



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:52 AM GMT

PDB ID : 3CFF
Title : Photoswitchable red fluorescent protein psRFP, on-state
Authors : Kachalova, G.S.; Gundel, S.; Bartunik, H.D.; Wiedenmann, J.
Deposited on : 2008-03-03
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

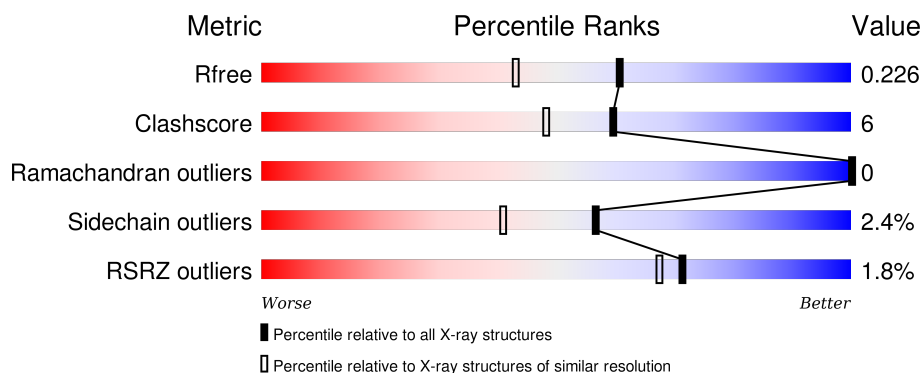
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	L	62	<div> <div>5%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	M	62	<div> <div>3%</div> <div>81%</div> <div>11%</div> <div>6%</div> </div>
1	R	62	<div> <div>3%</div> <div>79%</div> <div>11%</div> <div>6%</div> </div>
1	S	62	<div> <div>2%</div> <div>79%</div> <div>13%</div> <div>6%</div> </div>
2	A	167	<div> <div>0%</div> <div>92%</div> <div>7%</div> <div>0%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	167	<div><div><div>%</div><div><div></div></div><div>89%</div><div>11%</div><div>.</div></div></div>
2	G	167	<div><div><div>%</div><div><div></div></div><div>91%</div><div>9%</div><div></div></div></div>
2	H	167	<div><div><div>2%</div><div><div></div></div><div>95%</div><div></div><div>..</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8441 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 GFP-like photoswitchable fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	58	Total	C	N	O	S	0	9	0
			504	318	82	95	9			
1	M	58	Total	C	N	O	S	0	8	0
			501	314	82	98	7			
1	R	58	Total	C	N	O	S	0	9	0
			497	316	81	91	9			
1	S	58	Total	C	N	O	S	0	5	0
			477	301	77	91	8			

- Molecule 2 is a protein called GFP-like photoswitchable fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	167	Total	C	N	O	S	0	7	0
			1378	878	232	253	15			
2	B	167	Total	C	N	O	S	0	9	0
			1392	889	234	254	15			
2	G	167	Total	C	N	O	S	0	9	0
			1389	886	232	256	15			
2	H	167	Total	C	N	O	S	0	7	0
			1386	882	233	256	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	SER	ENGINEERED	PDB 3CFF
B	143	GLY	SER	ENGINEERED	PDB 3CFF
G	143	GLY	SER	ENGINEERED	PDB 3CFF
H	143	GLY	SER	ENGINEERED	PDB 3CFF

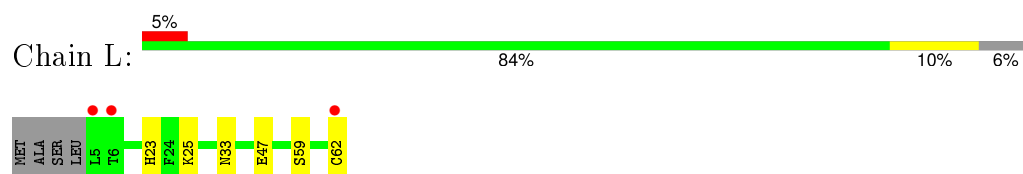
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	57	Total 57	O 57	0	0
3	A	186	Total 186	O 186	0	0
3	M	41	Total 41	O 41	0	0
3	B	161	Total 161	O 161	0	0
3	R	68	Total 68	O 68	0	0
3	G	193	Total 193	O 193	0	0
3	S	38	Total 38	O 38	0	0
3	H	173	Total 173	O 173	0	1

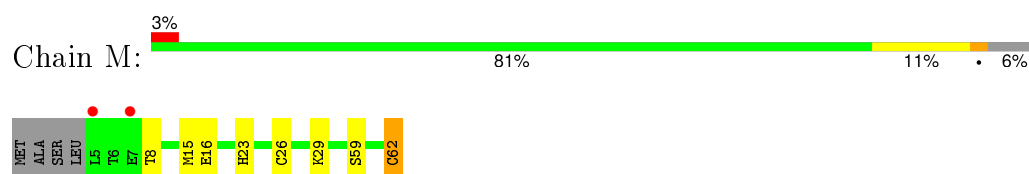
3 Residue-property plots [i](#)

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

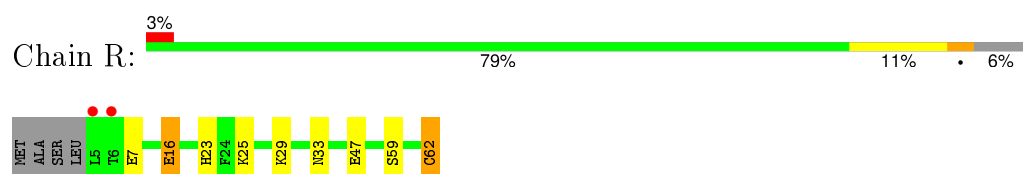
- Molecule 1: GFP-like photoswitchable fluorescent protein



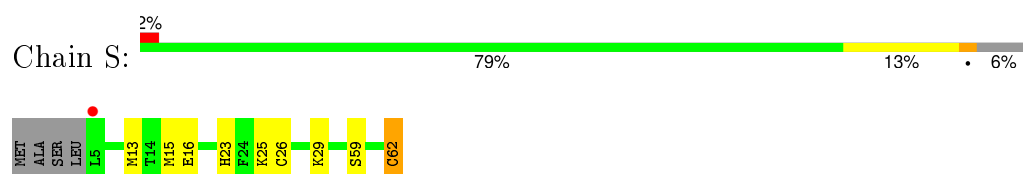
- Molecule 1: GFP-like photoswitchable fluorescent protein



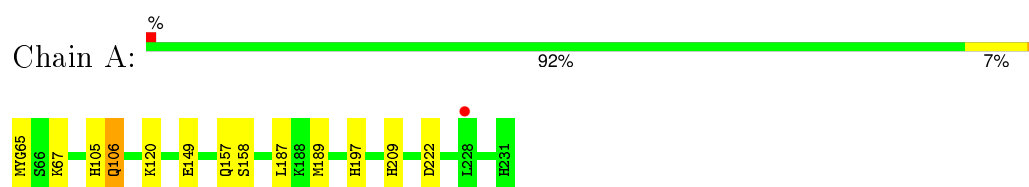
- Molecule 1: GFP-like photoswitchable fluorescent protein




- Molecule 1: GFP-like photoswitchable fluorescent protein

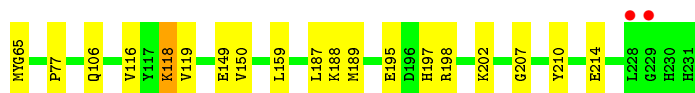


- Molecule 2: GFP-like photoswitchable fluorescent protein

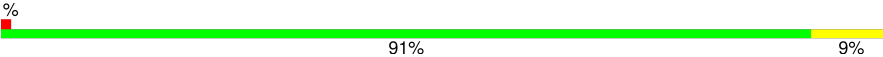


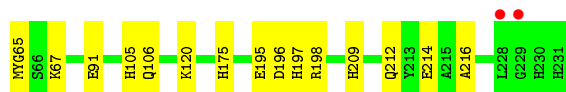
- Molecule 2: GFP-like photoswitchable fluorescent protein

Chain B:  89% 11%



- Molecule 2: GFP-like photoswitchable fluorescent protein

Chain G:  91% 9%



- Molecule 2: GFP-like photoswitchable fluorescent protein

Chain H:  95% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.42Å 98.36Å 242.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.27 – 1.80 19.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (12.27-1.80) 96.9 (19.90-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.224 0.197 , 0.226	Depositor DCC
R_{free} test set	5260 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.476 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105607 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8441	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	L	0.41	0/534	0.53	0/716
1	M	0.52	1/525 (0.2%)	0.57	0/704
1	R	0.44	1/534 (0.2%)	0.55	0/715
1	S	0.55	1/498 (0.2%)	0.54	0/667
2	A	0.37	0/1388	0.55	0/1867
2	B	0.35	0/1409	0.53	0/1896
2	G	0.37	0/1402	0.53	0/1888
2	H	0.34	0/1392	0.53	0/1871
All	All	0.40	3/7682 (0.0%)	0.54	0/10324

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	62	CYS	C-OXT	9.23	1.40	1.23
1	M	62	CYS	C-OXT	8.30	1.39	1.23
1	R	62	CYS	C-OXT	6.08	1.34	1.23

There are no bond angle outliers.

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	L	504	0	491	5	0
1	M	501	0	477	7	0
1	R	497	0	495	8	0
1	S	477	0	457	17	0
2	A	1378	0	1337	14	0
2	B	1392	0	1354	17	0
2	G	1389	0	1347	16	0
2	H	1386	0	1337	10	0
3	A	186	0	0	6	0
3	B	161	0	0	1	0
3	G	193	0	0	6	0
3	H	173	0	0	0	0
3	L	57	0	0	4	0
3	M	41	0	0	1	0
3	R	68	0	0	3	0
3	S	38	0	0	0	0
All	All	8441	0	7295	84	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 6.

All (84) 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:S:13[B]:MET:CE	1:S:15[B]:MET:HB2	1.59	1.31
1:S:13[B]:MET:HE2	1:S:15[B]:MET:HB2	1.24	1.14
2:H:168:ARG:HH11	2:H:168:ARG:HG3	1.07	1.09
2:G:195[A]:GLU:OE2	3:G:360:HOH:O	1.83	0.97
1:S:13[B]:MET:CE	1:S:15[B]:MET:CB	2.42	0.95
2:A:197:HIS:HE1	3:A:416:HOH:O	1.51	0.94
1:S:16[B]:GLU:OE1	1:S:23[B]:HIS:CE1	2.25	0.90
1:M:16[B]:GLU:OE2	1:M:23[B]:HIS:CE1	2.27	0.87
2:H:168:ARG:NH1	2:H:168:ARG:HG3	1.86	0.86
1:M:16[B]:GLU:OE2	1:M:23[B]:HIS:HE1	1.63	0.82
1:S:16[B]:GLU:OE2	1:S:23[B]:HIS:HE1	1.63	0.82
2:H:168:ARG:HH11	2:H:168:ARG:CG	1.93	0.80
1:R:62:CYS:O	2:G:65:NRQ:N1	2.14	0.80
2:B:149:GLU:HB2	2:B:189[A]:MET:HE2	1.63	0.79
2:A:149:GLU:HB2	2:A:189[A]:MET:HE2	1.65	0.78
1:S:13[B]:MET:HE1	1:S:15[B]:MET:HB2	1.66	0.77
1:L:62:CYS:O	2:A:65:NRQ:N1	2.17	0.77
2:B:149:GLU:HB2	2:B:189[A]:MET:CE	2.16	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:13[B]:MET:HE1	1:S:15[B]:MET:CB	2.17	0.74
1:M:62:CYS:O	2:B:65:NRQ:N1	2.21	0.73
1:S:62:CYS:O	2:H:65:NRQ:N1	2.21	0.72
2:A:149:GLU:HB2	2:A:189[A]:MET:CE	2.20	0.71
2:A:105:HIS:HB2	3:A:398:HOH:O	1.92	0.70
2:B:195[A]:GLU:OE1	3:B:380:HOH:O	2.09	0.69
1:S:16[B]:GLU:CD	1:S:23[B]:HIS:HE1	1.95	0.69
1:L:33[B]:ASN:OD1	3:L:102:HOH:O	2.12	0.67
1:R:33[B]:ASN:OD1	3:R:107:HOH:O	2.13	0.67
1:S:16[B]:GLU:CD	1:S:23[B]:HIS:CE1	2.72	0.61
1:L:25:LYS:HB2	1:L:47:GLU:HB2	1.82	0.61
1:R:23[B]:HIS:CD2	3:R:113:HOH:O	2.54	0.60
3:L:89:HOH:O	2:G:120:LYS:HE3	2.01	0.60
1:R:25[B]:LYS:HB2	1:R:47:GLU:HB2	1.84	0.60
1:M:59:SER:O	2:B:65:NRQ:HB11	2.04	0.58
2:A:65:NRQ:N1	2:A:65:NRQ:HA31	2.20	0.57
2:G:65:NRQ:HA31	2:G:65:NRQ:N1	2.21	0.56
1:S:15[A]:MET:HB3	1:S:26:CYS:HB2	1.88	0.55
2:G:67:LYS:HD2	3:G:315:HOH:O	2.05	0.55
1:R:25[A]:LYS:HB2	1:R:47:GLU:HB2	1.89	0.55
1:L:59:SER:O	2:A:65:NRQ:HB11	2.08	0.54
2:G:197:HIS:HE1	3:G:315:HOH:O	1.89	0.54
2:A:67:LYS:HD2	3:A:416:HOH:O	2.08	0.54
2:A:65:NRQ:N1	2:A:65:NRQ:CA3	2.71	0.53
2:G:65:NRQ:N1	2:G:65:NRQ:CA3	2.72	0.53
1:R:59:SER:O	2:G:65:NRQ:HB11	2.09	0.53
2:B:65:NRQ:N1	2:B:65:NRQ:HA31	2.25	0.52
2:B:197[A]:HIS:HD2	2:B:214:GLU:OE2	1.92	0.51
3:A:406:HOH:O	2:G:175:HIS:HD2	1.93	0.51
1:S:13[B]:MET:HE1	1:S:15[B]:MET:HB3	1.92	0.50
1:M:8[A]:THR:HG22	3:M:98:HOH:O	2.10	0.50
2:H:65:NRQ:N1	2:H:65:NRQ:HA31	2.27	0.49
1:S:59:SER:O	2:H:65:NRQ:HB11	2.12	0.49
1:M:15:MET:HB3	1:M:26:CYS:HB2	1.94	0.49
1:M:15:MET:HG3	2:B:119[B]:VAL:CG2	2.44	0.48
1:S:15[B]:MET:HB3	1:S:26:CYS:HB2	1.95	0.47
3:R:77:HOH:O	2:G:209:HIS:HD2	1.97	0.47
2:B:65:NRQ:N1	2:B:65:NRQ:CA3	2.78	0.47
2:A:120[B]:LYS:NZ	3:A:375:HOH:O	2.21	0.47
2:B:116:VAL:HG12	2:B:118[A]:LYS:HE2	1.97	0.47
1:R:16:GLU:HB2	1:R:25[A]:LYS:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:16[B]:GLU:OE2	1:S:23[B]:HIS:CE1	2.55	0.46
2:B:198:ARG:O	2:B:214:GLU:HA	2.15	0.46
3:L:76:HOH:O	2:A:209:HIS:HD2	1.98	0.46
1:L:23[B]:HIS:CD2	3:L:101:HOH:O	2.68	0.46
2:H:65:NRQ:N1	2:H:65:NRQ:CA3	2.79	0.45
2:B:77:PRO:HG2	2:B:188:LYS:HD2	1.99	0.45
1:S:16[B]:GLU:OE2	1:S:25:LYS:HE2	2.18	0.44
1:S:13[B]:MET:HE3	1:S:15[B]:MET:HB2	1.80	0.43
2:B:77:PRO:CG	2:B:188:LYS:HD2	2.48	0.43
2:H:65:NRQ:SD	2:H:214:GLU:HB2	2.58	0.43
2:G:198:ARG:O	2:G:214:GLU:HA	2.19	0.43
2:H:198:ARG:O	2:H:214:GLU:HA	2.18	0.42
2:A:157:GLN:HB3	2:B:159:LEU:HD13	1.99	0.42
2:G:65:NRQ:CE	3:G:417:HOH:O	2.68	0.42
2:G:105:HIS:HB2	3:G:382:HOH:O	2.19	0.42
2:A:158[A]:SER:OG	3:A:391:HOH:O	2.21	0.42
1:R:16:GLU:HB2	1:R:25[B]:LYS:HG2	2.01	0.42
2:A:106:GLN:C	2:A:106:GLN:HE21	2.23	0.42
2:B:149:GLU:HB2	2:B:189[A]:MET:HE1	1.97	0.41
2:H:120:LYS:HD3	2:H:120:LYS:HA	1.78	0.41
2:G:196:ASP:O	2:G:216:ALA:HA	2.21	0.41
2:B:207:GLY:HA2	2:B:210:TYR:OH	2.21	0.40
2:G:91:GLU:CB	3:G:382:HOH:O	2.69	0.40
2:G:65:NRQ:HB11	2:G:212:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	65/62 (105%)	64 (98%)	1 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	64/62 (103%)	63 (98%)	1 (2%)	0	100	100
1	R	65/62 (105%)	64 (98%)	1 (2%)	0	100	100
1	S	61/62 (98%)	60 (98%)	1 (2%)	0	100	100
2	A	169/167 (101%)	167 (99%)	2 (1%)	0	100	100
2	B	171/167 (102%)	167 (98%)	4 (2%)	0	100	100
2	G	171/167 (102%)	166 (97%)	5 (3%)	0	100	100
2	H	169/167 (101%)	166 (98%)	3 (2%)	0	100	100
All	All	935/916 (102%)	917 (98%)	18 (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	L	58/52 (112%)	58 (100%)	0	100	100
1	M	57/52 (110%)	56 (98%)	1 (2%)	66	54
1	R	58/52 (112%)	55 (95%)	3 (5%)	29	12
1	S	54/52 (104%)	53 (98%)	1 (2%)	65	52
2	A	144/137 (105%)	141 (98%)	3 (2%)	61	47
2	B	146/137 (107%)	140 (96%)	6 (4%)	37	19
2	G	146/137 (107%)	145 (99%)	1 (1%)	88	86
2	H	144/137 (105%)	140 (97%)	4 (3%)	51	35
All	All	807/756 (107%)	788 (98%)	19 (2%)	57	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	106	GLN
2	A	187	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	222	ASP
1	M	29	LYS
2	B	106	GLN
2	B	118[A]	LYS
2	B	118[B]	LYS
2	B	150	VAL
2	B	187	LEU
2	B	202	LYS
1	R	7	GLU
1	R	16	GLU
1	R	29	LYS
2	G	106	GLN
1	S	29	LYS
2	H	106	GLN
2	H	168	ARG
2	H	187	LEU
2	H	206	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	105	HIS
2	A	106	GLN
2	A	175	HIS
2	B	105	HIS
2	B	106	GLN
2	B	175	HIS
2	G	105	HIS
2	G	106	GLN
2	G	175	HIS
2	H	105	HIS
2	H	106	GLN
2	H	175	HIS
2	H	205	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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$
2	CME	A	114	2	8,9,10	0.81	0	6,9,11	1.14	0
2	CME	A	221	2	8,9,10	0.70	0	6,9,11	1.06	0
2	NRQ	A	65	2	23,24,25	2.95	6 (26%)	23,32,34	5.60	9 (39%)
2	CME	B	114	2	8,9,10	0.76	0	6,9,11	1.22	0
2	CME	B	221	2	8,9,10	0.71	0	6,9,11	1.04	0
2	NRQ	B	65	2	23,24,25	2.91	6 (26%)	23,32,34	5.57	9 (39%)
2	CME	G	114	2	8,9,10	0.77	0	6,9,11	1.07	0
2	CME	G	221	2	8,9,10	0.70	0	6,9,11	1.07	0
2	NRQ	G	65	2	23,24,25	2.91	5 (21%)	23,32,34	5.52	10 (43%)
2	CME	H	114	2	8,9,10	0.79	0	6,9,11	1.01	0
2	CME	H	221	2	8,9,10	0.70	0	6,9,11	0.98	0
2	NRQ	H	65	2	23,24,25	2.90	6 (26%)	23,32,34	5.60	9 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CME	A	114	2	-	0/5/8/10	0/0/0/0
2	CME	A	221	2	-	0/5/8/10	0/0/0/0
2	NRQ	A	65	2	-	0/9/31/32	0/2/2/2
2	CME	B	114	2	-	0/5/8/10	0/0/0/0
2	CME	B	221	2	-	0/5/8/10	0/0/0/0
2	NRQ	B	65	2	-	0/9/31/32	0/2/2/2
2	CME	G	114	2	-	0/5/8/10	0/0/0/0
2	CME	G	221	2	-	0/5/8/10	0/0/0/0
2	NRQ	G	65	2	-	0/9/31/32	0/2/2/2
2	CME	H	114	2	-	0/5/8/10	0/0/0/0
2	CME	H	221	2	-	0/5/8/10	0/0/0/0
2	NRQ	H	65	2	-	0/9/31/32	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	65	NRQ	CA2-C2	-6.36	1.41	1.48
2	A	65	NRQ	CA2-C2	-6.25	1.41	1.48
2	H	65	NRQ	CA2-C2	-6.13	1.41	1.48
2	B	65	NRQ	CA2-C2	-5.76	1.42	1.48
2	B	65	NRQ	OH-CZ	-4.71	1.25	1.37
2	H	65	NRQ	OH-CZ	-4.70	1.25	1.37
2	A	65	NRQ	OH-CZ	-4.68	1.25	1.37
2	G	65	NRQ	OH-CZ	-4.67	1.25	1.37
2	G	65	NRQ	C2-N3	-4.07	1.31	1.39
2	A	65	NRQ	C2-N3	-3.96	1.31	1.39
2	H	65	NRQ	C2-N3	-3.72	1.31	1.39
2	B	65	NRQ	C2-N3	-3.70	1.31	1.39
2	A	65	NRQ	O2-C2	2.11	1.27	1.23
2	B	65	NRQ	O2-C2	2.31	1.28	1.23
2	H	65	NRQ	O2-C2	2.42	1.28	1.23
2	B	65	NRQ	C1-N2	3.26	1.39	1.33
2	H	65	NRQ	C1-N2	3.38	1.40	1.33
2	G	65	NRQ	C1-N2	3.38	1.40	1.33
2	A	65	NRQ	C1-N2	3.48	1.40	1.33
2	H	65	NRQ	CB2-CA2	9.65	1.43	1.35
2	G	65	NRQ	CB2-CA2	9.66	1.43	1.35
2	A	65	NRQ	CB2-CA2	9.94	1.43	1.35
2	B	65	NRQ	CB2-CA2	10.00	1.44	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	65	NRQ	O2-C2-CA2	-16.65	121.96	130.95
2	A	65	NRQ	O2-C2-CA2	-16.32	122.13	130.95
2	B	65	NRQ	O2-C2-CA2	-15.85	122.39	130.95
2	G	65	NRQ	O2-C2-CA2	-15.67	122.48	130.95
2	H	65	NRQ	CB1-CA1-N1	-7.86	110.50	124.94
2	A	65	NRQ	CB1-CA1-N1	-7.79	110.62	124.94
2	B	65	NRQ	CB1-CA1-N1	-7.79	110.63	124.94
2	G	65	NRQ	CB1-CA1-N1	-7.57	111.03	124.94
2	B	65	NRQ	C2-CA2-N2	-4.58	105.25	108.91
2	A	65	NRQ	C2-CA2-N2	-4.30	105.48	108.91
2	H	65	NRQ	C2-CA2-N2	-4.25	105.52	108.91
2	G	65	NRQ	C2-CA2-N2	-4.06	105.67	108.91
2	H	65	NRQ	N3-C1-N2	-3.37	109.44	113.26
2	B	65	NRQ	N3-C1-N2	-3.20	109.64	113.26
2	A	65	NRQ	N3-C1-N2	-3.17	109.67	113.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	65	NRQ	N3-C1-N2	-2.76	110.14	113.26
2	B	65	NRQ	CB1-CG1-SD	2.02	117.83	112.88
2	A	65	NRQ	CD1-CG2-CD2	2.08	120.81	117.64
2	H	65	NRQ	CD1-CG2-CD2	2.10	120.84	117.64
2	G	65	NRQ	CA3-N3-C2	2.14	127.47	123.99
2	A	65	NRQ	CA3-N3-C2	2.20	127.56	123.99
2	G	65	NRQ	CB1-CG1-SD	2.27	118.46	112.88
2	G	65	NRQ	CD1-CG2-CD2	2.27	121.12	117.64
2	H	65	NRQ	CA3-N3-C2	2.28	127.70	123.99
2	B	65	NRQ	CA3-N3-C2	2.33	127.78	123.99
2	A	65	NRQ	CG2-CB2-CA2	2.55	133.53	130.22
2	H	65	NRQ	CG2-CB2-CA2	2.73	133.75	130.22
2	G	65	NRQ	CG2-CB2-CA2	3.02	134.14	130.22
2	B	65	NRQ	CG2-CB2-CA2	3.23	134.41	130.22
2	A	65	NRQ	C3-CA3-N3	4.23	122.25	113.00
2	G	65	NRQ	C3-CA3-N3	4.31	122.44	113.00
2	H	65	NRQ	C3-CA3-N3	4.81	123.54	113.00
2	B	65	NRQ	C3-CA3-N3	5.15	124.28	113.00
2	H	65	NRQ	CA2-C2-N3	17.35	112.10	103.40
2	B	65	NRQ	CA2-C2-N3	17.62	112.23	103.40
2	A	65	NRQ	CA2-C2-N3	17.87	112.36	103.40
2	G	65	NRQ	CA2-C2-N3	17.97	112.41	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	65	NRQ	4	0
2	B	65	NRQ	4	0
2	G	65	NRQ	6	0
2	H	65	NRQ	5	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	L	58/62 (93%)	0.06	3 (5%) 31 25	24, 32, 42, 49	2 (3%)
1	M	58/62 (93%)	0.16	2 (3%) 49 43	29, 40, 54, 59	0
1	R	58/62 (93%)	-0.08	2 (3%) 49 43	23, 32, 41, 47	0
1	S	58/62 (93%)	0.15	1 (1%) 73 69	29, 40, 53, 59	1 (1%)
2	A	164/167 (98%)	-0.21	1 (0%) 90 88	21, 29, 46, 61	0
2	B	164/167 (98%)	-0.09	2 (1%) 81 78	24, 37, 49, 67	0
2	G	164/167 (98%)	-0.22	2 (1%) 81 78	20, 29, 46, 63	0
2	H	164/167 (98%)	-0.11	3 (1%) 71 67	24, 36, 49, 65	0
All	All	888/916 (96%)	-0.10	16 (1%) 71 67	20, 33, 49, 67	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	228	LEU	4.8
1	L	62	CYS	4.3
2	A	228	LEU	4.1
2	H	229	GLY	4.1
2	B	229	GLY	3.9
2	B	228	LEU	3.4
2	G	229	GLY	3.3
1	R	5	LEU	3.3
2	H	228	LEU	3.3
1	S	5	LEU	3.2
1	M	5	LEU	2.8
1	L	5	LEU	2.7
1	L	6	THR	2.7
1	R	6	THR	2.5
2	H	230	HIS	2.2
1	M	7	GLU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CME	H	114	10/11	0.94	0.10	-	42,43,47,48	3
2	CME	H	221	10/11	0.90	0.11	-	42,43,44,44	0
2	CME	A	114	10/11	0.93	0.10	-	34,35,41,42	3
2	NRQ	H	65	23/24	0.83	0.19	-	40,44,48,50	0
2	NRQ	B	65	23/24	0.85	0.16	-	41,45,49,51	0
2	CME	B	221	10/11	0.94	0.10	-	42,43,44,44	0
2	CME	G	114	10/11	0.91	0.13	-	33,35,37,38	4
2	CME	B	114	10/11	0.91	0.11	-	42,44,45,46	4
2	NRQ	G	65	23/24	0.86	0.14	-	31,37,40,42	0
2	CME	A	221	10/11	0.92	0.08	-	37,41,42,43	0
2	NRQ	A	65	23/24	0.86	0.16	-	31,36,40,44	0
2	CME	G	221	10/11	0.94	0.07	-	37,40,41,41	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.