



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:26 am GMT

PDB ID : 3CFA  
Title : Anemonia sulcata red fluorescent protein asRFP  
Authors : Kachalova, G.S.; Gundel, S.; Wiedenmann, J.; Bartunik, H.D.  
Deposited on : 2008-03-03  
Resolution : 1.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

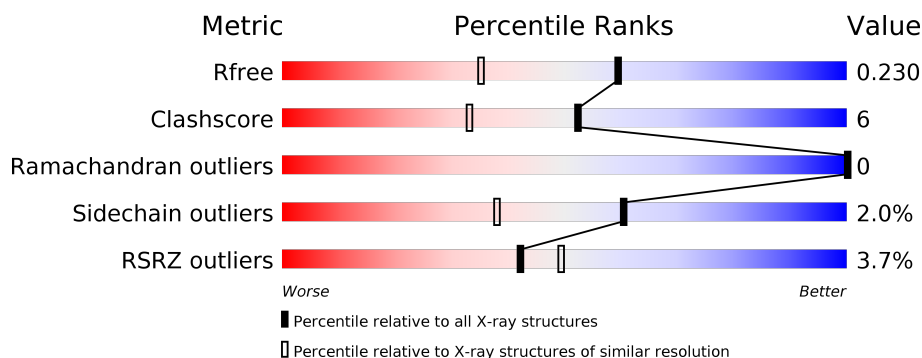
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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	L	62	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>6%</div> </div> </div>
1	M	62	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>5%</div> </div> </div>
1	R	62	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>6%</div> </div> </div>
1	S	62	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>5%</div> </div> </div>
2	A	167	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	B	167	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	167	<div><div></div><div>5%</div><div>90%</div><div>10%</div></div>
2	H	167	<div><div></div><div>4%</div><div>91%</div><div>8%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8488 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 fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	58	Total	C	N	O	S	0	8	0
			494	312	79	94	9			
1	M	59	Total	C	N	O	S	0	7	0
			497	314	79	97	7			
1	R	58	Total	C	N	O	S	0	5	0
			475	298	77	92	8			
1	S	59	Total	C	N	O	S	0	5	0
			485	307	78	92	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	167	Total	C	N	O	S	0	8	0
			1384	881	232	256	15			
2	B	167	Total	C	N	O	S	0	8	0
			1381	881	232	253	15			
2	G	167	Total	C	N	O	S	0	8	0
			1387	885	232	255	15			
2	H	167	Total	C	N	O	S	0	6	0
			1381	878	232	256	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	69	Total	O	0	0
			69	69		
3	A	195	Total	O	0	0
			195	195		
3	M	51	Total	O	0	0
			51	51		
3	B	181	Total	O	0	0
			181	181		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	62	Total 62	O 62	0	0
3	G	217	Total 217	O 217	0	0
3	S	47	Total 47	O 47	0	0
3	H	182	Total 182	O 182	0	1

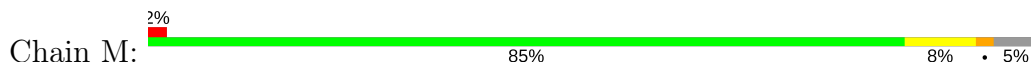
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

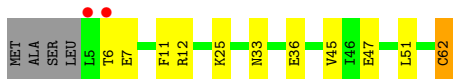
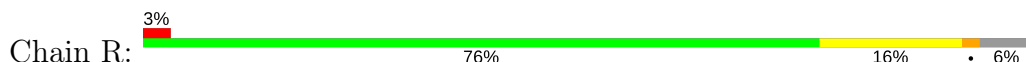
- Molecule 1: GFP-like fluorescent protein



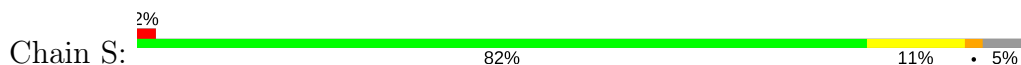
- Molecule 1: GFP-like fluorescent protein



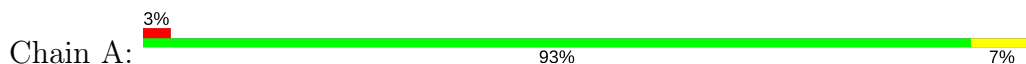
- Molecule 1: GFP-like fluorescent protein




- Molecule 1: GFP-like fluorescent protein

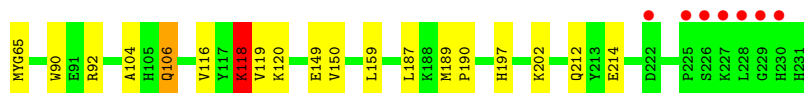


- Molecule 2: GFP-like fluorescent protein




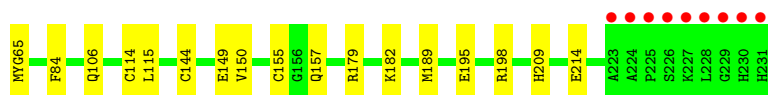
- Molecule 2: GFP-like fluorescent protein

Chain B:  4% 89% 10% ..

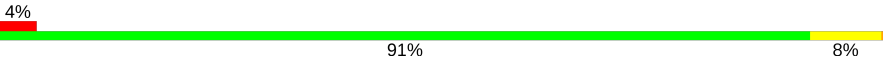


- Molecule 2: GFP-like fluorescent protein

Chain G:  5% 90% 10%



- Molecule 2: GFP-like fluorescent protein

Chain H:  4% 91% 8% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.45Å 98.54Å 241.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.39 – 1.75 19.85 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (12.39-1.75) 96.7 (19.85-1.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.204 , 0.231 0.203 , 0.230	Depositor DCC
$R_{free}$ test set	5732 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.469 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8488	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/523	0.55	0/700
1	M	0.53	1/523 (0.2%)	0.55	0/701
1	R	0.50	1/495 (0.2%)	0.57	0/663
1	S	0.47	1/506 (0.2%)	0.53	0/678
2	A	0.36	0/1399	0.52	0/1882
2	B	0.47	2/1391 (0.1%)	0.59	2/1872 (0.1%)
2	G	0.36	0/1397	0.53	0/1883
2	H	0.35	0/1384	0.53	1/1863 (0.1%)
All	All	0.41	5/7618 (0.1%)	0.55	3/10242 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	62	CYS	C-OXT	8.65	1.39	1.23
1	R	62	CYS	C-OXT	7.63	1.37	1.23
1	S	62	CYS	C-OXT	6.90	1.36	1.23
2	B	118[A]	LYS	CD-CE	5.32	1.64	1.51
2	B	118[B]	LYS	CD-CE	5.32	1.64	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	118[A]	LYS	CG-CD-CE	5.38	128.05	111.90
2	B	118[B]	LYS	CG-CD-CE	5.38	128.05	111.90
2	H	187	LEU	CA-CB-CG	5.07	126.96	115.30

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	494	0	484	14	0
1	M	497	0	484	5	0
1	R	475	0	458	12	0
1	S	485	0	467	5	0
2	A	1384	0	1341	11	0
2	B	1381	0	1343	24	0
2	G	1387	0	1345	21	0
2	H	1381	0	1327	17	0
3	A	195	0	0	2	0
3	B	181	0	0	8	0
3	G	217	0	0	3	0
3	H	182	0	0	6	0
3	L	69	0	0	5	0
3	M	51	0	0	0	0
3	R	62	0	0	4	0
3	S	47	0	0	0	0
All	All	8488	0	7249	91	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 (91) 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)
2:H:65:NRQ:HG11	2:H:214:GLU:OE1	1.67	0.93
2:H:92:ARG:HB3	3:H:551:HOH:O	1.74	0.88
1:R:62:CYS:O	2:G:65:NRQ:N1	2.09	0.86
2:G:195[A]:GLU:OE2	3:G:367:HOH:O	1.94	0.84
2:A:195[A]:GLU:OE2	3:A:319:HOH:O	1.99	0.81
1:S:33:ASN:HB3	1:S:36:GLU:HG2	1.62	0.81
2:B:106:GLN:HG2	2:B:119[B]:VAL:HG12	1.61	0.81
1:L:6:THR:OG1	3:L:120:HOH:O	1.99	0.79
2:G:65:NRQ:HE2	3:G:443:HOH:O	1.85	0.76
1:M:62:CYS:O	2:B:65:NRQ:N1	2.19	0.76
1:L:62:CYS:O	2:A:65:NRQ:N1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:MET:HG3	3:H:558:HOH:O	1.87	0.73
1:L:33[A]:ASN:OD1	3:L:113:HOH:O	2.05	0.73
2:B:90:TRP:HZ3	3:B:431:HOH:O	1.71	0.72
2:B:92:ARG:HB3	3:B:431:HOH:O	1.90	0.72
2:B:65:NRQ:HG12	2:B:212:GLN:NE2	2.04	0.72
1:S:62:CYS:O	2:H:65:NRQ:N1	2.24	0.70
2:B:118[A]:LYS:HD3	3:B:324:HOH:O	1.90	0.70
2:G:144[A]:CYS:HG	2:H:144[A]:CYS:CB	2.04	0.69
1:R:33[A]:ASN:ND2	1:R:36[A]:GLU:CD	2.46	0.69
1:L:23[B]:HIS:HD2	3:L:114:HOH:O	1.77	0.66
2:B:106:GLN:CG	2:B:119[B]:VAL:HG12	2.26	0.66
2:B:149:GLU:HB2	2:B:189[A]:MET:HE2	1.78	0.66
2:H:104:ALA:HB3	3:H:551:HOH:O	1.95	0.65
2:H:90:TRP:HZ3	3:H:551:HOH:O	1.78	0.65
2:G:150[B]:VAL:CG2	2:G:155[B]:CYS:HB2	2.28	0.64
1:R:33[A]:ASN:OD1	3:R:110:HOH:O	2.15	0.63
2:G:65:NRQ:HA31	2:G:65:NRQ:N1	2.14	0.63
1:R:33[A]:ASN:ND2	1:R:36[A]:GLU:OE2	2.32	0.63
2:A:189[A]:MET:HE3	2:A:190:PRO:HD2	1.81	0.63
2:G:150[B]:VAL:HG21	2:G:155[B]:CYS:HB2	1.82	0.62
2:G:144[A]:CYS:CB	2:H:144[A]:CYS:HG	2.12	0.61
2:B:116:VAL:HG12	2:B:118[A]:LYS:HE2	1.82	0.60
1:L:41[B]:MET:CE	1:L:62:CYS:HB3	2.33	0.59
2:B:149:GLU:HB2	2:B:189[A]:MET:CE	2.33	0.59
2:H:65:NRQ:N1	2:H:65:NRQ:HA31	2.19	0.58
2:B:65:NRQ:HG12	2:B:212:GLN:HE21	1.69	0.57
2:B:197:HIS:HD2	3:B:429:HOH:O	1.87	0.57
1:M:15:MET:HG3	2:B:119[B]:VAL:HG23	1.87	0.56
2:B:65:NRQ:CG1	2:B:212:GLN:HE21	2.20	0.55
2:G:84:PHE:O	2:G:182:LYS:NZ	2.40	0.55
2:A:65:NRQ:N1	2:A:65:NRQ:HA31	2.22	0.55
2:B:65:NRQ:HB12	2:B:214:GLU:OE1	2.06	0.55
1:L:15[B]:MET:HB3	1:L:26:CYS:HB2	1.88	0.55
1:L:41[B]:MET:HE1	1:L:62:CYS:HB3	1.90	0.54
2:G:144[A]:CYS:HG	2:H:144[A]:CYS:HB2	1.72	0.54
1:R:12[A]:ARG:HD3	2:G:114:CME:SG	2.47	0.53
2:G:65:NRQ:N1	2:G:65:NRQ:CA3	2.72	0.53
2:B:65:NRQ:N1	2:B:65:NRQ:HA31	2.24	0.52
2:B:104:ALA:HB3	3:B:431:HOH:O	2.10	0.52
1:R:7:GLU:HA	3:R:110:HOH:O	2.08	0.52
1:R:6:THR:HG23	3:R:98:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:MET:HG3	2:B:119[B]:VAL:CG2	2.42	0.49
1:L:25:LYS:HB2	1:L:47:GLU:HB2	1.94	0.49
2:A:65:NRQ:N1	2:A:65:NRQ:CA3	2.77	0.48
2:G:149:GLU:OE1	2:G:189[B]:MET:HG2	2.14	0.48
2:H:104:ALA:HB2	2:H:121:ILE:HD13	1.95	0.48
2:H:174:LEU:HD13	3:H:558:HOH:O	2.14	0.47
2:B:90:TRP:CZ3	3:B:431:HOH:O	2.56	0.47
2:A:209:HIS:HD2	3:A:303:HOH:O	1.98	0.47
1:L:33[A]:ASN:CG	1:L:36[A]:GLU:HB2	2.35	0.46
2:B:189[A]:MET:HE3	2:B:190:PRO:HD2	1.98	0.46
2:H:158:SER:HB3	3:H:558:HOH:O	2.15	0.46
2:B:65:NRQ:HE2	3:B:427:HOH:O	2.16	0.46
2:A:149:GLU:HB2	2:A:189[A]:MET:HE2	1.97	0.45
1:M:25:LYS:HB2	1:M:47:GLU:HB2	1.99	0.45
1:L:11:PHE:HB3	2:A:115:LEU:HB2	1.97	0.45
2:B:65:NRQ:N1	2:B:65:NRQ:CA3	2.80	0.44
2:B:92:ARG:N	3:B:431:HOH:O	2.50	0.44
1:R:12[A]:ARG:CD	2:G:114:CME:HE3	2.47	0.44
1:S:11:PHE:HB3	2:H:115:LEU:HB2	1.99	0.44
2:A:149:GLU:HB2	2:A:189[A]:MET:CE	2.49	0.43
1:R:45:VAL:HG21	1:R:51:LEU:HG	2.00	0.43
3:R:73:HOH:O	2:G:209:HIS:HD2	2.01	0.43
2:H:65:NRQ:N1	2:H:65:NRQ:CA3	2.81	0.43
1:M:15:MET:HB3	1:M:26:CYS:HB2	2.00	0.42
2:A:157:GLN:HB3	2:B:159:LEU:HD13	2.02	0.42
2:G:157:GLN:HB3	2:H:159:LEU:HD13	2.02	0.42
1:R:25:LYS:HB2	1:R:47:GLU:HB2	2.00	0.42
1:R:12[A]:ARG:HG3	2:G:114:CME:CE	2.49	0.42
1:S:39:GLN:HE22	2:H:66:SER:HB3	1.85	0.41
1:L:8:THR:C	3:L:120:HOH:O	2.58	0.41
2:G:179:ARG:NH1	3:G:436:HOH:O	2.53	0.41
1:L:11:PHE:HE1	1:L:41[B]:MET:SD	2.42	0.41
2:G:198:ARG:O	2:G:214:GLU:HA	2.21	0.41
1:R:11:PHE:HB3	2:G:115:LEU:HB2	2.02	0.41
2:G:150[A]:VAL:HB	2:G:155[A]:CYS:SG	2.61	0.40
1:L:49:GLY:HA2	1:L:50:PRO:C	2.41	0.40
2:A:189[A]:MET:HE3	2:A:190:PRO:CD	2.51	0.40
1:S:45:VAL:HG21	1:S:51:LEU:HG	2.04	0.40
1:L:12[A]:ARG:NH1	3:L:95:HOH:O	2.53	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	L	64/62 (103%)	63 (98%)	1 (2%)	0	100	100
1	M	64/62 (103%)	63 (98%)	1 (2%)	0	100	100
1	R	61/62 (98%)	59 (97%)	2 (3%)	0	100	100
1	S	62/62 (100%)	61 (98%)	1 (2%)	0	100	100
2	A	170/167 (102%)	166 (98%)	4 (2%)	0	100	100
2	B	169/167 (101%)	166 (98%)	3 (2%)	0	100	100
2	G	170/167 (102%)	165 (97%)	5 (3%)	0	100	100
2	H	168/167 (101%)	164 (98%)	4 (2%)	0	100	100
All	All	928/916 (101%)	907 (98%)	21 (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	57/52 (110%)	57 (100%)	0	100	100
1	M	57/52 (110%)	55 (96%)	2 (4%)	41	16
1	R	54/52 (104%)	54 (100%)	0	100	100
1	S	55/52 (106%)	53 (96%)	2 (4%)	40	15
2	A	146/138 (106%)	142 (97%)	4 (3%)	50	25
2	B	145/138 (105%)	137 (94%)	8 (6%)	25	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	146/138 (106%)	145 (99%)	1 (1%)	87	78
2	H	144/138 (104%)	142 (99%)	2 (1%)	71	56
All	All	804/760 (106%)	785 (98%)	19 (2%)	60	30

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

Mol	Chain	Res	Type
2	A	106	GLN
2	A	118	LYS
2	A	129	ASP
2	A	202	LYS
1	M	7[A]	GLU
1	M	7[B]	GLU
2	B	106	GLN
2	B	118[A]	LYS
2	B	118[B]	LYS
2	B	120[A]	LYS
2	B	120[B]	LYS
2	B	150	VAL
2	B	187	LEU
2	B	202	LYS
2	G	106	GLN
1	S	7[A]	GLU
1	S	7[B]	GLU
2	H	106	GLN
2	H	187	LEU

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	A	209	HIS
2	B	105	HIS
2	B	106	GLN
2	G	105	HIS
2	G	106	GLN
2	G	175	HIS
2	G	209	HIS

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Mol	Chain	Res	Type
1	S	39	GLN
2	H	105	HIS
2	H	106	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	9,9,10	0.76	0	6,9,11	1.07	0
2	CME	A	221	2	9,9,10	0.72	0	6,9,11	0.85	0
2	NRQ	A	65	2	23,24,25	2.93	6 (26%)	25,32,34	5.58	8 (32%)
2	CME	B	114	2	9,9,10	0.76	0	6,9,11	1.03	0
2	CME	B	221	2	9,9,10	0.69	0	6,9,11	0.91	0
2	NRQ	B	65	2	23,24,25	2.85	6 (26%)	25,32,34	5.43	8 (32%)
2	CME	G	114	2	9,9,10	0.80	0	6,9,11	0.98	0
2	CME	G	221	2	9,9,10	0.70	0	6,9,11	0.85	0
2	NRQ	G	65	2	23,24,25	2.94	6 (26%)	25,32,34	5.59	8 (32%)
2	CME	H	114	2	9,9,10	0.77	0	6,9,11	0.88	0
2	CME	H	221	2	9,9,10	0.71	0	6,9,11	0.86	0
2	NRQ	H	65	2	23,24,25	2.93	6 (26%)	25,32,34	5.56	9 (36%)

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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	65	NRQ	CA2-C2	-6.67	1.41	1.48
2	A	65	NRQ	CA2-C2	-6.52	1.42	1.48
2	B	65	NRQ	CA2-C2	-6.47	1.42	1.48
2	H	65	NRQ	CA2-C2	-6.41	1.42	1.48
2	A	65	NRQ	OH-CZ	-5.12	1.25	1.37
2	G	65	NRQ	OH-CZ	-4.99	1.25	1.37
2	H	65	NRQ	OH-CZ	-4.93	1.25	1.37
2	B	65	NRQ	OH-CZ	-4.83	1.25	1.37
2	G	65	NRQ	C2-N3	-3.41	1.31	1.39
2	A	65	NRQ	C2-N3	-3.33	1.31	1.39
2	B	65	NRQ	C2-N3	-3.28	1.31	1.39
2	H	65	NRQ	C2-N3	-3.14	1.32	1.39
2	H	65	NRQ	O2-C2	2.16	1.27	1.23
2	B	65	NRQ	O2-C2	2.28	1.28	1.23
2	A	65	NRQ	O2-C2	2.38	1.28	1.23
2	G	65	NRQ	O2-C2	2.40	1.28	1.23
2	B	65	NRQ	C1-N2	3.33	1.39	1.33
2	A	65	NRQ	C1-N2	3.52	1.40	1.33
2	H	65	NRQ	C1-N2	3.52	1.40	1.33
2	G	65	NRQ	C1-N2	3.64	1.40	1.33
2	B	65	NRQ	CB2-CA2	9.29	1.43	1.35
2	A	65	NRQ	CB2-CA2	9.56	1.43	1.35
2	G	65	NRQ	CB2-CA2	9.60	1.43	1.35
2	H	65	NRQ	CB2-CA2	9.79	1.43	1.35

All (33) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	65	NRQ	O2-C2-CA2	-16.53	122.06	130.97
2	G	65	NRQ	O2-C2-CA2	-16.51	122.07	130.97
2	B	65	NRQ	O2-C2-CA2	-16.12	122.28	130.97
2	H	65	NRQ	O2-C2-CA2	-15.88	122.41	130.97
2	G	65	NRQ	CG1-CB1-CA1	-6.17	101.82	112.67
2	A	65	NRQ	CG1-CB1-CA1	-6.07	101.99	112.67
2	H	65	NRQ	CG1-CB1-CA1	-5.72	102.61	112.67
2	H	65	NRQ	C2-CA2-N2	-5.08	105.22	108.93
2	B	65	NRQ	C2-CA2-N2	-4.55	105.60	108.93
2	G	65	NRQ	CB1-CA1-N1	-4.47	109.94	125.34
2	A	65	NRQ	CB1-CA1-N1	-4.44	110.03	125.34
2	A	65	NRQ	C2-CA2-N2	-4.28	105.80	108.93
2	H	65	NRQ	CB1-CA1-N1	-4.07	111.28	125.34
2	G	65	NRQ	C2-CA2-N2	-4.04	105.97	108.93
2	B	65	NRQ	CB1-CA1-N1	-3.97	111.63	125.34
2	B	65	NRQ	CG1-CB1-CA1	-3.60	106.33	112.67
2	A	65	NRQ	N3-C1-N2	-2.90	109.59	113.31
2	H	65	NRQ	N3-C1-N2	-2.86	109.63	113.31
2	G	65	NRQ	N3-C1-N2	-2.85	109.65	113.31
2	B	65	NRQ	N3-C1-N2	-2.75	109.77	113.31
2	H	65	NRQ	CD1-CG2-CD2	2.09	120.76	117.63
2	H	65	NRQ	CB2-CA2-C2	2.17	125.04	122.32
2	B	65	NRQ	CD1-CG2-CD2	2.27	121.03	117.63
2	A	65	NRQ	CD1-CG2-CD2	2.33	121.12	117.63
2	G	65	NRQ	CD1-CG2-CD2	2.44	121.29	117.63
2	H	65	NRQ	CG2-CB2-CA2	3.69	134.49	130.19
2	B	65	NRQ	CG2-CB2-CA2	4.41	135.31	130.19
2	A	65	NRQ	CG2-CB2-CA2	5.20	136.24	130.19
2	G	65	NRQ	CG2-CB2-CA2	5.72	136.84	130.19
2	G	65	NRQ	CA2-C2-N3	19.17	111.86	103.30
2	A	65	NRQ	CA2-C2-N3	19.26	111.89	103.30
2	B	65	NRQ	CA2-C2-N3	19.46	111.98	103.30
2	H	65	NRQ	CA2-C2-N3	19.99	112.22	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	65	NRQ	3	0
2	B	65	NRQ	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	114	CME	3	0
2	G	65	NRQ	4	0
2	H	65	NRQ	4	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	L	58/62 (93%)	0.35	2 (3%) 46 52	18, 26, 35, 41	1 (1%)
1	M	59/62 (95%)	0.34	1 (1%) 70 78	21, 28, 38, 42	0
1	R	58/62 (93%)	0.23	2 (3%) 46 52	19, 27, 35, 41	2 (3%)
1	S	59/62 (95%)	0.38	1 (1%) 70 78	20, 30, 39, 43	0
2	A	164/167 (98%)	0.20	5 (3%) 51 57	15, 23, 39, 68	0
2	B	164/167 (98%)	0.21	7 (4%) 36 43	16, 26, 40, 70	0
2	G	164/167 (98%)	0.23	9 (5%) 26 32	15, 23, 39, 72	0
2	H	164/167 (98%)	0.22	6 (3%) 42 49	16, 26, 40, 73	0
All	All	890/916 (97%)	0.24	33 (3%) 42 49	15, 26, 40, 73	3 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	229	GLY	11.3
2	H	229	GLY	10.6
2	G	228	LEU	9.7
2	A	228	LEU	9.4
2	A	229	GLY	8.7
2	H	228	LEU	6.8
2	G	229	GLY	5.5
2	G	230	HIS	4.4
2	B	230	HIS	4.1
2	G	224	ALA	4.1
2	H	230	HIS	4.0
2	A	230	HIS	3.9
2	G	226	SER	3.9
2	H	231	HIS	3.8
2	B	228	LEU	3.8
2	H	226	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	6	THR	3.5
1	L	5	LEU	3.4
2	B	227	LYS	3.2
2	H	227	LYS	3.1
2	G	231	HIS	3.1
2	A	224	ALA	3.0
1	R	5	LEU	2.8
1	R	6	THR	2.7
2	B	226	SER	2.6
2	B	225	PRO	2.5
2	G	225	PRO	2.5
2	G	227	LYS	2.4
2	A	226	SER	2.3
2	B	222	ASP	2.3
1	M	4	LEU	2.2
1	S	4	LEU	2.2
2	G	223	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NRQ	H	65	23/24	0.81	0.14	-	28,32,38,43	0
2	CME	B	114	10/11	0.94	0.11	-	30,33,34,34	4
2	CME	H	221	10/11	0.93	0.11	-	31,33,34,35	0
2	CME	G	221	10/11	0.92	0.10	-	29,31,33,33	0
2	NRQ	A	65	23/24	0.84	0.14	-	26,30,35,40	0
2	CME	A	221	10/11	0.89	0.12	-	28,31,32,33	0
2	NRQ	G	65	23/24	0.80	0.16	-	26,31,36,40	0
2	CME	G	114	10/11	0.90	0.12	-	28,30,32,32	4
2	CME	H	114	10/11	0.91	0.12	-	31,33,37,37	3
2	CME	A	114	10/11	0.94	0.10	-	27,29,31,31	4
2	CME	B	221	10/11	0.93	0.11	-	31,33,34,34	0
2	NRQ	B	65	23/24	0.83	0.14	-	28,31,37,41	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.