



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:06 PM UTC

PDB ID : 7DIG / pdb_00007dig
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 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

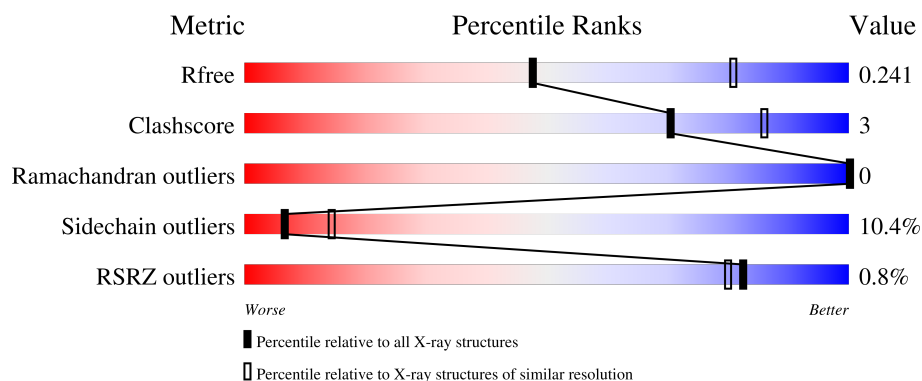
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

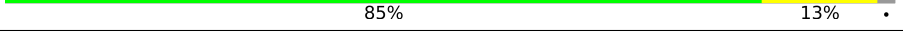
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	 81% 16% . .
1	B	223	 75% 21% . .
1	C	223	 2% 74% 22% . .
1	D	223	 81% 17% .
1	E	223	 85% 13% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	223	 85% 13% .
1	G	223	 81% 16% ..
1	H	223	 78% 17% ..

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

Continued on next page...

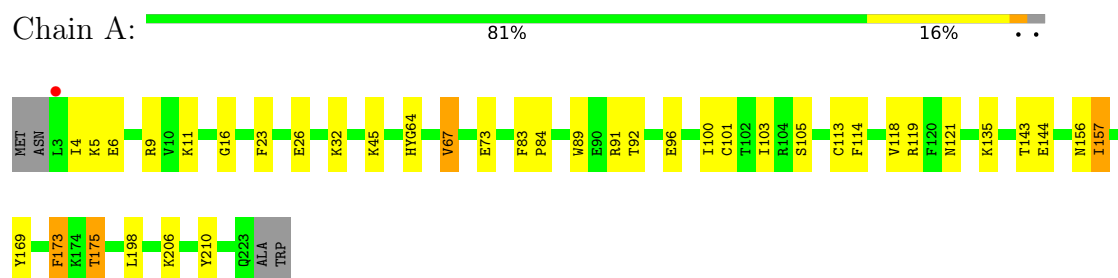
Continued from previous page...

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

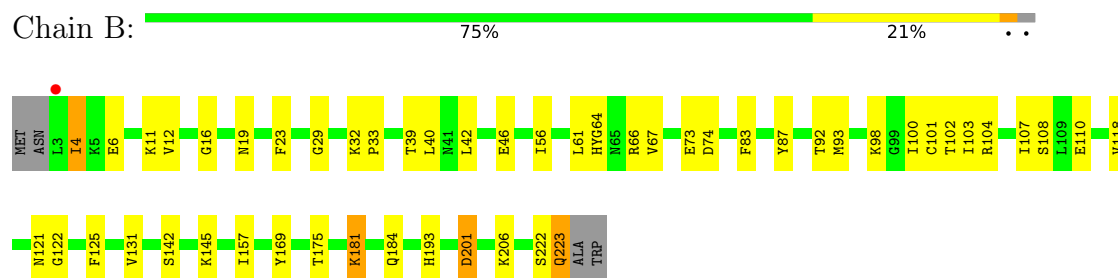
3 Residue-property plots

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.

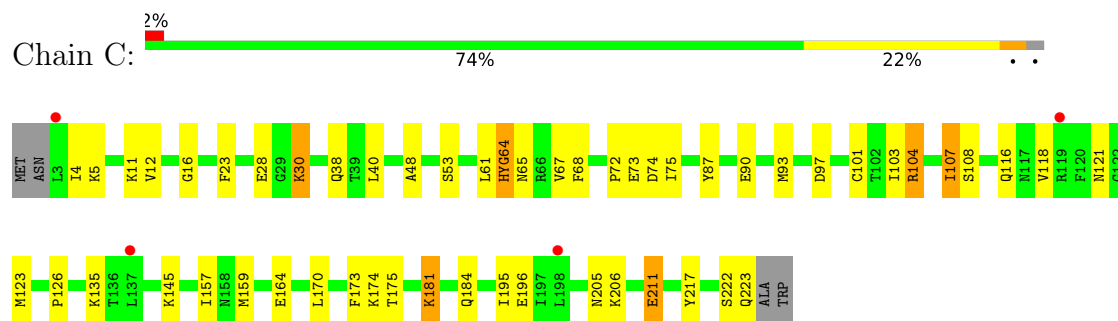
- Molecule 1: Green fluorescent protein



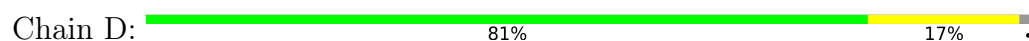
- Molecule 1: Green fluorescent protein

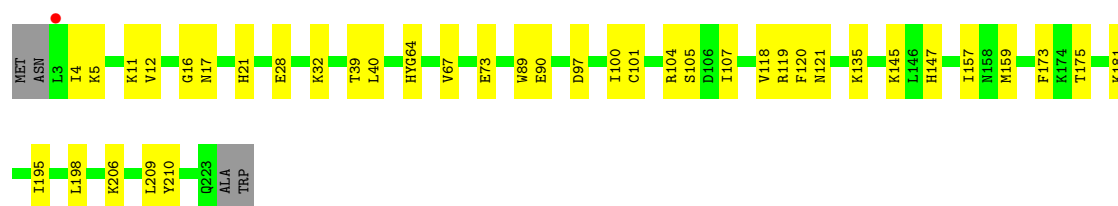


- Molecule 1: Green fluorescent protein

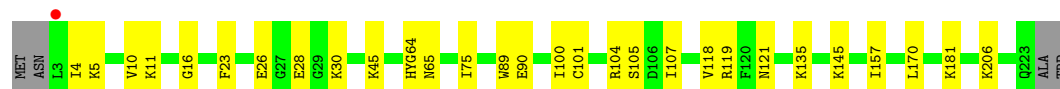
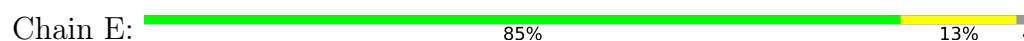


- Molecule 1: Green fluorescent protein

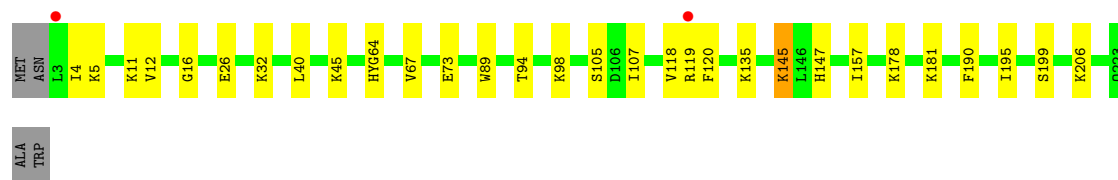
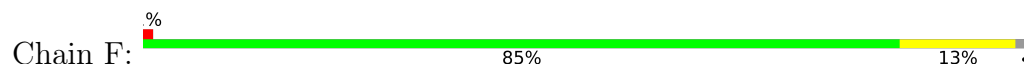




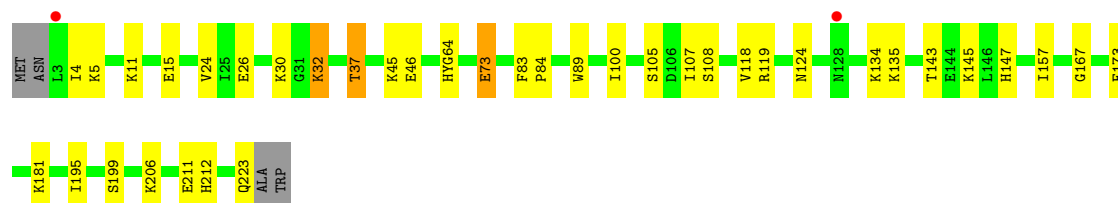
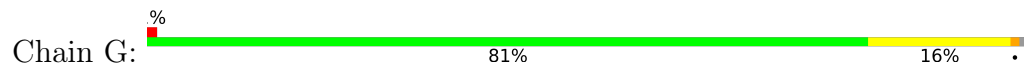
- Molecule 1: Green fluorescent protein



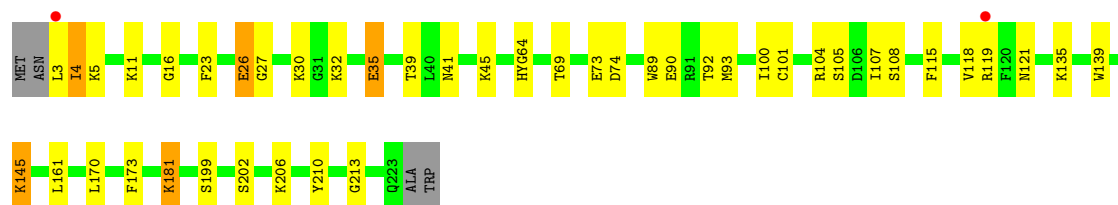
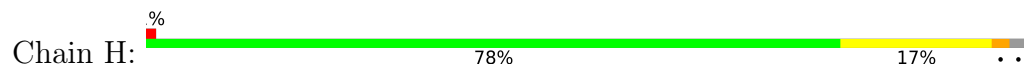
- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein



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 48.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.70-2.60) 95.1 (48.70-2.60)	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 (4.79%)	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 , 11.1	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	0.93	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 [i](#)

5.1 Standard geometry [i](#)

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	0.97	0/1803	1.28	0/2437
1	B	0.96	0/1803	1.25	4/2437 (0.2%)
1	C	1.01	0/1803	1.25	1/2437 (0.0%)
1	D	0.99	0/1803	1.26	1/2437 (0.0%)
1	E	0.99	1/1803 (0.1%)	1.28	0/2437
1	F	0.98	0/1803	1.27	0/2437
1	G	0.99	0/1803	1.27	1/2437 (0.0%)
1	H	0.99	0/1803	1.25	0/2437
All	All	0.99	1/14424 (0.0%)	1.26	7/19496 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	ILE	N-CA	5.19	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LEU	CA-C-O	-5.85	110.86	120.80
1	B	201	ASP	CB-CA-C	5.63	119.83	109.46
1	B	83	PHE	CB-CA-C	5.59	117.50	109.11
1	B	61	LEU	CA-C-O	-5.36	111.69	120.80
1	B	169	TYR	CB-CA-C	5.20	118.47	110.62
1	G	167	GLY	CA-C-O	-5.20	117.79	122.57
1	D	97	ASP	CA-CB-CG	5.17	117.77	112.60

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	1783	0	1723	16	0
1	B	1783	0	1723	16	0
1	C	1783	0	1723	20	0
1	D	1783	0	1723	10	0
1	E	1783	0	1723	6	0
1	F	1783	0	1723	7	0
1	G	1783	0	1723	10	0
1	H	1783	0	1723	17	0
All	All	14264	0	13784	94	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 3.

All (94) 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: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
1:C:72:PRO:HB2	1:C:74:ASP:OD1	2.05	0.57
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:G:83:PHE:HA	1:G:84:PRO:C	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:THR:HB	1:B:145:LYS:HZ1	1.76	0.50
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:C:170:LEU:HD11	1:D:147:HIS:CE1	2.48	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:C:222:SER:C	1:C:223:GLN:HG2	2.37	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: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:A:83:PHE:HA	1:A:84:PRO:C	2.41	0.47
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:B:222:SER:C	1:B:223:GLN:HG2	2.38	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:MET:HE2	1:C:103:ILE:HD11	1.99	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: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: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:G:32:LYS:HE2	1:G:32:LYS:HB3	1.95	0.41
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:B:56:ILE:O	1:B:93:MET:HE1	2.21	0.41
1:H:32:LYS:HB3	1:H:35:GLU:HG3	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	214/223 (96%)	207 (97%)	7 (3%)	0	100	100
1	B	214/223 (96%)	208 (97%)	6 (3%)	0	100	100
1	C	214/223 (96%)	212 (99%)	2 (1%)	0	100	100
1	D	214/223 (96%)	208 (97%)	6 (3%)	0	100	100
1	E	214/223 (96%)	211 (99%)	3 (1%)	0	100	100
1	F	214/223 (96%)	212 (99%)	2 (1%)	0	100	100
1	G	214/223 (96%)	207 (97%)	7 (3%)	0	100	100
1	H	214/223 (96%)	211 (99%)	3 (1%)	0	100	100
All	All	1712/1784 (96%)	1676 (98%)	36 (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%)	179 (92%)	15 (8%)	12	27
1	B	194/197 (98%)	169 (87%)	25 (13%)	4	8
1	C	194/197 (98%)	169 (87%)	25 (13%)	4	8
1	D	194/197 (98%)	176 (91%)	18 (9%)	8	18
1	E	194/197 (98%)	178 (92%)	16 (8%)	10	24
1	F	194/197 (98%)	175 (90%)	19 (10%)	7	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	194/197 (98%)	170 (88%)	24 (12%)	4	9
1	H	194/197 (98%)	174 (90%)	20 (10%)	7	15
All	All	1552/1576 (98%)	1390 (90%)	162 (10%)	7	14

All (162) 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	67	VAL
1	A	73	GLU
1	A	92	THR
1	A	100	ILE
1	A	103	ILE
1	A	118	VAL
1	A	119	ARG
1	A	135	LYS
1	A	157	ILE
1	A	173	PHE
1	A	175	THR
1	A	206	LYS
1	B	4	ILE
1	B	6	GLU
1	B	11	LYS
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	98	LYS
1	B	100	ILE
1	B	102	THR
1	B	103	ILE
1	B	104	ARG
1	B	108	SER
1	B	110	GLU
1	B	118	VAL
1	B	157	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	175	THR
1	B	181	LYS
1	B	184	GLN
1	B	201	ASP
1	B	206	LYS
1	B	223	GLN
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	67	VAL
1	C	73	GLU
1	C	104	ARG
1	C	107	ILE
1	C	108	SER
1	C	118	VAL
1	C	123	MET
1	C	135	LYS
1	C	145	LYS
1	C	157	ILE
1	C	164	GLU
1	C	174	LYS
1	C	175	THR
1	C	181	LYS
1	C	184	GLN
1	C	195	ILE
1	C	196	GLU
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
1	D	67	VAL
1	D	73	GLU
1	D	100	ILE
1	D	107	ILE
1	D	118	VAL
1	D	119	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	135	LYS
1	D	145	LYS
1	D	157	ILE
1	D	175	THR
1	D	181	LYS
1	D	195	ILE
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	100	ILE
1	E	107	ILE
1	E	118	VAL
1	E	119	ARG
1	E	135	LYS
1	E	145	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	32	LYS
1	F	67	VAL
1	F	73	GLU
1	F	94	THR
1	F	98	LYS
1	F	107	ILE
1	F	118	VAL
1	F	119	ARG
1	F	135	LYS
1	F	145	LYS
1	F	157	ILE
1	F	178	LYS
1	F	181	LYS
1	F	195	ILE
1	F	199	SER
1	F	206	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	4	ILE
1	G	5	LYS
1	G	11	LYS
1	G	30	LYS
1	G	32	LYS
1	G	37	THR
1	G	46	GLU
1	G	73	GLU
1	G	100	ILE
1	G	107	ILE
1	G	108	SER
1	G	118	VAL
1	G	119	ARG
1	G	124	ASN
1	G	134	LYS
1	G	135	LYS
1	G	145	LYS
1	G	157	ILE
1	G	173	PHE
1	G	181	LYS
1	G	195	ILE
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	30	LYS
1	H	35	GLU
1	H	39	THR
1	H	73	GLU
1	H	74	ASP
1	H	92	THR
1	H	100	ILE
1	H	107	ILE
1	H	118	VAL
1	H	119	ARG
1	H	135	LYS
1	H	145	LYS
1	H	181	LYS
1	H	199	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	202	SER
1	H	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	116	GLN
1	A	133	GLN
1	A	205	ASN
1	B	116	GLN
1	B	133	GLN
1	B	147	HIS
1	B	212	HIS
1	C	21	HIS
1	C	128	ASN
1	C	147	HIS
1	D	13	HIS
1	D	38	GLN
1	D	117	ASN
1	D	147	HIS
1	E	21	HIS
1	E	41	ASN
1	E	121	ASN
1	E	128	ASN
1	E	133	GLN
1	F	13	HIS
1	F	21	HIS
1	F	147	HIS
1	G	21	HIS
1	G	124	ASN
1	G	147	HIS
1	G	212	HIS
1	H	41	ASN
1	H	116	GLN
1	H	133	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	D	64	1	25,27,28	1.86	5 (20%)	24,37,39	1.89	10 (41%)
1	CR8	G	64	1	25,27,28	1.97	7 (28%)	24,37,39	1.91	7 (29%)
1	CR8	E	64	1	25,27,28	2.02	6 (24%)	24,37,39	1.93	6 (25%)
1	CR8	C	64	1	25,27,28	1.97	7 (28%)	24,37,39	1.76	6 (25%)
1	CR8	H	64	1	25,27,28	2.09	6 (24%)	24,37,39	2.03	9 (37%)
1	CR8	A	64	1	25,27,28	1.97	8 (32%)	24,37,39	2.00	7 (29%)
1	CR8	B	64	1	25,27,28	1.94	5 (20%)	24,37,39	1.89	5 (20%)
1	CR8	F	64	1	25,27,28	1.91	6 (24%)	24,37,39	1.73	5 (20%)

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	D	64	1	-	4/12/25/26	0/3/3/3
1	CR8	G	64	1	-	4/12/25/26	0/3/3/3
1	CR8	E	64	1	-	4/12/25/26	0/3/3/3
1	CR8	C	64	1	-	4/12/25/26	0/3/3/3
1	CR8	H	64	1	-	4/12/25/26	0/3/3/3
1	CR8	A	64	1	-	4/12/25/26	0/3/3/3
1	CR8	B	64	1	-	3/12/25/26	0/3/3/3
1	CR8	F	64	1	-	4/12/25/26	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	64	CR8	C1-N2	6.45	1.41	1.32
1	B	64	CR8	C1-N2	6.05	1.41	1.32
1	C	64	CR8	C1-N2	5.88	1.40	1.32
1	A	64	CR8	C1-N2	5.84	1.40	1.32
1	G	64	CR8	C1-N2	5.53	1.40	1.32
1	E	64	CR8	C1-N2	5.52	1.40	1.32
1	D	64	CR8	C1-N2	5.39	1.40	1.32
1	F	64	CR8	C1-N2	4.84	1.39	1.32
1	H	64	CR8	C8-CA2	4.14	1.50	1.40
1	E	64	CR8	C8-CA2	4.08	1.50	1.40
1	C	64	CR8	C8-CA2	3.91	1.49	1.40
1	G	64	CR8	C8-CA2	3.84	1.49	1.40
1	F	64	CR8	C4-C11	-3.83	1.36	1.46
1	F	64	CR8	C8-CA2	3.47	1.48	1.40
1	G	64	CR8	C4-C11	-3.43	1.37	1.46
1	B	64	CR8	C8-CA2	3.39	1.48	1.40
1	E	64	CR8	C8-C7	3.36	1.47	1.39
1	H	64	CR8	C8-C7	3.35	1.47	1.39
1	D	64	CR8	C8-CA2	3.19	1.48	1.40
1	E	64	CR8	C4-C11	-3.18	1.38	1.46
1	D	64	CR8	C4-C11	-3.16	1.38	1.46
1	E	64	CR8	C12-C11	-3.13	1.38	1.46
1	F	64	CR8	C8-C7	3.10	1.46	1.39
1	C	64	CR8	C8-C7	3.07	1.46	1.39
1	G	64	CR8	C8-C7	3.04	1.46	1.39
1	A	64	CR8	C8-CA2	3.03	1.47	1.40
1	A	64	CR8	C8-C7	2.91	1.46	1.39
1	F	64	CR8	C12-C11	-2.89	1.38	1.46
1	H	64	CR8	C20-C21	2.83	1.53	1.49
1	B	64	CR8	C4-C11	-2.81	1.39	1.46
1	B	64	CR8	C8-C7	2.79	1.46	1.39
1	A	64	CR8	C4-C11	-2.76	1.39	1.46
1	C	64	CR8	C12-C11	-2.66	1.39	1.46
1	D	64	CR8	C12-C11	-2.63	1.39	1.46
1	D	64	CR8	C8-C7	2.60	1.45	1.39
1	H	64	CR8	C4-C11	-2.56	1.39	1.46
1	H	64	CR8	C12-C11	-2.53	1.39	1.46
1	E	64	CR8	C20-C21	2.51	1.53	1.49
1	A	64	CR8	C12-C11	-2.47	1.39	1.46
1	A	64	CR8	C20-C21	2.34	1.53	1.49
1	B	64	CR8	C12-C11	-2.33	1.40	1.46
1	C	64	CR8	C20-C21	2.30	1.53	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	64	CR8	C12-C11	-2.28	1.40	1.46
1	A	64	CR8	C23-C21	2.25	1.40	1.35
1	C	64	CR8	C4-C11	-2.22	1.40	1.46
1	F	64	CR8	C20-C21	2.10	1.52	1.49
1	G	64	CR8	C21-N22	-2.08	1.34	1.37
1	G	64	CR8	C6-C12	2.05	1.40	1.35
1	C	64	CR8	C21-N22	-2.04	1.34	1.37
1	A	64	CR8	C21-N22	-2.01	1.34	1.37

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	64	CR8	C12-C6-C7	-4.83	117.53	122.10
1	A	64	CR8	C3-CA3-N3	4.38	122.39	112.43
1	A	64	CR8	C12-C6-C7	-4.33	118.00	122.10
1	B	64	CR8	C12-C6-C7	-4.24	118.09	122.10
1	E	64	CR8	C3-CA3-N3	4.12	121.80	112.43
1	D	64	CR8	C12-C6-C7	-4.05	118.27	122.10
1	C	64	CR8	C8-CA2-C2	-3.78	121.62	129.19
1	B	64	CR8	C3-CA3-N3	3.77	121.02	112.43
1	A	64	CR8	C8-CA2-C2	-3.75	121.68	129.19
1	H	64	CR8	CA2-N2-C1	3.70	108.69	105.80
1	G	64	CR8	C3-CA3-N3	3.57	120.55	112.43
1	H	64	CR8	C3-CA3-N3	3.54	120.49	112.43
1	B	64	CR8	C8-CA2-C2	-3.53	122.12	129.19
1	E	64	CR8	CA2-N2-C1	3.48	108.52	105.80
1	F	64	CR8	C12-C6-C7	-3.46	118.83	122.10
1	H	64	CR8	N3-C1-N2	-3.42	108.79	111.48
1	H	64	CR8	C12-C6-C7	-3.40	118.88	122.10
1	C	64	CR8	C12-C6-C7	-3.24	119.03	122.10
1	E	64	CR8	C12-C6-C7	-3.21	119.07	122.10
1	E	64	CR8	N3-C1-N2	-3.19	108.97	111.48
1	G	64	CR8	C8-CA2-C2	-3.15	122.87	129.19
1	D	64	CR8	C8-CA2-C2	-3.14	122.89	129.19
1	F	64	CR8	C3-CA3-N3	3.09	119.47	112.43
1	F	64	CR8	O3-C3-CA3	-2.99	112.00	125.47
1	H	64	CR8	C8-CA2-C2	-2.98	123.21	129.19
1	C	64	CR8	C3-CA3-N3	2.88	118.97	112.43
1	E	64	CR8	O3-C3-CA3	-2.79	112.93	125.47
1	A	64	CR8	O3-C3-CA3	-2.76	113.07	125.47
1	A	64	CR8	CA1-C20-C21	2.74	117.79	113.23
1	E	64	CR8	C8-CA2-C2	-2.72	123.75	129.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	CR8	N3-C1-N2	-2.70	109.35	111.48
1	D	64	CR8	C6-C7-C5	2.69	121.66	115.81
1	F	64	CR8	C8-CA2-C2	-2.68	123.82	129.19
1	D	64	CR8	C4-C5-C7	-2.60	119.64	122.10
1	G	64	CR8	O3-C3-CA3	-2.58	113.86	125.47
1	C	64	CR8	C4-C5-C7	-2.56	119.68	122.10
1	C	64	CR8	CA1-C20-C21	2.52	117.41	113.23
1	G	64	CR8	C5-C4-C11	-2.51	117.83	121.25
1	B	64	CR8	O3-C3-CA3	-2.49	114.26	125.47
1	B	64	CR8	C6-C7-C5	2.44	121.12	115.81
1	F	64	CR8	O13-C11-C4	-2.42	117.66	121.56
1	A	64	CR8	C6-C7-C5	2.39	121.02	115.81
1	D	64	CR8	O3-C3-CA3	-2.34	114.95	125.47
1	H	64	CR8	O3-C3-CA3	-2.31	115.08	125.47
1	H	64	CR8	CA1-C20-C21	2.25	116.97	113.23
1	A	64	CR8	C23-C21-N22	2.25	108.31	105.65
1	C	64	CR8	C6-C7-C5	2.24	120.70	115.81
1	H	64	CR8	C10-N22-C21	2.21	110.78	107.91
1	H	64	CR8	N22-C10-N11	-2.20	106.92	111.00
1	G	64	CR8	CA1-C20-C21	2.19	116.86	113.23
1	D	64	CR8	C4-C11-C12	2.19	120.73	116.67
1	D	64	CR8	CA1-C1-N3	2.11	127.59	124.84
1	D	64	CR8	O13-C11-C4	-2.03	118.29	121.56
1	D	64	CR8	CA2-N2-C1	2.01	107.37	105.80
1	G	64	CR8	C6-C7-C5	2.00	120.17	115.81

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	CR8	C3-CA3-N3-C2
1	A	64	CR8	C3-CA3-N3-C1
1	B	64	CR8	C3-CA3-N3-C2
1	B	64	CR8	C3-CA3-N3-C1
1	C	64	CR8	C3-CA3-N3-C2
1	C	64	CR8	C3-CA3-N3-C1
1	C	64	CR8	C21-C20-CA1-N1
1	D	64	CR8	C3-CA3-N3-C2
1	D	64	CR8	C3-CA3-N3-C1
1	E	64	CR8	C3-CA3-N3-C2
1	E	64	CR8	C3-CA3-N3-C1
1	F	64	CR8	C3-CA3-N3-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	F	64	CR8	C3-CA3-N3-C1
1	G	64	CR8	C3-CA3-N3-C2
1	G	64	CR8	C3-CA3-N3-C1
1	H	64	CR8	C3-CA3-N3-C2
1	H	64	CR8	C3-CA3-N3-C1
1	E	64	CR8	CA1-C20-C21-N22
1	E	64	CR8	CA1-C20-C21-C23
1	C	64	CR8	C21-C20-CA1-C1
1	H	64	CR8	CA1-C20-C21-N22
1	H	64	CR8	CA1-C20-C21-C23
1	F	64	CR8	CA1-C20-C21-C23
1	F	64	CR8	CA1-C20-C21-N22
1	D	64	CR8	CA1-C20-C21-N22
1	G	64	CR8	CA1-C20-C21-N22
1	D	64	CR8	CA1-C20-C21-C23
1	A	64	CR8	CA1-C20-C21-N22
1	A	64	CR8	CA1-C20-C21-C23
1	B	64	CR8	CA1-C20-C21-C23
1	G	64	CR8	CA1-C20-C21-C23

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	64	CR8	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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	218/223 (97%)	-0.19	1 (0%) 87 85	24, 38, 56, 66	2 (0%)
1	B	218/223 (97%)	-0.08	1 (0%) 87 85	25, 43, 63, 80	2 (0%)
1	C	218/223 (97%)	0.29	4 (1%) 67 63	35, 56, 77, 88	2 (0%)
1	D	218/223 (97%)	0.00	1 (0%) 87 85	23, 42, 63, 74	2 (0%)
1	E	218/223 (97%)	-0.17	1 (0%) 87 85	22, 39, 59, 79	2 (0%)
1	F	218/223 (97%)	-0.28	2 (0%) 81 78	21, 33, 51, 63	2 (0%)
1	G	218/223 (97%)	-0.15	2 (0%) 81 78	22, 39, 60, 73	2 (0%)
1	H	218/223 (97%)	-0.20	2 (0%) 81 78	25, 40, 58, 76	2 (0%)
All	All	1744/1784 (97%)	-0.10	14 (0%) 82 80	21, 41, 65, 88	16 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	4.4
1	G	3	LEU	3.6
1	E	3	LEU	3.1
1	C	3	LEU	2.7
1	A	3	LEU	2.6
1	C	119	ARG	2.6
1	F	119	ARG	2.4
1	H	3	LEU	2.4
1	F	3	LEU	2.3
1	D	3	LEU	2.1
1	C	198	LEU	2.1
1	G	128	ASN	2.0
1	H	119	ARG	2.0
1	C	137	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, 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	CR8	C	64	25/26	0.84	0.11	45,61,68,72	0
1	CR8	B	64	25/26	0.88	0.10	41,52,57,59	0
1	CR8	H	64	25/26	0.89	0.10	39,47,51,57	0
1	CR8	G	64	25/26	0.91	0.09	30,40,44,49	0
1	CR8	F	64	25/26	0.92	0.09	35,38,43,50	0
1	CR8	D	64	25/26	0.92	0.08	34,42,49,51	0
1	CR8	E	64	25/26	0.92	0.08	34,40,49,52	0
1	CR8	A	64	25/26	0.94	0.07	32,34,38,38	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.