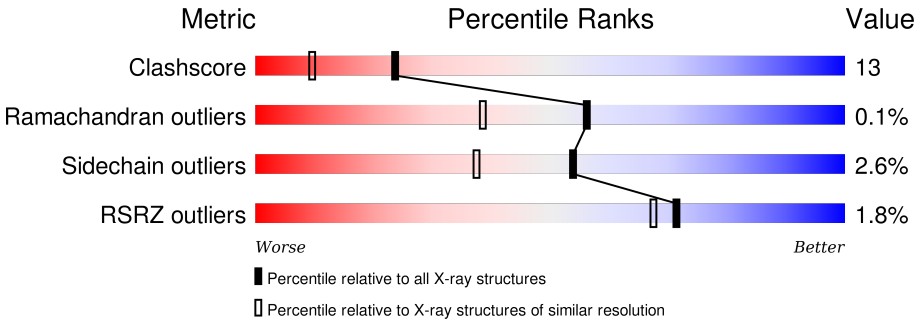
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	233	79% 16%
1	B	233	% 75% 21%
1	C	233	2% 70% 24%
1	D	233	% 71% 24%
1	E	233	% 74% 22%
1	F	233	2% 73% 23%
1	G	233	4% 72% 24%

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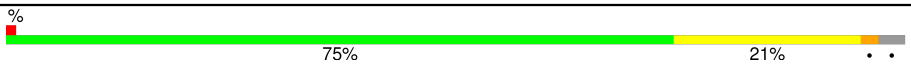
Mol	Chain	Length	Quality of chain
1	H	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	2001	-	-	X	-
2	PO4	D	2012	-	-	-	X
2	PO4	E	2013	-	-	-	X
2	PO4	H	2005	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15792 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 Chromo protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	B	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	C	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	D	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	E	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	F	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	G	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			
1	H	226	Total	C	N	O	S	Se	0	0	0
			1798	1132	308	340	11	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
A	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
A	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
A	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
A	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
A	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
B	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
B	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
B	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
B	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
B	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
B	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
C	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7

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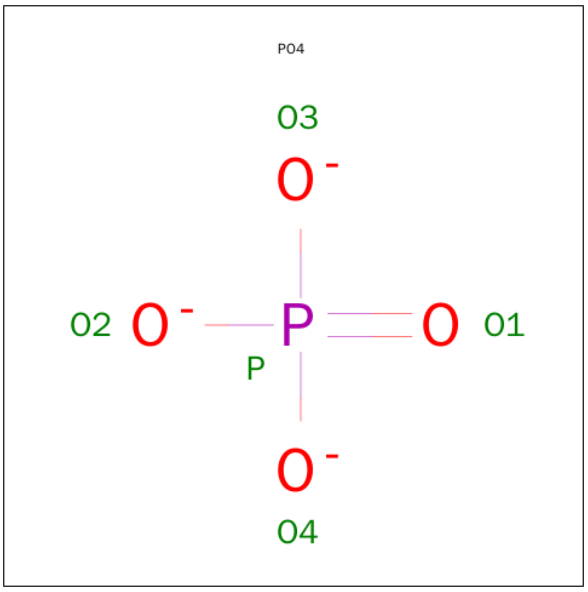
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
C	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
C	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
C	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
C	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
D	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
D	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
D	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
D	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
D	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
D	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
E	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
E	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
E	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
E	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
E	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
E	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
F	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
F	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
F	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
F	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
F	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
F	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
G	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
G	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
G	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
G	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
G	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
G	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7
H	-2	GLY	-	EXPRESSION TAG	UNP A0AQQ7
H	-1	SER	-	EXPRESSION TAG	UNP A0AQQ7
H	0	HIS	-	EXPRESSION TAG	UNP A0AQQ7
H	65	CRQ	GLN	CHROMOPHORE	UNP A0AQQ7
H	65	CRQ	TYR	CHROMOPHORE	UNP A0AQQ7
H	65	CRQ	GLY	CHROMOPHORE	UNP A0AQQ7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

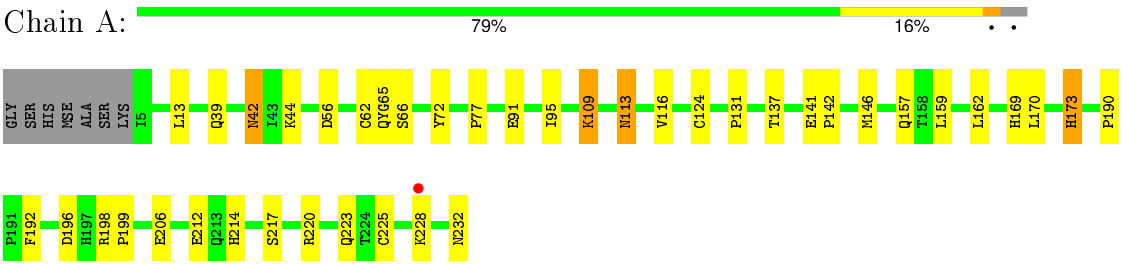
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	198	Total O 198 198	0	0
3	B	174	Total O 174 174	0	0
3	C	183	Total O 183 183	0	0
3	D	182	Total O 182 182	0	0
3	E	151	Total O 151 151	0	0
3	F	136	Total O 136 136	0	0
3	G	141	Total O 141 141	0	0
3	H	163	Total O 163 163	0	0

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.

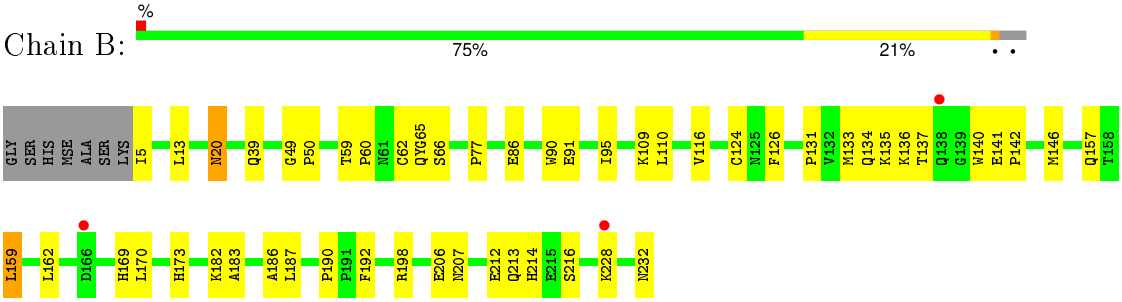
- Molecule 1: Chromo protein

Chain A:



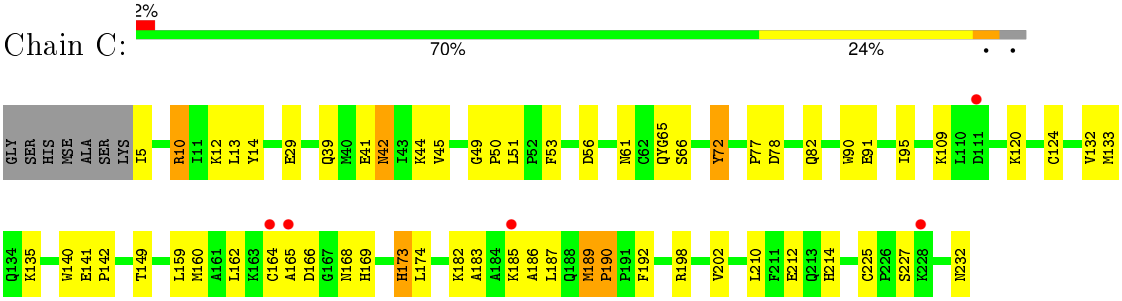
- Molecule 1: Chromo protein

Chain B:



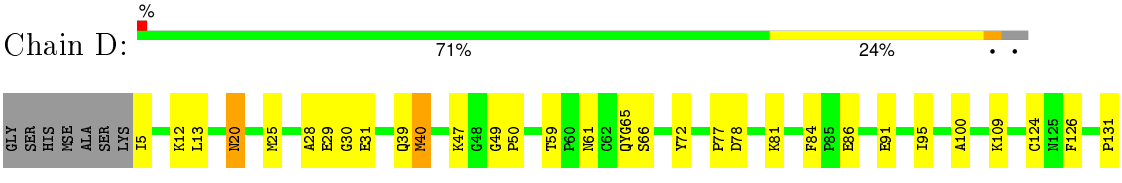
- Molecule 1: Chromo protein

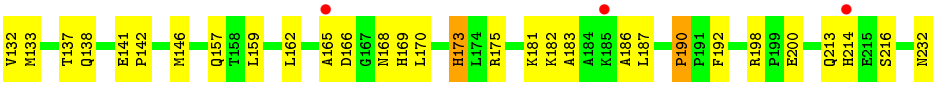
Chain C:



- Molecule 1: Chromo protein

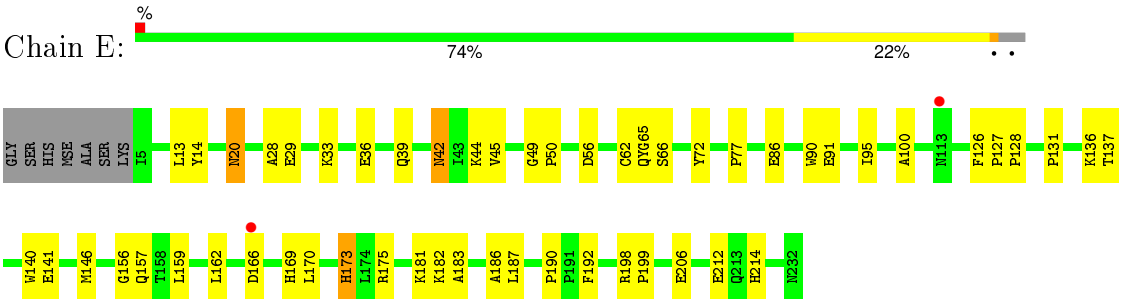
Chain D:





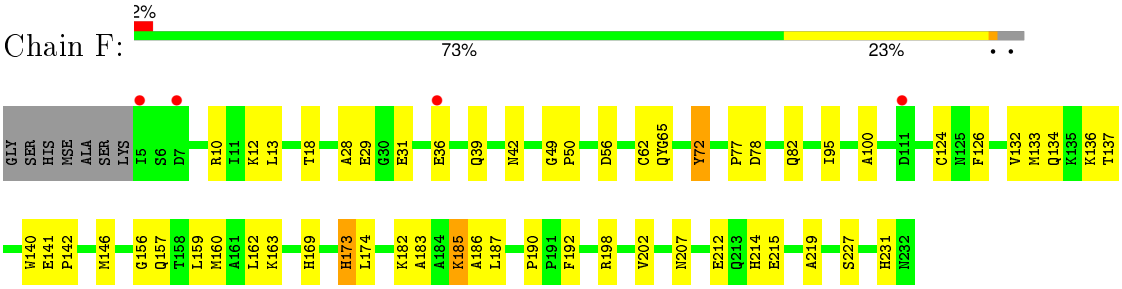
• Molecule 1: Chromo protein

Chain E:



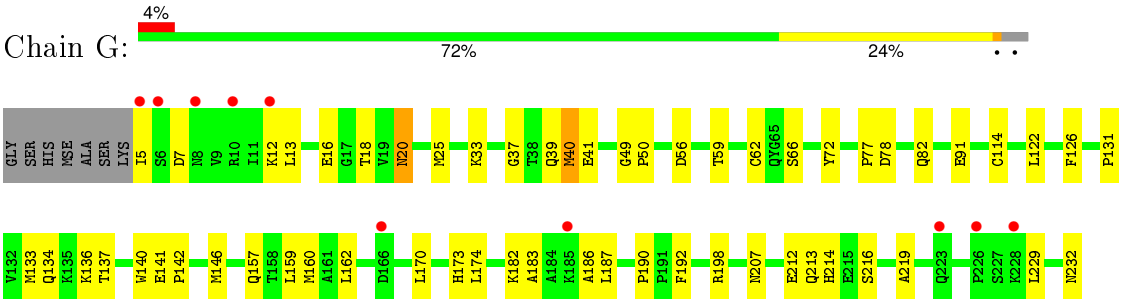
• Molecule 1: Chromo protein

Chain F:



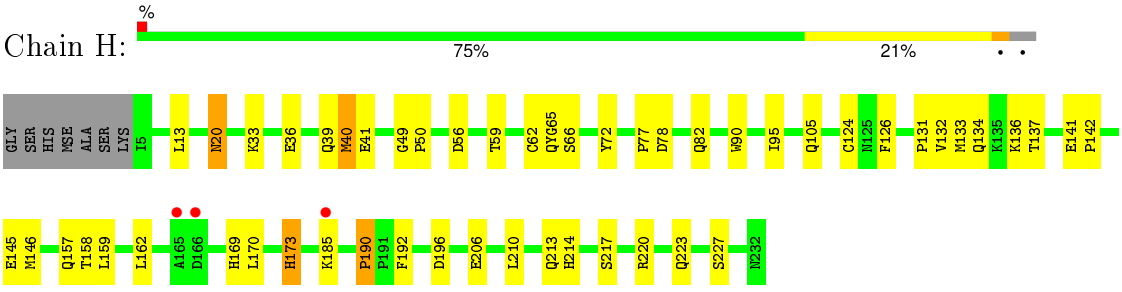
• Molecule 1: Chromo protein

Chain G:



• Molecule 1: Chromo protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.86Å 126.85Å 100.51Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 45.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.80) 99.4 (45.82-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.03 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.225 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.777	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 331473 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15792	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.59% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.38	0/1811	0.72	1/2436 (0.0%)
1	B	0.35	0/1811	0.69	1/2436 (0.0%)
1	C	0.36	0/1811	0.75	4/2436 (0.2%)
1	D	0.37	0/1811	0.73	1/2436 (0.0%)
1	E	0.34	0/1811	0.68	1/2436 (0.0%)
1	F	0.33	0/1811	0.66	1/2436 (0.0%)
1	G	0.33	0/1811	0.64	1/2436 (0.0%)
1	H	0.37	0/1811	0.69	2/2436 (0.1%)
All	All	0.35	0/14488	0.70	12/19488 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	ASN	O-C-N	-7.17	111.23	122.70
1	C	72	TYR	N-CA-CB	-6.87	98.23	110.60
1	C	90	TRP	CA-CB-CG	6.59	126.22	113.70
1	H	90	TRP	CA-CB-CG	6.24	125.55	113.70
1	B	62	CYS	N-CA-C	5.81	126.70	111.00
1	F	62	CYS	N-CA-C	5.78	126.60	111.00
1	H	62	CYS	N-CA-C	5.75	126.54	111.00
1	C	72	TYR	CB-CA-C	5.52	121.43	110.40
1	A	62	CYS	N-CA-C	5.38	125.53	111.00
1	E	62	CYS	N-CA-C	5.25	125.19	111.00
1	G	62	CYS	N-CA-C	5.25	125.18	111.00
1	C	61	ASN	O-C-N	-5.24	114.32	122.70

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	1798	0	1730	42	0
1	B	1798	0	1730	57	0
1	C	1798	0	1730	59	0
1	D	1798	0	1730	60	0
1	E	1798	0	1730	54	0
1	F	1798	0	1730	56	0
1	G	1798	0	1730	55	0
1	H	1798	0	1730	49	0
2	A	15	0	0	2	0
2	B	15	0	0	1	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	15	0	0	1	0
2	G	10	0	0	0	0
2	H	10	0	0	2	0
3	A	198	0	0	4	0
3	B	174	0	0	2	1
3	C	183	0	0	5	0
3	D	182	0	0	4	1
3	E	151	0	0	5	0
3	F	136	0	0	2	0
3	G	141	0	0	9	0
3	H	163	0	0	4	0
All	All	15792	0	13840	373	1

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 13.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:MSE:CE	3:G:2155:HOH:O	1.78	1.26
3:G:2046:HOH:O	1:H:124:CYS:HB3	1.53	1.04
1:E:182:LYS:HB3	1:E:187:LEU:HD11	1.44	0.97
1:F:160:MSE:HE2	1:F:174:LEU:HD11	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LYS:HB3	1:C:187:LEU:HD21	1.46	0.95
1:B:182:LYS:HB3	1:B:187:LEU:HD21	1.48	0.94
1:B:136:LYS:HG2	1:E:136:LYS:HG2	1.49	0.92
1:G:160:MSE:HE2	1:G:174:LEU:HD11	1.49	0.92
1:A:192:PHE:CD2	1:D:141:GLU:HG2	2.08	0.89
1:A:141:GLU:HG3	1:A:142:PRO:HD2	1.53	0.89
1:B:141:GLU:HG2	1:C:192:PHE:CD2	2.08	0.89
1:E:175:ARG:NH1	3:E:2160:HOH:O	2.04	0.88
1:C:160:MSE:HE2	1:C:174:LEU:HD11	1.54	0.87
1:D:200:GLU:HB2	1:D:214:HIS:CE1	2.10	0.86
1:F:141:GLU:HG2	1:G:192:PHE:CD2	2.10	0.86
1:F:141:GLU:HG3	1:F:142:PRO:HD2	1.56	0.86
1:B:141:GLU:HG3	1:B:142:PRO:HD2	1.58	0.86
1:A:141:GLU:HG2	1:D:192:PHE:CD2	2.10	0.85
1:F:192:PHE:CD2	1:G:141:GLU:HG2	2.11	0.85
1:H:39:GLN:NE2	1:H:65:CRQ:HE11	1.77	0.83
1:D:141:GLU:HG3	1:D:142:PRO:HD2	1.61	0.82
1:C:182:LYS:CB	1:C:187:LEU:HD21	2.09	0.81
1:E:182:LYS:CB	1:E:187:LEU:HD11	2.09	0.81
1:G:141:GLU:HG3	1:G:142:PRO:HD2	1.62	0.81
1:A:141:GLU:HG2	1:D:192:PHE:CE2	2.17	0.80
1:A:198:ARG:HH22	1:D:232:ASN:C	1.86	0.78
1:E:192:PHE:CD2	1:H:141:GLU:HG2	2.19	0.78
1:D:39:GLN:NE2	1:D:65:CRQ:HE11	1.82	0.77
1:D:182:LYS:HB3	1:D:187:LEU:HD11	1.67	0.76
1:F:10:ARG:NH2	1:F:29:GLU:HG3	2.00	0.76
1:B:192:PHE:CD2	1:C:141:GLU:HG2	2.20	0.76
1:D:39:GLN:HE21	1:D:65:CRQ:HE11	1.33	0.76
2:E:2013:PO4:O2	3:E:2159:HOH:O	2.05	0.75
1:G:20:ASN:HD21	1:G:126:PHE:H	1.34	0.75
1:F:10:ARG:HH22	1:F:29:GLU:HG3	1.50	0.74
1:B:20:ASN:HD21	1:B:126:PHE:H	1.34	0.74
1:B:86:GLU:OE2	1:B:182:LYS:HE3	1.88	0.74
1:E:183:ALA:O	1:E:187:LEU:HD13	1.88	0.74
1:B:131:PRO:HG2	1:B:170:LEU:HD22	1.68	0.74
1:B:141:GLU:HG2	1:C:192:PHE:CE2	2.23	0.73
1:G:134:GLN:HB2	1:G:136:LYS:HE2	1.71	0.73
1:G:160:MSE:HE1	3:G:2155:HOH:O	1.61	0.72
1:D:20:ASN:HD21	1:D:126:PHE:H	1.35	0.72
1:H:39:GLN:HE21	1:H:65:CRQ:HE11	1.34	0.72
1:A:228:LYS:HB2	1:D:214:HIS:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:PHE:CE2	1:H:141:GLU:HG2	2.24	0.72
1:H:141:GLU:HG3	1:H:142:PRO:HD2	1.72	0.72
1:A:198:ARG:NH2	1:D:232:ASN:O	2.23	0.71
1:B:206:GLU:OE2	1:H:185:LYS:HD2	1.90	0.71
1:H:20:ASN:HD21	1:H:126:PHE:H	1.38	0.71
1:F:198:ARG:HH22	1:G:232:ASN:C	1.94	0.70
1:D:157:GLN:HE21	1:D:173:HIS:CE1	2.10	0.70
1:C:182:LYS:HB3	1:C:187:LEU:CD2	2.21	0.70
1:A:192:PHE:CE2	1:D:141:GLU:HG2	2.27	0.70
1:F:77:PRO:HG2	1:F:190:PRO:HA	1.73	0.69
1:E:20:ASN:HD21	1:E:126:PHE:H	1.40	0.69
1:G:182:LYS:HB3	1:G:187:LEU:HD21	1.74	0.69
1:C:164:CYS:HB2	1:C:168:ASN:C	2.13	0.69
1:H:40:MSE:HE2	1:H:41:GLU:CA	2.22	0.69
1:H:134:GLN:HB2	1:H:136:LYS:HE2	1.75	0.69
1:E:182:LYS:HB3	1:E:187:LEU:CD1	2.22	0.69
1:F:141:GLU:HG2	1:G:192:PHE:CE2	2.28	0.69
1:B:77:PRO:HG2	1:B:190:PRO:HA	1.75	0.69
1:A:39:GLN:NE2	1:A:65:CRQ:HE11	1.91	0.68
1:B:228:LYS:O	1:B:228:LYS:HD3	1.92	0.68
1:F:215:GLU:OE2	3:F:2150:HOH:O	2.12	0.68
1:B:192:PHE:CE2	1:C:141:GLU:HG2	2.29	0.68
1:D:30:GLY:HA2	1:D:40:MSE:HE3	1.74	0.67
1:D:157:GLN:HE21	1:D:173:HIS:HE1	1.42	0.67
1:A:232:ASN:C	1:D:198:ARG:HH22	1.97	0.67
1:C:183:ALA:O	1:C:187:LEU:HD23	1.95	0.66
1:H:33:LYS:HE2	1:H:36:GLU:HG3	1.77	0.66
1:F:227:SER:HB2	1:G:198:ARG:HE	1.60	0.66
1:G:137:THR:HG21	1:G:162:LEU:HD13	1.77	0.66
1:B:228:LYS:HD2	1:C:202:VAL:HG11	1.78	0.65
1:F:198:ARG:NH2	1:G:232:ASN:O	2.29	0.65
1:H:131:PRO:HA	1:H:136:LYS:HE3	1.79	0.64
1:A:232:ASN:O	1:D:198:ARG:NH2	2.29	0.64
1:B:39:GLN:NE2	1:B:65:CRQ:HE11	1.95	0.64
1:B:232:ASN:O	1:C:198:ARG:NH2	2.28	0.64
1:F:192:PHE:CE2	1:G:141:GLU:HG2	2.33	0.64
1:C:132:VAL:HG12	1:C:133:MSE:HE2	1.80	0.64
1:F:12:LYS:NZ	1:F:12:LYS:HB3	2.13	0.64
1:E:146:MSE:HG3	1:E:192:PHE:CZ	2.33	0.63
1:B:169:HIS:HD2	3:C:277:HOH:O	1.81	0.63
1:E:44:LYS:HD3	1:E:45:VAL:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LYS:CB	1:D:187:LEU:HD11	2.28	0.63
1:G:91:GLU:HB2	3:G:2046:HOH:O	1.97	0.63
1:A:212:GLU:OE2	1:A:214:HIS:HE1	1.82	0.63
1:E:131:PRO:HG2	1:E:170:LEU:HD22	1.81	0.62
1:H:40:MSE:HE2	1:H:41:GLU:HA	1.80	0.62
1:G:160:MSE:HE2	3:G:2155:HOH:O	1.69	0.62
1:H:132:VAL:HG12	1:H:133:MSE:HE2	1.81	0.61
1:D:200:GLU:HB2	1:D:214:HIS:HE1	1.65	0.61
3:E:2029:HOH:O	1:H:169:HIS:HD2	1.84	0.61
1:D:30:GLY:HA2	1:D:40:MSE:CE	2.30	0.61
1:D:25:MSE:SE	1:D:47:LYS:HD3	2.51	0.61
1:A:146:MSE:HG3	1:A:192:PHE:CZ	2.35	0.61
1:H:146:MSE:HG3	1:H:192:PHE:CZ	2.36	0.61
1:D:183:ALA:O	1:D:187:LEU:HD13	2.01	0.60
1:B:77:PRO:HG2	1:B:190:PRO:CA	2.31	0.60
1:B:198:ARG:HH22	1:C:232:ASN:C	2.05	0.60
1:D:137:THR:HG21	1:D:162:LEU:HD13	1.84	0.60
1:F:39:GLN:NE2	1:F:65:CRQ:HE11	2.00	0.60
1:B:65:CRQ:HA31	1:B:65:CRQ:N	2.17	0.59
1:F:183:ALA:O	1:F:187:LEU:HD23	2.02	0.59
1:B:232:ASN:C	1:C:198:ARG:HH22	2.04	0.59
1:E:137:THR:HG21	1:E:162:LEU:HD13	1.83	0.59
1:E:39:GLN:NE2	1:E:65:CRQ:HE11	2.00	0.59
1:A:169:HIS:HD2	3:A:2019:HOH:O	1.85	0.59
1:C:39:GLN:NE2	1:C:65:CRQ:HE11	2.01	0.59
1:C:53:PHE:N	1:C:135:LYS:HZ3	2.00	0.58
1:F:182:LYS:CB	1:F:187:LEU:HD21	2.33	0.58
1:A:77:PRO:HG2	1:A:190:PRO:HA	1.85	0.58
1:G:12:LYS:HG3	1:G:114:CYS:SG	2.42	0.58
1:D:77:PRO:HG2	1:D:190:PRO:HA	1.84	0.58
1:F:182:LYS:HB3	1:F:187:LEU:HD21	1.85	0.58
1:C:77:PRO:HG2	1:C:190:PRO:HA	1.86	0.58
1:F:10:ARG:HH11	1:F:10:ARG:HG3	1.68	0.58
1:C:77:PRO:HG2	1:C:190:PRO:HB3	1.85	0.58
1:C:141:GLU:HG3	1:C:142:PRO:HD2	1.84	0.58
1:A:77:PRO:HG2	1:A:190:PRO:CA	2.33	0.58
1:A:137:THR:HG21	1:A:162:LEU:HD13	1.84	0.58
1:F:77:PRO:HG2	1:F:190:PRO:CA	2.33	0.58
1:C:77:PRO:HG2	1:C:190:PRO:CA	2.33	0.58
1:B:182:LYS:CB	1:B:187:LEU:HD21	2.27	0.57
1:H:77:PRO:HG2	1:H:190:PRO:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:HG2	1:E:136:LYS:CG	2.29	0.57
1:G:77:PRO:HG2	1:G:190:PRO:HB3	1.86	0.57
1:E:169:HIS:HD2	3:H:2031:HOH:O	1.86	0.57
1:B:65:CRQ:CA3	1:B:65:CRQ:N	2.68	0.56
1:C:44:LYS:HD3	1:C:45:VAL:N	2.18	0.56
1:C:12:LYS:HE3	1:C:29:GLU:OE2	2.05	0.56
1:F:10:ARG:HH22	1:F:29:GLU:CG	2.18	0.56
1:H:77:PRO:HG2	1:H:190:PRO:CA	2.35	0.56
1:A:39:GLN:HE21	1:A:65:CRQ:HE11	1.52	0.56
1:A:225:CYS:HB3	1:D:216:SER:OG	2.05	0.56
1:B:183:ALA:O	1:B:187:LEU:HD23	2.06	0.56
1:E:198:ARG:NH2	1:H:227:SER:HB2	2.19	0.56
1:D:78:ASP:OD1	1:D:81:LYS:HD3	2.06	0.56
1:D:165:ALA:HB3	3:D:2065:HOH:O	2.05	0.56
1:E:77:PRO:HG2	1:E:190:PRO:CA	2.36	0.55
1:B:65:CRQ:HA32	1:B:90:TRP:CZ2	2.41	0.55
1:C:189:MSE:HE2	3:C:397:HOH:O	2.07	0.55
1:G:40:MSE:HE2	1:G:41:GLU:C	2.26	0.55
1:G:5:ILE:N	3:G:2090:HOH:O	2.39	0.55
1:F:13:LEU:HB3	1:F:28:ALA:HB3	1.87	0.55
3:B:2060:HOH:O	1:C:169:HIS:HD2	1.89	0.55
1:D:13:LEU:HD23	1:D:13:LEU:C	2.27	0.55
1:A:228:LYS:HB2	1:D:214:HIS:HE2	1.70	0.55
1:C:56:ASP:HB3	1:C:162:LEU:HD21	1.88	0.55
1:C:10:ARG:HD3	3:C:384:HOH:O	2.07	0.55
1:G:77:PRO:HG2	1:G:190:PRO:CA	2.37	0.55
1:E:77:PRO:HG2	1:E:190:PRO:HA	1.88	0.55
1:G:131:PRO:HG2	1:G:170:LEU:HD22	1.88	0.55
1:E:186:ALA:C	1:E:187:LEU:HD12	2.28	0.54
1:B:146:MSE:HG3	1:B:192:PHE:CZ	2.42	0.54
1:D:59:THR:HG23	1:D:213:GLN:NE2	2.22	0.54
1:G:59:THR:HG23	1:G:213:GLN:NE2	2.22	0.54
1:A:131:PRO:HG2	1:A:170:LEU:HD22	1.89	0.54
1:C:124:CYS:HB2	1:D:91:GLU:HG3	1.89	0.54
1:G:146:MSE:HG3	1:G:192:PHE:CZ	2.43	0.54
1:F:186:ALA:C	1:F:187:LEU:HD22	2.28	0.53
1:G:77:PRO:HG2	1:G:190:PRO:HA	1.90	0.53
1:G:18:THR:HG21	1:H:105:GLN:HG2	1.89	0.53
1:F:137:THR:HG21	1:F:162:LEU:HD13	1.90	0.53
1:A:113:ASN:H	1:A:113:ASN:HD22	1.56	0.53
1:B:39:GLN:HE21	1:B:65:CRQ:HE11	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:GLN:HE22	1:D:66:SER:CB	2.21	0.53
1:F:212:GLU:OE2	1:F:214:HIS:HE1	1.91	0.53
1:G:40:MSE:HE3	1:G:212:GLU:HG3	1.89	0.53
1:C:13:LEU:HD23	1:C:13:LEU:C	2.30	0.53
1:H:77:PRO:HG2	1:H:190:PRO:HB3	1.90	0.53
1:E:29:GLU:HG3	3:E:2151:HOH:O	2.09	0.53
2:B:2002:PO4:O2	1:C:173:HIS:HD2	1.91	0.52
3:A:2046:HOH:O	1:D:169:HIS:HD2	1.92	0.52
1:G:78:ASP:O	1:G:82:GLN:HG3	2.09	0.52
1:D:86:GLU:O	1:D:181:LYS:HD2	2.10	0.52
1:A:109:LYS:HB2	1:A:109:LYS:NZ	2.25	0.52
1:A:109:LYS:HG2	1:A:116:VAL:HB	1.92	0.52
1:C:77:PRO:HG2	1:C:190:PRO:CB	2.39	0.52
1:H:95:ILE:HD13	3:H:2159:HOH:O	2.09	0.52
1:F:169:HIS:HD2	3:G:2041:HOH:O	1.93	0.52
1:E:33:LYS:HE2	1:E:36:GLU:HG3	1.91	0.52
1:B:198:ARG:NH2	1:C:232:ASN:O	2.43	0.52
1:C:12:LYS:HD3	1:C:13:LEU:N	2.25	0.52
1:A:77:PRO:HG2	1:A:190:PRO:HB3	1.92	0.52
1:E:56:ASP:HB3	1:E:162:LEU:HD21	1.92	0.51
1:B:137:THR:HG21	1:B:162:LEU:HD13	1.92	0.51
1:H:131:PRO:HA	1:H:136:LYS:CE	2.40	0.51
1:G:212:GLU:OE2	1:G:214:HIS:HE1	1.93	0.51
1:E:13:LEU:C	1:E:13:LEU:HD23	2.31	0.51
1:D:13:LEU:HB3	1:D:28:ALA:HB3	1.93	0.51
1:B:212:GLU:OE2	1:B:214:HIS:HE1	1.92	0.51
1:C:212:GLU:OE2	1:C:214:HIS:HE1	1.93	0.51
1:C:164:CYS:HB2	1:C:168:ASN:O	2.09	0.51
1:E:77:PRO:HG2	1:E:190:PRO:HB3	1.93	0.51
1:D:77:PRO:HG2	1:D:190:PRO:CA	2.41	0.51
1:B:131:PRO:CG	1:B:170:LEU:HD22	2.39	0.50
2:A:2001:PO4:O2	1:D:173:HIS:HD2	1.94	0.50
1:B:39:GLN:HE22	1:B:66:SER:CB	2.23	0.50
1:H:173:HIS:HD2	2:H:2005:PO4:O1	1.94	0.50
1:A:109:LYS:CG	1:A:116:VAL:HB	2.42	0.50
1:H:137:THR:HG21	1:H:162:LEU:HD13	1.93	0.50
1:C:149:THR:HG21	1:C:189:MSE:HG3	1.93	0.50
1:G:13:LEU:C	1:G:13:LEU:HD23	2.32	0.50
1:H:206:GLU:OE2	1:H:210:LEU:HD22	2.11	0.50
1:H:33:LYS:CE	1:H:36:GLU:HG3	2.41	0.49
1:D:186:ALA:C	1:D:187:LEU:HD12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASN:ND2	3:A:2089:HOH:O	2.44	0.49
1:F:163:LYS:HB3	1:F:163:LYS:NZ	2.27	0.49
1:D:5:ILE:N	3:D:2076:HOH:O	2.44	0.49
1:A:39:GLN:HE22	1:A:66:SER:CB	2.25	0.49
1:D:30:GLY:CA	1:D:40:MSE:HE3	2.41	0.49
1:C:39:GLN:HE22	1:C:66:SER:CB	2.25	0.49
3:E:2119:HOH:O	1:F:18:THR:HG21	2.13	0.49
1:C:186:ALA:C	1:C:187:LEU:HD22	2.33	0.49
1:H:77:PRO:HG2	1:H:190:PRO:CB	2.43	0.49
1:A:220:ARG:HD2	1:A:223:GLN:HE21	1.77	0.49
1:A:173:HIS:HD2	2:A:2001:PO4:O3	1.96	0.49
1:A:124:CYS:HB2	1:B:91:GLU:HG3	1.95	0.49
1:F:13:LEU:HD23	1:F:13:LEU:C	2.33	0.49
1:F:72:TYR:HA	1:F:219:ALA:HB3	1.95	0.49
1:G:91:GLU:HG3	1:H:124:CYS:HB2	1.95	0.48
1:E:141:GLU:OE2	1:E:169:HIS:HE1	1.96	0.48
1:B:140:TRP:CZ3	1:B:162:LEU:HG	2.49	0.48
1:F:49:GLY:HA2	1:F:50:PRO:C	2.33	0.48
1:B:157:GLN:HB3	1:C:159:LEU:HD13	1.95	0.48
1:F:159:LEU:HD13	1:G:157:GLN:HB3	1.96	0.48
1:G:186:ALA:C	1:G:187:LEU:HD22	2.34	0.48
1:F:36:GLU:HG2	3:F:2103:HOH:O	2.13	0.48
1:H:41:GLU:HG3	1:H:65:CRQ:NE1	2.29	0.48
1:G:77:PRO:HG2	1:G:190:PRO:CB	2.43	0.48
1:B:109:LYS:CG	1:B:116:VAL:HB	2.43	0.48
1:H:220:ARG:HD2	1:H:223:GLN:HE21	1.78	0.47
1:C:53:PHE:N	1:C:135:LYS:NZ	2.62	0.47
1:C:12:LYS:HD2	1:C:14:TYR:CE1	2.49	0.47
1:C:49:GLY:HA2	1:C:50:PRO:C	2.34	0.47
1:D:109:LYS:HD3	3:D:2183:HOH:O	2.15	0.47
1:B:126:PHE:HB2	1:B:133:MSE:HE3	1.96	0.47
1:G:183:ALA:O	1:G:187:LEU:HD23	2.14	0.47
1:D:49:GLY:HA2	1:D:50:PRO:C	2.35	0.47
1:E:159:LEU:HD13	1:H:157:GLN:HB3	1.96	0.47
1:C:109:LYS:HG2	3:C:376:HOH:O	2.13	0.47
1:F:10:ARG:NH1	1:F:10:ARG:HG3	2.30	0.47
1:A:13:LEU:C	1:A:13:LEU:HD23	2.36	0.47
1:E:39:GLN:HE21	1:E:65:CRQ:HE11	1.62	0.47
1:D:138:GLN:HE22	1:D:165:ALA:CA	2.27	0.47
1:D:131:PRO:HG2	1:D:170:LEU:HD22	1.97	0.46
1:G:229:LEU:HA	3:G:2115:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:THR:HG22	1:G:122:LEU:HD23	1.97	0.46
1:A:228:LYS:CB	1:D:214:HIS:NE2	2.76	0.46
1:F:140:TRP:CH2	1:F:162:LEU:HG	2.50	0.46
1:B:13:LEU:C	1:B:13:LEU:HD23	2.36	0.46
1:F:56:ASP:HB3	1:F:162:LEU:HD21	1.98	0.46
1:C:42:ASN:ND2	1:C:210:LEU:HD11	2.30	0.46
1:E:159:LEU:HG	1:H:159:LEU:HG	1.97	0.46
1:F:202:VAL:HG12	1:G:229:LEU:HD21	1.97	0.46
1:G:39:GLN:HE22	1:G:66:SER:CB	2.28	0.46
1:A:77:PRO:HG2	1:A:190:PRO:CB	2.46	0.46
1:B:186:ALA:C	1:B:187:LEU:HD22	2.37	0.46
1:A:159:LEU:HD13	1:D:157:GLN:HB3	1.98	0.46
1:E:65:CRQ:HA31	1:E:90:TRP:CZ2	2.51	0.46
1:C:91:GLU:HG3	1:D:124:CYS:HB2	1.97	0.46
1:C:53:PHE:CA	1:C:135:LYS:HZ3	2.29	0.45
1:A:157:GLN:HB3	1:D:159:LEU:HD13	1.97	0.45
1:H:49:GLY:HA2	1:H:50:PRO:C	2.37	0.45
1:H:13:LEU:C	1:H:13:LEU:HD23	2.37	0.45
1:H:214:HIS:HD2	3:H:2032:HOH:O	1.99	0.45
1:G:140:TRP:CH2	1:G:162:LEU:HG	2.52	0.45
1:B:198:ARG:NH2	1:C:227:SER:HB2	2.31	0.45
1:C:51:LEU:O	1:C:135:LYS:NZ	2.34	0.45
1:E:42:ASN:HA	1:E:42:ASN:HD22	1.60	0.45
1:G:126:PHE:CB	1:G:133:MSE:HE3	2.46	0.45
1:E:198:ARG:CZ	1:H:227:SER:HB2	2.47	0.45
1:H:39:GLN:HE22	1:H:66:SER:CB	2.29	0.45
1:G:56:ASP:HB3	1:G:162:LEU:HD21	1.99	0.45
1:E:39:GLN:HE22	1:E:66:SER:CB	2.30	0.45
1:B:159:LEU:HD13	1:C:159:LEU:HD11	1.98	0.45
1:F:146:MSE:HG3	1:F:192:PHE:CZ	2.52	0.45
1:H:39:GLN:NE2	1:H:65:CRQ:NE1	2.57	0.45
1:E:77:PRO:HG2	1:E:190:PRO:CB	2.47	0.45
1:C:185:LYS:HG2	1:E:206:GLU:OE2	2.16	0.44
1:F:134:GLN:CB	1:F:136:LYS:HE2	2.48	0.44
1:C:41:GLU:HG3	1:C:65:CRQ:NE1	2.32	0.44
1:E:91:GLU:HG3	1:F:124:CYS:HB2	2.00	0.44
1:E:157:GLN:HB3	1:H:159:LEU:HD13	1.99	0.44
1:G:49:GLY:HA2	1:G:50:PRO:C	2.37	0.44
1:D:100:ALA:HB2	1:D:126:PHE:HA	1.99	0.44
1:B:198:ARG:CZ	1:C:227:SER:HB2	2.48	0.44
1:E:95:ILE:N	1:E:95:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:PRO:CG	1:F:190:PRO:HA	2.45	0.44
1:G:198:ARG:CZ	3:G:2019:HOH:O	2.66	0.44
1:F:140:TRP:CZ3	1:F:162:LEU:HG	2.52	0.44
1:G:59:THR:HG23	1:G:213:GLN:CD	2.38	0.44
1:C:5:ILE:N	3:C:353:HOH:O	2.50	0.44
1:A:95:ILE:HD13	3:A:2070:HOH:O	2.17	0.44
1:G:131:PRO:HA	1:G:136:LYS:CE	2.48	0.43
1:E:131:PRO:CG	1:E:170:LEU:HD22	2.46	0.43
1:E:173:HIS:HD2	2:H:2005:PO4:O4	2.01	0.43
1:F:157:GLN:HB3	1:G:159:LEU:HD13	2.00	0.43
1:B:134:GLN:HB3	1:E:136:LYS:HD3	2.00	0.43
1:F:185:LYS:HD2	1:F:186:ALA:N	2.34	0.43
1:D:59:THR:HG23	1:D:213:GLN:CD	2.39	0.43
1:E:86:GLU:O	1:E:181:LYS:HD2	2.18	0.43
1:C:120:LYS:HE2	3:D:2045:HOH:O	2.18	0.43
1:F:12:LYS:HZ2	1:F:12:LYS:HB3	1.80	0.43
1:F:132:VAL:HG12	1:F:133:MSE:HE2	2.00	0.43
1:B:135:LYS:HD3	1:E:166:ASP:OD2	2.18	0.43
1:B:216:SER:OG	1:C:225:CYS:HB3	2.19	0.43
1:A:141:GLU:HG3	1:A:142:PRO:CD	2.36	0.43
1:D:146:MSE:HG3	1:D:192:PHE:CZ	2.54	0.43
1:D:132:VAL:HG12	1:D:133:MSE:HE2	1.99	0.43
1:F:182:LYS:HB2	1:F:187:LEU:HD21	2.00	0.43
1:F:100:ALA:HB2	1:F:126:PHE:HA	2.01	0.43
1:D:166:ASP:HB2	1:D:168:ASN:HD22	1.83	0.43
1:A:44:LYS:HE2	1:A:206:GLU:OE1	2.18	0.43
1:H:78:ASP:O	1:H:82:GLN:HG3	2.18	0.43
1:H:145:GLU:HG3	1:H:158:THR:OG1	2.19	0.43
1:C:182:LYS:HB2	1:C:187:LEU:HD21	1.96	0.43
1:D:138:GLN:HE22	1:D:165:ALA:HA	1.83	0.43
1:G:37:GLY:O	1:G:216:SER:HA	2.18	0.43
1:D:126:PHE:CB	1:D:133:MSE:HE3	2.48	0.43
1:H:59:THR:HG23	1:H:213:GLN:NE2	2.34	0.43
1:B:109:LYS:HG2	1:B:116:VAL:HB	2.01	0.43
1:C:140:TRP:CH2	1:C:162:LEU:HG	2.54	0.42
1:B:59:THR:HG23	1:B:213:GLN:NE2	2.34	0.42
1:F:173:HIS:HD2	2:F:2007:PO4:O2	2.01	0.42
1:F:160:MSE:HE2	1:F:174:LEU:CD1	2.34	0.42
1:E:100:ALA:HB2	1:E:126:PHE:HA	2.01	0.42
1:E:140:TRP:CZ3	1:E:162:LEU:HG	2.54	0.42
1:A:56:ASP:HB3	1:A:162:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ASP:O	1:F:82:GLN:HG3	2.20	0.42
1:D:95:ILE:HD12	1:D:95:ILE:N	2.33	0.42
1:G:146:MSE:HE2	1:G:157:GLN:HB2	2.01	0.42
1:B:60:PRO:O	1:B:65:CRQ:C2	2.67	0.42
1:D:12:LYS:HE2	1:D:29:GLU:OE1	2.18	0.42
1:B:126:PHE:CB	1:B:133:MSE:HE3	2.48	0.42
1:E:166:ASP:O	1:E:166:ASP:OD1	2.38	0.42
1:G:16:GLU:HG3	1:G:25:MSE:HG2	2.01	0.42
1:B:50:PRO:HG3	1:B:207:ASN:O	2.19	0.42
1:B:49:GLY:HA2	1:B:50:PRO:C	2.41	0.42
1:H:126:PHE:CB	1:H:133:MSE:HE3	2.49	0.42
1:G:7:ASP:O	1:G:33:LYS:HA	2.19	0.42
1:E:49:GLY:HA2	1:E:50:PRO:C	2.40	0.42
1:F:231:HIS:HB2	1:G:198:ARG:HH21	1.84	0.41
1:D:146:MSE:CG	1:D:192:PHE:CZ	3.02	0.41
1:F:95:ILE:N	1:F:95:ILE:HD12	2.36	0.41
1:E:146:MSE:O	1:E:156:GLY:HA2	2.20	0.41
1:E:212:GLU:OE2	1:E:214:HIS:HE1	2.04	0.41
1:H:196:ASP:O	1:H:217:SER:HA	2.21	0.41
1:H:56:ASP:HB3	1:H:162:LEU:HD21	2.01	0.41
1:G:131:PRO:HA	1:G:136:LYS:HE3	2.02	0.41
1:H:131:PRO:HG2	1:H:170:LEU:HD22	2.01	0.41
1:E:140:TRP:CH2	1:E:162:LEU:HG	2.56	0.41
1:E:198:ARG:HH21	1:H:227:SER:HB2	1.85	0.41
1:F:50:PRO:HG3	1:F:207:ASN:O	2.21	0.41
1:B:131:PRO:HA	1:B:136:LYS:HD3	2.03	0.41
1:D:84:PHE:O	1:D:182:LYS:NZ	2.54	0.41
1:E:13:LEU:HB3	1:E:28:ALA:HB3	2.03	0.41
1:E:13:LEU:HD23	1:E:14:TYR:N	2.36	0.41
1:C:95:ILE:N	1:C:95:ILE:HD12	2.35	0.41
1:A:196:ASP:O	1:A:217:SER:HA	2.21	0.41
1:G:72:TYR:HA	1:G:219:ALA:HB3	2.03	0.41
1:F:42:ASN:HA	1:F:42:ASN:HD22	1.69	0.41
1:C:78:ASP:O	1:C:82:GLN:HG3	2.21	0.41
1:H:33:LYS:HD2	3:H:2125:HOH:O	2.21	0.40
1:B:77:PRO:HG2	1:B:190:PRO:CB	2.52	0.40
1:A:91:GLU:HG3	1:B:124:CYS:HB2	2.03	0.40
1:B:95:ILE:HD12	1:B:95:ILE:N	2.36	0.40
1:F:146:MSE:O	1:F:156:GLY:HA2	2.22	0.40
1:E:127:PRO:HA	1:E:128:PRO:HD2	1.97	0.40
1:B:5:ILE:N	3:B:2162:HOH:O	2.55	0.40

All (1) 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)
3:B:2184:HOH:O	3:D:2192:HOH:O[2_645]	0.17	2.03

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	223/233 (96%)	221 (99%)	2 (1%)	0	100 100
1	B	223/233 (96%)	221 (99%)	2 (1%)	0	100 100
1	C	223/233 (96%)	218 (98%)	3 (1%)	2 (1%)	21 7
1	D	223/233 (96%)	220 (99%)	3 (1%)	0	100 100
1	E	223/233 (96%)	221 (99%)	2 (1%)	0	100 100
1	F	223/233 (96%)	220 (99%)	3 (1%)	0	100 100
1	G	223/233 (96%)	219 (98%)	4 (2%)	0	100 100
1	H	223/233 (96%)	219 (98%)	4 (2%)	0	100 100
All	All	1784/1864 (96%)	1759 (99%)	23 (1%)	2 (0%)	56 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA
1	C	166	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	197/195 (101%)	191 (97%)	6 (3%)	48	31
1	B	197/195 (101%)	193 (98%)	4 (2%)	63	49
1	C	197/195 (101%)	191 (97%)	6 (3%)	48	31
1	D	197/195 (101%)	190 (96%)	7 (4%)	42	24
1	E	197/195 (101%)	192 (98%)	5 (2%)	55	39
1	F	197/195 (101%)	193 (98%)	4 (2%)	63	49
1	G	197/195 (101%)	193 (98%)	4 (2%)	63	49
1	H	197/195 (101%)	192 (98%)	5 (2%)	55	39
All	All	1576/1560 (101%)	1535 (97%)	41 (3%)	54	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	72	TYR
1	A	109	LYS
1	A	113	ASN
1	A	173	HIS
1	A	199	PRO
1	B	20	ASN
1	B	110	LEU
1	B	159	LEU
1	B	173	HIS
1	C	10	ARG
1	C	42	ASN
1	C	72	TYR
1	C	173	HIS
1	C	189	MSE
1	C	190	PRO
1	D	20	ASN
1	D	31	GLU
1	D	40	MSE
1	D	72	TYR
1	D	173	HIS
1	D	175	ARG
1	D	190	PRO
1	E	20	ASN

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Mol	Chain	Res	Type
1	E	42	ASN
1	E	72	TYR
1	E	173	HIS
1	E	199	PRO
1	F	31	GLU
1	F	72	TYR
1	F	173	HIS
1	F	185	LYS
1	G	20	ASN
1	G	40	MSE
1	G	173	HIS
1	G	207	ASN
1	H	20	ASN
1	H	40	MSE
1	H	72	TYR
1	H	173	HIS
1	H	190	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	22	HIS
1	A	39	GLN
1	A	42	ASN
1	A	113	ASN
1	A	157	GLN
1	A	169	HIS
1	A	173	HIS
1	A	214	HIS
1	A	223	GLN
1	A	232	ASN
1	B	20	ASN
1	B	21	ASN
1	B	22	HIS
1	B	23	HIS
1	B	39	GLN
1	B	105	GLN
1	B	125	ASN
1	B	129	ASN
1	B	157	GLN
1	B	169	HIS

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Mol	Chain	Res	Type
1	B	173	HIS
1	B	231	HIS
1	C	21	ASN
1	C	22	HIS
1	C	23	HIS
1	C	39	GLN
1	C	42	ASN
1	C	138	GLN
1	C	157	GLN
1	C	169	HIS
1	C	173	HIS
1	C	214	HIS
1	D	20	ASN
1	D	22	HIS
1	D	23	HIS
1	D	39	GLN
1	D	42	ASN
1	D	129	ASN
1	D	138	GLN
1	D	168	ASN
1	D	169	HIS
1	D	173	HIS
1	D	223	GLN
1	D	232	ASN
1	E	20	ASN
1	E	21	ASN
1	E	39	GLN
1	E	42	ASN
1	E	157	GLN
1	E	169	HIS
1	E	173	HIS
1	F	21	ASN
1	F	39	GLN
1	F	42	ASN
1	F	118	ASN
1	F	138	GLN
1	F	157	GLN
1	F	169	HIS
1	F	173	HIS
1	F	223	GLN
1	F	232	ASN
1	G	20	ASN

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Mol	Chain	Res	Type
1	G	23	HIS
1	G	39	GLN
1	G	113	ASN
1	G	138	GLN
1	G	157	GLN
1	G	169	HIS
1	G	173	HIS
1	G	207	ASN
1	G	214	HIS
1	G	223	GLN
1	G	231	HIS
1	G	232	ASN
1	H	8	ASN
1	H	20	ASN
1	H	21	ASN
1	H	23	HIS
1	H	39	GLN
1	H	138	GLN
1	H	157	GLN
1	H	168	ASN
1	H	169	HIS
1	H	173	HIS
1	H	214	HIS
1	H	223	GLN
1	H	232	ASN

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	A	65	1	24,25,26	3.55	5 (20%)	25,34,36	4.77	7 (28%)
1	CRQ	B	65	1	24,25,26	3.70	6 (25%)	25,34,36	6.04	8 (32%)
1	CRQ	C	65	1	24,25,26	3.19	5 (20%)	25,34,36	5.10	6 (24%)
1	CRQ	D	65	1	24,25,26	2.29	4 (16%)	25,34,36	5.46	8 (32%)
1	CRQ	E	65	1	24,25,26	3.55	3 (12%)	25,34,36	5.54	7 (28%)
1	CRQ	F	65	1	24,25,26	4.29	5 (20%)	25,34,36	5.82	7 (28%)
1	CRQ	G	65	1	24,25,26	4.05	4 (16%)	25,34,36	5.43	9 (36%)
1	CRQ	H	65	1	24,25,26	4.33	3 (12%)	25,34,36	4.88	7 (28%)

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	A	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	B	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	C	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	E	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	F	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	G	65	1	-	0/10/32/33	0/2/2/2
1	CRQ	H	65	1	-	0/10/32/33	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	CRQ	CA3-N3	-3.88	1.40	1.47
1	B	65	CRQ	CA3-N3	-2.42	1.43	1.47
1	F	65	CRQ	CA3-N3	-2.26	1.43	1.47
1	C	65	CRQ	CA3-N3	-2.18	1.43	1.47
1	C	65	CRQ	CA2-C2	2.10	1.50	1.48
1	G	65	CRQ	C2-N3	2.26	1.44	1.39
1	E	65	CRQ	CA2-C2	2.31	1.51	1.48
1	A	65	CRQ	C1-N3	2.35	1.43	1.38
1	H	65	CRQ	C1-N3	2.37	1.43	1.38
1	D	65	CRQ	CA2-C2	2.37	1.51	1.48
1	F	65	CRQ	C1-N3	2.47	1.43	1.38
1	D	65	CRQ	C1-N3	2.49	1.43	1.38
1	C	65	CRQ	C2-N3	2.56	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	CRQ	C1-N3	2.58	1.43	1.38
1	F	65	CRQ	CA2-C2	2.75	1.51	1.48
1	B	65	CRQ	CA2-C2	2.94	1.51	1.48
1	G	65	CRQ	CA2-C2	3.33	1.52	1.48
1	B	65	CRQ	C2-N3	3.84	1.47	1.39
1	A	65	CRQ	CA2-C2	4.16	1.53	1.48
1	A	65	CRQ	CA1-N	5.58	1.45	1.28
1	H	65	CRQ	CA1-N	5.91	1.46	1.28
1	D	65	CRQ	CA1-N	5.92	1.46	1.28
1	E	65	CRQ	CA1-N	5.92	1.46	1.28
1	F	65	CRQ	CA1-N	5.93	1.46	1.28
1	C	65	CRQ	CA1-N	5.93	1.46	1.28
1	G	65	CRQ	CA1-N	5.95	1.46	1.28
1	B	65	CRQ	CA1-N	5.96	1.46	1.28
1	D	65	CRQ	CB2-CA2	8.28	1.42	1.35
1	C	65	CRQ	CB2-CA2	13.59	1.47	1.35
1	A	65	CRQ	CB2-CA2	14.89	1.48	1.35
1	E	65	CRQ	CB2-CA2	15.76	1.49	1.35
1	B	65	CRQ	CB2-CA2	15.83	1.49	1.35
1	G	65	CRQ	CB2-CA2	18.15	1.51	1.35
1	F	65	CRQ	CB2-CA2	19.49	1.52	1.35
1	H	65	CRQ	CB2-CA2	19.90	1.52	1.35

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	65	CRQ	CA3-N3-C2	-16.88	96.51	123.99
1	B	65	CRQ	O2-C2-CA2	-16.83	121.86	130.95
1	E	65	CRQ	CA3-N3-C2	-16.29	97.47	123.99
1	G	65	CRQ	CA3-N3-C2	-15.72	98.39	123.99
1	C	65	CRQ	CA3-N3-C2	-15.30	99.08	123.99
1	A	65	CRQ	CA3-N3-C2	-14.94	99.67	123.99
1	D	65	CRQ	CA3-N3-C2	-14.46	100.45	123.99
1	F	65	CRQ	CB2-CA2-N2	-13.58	104.39	128.67
1	B	65	CRQ	CB2-CA2-N2	-12.91	105.59	128.67
1	H	65	CRQ	CA3-N3-C2	-12.34	103.89	123.99
1	G	65	CRQ	CB2-CA2-N2	-12.04	107.15	128.67
1	E	65	CRQ	CB2-CA2-N2	-11.85	107.48	128.67
1	H	65	CRQ	CB2-CA2-N2	-11.79	107.59	128.67
1	B	65	CRQ	CG2-CB2-CA2	-11.64	115.10	130.22
1	E	65	CRQ	CG2-CB2-CA2	-10.77	116.23	130.22
1	F	65	CRQ	CG2-CB2-CA2	-10.68	116.35	130.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	65	CRQ	CG2-CB2-CA2	-10.43	116.67	130.22
1	C	65	CRQ	CG2-CB2-CA2	-10.04	117.17	130.22
1	D	65	CRQ	CG2-CB2-CA2	-9.98	117.26	130.22
1	D	65	CRQ	N3-C1-N2	-9.68	102.29	113.26
1	H	65	CRQ	CG2-CB2-CA2	-9.39	118.02	130.22
1	A	65	CRQ	CG2-CB2-CA2	-9.31	118.12	130.22
1	D	65	CRQ	C2-CA2-N2	-9.17	101.59	108.91
1	B	65	CRQ	CA2-C2-N3	-8.48	99.15	103.40
1	C	65	CRQ	CB2-CA2-N2	-8.17	114.06	128.67
1	A	65	CRQ	CB2-CA2-N2	-8.08	114.24	128.67
1	C	65	CRQ	N3-C1-N2	-7.68	104.56	113.26
1	D	65	CRQ	CB2-CA2-N2	-7.11	115.96	128.67
1	H	65	CRQ	CA2-C2-N3	-6.45	100.17	103.40
1	G	65	CRQ	CA2-C2-N3	-6.35	100.22	103.40
1	F	65	CRQ	CA2-C2-N3	-6.15	100.31	103.40
1	A	65	CRQ	N3-C1-N2	-5.44	107.10	113.26
1	E	65	CRQ	O2-C2-CA2	-4.99	128.25	130.95
1	C	65	CRQ	C2-CA2-N2	-4.83	105.06	108.91
1	A	65	CRQ	C2-CA2-N2	-3.54	106.09	108.91
1	E	65	CRQ	CA2-C2-N3	-2.52	102.13	103.40
1	F	65	CRQ	C-CA3-N3	-2.28	108.02	113.00
1	G	65	CRQ	O2-C2-CA2	-2.21	129.75	130.95
1	B	65	CRQ	N3-C1-N2	-2.15	110.82	113.26
1	G	65	CRQ	C-CA3-N3	-2.12	108.36	113.00
1	D	65	CRQ	O2-C2-CA2	-2.02	129.85	130.95
1	A	65	CRQ	CB1-CA1-N	2.21	128.99	124.94
1	H	65	CRQ	O2-C2-N3	2.22	129.28	124.50
1	E	65	CRQ	O2-C2-N3	2.37	129.61	124.50
1	G	65	CRQ	O2-C2-N3	2.55	129.99	124.50
1	D	65	CRQ	CA2-C2-N3	3.28	105.04	103.40
1	G	65	CRQ	C2-CA2-N2	3.37	111.60	108.91
1	B	65	CRQ	C2-CA2-N2	3.97	112.08	108.91
1	H	65	CRQ	C2-CA2-N2	4.83	112.76	108.91
1	F	65	CRQ	C2-CA2-N2	5.82	113.56	108.91
1	B	65	CRQ	O2-C2-N3	6.72	138.99	124.50
1	A	65	CRQ	CB2-CA2-C2	11.79	139.63	122.36
1	H	65	CRQ	CB2-CA2-C2	11.79	139.63	122.36
1	C	65	CRQ	CB2-CA2-C2	12.59	140.79	122.36
1	G	65	CRQ	CB2-CA2-C2	12.83	141.14	122.36
1	F	65	CRQ	CB2-CA2-C2	13.42	142.01	122.36
1	B	65	CRQ	CB2-CA2-C2	13.60	142.27	122.36
1	D	65	CRQ	CB2-CA2-C2	13.70	142.43	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	65	CRQ	CB2-CA2-C2	14.07	142.96	122.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	CRQ	2	0
1	B	65	CRQ	6	0
1	C	65	CRQ	2	0
1	D	65	CRQ	2	0
1	E	65	CRQ	3	0
1	F	65	CRQ	1	0
1	H	65	CRQ	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

16 ligands 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	$\#\|Z\| > 2$
2	PO4	A	2001	-	4,4,4	1.18	0	6,6,6	0.27	0
2	PO4	A	2004	-	4,4,4	1.17	0	6,6,6	0.27	0
2	PO4	A	2009	-	4,4,4	1.09	0	6,6,6	0.27	0
2	PO4	B	2002	-	4,4,4	1.18	0	6,6,6	0.27	0
2	PO4	B	2010	-	4,4,4	1.10	0	6,6,6	0.27	0
2	PO4	B	2011	-	4,4,4	1.10	0	6,6,6	0.27	0
2	PO4	D	2003	-	4,4,4	1.16	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	D	2012	-	4,4,4	1.08	0	6,6,6	0.27	0
2	PO4	E	2013	-	4,4,4	1.11	0	6,6,6	0.27	0
2	PO4	F	2007	-	4,4,4	1.18	0	6,6,6	0.27	0
2	PO4	F	2008	-	4,4,4	1.19	0	6,6,6	0.27	0
2	PO4	F	2015	-	4,4,4	1.08	0	6,6,6	0.27	0
2	PO4	G	2006	-	4,4,4	1.16	0	6,6,6	0.27	0
2	PO4	G	2016	-	4,4,4	1.11	0	6,6,6	0.27	0
2	PO4	H	2005	-	4,4,4	1.15	0	6,6,6	0.27	0
2	PO4	H	2014	-	4,4,4	1.08	0	6,6,6	0.27	0

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
2	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2004	-	-	0/0/0/0	0/0/0/0
2	PO4	A	2009	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2010	-	-	0/0/0/0	0/0/0/0
2	PO4	B	2011	-	-	0/0/0/0	0/0/0/0
2	PO4	D	2003	-	-	0/0/0/0	0/0/0/0
2	PO4	D	2012	-	-	0/0/0/0	0/0/0/0
2	PO4	E	2013	-	-	0/0/0/0	0/0/0/0
2	PO4	F	2007	-	-	0/0/0/0	0/0/0/0
2	PO4	F	2008	-	-	0/0/0/0	0/0/0/0
2	PO4	F	2015	-	-	0/0/0/0	0/0/0/0
2	PO4	G	2006	-	-	0/0/0/0	0/0/0/0
2	PO4	G	2016	-	-	0/0/0/0	0/0/0/0
2	PO4	H	2005	-	-	0/0/0/0	0/0/0/0
2	PO4	H	2014	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	PO4	2	0
2	B	2002	PO4	1	0
2	E	2013	PO4	1	0
2	F	2007	PO4	1	0
2	H	2005	PO4	2	0

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	218/233 (93%)	-0.30	1 (0%)	91 90	8, 13, 26, 39	0
1	B	218/233 (93%)	-0.21	3 (1%)	78 74	9, 15, 29, 43	0
1	C	218/233 (93%)	-0.16	5 (2%)	64 59	8, 14, 28, 40	0
1	D	218/233 (93%)	-0.26	3 (1%)	78 74	8, 14, 28, 41	0
1	E	218/233 (93%)	-0.09	2 (0%)	85 83	11, 19, 31, 37	0
1	F	218/233 (93%)	0.03	4 (1%)	71 67	10, 20, 32, 42	0
1	G	218/233 (93%)	0.16	10 (4%)	36 30	12, 22, 36, 46	0
1	H	218/233 (93%)	-0.15	3 (1%)	78 74	10, 17, 31, 48	0
All	All	1744/1864 (93%)	-0.12	31 (1%)	71 67	8, 17, 31, 48	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	165	ALA	5.6
1	C	164	CYS	5.0
1	C	165	ALA	4.7
1	D	165	ALA	4.2
1	H	166	ASP	3.9
1	D	214	HIS	3.9
1	B	166	ASP	3.2
1	G	8	ASN	3.1
1	G	185	LYS	3.1
1	G	166	ASP	2.8
1	F	111	ASP	2.7
1	D	185	LYS	2.7
1	G	10	ARG	2.7
1	C	111	ASP	2.6
1	G	228	LYS	2.6
1	E	166	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	228	LYS	2.5
1	F	5	ILE	2.4
1	B	138	GLN	2.3
1	A	228	LYS	2.3
1	B	228	LYS	2.3
1	C	185	LYS	2.3
1	H	185	LYS	2.2
1	G	226	PRO	2.2
1	G	223	GLN	2.2
1	G	6	SER	2.2
1	F	36	GLU	2.1
1	F	7	ASP	2.1
1	G	12	LYS	2.0
1	E	113	ASN	2.0
1	G	5	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	CRQ	A	65	24/25	0.85	0.14	-	11,19,29,30	0
1	CRQ	G	65	24/25	0.86	0.14	-	11,19,29,30	0
1	CRQ	E	65	24/25	0.84	0.14	-	11,19,29,30	0
1	CRQ	D	65	24/25	0.85	0.16	-	11,19,29,30	0
1	CRQ	B	65	24/25	0.87	0.12	-	11,19,29,30	0
1	CRQ	H	65	24/25	0.86	0.14	-	11,19,29,30	0
1	CRQ	F	65	24/25	0.82	0.14	-	11,19,29,30	0
1	CRQ	C	65	24/25	0.87	0.13	-	11,19,29,30	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	E	2013	5/5	0.66	0.34	7.28	58,60,61,61	0
2	PO4	D	2012	5/5	0.94	0.18	2.39	22,26,29,31	0
2	PO4	G	2016	5/5	0.87	0.18	1.65	47,48,52,52	0
2	PO4	A	2009	5/5	0.95	0.14	1.21	17,24,27,27	0
2	PO4	H	2014	5/5	0.89	0.18	1.10	22,22,30,31	0
2	PO4	F	2007	5/5	0.95	0.14	0.43	21,23,26,26	0
2	PO4	H	2005	5/5	0.91	0.13	-0.17	22,23,24,25	0
2	PO4	G	2006	5/5	0.99	0.12	-0.45	16,16,20,20	0
2	PO4	B	2010	5/5	0.93	0.12	-0.63	23,27,32,32	0
2	PO4	A	2001	5/5	0.97	0.12	-0.66	20,20,25,27	0
2	PO4	B	2002	5/5	0.96	0.11	-1.06	20,20,24,25	0
2	PO4	D	2003	5/5	0.99	0.11	-1.72	13,13,15,16	0
2	PO4	A	2004	5/5	0.99	0.09	-4.46	14,14,18,19	0
2	PO4	F	2015	5/5	0.78	0.27	-	38,40,45,45	0
2	PO4	F	2008	5/5	0.98	0.11	-	16,16,19,21	0
2	PO4	B	2011	5/5	0.79	0.24	-	27,32,37,37	0

6.5 Other polymers

There are no such residues in this entry.