



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:17 am BST

PDB ID : 1ZGO
Title : High Resolution Crystal Structure of the Discosoma Red Fluorescent Protein (DsRed)
Authors : Tubbs, J.L.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2005-04-21
Resolution : 1.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

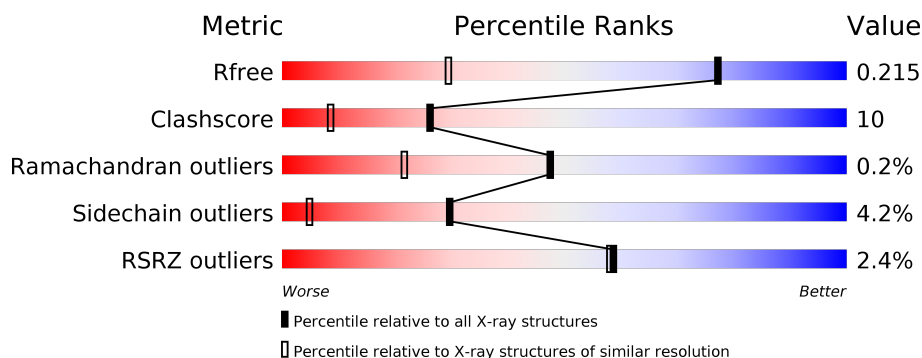
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>••</div> </div> </div>
1	B	223	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>••</div> </div> </div>
1	C	223	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>••</div> </div> </div>
1	D	223	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>5%</div> <div>•</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7754 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 Red fluorescent protein drFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	4	0
			1805	1166	301	331	7			
1	B	218	Total	C	N	O	S	0	3	0
			1802	1164	301	330	7			
1	C	218	Total	C	N	O	S	0	5	0
			1807	1167	301	331	8			
1	D	218	Total	C	N	O	S	0	4	0
			1805	1166	301	331	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
A	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
A	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	136	Total	O	0	0
			136	136		
2	B	129	Total	O	0	0
			129	129		

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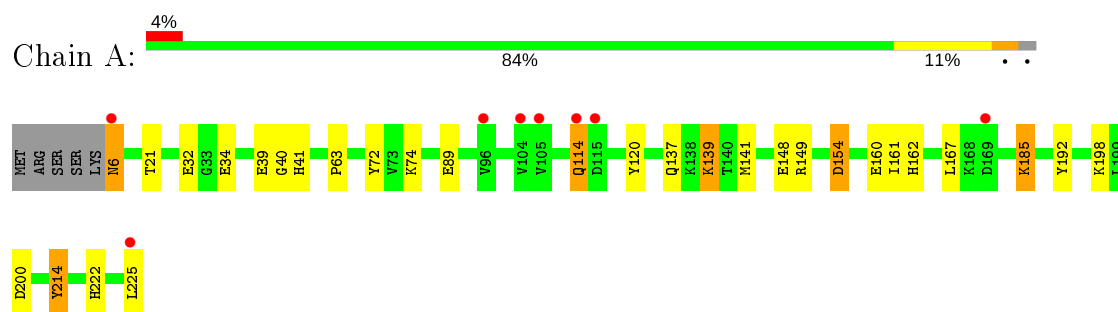
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	137	Total 137	O 137	0	0
2	D	133	Total 133	O 133	0	0

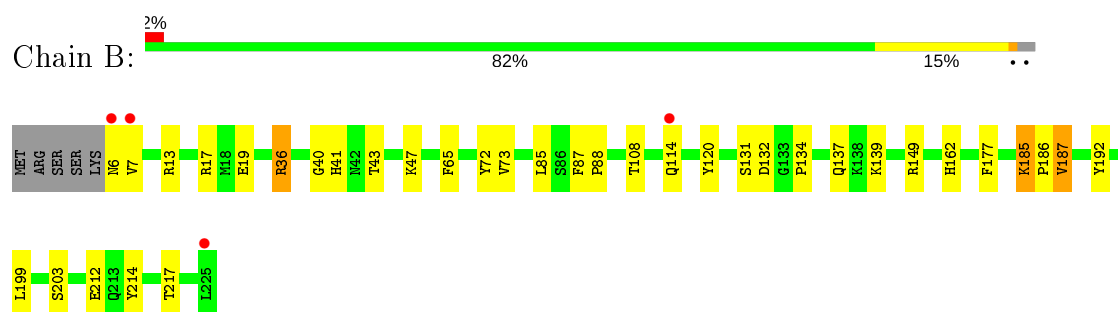
3 Residue-property plots [i](#)

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.

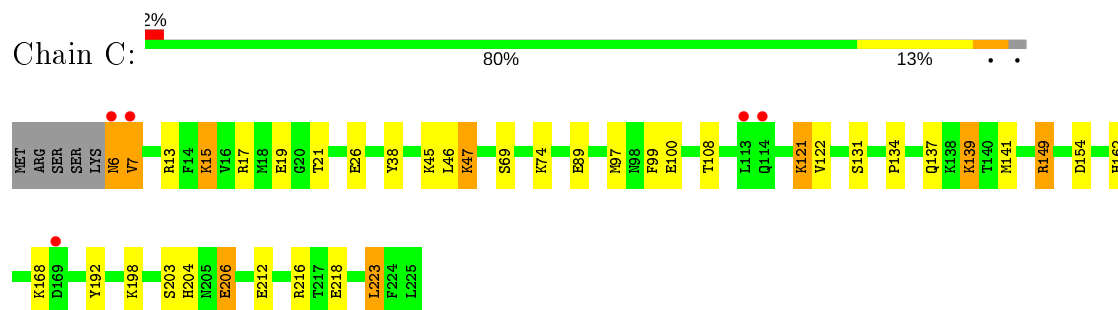
- Molecule 1: Red fluorescent protein drFP583



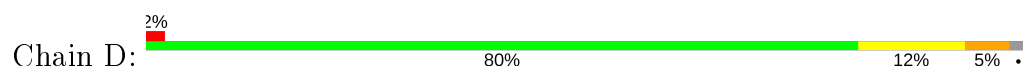
- Molecule 1: Red fluorescent protein drFP583

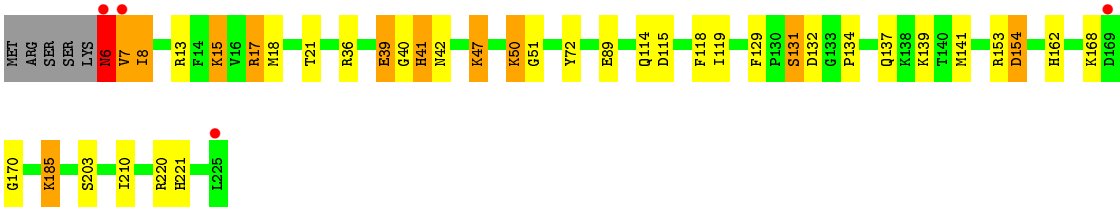


- Molecule 1: Red fluorescent protein drFP583



- Molecule 1: Red fluorescent protein drFP583





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.72Å 127.22Å 57.12Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	40.00 – 1.40 36.10 – 1.40	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.00-1.40) 90.9 (36.10-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.40Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.143 , 0.206 0.153 , 0.215	Depositor DCC
R_{free} test set	7412 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7754	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.78 % 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 5.3452e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/1840	1.14	4/2476 (0.2%)
1	B	0.52	0/1833	1.15	7/2466 (0.3%)
1	C	0.49	0/1846	1.10	4/2484 (0.2%)
1	D	0.52	0/1840	1.17	7/2476 (0.3%)
All	All	0.51	0/7359	1.14	22/9902 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	ARG	NE-CZ-NH1	-8.69	115.96	120.30
1	A	192	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	B	36	ARG	CD-NE-CZ	6.33	132.46	123.60
1	B	65[A]	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	B	65[B]	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	D	153	ARG	CD-NE-CZ	-6.19	114.93	123.60
1	B	13	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	D	36	ARG	NE-CZ-NH2	6.09	123.35	120.30
1	C	149	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	214	TYR	CB-CG-CD1	5.86	124.52	121.00
1	B	120	TYR	CB-CG-CD1	5.84	124.50	121.00
1	C	216	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	C	38	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	D	153	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	120	TYR	CB-CG-CD1	5.58	124.35	121.00
1	D	13	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	D	6	ASN	C-N-CA	5.49	135.42	121.70
1	D	129	PHE	CB-CG-CD1	5.25	124.47	120.80
1	B	177	PHE	CB-CG-CD1	5.21	124.45	120.80
1	A	192	TYR	CB-CG-CD2	5.21	124.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	36	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	A	1805	0	1745	26	3
1	B	1802	0	1744	33	3
1	C	1807	0	1748	49	0
1	D	1805	0	1747	54	0
2	A	136	0	0	4	0
2	B	129	0	0	2	0
2	C	137	0	0	5	0
2	D	133	0	0	2	0
All	All	7754	0	6984	148	3

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 10.

All (148) 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:C:141:MET:SD	1:C:168:LYS:HA	1.49	1.51
1:D:134:PRO:CA	1:D:139:LYS:HE3	1.69	1.23
1:C:6:ASN:ND2	1:C:7:VAL:HG13	1.57	1.20
1:D:134:PRO:HA	1:D:139:LYS:CE	1.73	1.18
1:A:6:ASN:O	1:A:6:ASN:OD1	1.62	1.18
1:C:6:ASN:CG	1:C:7:VAL:H	1.51	1.12
1:C:108:THR:HG21	1:D:21[B]:THR:HG21	1.33	1.10
1:C:141:MET:SD	1:C:168:LYS:CA	2.40	1.09
1:A:21[B]:THR:HG21	1:B:108:THR:HG21	1.37	1.06
1:B:185:LYS:HE2	1:B:187:VAL:CG2	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:PRO:HA	1:D:139:LYS:HE3	1.23	1.05
1:C:141:MET:HG2	1:C:168:LYS:HG2	1.34	1.05
1:C:131:SER:OG	1:D:154:ASP:OD1	1.75	1.01
1:C:154:ASP:OD1	1:D:131:SER:OG	1.82	0.97
2:C:301:HOH:O	1:D:21[B]:THR:HG23	1.68	0.94
1:A:154:ASP:OD1	1:B:131:SER:HB3	1.66	0.94
1:C:6:ASN:HD21	1:C:7:VAL:HG13	1.19	0.93
1:D:141:MET:SD	1:D:168:LYS:HA	2.09	0.92
1:C:134:PRO:HA	1:C:139:LYS:HD3	1.51	0.91
1:C:141:MET:CG	1:C:168:LYS:HG2	1.99	0.91
1:B:41:HIS:ND1	1:B:214:TYR:OH	2.03	0.91
1:C:19:GLU:OE2	1:C:121:LYS:NZ	2.03	0.90
1:C:137:GLN:HB2	1:C:139:LYS:HD2	1.52	0.90
1:C:6:ASN:CG	1:C:7:VAL:N	2.25	0.88
1:B:185:LYS:HE2	1:B:187:VAL:HG23	1.57	0.86
1:C:141:MET:HG2	1:C:168:LYS:CG	2.07	0.85
1:B:47:LYS:NZ	2:B:352:HOH:O	2.02	0.84
1:A:41:HIS:ND1	1:A:214:TYR:OH	2.12	0.83
1:B:185:LYS:HE2	1:B:187:VAL:HG21	1.58	0.83
1:C:6:ASN:ND2	1:C:7:VAL:H	1.75	0.83
1:D:134:PRO:HA	1:D:139:LYS:HE2	1.63	0.79
1:D:8:ILE:HD13	1:D:118:PHE:HZ	1.46	0.79
1:B:185:LYS:CE	1:B:187:VAL:HG23	2.13	0.78
1:A:154:ASP:OD1	1:B:131:SER:CB	2.32	0.76
1:C:154:ASP:CG	1:D:131:SER:OG	2.25	0.75
1:D:134:PRO:N	1:D:139:LYS:HE3	2.02	0.75
1:D:134:PRO:CA	1:D:139:LYS:CE	2.46	0.75
1:B:137:GLN:HB2	1:B:139:LYS:HE3	1.69	0.74
1:A:34:GLU:OE1	2:A:334:HOH:O	2.06	0.74
1:B:185:LYS:CE	1:B:187:VAL:CG2	2.68	0.71
1:D:6:ASN:O	1:D:7:VAL:HG22	1.90	0.70
1:D:139:LYS:HA	1:D:168:LYS:HD2	1.74	0.70
1:B:185:LYS:CD	1:B:187:VAL:HG23	2.21	0.70
1:D:15:LYS:NZ	1:D:119:ILE:CD1	2.56	0.69
1:C:74:LYS:HB3	1:C:218:GLU:HG2	1.75	0.69
1:D:39:GLU:HB3	1:D:41:HIS:CE1	2.28	0.68
1:C:137:GLN:CB	1:C:139:LYS:HD2	2.24	0.67
1:D:6:ASN:C	1:D:7:VAL:HG22	2.15	0.67
1:D:137:GLN:HB2	1:D:139:LYS:HE2	1.77	0.67
1:C:141:MET:SD	1:C:168:LYS:HG2	2.35	0.66
1:C:108:THR:CG2	1:D:21[B]:THR:HG21	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:MET:HE3	1:C:99:PHE:CE1	2.32	0.65
1:C:141:MET:CG	1:C:168:LYS:CG	2.72	0.64
1:A:6:ASN:O	1:A:6:ASN:CG	2.32	0.64
1:B:185:LYS:HD3	1:B:187:VAL:HG23	1.78	0.63
1:D:15:LYS:NZ	1:D:119:ILE:HD11	2.14	0.63
1:C:198:LYS:HE2	2:C:327:HOH:O	1.97	0.63
1:D:15:LYS:HZ2	1:D:119:ILE:HD12	1.64	0.63
1:D:15:LYS:HZ2	1:D:119:ILE:CD1	2.12	0.62
1:C:97:MET:HE3	1:C:99:PHE:CZ	2.37	0.59
1:A:40:GLY:HA2	1:A:72:TYR:O	2.01	0.59
1:A:185:LYS:O	1:A:185:LYS:HG2	2.04	0.58
1:D:141:MET:SD	1:D:168:LYS:HG2	2.43	0.58
1:D:15:LYS:HZ1	1:D:119:ILE:HD11	1.69	0.57
1:D:134:PRO:CB	1:D:139:LYS:HE3	2.32	0.57
1:D:50:LYS:CD	1:D:51:GLY:N	2.67	0.57
1:B:6:ASN:CG	1:B:7:VAL:H	2.09	0.56
1:D:89:GLU:OE1	1:D:185:LYS:HE2	2.05	0.56
1:D:17:ARG:HG2	1:D:18:MET:N	2.19	0.55
1:C:45:LYS:HG3	1:C:212:GLU:HG2	1.89	0.55
1:D:50:LYS:HD3	1:D:51:GLY:H	1.72	0.55
1:D:50:LYS:HD2	1:D:51:GLY:N	2.22	0.54
1:C:45:LYS:HE2	1:C:47:LYS:HE3	1.90	0.54
1:B:85:LEU:HB2	1:B:187:VAL:HG11	1.89	0.53
1:C:17:ARG:O	1:C:121:LYS:HE3	2.09	0.53
1:A:137:GLN:CB	1:A:139:LYS:NZ	2.71	0.53
1:B:212:GLU:HG2	2:B:335:HOH:O	2.09	0.53
1:C:21[A]:THR:HG22	1:C:26:GLU:HG2	1.90	0.53
1:B:40:GLY:HA2	1:B:72:TYR:O	2.09	0.52
1:D:134:PRO:N	1:D:139:LYS:CE	2.69	0.52
1:C:100:GLU:O	2:C:335:HOH:O	2.18	0.52
1:B:43:THR:HG22	1:B:214:TYR:HD1	1.75	0.52
1:C:203:SER:C	2:C:318:HOH:O	2.49	0.52
1:D:47:LYS:HD2	1:D:210:ILE:HG12	1.91	0.52
1:C:206:GLU:O	1:C:206:GLU:HG3	2.10	0.51
1:A:141:MET:HE3	2:A:335:HOH:O	2.10	0.51
1:A:21[B]:THR:HG21	1:B:108:THR:CG2	2.25	0.51
1:A:6:ASN:OD1	1:A:6:ASN:C	2.43	0.51
1:C:131:SER:OG	1:D:154:ASP:CG	2.48	0.51
1:D:8:ILE:HD13	1:D:118:PHE:CZ	2.37	0.51
1:A:137:GLN:HB3	1:A:139:LYS:NZ	2.26	0.51
1:A:185:LYS:H	1:A:185:LYS:NZ	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:HIS:CE1	2:D:338:HOH:O	2.64	0.50
1:A:149:ARG:HD2	1:A:149:ARG:C	2.32	0.50
1:B:185:LYS:HD3	1:B:187:VAL:CG2	2.41	0.50
1:D:203:SER:OG	2:D:357:HOH:O	2.01	0.50
1:D:15:LYS:HZ1	1:D:119:ILE:CD1	2.23	0.49
1:D:114:GLN:O	1:D:115:ASP:C	2.50	0.49
1:D:6:ASN:O	1:D:7:VAL:CG2	2.61	0.48
1:D:141:MET:SD	1:D:168:LYS:CA	2.93	0.48
1:D:50:LYS:CD	1:D:51:GLY:H	2.26	0.48
1:A:222:HIS:HB3	1:A:225:LEU:HG	1.95	0.48
1:C:6:ASN:ND2	1:C:7:VAL:CG1	2.52	0.48
1:C:131:SER:HG	1:D:154:ASP:CG	2.14	0.48
1:C:6:ASN:ND2	1:C:7:VAL:N	2.52	0.47
1:C:121:LYS:HE3	1:C:122:VAL:H	1.78	0.47
1:D:6:ASN:HD22	1:D:6:ASN:C	2.17	0.47
1:A:74:LYS:HE2	2:A:359:HOH:O	2.13	0.47
1:A:198:LYS:NZ	1:A:200:ASP:OD1	2.48	0.47
1:B:17:ARG:NH1	1:B:19:GLU:OE2	2.46	0.47
1:B:132:ASP:OD2	1:B:132:ASP:N	2.46	0.47
1:B:87:PHE:HB3	1:B:88:PRO:HA	1.97	0.47
1:D:50:LYS:HD3	1:D:51:GLY:N	2.31	0.46
1:C:121:LYS:HE2	1:C:122:VAL:N	2.31	0.46
1:C:154:ASP:OD2	1:D:131:SER:OG	2.33	0.45
1:C:149:ARG:HD3	1:C:192:TYR:CZ	2.52	0.45
1:D:141:MET:SD	1:D:168:LYS:CG	3.04	0.45
1:B:149:ARG:HD3	1:B:192:TYR:CZ	2.52	0.45
1:C:89:GLU:H	1:C:89:GLU:CD	2.18	0.45
1:B:134:PRO:N	1:B:139:LYS:HZ2	2.15	0.45
1:B:6:ASN:ND2	1:B:7:VAL:HG22	2.32	0.44
1:D:132:ASP:OD1	1:D:132:ASP:N	2.46	0.44
1:A:149:ARG:NH2	1:A:160:GLU:OE1	2.35	0.43
1:A:41:HIS:CE1	1:A:214:TYR:OH	2.71	0.43
1:B:137:GLN:CB	1:B:139:LYS:HE3	2.45	0.43
1:A:114:GLN:HE21	1:A:114:GLN:HB2	1.55	0.43
1:A:162:HIS:CE1	1:C:162:HIS:CE1	3.06	0.43
1:D:6:ASN:C	1:D:7:VAL:CG2	2.85	0.42
1:C:141:MET:SD	1:C:168:LYS:CG	3.06	0.42
1:B:85:LEU:HB2	1:B:187:VAL:CG1	2.50	0.42
1:B:203:SER:HB3	1:B:212:GLU:HB3	2.01	0.42
1:D:15:LYS:HB3	1:D:15:LYS:HE3	1.44	0.42
1:B:199:LEU:C	1:B:199:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LYS:CE	1:C:122:VAL:H	2.32	0.42
1:B:185:LYS:HG2	1:B:186:PRO:N	2.35	0.41
1:C:121:LYS:HB3	1:C:121:LYS:HE2	1.84	0.41
1:D:50:LYS:HA	1:D:50:LYS:HD3	1.93	0.41
1:B:162:HIS:CE1	1:D:162:HIS:CE1	3.09	0.41
1:C:97:MET:CE	1:C:99:PHE:CZ	3.04	0.41
1:B:73:VAL:HA	1:B:217:THR:HG23	2.03	0.41
1:C:204:HIS:N	2:C:318:HOH:O	2.54	0.41
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.91	0.41
1:A:148:GLU:HG3	1:A:161:ILE:HG12	2.03	0.41
1:C:15:LYS:NZ	1:C:15:LYS:HB3	2.36	0.41
1:D:40:GLY:HA2	1:D:72:TYR:O	2.21	0.41
1:A:167:LEU:HB3	2:A:315:HOH:O	2.22	0.40
1:D:39:GLU:HB3	1:D:41:HIS:NE2	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:OE2	1:B:36:ARG:NH2[1_656]	1.74	0.46
1:A:39:GLU:OE1	1:B:36:ARG:NH2[1_656]	2.03	0.17
1:A:39:GLU:CD	1:B:36:ARG:NH2[1_656]	2.15	0.05

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	218/223 (98%)	214 (98%)	4 (2%)	0	100	100
1	B	217/223 (97%)	213 (98%)	4 (2%)	0	100	100
1	C	219/223 (98%)	214 (98%)	5 (2%)	0	100	100
1	D	218/223 (98%)	209 (96%)	7 (3%)	2 (1%)	17	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	872/892 (98%)	850 (98%)	20 (2%)	2 (0%)	47 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	7	VAL
1	D	170	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/196 (99%)	187 (96%)	7 (4%)	35 7
1	B	193/196 (98%)	190 (98%)	3 (2%)	62 33
1	C	195/196 (100%)	184 (94%)	11 (6%)	21 2
1	D	194/196 (99%)	182 (94%)	12 (6%)	18 1
All	All	776/784 (99%)	743 (96%)	33 (4%)	30 4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	32	GLU
1	A	89	GLU
1	A	114	GLN
1	A	139	LYS
1	A	154	ASP
1	A	185	LYS
1	B	114	GLN
1	B	185	LYS
1	B	187	VAL
1	C	6	ASN
1	C	7	VAL
1	C	15	LYS

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Mol	Chain	Res	Type
1	C	46	LEU
1	C	47	LYS
1	C	69[A]	SER
1	C	69[B]	SER
1	C	121	LYS
1	C	139	LYS
1	C	206	GLU
1	C	223	LEU
1	D	6	ASN
1	D	8	ILE
1	D	15	LYS
1	D	17	ARG
1	D	39	GLU
1	D	41	HIS
1	D	42	ASN
1	D	47	LYS
1	D	50	LYS
1	D	131	SER
1	D	154	ASP
1	D	185	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	B	6	ASN
1	C	41	HIS
1	C	114	GLN
1	D	6	ASN
1	D	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRQ	A	66[B]	1	24,25,26	2.50	4 (16%)	27,34,36	3.12	9 (33%)
1	CRQ	D	66[A]	1	24,25,26	2.45	8 (33%)	27,34,36	2.87	9 (33%)
1	CRQ	D	66[B]	1	24,25,26	2.15	5 (20%)	27,34,36	3.50	11 (40%)
1	CRQ	B	66[B]	1	24,25,26	2.34	5 (20%)	27,34,36	3.22	9 (33%)
1	CRQ	C	66[B]	1	24,25,26	2.20	5 (20%)	27,34,36	3.00	9 (33%)
1	CRQ	B	66[A]	1	24,25,26	2.64	8 (33%)	27,34,36	2.97	9 (33%)
1	CRQ	A	66[A]	1	24,25,26	2.77	8 (33%)	27,34,36	2.49	6 (22%)
1	CRQ	C	66[A]	1	24,25,26	2.52	8 (33%)	27,34,36	2.34	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	A	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	D	66[A]	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	B	66[B]	1	-	2/10/32/33	0/2/2/2
1	CRQ	C	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	B	66[A]	1	-	0/10/32/33	0/2/2/2
1	CRQ	A	66[A]	1	-	1/10/32/33	0/2/2/2
1	CRQ	C	66[A]	1	-	1/10/32/33	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66[B]	CRQ	CA2-C2	-8.30	1.40	1.48
1	A	66[A]	CRQ	CA2-C2	-8.30	1.40	1.48
1	B	66[B]	CRQ	CA2-C2	-7.77	1.41	1.48
1	B	66[A]	CRQ	CA2-C2	-7.77	1.41	1.48
1	C	66[B]	CRQ	CA2-C2	-7.61	1.41	1.48
1	C	66[A]	CRQ	CA2-C2	-7.61	1.41	1.48
1	D	66[A]	CRQ	CA2-C2	-6.99	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66[B]	CRQ	CA2-C2	-6.99	1.41	1.48
1	A	66[B]	CRQ	OH-CZ	-5.22	1.24	1.37
1	A	66[A]	CRQ	OH-CZ	-5.22	1.24	1.37
1	B	66[A]	CRQ	C1-N3	-4.78	1.30	1.38
1	B	66[B]	CRQ	CG2-CB2	-4.61	1.38	1.46
1	B	66[A]	CRQ	CG2-CB2	-4.61	1.38	1.46
1	A	66[B]	CRQ	CG2-CB2	-4.42	1.38	1.46
1	A	66[A]	CRQ	CG2-CB2	-4.42	1.38	1.46
1	C	66[B]	CRQ	OH-CZ	-4.41	1.26	1.37
1	C	66[A]	CRQ	OH-CZ	-4.41	1.26	1.37
1	B	66[B]	CRQ	OH-CZ	-4.38	1.26	1.37
1	B	66[A]	CRQ	OH-CZ	-4.38	1.26	1.37
1	D	66[A]	CRQ	OH-CZ	-4.28	1.27	1.37
1	D	66[B]	CRQ	OH-CZ	-4.28	1.27	1.37
1	C	66[A]	CRQ	C1-N3	-4.24	1.31	1.38
1	D	66[A]	CRQ	C1-N3	-4.03	1.31	1.38
1	A	66[A]	CRQ	C1-N3	-3.89	1.31	1.38
1	D	66[A]	CRQ	CG2-CB2	-3.85	1.39	1.46
1	D	66[B]	CRQ	CG2-CB2	-3.85	1.39	1.46
1	C	66[B]	CRQ	CG2-CB2	-3.80	1.39	1.46
1	C	66[A]	CRQ	CG2-CB2	-3.80	1.39	1.46
1	B	66[B]	CRQ	O-C	3.50	1.39	1.19
1	B	66[A]	CRQ	O-C	3.50	1.39	1.19
1	D	66[A]	CRQ	CA1-N	3.46	1.35	1.27
1	A	66[A]	CRQ	CA1-N	3.44	1.35	1.27
1	A	66[B]	CRQ	O-C	3.44	1.39	1.19
1	A	66[A]	CRQ	O-C	3.44	1.39	1.19
1	A	66[A]	CRQ	CB1-CA1	3.37	1.59	1.50
1	C	66[A]	CRQ	CA1-N	3.36	1.35	1.27
1	B	66[A]	CRQ	CA1-N	3.33	1.35	1.27
1	C	66[B]	CRQ	O-C	3.29	1.38	1.19
1	C	66[A]	CRQ	O-C	3.29	1.38	1.19
1	C	66[A]	CRQ	CB1-CA1	3.21	1.59	1.50
1	D	66[A]	CRQ	CB1-CA1	3.18	1.59	1.50
1	D	66[A]	CRQ	O-C	3.06	1.37	1.19
1	D	66[B]	CRQ	O-C	3.06	1.37	1.19
1	B	66[A]	CRQ	CB1-CA1	3.01	1.58	1.50
1	B	66[B]	CRQ	C1-N3	-2.96	1.33	1.38
1	D	66[B]	CRQ	C1-N3	-2.27	1.34	1.38
1	C	66[B]	CRQ	C1-N3	-2.15	1.34	1.38
1	B	66[A]	CRQ	C2-N3	-2.14	1.34	1.39
1	A	66[A]	CRQ	C2-N3	-2.12	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66[A]	CRQ	C2-N3	-2.09	1.34	1.39
1	C	66[A]	CRQ	C2-N3	-2.04	1.35	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66[B]	CRQ	CG2-CB2-CA2	9.09	141.08	129.94
1	B	66[A]	CRQ	CG2-CB2-CA2	9.09	141.08	129.94
1	D	66[A]	CRQ	CA2-C2-N3	8.64	107.46	103.37
1	A	66[A]	CRQ	CA2-C2-N3	8.23	107.26	103.37
1	D	66[B]	CRQ	C2-CA2-N2	-8.20	103.19	108.93
1	B	66[A]	CRQ	CA2-C2-N3	8.02	107.17	103.37
1	D	66[B]	CRQ	CA2-C2-N3	8.02	107.16	103.37
1	D	66[A]	CRQ	CG2-CB2-CA2	7.51	139.14	129.94
1	D	66[B]	CRQ	CG2-CB2-CA2	7.51	139.14	129.94
1	A	66[B]	CRQ	CA2-C2-N3	7.44	106.89	103.37
1	C	66[B]	CRQ	C2-CA2-N2	-7.14	103.93	108.93
1	C	66[A]	CRQ	CA2-C2-N3	6.95	106.66	103.37
1	A	66[B]	CRQ	C2-CA2-N2	-6.91	104.09	108.93
1	A	66[B]	CRQ	N3-C1-N2	-6.80	104.30	113.28
1	D	66[B]	CRQ	N3-C1-N2	-6.59	104.58	113.28
1	C	66[B]	CRQ	N3-C1-N2	-6.56	104.62	113.28
1	B	66[B]	CRQ	C2-CA2-N2	-6.33	104.50	108.93
1	A	66[B]	CRQ	CG2-CB2-CA2	6.25	137.60	129.94
1	A	66[A]	CRQ	CG2-CB2-CA2	6.25	137.60	129.94
1	C	66[B]	CRQ	CA2-C2-N3	6.25	106.32	103.37
1	B	66[B]	CRQ	CA2-C2-N3	6.24	106.32	103.37
1	C	66[B]	CRQ	CG2-CB2-CA2	5.82	137.08	129.94
1	C	66[A]	CRQ	CG2-CB2-CA2	5.82	137.08	129.94
1	B	66[B]	CRQ	N3-C1-N2	-5.69	105.77	113.28
1	D	66[B]	CRQ	CA2-N2-C1	5.08	113.63	104.33
1	C	66[B]	CRQ	CA2-N2-C1	4.85	113.21	104.33
1	A	66[B]	CRQ	CA2-N2-C1	4.77	113.05	104.33
1	A	66[B]	CRQ	O2-C2-CA2	-4.53	128.42	130.96
1	A	66[A]	CRQ	O2-C2-CA2	-4.53	128.42	130.96
1	B	66[B]	CRQ	CB2-CA2-C2	4.37	127.49	122.28
1	B	66[A]	CRQ	CB2-CA2-C2	4.37	127.49	122.28
1	B	66[B]	CRQ	CA2-N2-C1	4.11	111.84	104.33
1	C	66[A]	CRQ	CG1-CB1-CA1	-3.78	101.80	113.53
1	D	66[A]	CRQ	O2-C2-CA2	-3.75	128.85	130.96
1	D	66[B]	CRQ	O2-C2-CA2	-3.75	128.85	130.96
1	B	66[B]	CRQ	O-C-CA3	-3.55	115.66	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66[A]	CRQ	O-C-CA3	-3.55	115.66	126.39
1	A	66[A]	CRQ	CG1-CB1-CA1	-3.52	102.61	113.53
1	B	66[B]	CRQ	CD1-CE1-CZ	3.46	123.67	119.88
1	B	66[A]	CRQ	CD1-CE1-CZ	3.46	123.67	119.88
1	D	66[A]	CRQ	O-C-CA3	-3.37	116.21	126.39
1	D	66[B]	CRQ	O-C-CA3	-3.37	116.21	126.39
1	B	66[A]	CRQ	CB2-CA2-N2	-3.34	124.19	128.83
1	A	66[B]	CRQ	O-C-CA3	-3.30	116.41	126.39
1	A	66[A]	CRQ	O-C-CA3	-3.30	116.41	126.39
1	D	66[A]	CRQ	CA3-N3-C1	3.26	134.60	128.22
1	C	66[B]	CRQ	O-C-CA3	-3.22	116.67	126.39
1	C	66[A]	CRQ	O-C-CA3	-3.22	116.67	126.39
1	C	66[B]	CRQ	CD1-CE1-CZ	3.19	123.37	119.88
1	C	66[A]	CRQ	CD1-CE1-CZ	3.19	123.37	119.88
1	D	66[A]	CRQ	CD2-CE2-CZ	3.08	123.25	119.88
1	D	66[B]	CRQ	CD2-CE2-CZ	3.08	123.25	119.88
1	D	66[A]	CRQ	CE2-CZ-CE1	-2.75	115.14	119.77
1	D	66[B]	CRQ	CE2-CZ-CE1	-2.75	115.14	119.77
1	D	66[A]	CRQ	CG1-CB1-CA1	-2.65	105.30	113.53
1	A	66[B]	CRQ	CB2-CA2-C2	2.55	125.32	122.28
1	A	66[A]	CRQ	CB2-CA2-C2	2.55	125.32	122.28
1	C	66[B]	CRQ	CE2-CZ-CE1	-2.44	115.66	119.77
1	C	66[A]	CRQ	CE2-CZ-CE1	-2.44	115.66	119.77
1	B	66[A]	CRQ	CG1-CB1-CA1	-2.42	106.01	113.53
1	D	66[A]	CRQ	CB2-CA2-C2	2.31	125.03	122.28
1	D	66[B]	CRQ	CB2-CA2-C2	2.31	125.03	122.28
1	A	66[B]	CRQ	CA3-N3-C1	-2.20	123.91	128.22
1	B	66[A]	CRQ	N3-C1-N2	2.12	116.08	113.28
1	C	66[B]	CRQ	CB2-CA2-N2	2.09	131.73	128.83
1	D	66[B]	CRQ	CB2-CA2-N2	2.08	131.71	128.83
1	B	66[B]	CRQ	CB1-CG1-CD3	2.02	124.29	114.16
1	C	66[A]	CRQ	CA3-N3-C1	2.02	132.18	128.22
1	B	66[A]	CRQ	CA3-N3-C1	2.01	132.17	128.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66[B]	CRQ	C1-CA1-CB1-CG1
1	D	66[B]	CRQ	C1-CA1-CB1-CG1
1	B	66[B]	CRQ	C1-CA1-CB1-CG1
1	C	66[B]	CRQ	C1-CA1-CB1-CG1

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Mol	Chain	Res	Type	Atoms
1	A	66[A]	CRQ	C1-CA1-CB1-CG1
1	B	66[B]	CRQ	CA1-CB1-CG1-CD3
1	C	66[A]	CRQ	C1-CA1-CB1-CG1

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	217/223 (97%)	0.07	8 (3%)	41 41	12, 17, 31, 54	2 (0%)
1	B	217/223 (97%)	0.03	4 (1%)	68 68	12, 17, 30, 57	6 (2%)
1	C	217/223 (97%)	0.22	5 (2%)	60 60	12, 19, 35, 70	2 (0%)
1	D	217/223 (97%)	0.10	4 (1%)	68 68	12, 18, 33, 66	3 (1%)
All	All	868/892 (97%)	0.11	21 (2%)	59 58	12, 18, 33, 70	13 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	ASN	7.5
1	D	7	VAL	6.2
1	D	6	ASN	5.9
1	A	6	ASN	4.7
1	B	6	ASN	4.4
1	D	225	LEU	3.5
1	A	115	ASP	3.4
1	D	169	ASP	3.3
1	A	114	GLN	3.2
1	C	114	GLN	2.4
1	A	104	VAL	2.3
1	B	225	LEU	2.3
1	C	113	LEU	2.3
1	C	7	VAL	2.3
1	A	225	LEU	2.2
1	A	96	VAL	2.2
1	C	169	ASP	2.2
1	B	7	VAL	2.1
1	A	169	ASP	2.1
1	B	114	GLN	2.0
1	A	105	VAL	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(\AA^2)	Q<0.9
1	CRQ	A	66[B]	24/25	0.94	0.08	14,16,17,22	6
1	CRQ	D	66[A]	24/25	0.94	0.09	13,16,20,23	6
1	CRQ	D	66[B]	24/25	0.94	0.09	13,16,18,23	6
1	CRQ	C	66[B]	24/25	0.94	0.09	14,17,19,21	6
1	CRQ	A	66[A]	24/25	0.94	0.08	14,16,18,22	6
1	CRQ	C	66[A]	24/25	0.94	0.09	14,17,20,21	6
1	CRQ	B	66[B]	24/25	0.95	0.08	13,17,19,23	6
1	CRQ	B	66[A]	24/25	0.95	0.08	13,17,19,23	6

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.