



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3CFA / pdb_00003cfa
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

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

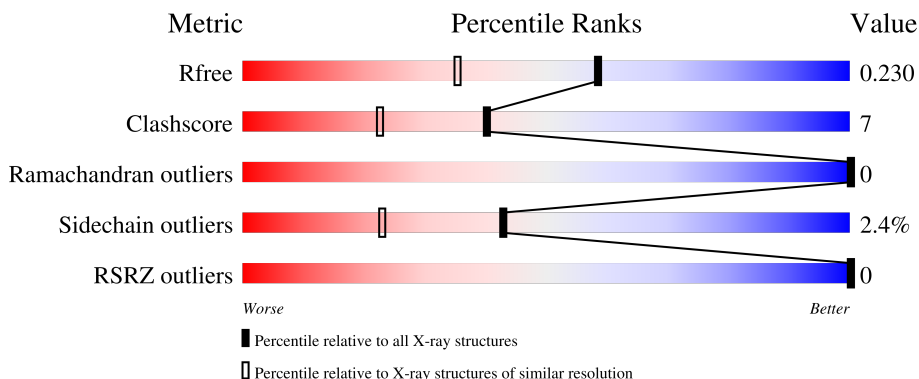
1 Overall quality at a glance i

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	L	62	 68% 26% 6%
1	M	62	 84% 10% • 5%
1	R	62	 73% 19% • 6%
1	S	62	 82% 11% • 5%
2	A	167	 93% 5% •

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Mol	Chain	Length	Quality of chain
2	B	167	 89% 10% .
2	G	167	 89% 10% .
2	H	167	 90% 8% .

2 Entry composition [i](#)

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

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

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

- Molecule 3 is water.

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

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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, 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: GFP-like fluorescent protein

Chain L: 



- Molecule 1: GFP-like fluorescent protein

Chain M: 




- Molecule 1: GFP-like fluorescent protein

Chain R: 



- Molecule 1: GFP-like fluorescent protein

Chain S: 




- Molecule 2: GFP-like fluorescent protein

Chain A: 



- Molecule 2: GFP-like fluorescent protein

Chain B: 



- Molecule 2: GFP-like fluorescent protein

Chain G: 89% 10%



- Molecule 2: GFP-like fluorescent protein

Chain H: 90% 8%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.45Å 98.54Å 241.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.39 – 1.75 12.39 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (12.39-1.75) 96.8 (12.39-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.76Å)	Xtrriage
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 (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtrriage
Anisotropy	0.480	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.469 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8488	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage'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.*

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: 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	0/523	0.64	0/700
1	M	0.52	1/523 (0.2%)	0.62	0/701
1	R	0.52	1/495 (0.2%)	0.67	0/663
1	S	0.49	1/506 (0.2%)	0.62	0/678
2	A	0.40	0/1399	0.64	0/1882
2	B	0.39	0/1391	0.66	0/1872
2	G	0.41	0/1397	0.65	0/1883
2	H	0.39	0/1384	0.65	0/1863
All	All	0.42	3/7618 (0.0%)	0.65	0/10242

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	62	CYS	C-OXT	8.12	1.39	1.23
1	R	62	CYS	C-OXT	7.15	1.37	1.23
1	S	62	CYS	C-OXT	6.46	1.36	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	L	494	0	484	15	0
1	M	497	0	484	5	0
1	R	475	0	458	11	0
1	S	485	0	467	5	0
2	A	1384	0	1341	12	0
2	B	1381	0	1343	25	0
2	G	1387	0	1345	20	0
2	H	1381	0	1327	18	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	95	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 7.

All (95) 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:B:149:GLU:HB2	2:B:189[A]:MET:HE2	1.38	1.03
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
2:A:149:GLU:HB2	2:A:189[A]:MET:HE2	1.55	0.87
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
1:R:33[A]:ASN:ND2	1:R:36[A]:GLU:CD	2.46	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:N1	2:G:65:NRQ:HA31	2.14	0.63
1:R:33[A]:ASN:ND2	1:R:36[A]:GLU:OE2	2.32	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
1:L:41[B]:MET:HE1	1:L:62:CYS:HB3	1.82	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
2:B:154:LEU:HD13	2:B:189[A]:MET:HE1	1.88	0.56
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
2:A:154:LEU:HD13	2:A:189[A]:MET:HE1	1.88	0.55
2:A:149:GLU:CB	2:A:189[A]:MET:HE2	2.34	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:L:33[A]:ASN:CG	1:L:36[A]:GLU:HB2	2.35	0.51
1:R:6:THR:HG23	3:R:98:HOH:O	2.12	0.50
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
1:L:41[A]:MET:HE2	1:L:43:ILE:HG13	1.94	0.49
2:A:65:NRQ:N1	2:A:65:NRQ:CA3	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:149:GLU:CB	2:B:189[A]:MET:HE2	2.25	0.47
2:A:189[A]:MET:HE3	2:A:190:PRO:HD2	1.96	0.47
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:8:THR:C	3:L:120:HOH:O	2.58	0.46
1:L:49:GLY:HA2	1:L:50:PRO:C	2.41	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
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:A:106:GLN:C	2:A:106:GLN:HE21	2.24	0.44
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:S:11:PHE:HB3	2:H:115:LEU:HB2	1.99	0.44
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
1:R:25:LYS:HB2	1:R:47:GLU:HB2	2.00	0.42
2:G:157:GLN:HB3	2:H:159:LEU:HD13	2.02	0.42
1:S:39:GLN:HE22	2:H:66:SER:HB3	1.85	0.41
1:L:11:PHE:HE1	1:L:41[B]:MET:SD	2.42	0.41
2:G:179:ARG:NH1	3:G:436:HOH:O	2.53	0.41
2:H:106:GLN:C	2:H:106:GLN:HE21	2.28	0.41
1:R:11:PHE:HB3	2:G:115:LEU:HB2	2.02	0.41
1:R:49:GLY:HA2	1:R:50:PRO:C	2.45	0.41
2:G:198:ARG:O	2:G:214:GLU:HA	2.21	0.41
2:B:106:GLN:HE21	2:B:106:GLN:C	2.30	0.40
2:G:150[A]:VAL:HB	2:G:155[A]:CYS:SG	2.61	0.40
2:G:106:GLN:HE21	2:G:106:GLN:C	2.29	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 [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	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 [i](#)

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%)	54 (95%)	3 (5%)	20	5
1	R	54/52 (104%)	54 (100%)	0	100	100
1	S	55/52 (106%)	53 (96%)	2 (4%)	31	11
2	A	146/138 (106%)	141 (97%)	5 (3%)	32	13
2	B	145/138 (105%)	137 (94%)	8 (6%)	19	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	146/138 (106%)	144 (99%)	2 (1%)	59	44
2	H	144/138 (104%)	141 (98%)	3 (2%)	47	27
All	All	804/760 (106%)	781 (97%)	23 (3%)	43	17

All (23) 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	195[A]	GLU
2	A	195[B]	GLU
1	M	4	LEU
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
2	G	119	VAL
1	S	7[A]	GLU
1	S	7[B]	GLU
2	H	106	GLN
2	H	187	LEU
2	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
2	A	105	HIS
2	A	106	GLN
2	A	134	GLN
2	A	175	HIS
2	A	209	HIS
1	M	39	GLN

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Mol	Chain	Res	Type
2	B	106	GLN
2	B	175	HIS
2	B	212	GLN
2	G	105	HIS
2	G	106	GLN
2	G	175	HIS
2	G	209	HIS
1	S	39	GLN
2	H	105	HIS
2	H	106	GLN
2	H	134	GLN
2	H	175	HIS
2	H	230	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	H	221	2	8,9,10	0.81	0	6,9,11	0.65	0
2	CME	G	221	2	8,9,10	0.79	0	6,9,11	0.62	0
2	CME	G	114	2	8,9,10	0.93	0	6,9,11	0.73	0
2	NRQ	G	65	2	24,24,25	2.78	6 (25%)	24,32,34	4.07	8 (33%)
2	NRQ	A	65	2	24,24,25	2.77	6 (25%)	24,32,34	4.07	7 (29%)
2	CME	A	114	2	8,9,10	0.87	0	6,9,11	0.83	0
2	CME	A	221	2	8,9,10	0.82	0	6,9,11	0.62	0
2	CME	H	114	2	8,9,10	0.88	0	6,9,11	0.63	0
2	CME	B	114	2	8,9,10	0.89	0	6,9,11	0.77	0
2	NRQ	B	65	2	24,24,25	2.70	6 (25%)	24,32,34	4.02	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CME	B	221	2	8,9,10	0.79	0	6,9,11	0.71	0
2	NRQ	H	65	2	24,24,25	2.76	6 (25%)	24,32,34	3.99	9 (37%)

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	H	221	2	-	1/5/8/10	-
2	CME	G	221	2	-	1/5/8/10	-
2	CME	G	114	2	-	1/5/8/10	-
2	NRQ	G	65	2	-	1/9/31/32	0/2/2/2
2	NRQ	A	65	2	-	1/9/31/32	0/2/2/2
2	CME	A	114	2	-	1/5/8/10	-
2	CME	A	221	2	-	1/5/8/10	-
2	CME	H	114	2	-	2/5/8/10	-
2	CME	B	114	2	-	0/5/8/10	-
2	NRQ	B	65	2	-	2/9/31/32	0/2/2/2
2	CME	B	221	2	-	1/5/8/10	-
2	NRQ	H	65	2	-	3/9/31/32	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	65	NRQ	CB2-CA2	8.99	1.43	1.35
2	G	65	NRQ	CB2-CA2	8.81	1.43	1.35
2	A	65	NRQ	CB2-CA2	8.78	1.43	1.35
2	B	65	NRQ	CB2-CA2	8.53	1.43	1.35
2	G	65	NRQ	CA2-C2	-6.20	1.41	1.48
2	A	65	NRQ	CA2-C2	-6.06	1.42	1.48
2	B	65	NRQ	CA2-C2	-6.02	1.42	1.48
2	H	65	NRQ	CA2-C2	-5.96	1.42	1.48
2	A	65	NRQ	OH-CZ	-5.29	1.25	1.37
2	G	65	NRQ	OH-CZ	-5.15	1.25	1.37
2	H	65	NRQ	OH-CZ	-5.10	1.25	1.37
2	B	65	NRQ	OH-CZ	-4.99	1.25	1.37
2	G	65	NRQ	C2-N3	-3.70	1.31	1.40
2	A	65	NRQ	C2-N3	-3.62	1.31	1.40
2	B	65	NRQ	C2-N3	-3.57	1.31	1.40
2	H	65	NRQ	C2-N3	-3.42	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	65	NRQ	C1-N2	3.33	1.40	1.33
2	H	65	NRQ	C1-N2	3.22	1.40	1.33
2	A	65	NRQ	C1-N2	3.21	1.40	1.33
2	B	65	NRQ	C1-N2	3.04	1.39	1.33
2	G	65	NRQ	O2-C2	2.60	1.28	1.23
2	A	65	NRQ	O2-C2	2.58	1.28	1.23
2	B	65	NRQ	O2-C2	2.47	1.28	1.23
2	H	65	NRQ	O2-C2	2.35	1.27	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	65	NRQ	O2-C2-CA2	-14.05	122.06	131.02
2	G	65	NRQ	O2-C2-CA2	-14.03	122.07	131.02
2	B	65	NRQ	O2-C2-CA2	-13.70	122.28	131.02
2	H	65	NRQ	O2-C2-CA2	-13.49	122.41	131.02
2	H	65	NRQ	CA2-C2-N3	10.38	112.22	103.50
2	B	65	NRQ	CA2-C2-N3	10.10	111.98	103.50
2	A	65	NRQ	CA2-C2-N3	9.99	111.89	103.50
2	G	65	NRQ	CA2-C2-N3	9.95	111.86	103.50
2	G	65	NRQ	CG2-CB2-CA2	5.87	136.84	129.87
2	A	65	NRQ	CG2-CB2-CA2	5.36	136.24	129.87
2	B	65	NRQ	C3-CA3-N3	5.24	124.34	112.43
2	H	65	NRQ	C2-CA2-N2	-5.21	105.22	108.95
2	B	65	NRQ	C2-CA2-N2	-4.68	105.60	108.95
2	A	65	NRQ	C3-CA3-N3	4.61	122.92	112.43
2	B	65	NRQ	CG2-CB2-CA2	4.58	135.31	129.87
2	A	65	NRQ	C2-CA2-N2	-4.39	105.80	108.95
2	G	65	NRQ	C3-CA3-N3	4.31	122.24	112.43
2	H	65	NRQ	C3-CA3-N3	4.31	122.23	112.43
2	G	65	NRQ	C2-CA2-N2	-4.16	105.97	108.95
2	H	65	NRQ	CG2-CB2-CA2	3.89	134.49	129.87
2	A	65	NRQ	N3-C1-N2	-2.56	109.59	112.62
2	H	65	NRQ	N3-C1-N2	-2.52	109.63	112.62
2	G	65	NRQ	N3-C1-N2	-2.50	109.65	112.62
2	G	65	NRQ	CD1-CG2-CD2	2.45	121.29	117.65
2	B	65	NRQ	N3-C1-N2	-2.40	109.77	112.62
2	A	65	NRQ	CD1-CG2-CD2	2.34	121.12	117.65
2	B	65	NRQ	CD1-CG2-CD2	2.28	121.03	117.65
2	H	65	NRQ	CB2-CA2-C2	2.22	125.04	122.36
2	G	65	NRQ	CB2-CA2-N2	2.10	131.62	128.76
2	H	65	NRQ	CD1-CG2-CD2	2.10	120.76	117.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	65	NRQ	CA3-N3-C2	2.07	128.22	123.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	65	NRQ	C1-CA1-CB1-CG1
2	A	114	CME	SD-CE-CZ-OH
2	B	65	NRQ	CA1-CB1-CG1-SD
2	G	65	NRQ	C1-CA1-CB1-CG1
2	H	65	NRQ	CA1-CB1-CG1-SD
2	G	114	CME	SD-CE-CZ-OH
2	H	65	NRQ	CB1-CG1-SD-CE
2	A	221	CME	CZ-CE-SD-SG
2	B	221	CME	CZ-CE-SD-SG
2	G	221	CME	CZ-CE-SD-SG
2	H	114	CME	CZ-CE-SD-SG
2	H	221	CME	CZ-CE-SD-SG
2	H	114	CME	CE-SD-SG-CB
2	B	65	NRQ	C1-CA1-CB1-CG1
2	H	65	NRQ	C1-CA1-CB1-CG1

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	114	CME	1	0
2	G	65	NRQ	4	0
2	A	65	NRQ	3	0
2	B	65	NRQ	8	0
2	H	65	NRQ	4	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 [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	L	58/62 (93%)	-1.13	0 100 100	11, 25, 33, 41	9 (15%)
1	M	59/62 (95%)	-1.11	0 100 100	13, 28, 34, 42	7 (11%)
1	R	58/62 (93%)	-1.12	0 100 100	11, 26, 32, 41	7 (12%)
1	S	59/62 (95%)	-1.09	0 100 100	13, 30, 37, 43	5 (8%)
2	A	164/167 (98%)	-1.26	0 100 100	11, 23, 39, 68	8 (4%)
2	B	164/167 (98%)	-1.20	0 100 100	13, 26, 40, 70	7 (4%)
2	G	164/167 (98%)	-1.24	0 100 100	9, 23, 39, 72	8 (4%)
2	H	164/167 (98%)	-1.20	0 100 100	14, 26, 40, 73	6 (3%)
All	All	890/916 (97%)	-1.19	0 100 100	9, 25, 40, 73	57 (6%)

There are no RSRZ outliers to report.

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
2	CME	G	114	10/11	0.97	0.06	28,30,32,32	4
2	NRQ	B	65	23/24	0.98	0.04	28,31,37,41	0
2	CME	B	114	10/11	0.98	0.06	30,33,34,34	4
2	NRQ	G	65	23/24	0.98	0.05	26,31,36,40	0
2	NRQ	A	65	23/24	0.98	0.04	26,30,35,40	0
2	NRQ	H	65	23/24	0.98	0.05	28,32,38,43	0
2	CME	H	114	10/11	0.98	0.06	31,33,37,37	3
2	CME	A	221	10/11	0.99	0.04	28,31,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CME	G	221	10/11	0.99	0.04	29,31,33,33	0
2	CME	B	221	10/11	0.99	0.06	31,33,34,34	0
2	CME	A	114	10/11	0.99	0.05	27,29,31,31	4
2	CME	H	221	10/11	0.99	0.05	31,33,34,35	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.