



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:32 AM UTC

PDB ID : 2WHS / pdb_00002whs
Title : Fluorescent Protein mKeima at pH 3.8
Authors : Violot, S.; Carpentier, P.; Blanchoin, L.; Bourgeois, D.
Deposited on : 2009-05-06
Resolution : 2.10 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

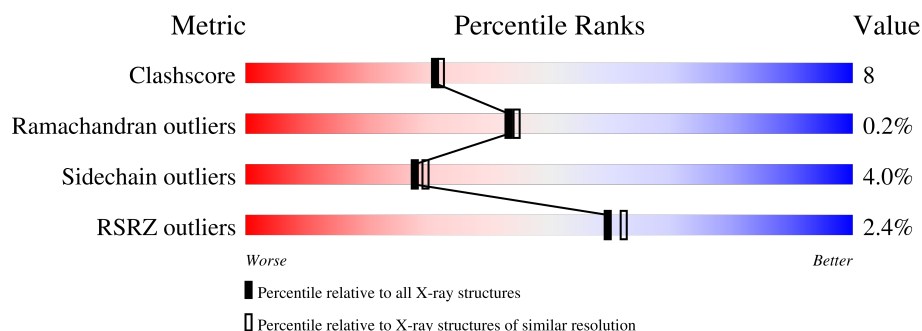
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	240	2% 74% 13% • 10%
1	B	240	3% 80% 14% • 5%
1	C	240	78% 10% • 10%
1	D	240	3% 79% 14% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	1221	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7919 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 LARGE STOKES SHIFT FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1740	1107	291	331	11			
1	B	227	Total	C	N	O	S	0	0	0
			1813	1153	306	342	12			
1	C	216	Total	C	N	O	S	0	0	0
			1733	1102	290	330	11			
1	D	227	Total	C	N	O	S	0	1	0
			1817	1155	306	344	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	CRQ	GLN	chromophore	UNP Q1JV70
A	62	CRQ	TYR	chromophore	UNP Q1JV70
A	62	CRQ	GLY	chromophore	UNP Q1JV70
B	62	CRQ	GLN	chromophore	UNP Q1JV70
B	62	CRQ	TYR	chromophore	UNP Q1JV70
B	62	CRQ	GLY	chromophore	UNP Q1JV70
C	62	CRQ	GLN	chromophore	UNP Q1JV70
C	62	CRQ	TYR	chromophore	UNP Q1JV70
C	62	CRQ	GLY	chromophore	UNP Q1JV70
D	62	CRQ	GLN	chromophore	UNP Q1JV70
D	62	CRQ	TYR	chromophore	UNP Q1JV70
D	62	CRQ	GLY	chromophore	UNP Q1JV70

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	159	Total	O	0	0
			159	159		

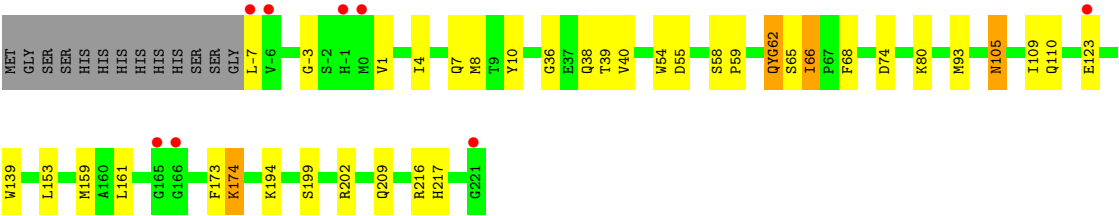
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	222	Total 222	O 222	0	0
3	C	166	Total 166	O 166	0	0
3	D	214	Total 214	O 214	0	0

• Molecule 1: LARGE STOKES SHIFT 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	92.57Å 98.10Å 123.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.70 – 2.10 76.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (76.70-2.10) 99.2 (76.70-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.248 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	1.084	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7919	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.90 % 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 1.0715e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRQ, SO4

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	0.92	0/1761	0.97	0/2379
1	B	0.91	0/1836	0.97	0/2480
1	C	0.93	0/1754	0.96	1/2369 (0.0%)
1	D	0.94	0/1843	0.99	2/2488 (0.1%)
All	All	0.93	0/7194	0.97	3/9716 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	ILE	CA-C-N	-6.09	113.86	119.82
1	D	66	ILE	C-N-CA	-6.09	113.86	119.82
1	C	66	ILE	N-CA-C	5.01	119.70	108.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Peptide

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	1740	0	1673	47	0
1	B	1813	0	1751	28	0
1	C	1733	0	1661	25	0
1	D	1817	0	1756	25	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	3	0
2	D	15	0	0	0	0
3	A	159	0	0	2	0
3	B	222	0	0	4	0
3	C	166	0	0	2	0
3	D	214	0	0	6	0
All	All	7919	0	6841	115	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 8.

All (115) 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:212:ILE:HD11	1:A:214:ILE:CD1	1.65	1.25
1:A:212:ILE:HD11	1:A:214:ILE:HD12	1.03	1.02
1:A:212:ILE:CD1	1:A:214:ILE:HD12	1.95	0.95
1:C:38:GLN:HE22	1:C:65:SER:HB3	1.29	0.94
1:D:7:GLN:HB2	3:D:2017:HOH:O	1.70	0.92
1:A:1:VAL:HG12	1:A:1:VAL:O	1.74	0.85
1:A:93:MET:HE3	1:A:173:PHE:CZ	2.12	0.84
1:B:36:GLY:HA2	1:B:68:PHE:O	1.78	0.83
1:D:93:MET:HE3	1:D:173:PHE:CE1	2.13	0.83
1:B:123:GLU:O	1:B:124:ASN:OD1	1.96	0.83
1:A:202:ARG:H	1:A:202:ARG:CD	1.95	0.80
1:C:38:GLN:HE22	1:C:65:SER:CB	1.95	0.78
1:A:54:TRP:HE1	1:A:209:GLN:HE21	1.29	0.76
1:A:212:ILE:CD1	1:A:214:ILE:CD1	2.57	0.75
1:C:154:ILE:CG2	1:C:174:LYS:HE2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:H	1:A:202:ARG:HD3	1.51	0.73
1:A:212:ILE:HD11	1:A:214:ILE:HD11	1.67	0.73
1:A:199:SER:HB3	1:A:208:GLU:HB2	1.69	0.73
1:A:38:GLN:HE22	1:A:65:SER:HB3	1.54	0.71
1:C:38:GLN:NE2	1:C:65:SER:HB3	2.03	0.70
1:D:93:MET:HE3	1:D:173:PHE:CZ	2.26	0.70
1:B:8:MET:HE1	1:B:109:ILE:HD11	1.74	0.69
1:D:54:TRP:HE1	1:D:209:GLN:HE21	1.41	0.69
1:A:219:LEU:C	1:A:219:LEU:HD22	2.20	0.67
1:A:219:LEU:HD23	1:B:212:ILE:HG21	1.77	0.67
1:A:38:GLN:NE2	1:A:65:SER:HB3	2.10	0.67
1:B:62:CRQ:HD1	3:B:2172:HOH:O	1.93	0.66
1:B:38:GLN:HE22	1:B:65:SER:HB3	1.61	0.66
1:C:21:HIS:HB2	2:C:1221:SO4:O4	1.96	0.66
1:A:219:LEU:HD21	1:B:212:ILE:HB	1.78	0.65
1:C:81:GLN:HE22	1:C:184:ARG:H	1.45	0.65
1:D:54:TRP:HE1	1:D:209:GLN:NE2	1.93	0.64
1:A:54:TRP:HE1	1:A:209:GLN:NE2	1.95	0.64
1:A:202:ARG:HD3	1:A:202:ARG:N	2.12	0.64
1:B:38:GLN:HE22	1:B:65:SER:CB	2.12	0.62
1:C:154:ILE:HG23	1:C:174:LYS:HE2	1.82	0.61
1:C:38:GLN:NE2	1:C:65:SER:CB	2.64	0.61
1:D:8:MET:HE1	1:D:109:ILE:HD11	1.82	0.60
1:B:-2:SER:HB2	1:B:0:MET:HE2	1.83	0.60
1:C:2:SER:O	1:C:3:VAL:HB	2.01	0.60
1:A:154:ILE:HG23	1:A:174:LYS:HE2	1.84	0.59
1:A:1:VAL:O	1:A:1:VAL:CG1	2.47	0.59
1:A:38:GLN:HE22	1:A:65:SER:CB	2.15	0.59
1:A:154:ILE:CG2	1:A:174:LYS:HE2	2.34	0.58
1:A:55:ASP:HB3	1:A:161:LEU:HD21	1.85	0.58
1:B:74:ASP:OD1	1:B:217:HIS:HE1	1.87	0.58
1:B:72:PRO:HG2	1:B:75:ILE:HD12	1.85	0.57
1:D:74:ASP:OD1	1:D:217:HIS:HE1	1.87	0.57
1:A:36:GLY:HA2	1:A:68:PHE:O	2.04	0.57
1:D:7:GLN:CB	3:D:2017:HOH:O	2.42	0.57
1:C:62:CRQ:HE2	1:C:195:LEU:HB2	1.87	0.56
1:B:54:TRP:HE1	1:B:209:GLN:NE2	2.05	0.55
1:B:200:HIS:HD2	1:B:201:ASN:O	1.89	0.55
1:A:214:ILE:HD13	1:B:219:LEU:HB2	1.88	0.54
1:B:65:SER:N	3:B:2091:HOH:O	2.41	0.54
1:A:38:GLN:NE2	1:A:65:SER:CB	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLU:C	1:B:124:ASN:OD1	2.52	0.53
1:C:216:ARG:HD3	1:D:216:ARG:NH2	2.24	0.53
1:C:110:GLN:NE2	3:C:2088:HOH:O	2.41	0.52
1:B:110:GLN:NE2	3:B:2129:HOH:O	2.42	0.52
1:A:202:ARG:H	1:A:202:ARG:NE	2.07	0.52
1:C:21:HIS:HB2	2:C:1221:SO4:S	2.50	0.52
1:D:194:LYS:HE3	3:D:2189:HOH:O	2.10	0.52
1:C:188:ARG:HG3	3:C:2142:HOH:O	2.10	0.51
1:A:62:CRQ:HD1	3:A:2116:HOH:O	2.10	0.50
1:A:93:MET:HE3	1:A:173:PHE:HZ	1.70	0.50
1:D:38:GLN:HE22	1:D:65:SER:HB3	1.77	0.50
1:A:1:VAL:C	1:A:2:SER:HG	2.20	0.49
1:A:137:GLN:NE2	1:A:164:GLU:HG2	2.28	0.49
1:A:67:PRO:HD3	1:A:87:TYR:OH	2.13	0.49
1:A:194:LYS:HB2	1:B:220:LEU:HG	1.95	0.48
1:A:219:LEU:CD2	1:B:212:ILE:HG21	2.42	0.48
1:C:81:GLN:HE22	1:C:184:ARG:HB2	1.77	0.48
1:B:67:PRO:HD3	1:B:87:TYR:OH	2.14	0.48
1:A:219:LEU:HD23	1:B:212:ILE:CG2	2.43	0.47
1:A:83:PHE:HB3	1:A:84:PRO:HA	1.97	0.47
1:A:210:CYS:SG	3:A:2153:HOH:O	2.53	0.47
1:D:65:SER:N	3:D:2077:HOH:O	2.48	0.46
1:A:219:LEU:CD2	1:B:212:ILE:CG2	2.94	0.46
1:A:20:GLY:O	1:D:-3:GLY:HA2	2.15	0.46
1:B:55:ASP:HB3	1:B:161:LEU:HD21	1.98	0.46
1:A:212:ILE:CD1	1:A:214:ILE:HD11	2.38	0.45
1:A:202:ARG:CD	1:A:202:ARG:N	2.67	0.45
1:C:195:LEU:HD23	1:C:196:ASP:N	2.31	0.45
1:D:139:TRP:CE3	1:D:159:MET:HE3	2.52	0.45
1:D:36:GLY:HA2	1:D:68:PHE:O	2.18	0.44
1:C:105:ASN:ND2	1:C:105:ASN:C	2.76	0.44
1:C:66:ILE:HG22	1:C:66:ILE:O	2.17	0.44
1:C:139:TRP:CE3	1:C:159:MET:HE3	2.53	0.44
1:D:59:PRO:O	1:D:62:CRQ:C2	2.66	0.44
1:B:58:SER:CB	1:B:209:GLN:HE22	2.31	0.43
1:B:139:TRP:CE3	1:B:159:MET:HE3	2.54	0.43
1:D:39:THR:HG23	3:D:2055:HOH:O	2.19	0.43
1:D:58:SER:OG	1:D:59:PRO:HD3	2.19	0.43
1:C:67:PRO:HD3	1:C:87:TYR:OH	2.19	0.43
1:D:55:ASP:HB3	1:D:161:LEU:HD21	2.01	0.43
1:A:1:VAL:O	1:A:2:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TYR:CE1	1:A:172:GLU:HG3	2.54	0.42
1:C:36:GLY:HA2	1:C:68:PHE:O	2.20	0.42
1:A:2:SER:OG	1:A:3:VAL:N	2.50	0.42
1:C:49:PRO:HB3	1:C:203:ASP:HB2	2.02	0.42
1:A:219:LEU:C	1:A:219:LEU:CD2	2.90	0.42
1:D:4:ILE:HD12	1:D:80:LYS:HG2	2.01	0.42
1:B:174:LYS:HB3	3:B:2168:HOH:O	2.20	0.41
1:D:10:TYR:OH	1:D:40:VAL:HB	2.20	0.41
1:D:174:LYS:HD3	1:D:174:LYS:HA	1.85	0.41
1:D:58:SER:HA	1:D:209:GLN:HE22	1.85	0.41
1:D:62:CRQ:HD1	3:D:2159:HOH:O	2.21	0.41
1:C:21:HIS:HB2	2:C:1221:SO4:O2	2.20	0.41
1:A:163:LEU:HD21	1:A:169:TYR:HB2	2.02	0.41
1:B:42:LEU:HG	1:B:61:LEU:HD13	2.03	0.41
1:C:55:ASP:HB3	1:C:161:LEU:HD21	2.02	0.40
1:D:105:ASN:ND2	1:D:105:ASN:C	2.79	0.40
1:A:219:LEU:HD21	1:B:212:ILE:CB	2.48	0.40
1:C:62:CRQ:HD2	1:C:195:LEU:HD12	2.04	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	212/240 (88%)	208 (98%)	3 (1%)	1 (0%)	24	22
1	B	222/240 (92%)	219 (99%)	3 (1%)	0	100	100
1	C	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	22
1	D	223/240 (93%)	220 (99%)	3 (1%)	0	100	100
All	All	868/960 (90%)	852 (98%)	14 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	C	3	VAL

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	188/207 (91%)	179 (95%)	9 (5%)	23	23
1	B	196/207 (95%)	191 (97%)	5 (3%)	40	46
1	C	187/207 (90%)	180 (96%)	7 (4%)	30	33
1	D	197/207 (95%)	187 (95%)	10 (5%)	21	21
All	All	768/828 (93%)	737 (96%)	31 (4%)	28	29

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	66	ILE
1	A	105	ASN
1	A	153	LEU
1	A	181	LYS
1	A	202	ARG
1	A	212	ILE
1	A	214	ILE
1	A	219	LEU
1	B	66	ILE
1	B	105	ASN
1	B	110	GLN
1	B	153	LEU
1	B	220	LEU
1	C	105	ASN
1	C	110	GLN
1	C	123	GLU
1	C	153	LEU
1	C	184	ARG
1	C	209	GLN

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Mol	Chain	Res	Type
1	C	216	ARG
1	D	-7	LEU
1	D	1	VAL
1	D	66	ILE
1	D	105	ASN
1	D	110	GLN
1	D	123	GLU
1	D	153	LEU
1	D	174	LYS
1	D	199	SER
1	D	202	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	94	ASN
1	A	105	ASN
1	A	112	ASN
1	A	124	ASN
1	A	200	HIS
1	A	209	GLN
1	B	38	GLN
1	B	105	ASN
1	B	110	GLN
1	B	112	ASN
1	B	128	ASN
1	B	137	GLN
1	B	200	HIS
1	B	209	GLN
1	B	217	HIS
1	C	38	GLN
1	C	81	GLN
1	C	94	ASN
1	C	105	ASN
1	C	110	GLN
1	C	112	ASN
1	C	124	ASN
1	C	200	HIS
1	D	38	GLN
1	D	105	ASN
1	D	110	GLN

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Mol	Chain	Res	Type
1	D	156	ASN
1	D	200	HIS
1	D	209	GLN
1	D	217	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	CRQ	D	62	1	25,25,26	3.44	7 (28%)	28,34,36	3.50	9 (32%)
1	CRQ	A	62	1	25,25,26	3.33	6 (24%)	28,34,36	3.28	6 (21%)
1	CRQ	B	62	1	25,25,26	3.29	6 (24%)	28,34,36	3.11	8 (28%)
1	CRQ	C	62	1	25,25,26	3.53	7 (28%)	28,34,36	3.71	7 (25%)

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	CRQ	D	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	A	62	1	-	2/10/32/33	0/2/2/2
1	CRQ	B	62	1	-	1/10/32/33	0/2/2/2
1	CRQ	C	62	1	-	1/10/32/33	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	CRQ	CB2-CA2	15.30	1.49	1.35
1	D	62	CRQ	CB2-CA2	14.77	1.49	1.35
1	A	62	CRQ	CB2-CA2	14.36	1.49	1.35
1	B	62	CRQ	CB2-CA2	13.81	1.48	1.35
1	B	62	CRQ	CA2-C2	-4.41	1.43	1.48
1	C	62	CRQ	C1-N2	4.06	1.41	1.33
1	B	62	CRQ	OH-CZ	-4.05	1.27	1.37
1	D	62	CRQ	OH-CZ	-4.03	1.27	1.37
1	C	62	CRQ	C2-N3	-3.96	1.30	1.40
1	D	62	CRQ	CA2-C2	-3.73	1.44	1.48
1	A	62	CRQ	C2-N3	-3.67	1.31	1.40
1	B	62	CRQ	C2-N3	-3.54	1.31	1.40
1	D	62	CRQ	C1-N2	3.46	1.40	1.33
1	C	62	CRQ	OH-CZ	-3.32	1.29	1.37
1	A	62	CRQ	C1-N2	3.28	1.40	1.33
1	B	62	CRQ	O2-C2	3.16	1.29	1.23
1	D	62	CRQ	C2-N3	-3.12	1.32	1.40
1	A	62	CRQ	OH-CZ	-3.06	1.30	1.37
1	B	62	CRQ	C1-N2	3.01	1.39	1.33
1	C	62	CRQ	CA2-C2	-2.97	1.45	1.48
1	A	62	CRQ	O2-C2	2.89	1.29	1.23
1	D	62	CRQ	O2-C2	2.87	1.28	1.23
1	A	62	CRQ	CA2-C2	-2.74	1.45	1.48
1	D	62	CRQ	C1-CA1	2.53	1.51	1.48
1	C	62	CRQ	O2-C2	2.10	1.27	1.23
1	C	62	CRQ	CE1-CD1	2.07	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	CRQ	O2-C2-CA2	-14.72	121.62	131.02
1	C	62	CRQ	O2-C2-CA2	-12.31	123.17	131.02
1	A	62	CRQ	O2-C2-CA2	-12.10	123.30	131.02
1	B	62	CRQ	O2-C2-CA2	-12.05	123.33	131.02
1	C	62	CRQ	CA2-C2-N3	11.60	113.24	103.50
1	A	62	CRQ	CA2-C2-N3	9.33	111.33	103.50
1	D	62	CRQ	CA2-C2-N3	7.73	109.99	103.50
1	B	62	CRQ	CA2-C2-N3	7.18	109.53	103.50
1	C	62	CRQ	C2-CA2-N2	-5.49	105.02	108.95
1	B	62	CRQ	C3-CA3-N3	4.92	123.61	112.43
1	C	62	CRQ	C3-CA3-N3	4.57	122.82	112.43
1	A	62	CRQ	C2-CA2-N2	-4.51	105.72	108.95
1	D	62	CRQ	C3-CA3-N3	3.84	121.16	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	CRQ	CA3-N3-C1	3.56	135.40	128.39
1	B	62	CRQ	CG1-CB1-CA1	-3.40	103.21	113.51
1	A	62	CRQ	C3-CA3-N3	3.21	119.73	112.43
1	D	62	CRQ	CD2-CG2-CD1	2.87	121.91	117.65
1	C	62	CRQ	CG1-CB1-CA1	-2.76	105.15	113.51
1	C	62	CRQ	CB2-CA2-N2	2.75	132.49	128.76
1	A	62	CRQ	CG1-CB1-CA1	-2.72	105.28	113.51
1	A	62	CRQ	CG2-CB2-CA2	2.52	132.86	129.87
1	B	62	CRQ	CD2-CG2-CD1	2.45	121.29	117.65
1	D	62	CRQ	CG1-CB1-CA1	-2.43	106.13	113.51
1	D	62	CRQ	CB2-CA2-N2	2.37	131.98	128.76
1	B	62	CRQ	C2-CA2-N2	-2.29	107.31	108.95
1	D	62	CRQ	C2-CA2-N2	-2.28	107.32	108.95
1	D	62	CRQ	CE1-CD1-CG2	-2.21	118.36	121.22
1	B	62	CRQ	CE2-CD2-CG2	-2.10	118.51	121.22
1	B	62	CRQ	O3-C3-CA3	-2.09	116.04	125.47
1	D	62	CRQ	O3-C3-CA3	-2.02	116.38	125.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	62	CRQ	C1-CA1-CB1-CG1
1	D	62	CRQ	C1-CA1-CB1-CG1
1	A	62	CRQ	CA1-CB1-CG1-CD3
1	A	62	CRQ	C3-CA3-N3-C1
1	C	62	CRQ	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	62	CRQ	2	0
1	A	62	CRQ	1	0
1	B	62	CRQ	1	0
1	C	62	CRQ	2	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 ligands 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	SO4	B	1222	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	C	1220	-	4,4,4	0.31	0	6,6,6	0.11	0
2	SO4	B	1223	-	4,4,4	0.30	0	6,6,6	0.19	0
2	SO4	C	1221	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	D	1223	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	D	1222	-	4,4,4	0.32	0	6,6,6	0.72	0
2	SO4	D	1224	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	A	1222	-	4,4,4	0.29	0	6,6,6	0.36	0
2	SO4	A	1221	-	4,4,4	0.21	0	6,6,6	0.22	0
2	SO4	A	1220	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	B	1224	-	4,4,4	0.25	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1221	SO4	3	0

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	A	216/240 (90%)	-0.06	4 (1%) 66 69	13, 21, 32, 39	1 (0%)
1	B	226/240 (94%)	0.00	8 (3%) 47 49	12, 20, 35, 52	2 (0%)
1	C	215/240 (89%)	-0.13	1 (0%) 87 88	11, 20, 30, 44	1 (0%)
1	D	226/240 (94%)	-0.00	8 (3%) 47 49	12, 21, 37, 49	3 (1%)
All	All	883/960 (91%)	-0.05	21 (2%) 59 62	11, 20, 34, 52	7 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-7	LEU	5.0
1	A	1	VAL	4.6
1	B	-7	LEU	3.9
1	D	221	GLY	3.8
1	B	123	GLU	3.6
1	D	165	GLY	3.3
1	B	221	GLY	3.3
1	C	2	SER	3.0
1	A	2	SER	2.9
1	D	123	GLU	2.7
1	B	165	GLY	2.7
1	D	-1	HIS	2.6
1	A	219	LEU	2.6
1	D	-6	VAL	2.6
1	D	0	MET	2.4
1	D	166	GLY	2.3
1	B	-1	HIS	2.3
1	B	-6	VAL	2.2
1	B	1	VAL	2.1
1	B	-3	GLY	2.1
1	A	165	GLY	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	CRQ	C	62	24/25	0.86	0.12	21,25,32,34	0
1	CRQ	A	62	24/25	0.88	0.11	18,22,29,31	0
1	CRQ	D	62	24/25	0.88	0.11	20,23,32,33	0
1	CRQ	B	62	24/25	0.90	0.10	19,21,29,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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	SO4	C	1221	5/5	0.68	0.19	93,94,94,95	0
2	SO4	A	1221	5/5	0.77	0.16	86,86,87,87	0
2	SO4	C	1220	5/5	0.80	0.16	88,88,88,89	0
2	SO4	A	1222	5/5	0.83	0.17	80,80,80,81	0
2	SO4	B	1223	5/5	0.83	0.15	90,91,91,91	0
2	SO4	D	1224	5/5	0.83	0.17	90,90,90,90	0
2	SO4	D	1223	5/5	0.86	0.14	70,71,72,73	0
2	SO4	A	1220	5/5	0.87	0.15	82,82,83,83	0
2	SO4	B	1224	5/5	0.88	0.12	79,79,79,79	0
2	SO4	D	1222	5/5	0.94	0.10	36,36,38,41	0
2	SO4	B	1222	5/5	0.97	0.11	34,36,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.