



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2019 – 09:06 PM EDT

PDB ID : 2C9J  
Title : Structure of the fluorescent protein cmFP512 at 1.35Å from Cerianthus membranaceus  
Authors : Renzi, F.; Nienhaus, K.; Wiedenmann, J.; Vallone, B.; Nienhaus, G.U.  
Deposited on : 2005-12-12  
Resolution : 1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

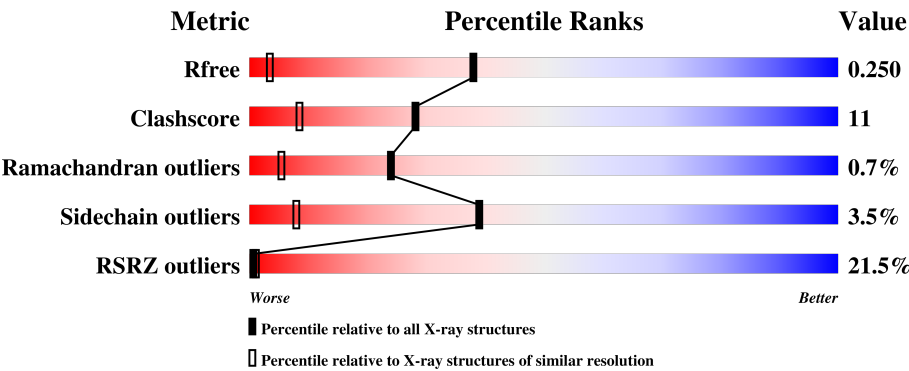
MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 1.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	111664	1197 (1.38-1.34)
Clashscore	122126	1232 (1.38-1.34)
Ramachandran outliers	120053	1215 (1.38-1.34)
Sidechain outliers	120020	1215 (1.38-1.34)
RSRZ outliers	108989	1177 (1.38-1.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	<div><div>32%</div><div><div></div><div>76%</div><div>18%</div><div>• •</div></div></div>
1	B	223	<div><div>17%</div><div><div></div><div>82%</div><div>14%</div><div>• •</div></div></div>
1	C	223	<div><div>22%</div><div><div></div><div>73%</div><div>23%</div><div>• •</div></div></div>
1	D	223	<div><div>23%</div><div><div></div><div>76%</div><div>19%</div><div>• •</div></div></div>
1	E	223	<div><div>19%</div><div><div></div><div>82%</div><div>15%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	223	
1	G	223	
1	H	223	

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
1	CRQ	A	62	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15518 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 GREEN FLUORESCENT PROTEIN FP512.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1715	1111	282	313	9			
1	B	218	Total	C	N	O	S	0	0	0
			1748	1131	288	320	9			
1	C	218	Total	C	N	O	S	0	2	0
			1760	1141	290	320	9			
1	D	219	Total	C	N	O	S	0	1	0
			1760	1141	289	321	9			
1	E	218	Total	C	N	O	S	0	0	0
			1747	1130	288	320	9			
1	F	216	Total	C	N	O	S	0	2	0
			1743	1132	287	315	9			
1	G	218	Total	C	N	O	S	0	0	0
			1747	1130	288	320	9			
1	H	219	Total	C	N	O	S	0	0	0
			1755	1136	289	321	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
A	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
A	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
B	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
B	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
B	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
C	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
C	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
C	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
D	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
D	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
D	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
E	62	CRQ	GLN	chromophore	UNP Q5ZQQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
E	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
F	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
F	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
F	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
G	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
G	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
G	62	CRQ	GLY	chromophore	UNP Q5ZQQ5
H	62	CRQ	GLN	chromophore	UNP Q5ZQQ5
H	62	CRQ	TYR	chromophore	UNP Q5ZQQ5
H	62	CRQ	GLY	chromophore	UNP Q5ZQQ5

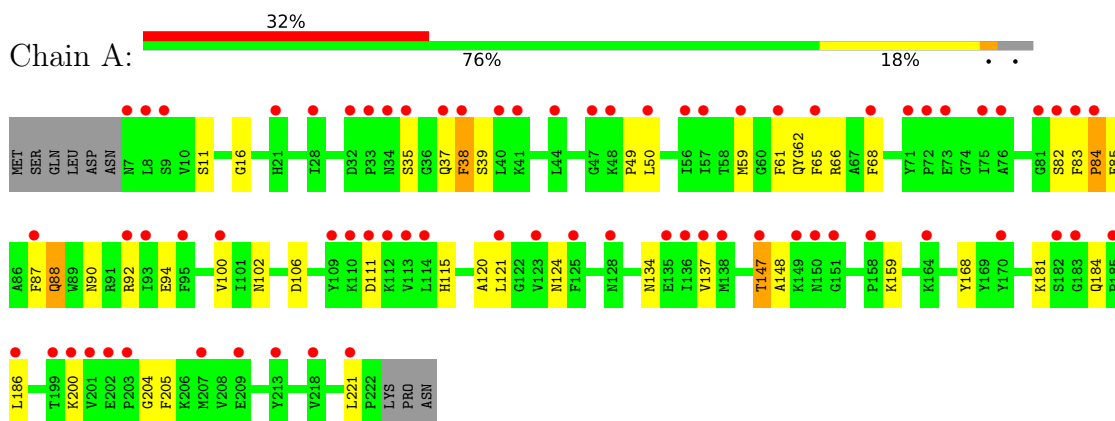
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	168	Total O 168 168	0	0
2	B	187	Total O 187 187	0	0
2	C	210	Total O 210 210	0	0
2	D	197	Total O 197 197	0	0
2	E	184	Total O 184 184	0	0
2	F	219	Total O 219 219	0	0
2	G	204	Total O 204 204	0	0
2	H	174	Total O 174 174	0	0

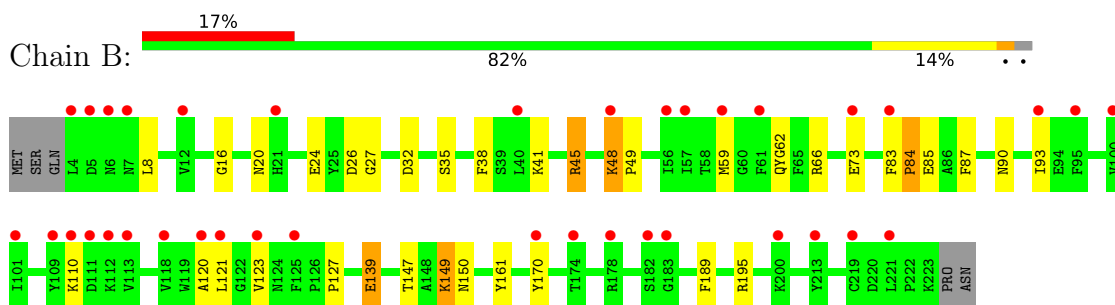
### 3 Residue-property plots [i](#)

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

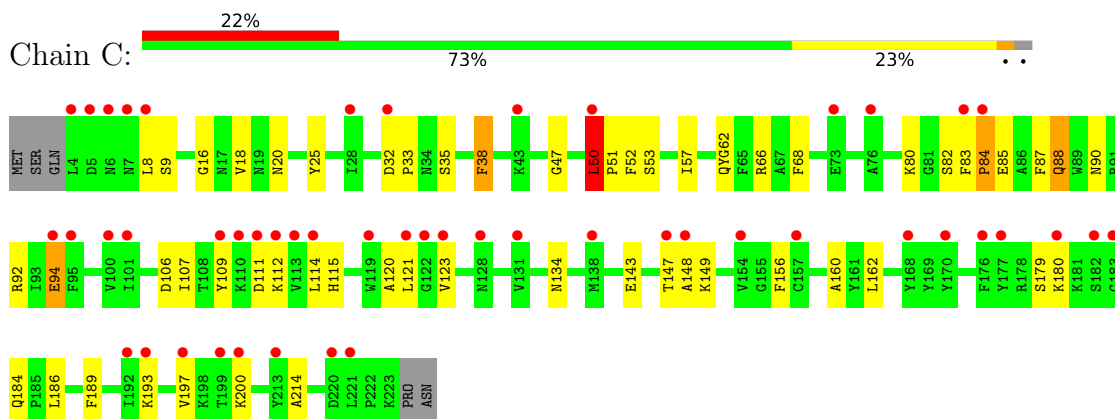
#### • Molecule 1: GREEN FLUORESCENT PROTEIN FP512



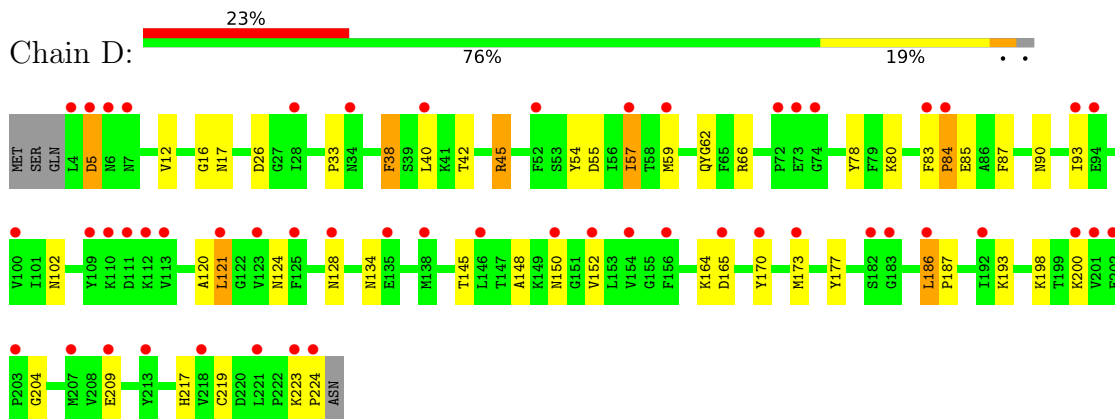
#### • Molecule 1: GREEN FLUORESCENT PROTEIN FP512



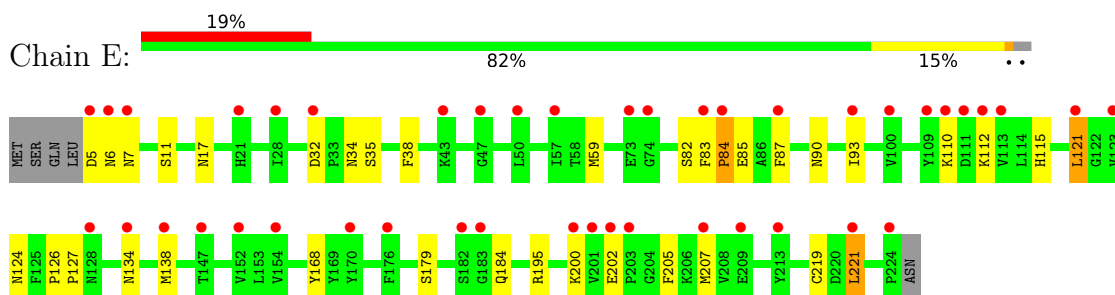
#### • Molecule 1: GREEN FLUORESCENT PROTEIN FP512



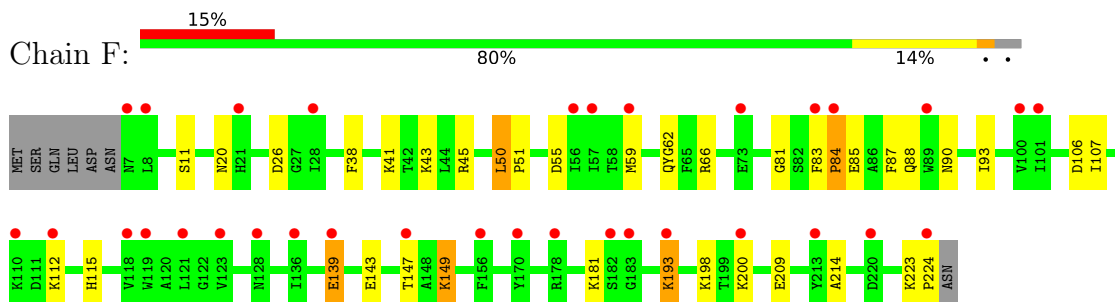
## ● Molecule 1: GREEN FLUORESCENT PROTEIN FP512



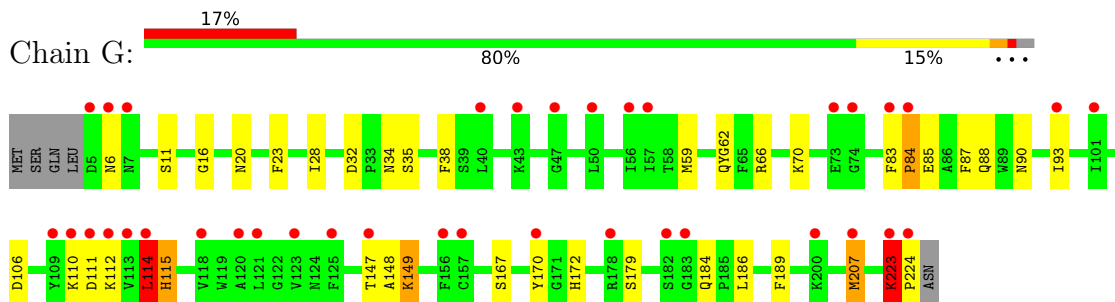
## ● Molecule 1: GREEN FLUORESCENT PROTEIN FP512



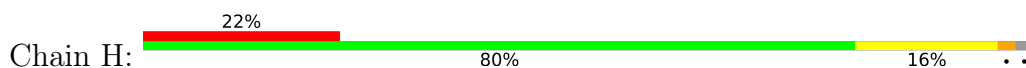
## ● Molecule 1: GREEN FLUORESCENT PROTEIN FP512

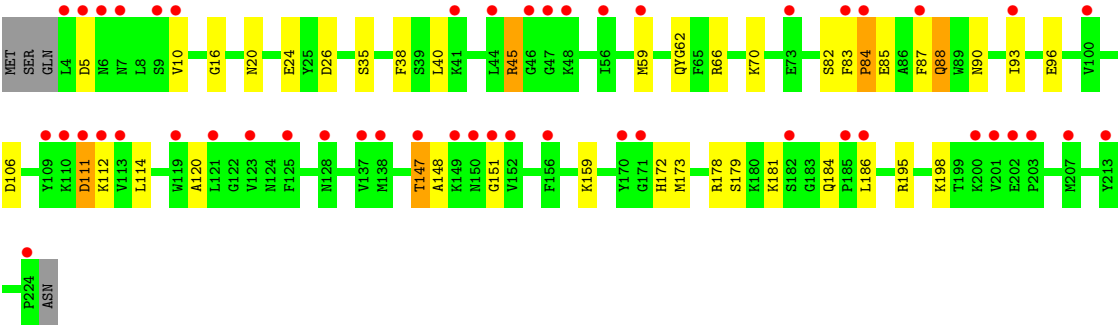


## ● Molecule 1: GREEN FLUORESCENT PROTEIN FP512



## ● Molecule 1: GREEN FLUORESCENT PROTEIN FP512







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.00Å 60.11Å 125.40Å 83.80° 89.98° 73.85°	Depositor
Resolution (Å)	55.00 – 1.35 34.02 – 1.35	Depositor EDS
% Data completeness (in resolution range)	91.0 (55.00-1.35) 90.9 (34.02-1.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.228 , 0.255 0.224 , 0.250	Depositor DCC
$R_{free}$ test set	15177 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.39	0/1741	0.60	1/2350 (0.0%)
1	B	0.42	0/1774	0.63	0/2394
1	C	0.43	0/1792	0.67	2/2416 (0.1%)
1	D	0.41	0/1790	0.65	0/2417
1	E	0.41	0/1774	0.63	0/2395
1	F	0.44	0/1776	0.64	0/2395
1	G	0.44	0/1774	0.67	3/2395 (0.1%)
1	H	0.41	0/1782	0.61	1/2406 (0.0%)
All	All	0.42	0/14203	0.64	7/19168 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	3
1	E	0	2
1	F	0	4
1	G	0	4
1	H	0	2
All	All	0	22

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	LEU	CA-CB-CG	6.40	130.03	115.30
1	G	115	HIS	N-CA-CB	6.34	122.00	110.60
1	G	114	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	88	GLN	N-CA-C	5.91	126.96	111.00
1	H	88	GLN	N-CA-C	5.71	126.42	111.00
1	C	88	GLN	N-CA-C	5.25	125.18	111.00
1	G	115	HIS	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PHE	Peptide
1	A	87	PHE	Peptide
1	B	83	PHE	Peptide
1	B	87	PHE	Peptide
1	C	50	LEU	Peptide
1	C	83	PHE	Peptide
1	C	87	PHE	Peptide
1	D	186	LEU	Peptide
1	D	83	PHE	Peptide
1	D	87	PHE	Peptide
1	E	83	PHE	Peptide
1	E	87	PHE	Peptide
1	F	223	LYS	Peptide
1	F	50	LEU	Peptide
1	F	83	PHE	Peptide
1	F	87	PHE	Peptide
1	G	110	LYS	Peptide
1	G	114	LEU	Peptide
1	G	83	PHE	Peptide
1	G	87	PHE	Peptide
1	H	83	PHE	Peptide
1	H	87	PHE	Peptide

## 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	1715	0	1649	47	0
1	B	1748	0	1682	32	0
1	C	1760	0	1710	57	0
1	D	1760	0	1702	60	0
1	E	1747	0	1678	26	0
1	F	1743	0	1696	37	0
1	G	1747	0	1680	33	0
1	H	1755	0	1691	47	0
2	A	168	0	0	3	0
2	B	187	0	0	3	0
2	C	210	0	0	13	0
2	D	197	0	0	3	0
2	E	184	0	0	1	0
2	F	219	0	0	4	0
2	G	204	0	0	3	0
2	H	174	0	0	2	0
All	All	15518	0	13488	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (292) 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:A:62:CRQ:C	1:A:65:PHE:N	1.84	1.40
1:E:219:CYS:SG	1:F:193[A]:LYS:HE3	1.62	1.38
1:H:59:MET:CE	1:H:173:MET:HE1	1.53	1.36
1:E:219:CYS:SG	1:F:193[A]:LYS:CE	2.19	1.30
1:A:61:PHE:C	1:A:62:CRQ:N	1.89	1.25
1:A:59:MET:CE	1:A:159:LYS:HE2	1.66	1.24
1:A:59:MET:HE3	1:A:159:LYS:HE2	1.12	1.07
1:H:59:MET:HE3	1:H:173:MET:CE	1.85	1.06
1:H:59:MET:CE	1:H:173:MET:CE	2.33	1.06
1:B:26:ASP:OD1	1:B:45:ARG:HD3	1.61	0.98
1:C:84:PRO:HD2	1:C:85:GLU:OE1	1.64	0.98
1:D:84:PRO:HD2	1:D:85:GLU:OE1	1.63	0.96
1:A:59:MET:CE	1:A:159:LYS:CE	2.46	0.94
1:F:26:ASP:OD1	1:F:45:ARG:HD3	1.68	0.94
1:C:193[A]:LYS:HE2	2:C:2180:HOH:O	1.69	0.91
1:E:84:PRO:HD2	1:E:85:GLU:OE1	1.71	0.91
1:D:26:ASP:OD2	1:D:45:ARG:HD3	1.69	0.90
1:A:148:ALA:HB1	1:A:186:LEU:HD13	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:VAL:CG2	1:H:40:LEU:HD21	2.01	0.90
1:G:147:THR:HG22	1:G:189:PHE:HD1	1.38	0.88
1:H:26:ASP:OD2	1:H:45:ARG:HD3	1.74	0.88
1:E:219:CYS:SG	1:F:193[A]:LYS:HE2	2.13	0.88
1:G:84:PRO:HD2	1:G:85:GLU:OE1	1.72	0.88
1:H:59:MET:HE3	1:H:173:MET:HE1	0.89	0.87
1:H:111:ASP:CG	1:H:112:LYS:H	1.77	0.87
1:F:84:PRO:HD2	1:F:85:GLU:OE1	1.75	0.86
1:D:93:ILE:HG12	1:D:173:MET:HE2	1.58	0.85
1:C:149:LYS:HB2	1:D:170:TYR:OH	1.77	0.85
1:G:223:LYS:HB3	1:G:224:PRO:CD	2.06	0.84
1:B:84:PRO:HD2	1:B:85:GLU:OE1	1.76	0.84
1:A:84:PRO:HD2	1:A:85:GLU:OE1	1.77	0.84
1:H:84:PRO:HD2	1:H:85:GLU:OE1	1.77	0.83
1:D:59:MET:CE	1:D:173:MET:SD	2.67	0.82
1:C:149:LYS:HD2	1:D:170:TYR:CE1	2.15	0.82
1:C:160:ALA:HB2	2:C:2149:HOH:O	1.81	0.81
1:C:193[A]:LYS:CG	2:C:2180:HOH:O	2.28	0.81
1:C:193[A]:LYS:HG2	2:C:2180:HOH:O	1.78	0.80
1:A:59:MET:HE1	1:A:159:LYS:CE	2.10	0.78
1:G:223:LYS:HB3	1:G:224:PRO:HD3	1.63	0.78
1:A:59:MET:HE3	1:A:159:LYS:CE	2.03	0.77
1:H:10:VAL:HG23	1:H:40:LEU:HD21	1.67	0.76
1:H:10:VAL:HG21	1:H:40:LEU:HD21	1.67	0.76
1:C:147:THR:HG22	1:C:189:PHE:HD1	1.51	0.76
1:A:100:VAL:HG23	1:C:92:ARG:HH11	1.52	0.74
1:H:111:ASP:CG	1:H:112:LYS:N	2.40	0.74
1:A:59:MET:HE1	1:A:159:LYS:NZ	2.03	0.73
1:B:48:LYS:HG3	2:B:2052:HOH:O	1.89	0.73
1:D:59:MET:HE1	1:D:173:MET:SD	2.29	0.72
1:C:197:VAL:HG11	1:D:224:PRO:HG3	1.70	0.72
1:G:207:MET:HB3	2:G:2185:HOH:O	1.90	0.72
2:C:2149:HOH:O	1:D:145:THR:HG21	1.89	0.71
1:G:147:THR:HG22	1:G:189:PHE:CD1	2.23	0.71
1:B:90:ASN:ND2	1:D:124:ASN:H	1.89	0.70
1:E:124:ASN:H	1:G:90:ASN:ND2	1.88	0.70
1:D:59:MET:HE2	1:D:173:MET:SD	2.32	0.70
1:A:84:PRO:HD2	1:A:85:GLU:H	1.58	0.69
1:F:139:GLU:OE2	2:F:2134:HOH:O	2.12	0.68
1:D:40[B]:LEU:HD21	1:D:42:THR:HG23	1.73	0.68
1:A:168:TYR:O	1:B:149:LYS:HE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:VAL:HG21	2:C:2056:HOH:O	1.94	0.67
1:C:57:ILE:HG23	2:C:2056:HOH:O	1.95	0.67
1:C:109:TYR:CE1	1:C:112:LYS:O	2.49	0.66
1:A:221:LEU:HB2	1:B:195:ARG:NH1	2.11	0.66
1:A:124:ASN:H	1:C:90:ASN:ND2	1.94	0.66
1:E:168:TYR:CG	1:F:147:THR:HG21	2.31	0.65
1:F:88:GLN:HA	2:F:2094:HOH:O	1.97	0.65
1:D:40[B]:LEU:HD21	1:D:42:THR:CG2	2.27	0.65
1:B:147:THR:CG2	1:B:189:PHE:HD1	2.10	0.65
1:D:54:TYR:HA	1:D:57:ILE:HD11	1.77	0.65
1:B:139:GLU:HG2	1:B:161:TYR:CE2	2.32	0.64
1:B:121:LEU:HD22	1:D:102:ASN:HB3	1.79	0.64
1:C:193[A]:LYS:CE	2:C:2180:HOH:O	2.36	0.63
1:F:26:ASP:OD1	1:F:45:ARG:CD	2.44	0.63
1:D:152:VAL:HG13	1:D:177:TYR:O	1.99	0.63
1:A:147:THR:HG21	1:B:170:TYR:CE2	2.34	0.62
1:A:100:VAL:CG2	1:C:92:ARG:HH11	2.11	0.62
1:H:148:ALA:HB1	1:H:186:LEU:HD13	1.82	0.61
1:H:59:MET:HE1	1:H:173:MET:CE	2.30	0.61
1:H:10:VAL:HG23	1:H:40:LEU:CD2	2.30	0.61
1:A:84:PRO:HD2	1:A:85:GLU:CD	2.21	0.61
1:A:62:CRQ:C	1:A:65:PHE:CA	2.76	0.61
1:A:221:LEU:HB2	1:B:195:ARG:HH12	1.66	0.60
1:A:61:PHE:C	1:A:62:CRQ:CA1	2.67	0.60
1:D:59:MET:SD	1:D:173:MET:CE	2.89	0.60
1:H:10:VAL:HG12	1:H:114:LEU:HB3	1.83	0.59
1:F:41:LYS:NZ	1:F:43[B]:LYS:HE2	2.17	0.59
1:H:93:ILE:HG12	1:H:173:MET:HE2	1.84	0.59
1:C:106:ASP:OD1	1:C:180:LYS:HE2	2.03	0.59
1:D:198:LYS:NZ	2:D:2170:HOH:O	2.36	0.59
1:G:223:LYS:CB	1:G:224:PRO:HD3	2.33	0.59
1:H:59:MET:SD	1:H:173:MET:CE	2.91	0.59
1:D:12:VAL:HG11	1:D:40[B]:LEU:HD11	1.85	0.58
1:F:11:SER:OG	1:F:115:HIS:HD2	1.86	0.58
1:G:170:TYR:CE1	1:H:147:THR:HG21	2.37	0.58
1:A:62:CRQ:CA3	1:A:65:PHE:N	2.63	0.58
1:E:90:ASN:HD22	1:G:20:ASN:ND2	2.01	0.58
1:H:151:GLY:C	1:H:186:LEU:HD11	2.24	0.58
1:F:55:ASP:OD1	1:F:198:LYS:CE	2.53	0.57
1:F:90:ASN:HD22	1:H:20:ASN:ND2	2.03	0.57
1:D:223:LYS:HB3	1:D:224:PRO:HD2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HD22	1:C:20:ASN:ND2	2.02	0.56
1:B:20:ASN:ND2	1:D:90:ASN:HD22	2.03	0.56
1:H:59:MET:SD	1:H:173:MET:HE1	2.45	0.56
1:A:84:PRO:CD	1:A:85:GLU:H	2.17	0.56
1:C:143:GLU:CD	1:C:193[A]:LYS:HD2	2.26	0.56
1:C:121:LEU:CD2	1:C:123:VAL:HG13	2.35	0.56
1:D:26:ASP:OD2	1:D:45:ARG:CD	2.50	0.56
1:E:17:ASN:HB3	1:E:121:LEU:HD23	1.87	0.56
1:A:134:ASN:HD21	1:A:205:PHE:HE1	1.55	0.55
1:D:134:ASN:O	1:D:164:LYS:HE2	2.05	0.55
1:D:84:PRO:HD2	1:D:85:GLU:H	1.70	0.55
1:E:82:SER:HA	1:E:184:GLN:HE22	1.73	0.54
1:A:62:CRQ:HB1	2:A:2134:HOH:O	2.07	0.54
1:C:156:PHE:HZ	1:D:170:TYR:CD1	2.25	0.54
1:F:20:ASN:ND2	1:H:90:ASN:HD22	2.06	0.53
1:G:6:ASN:HD22	1:G:34:ASN:HD22	1.56	0.53
1:E:219:CYS:SG	1:F:193[A]:LYS:NZ	2.80	0.53
1:H:88:GLN:OE1	1:H:178:ARG:NH1	2.42	0.53
1:E:134:ASN:HD21	1:E:205:PHE:HE1	1.57	0.53
1:G:84:PRO:HD2	1:G:85:GLU:H	1.74	0.53
1:H:84:PRO:HD2	1:H:85:GLU:H	1.75	0.52
1:C:149:LYS:HD2	1:D:170:TYR:HE1	1.68	0.52
1:D:59:MET:SD	1:D:173:MET:HE1	2.50	0.52
1:C:143:GLU:OE1	1:C:193[A]:LYS:HD3	2.10	0.52
1:F:55:ASP:OD1	1:F:198:LYS:HE3	2.10	0.52
1:D:40[B]:LEU:CD2	1:D:42:THR:HG23	2.40	0.52
1:D:200:LYS:HB2	1:D:209:GLU:HB2	1.92	0.51
1:B:147:THR:HG22	1:B:189:PHE:HD1	1.74	0.51
1:E:32:ASP:HB3	1:E:35:SER:OG	2.10	0.51
2:G:2148:HOH:O	1:H:172:HIS:HE1	1.92	0.51
1:E:202:GLU:HG3	1:E:207:MET:HB2	1.92	0.51
1:E:195:ARG:HD2	1:F:224:PRO:O	2.10	0.51
1:D:54:TYR:HA	1:D:57:ILE:CD1	2.41	0.51
1:B:127:PRO:HD2	1:D:150:ASN:OD1	2.11	0.51
1:D:223:LYS:CB	1:D:224:PRO:HD2	2.41	0.51
1:G:111:ASP:O	1:G:112:LYS:HB2	2.11	0.51
1:E:11:SER:OG	1:E:115:HIS:HD2	1.94	0.51
1:G:223:LYS:CB	1:G:224:PRO:CD	2.84	0.50
1:B:48:LYS:HD2	2:B:2024:HOH:O	2.12	0.50
1:D:59:MET:HE3	1:D:62:CRQ:CG2	2.42	0.50
1:E:219:CYS:HA	1:F:193[A]:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ASP:C	1:G:112:LYS:HD2	2.32	0.50
1:H:62:CRQ:HD2	1:H:62:CRQ:N2	2.27	0.50
1:D:84:PRO:CD	1:D:85:GLU:H	2.23	0.49
1:A:92:ARG:NH1	1:A:94:GLU:OE2	2.44	0.49
1:D:193:LYS:HG3	1:D:217:HIS:CD2	2.48	0.49
1:D:148:ALA:HB1	1:D:186:LEU:HD13	1.93	0.49
1:F:200:LYS:HB2	1:F:209:GLU:HB2	1.93	0.49
1:G:170:TYR:HE1	1:H:147:THR:HG21	1.78	0.49
1:C:32:ASP:HB3	1:C:35:SER:OG	2.12	0.49
1:D:59:MET:HE3	1:D:62:CRQ:CB2	2.43	0.49
1:F:143:GLU:OE2	1:F:193[A]:LYS:HG3	2.12	0.49
1:F:81:GLY:O	1:F:181:LYS:HE3	2.13	0.49
1:C:121:LEU:HD22	1:C:123:VAL:HG13	1.95	0.49
2:A:2069:HOH:O	1:C:94:GLU:HG2	2.12	0.49
1:G:149:LYS:HE2	1:H:96:GLU:OE1	2.12	0.49
1:A:90:ASN:HB2	1:C:123:VAL:HG12	1.95	0.48
1:B:59:MET:HE3	1:B:93:ILE:HD11	1.94	0.48
1:A:88:GLN:HG2	1:A:106:ASP:OD2	2.13	0.48
1:D:62:CRQ:HB1	2:D:2143:HOH:O	2.13	0.48
1:A:62:CRQ:N2	1:A:62:CRQ:HD2	2.28	0.48
1:H:59:MET:HG2	1:H:62:CRQ:CD2	2.43	0.48
1:E:90:ASN:HD22	1:G:20:ASN:HD21	1.60	0.48
1:A:102:ASN:HB3	1:C:121:LEU:HD22	1.95	0.47
1:C:57:ILE:CG2	2:C:2056:HOH:O	2.57	0.47
1:D:84:PRO:HD2	1:D:85:GLU:CD	2.31	0.47
1:C:143:GLU:OE1	1:C:193[A]:LYS:CD	2.63	0.47
1:A:90:ASN:HD22	1:C:20:ASN:HD21	1.62	0.47
1:D:17:ASN:HB3	1:D:121:LEU:HD23	1.95	0.47
1:D:12:VAL:CG1	1:D:40[B]:LEU:HD11	2.44	0.47
1:D:55:ASP:OD1	1:D:198:LYS:HE2	2.15	0.47
1:G:84:PRO:CD	1:G:85:GLU:H	2.27	0.47
1:C:85:GLU:O	1:C:180:LYS:HD3	2.15	0.47
1:C:197:VAL:HG21	1:D:224:PRO:HD3	1.97	0.47
1:C:162:LEU:HD11	2:C:2151:HOH:O	2.15	0.46
1:F:41:LYS:HZ3	1:F:43[B]:LYS:HE2	1.81	0.46
1:B:62:CRQ:HB1	2:B:2125:HOH:O	2.14	0.46
1:C:147:THR:HG22	1:C:189:PHE:CD1	2.40	0.46
1:B:66:ARG:NE	1:B:66:ARG:HA	2.31	0.46
1:H:84:PRO:CD	1:H:85:GLU:H	2.29	0.46
1:B:150:ASN:ND2	1:D:128:ASN:HD21	2.13	0.46
1:B:48:LYS:HD3	1:B:49:PRO:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:TYR:HB2	1:D:187:PRO:HD3	1.96	0.46
1:E:219:CYS:SG	1:E:221:LEU:HB2	2.56	0.46
1:H:88:GLN:HG2	1:H:106:ASP:OD2	2.16	0.46
1:H:151:GLY:CA	1:H:186:LEU:HD11	2.46	0.46
1:A:35:SER:OG	1:A:37:GLN:HG2	2.16	0.45
1:A:84:PRO:CD	1:A:85:GLU:N	2.79	0.45
2:C:2149:HOH:O	1:D:145:THR:CG2	2.57	0.45
1:D:5:ASP:N	1:D:5:ASP:OD1	2.39	0.45
1:C:82:SER:HA	1:C:184:GLN:NE2	2.31	0.45
1:A:100:VAL:HG23	1:C:92:ARG:NH1	2.26	0.45
1:G:32:ASP:HB3	1:G:35:SER:OG	2.17	0.45
1:E:6:ASN:ND2	1:E:34:ASN:HD22	2.14	0.45
1:A:66:ARG:HA	1:A:66:ARG:NE	2.31	0.45
1:F:90:ASN:HD22	1:H:20:ASN:HD21	1.65	0.45
1:F:59:MET:HE3	1:F:93:ILE:HD11	1.99	0.45
1:B:121:LEU:CD2	1:B:123:VAL:HG13	2.46	0.45
1:B:24:GLU:HB2	1:B:45:ARG:HG3	1.99	0.45
1:C:156:PHE:CZ	1:D:170:TYR:CD1	3.05	0.45
1:D:204:GLY:HA2	2:D:2050:HOH:O	2.17	0.45
1:B:20:ASN:HD21	1:D:90:ASN:HD22	1.65	0.45
1:H:24:GLU:HB2	1:H:45:ARG:HG3	1.99	0.45
1:G:148:ALA:HB1	1:G:186:LEU:HD13	1.98	0.44
1:D:59:MET:CE	1:D:62:CRQ:CD1	2.95	0.44
1:G:62:CRQ:N	1:G:62:CRQ:HA31	2.31	0.44
1:G:11:SER:HB3	1:G:115:HIS:HD2	1.81	0.44
1:A:38:PHE:CZ	1:A:62:CRQ:HB11	2.53	0.44
1:F:41:LYS:HZ2	1:F:43[B]:LYS:HE2	1.81	0.44
1:B:32:ASP:HB3	1:B:35:SER:OG	2.18	0.44
1:D:38:PHE:CZ	1:D:62:CRQ:HB11	2.53	0.44
1:F:50:LEU:HA	1:F:51:PRO:HD3	1.85	0.44
1:A:39:SER:HA	1:A:62:CRQ:HE12	1.82	0.44
1:F:149:LYS:HE2	1:F:149:LYS:HB2	1.60	0.44
1:H:16:GLY:HA2	1:H:120:ALA:O	2.18	0.44
1:H:173:MET:HB2	1:H:173:MET:HE2	1.49	0.44
1:H:179:SER:OG	1:H:184:GLN:NE2	2.51	0.44
1:E:6:ASN:HD22	1:E:34:ASN:HD22	1.66	0.43
1:B:84:PRO:HD2	1:B:85:GLU:H	1.82	0.43
1:C:53:SER:OG	1:C:134:ASN:HA	2.17	0.43
1:D:193:LYS:CG	1:D:217:HIS:CD2	3.01	0.43
1:D:62:CRQ:HD2	1:D:62:CRQ:N2	2.33	0.43
1:F:20:ASN:HD21	1:H:90:ASN:HD22	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:SER:O	1:A:115:HIS:HA	2.18	0.43
1:C:82:SER:HA	1:C:184:GLN:HE22	1.83	0.43
1:A:115:HIS:HE1	2:A:2094:HOH:O	2.02	0.43
1:A:59:MET:HG2	1:A:62:CRQ:CD2	2.49	0.43
1:C:62:CRQ:HD2	1:C:62:CRQ:N2	2.34	0.43
1:C:107:ILE:HA	1:C:115:HIS:O	2.18	0.43
1:H:59:MET:HE1	1:H:159:LYS:HE2	2.00	0.43
1:C:84:PRO:HD2	1:C:85:GLU:H	1.82	0.43
1:E:179:SER:OG	1:E:184:GLN:NE2	2.52	0.43
1:C:47:GLY:HA2	1:G:28:ILE:HG12	2.00	0.43
1:E:115:HIS:HE1	2:E:2098:HOH:O	2.00	0.43
1:E:82:SER:HA	1:E:184:GLN:NE2	2.32	0.42
1:G:66:ARG:NE	1:G:66:ARG:HA	2.33	0.42
1:C:66:ARG:NE	1:C:66:ARG:HA	2.35	0.42
1:D:84:PRO:CD	1:D:85:GLU:N	2.81	0.42
1:G:179:SER:OG	1:G:184:GLN:NE2	2.51	0.42
1:H:198:LYS:HB2	1:H:198:LYS:HE3	1.92	0.42
1:H:66:ARG:HA	1:H:66:ARG:NE	2.34	0.42
1:C:106:ASP:OD1	1:C:180:LYS:CE	2.66	0.42
1:C:33:PRO:HB2	1:C:80:LYS:HE3	2.01	0.42
1:F:139:GLU:OE1	2:F:2132:HOH:O	2.21	0.42
1:G:35:SER:HA	1:G:70:LYS:HE3	2.00	0.42
1:C:51:PRO:HD2	1:C:52:PHE:CD2	2.53	0.42
1:A:49:PRO:HB3	1:A:204:GLY:HA3	2.01	0.42
1:C:148:ALA:HB1	1:C:186:LEU:HD13	2.02	0.42
1:A:38:PHE:HB3	1:A:68:PHE:CD2	2.55	0.42
1:B:27:GLY:HA2	1:B:41:LYS:O	2.20	0.42
1:B:84:PRO:CD	1:B:85:GLU:H	2.32	0.42
1:D:33:PRO:HB2	1:D:80:LYS:HE3	2.02	0.42
1:G:172:HIS:HE1	2:H:2133:HOH:O	2.01	0.42
1:F:62:CRQ:N2	1:F:62:CRQ:HD2	2.35	0.42
1:D:198:LYS:HB2	1:D:198:LYS:HE3	1.85	0.42
2:C:2180:HOH:O	1:D:219:CYS:SG	2.01	0.42
1:C:38:PHE:HB3	1:C:68:PHE:CD2	2.55	0.41
1:C:88:GLN:HG2	1:C:106:ASP:OD1	2.19	0.41
1:F:43[A]:LYS:HD3	2:F:2019:HOH:O	2.19	0.41
1:G:88:GLN:HG2	1:G:106:ASP:OD1	2.20	0.41
1:G:115:HIS:HE1	2:G:2106:HOH:O	2.02	0.41
1:C:84:PRO:CD	1:C:85:GLU:H	2.32	0.41
1:E:59:MET:HE3	1:E:93:ILE:HD11	2.01	0.41
1:E:168:TYR:CD1	1:F:147:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:MET:HE3	1:G:93:ILE:HD11	2.02	0.41
1:H:84:PRO:HD2	1:H:85:GLU:CD	2.38	0.41
1:A:147:THR:CG2	1:B:170:TYR:CE2	3.02	0.41
1:H:35:SER:HA	1:H:70:LYS:HD2	2.01	0.41
1:D:66:ARG:NE	1:D:66:ARG:HA	2.35	0.41
1:F:66:ARG:NE	1:F:66:ARG:HA	2.36	0.41
1:A:82:SER:HA	1:A:184:GLN:NE2	2.35	0.41
1:C:25:TYR:OH	1:C:50:LEU:HG	2.20	0.41
1:H:10:VAL:CG2	1:H:40:LEU:CD2	2.83	0.41
1:C:179:SER:OG	1:C:184:GLN:NE2	2.53	0.41
1:F:88:GLN:HG2	1:F:106:ASP:OD2	2.20	0.41
1:F:38:PHE:CZ	1:F:62:CRQ:HB11	2.56	0.41
1:H:82:SER:HA	1:H:184:GLN:NE2	2.36	0.41
1:G:224:PRO:HD2	1:H:195:ARG:HD3	2.03	0.41
1:H:62:CRQ:HB1	2:H:2135:HOH:O	2.20	0.41
1:F:107:ILE:HA	1:F:115:HIS:O	2.20	0.41
1:C:16:GLY:HA2	1:C:120:ALA:O	2.21	0.40
1:A:221:LEU:O	1:B:195:ARG:NH1	2.54	0.40
1:C:193[A]:LYS:CD	2:C:2180:HOH:O	2.57	0.40
1:D:16:GLY:HA2	1:D:120:ALA:O	2.21	0.40
1:B:147:THR:CG2	1:B:189:PHE:CD1	2.99	0.40
1:A:16:GLY:HA2	1:A:120:ALA:O	2.21	0.40
1:G:16:GLY:HA3	1:G:23:PHE:CZ	2.57	0.40
1:B:16:GLY:HA2	1:B:120:ALA:O	2.21	0.40
1:B:147:THR:HG23	1:B:189:PHE:HD1	1.82	0.40
1:E:126:PRO:HA	1:E:127:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

## 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	211/223 (95%)	205 (97%)	4 (2%)	2 (1%)	19	3
1	B	215/223 (96%)	209 (97%)	5 (2%)	1 (0%)	31	8
1	C	217/223 (97%)	209 (96%)	6 (3%)	2 (1%)	19	3
1	D	217/223 (97%)	211 (97%)	5 (2%)	1 (0%)	31	8
1	E	215/223 (96%)	209 (97%)	4 (2%)	2 (1%)	19	3
1	F	215/223 (96%)	211 (98%)	3 (1%)	1 (0%)	31	8
1	G	215/223 (96%)	209 (97%)	4 (2%)	2 (1%)	19	3
1	H	216/223 (97%)	211 (98%)	4 (2%)	1 (0%)	31	8
All	All	1721/1784 (96%)	1674 (97%)	35 (2%)	12 (1%)	24	5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	112	LYS
1	G	223	LYS
1	A	84	PRO
1	H	84	PRO
1	B	84	PRO
1	C	84	PRO
1	C	111	ASP
1	D	84	PRO
1	E	84	PRO
1	G	84	PRO
1	A	111	ASP
1	F	84	PRO

### 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	180/189 (95%)	173 (96%)	7 (4%)	35	5
1	B	184/189 (97%)	176 (96%)	8 (4%)	32	4
1	C	186/189 (98%)	179 (96%)	7 (4%)	36	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	186/189 (98%)	180 (97%)	6 (3%)	42	9
1	E	184/189 (97%)	176 (96%)	8 (4%)	32	4
1	F	184/189 (97%)	179 (97%)	5 (3%)	48	13
1	G	184/189 (97%)	178 (97%)	6 (3%)	41	8
1	H	185/189 (98%)	179 (97%)	6 (3%)	42	9
All	All	1473/1512 (97%)	1420 (96%)	53 (4%)	39	7

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PHE
1	A	50	LEU
1	A	121	LEU
1	A	137	VAL
1	A	147	THR
1	A	181	LYS
1	A	200	LYS
1	B	8	LEU
1	B	38	PHE
1	B	45	ARG
1	B	48	LYS
1	B	73	GLU
1	B	110	LYS
1	B	139	GLU
1	B	149	LYS
1	C	8	LEU
1	C	9	SER
1	C	38	PHE
1	C	50	LEU
1	C	94	GLU
1	C	114	LEU
1	C	200	LYS
1	D	5	ASP
1	D	38	PHE
1	D	45	ARG
1	D	57	ILE
1	D	121	LEU
1	D	165	ASP
1	E	5	ASP
1	E	7	ASN

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Mol	Chain	Res	Type
1	E	38	PHE
1	E	110	LYS
1	E	121	LEU
1	E	138	MET
1	E	200	LYS
1	E	221	LEU
1	F	112	LYS
1	F	139	GLU
1	F	149	LYS
1	F	193[A]	LYS
1	F	193[B]	LYS
1	G	38	PHE
1	G	114	LEU
1	G	149	LYS
1	G	167	SER
1	G	207	MET
1	G	223	LYS
1	H	5	ASP
1	H	38	PHE
1	H	45	ARG
1	H	111	ASP
1	H	147	THR
1	H	181	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	37	GLN
1	A	115	HIS
1	A	124	ASN
1	A	184	GLN
1	B	20	ASN
1	B	37	GLN
1	B	90	ASN
1	B	150	ASN
1	C	6	ASN
1	C	20	ASN
1	C	37	GLN
1	C	90	ASN
1	C	134	ASN
1	C	150	ASN

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Mol	Chain	Res	Type
1	C	184	GLN
1	D	20	ASN
1	D	37	GLN
1	D	184	GLN
1	E	6	ASN
1	E	20	ASN
1	E	37	GLN
1	E	115	HIS
1	E	150	ASN
1	E	184	GLN
1	F	20	ASN
1	F	115	HIS
1	F	150	ASN
1	G	6	ASN
1	G	20	ASN
1	G	90	ASN
1	G	115	HIS
1	G	134	ASN
1	G	172	HIS
1	G	184	GLN
1	H	20	ASN
1	H	37	GLN
1	H	172	HIS
1	H	184	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CRQ	A	62	-	24,25,26	3.04	5 (20%)	27,34,36	6.17	9 (33%)
1	CRQ	B	62	1	24,25,26	3.03	6 (25%)	27,34,36	5.86	10 (37%)
1	CRQ	C	62	1	24,25,26	3.05	9 (37%)	27,34,36	5.56	10 (37%)
1	CRQ	D	62	1	24,25,26	3.01	6 (25%)	27,34,36	5.78	9 (33%)
1	CRQ	E	62	1	24,25,26	3.06	7 (29%)	27,34,36	5.78	8 (29%)
1	CRQ	F	62	1	24,25,26	3.06	7 (29%)	27,34,36	5.73	8 (29%)
1	CRQ	G	62	1	24,25,26	3.02	7 (29%)	27,34,36	5.75	10 (37%)
1	CRQ	H	62	1	24,25,26	3.07	6 (25%)	27,34,36	5.94	8 (29%)

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	62	-	-	4/10/32/33	0/2/2/2
1	CRQ	B	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	C	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	D	62	1	-	4/10/32/33	0/2/2/2
1	CRQ	E	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	F	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	G	62	1	-	3/10/32/33	0/2/2/2
1	CRQ	H	62	1	-	3/10/32/33	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	62	CRQ	CB2-CA2	10.00	1.43	1.35
1	A	62	CRQ	CB2-CA2	9.64	1.43	1.35
1	H	62	CRQ	CB2-CA2	9.51	1.43	1.35
1	D	62	CRQ	CB2-CA2	9.46	1.43	1.35
1	C	62	CRQ	CB2-CA2	9.31	1.43	1.35
1	B	62	CRQ	CB2-CA2	9.29	1.43	1.35
1	F	62	CRQ	CB2-CA2	9.18	1.42	1.35
1	G	62	CRQ	CB2-CA2	8.82	1.42	1.35
1	G	62	CRQ	CA2-C2	-7.15	1.41	1.48
1	F	62	CRQ	CA2-C2	-6.94	1.41	1.48
1	H	62	CRQ	CA2-C2	-6.85	1.41	1.48
1	A	62	CRQ	CA2-C2	-6.71	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	CRQ	CA2-C2	-6.70	1.41	1.48
1	D	62	CRQ	CA2-C2	-6.58	1.42	1.48
1	C	62	CRQ	CA2-C2	-6.42	1.42	1.48
1	E	62	CRQ	CA2-C2	-6.24	1.42	1.48
1	H	62	CRQ	OH-CZ	-6.12	1.22	1.37
1	A	62	CRQ	OH-CZ	-6.03	1.22	1.37
1	C	62	CRQ	OH-CZ	-6.02	1.22	1.37
1	F	62	CRQ	OH-CZ	-6.00	1.22	1.37
1	D	62	CRQ	OH-CZ	-5.98	1.22	1.37
1	B	62	CRQ	OH-CZ	-5.91	1.23	1.37
1	E	62	CRQ	OH-CZ	-5.90	1.23	1.37
1	G	62	CRQ	OH-CZ	-5.84	1.23	1.37
1	B	62	CRQ	C1-N2	3.92	1.40	1.33
1	A	62	CRQ	C1-N2	3.87	1.40	1.33
1	H	62	CRQ	C1-N2	3.79	1.40	1.33
1	E	62	CRQ	C1-N2	3.72	1.40	1.33
1	A	62	CRQ	CD3-NE1	3.71	1.44	1.32
1	F	62	CRQ	C1-N2	3.71	1.40	1.33
1	D	62	CRQ	C1-N2	3.64	1.39	1.33
1	C	62	CRQ	C1-N2	3.64	1.39	1.33
1	D	62	CRQ	CD3-NE1	3.55	1.44	1.32
1	H	62	CRQ	CD3-NE1	3.51	1.44	1.32
1	G	62	CRQ	C1-N2	3.51	1.39	1.33
1	E	62	CRQ	CD3-NE1	3.44	1.44	1.32
1	C	62	CRQ	CD3-NE1	3.40	1.43	1.32
1	F	62	CRQ	CD3-NE1	3.38	1.43	1.32
1	B	62	CRQ	CD3-NE1	3.31	1.43	1.32
1	G	62	CRQ	CD3-NE1	3.29	1.43	1.32
1	G	62	CRQ	CA1-N	2.39	1.33	1.27
1	B	62	CRQ	CB1-CA1	-2.23	1.44	1.50
1	C	62	CRQ	CG1-CD3	-2.23	1.42	1.51
1	E	62	CRQ	CA1-N	2.21	1.32	1.27
1	E	62	CRQ	CB1-CA1	-2.21	1.44	1.50
1	C	62	CRQ	CG1-CB1	-2.18	1.45	1.52
1	F	62	CRQ	CB1-CA1	-2.16	1.44	1.50
1	D	62	CRQ	CA1-N	2.08	1.32	1.27
1	C	62	CRQ	CB1-CA1	-2.08	1.44	1.50
1	C	62	CRQ	CA1-N	2.06	1.32	1.27
1	H	62	CRQ	CG1-CD3	-2.06	1.43	1.51
1	G	62	CRQ	CE1-CD1	-2.04	1.35	1.38
1	F	62	CRQ	CA1-N	2.03	1.32	1.27

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	62	CRQ	CA2-C2-N3	20.86	113.34	103.35
1	B	62	CRQ	CA2-C2-N3	20.84	113.33	103.35
1	A	62	CRQ	CA2-C2-N3	20.84	113.33	103.35
1	E	62	CRQ	CA2-C2-N3	20.42	113.13	103.35
1	D	62	CRQ	CA2-C2-N3	20.16	113.00	103.35
1	G	62	CRQ	CA2-C2-N3	20.16	113.00	103.35
1	F	62	CRQ	CA2-C2-N3	20.13	112.98	103.35
1	C	62	CRQ	CA2-C2-N3	19.73	112.80	103.35
1	A	62	CRQ	CG1-CB1-CA1	15.32	163.35	113.55
1	B	62	CRQ	CG1-CB1-CA1	14.20	159.68	113.55
1	G	62	CRQ	CG1-CB1-CA1	13.96	158.91	113.55
1	E	62	CRQ	CG1-CB1-CA1	13.94	158.85	113.55
1	D	62	CRQ	CG1-CB1-CA1	13.76	158.28	113.55
1	F	62	CRQ	CG1-CB1-CA1	13.76	158.26	113.55
1	H	62	CRQ	CG1-CB1-CA1	13.56	157.63	113.55
1	C	62	CRQ	CG1-CB1-CA1	13.50	157.43	113.55
1	A	62	CRQ	O2-C2-CA2	-10.88	124.85	130.96
1	B	62	CRQ	CB1-CG1-CD3	10.48	169.36	114.26
1	H	62	CRQ	CB1-CG1-CD3	10.44	169.17	114.26
1	C	62	CRQ	CB1-CG1-CD3	10.34	168.65	114.26
1	G	62	CRQ	CB1-CG1-CD3	10.22	168.02	114.26
1	E	62	CRQ	CB1-CG1-CD3	10.20	167.90	114.26
1	D	62	CRQ	CB1-CG1-CD3	10.18	167.79	114.26
1	H	62	CRQ	O2-C2-CA2	-10.09	125.30	130.96
1	A	62	CRQ	CB1-CG1-CD3	9.98	166.78	114.26
1	F	62	CRQ	CB1-CG1-CD3	9.92	166.46	114.26
1	E	62	CRQ	O2-C2-CA2	-8.57	126.15	130.96
1	D	62	CRQ	O2-C2-CA2	-8.55	126.16	130.96
1	F	62	CRQ	O2-C2-CA2	-8.47	126.21	130.96
1	G	62	CRQ	O2-C2-CA2	-7.71	126.63	130.96
1	B	62	CRQ	O2-C2-CA2	-7.64	126.67	130.96
1	A	62	CRQ	C2-CA2-N2	-6.96	104.05	108.92
1	A	62	CRQ	CG2-CB2-CA2	-6.72	121.80	130.01
1	B	62	CRQ	C2-CA2-N2	-6.62	104.28	108.92
1	H	62	CRQ	CG2-CB2-CA2	-6.59	121.95	130.01
1	G	62	CRQ	C2-CA2-N2	-6.59	104.30	108.92
1	D	62	CRQ	CG2-CB2-CA2	-6.32	122.29	130.01
1	D	62	CRQ	C2-CA2-N2	-6.30	104.51	108.92
1	F	62	CRQ	C2-CA2-N2	-6.19	104.58	108.92
1	E	62	CRQ	C2-CA2-N2	-6.14	104.61	108.92
1	C	62	CRQ	CG2-CB2-CA2	-5.99	122.68	130.01
1	H	62	CRQ	C2-CA2-N2	-5.98	104.73	108.92
1	C	62	CRQ	C2-CA2-N2	-5.91	104.78	108.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	CRQ	O2-C2-CA2	-5.90	127.65	130.96
1	B	62	CRQ	CG2-CB2-CA2	-5.89	122.81	130.01
1	G	62	CRQ	CG2-CB2-CA2	-5.75	122.98	130.01
1	F	62	CRQ	CG2-CB2-CA2	-5.72	123.01	130.01
1	E	62	CRQ	CG2-CB2-CA2	-5.41	123.39	130.01
1	F	62	CRQ	OE1-CD3-CG1	-4.07	109.10	121.05
1	C	62	CRQ	OE1-CD3-CG1	-3.59	110.50	121.05
1	G	62	CRQ	OE1-CD3-CG1	-3.48	110.83	121.05
1	E	62	CRQ	OE1-CD3-CG1	-3.47	110.86	121.05
1	A	62	CRQ	CB2-CA2-C2	3.28	126.25	122.28
1	H	62	CRQ	OE1-CD3-CG1	-3.15	111.80	121.05
1	E	62	CRQ	CA3-N3-C2	3.12	130.99	123.83
1	D	62	CRQ	CA3-N3-C2	3.06	130.83	123.83
1	D	62	CRQ	OE1-CD3-CG1	-3.03	112.15	121.05
1	A	62	CRQ	CA3-N3-C2	3.01	130.73	123.83
1	H	62	CRQ	CA3-N3-C2	2.94	130.57	123.83
1	B	62	CRQ	OE1-CD3-CG1	-2.64	113.30	121.05
1	D	62	CRQ	CB2-CA2-C2	2.59	125.41	122.28
1	A	62	CRQ	OE1-CD3-CG1	-2.50	113.69	121.05
1	C	62	CRQ	CA3-N3-C2	2.43	129.40	123.83
1	C	62	CRQ	O2-C2-N3	-2.35	119.53	124.31
1	F	62	CRQ	CA3-N3-C2	2.22	128.92	123.83
1	B	62	CRQ	O2-C2-N3	-2.13	119.99	124.31
1	G	62	CRQ	CA3-N3-C2	2.10	128.64	123.83
1	C	62	CRQ	O-C-CA3	-2.08	120.10	126.39
1	B	62	CRQ	CG1-CD3-NE1	-2.07	110.07	116.53
1	G	62	CRQ	CB2-CA2-C2	2.06	124.77	122.28
1	B	62	CRQ	CA3-N3-C2	2.02	128.46	123.83
1	G	62	CRQ	CD2-CG2-CB2	2.00	128.07	121.22

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	62	CRQ	C1-CA1-CB1-CG1
1	B	62	CRQ	CA1-CB1-CG1-CD3
1	B	62	CRQ	C2-CA2-CB2-CG2
1	A	62	CRQ	C-CA3-N3-C2
1	A	62	CRQ	C2-CA2-CB2-CG2
1	H	62	CRQ	C-CA3-N3-C2
1	D	62	CRQ	CA1-CB1-CG1-CD3
1	G	62	CRQ	CA1-CB1-CG1-CD3

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Mol	Chain	Res	Type	Atoms
1	F	62	CRQ	CA1-CB1-CG1-CD3
1	E	62	CRQ	CA1-CB1-CG1-CD3
1	H	62	CRQ	CA1-CB1-CG1-CD3
1	D	62	CRQ	C-CA3-N3-C2
1	E	62	CRQ	C-CA3-N3-C2
1	D	62	CRQ	C2-CA2-CB2-CG2
1	H	62	CRQ	C2-CA2-CB2-CG2
1	C	62	CRQ	CA1-CB1-CG1-CD3
1	G	62	CRQ	C2-CA2-CB2-CG2
1	C	62	CRQ	C-CA3-N3-C2
1	F	62	CRQ	C2-CA2-CB2-CG2
1	C	62	CRQ	C2-CA2-CB2-CG2
1	A	62	CRQ	CA1-CB1-CG1-CD3
1	A	62	CRQ	C-CA3-N3-C1
1	D	62	CRQ	C1-CA1-CB1-CG1
1	G	62	CRQ	C1-CA1-CB1-CG1
1	F	62	CRQ	C1-CA1-CB1-CG1

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	62	CRQ	10	0
1	B	62	CRQ	1	0
1	C	62	CRQ	1	0
1	D	62	CRQ	6	0
1	F	62	CRQ	2	0
1	G	62	CRQ	1	0
1	H	62	CRQ	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	2
1	A	2
1	D	2
1	E	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	61:PHE	C	62:CRQ	N	1.89
1	A	62:CRQ	C	65:PHE	N	1.84
1	D	61:PHE	C	62:CRQ	N	1.67
1	H	62:CRQ	C	65:PHE	N	1.65
1	D	62:CRQ	C	65:PHE	N	1.63
1	H	61:PHE	C	62:CRQ	N	1.63
1	B	61:PHE	C	62:CRQ	N	1.62
1	E	62:CRQ	C	65:PHE	N	1.62
1	E	61:PHE	C	62:CRQ	N	1.61

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	213/223 (95%)	1.84	72 (33%) 0 0	12, 20, 29, 35	3 (1%)
1	B	217/223 (97%)	1.37	37 (17%) 1 2	10, 16, 25, 36	1 (0%)
1	C	217/223 (97%)	1.40	49 (22%) 0 1	12, 16, 25, 40	0
1	D	218/223 (97%)	1.52	52 (23%) 0 1	10, 17, 25, 36	2 (0%)
1	E	217/223 (97%)	1.35	43 (19%) 1 1	11, 16, 24, 32	3 (1%)
1	F	215/223 (96%)	1.20	33 (15%) 2 2	11, 15, 21, 27	1 (0%)
1	G	217/223 (97%)	1.30	37 (17%) 1 2	10, 15, 23, 33	1 (0%)
1	H	218/223 (97%)	1.52	49 (22%) 0 1	11, 18, 27, 34	0
All	All	1732/1784 (97%)	1.44	372 (21%) 1 1	10, 16, 27, 40	11 (0%)

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	4	LEU	12.7
1	D	224	PRO	11.3
1	C	4	LEU	10.1
1	A	112	LYS	10.1
1	D	170	TYR	9.5
1	H	112	LYS	9.3
1	A	111	ASP	9.0
1	G	224	PRO	9.0
1	E	111	ASP	8.4
1	B	182	SER	8.0
1	B	112	LYS	7.6
1	C	111	ASP	7.6
1	H	113	VAL	7.4
1	A	109	TYR	7.2
1	A	113	VAL	6.9
1	H	111	ASP	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	111	ASP	6.8
1	A	7	ASN	6.7
1	E	109	TYR	6.6
1	D	111	ASP	6.5
1	E	5	ASP	6.4
1	G	111	ASP	6.4
1	C	5	ASP	6.2
1	H	5	ASP	6.2
1	F	224	PRO	6.0
1	C	183	GLY	6.0
1	H	109	TYR	5.9
1	A	110	LYS	5.8
1	B	5	ASP	5.8
1	A	151	GLY	5.7
1	E	170	TYR	5.7
1	B	73	GLU	5.6
1	G	112	LYS	5.5
1	C	73	GLU	5.5
1	G	110	LYS	5.5
1	A	73	GLU	5.4
1	A	182	SER	5.3
1	G	83	PHE	5.3
1	A	150	ASN	5.3
1	E	7	ASN	5.2
1	G	5	ASP	5.2
1	B	4	LEU	5.2
1	E	110	LYS	5.1
1	G	73	GLU	5.0
1	E	74	GLY	5.0
1	A	28	ILE	5.0
1	B	170	TYR	5.0
1	D	112	LYS	5.0
1	E	83	PHE	4.9
1	H	7	ASN	4.9
1	D	213	TYR	4.9
1	G	170	TYR	4.9
1	G	47	GLY	4.8
1	B	6	ASN	4.8
1	C	112	LYS	4.7
1	B	83	PHE	4.7
1	G	6	ASN	4.6
1	E	183	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	110	LYS	4.6
1	D	7	ASN	4.6
1	A	207	MET	4.6
1	B	7	ASN	4.6
1	H	128	ASN	4.6
1	A	83	PHE	4.5
1	D	109	TYR	4.5
1	H	83	PHE	4.5
1	A	121	LEU	4.5
1	G	109	TYR	4.5
1	H	151	GLY	4.5
1	H	110	LYS	4.4
1	D	40[A]	LEU	4.4
1	E	84	PRO	4.3
1	C	100	VAL	4.3
1	C	220	ASP	4.3
1	E	112	LYS	4.3
1	F	100	VAL	4.2
1	A	183	GLY	4.2
1	C	7	ASN	4.2
1	A	213	TYR	4.2
1	A	201	VAL	4.1
1	D	165	ASP	4.1
1	B	213	TYR	4.1
1	H	213	TYR	4.1
1	D	74	GLY	4.1
1	B	93	ILE	4.1
1	H	170	TYR	4.1
1	D	4	LEU	4.0
1	D	100	VAL	4.0
1	D	203	PRO	4.0
1	H	150	ASN	4.0
1	A	200	LYS	4.0
1	A	37	GLN	4.0
1	G	223	LYS	3.9
1	G	93	ILE	3.9
1	D	83	PHE	3.9
1	F	83	PHE	3.9
1	C	121	LEU	3.9
1	D	186	LEU	3.9
1	F	200	LYS	3.9
1	B	48	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	84	PRO	3.8
1	D	6	ASN	3.8
1	G	183	GLY	3.8
1	C	6	ASN	3.8
1	E	100	VAL	3.8
1	D	110	LYS	3.8
1	A	170	TYR	3.7
1	A	48	LYS	3.7
1	H	73	GLU	3.7
1	D	57	ILE	3.7
1	H	93	ILE	3.7
1	C	213	TYR	3.7
1	D	5	ASP	3.7
1	A	128	ASN	3.7
1	A	21	HIS	3.7
1	D	207	MET	3.6
1	A	202	GLU	3.6
1	E	121	LEU	3.6
1	H	202	GLU	3.6
1	D	121	LEU	3.6
1	D	28	ILE	3.5
1	F	28	ILE	3.5
1	A	32	ASP	3.5
1	B	21	HIS	3.5
1	D	150	ASN	3.5
1	C	110	LYS	3.5
1	D	113	VAL	3.5
1	B	200	LYS	3.5
1	E	21	HIS	3.5
1	H	6	ASN	3.4
1	C	170	TYR	3.4
1	F	73	GLU	3.4
1	F	121	LEU	3.4
1	E	134	ASN	3.3
1	A	93	ILE	3.3
1	C	94	GLU	3.3
1	B	121	LEU	3.3
1	B	109	TYR	3.3
1	F	101	ILE	3.3
1	D	84	PRO	3.3
1	A	123	VAL	3.3
1	H	100	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	110	LYS	3.2
1	A	50	LEU	3.2
1	H	84	PRO	3.2
1	D	59	MET	3.2
1	F	21	HIS	3.2
1	B	183	GLY	3.2
1	E	221	LEU	3.2
1	D	73	GLU	3.1
1	H	47	GLY	3.1
1	E	207	MET	3.1
1	H	121	LEU	3.1
1	D	202	GLU	3.1
1	G	101	ILE	3.1
1	A	68	PHE	3.1
1	G	7	ASN	3.1
1	A	47	GLY	3.1
1	C	50	LEU	3.1
1	E	182	SER	3.1
1	H	200	LYS	3.1
1	B	57	ILE	3.1
1	A	34	ASN	3.1
1	E	203	PRO	3.1
1	A	186	LEU	3.0
1	E	73	GLU	3.0
1	G	207	MET	3.0
1	C	28	ILE	3.0
1	A	59	MET	3.0
1	F	220	ASP	3.0
1	F	183	GLY	3.0
1	E	147	THR	3.0
1	F	147	THR	3.0
1	C	84	PRO	2.9
1	F	178	ARG	2.9
1	E	28	ILE	2.9
1	E	152	VAL	2.9
1	E	213	TYR	2.9
1	B	123	VAL	2.9
1	H	224	PRO	2.9
1	C	128	ASN	2.9
1	A	33	PRO	2.9
1	A	164	LYS	2.9
1	H	87	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	113	VAL	2.8
1	C	138	MET	2.8
1	H	56	ILE	2.8
1	G	182	SER	2.8
1	E	200	LYS	2.8
1	B	118	VAL	2.8
1	B	101	ILE	2.8
1	D	93	ILE	2.8
1	D	192	ILE	2.8
1	B	125	PHE	2.8
1	H	149	LYS	2.8
1	G	123	VAL	2.8
1	G	178	ARG	2.8
1	F	170	TYR	2.7
1	F	7	ASN	2.7
1	A	72	PRO	2.7
1	D	218	VAL	2.7
1	E	113	VAL	2.7
1	G	118	VAL	2.7
1	C	200	LYS	2.7
1	F	112	LYS	2.7
1	A	221	LEU	2.7
1	A	100	VAL	2.7
1	H	147	THR	2.7
1	F	57	ILE	2.7
1	C	148	ALA	2.7
1	A	41	LYS	2.7
1	E	50	LEU	2.7
1	D	183	GLY	2.7
1	H	46	GLY	2.7
1	C	123	VAL	2.7
1	F	123	VAL	2.7
1	E	138	MET	2.7
1	H	203	PRO	2.7
1	H	207	MET	2.7
1	D	200	LYS	2.6
1	F	193[A]	LYS	2.6
1	B	221	LEU	2.6
1	D	138	MET	2.6
1	C	83	PHE	2.6
1	F	213	TYR	2.6
1	D	156	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	113	VAL	2.6
1	G	157	CYS	2.6
1	H	123	VAL	2.6
1	F	119	TRP	2.6
1	H	185	PRO	2.6
1	E	128	ASN	2.6
1	C	199	THR	2.5
1	G	120	ALA	2.5
1	A	71	TYR	2.5
1	C	192	ILE	2.5
1	C	147	THR	2.5
1	A	82	SER	2.5
1	C	8	LEU	2.5
1	E	123	VAL	2.5
1	C	95	PHE	2.5
1	B	219	CYS	2.5
1	F	59	MET	2.5
1	A	147	THR	2.5
1	C	109	TYR	2.5
1	A	35	SER	2.5
1	A	81	GLY	2.5
1	B	100	VAL	2.5
1	E	87	PHE	2.5
1	F	156	PHE	2.5
1	F	84	PRO	2.4
1	E	47	GLY	2.4
1	H	44	LEU	2.4
1	D	128	ASN	2.4
1	D	123	VAL	2.4
1	A	87	PHE	2.4
1	H	125	PHE	2.4
1	E	93	ILE	2.4
1	G	200	LYS	2.4
1	H	48	LYS	2.4
1	A	44	LEU	2.4
1	G	50	LEU	2.4
1	G	121	LEU	2.4
1	H	201	VAL	2.4
1	A	92	ARG	2.4
1	A	38	PHE	2.4
1	C	101	ILE	2.4
1	G	57	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	89	TRP	2.4
1	A	114	LEU	2.4
1	A	158	PRO	2.4
1	E	43	LYS	2.4
1	H	138	MET	2.4
1	D	152	VAL	2.4
1	A	95	PHE	2.4
1	G	156	PHE	2.4
1	A	9	SER	2.3
1	D	146	LEU	2.3
1	D	201	VAL	2.3
1	H	171	GLY	2.3
1	G	84	PRO	2.3
1	B	95	PHE	2.3
1	H	41	LYS	2.3
1	A	75	ILE	2.3
1	F	136	ILE	2.3
1	E	202	GLU	2.3
1	C	76	ALA	2.3
1	C	193[A]	LYS	2.3
1	C	154	VAL	2.3
1	D	182	SER	2.3
1	A	65	PHE	2.3
1	G	125	PHE	2.3
1	A	209	GLU	2.3
1	D	135	GLU	2.3
1	E	57	ILE	2.3
1	C	119	TRP	2.3
1	D	221	LEU	2.3
1	G	114	LEU	2.3
1	H	59	MET	2.3
1	A	199	THR	2.3
1	G	74	GLY	2.3
1	G	147	THR	2.3
1	C	168	TYR	2.3
1	A	185	PRO	2.2
1	D	34	ASN	2.2
1	A	76	ALA	2.2
1	D	173	MET	2.2
1	A	136	ILE	2.2
1	H	119	TRP	2.2
1	F	182	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	131	VAL	2.2
1	C	43[A]	LYS	2.2
1	B	59	MET	2.2
1	D	52	PHE	2.2
1	E	32	ASP	2.2
1	C	180	LYS	2.2
1	A	40	LEU	2.2
1	B	56	ILE	2.2
1	F	139	GLU	2.2
1	A	218	VAL	2.2
1	H	137	VAL	2.2
1	A	61	PHE	2.2
1	G	40	LEU	2.2
1	C	182	SER	2.2
1	A	56	ILE	2.2
1	F	56	ILE	2.2
1	G	56	ILE	2.2
1	E	154	VAL	2.2
1	B	178	ARG	2.2
1	D	72	PRO	2.2
1	B	61	PHE	2.1
1	C	221	LEU	2.1
1	A	57	ILE	2.1
1	F	118	VAL	2.1
1	H	152	VAL	2.1
1	F	128	ASN	2.1
1	B	174	THR	2.1
1	A	149	LYS	2.1
1	A	125	PHE	2.1
1	C	176	PHE	2.1
1	D	125	PHE	2.1
1	C	114	LEU	2.1
1	A	138	MET	2.1
1	B	12	VAL	2.1
1	D	154	VAL	2.1
1	H	10	VAL	2.1
1	A	203	PRO	2.1
1	H	9	SER	2.1
1	D	223	LYS	2.1
1	E	176	PHE	2.1
1	C	122	GLY	2.1
1	C	32	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	197	VAL	2.1
1	E	201	VAL	2.1
1	A	135	GLU	2.0
1	D	209	GLU	2.0
1	E	209	GLU	2.0
1	A	8	LEU	2.0
1	B	40	LEU	2.0
1	E	224	PRO	2.0
1	D	94	GLU	2.0
1	A	137	VAL	2.0
1	G	43	LYS	2.0
1	G	113	VAL	2.0
1	B	120	ALA	2.0
1	E	6	ASN	2.0
1	C	157	CYS	2.0
1	H	182	SER	2.0
1	C	177	TYR	2.0
1	H	156	PHE	2.0
1	F	8	LEU	2.0
1	H	186	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CRQ	D	62	24/25	0.85	0.14	14,17,18,19	0
1	CRQ	E	62	24/25	0.86	0.14	14,16,17,18	0
1	CRQ	A	62	24/25	0.86	0.15	18,20,22,23	0
1	CRQ	C	62	24/25	0.87	0.15	12,15,16,17	0
1	CRQ	H	62	24/25	0.87	0.14	15,17,18,19	0
1	CRQ	B	62	24/25	0.88	0.15	11,15,17,18	0
1	CRQ	G	62	24/25	0.90	0.14	11,14,16,17	0
1	CRQ	F	62	24/25	0.91	0.13	12,16,17,18	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.