



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2021 – 02:16 PM JST

PDB ID : 7DIG
Title : Green fluorescent protein from Dendronephthya sp. SSAL-2002
Authors : Nam, K.H.
Deposited on : 2020-11-19
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

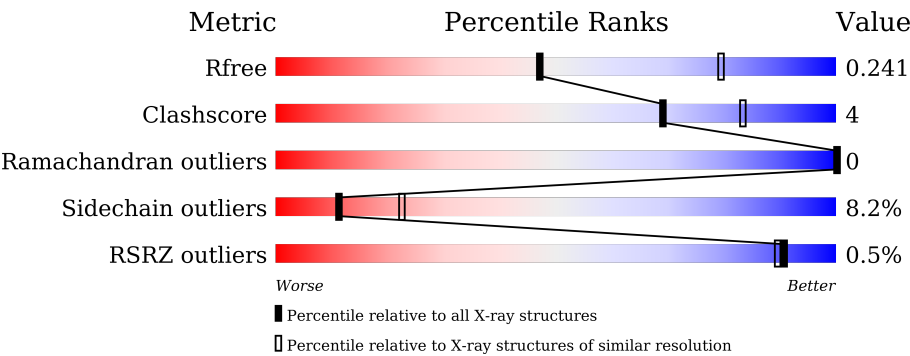
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	223	<div><div></div><div>81%16%..</div></div>
1	B	223	<div><div></div><div>78%18%..</div></div>
1	C	223	<div><div>2%</div><div></div><div>76%20%..</div></div>
1	D	223	<div><div>%</div><div></div><div>82%16%. </div></div>
1	E	223	<div><div></div><div>85%13%. </div></div>
1	F	223	<div><div></div><div>86%12%. </div></div>

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Mol	Chain	Length	Quality of chain
1	G	223	<div><div></div><div>83%</div><div>13%</div><div>..</div></div>
1	H	223	<div><div></div><div>77%</div><div>20%</div><div>..</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14264 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	B	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	C	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	D	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	E	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	F	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	G	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			
1	H	219	Total	C	N	O	S	0	0	0
			1783	1143	299	332	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	CR8	HIS	chromophore	UNP Q8T6U0
A	64	CR8	TYR	chromophore	UNP Q8T6U0
A	64	CR8	GLY	chromophore	UNP Q8T6U0
B	64	CR8	HIS	chromophore	UNP Q8T6U0
B	64	CR8	TYR	chromophore	UNP Q8T6U0
B	64	CR8	GLY	chromophore	UNP Q8T6U0
C	64	CR8	HIS	chromophore	UNP Q8T6U0
C	64	CR8	TYR	chromophore	UNP Q8T6U0
C	64	CR8	GLY	chromophore	UNP Q8T6U0
D	64	CR8	HIS	chromophore	UNP Q8T6U0
D	64	CR8	TYR	chromophore	UNP Q8T6U0
D	64	CR8	GLY	chromophore	UNP Q8T6U0
E	64	CR8	HIS	chromophore	UNP Q8T6U0

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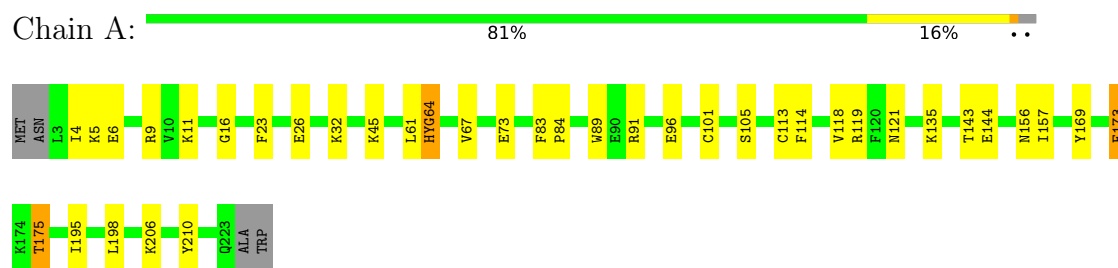
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Chain	Residue	Modelled	Actual	Comment	Reference
E	64	CR8	TYR	chromophore	UNP Q8T6U0
E	64	CR8	GLY	chromophore	UNP Q8T6U0
F	64	CR8	HIS	chromophore	UNP Q8T6U0
F	64	CR8	TYR	chromophore	UNP Q8T6U0
F	64	CR8	GLY	chromophore	UNP Q8T6U0
G	64	CR8	HIS	chromophore	UNP Q8T6U0
G	64	CR8	TYR	chromophore	UNP Q8T6U0
G	64	CR8	GLY	chromophore	UNP Q8T6U0
H	64	CR8	HIS	chromophore	UNP Q8T6U0
H	64	CR8	TYR	chromophore	UNP Q8T6U0
H	64	CR8	GLY	chromophore	UNP Q8T6U0

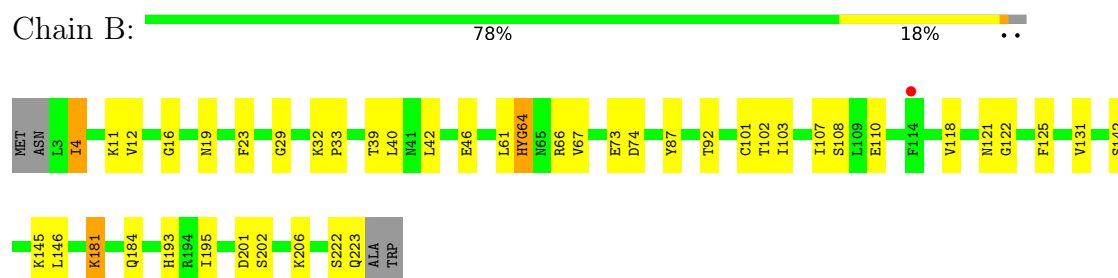
3 Residue-property plots [i](#)

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.

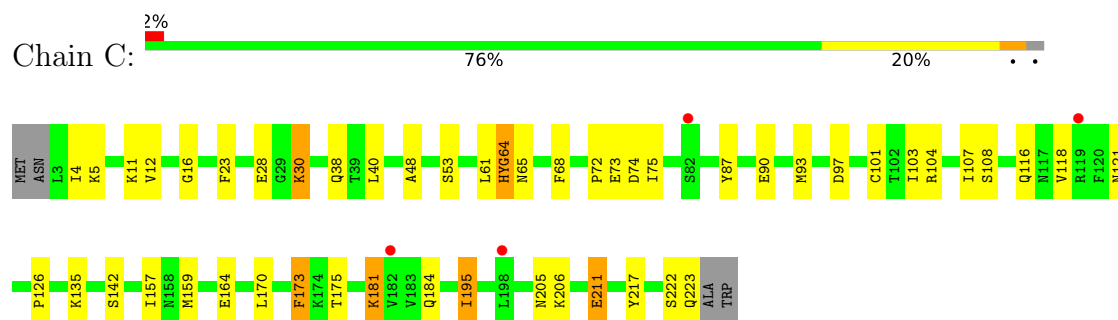
- Molecule 1: Green fluorescent protein



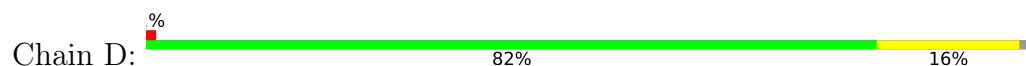
- Molecule 1: Green fluorescent protein

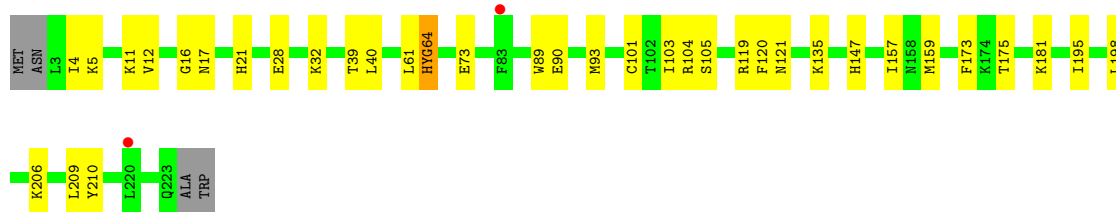


- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein





- Molecule 1: Green fluorescent protein

Chain E: 85% 13% 2%



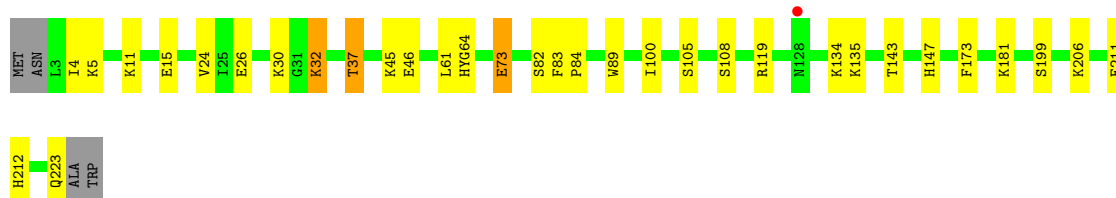
- Molecule 1: Green fluorescent protein

Chain F: 86% 12% 2%



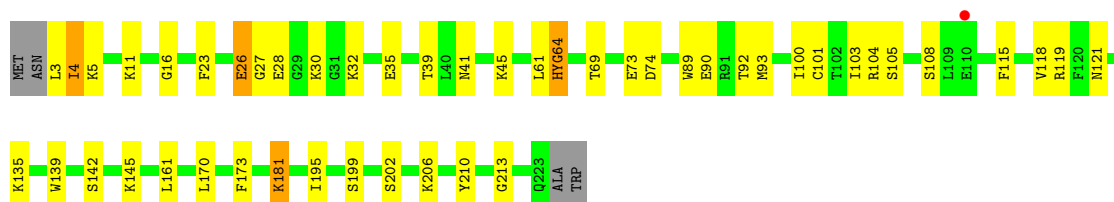
- Molecule 1: Green fluorescent protein

Chain G: 83% 13% 4%



- Molecule 1: Green fluorescent protein

Chain H: 77% 20% 3%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.83Å 124.74Å 129.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.60 48.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.70-2.60) 95.1 (48.65-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.281 0.237 , 0.241	Depositor DCC
R_{free} test set	2782 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 18.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14264	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8614e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CR8

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	0.64	0/1803	0.82	0/2437
1	B	0.63	0/1803	0.81	0/2437
1	C	0.66	0/1803	0.80	0/2437
1	D	0.65	0/1803	0.81	0/2437
1	E	0.64	0/1803	0.81	0/2437
1	F	0.64	0/1803	0.82	0/2437
1	G	0.65	0/1803	0.80	0/2437
1	H	0.64	0/1803	0.79	0/2437
All	All	0.64	0/14424	0.81	0/19496

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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	LEU	Mainchain
1	B	61	LEU	Mainchain
1	C	61	LEU	Mainchain
1	D	61	LEU	Mainchain
1	E	61	LEU	Mainchain
1	F	61	LEU	Mainchain
1	G	61	LEU	Mainchain
1	H	61	LEU	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1783	0	1733	17	0
1	B	1783	0	1733	16	0
1	C	1783	0	1734	23	0
1	D	1783	0	1733	12	0
1	E	1783	0	1732	8	0
1	F	1783	0	1733	7	0
1	G	1783	0	1734	10	0
1	H	1783	0	1733	20	0
All	All	14264	0	13865	105	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 4.

All (105) 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:C:64:CR8:H2	1:C:195:ILE:HB	1.75	0.69
1:A:26:GLU:HG3	1:A:45:LYS:HG3	1.76	0.68
1:E:26:GLU:HG3	1:E:45:LYS:HG3	1.77	0.66
1:G:26:GLU:HG3	1:G:45:LYS:HG3	1.81	0.62
1:B:122:GLY:O	1:C:104:ARG:NH1	2.33	0.62
1:E:101:CYS:HA	1:E:121:ASN:O	1.99	0.61
1:A:16:GLY:HA3	1:A:23:PHE:CZ	2.35	0.61
1:F:16:GLY:HA2	1:F:120:PHE:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:HB2	1:C:74:ASP:OD1	2.05	0.57
1:C:64:CR8:H16	1:C:64:CR8:C	2.35	0.56
1:H:64:CR8:H4	1:H:142:SER:OG	2.07	0.55
1:D:12:VAL:HG21	1:D:40:LEU:HD21	1.89	0.54
1:H:26:GLU:HG3	1:H:45:LYS:HG3	1.89	0.53
1:A:16:GLY:HA3	1:A:23:PHE:CE1	2.42	0.53
1:A:26:GLU:CG	1:A:45:LYS:HG3	2.38	0.53
1:G:15:GLU:HG2	1:G:24:VAL:HG22	1.90	0.53
1:D:89:TRP:CE2	1:D:105:SER:HB3	2.44	0.52
1:G:147:HIS:CE1	1:H:170:LEU:HD11	2.44	0.52
1:C:159:MET:HG3	1:C:173:PHE:CD1	2.44	0.52
1:C:87:TYR:CZ	1:C:107:ILE:HG13	2.45	0.52
1:H:27:GLY:HA2	1:H:41:ASN:O	2.10	0.52
1:F:26:GLU:HG3	1:F:45:LYS:HG3	1.93	0.51
1:B:40:LEU:HD23	1:B:42:LEU:HD21	1.93	0.51
1:E:16:GLY:HA3	1:E:23:PHE:CZ	2.45	0.51
1:C:65:ASN:HB2	1:C:116:GLN:OE1	2.10	0.51
1:C:64:CR8:N22	1:C:211:GLU:HB2	2.26	0.51
1:G:223:GLN:HG3	1:H:210:TYR:CE2	2.46	0.51
1:A:101:CYS:HA	1:A:121:ASN:O	2.12	0.50
1:B:12:VAL:HG21	1:B:40:LEU:HD21	1.93	0.50
1:D:17:ASN:HA	1:D:21:HIS:O	2.11	0.50
1:A:67:VAL:HG11	1:A:114:PHE:CZ	2.47	0.50
1:A:64:CR8:H2	1:A:195:ILE:HB	1.95	0.49
1:A:143:THR:HB	1:B:145:LYS:HZ1	1.77	0.49
1:C:170:LEU:HD11	1:D:147:HIS:CE1	2.48	0.49
1:H:64:CR8:H2	1:H:195:ILE:HB	1.94	0.49
1:B:101:CYS:HA	1:B:121:ASN:O	2.13	0.49
1:C:38:GLN:NE2	1:C:68:PHE:HB2	2.27	0.49
1:B:29:GLY:HA3	1:B:40:LEU:HD12	1.95	0.49
1:E:64:CR8:H2	1:E:195:ILE:HB	1.94	0.48
1:G:143:THR:H	1:H:145:LYS:HE3	1.79	0.48
1:B:19:ASN:HA	1:C:90:GLU:OE2	2.13	0.48
1:C:90:GLU:HG2	1:C:104:ARG:HG3	1.95	0.48
1:D:90:GLU:HG2	1:D:104:ARG:HG2	1.96	0.48
1:A:89:TRP:CE2	1:A:105:SER:HB3	2.49	0.47
1:E:64:CR8:H4	1:E:142:SER:OG	2.14	0.47
1:H:90:GLU:OE2	1:H:104:ARG:NH1	2.47	0.47
1:H:89:TRP:CE2	1:H:105:SER:HB3	2.50	0.47
1:G:83:PHE:HA	1:G:84:PRO:C	2.35	0.47
1:C:64:CR8:H4	1:C:142:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ASP:HB2	1:C:126:PRO:HG2	1.97	0.46
1:C:101:CYS:HA	1:C:121:ASN:O	2.15	0.46
1:E:90:GLU:HG2	1:E:104:ARG:HD2	1.97	0.46
1:H:181:LYS:HB3	1:H:181:LYS:HE2	1.64	0.46
1:C:48:ALA:HB1	1:C:205:ASN:HD21	1.81	0.46
1:B:125:PHE:CE1	1:B:131:VAL:HG21	2.50	0.46
1:A:198:LEU:HD11	1:A:210:TYR:HB2	1.98	0.45
1:F:89:TRP:CE2	1:F:105:SER:HB3	2.52	0.45
1:G:37:THR:HG23	1:G:212:HIS:CD2	2.51	0.45
1:B:4:ILE:HG22	1:B:33:PRO:HG2	1.98	0.45
1:H:93:MET:SD	1:H:173:PHE:CZ	3.09	0.45
1:B:181:LYS:HB3	1:B:181:LYS:HE2	1.61	0.45
1:F:145:LYS:HD3	1:F:190:PHE:CE1	2.51	0.45
1:E:89:TRP:CE2	1:E:105:SER:HB3	2.52	0.45
1:E:170:LEU:HD11	1:F:147:HIS:CE1	2.52	0.45
1:G:89:TRP:CE2	1:G:105:SER:HB3	2.51	0.44
1:B:64:CR8:H2	1:B:195:ILE:HB	1.99	0.44
1:G:73:GLU:H	1:G:73:GLU:HG3	1.55	0.44
1:F:145:LYS:HD3	1:F:190:PHE:HE1	1.82	0.44
1:C:181:LYS:HE2	1:C:181:LYS:HB3	1.57	0.44
1:C:12:VAL:HG21	1:C:40:LEU:HD21	2.00	0.44
1:B:16:GLY:HA3	1:B:23:PHE:CZ	2.53	0.44
1:H:108:SER:OG	1:H:115:PHE:HB3	2.18	0.43
1:C:222:SER:C	1:C:223:GLN:HG2	2.37	0.43
1:D:198:LEU:HD11	1:D:210:TYR:HB2	2.01	0.43
1:H:69:THR:HA	1:H:213:GLY:O	2.19	0.43
1:D:159:MET:HG3	1:D:173:PHE:CD1	2.54	0.43
1:C:93:MET:HE2	1:C:103:ILE:HD11	2.00	0.42
1:H:16:GLY:HA3	1:H:23:PHE:CZ	2.55	0.42
1:A:6:GLU:O	1:A:32:LYS:HA	2.19	0.42
1:A:96:GLU:OE2	1:A:169:TYR:HA	2.20	0.42
1:B:222:SER:C	1:B:223:GLN:HG2	2.38	0.42
1:A:83:PHE:HA	1:A:84:PRO:C	2.41	0.42
1:D:64:CR8:H2	1:D:195:ILE:HB	2.00	0.42
1:A:156:ASN:HA	1:A:173:PHE:O	2.20	0.41
1:D:39:THR:HA	1:D:209:LEU:O	2.19	0.41
1:C:16:GLY:HA3	1:C:23:PHE:CZ	2.55	0.41
1:C:75:ILE:HG12	1:C:217:TYR:CZ	2.55	0.41
1:D:16:GLY:HA2	1:D:120:PHE:O	2.20	0.41
1:H:93:MET:HE2	1:H:103:ILE:HD11	2.03	0.41
1:G:32:LYS:HE2	1:G:32:LYS:HB3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:TYR:CZ	1:B:107:ILE:HG13	2.56	0.41
1:H:26:GLU:HG3	1:H:45:LYS:CG	2.50	0.41
1:H:139:TRP:CZ3	1:H:161:LEU:HG	2.56	0.41
1:F:12:VAL:HG21	1:F:40:LEU:HD21	2.03	0.41
1:A:144:GLU:HG3	1:A:157:ILE:HG12	2.02	0.41
1:B:66:ARG:HA	1:B:66:ARG:CZ	2.51	0.41
1:A:9:ARG:O	1:A:113:CYS:HA	2.21	0.41
1:A:91:ARG:HB2	1:A:175:THR:HG23	2.03	0.41
1:H:32:LYS:HB3	1:H:35:GLU:HG3	2.02	0.40
1:D:93:MET:HE2	1:D:103:ILE:HD11	2.02	0.40
1:H:3:LEU:HG	1:H:4:ILE:N	2.36	0.40
1:H:101:CYS:HA	1:H:121:ASN:O	2.20	0.40
1:C:30:LYS:HB2	1:C:30:LYS:HE3	1.96	0.40
1:B:142:SER:OG	1:B:193:HIS:HB2	2.21	0.40
1:D:101:CYS:HA	1:D:121:ASN:O	2.21	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	216/223 (97%)	208 (96%)	8 (4%)	0	100	100
1	B	216/223 (97%)	210 (97%)	6 (3%)	0	100	100
1	C	216/223 (97%)	214 (99%)	2 (1%)	0	100	100
1	D	216/223 (97%)	210 (97%)	6 (3%)	0	100	100
1	E	216/223 (97%)	213 (99%)	3 (1%)	0	100	100
1	F	216/223 (97%)	214 (99%)	2 (1%)	0	100	100
1	G	216/223 (97%)	209 (97%)	7 (3%)	0	100	100
1	H	216/223 (97%)	213 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1728/1784 (97%)	1691 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	194/197 (98%)	184 (95%)	10 (5%)	23	46
1	B	194/197 (98%)	174 (90%)	20 (10%)	7	13
1	C	194/197 (98%)	175 (90%)	19 (10%)	8	15
1	D	194/197 (98%)	182 (94%)	12 (6%)	18	37
1	E	194/197 (98%)	180 (93%)	14 (7%)	14	29
1	F	194/197 (98%)	178 (92%)	16 (8%)	11	22
1	G	194/197 (98%)	175 (90%)	19 (10%)	8	15
1	H	194/197 (98%)	176 (91%)	18 (9%)	9	17
All	All	1552/1576 (98%)	1424 (92%)	128 (8%)	11	22

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	LYS
1	A	11	LYS
1	A	73	GLU
1	A	118	VAL
1	A	119	ARG
1	A	135	LYS
1	A	173	PHE
1	A	175	THR
1	A	206	LYS
1	B	4	ILE
1	B	11	LYS

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Mol	Chain	Res	Type
1	B	32	LYS
1	B	39	THR
1	B	46	GLU
1	B	67	VAL
1	B	73	GLU
1	B	74	ASP
1	B	92	THR
1	B	102	THR
1	B	103	ILE
1	B	108	SER
1	B	110	GLU
1	B	118	VAL
1	B	146	LEU
1	B	181	LYS
1	B	184	GLN
1	B	201	ASP
1	B	202	SER
1	B	206	LYS
1	C	4	ILE
1	C	5	LYS
1	C	11	LYS
1	C	28	GLU
1	C	30	LYS
1	C	53	SER
1	C	73	GLU
1	C	108	SER
1	C	118	VAL
1	C	135	LYS
1	C	157	ILE
1	C	164	GLU
1	C	173	PHE
1	C	175	THR
1	C	181	LYS
1	C	184	GLN
1	C	195	ILE
1	C	206	LYS
1	C	211	GLU
1	D	4	ILE
1	D	5	LYS
1	D	11	LYS
1	D	28	GLU
1	D	32	LYS

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Mol	Chain	Res	Type
1	D	73	GLU
1	D	119	ARG
1	D	135	LYS
1	D	157	ILE
1	D	175	THR
1	D	181	LYS
1	D	206	LYS
1	E	4	ILE
1	E	5	LYS
1	E	10	VAL
1	E	11	LYS
1	E	28	GLU
1	E	30	LYS
1	E	65	ASN
1	E	107	ILE
1	E	118	VAL
1	E	119	ARG
1	E	135	LYS
1	E	157	ILE
1	E	181	LYS
1	E	206	LYS
1	F	4	ILE
1	F	5	LYS
1	F	11	LYS
1	F	28	GLU
1	F	30	LYS
1	F	67	VAL
1	F	73	GLU
1	F	94	THR
1	F	98	LYS
1	F	107	ILE
1	F	119	ARG
1	F	145	LYS
1	F	157	ILE
1	F	181	LYS
1	F	199	SER
1	F	211	GLU
1	G	4	ILE
1	G	5	LYS
1	G	11	LYS
1	G	30	LYS
1	G	32	LYS

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Mol	Chain	Res	Type
1	G	37	THR
1	G	46	GLU
1	G	73	GLU
1	G	82	SER
1	G	100	ILE
1	G	108	SER
1	G	119	ARG
1	G	134	LYS
1	G	135	LYS
1	G	173	PHE
1	G	181	LYS
1	G	199	SER
1	G	206	LYS
1	G	211	GLU
1	H	4	ILE
1	H	5	LYS
1	H	11	LYS
1	H	26	GLU
1	H	28	GLU
1	H	30	LYS
1	H	39	THR
1	H	73	GLU
1	H	74	ASP
1	H	92	THR
1	H	100	ILE
1	H	118	VAL
1	H	119	ARG
1	H	135	LYS
1	H	181	LYS
1	H	199	SER
1	H	202	SER
1	H	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	116	GLN
1	B	147	HIS
1	C	21	HIS
1	C	128	ASN
1	C	133	GLN
1	C	147	HIS

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Mol	Chain	Res	Type
1	D	147	HIS
1	E	21	HIS
1	E	121	ASN
1	F	21	HIS
1	F	116	GLN
1	F	147	HIS
1	G	21	HIS
1	G	124	ASN
1	G	147	HIS
1	G	212	HIS
1	H	116	GLN
1	H	147	HIS
1	H	212	HIS

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	CR8	G	64	1	20,27,28	2.05	7 (35%)	17,37,39	2.96	8 (47%)
1	CR8	B	64	1	20,27,28	1.92	5 (25%)	17,37,39	2.71	6 (35%)
1	CR8	F	64	1	20,27,28	2.02	5 (25%)	17,37,39	2.72	8 (47%)
1	CR8	E	64	1	20,27,28	2.05	6 (30%)	17,37,39	2.60	4 (23%)
1	CR8	C	64	1	20,27,28	1.86	6 (30%)	17,37,39	2.23	7 (41%)
1	CR8	H	64	1	20,27,28	2.07	6 (30%)	17,37,39	2.42	4 (23%)
1	CR8	D	64	1	20,27,28	1.95	6 (30%)	17,37,39	2.57	9 (52%)
1	CR8	A	64	1	20,27,28	1.95	5 (25%)	17,37,39	2.79	7 (41%)

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	CR8	G	64	1	-	2/8/25/26	0/3/3/3
1	CR8	B	64	1	-	1/8/25/26	0/3/3/3
1	CR8	F	64	1	-	2/8/25/26	0/3/3/3
1	CR8	E	64	1	-	1/8/25/26	0/3/3/3
1	CR8	C	64	1	-	3/8/25/26	0/3/3/3
1	CR8	H	64	1	-	2/8/25/26	0/3/3/3
1	CR8	D	64	1	-	2/8/25/26	0/3/3/3
1	CR8	A	64	1	-	1/8/25/26	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	64	CR8	C14-N15	4.59	1.41	1.34
1	E	64	CR8	C8-C7	4.56	1.47	1.36
1	H	64	CR8	C8-C7	4.55	1.47	1.36
1	F	64	CR8	C8-C7	4.29	1.46	1.36
1	C	64	CR8	C8-C7	4.26	1.46	1.36
1	G	64	CR8	C8-C7	4.23	1.46	1.36
1	B	64	CR8	C14-N15	4.19	1.41	1.34
1	F	64	CR8	C4-C1	-4.15	1.36	1.45
1	A	64	CR8	C8-C7	4.09	1.46	1.36
1	C	64	CR8	C14-N15	4.02	1.40	1.34
1	A	64	CR8	C14-N15	3.98	1.40	1.34
1	B	64	CR8	C8-C7	3.97	1.46	1.36
1	D	64	CR8	C8-C7	3.77	1.45	1.36
1	G	64	CR8	C4-C1	-3.71	1.37	1.45
1	G	64	CR8	C14-N15	3.68	1.40	1.34
1	E	64	CR8	C14-N15	3.67	1.40	1.34
1	G	64	CR8	C12-N13	-3.57	1.30	1.36
1	D	64	CR8	C14-N15	3.54	1.40	1.34
1	E	64	CR8	C4-C1	-3.45	1.38	1.45
1	D	64	CR8	C4-C1	-3.42	1.38	1.45
1	E	64	CR8	C2-C1	-3.39	1.38	1.45
1	D	64	CR8	C12-N13	-3.34	1.31	1.36
1	F	64	CR8	C12-N13	-3.30	1.31	1.36
1	F	64	CR8	C2-C1	-3.13	1.38	1.45
1	A	64	CR8	C12-N13	-3.11	1.31	1.36
1	B	64	CR8	C4-C1	-3.04	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	64	CR8	C14-N15	2.99	1.39	1.34
1	A	64	CR8	C4-C1	-2.99	1.39	1.45
1	C	64	CR8	C2-C1	-2.88	1.39	1.45
1	D	64	CR8	C2-C1	-2.85	1.39	1.45
1	H	64	CR8	C4-C1	-2.77	1.39	1.45
1	H	64	CR8	C2-C1	-2.73	1.39	1.45
1	B	64	CR8	C12-N13	-2.73	1.31	1.36
1	A	64	CR8	C2-C1	-2.67	1.39	1.45
1	B	64	CR8	C2-C1	-2.52	1.40	1.45
1	G	64	CR8	C2-C1	-2.46	1.40	1.45
1	C	64	CR8	C4-C1	-2.41	1.40	1.45
1	C	64	CR8	C12-N13	-2.39	1.32	1.36
1	H	64	CR8	C9-C8	2.34	1.50	1.41
1	E	64	CR8	C12-N13	-2.31	1.32	1.36
1	E	64	CR8	C9-C8	2.30	1.50	1.41
1	C	64	CR8	C9-C8	2.20	1.49	1.41
1	G	64	CR8	C9-C8	2.16	1.49	1.41
1	G	64	CR8	C6-C2	2.14	1.40	1.35
1	H	64	CR8	C12-N13	-2.13	1.32	1.36
1	D	64	CR8	C17-N13	-2.12	1.45	1.49

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	CR8	C-C17-N13	6.91	122.39	111.92
1	E	64	CR8	C-C17-N13	6.52	121.80	111.92
1	B	64	CR8	C-C17-N13	6.00	121.02	111.92
1	G	64	CR8	C-C17-N13	5.69	120.55	111.92
1	H	64	CR8	C-C17-N13	5.65	120.49	111.92
1	F	64	CR8	C17-N13-C12	-5.57	115.24	124.32
1	G	64	CR8	C17-N13-C12	-5.57	115.25	124.32
1	D	64	CR8	C17-N13-C12	-5.34	115.62	124.32
1	B	64	CR8	C17-N13-C12	-5.20	115.83	124.32
1	G	64	CR8	C2-C6-C7	-5.20	117.53	121.95
1	F	64	CR8	O19-C-C17	-5.04	112.00	126.32
1	F	64	CR8	C-C17-N13	4.98	119.47	111.92
1	E	64	CR8	C17-N13-C12	-4.82	116.46	124.32
1	E	64	CR8	O19-C-C17	-4.71	112.93	126.32
1	A	64	CR8	O19-C-C17	-4.66	113.07	126.32
1	C	64	CR8	C-C17-N13	4.65	118.97	111.92
1	A	64	CR8	C2-C6-C7	-4.64	118.00	121.95
1	B	64	CR8	C2-C6-C7	-4.54	118.09	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	64	CR8	C17-N13-C12	-4.51	116.96	124.32
1	G	64	CR8	O19-C-C17	-4.38	113.86	126.32
1	D	64	CR8	C2-C6-C7	-4.33	118.27	121.95
1	B	64	CR8	O19-C-C17	-4.24	114.26	126.32
1	D	64	CR8	O19-C-C17	-4.00	114.95	126.32
1	H	64	CR8	O19-C-C17	-3.95	115.08	126.32
1	F	64	CR8	C2-C6-C7	-3.68	118.83	121.95
1	H	64	CR8	C2-C6-C7	-3.61	118.88	121.95
1	C	64	CR8	C17-N13-C12	-3.53	118.56	124.32
1	C	64	CR8	C2-C6-C7	-3.43	119.03	121.95
1	E	64	CR8	C2-C6-C7	-3.39	119.07	121.95
1	A	64	CR8	C20-C16-C14	-3.37	105.18	110.62
1	G	64	CR8	C20-C16-C14	-3.36	105.19	110.62
1	C	64	CR8	O19-C-C17	-3.31	116.92	126.32
1	D	64	CR8	C-C17-N13	3.07	116.57	111.92
1	A	64	CR8	C17-N13-C12	-2.80	119.76	124.32
1	D	64	CR8	C5-C7-C8	-2.74	114.15	121.90
1	D	64	CR8	C4-C5-C7	-2.71	119.64	121.95
1	C	64	CR8	C4-C5-C7	-2.67	119.68	121.95
1	D	64	CR8	C6-C7-C5	2.60	121.66	116.20
1	C	64	CR8	C20-C16-C14	-2.55	106.51	110.62
1	G	64	CR8	C5-C7-C8	-2.50	114.84	121.90
1	G	64	CR8	C5-C4-C1	-2.46	117.83	121.23
1	F	64	CR8	O3-C1-C4	-2.42	117.66	121.56
1	F	64	CR8	C5-C7-C8	-2.42	115.07	121.90
1	A	64	CR8	C5-C7-C8	-2.38	115.19	121.90
1	B	64	CR8	C6-C7-C5	2.34	121.12	116.20
1	D	64	CR8	C4-C1-C2	2.33	120.73	116.62
1	A	64	CR8	C6-C7-C5	2.29	121.02	116.20
1	F	64	CR8	C20-C16-C14	-2.18	107.10	110.62
1	B	64	CR8	C5-C7-C8	-2.17	115.76	121.90
1	C	64	CR8	C6-C7-C5	2.14	120.70	116.20
1	F	64	CR8	C4-C1-C2	2.05	120.24	116.62
1	G	64	CR8	C4-C1-C2	2.04	120.21	116.62
1	D	64	CR8	O3-C1-C4	-2.03	118.29	121.56

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	CR8	C16-C20-C21-N22
1	B	64	CR8	C16-C20-C21-N22

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Mol	Chain	Res	Type	Atoms
1	C	64	CR8	C14-C16-C20-C21
1	C	64	CR8	N-C16-C20-C21
1	E	64	CR8	C16-C20-C21-N22
1	G	64	CR8	C16-C20-C21-N22
1	C	64	CR8	C16-C20-C21-N22
1	D	64	CR8	C16-C20-C21-N22
1	F	64	CR8	C16-C20-C21-N22
1	H	64	CR8	C16-C20-C21-N22
1	D	64	CR8	C16-C20-C21-C23
1	F	64	CR8	C16-C20-C21-C23
1	G	64	CR8	C16-C20-C21-C23
1	H	64	CR8	C16-C20-C21-C23

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	64	CR8	1	0
1	E	64	CR8	2	0
1	C	64	CR8	4	0
1	H	64	CR8	2	0
1	D	64	CR8	1	0
1	A	64	CR8	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	218/223 (97%)	-0.32	0 100 100	24, 38, 56, 66	2 (0%)
1	B	218/223 (97%)	-0.22	1 (0%) 91 89	25, 43, 63, 80	2 (0%)
1	C	218/223 (97%)	0.05	4 (1%) 68 64	35, 56, 77, 88	2 (0%)
1	D	218/223 (97%)	-0.17	2 (0%) 84 82	28, 42, 63, 74	2 (0%)
1	E	218/223 (97%)	-0.27	0 100 100	22, 39, 59, 79	2 (0%)
1	F	218/223 (97%)	-0.36	0 100 100	22, 34, 51, 63	2 (0%)
1	G	218/223 (97%)	-0.25	1 (0%) 91 89	22, 39, 60, 73	2 (0%)
1	H	218/223 (97%)	-0.31	1 (0%) 91 89	25, 41, 58, 76	2 (0%)
All	All	1744/1784 (97%)	-0.23	9 (0%) 91 89	22, 41, 65, 88	16 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	SER	3.1
1	H	110	GLU	3.0
1	C	198	LEU	2.7
1	G	128	ASN	2.5
1	D	220	LEU	2.5
1	C	182	VAL	2.5
1	B	114	PHE	2.1
1	D	83	PHE	2.1
1	C	119	ARG	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, 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(\AA^2)	Q<0.9
1	CR8	C	64	25/26	0.86	0.15	45,61,68,72	0
1	CR8	B	64	25/26	0.90	0.14	41,52,57,59	0
1	CR8	H	64	25/26	0.92	0.15	39,47,51,57	0
1	CR8	D	64	25/26	0.93	0.14	34,42,49,51	0
1	CR8	F	64	25/26	0.93	0.16	35,38,43,50	0
1	CR8	G	64	25/26	0.93	0.15	30,40,44,49	0
1	CR8	A	64	25/26	0.93	0.14	32,34,38,38	0
1	CR8	E	64	25/26	0.94	0.13	34,40,49,52	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.