



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:29 PM UTC

PDB ID : 2IB5 / pdb_00002ib5
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

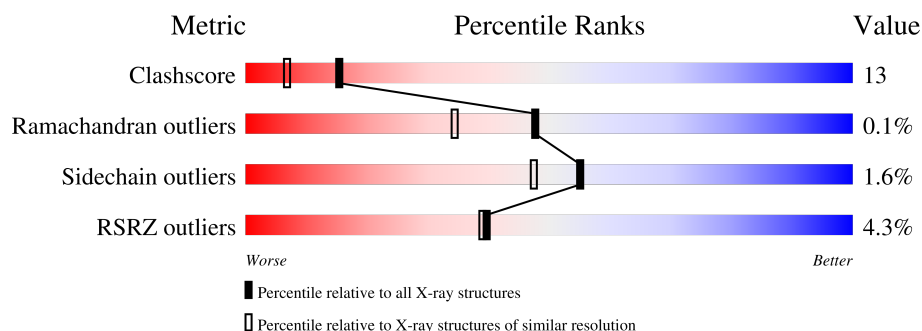
1 Overall quality at a glance

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.



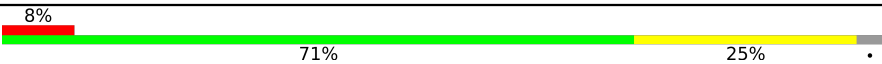
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	3% 78% 17% • •
1	B	233	4% 74% 22% • •
1	C	233	4% 67% 26% • •
1	D	233	2% 70% 25% • •
1	E	233	3% 73% 22% • •
1	F	233	4% 71% 25% • •

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Mol	Chain	Length	Quality of chain
1	G	233	
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	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 (CCD ID: PO4) (formula: O₄P).



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

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

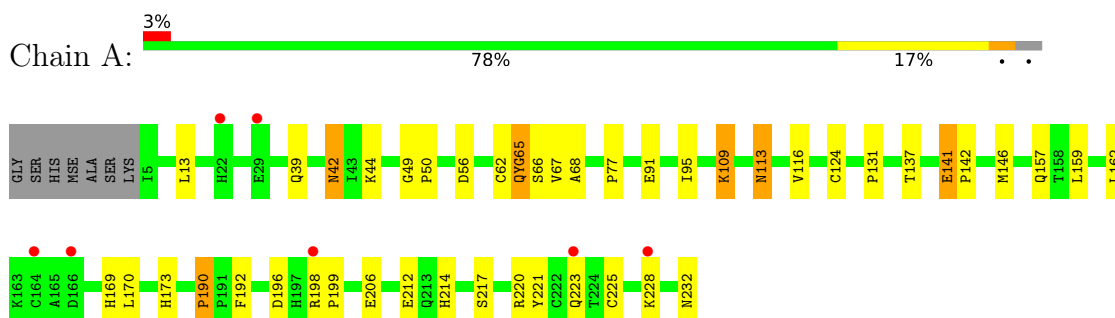
- Molecule 3 is water.

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

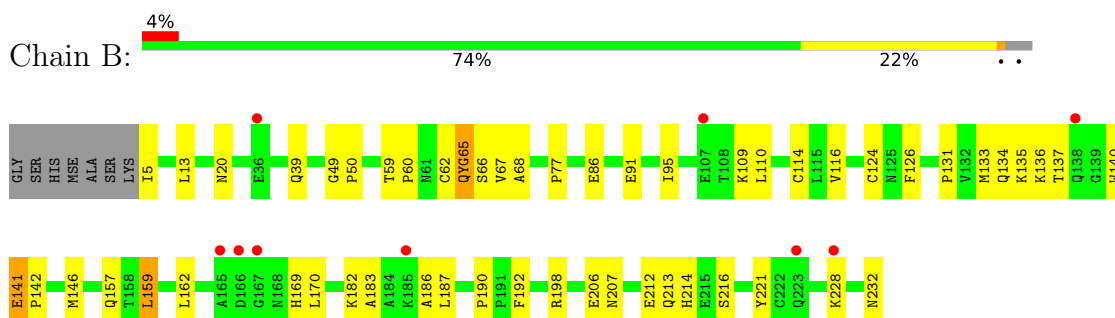
3 Residue-property plots [i](#)

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.

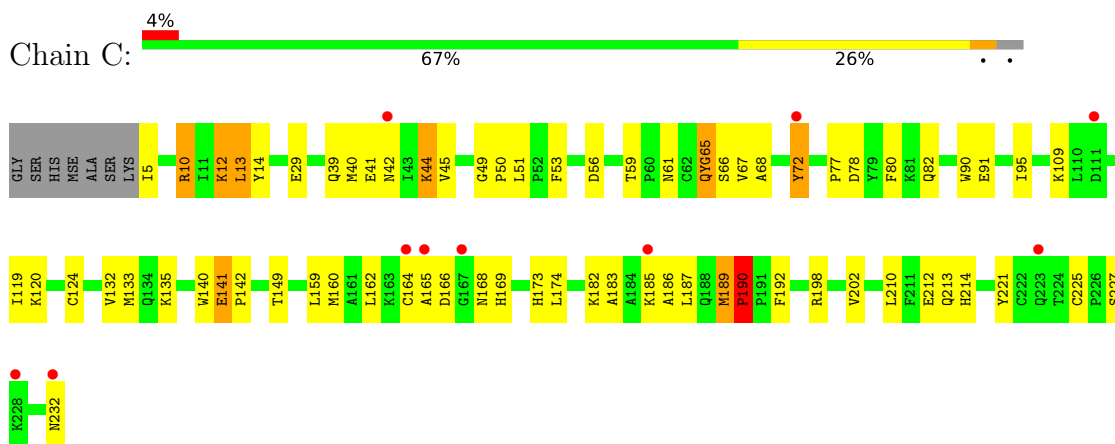
• Molecule 1: Chromo protein



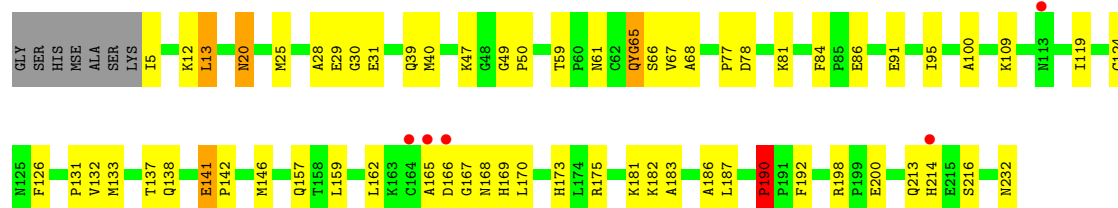
• Molecule 1: Chromo protein



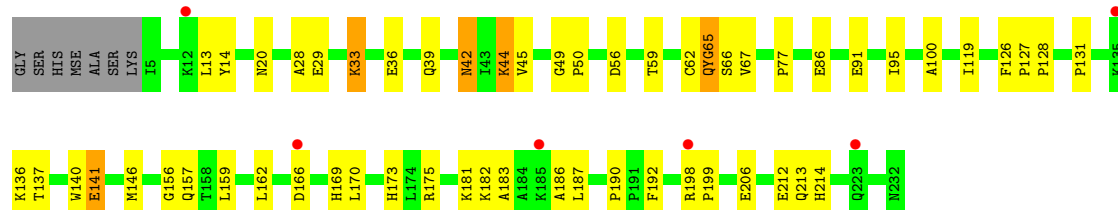
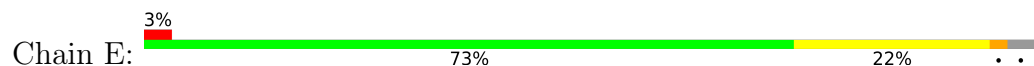
• Molecule 1: Chromo protein



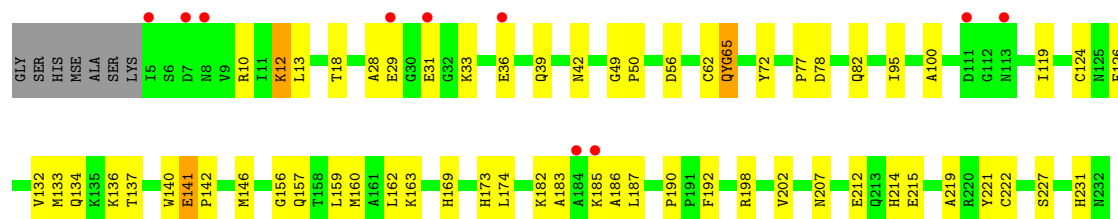
• Molecule 1: Chromo protein



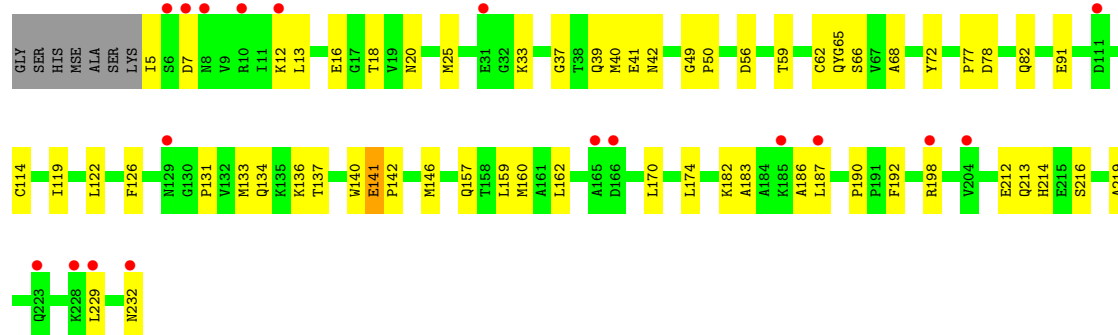
• Molecule 1: Chromo protein



• Molecule 1: Chromo protein

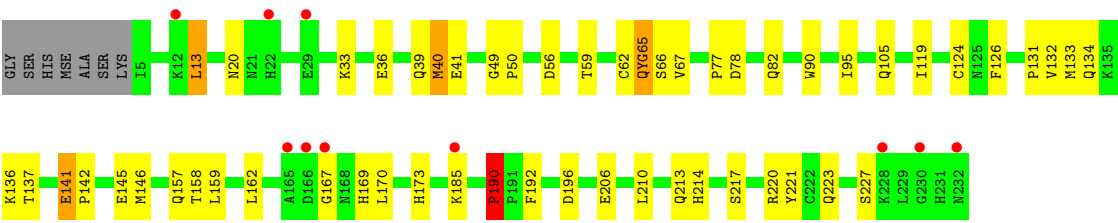


• Molecule 1: Chromo protein



• Molecule 1: Chromo protein





4 Data and refinement statistics

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 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.80) 98.3 (50.00-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.195 , 0.225 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.776	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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 14.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRQ, PO4

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	0.43	0/1811	0.97	6/2436 (0.2%)
1	B	0.37	0/1811	0.93	6/2436 (0.2%)
1	C	0.41	0/1811	1.01	12/2436 (0.5%)
1	D	0.43	0/1811	0.99	9/2436 (0.4%)
1	E	0.39	0/1811	0.94	6/2436 (0.2%)
1	F	0.36	0/1811	0.90	7/2436 (0.3%)
1	G	0.37	0/1811	0.88	4/2436 (0.2%)
1	H	0.41	0/1811	0.94	8/2436 (0.3%)
All	All	0.40	0/14488	0.95	58/19488 (0.3%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ASN	O-C-N	-7.87	111.23	122.41
1	C	72	TYR	N-CA-CB	-7.36	98.23	110.37
1	H	190	PRO	N-CA-C	7.06	119.31	110.70
1	D	141	GLU	N-CA-C	-7.02	100.96	110.36
1	D	190	PRO	N-CA-C	6.96	119.19	110.70
1	C	190	PRO	N-CA-C	6.92	119.14	110.70
1	C	72	TYR	CB-CA-C	6.66	121.43	110.78
1	C	90	TRP	CA-CB-CG	6.64	126.22	113.60
1	C	80	PHE	CA-CB-CG	-6.51	107.29	113.80
1	H	141	GLU	N-CA-C	-6.42	100.77	110.39
1	C	141	GLU	N-CA-C	-6.33	100.89	110.39
1	H	90	TRP	CA-CB-CG	6.29	125.55	113.60
1	D	68	ALA	N-CA-C	-6.27	105.60	113.18
1	C	61	ASN	O-C-N	-6.18	114.32	122.42
1	G	141	GLU	N-CA-C	-6.16	102.11	110.36
1	B	141	GLU	N-CA-C	-5.99	101.40	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLU	N-CA-C	-5.89	101.56	110.39
1	A	68	ALA	N-CA-C	-5.81	105.68	112.89
1	D	167	GLY	N-CA-C	-5.81	107.08	115.27
1	H	167	GLY	N-CA-C	-5.72	107.49	114.92
1	E	67	VAL	N-CA-C	5.67	120.36	113.00
1	H	67	VAL	N-CA-C	5.64	121.08	109.34
1	D	119	ILE	N-CA-C	5.64	116.60	108.48
1	E	141	GLU	N-CA-C	-5.63	101.94	110.39
1	B	68	ALA	N-CA-C	-5.62	106.38	113.18
1	B	62	CYS	N-CA-C	5.61	126.70	111.00
1	F	62	CYS	N-CA-C	5.57	126.60	111.00
1	H	62	CYS	N-CA-C	5.55	126.54	111.00
1	E	33	LYS	CA-C-N	5.49	125.58	119.32
1	E	33	LYS	C-N-CA	5.49	125.58	119.32
1	G	68	ALA	N-CA-C	-5.44	106.14	112.89
1	B	221	TYR	N-CA-C	-5.42	101.99	110.17
1	B	67	VAL	N-CA-C	5.40	120.58	109.34
1	A	190	PRO	N-CA-C	5.36	117.24	110.70
1	D	67	VAL	N-CA-C	5.36	120.48	109.34
1	C	67	VAL	N-CA-C	5.34	120.45	109.34
1	F	141	GLU	N-CA-C	-5.34	102.38	110.39
1	B	114	CYS	N-CA-C	5.32	117.57	108.90
1	A	67	VAL	N-CA-C	5.30	120.37	109.34
1	G	119	ILE	N-CA-C	5.26	116.06	108.48
1	F	221	TYR	N-CA-C	-5.20	102.50	110.14
1	F	119	ILE	N-CA-C	5.20	115.96	108.48
1	C	119	ILE	N-CA-C	5.20	115.96	108.48
1	A	62	CYS	N-CA-C	5.19	125.53	111.00
1	F	33	LYS	CA-C-N	5.19	125.23	119.32
1	F	33	LYS	C-N-CA	5.19	125.23	119.32
1	C	72	TYR	CA-C-O	5.18	125.92	120.54
1	E	119	ILE	N-CA-C	5.17	115.93	108.48
1	D	61	ASN	CA-C-N	5.16	130.99	121.70
1	D	61	ASN	C-N-CA	5.16	130.99	121.70
1	H	119	ILE	N-CA-C	5.16	115.91	108.48
1	A	221	TYR	N-CA-C	-5.15	102.39	110.17
1	C	221	TYR	N-CA-C	-5.15	102.54	109.95
1	F	222	CYS	N-CA-C	-5.14	102.24	109.96
1	E	62	CYS	N-CA-C	5.07	125.19	111.00
1	G	62	CYS	N-CA-C	5.07	125.18	111.00
1	C	68	ALA	N-CA-C	-5.05	106.63	112.89
1	H	221	TYR	N-CA-C	-5.02	102.59	110.17

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	1798	0	1727	42	0
1	B	1798	0	1727	57	0
1	C	1798	0	1727	61	0
1	D	1798	0	1727	59	0
1	E	1798	0	1727	55	0
1	F	1798	0	1727	59	0
1	G	1798	0	1727	55	0
1	H	1798	0	1727	52	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	13816	381	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 (381) 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
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:141:GLU:HG3	1:A:142:PRO:HD2	1.53	0.89
1:A:192:PHE:CD2	1:D:141:GLU:HG2	2.08	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:A:198:ARG:HH22	1:D:232:ASN:C	1.86	0.82
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: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:198:ARG:HH22	1:G:232:ASN:C	1.94	0.75
1:B:20:ASN:HD21	1:B:126:PHE:H	1.34	0.74
1:F:10:ARG:HH22	1:F:29:GLU:HG3	1.50	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:C:164:CYS:HB2	1:C:168:ASN:C	2.13	0.74
1:B:141:GLU:HG2	1:C:192:PHE:CE2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:232:ASN:C	1:D:198:ARG:HH22	1.97	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: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: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:C:183:ALA:O	1:C:187:LEU:HD23	1.95	0.66
1:F:227:SER:HB2	1:G:198:ARG:HE	1.60	0.66
1:H:33:LYS:HE2	1:H:36:GLU:HG3	1.77	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:B:198:ARG:HH22	1:C:232:ASN:C	2.05	0.65
1:A:232:ASN:O	1:D:198:ARG:NH2	2.29	0.64
1:H:131:PRO:HA	1:H:136:LYS:HE3	1.79	0.64
1:B:39:GLN:NE2	1:B:65:CRQ:HE11	1.95	0.64
1:B:232:ASN:C	1:C:198:ARG:HH22	2.04	0.64
1:B:232:ASN:O	1:C:198:ARG:NH2	2.28	0.64
1:C:132:VAL:HG12	1:C:133:MSE:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:PHE:CE2	1:G:141:GLU:HG2	2.33	0.64
1:F:12:LYS:NZ	1:F:12:LYS:HB3	2.13	0.64
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
1:E:146:MSE:HG3	1:E:192:PHE:CZ	2.33	0.63
1:D:182:LYS:CB	1:D:187:LEU:HD11	2.28	0.63
1:A:212:GLU:OE2	1:A:214:HIS:HE1	1.82	0.63
1:G:91:GLU:HB2	3:G:2046:HOH:O	1.97	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:25:MSE:SE	1:D:47:LYS:HD3	2.51	0.61
1:D:30:GLY:HA2	1:D:40:MSE:CE	2.30	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:G:40:MSE:HE2	1:G:41:GLU:C	2.26	0.60
1:B:77:PRO:HG2	1:B:190:PRO:CA	2.31	0.60
1:D:13:LEU:C	1:D:13:LEU:HD23	2.27	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:F:183:ALA:O	1:F:187:LEU:HD23	2.02	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:E:186:ALA:C	1:E:187:LEU:HD12	2.28	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:A:77:PRO:HG2	1:A:190:PRO:HA	1.85	0.58
1:F:182:LYS:CB	1:F:187:LEU:HD21	2.33	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:C:77:PRO:HG2	1:C:190:PRO:HA	1.86	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:HB3	1.85	0.58
1:F:10:ARG:HG3	1:F:10:ARG:HH11	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PRO:HG2	1:C:190:PRO:CA	2.33	0.58
1:F:77:PRO:HG2	1:F:190:PRO:CA	2.33	0.58
1:B:182:LYS:CB	1:B:187:LEU:HD21	2.27	0.57
1:C:13:LEU:HD23	1:C:13:LEU:C	2.30	0.57
1:F:186:ALA:C	1:F:187:LEU:HD22	2.28	0.57
1:H:77:PRO:HG2	1:H:190:PRO:HA	1.85	0.57
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:N1	2.68	0.56
1:C:12:LYS:HE3	1:C:29:GLU:OE2	2.05	0.56
1:C:44:LYS:HD3	1:C:45:VAL:N	2.18	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:D:78:ASP:OD1	1:D:81:LYS:HD3	2.06	0.56
1:E:13:LEU:C	1:E:13:LEU:HD23	2.31	0.56
1:E:198:ARG:NH2	1:H:227:SER:HB2	2.19	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:C:189:MSE:HE2	3:C:397:HOH:O	2.07	0.55
1:F:13:LEU:HB3	1:F:28:ALA:HB3	1.87	0.55
1:G:5:ILE:N	3:G:2090:HOH:O	2.39	0.55
3:B:2060:HOH:O	1:C:169:HIS:HD2	1.89	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:E:77:PRO:HG2	1:E:190:PRO:HA	1.88	0.55
1:G:77:PRO:HG2	1:G:190:PRO:CA	2.37	0.55
1:G:131:PRO:HG2	1:G:170:LEU:HD22	1.88	0.55
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:13:LEU:C	1:G:13:LEU:HD23	2.32	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:D:186:ALA:C	1:D:187:LEU:HD12	2.33	0.54
1:C:124:CYS:HB2	1:D:91:GLU:HG3	1.89	0.54
1:C:186:ALA:C	1:C:187:LEU:HD22	2.33	0.54
1:G:146:MSE:HG3	1:G:192:PHE:CZ	2.43	0.54
1:G:18:THR:HG21	1:H:105:GLN:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:PRO:HG2	1:G:190:PRO:HA	1.90	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
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:F:49:GLY:HA2	1:F:50:PRO:C	2.33	0.53
1:G:40:MSE:HE3	1:G:212:GLU:HG3	1.89	0.53
1:E:29:GLU:HG3	3:E:2151:HOH:O	2.09	0.53
1:G:186:ALA:C	1:G:187:LEU:HD22	2.34	0.53
1:H:77:PRO:HG2	1:H:190:PRO:HB3	1.90	0.53
3:A:2046:HOH:O	1:D:169:HIS:HD2	1.92	0.52
2:B:2002:PO4:O2	1:C:173:HIS:HD2	1.91	0.52
1:F:13:LEU:C	1:F:13:LEU:HD23	2.33	0.52
1:D:86:GLU:O	1:D:181:LYS:HD2	2.10	0.52
1:G:78:ASP:O	1:G:82:GLN:HG3	2.09	0.52
1:A:109:LYS:HB2	1:A:109:LYS:NZ	2.25	0.52
1:C:49:GLY:HA2	1:C:50:PRO:C	2.34	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:E:33:LYS:HE2	1:E:36:GLU:HG3	1.91	0.52
1:F:169:HIS:HD2	3:G:2041:HOH:O	1.93	0.52
1:B:198:ARG:NH2	1:C:232:ASN:O	2.43	0.52
1:D:49:GLY:HA2	1:D:50:PRO:C	2.35	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:A:13:LEU:HD23	1:A:13:LEU:C	2.36	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:D:13:LEU:HB3	1:D:28:ALA:HB3	1.93	0.51
1:B:13:LEU:C	1:B:13:LEU:HD23	2.36	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:C:53:PHE:N	1:C:135:LYS:HZ3	2.08	0.50
2:A:2001:PO4:O2	1:D:173:HIS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLN:HE22	1:B:66:SER:CB	2.23	0.50
1:B:131:PRO:CG	1:B:170:LEU:HD22	2.39	0.50
1:B:186:ALA:C	1:B:187:LEU:HD22	2.37	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:H:13:LEU:HD23	1:H:13:LEU:C	2.37	0.50
1:H:49:GLY:HA2	1:H:50:PRO:C	2.37	0.50
1:C:149:THR:HG21	1:C:189:MSE:HG3	1.93	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:A:42:ASN:ND2	3:A:2089:HOH:O	2.44	0.49
1:D:5:ILE:N	3:D:2076:HOH:O	2.44	0.49
1:F:163:LYS:HB3	1:F:163:LYS:NZ	2.27	0.49
1:A:39:GLN:HE22	1:A:66:SER:CB	2.25	0.49
1:C:39:GLN:HE22	1:C:66:SER:CB	2.25	0.49
1:D:30:GLY:CA	1:D:40:MSE:HE3	2.41	0.49
3:E:2119:HOH:O	1:F:18:THR:HG21	2.13	0.49
1:A:220:ARG:HD2	1:A:223:GLN:HE21	1.77	0.49
1:H:77:PRO:HG2	1:H:190:PRO:CB	2.43	0.49
1:A:124:CYS:HB2	1:B:91:GLU:HG3	1.95	0.49
1:A:173:HIS:HD2	2:A:2001:PO4:O3	1.96	0.49
1:F:72:TYR:HA	1:F:219:ALA:HB3	1.95	0.49
1:G:49:GLY:HA2	1:G:50:PRO:C	2.37	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:G:59:THR:HG23	1:G:213:GLN:CD	2.38	0.48
1:B:140:TRP:CZ3	1:B:162:LEU:HG	2.49	0.48
1:B:157:GLN:HB3	1:C:159:LEU:HD13	1.95	0.48
1:D:59:THR:HG23	1:D:213:GLN:CD	2.39	0.48
1:F:36:GLU:HG2	3:F:2103:HOH:O	2.13	0.48
1:F:159:LEU:HD13	1:G:157:GLN:HB3	1.96	0.48
1:B:109:LYS:CG	1:B:116:VAL:HB	2.43	0.48
1:G:77:PRO:HG2	1:G:190:PRO:CB	2.43	0.48
1:H:41:GLU:HG3	1:H:65:CRQ:NE1	2.29	0.48
1:H:220:ARG:HD2	1:H:223:GLN:HE21	1.78	0.47
1:C:12:LYS:HD2	1:C:14:TYR:CE1	2.49	0.47
1:C:53:PHE:N	1:C:135:LYS:NZ	2.62	0.47
1:F:12:LYS:HB3	1:F:12:LYS:HZ2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:ALA:O	1:G:187:LEU:HD23	2.14	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:HG3	1:F:10:ARG:NH1	2.30	0.47
1:F:31:GLU:C	1:F:31:GLU:CD	2.83	0.47
1:D:138:GLN:HE22	1:D:165:ALA:CA	2.27	0.47
1:E:39:GLN:HE21	1:E:65:CRQ:HE11	1.62	0.47
1:B:49:GLY:HA2	1:B:50:PRO:C	2.41	0.46
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
1:E:49:GLY:HA2	1:E:50:PRO:C	2.40	0.46
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:C:42:ASN:ND2	1:C:210:LEU:HD11	2.30	0.46
1:F:56:ASP:HB3	1:F:162:LEU:HD21	1.98	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:A:159:LEU:HD13	1:D:157:GLN:HB3	1.98	0.46
1:C:91:GLU:HG3	1:D:124:CYS:HB2	1.97	0.46
1:A:157:GLN:HB3	1:D:159:LEU:HD13	1.97	0.45
1:H:214:HIS:HD2	3:H:2032:HOH:O	1.99	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:HD22	1:E:42:ASN:HA	1.60	0.45
1:G:140:TRP:CH2	1:G:162:LEU:HG	2.52	0.45
1:E:198:ARG:CZ	1:H:227:SER:HB2	2.47	0.45
1:G:126:PHE:CB	1:G:133:MSE:HE3	2.46	0.45
1:B:159:LEU:HD13	1:C:159:LEU:HD11	1.98	0.45
1:E:39:GLN:HE22	1:E:66:SER:CB	2.30	0.45
1:G:56:ASP:HB3	1:G:162:LEU:HD21	1.99	0.45
1:H:39:GLN:HE22	1:H:66:SER:CB	2.29	0.45
1:E:77:PRO:HG2	1:E:190:PRO:CB	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLY:HA2	1:A:50:PRO:C	2.41	0.44
1:E:157:GLN:HB3	1:H:159:LEU:HD13	1.99	0.44
1:B:198:ARG:CZ	1:C:227:SER:HB2	2.48	0.44
1:D:100:ALA:HB2	1:D:126:PHE:HA	1.99	0.44
1:E:95:ILE:N	1:E:95:ILE:HD12	2.32	0.44
1:F:77:PRO:CG	1:F:190:PRO:HA	2.45	0.44
1:F:140:TRP:CZ3	1:F:162:LEU:HG	2.52	0.44
1:G:198:ARG:CZ	3:G:2019:HOH:O	2.66	0.44
1:A:95:ILE:HD13	3:A:2070:HOH:O	2.17	0.44
1:C:5:ILE:N	3:C:353:HOH:O	2.50	0.44
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:G:131:PRO:HA	1:G:136:LYS:CE	2.48	0.43
1:B:134:GLN:HB3	1:E:136:LYS:HD3	2.00	0.43
1:H:59:THR:HG23	1:H:213:GLN:CD	2.43	0.43
1:C:53:PHE:CA	1:C:135:LYS:HZ3	2.31	0.43
1:E:59:THR:HG23	1:E:213:GLN:CD	2.43	0.43
1:E:86:GLU:O	1:E:181:LYS:HD2	2.18	0.43
1:F:185:LYS:HD2	1:F:186:ALA:N	2.34	0.43
1:C:120:LYS:HE2	3:D:2045:HOH:O	2.18	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:F:132:VAL:HG12	1:F:133:MSE:HE2	2.00	0.43
1:H:40:MSE:HE2	1:H:41:GLU:C	2.42	0.43
1:A:44:LYS:HE2	1:A:206:GLU:OE1	2.18	0.43
1:A:141:GLU:HG3	1:A:142:PRO:CD	2.36	0.43
1:D:132:VAL:HG12	1:D:133:MSE:HE2	1.99	0.43
1:D:146:MSE:HG3	1:D:192:PHE:CZ	2.54	0.43
1:D:166:ASP:HB2	1:D:168:ASN:HD22	1.83	0.43
1:F:100:ALA:HB2	1:F:126:PHE:HA	2.01	0.43
1:F:182:LYS:HB2	1:F:187:LEU:HD21	2.00	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:40:MSE:SE	1:C:40:MSE:C	3.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:56:ASP:HB3	1:A:162:LEU:HD21	2.01	0.42
1:D:95:ILE:HD12	1:D:95:ILE:N	2.33	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:F:78:ASP:O	1:F:82:GLN:HG3	2.20	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:G:146:MSE:HE2	1:G:157:GLN:HB2	2.01	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:E:44:LYS:HD3	1:E:44:LYS:C	2.45	0.42
1:F:10:ARG:HH22	1:F:29:GLU:CD	2.28	0.42
1:G:7:ASP:O	1:G:33:LYS:HA	2.19	0.42
1:H:126:PHE:CB	1:H:133:MSE:HE3	2.49	0.42
1:B:59:THR:HG23	1:B:213:GLN:CD	2.45	0.41
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:C:59:THR:HG23	1:C:213:GLN:CD	2.46	0.41
1:H:56:ASP:HB3	1:H:162:LEU:HD21	2.01	0.41
1:E:140:TRP:CH2	1:E:162:LEU:HG	2.56	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: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:A:196:ASP:O	1:A:217:SER:HA	2.21	0.41
1:B:131:PRO:HA	1:B:136:LYS:HD3	2.03	0.41
1:C:95:ILE:N	1:C:95:ILE:HD12	2.35	0.41
1:D:84:PHE:O	1:D:182:LYS:NZ	2.54	0.41
1:E:13:LEU:HD23	1:E:14:TYR:N	2.36	0.41
1:E:13:LEU:HB3	1:E:28:ALA:HB3	2.03	0.41
1:F:185:LYS:HD2	1:F:185:LYS:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:TYR:HA	1:G:219:ALA:HB3	2.03	0.41
1:C:78:ASP:O	1:C:82:GLN:HG3	2.21	0.41
1:F:42:ASN:HD22	1:F:42:ASN:HA	1.69	0.41
1:H:33:LYS:HD2	3:H:2125:HOH:O	2.21	0.40
1:A:91:GLU:HG3	1:B:124:CYS:HB2	2.03	0.40
1:B:77:PRO:HG2	1:B:190:PRO:CB	2.52	0.40
1:B:95:ILE:HD12	1:B:95:ILE:N	2.36	0.40
1:E:127:PRO:HA	1:E:128:PRO:HD2	1.97	0.40
1:F:146:MSE:O	1:F:156:GLY:HA2	2.22	0.40
1:B:5:ILE:N	3:B:2162:HOH:O	2.55	0.40
1:B:206:GLU:CD	1:H:185:LYS:HD2	2.46	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/233 (95%)	220 (100%)	1 (0%)	0	100	100
1	B	221/233 (95%)	220 (100%)	1 (0%)	0	100	100
1	C	221/233 (95%)	217 (98%)	2 (1%)	2 (1%)	14	5
1	D	221/233 (95%)	219 (99%)	2 (1%)	0	100	100
1	E	221/233 (95%)	220 (100%)	1 (0%)	0	100	100
1	F	221/233 (95%)	219 (99%)	2 (1%)	0	100	100
1	G	221/233 (95%)	218 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
All	All	1768/1864 (95%)	1751 (99%)	15 (1%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	165	ALA
1	C	166	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/195 (101%)	193 (98%)	4 (2%)	48	38
1	B	197/195 (101%)	195 (99%)	2 (1%)	68	64
1	C	197/195 (101%)	190 (96%)	7 (4%)	31	18
1	D	197/195 (101%)	192 (98%)	5 (2%)	42	30
1	E	197/195 (101%)	194 (98%)	3 (2%)	57	49
1	F	197/195 (101%)	196 (100%)	1 (0%)	81	80
1	G	197/195 (101%)	196 (100%)	1 (0%)	81	80
1	H	197/195 (101%)	194 (98%)	3 (2%)	57	49
All	All	1576/1560 (101%)	1550 (98%)	26 (2%)	55	47

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	109	LYS
1	A	113	ASN
1	A	199	PRO
1	B	110	LEU
1	B	159	LEU

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Mol	Chain	Res	Type
1	C	10	ARG
1	C	12	LYS
1	C	13	LEU
1	C	44	LYS
1	C	72	TYR
1	C	189	MSE
1	C	190	PRO
1	D	13	LEU
1	D	20	ASN
1	D	31	GLU
1	D	175	ARG
1	D	190	PRO
1	E	42	ASN
1	E	44	LYS
1	E	199	PRO
1	F	12	LYS
1	G	42	ASN
1	H	13	LEU
1	H	40	MSE
1	H	190	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) 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	134	GLN
1	A	169	HIS
1	A	173	HIS
1	A	214	HIS
1	A	223	GLN
1	A	231	HIS
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

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Mol	Chain	Res	Type
1	B	125	ASN
1	B	129	ASN
1	B	169	HIS
1	B	173	HIS
1	C	21	ASN
1	C	22	HIS
1	C	23	HIS
1	C	39	GLN
1	C	42	ASN
1	C	105	GLN
1	C	118	ASN
1	C	129	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	21	ASN
1	D	22	HIS
1	D	23	HIS
1	D	39	GLN
1	D	42	ASN
1	D	134	GLN
1	D	138	GLN
1	D	157	GLN
1	D	168	ASN
1	D	169	HIS
1	D	173	HIS
1	D	232	ASN
1	E	8	ASN
1	E	20	ASN
1	E	23	HIS
1	E	39	GLN
1	E	42	ASN
1	E	129	ASN
1	E	134	GLN
1	E	169	HIS
1	E	173	HIS
1	E	232	ASN
1	F	21	ASN
1	F	39	GLN

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Mol	Chain	Res	Type
1	F	42	ASN
1	F	118	ASN
1	F	134	GLN
1	F	138	GLN
1	F	169	HIS
1	F	173	HIS
1	F	232	ASN
1	G	20	ASN
1	G	21	ASN
1	G	23	HIS
1	G	39	GLN
1	G	129	ASN
1	G	138	GLN
1	G	168	ASN
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	23	HIS
1	H	39	GLN
1	H	129	ASN
1	H	138	GLN
1	H	168	ASN
1	H	169	HIS
1	H	173	HIS
1	H	214	HIS
1	H	223	GLN
1	H	231	HIS
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	25,25,26	3.49	5 (20%)	28,34,36	5.14	8 (28%)
1	CRQ	C	65	1	25,25,26	3.23	6 (24%)	28,34,36	5.40	8 (28%)
1	CRQ	F	65	1	25,25,26	4.22	6 (24%)	28,34,36	6.34	8 (28%)
1	CRQ	E	65	1	25,25,26	3.55	5 (20%)	28,34,36	6.05	8 (28%)
1	CRQ	H	65	1	25,25,26	4.20	4 (16%)	28,34,36	5.25	8 (28%)
1	CRQ	D	65	1	25,25,26	2.60	5 (20%)	28,34,36	5.87	8 (28%)
1	CRQ	B	65	1	25,25,26	3.68	7 (28%)	28,34,36	6.07	8 (28%)
1	CRQ	G	65	1	25,25,26	3.94	5 (20%)	28,34,36	5.84	8 (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	-	5/10/32/33	0/2/2/2
1	CRQ	C	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	F	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	E	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	H	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	D	65	1	-	5/10/32/33	0/2/2/2
1	CRQ	B	65	1	-	3/10/32/33	0/2/2/2
1	CRQ	G	65	1	-	5/10/32/33	0/2/2/2

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	65	CRQ	CB2-CA2	18.34	1.52	1.35
1	F	65	CRQ	CB2-CA2	17.96	1.52	1.35
1	G	65	CRQ	CB2-CA2	16.72	1.51	1.35
1	B	65	CRQ	CB2-CA2	14.57	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	65	CRQ	CB2-CA2	14.50	1.49	1.35
1	A	65	CRQ	CB2-CA2	13.69	1.48	1.35
1	C	65	CRQ	CB2-CA2	12.49	1.47	1.35
1	B	65	CRQ	CA1-N1	8.54	1.46	1.27
1	G	65	CRQ	CA1-N1	8.52	1.46	1.27
1	C	65	CRQ	CA1-N1	8.50	1.46	1.27
1	F	65	CRQ	CA1-N1	8.49	1.46	1.27
1	E	65	CRQ	CA1-N1	8.49	1.46	1.27
1	D	65	CRQ	CA1-N1	8.48	1.46	1.27
1	H	65	CRQ	CA1-N1	8.48	1.46	1.27
1	A	65	CRQ	CA1-N1	8.01	1.45	1.27
1	D	65	CRQ	CB2-CA2	7.56	1.42	1.35
1	F	65	CRQ	C1-CA1	4.25	1.54	1.48
1	A	65	CRQ	CA2-C2	4.17	1.53	1.48
1	D	65	CRQ	C1-CA1	-3.50	1.42	1.48
1	B	65	CRQ	C1-N3	3.50	1.43	1.38
1	A	65	CRQ	CA3-N3	-3.48	1.40	1.47
1	B	65	CRQ	C2-N3	3.43	1.47	1.40
1	D	65	CRQ	C1-N3	3.39	1.43	1.38
1	F	65	CRQ	C1-N3	3.37	1.43	1.38
1	G	65	CRQ	CA2-C2	3.34	1.52	1.48
1	H	65	CRQ	C1-N3	3.25	1.43	1.38
1	A	65	CRQ	C1-N3	3.23	1.43	1.38
1	E	65	CRQ	C1-CA1	3.19	1.52	1.48
1	B	65	CRQ	CA2-C2	2.95	1.51	1.48
1	H	65	CRQ	C1-CA1	2.95	1.52	1.48
1	B	65	CRQ	C1-CA1	2.91	1.52	1.48
1	G	65	CRQ	C1-N3	2.78	1.42	1.38
1	F	65	CRQ	CA2-C2	2.76	1.51	1.48
1	E	65	CRQ	C1-N3	2.61	1.42	1.38
1	C	65	CRQ	C1-CA1	-2.58	1.44	1.48
1	D	65	CRQ	CA2-C2	2.38	1.51	1.48
1	E	65	CRQ	CA2-C2	2.32	1.51	1.48
1	C	65	CRQ	C2-N3	2.26	1.45	1.40
1	C	65	CRQ	C1-N3	2.23	1.41	1.38
1	G	65	CRQ	C1-CA1	2.16	1.51	1.48
1	B	65	CRQ	CA3-N3	-2.16	1.43	1.47
1	C	65	CRQ	CA2-C2	2.10	1.50	1.48
1	F	65	CRQ	CA3-N3	-2.02	1.43	1.47

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	65	CRQ	CB2-CA2-N2	-17.95	104.39	128.76
1	B	65	CRQ	CB2-CA2-N2	-17.06	105.59	128.76
1	E	65	CRQ	CB2-CA2-C2	17.00	142.96	122.36
1	D	65	CRQ	CB2-CA2-C2	16.56	142.43	122.36
1	B	65	CRQ	CB2-CA2-C2	16.43	142.27	122.36
1	F	65	CRQ	CB2-CA2-C2	16.21	142.01	122.36
1	G	65	CRQ	CB2-CA2-N2	-15.92	107.15	128.76
1	E	65	CRQ	CB2-CA2-N2	-15.67	107.48	128.76
1	H	65	CRQ	CB2-CA2-N2	-15.59	107.59	128.76
1	G	65	CRQ	CB2-CA2-C2	15.50	141.14	122.36
1	C	65	CRQ	CB2-CA2-C2	15.21	140.79	122.36
1	B	65	CRQ	O2-C2-CA2	-14.35	121.86	131.02
1	H	65	CRQ	CB2-CA2-C2	14.25	139.63	122.36
1	A	65	CRQ	CB2-CA2-C2	14.25	139.63	122.36
1	F	65	CRQ	CA3-N3-C1	13.79	155.58	128.39
1	E	65	CRQ	CA3-N3-C1	13.22	154.46	128.39
1	G	65	CRQ	CA3-N3-C1	12.44	152.92	128.39
1	B	65	CRQ	CG2-CB2-CA2	-12.43	115.10	129.87
1	F	65	CRQ	CA3-N3-C2	-12.36	96.51	123.67
1	E	65	CRQ	CA3-N3-C2	-11.93	97.47	123.67
1	G	65	CRQ	CA3-N3-C2	-11.51	98.39	123.67
1	E	65	CRQ	CG2-CB2-CA2	-11.47	116.23	129.87
1	F	65	CRQ	CG2-CB2-CA2	-11.37	116.35	129.87
1	A	65	CRQ	CA3-N3-C1	11.26	150.59	128.39
1	C	65	CRQ	CA3-N3-C2	-11.19	99.08	123.67
1	G	65	CRQ	CG2-CB2-CA2	-11.10	116.67	129.87
1	A	65	CRQ	CA3-N3-C2	-10.92	99.67	123.67
1	C	65	CRQ	CB2-CA2-N2	-10.83	114.06	128.76
1	A	65	CRQ	CB2-CA2-N2	-10.70	114.24	128.76
1	C	65	CRQ	CG2-CB2-CA2	-10.68	117.17	129.87
1	D	65	CRQ	CG2-CB2-CA2	-10.61	117.26	129.87
1	D	65	CRQ	CA3-N3-C2	-10.57	100.45	123.67
1	D	65	CRQ	CA3-N3-C1	10.32	148.75	128.39
1	D	65	CRQ	C2-CA2-N2	-10.27	101.59	108.95
1	C	65	CRQ	CA3-N3-C1	10.15	148.40	128.39
1	H	65	CRQ	CG2-CB2-CA2	-9.97	118.02	129.87
1	A	65	CRQ	CG2-CB2-CA2	-9.88	118.12	129.87
1	D	65	CRQ	CB2-CA2-N2	-9.43	115.96	128.76
1	H	65	CRQ	CA3-N3-C1	9.42	146.97	128.39
1	H	65	CRQ	CA3-N3-C2	-9.00	103.89	123.67
1	D	65	CRQ	CA2-N2-C1	8.80	120.29	104.09
1	D	65	CRQ	N3-C1-N2	-8.70	102.29	112.62
1	B	65	CRQ	O2-C2-N3	7.04	138.99	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	CRQ	N3-C1-N2	-6.79	104.56	112.62
1	C	65	CRQ	CA2-N2-C1	6.69	116.40	104.09
1	F	65	CRQ	C2-CA2-N2	6.42	113.56	108.95
1	A	65	CRQ	CA2-N2-C1	5.79	114.74	104.09
1	C	65	CRQ	C2-CA2-N2	-5.43	105.06	108.95
1	H	65	CRQ	C2-CA2-N2	5.32	112.76	108.95
1	B	65	CRQ	CA2-C2-N3	-5.18	99.15	103.50
1	A	65	CRQ	N3-C1-N2	-4.65	107.10	112.62
1	B	65	CRQ	C2-CA2-N2	4.36	112.08	108.95
1	E	65	CRQ	O2-C2-CA2	-4.34	128.25	131.02
1	A	65	CRQ	C2-CA2-N2	-4.00	106.09	108.95
1	H	65	CRQ	CA2-C2-N3	-3.97	100.17	103.50
1	G	65	CRQ	CA2-C2-N3	-3.92	100.22	103.50
1	F	65	CRQ	CA2-C2-N3	-3.80	100.31	103.50
1	G	65	CRQ	C2-CA2-N2	3.70	111.60	108.95
1	G	65	CRQ	O2-C2-N3	2.72	129.99	124.31
1	E	65	CRQ	CA2-N2-C1	2.69	109.05	104.09
1	E	65	CRQ	O2-C2-N3	2.54	129.61	124.31
1	H	65	CRQ	O2-C2-N3	2.38	129.28	124.31
1	B	65	CRQ	CA2-N2-C1	2.32	108.36	104.09
1	F	65	CRQ	O2-C2-N3	2.13	128.75	124.31

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	CRQ	C3-CA3-N3-C1
1	A	65	CRQ	C3-CA3-N3-C2
1	C	65	CRQ	C3-CA3-N3-C1
1	C	65	CRQ	C3-CA3-N3-C2
1	D	65	CRQ	C3-CA3-N3-C1
1	D	65	CRQ	C3-CA3-N3-C2
1	E	65	CRQ	C3-CA3-N3-C1
1	E	65	CRQ	C3-CA3-N3-C2
1	F	65	CRQ	C3-CA3-N3-C1
1	F	65	CRQ	C3-CA3-N3-C2
1	G	65	CRQ	C3-CA3-N3-C1
1	G	65	CRQ	C3-CA3-N3-C2
1	H	65	CRQ	C3-CA3-N3-C1
1	A	65	CRQ	C2-CA2-CB2-CG2
1	B	65	CRQ	C2-CA2-CB2-CG2
1	C	65	CRQ	C2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	D	65	CRQ	C2-CA2-CB2-CG2
1	E	65	CRQ	C2-CA2-CB2-CG2
1	F	65	CRQ	C2-CA2-CB2-CG2
1	G	65	CRQ	C2-CA2-CB2-CG2
1	H	65	CRQ	C2-CA2-CB2-CG2
1	H	65	CRQ	C3-CA3-N3-C2
1	A	65	CRQ	N2-CA2-CB2-CG2
1	B	65	CRQ	N2-CA2-CB2-CG2
1	C	65	CRQ	N2-CA2-CB2-CG2
1	D	65	CRQ	N2-CA2-CB2-CG2
1	E	65	CRQ	N2-CA2-CB2-CG2
1	F	65	CRQ	N2-CA2-CB2-CG2
1	G	65	CRQ	N2-CA2-CB2-CG2
1	H	65	CRQ	N2-CA2-CB2-CG2
1	A	65	CRQ	CA1-CB1-CG1-CD3
1	B	65	CRQ	CA1-CB1-CG1-CD3
1	C	65	CRQ	CA1-CB1-CG1-CD3
1	D	65	CRQ	CA1-CB1-CG1-CD3
1	E	65	CRQ	CA1-CB1-CG1-CD3
1	F	65	CRQ	CA1-CB1-CG1-CD3
1	G	65	CRQ	CA1-CB1-CG1-CD3
1	H	65	CRQ	CA1-CB1-CG1-CD3

There are no ring outliers.

7 monomers are involved in 17 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	F	2007	-	4,4,4	1.78	2 (50%)	6,6,6	0.45	0
2	PO4	D	2003	-	4,4,4	1.75	2 (50%)	6,6,6	0.48	0
2	PO4	A	2004	-	4,4,4	1.76	1 (25%)	6,6,6	0.45	0
2	PO4	B	2002	-	4,4,4	1.78	1 (25%)	6,6,6	0.46	0
2	PO4	F	2008	-	4,4,4	1.80	2 (50%)	6,6,6	0.46	0
2	PO4	B	2010	-	4,4,4	1.67	0	6,6,6	0.45	0
2	PO4	A	2009	-	4,4,4	1.66	0	6,6,6	0.46	0
2	PO4	E	2013	-	4,4,4	1.69	0	6,6,6	0.46	0
2	PO4	B	2011	-	4,4,4	1.67	0	6,6,6	0.47	0
2	PO4	G	2006	-	4,4,4	1.75	1 (25%)	6,6,6	0.48	0
2	PO4	D	2012	-	4,4,4	1.66	0	6,6,6	0.47	0
2	PO4	G	2016	-	4,4,4	1.69	0	6,6,6	0.47	0
2	PO4	H	2005	-	4,4,4	1.73	1 (25%)	6,6,6	0.48	0
2	PO4	H	2014	-	4,4,4	1.66	0	6,6,6	0.44	0
2	PO4	A	2001	-	4,4,4	1.79	1 (25%)	6,6,6	0.45	0
2	PO4	F	2015	-	4,4,4	1.66	0	6,6,6	0.45	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2005	PO4	P-O2	-2.29	1.48	1.54
2	B	2002	PO4	P-O3	-2.25	1.48	1.54
2	D	2003	PO4	P-O3	-2.20	1.48	1.54
2	F	2008	PO4	P-O3	-2.19	1.48	1.54
2	F	2007	PO4	P-O4	-2.16	1.48	1.54
2	F	2008	PO4	P-O4	-2.16	1.48	1.54
2	G	2006	PO4	P-O2	-2.15	1.48	1.54
2	D	2003	PO4	P-O4	-2.13	1.48	1.54
2	A	2004	PO4	P-O2	-2.12	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2007	PO4	P-O2	-2.02	1.48	1.54
2	A	2001	PO4	P-O3	-2.02	1.48	1.54

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	F	2007	PO4	1	0
2	B	2002	PO4	1	0
2	E	2013	PO4	1	0
2	H	2005	PO4	2	0
2	A	2001	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, 95th 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%)	-0.12	7 (3%)	50	50	8, 13, 26, 39	0
1	B	218/233 (93%)	0.02	9 (4%)	41	41	9, 15, 29, 43	0
1	C	218/233 (93%)	0.05	10 (4%)	37	36	8, 14, 28, 40	0
1	D	218/233 (93%)	-0.04	5 (2%)	61	61	8, 14, 28, 41	0
1	E	218/233 (93%)	0.25	6 (2%)	55	55	11, 19, 31, 37	0
1	F	218/233 (93%)	0.40	10 (4%)	37	36	10, 20, 32, 42	0
1	G	218/233 (93%)	0.60	18 (8%)	17	15	12, 22, 36, 46	0
1	H	218/233 (93%)	0.17	10 (4%)	37	36	10, 17, 31, 48	0
All	All	1744/1864 (93%)	0.17	75 (4%)	40	39	8, 17, 31, 48	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	164	CYS	6.6
1	C	165	ALA	6.6
1	D	214	HIS	6.5
1	B	166	ASP	5.5
1	H	165	ALA	5.1
1	H	166	ASP	5.1
1	G	8	ASN	4.7
1	G	185	LYS	4.1
1	C	111	ASP	4.0
1	E	166	ASP	3.9
1	D	165	ALA	3.7
1	H	230	GLY	3.4
1	G	198	ARG	3.3
1	G	228	LYS	3.3
1	G	166	ASP	3.2
1	C	185	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	232	ASN	3.1
1	G	10	ARG	3.1
1	B	138	GLN	3.0
1	D	113	ASN	3.0
1	F	5	ILE	3.0
1	B	107	GLU	3.0
1	B	228	LYS	2.9
1	F	113	ASN	2.9
1	G	223	GLN	2.9
1	H	228	LYS	2.9
1	B	167	GLY	2.8
1	G	129	ASN	2.8
1	H	167	GLY	2.8
1	G	6	SER	2.7
1	C	228	LYS	2.6
1	H	185	LYS	2.6
1	C	167	GLY	2.6
1	B	36	GLU	2.6
1	F	8	ASN	2.6
1	G	7	ASP	2.6
1	H	22	HIS	2.5
1	F	29	GLU	2.5
1	G	187	LEU	2.5
1	G	232	ASN	2.5
1	B	223	GLN	2.5
1	G	31	GLU	2.5
1	G	165	ALA	2.5
1	E	12	LYS	2.5
1	A	228	LYS	2.4
1	D	164	CYS	2.4
1	H	29	GLU	2.4
1	D	166	ASP	2.4
1	B	185	LYS	2.4
1	A	166	ASP	2.4
1	F	111	ASP	2.4
1	A	223	GLN	2.4
1	G	229	LEU	2.3
1	A	164	CYS	2.3
1	C	72	TYR	2.3
1	A	22	HIS	2.3
1	A	29	GLU	2.2
1	C	42	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	135	LYS	2.2
1	H	232	ASN	2.2
1	F	184	ALA	2.2
1	A	198	ARG	2.2
1	F	31	GLU	2.1
1	F	36	GLU	2.1
1	E	185	LYS	2.1
1	F	7	ASP	2.1
1	G	111	ASP	2.1
1	F	185	LYS	2.1
1	G	204	VAL	2.1
1	E	223	GLN	2.1
1	H	12	LYS	2.0
1	B	165	ALA	2.0
1	E	198	ARG	2.0
1	G	12	LYS	2.0
1	C	223	GLN	2.0

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

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, 95th 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	D	65	24/25	0.84	0.14	11,19,29,30	0
1	CRQ	E	65	24/25	0.84	0.13	11,19,29,30	0
1	CRQ	F	65	24/25	0.84	0.12	11,19,29,30	0
1	CRQ	G	65	24/25	0.85	0.13	11,19,29,30	0
1	CRQ	B	65	24/25	0.87	0.11	11,19,29,30	0
1	CRQ	C	65	24/25	0.87	0.12	11,19,29,30	0
1	CRQ	A	65	24/25	0.87	0.12	11,19,29,30	0
1	CRQ	H	65	24/25	0.87	0.12	11,19,29,30	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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($\text{\AA}^2$)	Q<0.9
2	PO4	E	2013	5/5	0.54	0.18	58,60,61,61	0
2	PO4	F	2015	5/5	0.71	0.17	38,40,45,45	0
2	PO4	B	2011	5/5	0.77	0.24	27,32,37,37	0
2	PO4	G	2016	5/5	0.79	0.16	47,48,52,52	0
2	PO4	H	2005	5/5	0.89	0.11	22,23,24,25	0
2	PO4	H	2014	5/5	0.90	0.15	22,22,30,31	0
2	PO4	D	2012	5/5	0.91	0.14	22,26,29,31	0
2	PO4	B	2010	5/5	0.92	0.14	23,27,32,32	0
2	PO4	A	2001	5/5	0.93	0.09	20,20,25,27	0
2	PO4	A	2009	5/5	0.94	0.14	17,24,27,27	0
2	PO4	F	2007	5/5	0.94	0.09	21,23,26,26	0
2	PO4	B	2002	5/5	0.95	0.08	20,20,24,25	0
2	PO4	F	2008	5/5	0.98	0.05	16,16,19,21	0
2	PO4	D	2003	5/5	0.98	0.05	13,13,15,16	0
2	PO4	G	2006	5/5	0.98	0.05	16,16,20,20	0
2	PO4	A	2004	5/5	0.99	0.04	14,14,18,19	0

6.5 Other polymers

There are no such residues in this entry.