



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 10:11 pm GMT

PDB ID : 2VAE  
Title : Fast maturing red fluorescent protein, DsRed.T4  
Authors : Strongin, D.E.; Bevis, B.; Khuong, N.; Downing, M.E.; Strack, R.L.; Sundaram, K.; Glick, B.S.; Keenan, R.J.  
Deposited on : 2007-08-31  
Resolution : 1.64 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

<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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

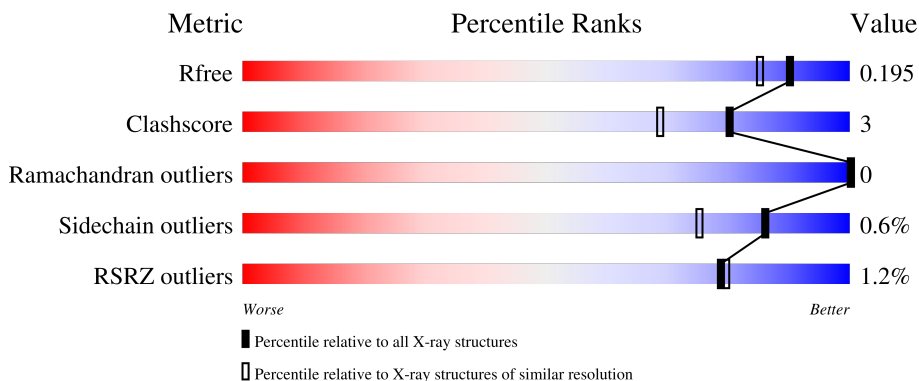
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

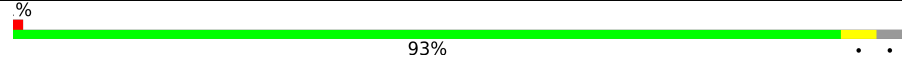
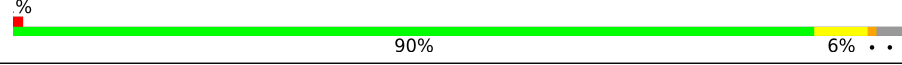
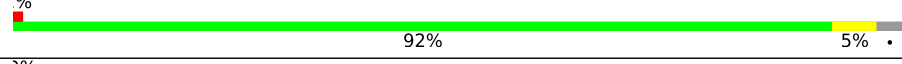
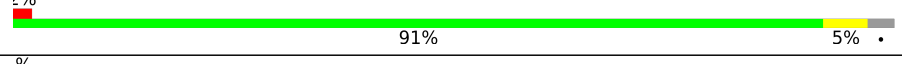

The reported resolution of this entry is 1.64 Å.

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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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  $\geq 3$ , 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	 93% . . .
1	B	223	 90% 6% . . .
1	C	223	 92% 5% . . .
1	D	223	 91% 5% . . .
1	E	223	 90% 7% . . .

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Mol	Chain	Length	Quality of chain
1	F	223	 91% 6% •
1	G	223	 2% 89% 7% ••
1	H	223	 88% 8% ••

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16703 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	Total 1848	C 1203	N 301	O 335	S 9	0	8	0
1	B	217	Total 1847	C 1202	N 301	O 336	S 8	0	8	0
1	C	217	Total 1848	C 1203	N 301	O 335	S 9	0	8	0
1	D	217	Total 1855	C 1208	N 302	O 337	S 8	0	9	0
1	E	217	Total 1852	C 1207	N 301	O 335	S 9	0	9	0
1	F	217	Total 1845	C 1201	N 301	O 335	S 8	0	7	0
1	G	217	Total 1855	C 1209	N 301	O 336	S 9	0	10	0
1	H	217	Total 1855	C 1209	N 301	O 336	S 9	0	10	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	219	Total O 219 219	0	0
3	B	226	Total O 226 226	0	0
3	C	211	Total O 211 211	0	0
3	D	235	Total O 235 235	0	0
3	E	232	Total O 232 232	0	0
3	F	230	Total O 230 230	0	0

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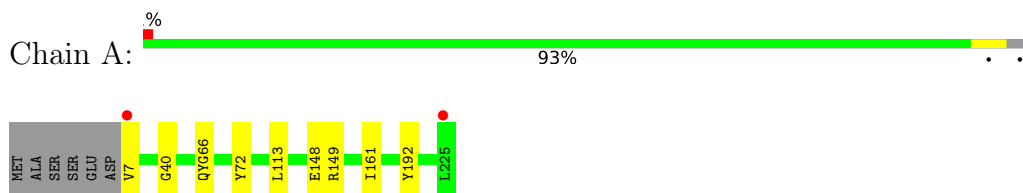
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	G	221	Total 221	O 221	0	0
3	H	216	Total 216	O 216	0	0

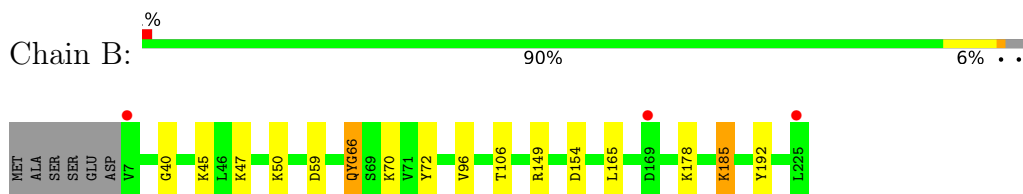
### 3 Residue-property plots [i](#)

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.

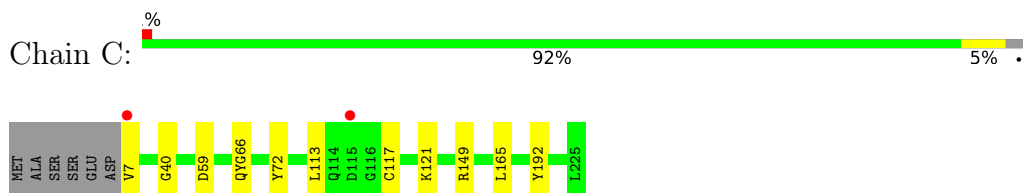
- Molecule 1: RED FLUORESCENT PROTEIN



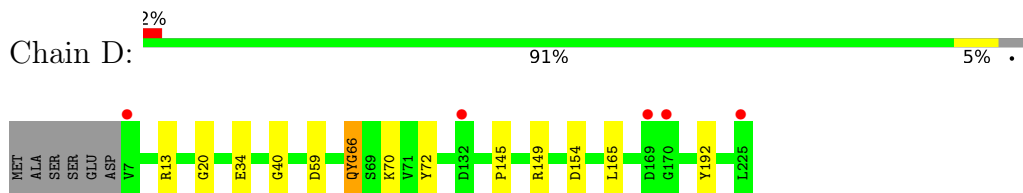
- Molecule 1: RED FLUORESCENT PROTEIN



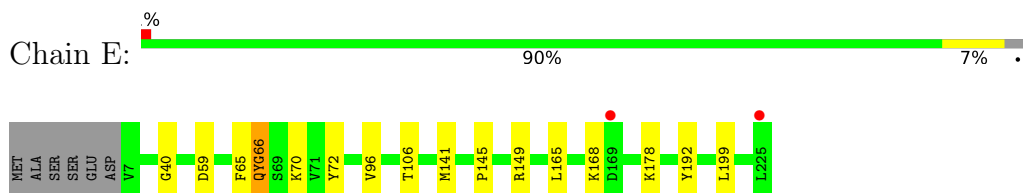
- Molecule 1: RED FLUORESCENT PROTEIN



- Molecule 1: RED FLUORESCENT PROTEIN



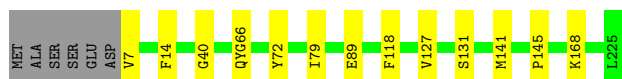
- Molecule 1: RED FLUORESCENT PROTEIN



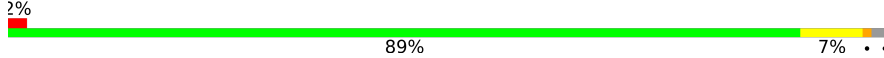
- Molecule 1: RED FLUORESCENT PROTEIN

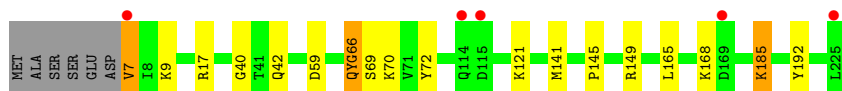


Chain F:  91% 6% .



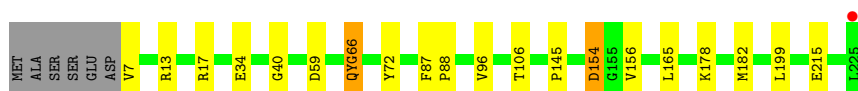
● Molecule 1: RED FLUORESCENT PROTEIN

Chain G:  89% 7% ..



● Molecule 1: RED FLUORESCENT PROTEIN

Chain H:  88% 8% ..



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.35Å 79.51Å 83.01Å 90.07° 96.87° 97.01°	Depositor
Resolution (Å)	32.44 – 1.64 32.44 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.9 (32.44-1.64) 91.6 (32.44-1.64)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 1.64Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.162 , 0.197 0.161 , 0.195	Depositor DCC
$R_{free}$ test set	10116 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	9.0	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.004 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	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 42.13 % 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 2.1339e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CRQ, EDO

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	0.73	0/1862	0.76	0/2505
1	B	0.74	0/1861	0.79	0/2504
1	C	0.72	0/1862	0.75	0/2505
1	D	0.72	0/1869	0.77	0/2515
1	E	0.75	0/1869	0.78	2/2515 (0.1%)
1	F	0.76	0/1856	0.75	0/2497
1	G	0.74	0/1875	0.76	0/2523
1	H	0.73	0/1875	0.75	0/2523
All	All	0.74	0/14929	0.76	2/20087 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65[A]	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	E	65[B]	PHE	CB-CG-CD1	-5.50	116.95	120.80

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	A	1848	0	1801	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1847	0	1799	10	0
1	C	1848	0	1801	6	0
1	D	1855	0	1809	7	0
1	E	1852	0	1808	10	0
1	F	1845	0	1796	7	0
1	G	1855	0	1814	19	0
1	H	1855	0	1815	14	0
2	A	12	0	18	0	0
2	B	16	0	24	0	0
2	C	16	0	24	0	0
2	D	12	0	18	1	0
2	E	8	0	12	0	0
2	F	16	0	24	1	0
2	G	8	0	12	0	0
2	H	20	0	30	1	0
3	A	219	0	0	0	0
3	B	226	0	0	2	0
3	C	211	0	0	2	0
3	D	235	0	0	1	0
3	E	232	0	0	1	0
3	F	230	0	0	1	0
3	G	221	0	0	6	0
3	H	216	0	0	4	0
All	All	16703	0	14605	81	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 3.

All (81) 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:G:141:MET:HE3	1:G:168:LYS:HG2	1.51	0.89
1:C:117[B]:CYS:SG	3:C:2008:HOH:O	2.31	0.88
1:H:96[B]:VAL:HG12	1:H:106:THR:HG22	1.58	0.86
1:F:40:GLY:HA2	1:F:72[B]:TYR:O	1.80	0.81
1:B:40:GLY:HA2	1:B:72[A]:TYR:O	1.80	0.80
1:D:40:GLY:HA2	1:D:72[A]:TYR:O	1.82	0.80
1:A:40:GLY:HA2	1:A:72[A]:TYR:O	1.82	0.78
1:G:141:MET:CE	1:G:168:LYS:HG2	2.12	0.78
1:G:40:GLY:HA2	1:G:72[A]:TYR:O	1.85	0.76
1:H:40:GLY:HA2	1:H:72[B]:TYR:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:PRO:HG2	3:H:2141:HOH:O	1.87	0.75
1:C:40:GLY:HA2	1:C:72[B]:TYR:O	1.88	0.74
1:E:40:GLY:HA2	1:E:72[B]:TYR:O	1.89	0.73
1:G:145:PRO:HG2	3:G:2143:HOH:O	1.92	0.69
1:G:7:VAL:HG12	1:G:9:LYS:NZ	2.12	0.65
1:A:7:VAL:CG2	1:A:113:LEU:HD21	2.27	0.64
1:F:145:PRO:HG2	3:F:2148:HOH:O	1.98	0.62
1:A:7:VAL:HG22	1:A:113:LEU:HD21	1.81	0.61
1:E:145:PRO:HG2	3:E:2150:HOH:O	2.02	0.59
1:E:96[B]:VAL:HG12	1:E:106:THR:HG22	1.86	0.58
1:G:17:ARG:HH22	1:G:121:LYS:HE2	1.69	0.57
1:B:96[B]:VAL:HG22	1:B:178:LYS:HB2	1.87	0.57
1:F:141:MET:HE3	1:F:168:LYS:HG2	1.86	0.56
1:H:17:ARG:NH2	3:H:2010:HOH:O	2.39	0.56
1:B:96[B]:VAL:HG12	1:B:106:THR:HG22	1.86	0.56
1:B:185:LYS:HD2	3:B:2097:HOH:O	2.05	0.55
1:E:96[B]:VAL:HG22	1:E:178:LYS:HB2	1.89	0.55
1:G:7:VAL:HG12	1:G:9:LYS:HZ3	1.74	0.53
1:C:7:VAL:HG22	1:C:113:LEU:HD21	1.91	0.52
1:G:185:LYS:HD3	3:G:2102:HOH:O	2.10	0.52
1:D:145:PRO:HG2	3:D:2152:HOH:O	2.11	0.51
1:D:13:ARG:NH1	1:D:34:GLU:OE2	2.42	0.51
1:H:13:ARG:NH1	1:H:34:GLU:OE2	2.42	0.51
1:G:7:VAL:HG22	3:G:2003:HOH:O	2.10	0.51
1:F:131:SER:OG	1:H:154:ASP:OD1	2.25	0.50
1:B:50:LYS:HG2	3:B:2022:HOH:O	2.10	0.49
1:G:42:GLN:HE22	1:G:69:SER:CB	2.26	0.49
1:A:7:VAL:HG21	1:A:113:LEU:CD2	2.42	0.49
2:H:1226:EDO:O1	3:H:2212:HOH:O	2.20	0.48
1:G:59:ASP:HB3	1:G:165:LEU:HD21	1.95	0.48
1:G:185:LYS:CD	3:G:2102:HOH:O	2.61	0.48
1:E:66[B]:CRQ:HE1	1:E:199[B]:LEU:HB2	1.96	0.48
1:A:40:GLY:HA2	1:A:72[B]:TYR:O	2.14	0.47
1:G:141:MET:HE3	1:G:141:MET:HB3	1.76	0.47
1:E:141:MET:SD	1:E:168:LYS:HA	2.55	0.47
1:H:154:ASP:CG	3:H:2153:HOH:O	2.52	0.47
1:B:66[B]:CRQ:CB2	1:B:70:LYS:HE2	2.46	0.46
1:E:149:ARG:HD3	1:E:192:TYR:CZ	2.51	0.46
1:E:66[B]:CRQ:CB2	1:E:70:LYS:HE2	2.47	0.45
1:E:66[A]:CRQ:CB2	1:E:70:LYS:HE2	2.47	0.45
1:H:66[A]:CRQ:HB11	1:H:215:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66[B]:CRQ:CB2	1:G:70:LYS:HE2	2.47	0.44
1:B:149:ARG:HD3	1:B:192:TYR:CZ	2.53	0.44
1:D:20:GLY:HA2	2:D:1226:EDO:H22	1.99	0.44
1:B:59:ASP:HB3	1:B:165:LEU:HD21	1.99	0.44
1:H:59:ASP:HB3	1:H:165:LEU:HD21	1.99	0.44
1:C:121:LYS:HE3	3:C:2113:HOH:O	2.17	0.44
1:G:66[A]:CRQ:CB2	1:G:70:LYS:HE2	2.48	0.43
1:C:59:ASP:HB3	1:C:165:LEU:HD21	1.99	0.43
1:A:149:ARG:HD3	1:A:192:TYR:CZ	2.53	0.43
1:E:59:ASP:HB3	1:E:165:LEU:HD21	2.00	0.43
1:B:66[A]:CRQ:CB2	1:B:70:LYS:HE2	2.47	0.43
1:H:96[B]:VAL:HG22	1:H:178:LYS:HB2	2.00	0.43
1:G:7:VAL:HA	3:G:2001:HOH:O	2.18	0.43
1:H:87:PHE:HB3	1:H:88:PRO:HA	2.02	0.42
1:C:149:ARG:HD3	1:C:192:TYR:CZ	2.55	0.42
1:G:149:ARG:HD3	1:G:192:TYR:CZ	2.55	0.42
1:D:149:ARG:HD3	1:D:192:TYR:CZ	2.55	0.42
1:A:7:VAL:CG2	1:A:113:LEU:CD2	2.95	0.41
1:A:7:VAL:HG21	1:A:113:LEU:HD21	2.00	0.41
1:H:156:VAL:HG11	1:H:182[A]:MET:HG2	2.03	0.41
1:D:59:ASP:HB3	1:D:165:LEU:HD21	2.01	0.41
1:F:14:PHE:HB3	1:F:118:PHE:HB2	2.03	0.41
1:G:7:VAL:CG1	1:G:9:LYS:NZ	2.82	0.41
1:F:79:ILE:HG12	2:F:1229:EDO:H21	2.03	0.41
1:H:66[B]:CRQ:HE1	1:H:199[B]:LEU:HB2	2.03	0.41
1:A:148:GLU:HG3	1:A:161:ILE:HG12	2.03	0.41
1:B:45:LYS:HE2	1:B:47:LYS:HE2	2.03	0.41
1:F:127:VAL:CG2	1:H:96[B]:VAL:HG13	2.51	0.41
1:D:66[B]:CRQ:CB2	1:D:70:LYS:HE2	2.50	0.41
1:G:185:LYS:HD2	3:G:2105:HOH:O	2.21	0.41

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	A	218/223 (98%)	212 (97%)	6 (3%)	0	100	100
1	B	218/223 (98%)	215 (99%)	3 (1%)	0	100	100
1	C	218/223 (98%)	216 (99%)	2 (1%)	0	100	100
1	D	219/223 (98%)	216 (99%)	3 (1%)	0	100	100
1	E	219/223 (98%)	218 (100%)	1 (0%)	0	100	100
1	F	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
1	G	220/223 (99%)	216 (98%)	4 (2%)	0	100	100
1	H	220/223 (99%)	217 (99%)	3 (1%)	0	100	100
All	All	1749/1784 (98%)	1724 (99%)	25 (1%)	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	A	196/194 (101%)	196 (100%)	0	100	100
1	B	196/194 (101%)	194 (99%)	2 (1%)	76	59
1	C	196/194 (101%)	196 (100%)	0	100	100
1	D	197/194 (102%)	196 (100%)	1 (0%)	88	80
1	E	197/194 (102%)	197 (100%)	0	100	100
1	F	195/194 (100%)	193 (99%)	2 (1%)	76	59
1	G	198/194 (102%)	196 (99%)	2 (1%)	76	59
1	H	198/194 (102%)	196 (99%)	2 (1%)	76	59
All	All	1573/1552 (101%)	1564 (99%)	9 (1%)	86	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	154	ASP
1	B	185	LYS
1	D	154	ASP
1	F	7	VAL
1	F	89	GLU
1	G	7	VAL
1	G	185	LYS
1	H	7	VAL
1	H	154	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	114	GLN
1	G	42	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

16 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	B	66[A]	1	24,25,26	2.78	6 (25%)	27,34,36	3.05	7 (25%)
1	CRQ	C	66[B]	1	24,25,26	2.46	6 (25%)	27,34,36	3.35	9 (33%)
1	CRQ	A	66[A]	1	24,25,26	2.78	6 (25%)	27,34,36	2.48	7 (25%)
1	CRQ	B	66[B]	1	24,25,26	2.55	5 (20%)	27,34,36	3.14	8 (29%)
1	CRQ	E	66[A]	1	24,25,26	2.89	6 (25%)	27,34,36	2.59	6 (22%)
1	CRQ	F	66[B]	1	24,25,26	2.45	5 (20%)	27,34,36	2.64	8 (29%)
1	CRQ	H	66[A]	1	24,25,26	2.88	6 (25%)	27,34,36	2.92	8 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CRQ	G	66[A]	1	24,25,26	2.51	6 (25%)	27,34,36	2.64	6 (22%)
1	CRQ	H	66[B]	1	24,25,26	2.69	5 (20%)	27,34,36	3.07	8 (29%)
1	CRQ	D	66[A]	1	24,25,26	2.68	6 (25%)	27,34,36	2.95	7 (25%)
1	CRQ	G	66[B]	1	24,25,26	2.35	4 (16%)	27,34,36	2.78	8 (29%)
1	CRQ	A	66[B]	1	24,25,26	2.57	5 (20%)	27,34,36	2.60	9 (33%)
1	CRQ	E	66[B]	1	24,25,26	2.62	6 (25%)	27,34,36	2.71	9 (33%)
1	CRQ	D	66[B]	1	24,25,26	2.40	5 (20%)	27,34,36	3.05	9 (33%)
1	CRQ	C	66[A]	1	24,25,26	2.62	6 (25%)	27,34,36	3.21	8 (29%)
1	CRQ	F	66[A]	1	24,25,26	2.66	6 (25%)	27,34,36	2.57	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	B	66[A]	1	-	3/10/32/33	0/2/2/2
1	CRQ	C	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	A	66[A]	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	E	66[A]	1	-	1/10/32/33	0/2/2/2
1	CRQ	F	66[B]	1	-	2/10/32/33	0/2/2/2
1	CRQ	H	66[A]	1	-	1/10/32/33	0/2/2/2
1	CRQ	G	66[A]	1	-	1/10/32/33	0/2/2/2
1	CRQ	H	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	D	66[A]	1	-	1/10/32/33	0/2/2/2
1	CRQ	G	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	A	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	E	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	D	66[B]	1	-	1/10/32/33	0/2/2/2
1	CRQ	C	66[A]	1	-	1/10/32/33	0/2/2/2
1	CRQ	F	66[A]	1	-	2/10/32/33	0/2/2/2

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	66[B]	CRQ	CA2-C2	-8.71	1.40	1.48
1	H	66[A]	CRQ	CA2-C2	-8.31	1.40	1.48
1	F	66[B]	CRQ	CA2-C2	-8.18	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	66[B]	CRQ	CA2-C2	-8.06	1.40	1.48
1	B	66[B]	CRQ	CA2-C2	-8.03	1.40	1.48
1	C	66[B]	CRQ	CA2-C2	-8.02	1.40	1.48
1	A	66[B]	CRQ	CB2-CA2	7.86	1.41	1.35
1	A	66[A]	CRQ	CB2-CA2	7.76	1.41	1.35
1	A	66[B]	CRQ	CA2-C2	-7.74	1.41	1.48
1	E	66[A]	CRQ	CA2-C2	-7.72	1.41	1.48
1	F	66[A]	CRQ	CA2-C2	-7.67	1.41	1.48
1	B	66[A]	CRQ	CA2-C2	-7.54	1.41	1.48
1	C	66[A]	CRQ	CA2-C2	-7.52	1.41	1.48
1	B	66[A]	CRQ	CB2-CA2	7.46	1.41	1.35
1	H	66[B]	CRQ	CB2-CA2	7.37	1.41	1.35
1	B	66[B]	CRQ	CB2-CA2	7.36	1.41	1.35
1	G	66[B]	CRQ	CA2-C2	-7.35	1.41	1.48
1	E	66[B]	CRQ	CB2-CA2	7.33	1.41	1.35
1	A	66[A]	CRQ	CA2-C2	-7.23	1.41	1.48
1	E	66[A]	CRQ	CB2-CA2	7.15	1.41	1.35
1	H	66[A]	CRQ	CB2-CA2	7.14	1.41	1.35
1	D	66[B]	CRQ	CA2-C2	-7.12	1.41	1.48
1	D	66[B]	CRQ	CB2-CA2	6.88	1.40	1.35
1	E	66[A]	CRQ	CA1-N1	6.80	1.44	1.27
1	G	66[A]	CRQ	CA2-C2	-6.78	1.41	1.48
1	D	66[A]	CRQ	CA1-N1	6.73	1.43	1.27
1	D	66[A]	CRQ	CA2-C2	-6.70	1.42	1.48
1	D	66[A]	CRQ	CB2-CA2	6.59	1.40	1.35
1	H	66[A]	CRQ	CA1-N1	6.47	1.43	1.27
1	F	66[B]	CRQ	CB2-CA2	6.32	1.40	1.35
1	C	66[B]	CRQ	CB2-CA2	6.28	1.40	1.35
1	A	66[A]	CRQ	CA1-N1	6.27	1.42	1.27
1	F	66[A]	CRQ	CB2-CA2	6.21	1.40	1.35
1	C	66[A]	CRQ	CA1-N1	6.18	1.42	1.27
1	G	66[B]	CRQ	CB2-CA2	6.18	1.40	1.35
1	F	66[A]	CRQ	CA1-N1	6.16	1.42	1.27
1	B	66[A]	CRQ	CA1-N1	6.09	1.42	1.27
1	C	66[A]	CRQ	CB2-CA2	6.01	1.40	1.35
1	G	66[A]	CRQ	CB2-CA2	5.94	1.40	1.35
1	G	66[A]	CRQ	CA1-N1	5.80	1.41	1.27
1	E	66[A]	CRQ	C2-N3	-3.30	1.32	1.39
1	H	66[A]	CRQ	O3-C3	3.26	1.38	1.19
1	H	66[B]	CRQ	O3-C3	3.23	1.38	1.19
1	D	66[A]	CRQ	O3-C3	3.21	1.38	1.19
1	E	66[B]	CRQ	O3-C3	3.19	1.38	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66[B]	CRQ	O3-C3	3.18	1.37	1.19
1	E	66[A]	CRQ	O3-C3	3.18	1.37	1.19
1	D	66[B]	CRQ	O3-C3	3.15	1.37	1.19
1	A	66[A]	CRQ	O3-C3	3.14	1.37	1.19
1	E	66[B]	CRQ	C2-N3	-3.14	1.32	1.39
1	C	66[A]	CRQ	O3-C3	3.13	1.37	1.19
1	C	66[B]	CRQ	O3-C3	3.12	1.37	1.19
1	G	66[A]	CRQ	O3-C3	3.08	1.37	1.19
1	G	66[B]	CRQ	O3-C3	3.04	1.37	1.19
1	F	66[A]	CRQ	O3-C3	3.01	1.36	1.19
1	F	66[B]	CRQ	O3-C3	2.97	1.36	1.19
1	B	66[B]	CRQ	O3-C3	2.92	1.36	1.19
1	E	66[B]	CRQ	CG2-CB2	-2.90	1.41	1.46
1	B	66[A]	CRQ	O3-C3	2.89	1.36	1.19
1	E	66[A]	CRQ	CG2-CB2	-2.85	1.41	1.46
1	F	66[A]	CRQ	C2-N3	-2.82	1.33	1.39
1	G	66[B]	CRQ	CG2-CB2	-2.81	1.41	1.46
1	G	66[A]	CRQ	CG2-CB2	-2.77	1.41	1.46
1	F	66[B]	CRQ	CG2-CB2	-2.67	1.41	1.46
1	F	66[A]	CRQ	CG2-CB2	-2.66	1.41	1.46
1	D	66[A]	CRQ	C2-N3	-2.64	1.33	1.39
1	H	66[B]	CRQ	CA1-N1	2.63	1.33	1.27
1	H	66[A]	CRQ	CG2-CB2	-2.61	1.41	1.46
1	C	66[A]	CRQ	CG2-CB2	-2.61	1.41	1.46
1	C	66[B]	CRQ	CG2-CB2	-2.60	1.41	1.46
1	F	66[B]	CRQ	C2-N3	-2.59	1.33	1.39
1	A	66[B]	CRQ	CG2-CB2	-2.58	1.41	1.46
1	C	66[B]	CRQ	CA1-N1	2.57	1.33	1.27
1	D	66[A]	CRQ	CG2-CB2	-2.55	1.41	1.46
1	B	66[B]	CRQ	CG2-CB2	-2.54	1.41	1.46
1	B	66[A]	CRQ	C2-N3	-2.52	1.33	1.39
1	B	66[A]	CRQ	CG2-CB2	-2.52	1.42	1.46
1	H	66[B]	CRQ	CG2-CB2	-2.52	1.42	1.46
1	A	66[A]	CRQ	CG2-CB2	-2.49	1.42	1.46
1	D	66[B]	CRQ	C2-N3	-2.46	1.34	1.39
1	D	66[B]	CRQ	CG2-CB2	-2.44	1.42	1.46
1	B	66[B]	CRQ	C2-N3	-2.35	1.34	1.39
1	C	66[A]	CRQ	C2-N3	-2.31	1.34	1.39
1	A	66[A]	CRQ	C2-N3	-2.21	1.34	1.39
1	G	66[A]	CRQ	C2-N3	-2.18	1.34	1.39
1	C	66[B]	CRQ	C2-N3	-2.12	1.34	1.39
1	A	66[B]	CRQ	C2-N3	-2.08	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	66[A]	CRQ	C2-N3	-2.02	1.35	1.39
1	E	66[B]	CRQ	CA2-N2	-2.01	1.34	1.38

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66[A]	CRQ	CA2-C2-N3	10.86	108.50	103.37
1	B	66[B]	CRQ	CA2-C2-N3	10.82	108.49	103.37
1	D	66[A]	CRQ	CA2-C2-N3	10.61	108.39	103.37
1	C	66[A]	CRQ	CA2-C2-N3	10.32	108.25	103.37
1	D	66[B]	CRQ	CA2-C2-N3	10.29	108.24	103.37
1	C	66[B]	CRQ	CA2-C2-N3	10.00	108.10	103.37
1	H	66[A]	CRQ	CA2-C2-N3	9.25	107.75	103.37
1	E	66[A]	CRQ	CA2-C2-N3	8.98	107.62	103.37
1	E	66[B]	CRQ	CA2-C2-N3	8.90	107.58	103.37
1	H	66[B]	CRQ	CA2-C2-N3	8.75	107.51	103.37
1	C	66[B]	CRQ	O2-C2-CA2	-8.67	126.09	130.96
1	F	66[A]	CRQ	CA2-C2-N3	8.47	107.38	103.37
1	F	66[B]	CRQ	CA2-C2-N3	8.20	107.25	103.37
1	G	66[A]	CRQ	CA2-C2-N3	8.20	107.25	103.37
1	G	66[B]	CRQ	O2-C2-CA2	-8.14	126.39	130.96
1	C	66[A]	CRQ	O2-C2-CA2	-8.11	126.41	130.96
1	G	66[B]	CRQ	CA2-C2-N3	7.85	107.08	103.37
1	B	66[B]	CRQ	O2-C2-CA2	-7.69	126.64	130.96
1	H	66[B]	CRQ	O2-C2-CA2	-7.65	126.67	130.96
1	G	66[A]	CRQ	O2-C2-CA2	-7.63	126.67	130.96
1	H	66[A]	CRQ	O2-C2-CA2	-7.41	126.80	130.96
1	B	66[A]	CRQ	O2-C2-CA2	-7.32	126.85	130.96
1	A	66[A]	CRQ	CA2-C2-N3	7.25	106.80	103.37
1	A	66[B]	CRQ	CA2-C2-N3	6.97	106.67	103.37
1	D	66[B]	CRQ	O2-C2-CA2	-6.73	127.18	130.96
1	D	66[A]	CRQ	O2-C2-CA2	-6.47	127.33	130.96
1	A	66[B]	CRQ	O2-C2-CA2	-6.33	127.41	130.96
1	F	66[B]	CRQ	O2-C2-CA2	-5.91	127.64	130.96
1	A	66[A]	CRQ	O3-C3-CA3	-5.85	108.71	126.39
1	A	66[B]	CRQ	O3-C3-CA3	-5.79	108.92	126.39
1	A	66[A]	CRQ	O2-C2-CA2	-5.73	127.74	130.96
1	H	66[B]	CRQ	O3-C3-CA3	-5.55	109.62	126.39
1	H	66[A]	CRQ	O3-C3-CA3	-5.53	109.70	126.39
1	F	66[A]	CRQ	O2-C2-CA2	-5.48	127.88	130.96
1	C	66[B]	CRQ	O3-C3-CA3	-5.42	110.02	126.39
1	F	66[A]	CRQ	O3-C3-CA3	-5.40	110.10	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66[B]	CRQ	O3-C3-CA3	-5.36	110.20	126.39
1	G	66[B]	CRQ	O3-C3-CA3	-5.34	110.27	126.39
1	C	66[A]	CRQ	O3-C3-CA3	-5.32	110.32	126.39
1	G	66[A]	CRQ	O3-C3-CA3	-5.29	110.40	126.39
1	E	66[B]	CRQ	O2-C2-CA2	-5.19	128.05	130.96
1	E	66[A]	CRQ	O3-C3-CA3	-5.00	111.29	126.39
1	E	66[B]	CRQ	O3-C3-CA3	-4.95	111.46	126.39
1	C	66[B]	CRQ	C2-CA2-N2	-4.91	105.49	108.93
1	D	66[A]	CRQ	O3-C3-CA3	-4.91	111.57	126.39
1	D	66[B]	CRQ	O3-C3-CA3	-4.86	111.72	126.39
1	B	66[A]	CRQ	O3-C3-CA3	-4.82	111.83	126.39
1	B	66[B]	CRQ	O3-C3-CA3	-4.78	111.96	126.39
1	C	66[B]	CRQ	CB2-CA2-N2	4.70	135.35	128.83
1	E	66[A]	CRQ	O2-C2-CA2	-4.52	128.42	130.96
1	D	66[B]	CRQ	CB2-CA2-N2	4.47	135.03	128.83
1	H	66[B]	CRQ	N3-C1-N2	-4.42	107.44	113.28
1	H	66[B]	CRQ	C2-CA2-N2	-4.39	105.86	108.93
1	H	66[B]	CRQ	CB2-CA2-N2	4.38	134.91	128.83
1	C	66[B]	CRQ	N3-C1-N2	-4.21	107.72	113.28
1	C	66[A]	CRQ	CB2-CA2-N2	4.20	134.65	128.83
1	E	66[B]	CRQ	CB2-CA2-N2	4.03	134.41	128.83
1	A	66[B]	CRQ	N3-C1-N2	-3.98	108.02	113.28
1	D	66[A]	CRQ	CB2-CA2-N2	3.94	134.29	128.83
1	D	66[B]	CRQ	C2-CA2-N2	-3.93	106.18	108.93
1	B	66[B]	CRQ	CB2-CA2-N2	3.87	134.19	128.83
1	H	66[A]	CRQ	CB2-CA2-N2	3.83	134.14	128.83
1	B	66[A]	CRQ	CB2-CA2-N2	3.82	134.12	128.83
1	C	66[A]	CRQ	C2-CA2-N2	-3.77	106.29	108.93
1	B	66[B]	CRQ	C2-CA2-N2	-3.72	106.32	108.93
1	F	66[B]	CRQ	N3-C1-N2	-3.68	108.43	113.28
1	E	66[A]	CRQ	CB2-CA2-N2	3.60	133.82	128.83
1	G	66[B]	CRQ	N3-C1-N2	-3.54	108.61	113.28
1	C	66[A]	CRQ	CG1-CB1-CA1	-3.51	102.66	113.53
1	E	66[B]	CRQ	N3-C1-N2	-3.39	108.80	113.28
1	A	66[A]	CRQ	CG1-CB1-CA1	-3.38	103.06	113.53
1	E	66[A]	CRQ	CG1-CB1-CA1	-3.31	103.28	113.53
1	G	66[B]	CRQ	CB2-CA2-N2	3.30	133.40	128.83
1	E	66[A]	CRQ	CB2-CA2-C2	-3.25	118.39	122.28
1	F	66[A]	CRQ	CG1-CB1-CA1	-3.15	103.76	113.53
1	H	66[A]	CRQ	C2-CA2-N2	-3.14	106.73	108.93
1	H	66[B]	CRQ	CA2-N2-C1	3.13	110.06	104.33
1	A	66[B]	CRQ	CB2-CA2-N2	3.13	133.17	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66[A]	CRQ	CB2-CA2-C2	-3.09	118.59	122.28
1	E	66[B]	CRQ	CB2-CA2-C2	-3.08	118.59	122.28
1	D	66[A]	CRQ	CG1-CB1-CA1	-3.08	103.98	113.53
1	D	66[B]	CRQ	N3-C1-N2	-3.05	109.25	113.28
1	B	66[B]	CRQ	N3-C1-N2	-3.02	109.29	113.28
1	C	66[B]	CRQ	CA2-N2-C1	3.01	109.84	104.33
1	B	66[A]	CRQ	C2-CA2-N2	-2.94	106.88	108.93
1	D	66[B]	CRQ	CB2-CA2-C2	-2.93	118.78	122.28
1	H	66[A]	CRQ	CG1-CB1-CA1	-2.93	104.45	113.53
1	F	66[B]	CRQ	CB2-CA2-N2	2.85	132.78	128.83
1	A	66[A]	CRQ	CB2-CA2-N2	2.83	132.75	128.83
1	E	66[B]	CRQ	C2-CA2-N2	-2.80	106.97	108.93
1	G	66[A]	CRQ	CG1-CB1-CA1	-2.79	104.88	113.53
1	C	66[A]	CRQ	CB2-CA2-C2	-2.77	118.97	122.28
1	F	66[B]	CRQ	C2-CA2-N2	-2.74	107.01	108.93
1	B	66[A]	CRQ	CB2-CA2-C2	-2.74	119.00	122.28
1	G	66[A]	CRQ	CB2-CA2-N2	2.73	132.62	128.83
1	F	66[A]	CRQ	CB2-CA2-N2	2.72	132.60	128.83
1	H	66[A]	CRQ	CB2-CA2-C2	-2.69	119.06	122.28
1	A	66[B]	CRQ	C2-CA2-N2	-2.66	107.07	108.93
1	C	66[B]	CRQ	CB2-CA2-C2	-2.65	119.11	122.28
1	A	66[B]	CRQ	CA2-N2-C1	2.65	109.18	104.33
1	D	66[A]	CRQ	C2-CA2-N2	-2.64	107.08	108.93
1	B	66[A]	CRQ	CG1-CB1-CA1	-2.63	105.37	113.53
1	H	66[B]	CRQ	CB2-CA2-C2	-2.59	119.18	122.28
1	G	66[B]	CRQ	CB2-CA2-C2	-2.44	119.36	122.28
1	G	66[B]	CRQ	C2-CA2-N2	-2.43	107.23	108.93
1	G	66[A]	CRQ	CB2-CA2-C2	-2.42	119.39	122.28
1	D	66[B]	CRQ	CG1-CB1-CA1	-2.41	106.05	113.53
1	C	66[A]	CRQ	N3-C1-N2	-2.40	110.11	113.28
1	A	66[A]	CRQ	CB2-CA2-C2	-2.38	119.44	122.28
1	G	66[B]	CRQ	CA2-N2-C1	2.35	108.63	104.33
1	B	66[B]	CRQ	CB2-CA2-C2	-2.34	119.48	122.28
1	D	66[B]	CRQ	CA2-N2-C1	2.33	108.59	104.33
1	E	66[B]	CRQ	CG1-CB1-CA1	-2.31	106.36	113.53
1	F	66[B]	CRQ	CA2-N2-C1	2.31	108.55	104.33
1	A	66[B]	CRQ	CG1-CB1-CA1	-2.31	106.38	113.53
1	B	66[B]	CRQ	CA2-N2-C1	2.29	108.53	104.33
1	A	66[A]	CRQ	N3-C1-N2	-2.27	110.28	113.28
1	H	66[A]	CRQ	N3-C1-N2	-2.23	110.33	113.28
1	F	66[B]	CRQ	CG1-CB1-CA1	-2.23	106.61	113.53
1	F	66[A]	CRQ	CB2-CA2-C2	-2.19	119.66	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66[B]	CRQ	CB2-CA2-C2	-2.16	119.70	122.28
1	F	66[A]	CRQ	N3-C1-N2	-2.10	110.50	113.28
1	C	66[B]	CRQ	CG1-CB1-CA1	-2.10	107.02	113.53
1	E	66[B]	CRQ	CA2-N2-C1	2.07	108.11	104.33

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66[A]	CRQ	C1-CA1-CB1-CG1
1	A	66[B]	CRQ	C1-CA1-CB1-CG1
1	B	66[A]	CRQ	C1-CA1-CB1-CG1
1	B	66[B]	CRQ	C1-CA1-CB1-CG1
1	C	66[A]	CRQ	C1-CA1-CB1-CG1
1	C	66[B]	CRQ	C1-CA1-CB1-CG1
1	D	66[A]	CRQ	C1-CA1-CB1-CG1
1	D	66[B]	CRQ	C1-CA1-CB1-CG1
1	E	66[A]	CRQ	C1-CA1-CB1-CG1
1	E	66[B]	CRQ	C1-CA1-CB1-CG1
1	F	66[A]	CRQ	C1-CA1-CB1-CG1
1	F	66[B]	CRQ	C1-CA1-CB1-CG1
1	G	66[A]	CRQ	C1-CA1-CB1-CG1
1	G	66[B]	CRQ	C1-CA1-CB1-CG1
1	H	66[A]	CRQ	C1-CA1-CB1-CG1
1	H	66[B]	CRQ	C1-CA1-CB1-CG1
1	F	66[A]	CRQ	C3-CA3-N3-C1
1	B	66[A]	CRQ	CA1-CB1-CG1-CD3
1	B	66[A]	CRQ	C3-CA3-N3-C1
1	F	66[B]	CRQ	C3-CA3-N3-C1
1	B	66[B]	CRQ	CA1-CB1-CG1-CD3

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66[A]	CRQ	1	0
1	B	66[B]	CRQ	1	0
1	E	66[A]	CRQ	1	0
1	H	66[A]	CRQ	1	0
1	G	66[A]	CRQ	1	0
1	H	66[B]	CRQ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	66[B]	CRQ	1	0
1	E	66[B]	CRQ	2	0
1	D	66[B]	CRQ	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

27 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	EDO	D	1228	-	3,3,3	0.38	0	2,2,2	0.40	0
2	EDO	H	1226	-	3,3,3	0.53	0	2,2,2	0.32	0
2	EDO	G	1226	-	3,3,3	0.38	0	2,2,2	0.11	0
2	EDO	A	1226	-	3,3,3	0.45	0	2,2,2	0.14	0
2	EDO	H	1228	-	3,3,3	0.53	0	2,2,2	0.42	0
2	EDO	A	1228	-	3,3,3	0.59	0	2,2,2	0.52	0
2	EDO	E	1227	-	3,3,3	0.56	0	2,2,2	0.25	0
2	EDO	F	1229	-	3,3,3	0.57	0	2,2,2	0.23	0
2	EDO	B	1227	-	3,3,3	0.53	0	2,2,2	0.12	0
2	EDO	C	1227	-	3,3,3	0.56	0	2,2,2	0.34	0
2	EDO	D	1226	-	3,3,3	0.69	0	2,2,2	0.47	0
2	EDO	C	1229	-	3,3,3	0.58	0	2,2,2	0.29	0
2	EDO	G	1227	-	3,3,3	0.61	0	2,2,2	0.24	0
2	EDO	A	1227	-	3,3,3	0.43	0	2,2,2	0.59	0
2	EDO	C	1226	-	3,3,3	0.48	0	2,2,2	0.37	0
2	EDO	D	1227	-	3,3,3	0.62	0	2,2,2	0.15	0
2	EDO	F	1227	-	3,3,3	0.38	0	2,2,2	0.54	0
2	EDO	F	1226	-	3,3,3	0.53	0	2,2,2	0.06	0
2	EDO	B	1226	-	3,3,3	0.36	0	2,2,2	0.39	0
2	EDO	H	1229	-	3,3,3	0.37	0	2,2,2	0.60	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	B	1228	-	3,3,3	0.47	0	2,2,2	0.19	0
2	EDO	H	1230	-	3,3,3	0.60	0	2,2,2	0.58	0
2	EDO	B	1229	-	3,3,3	0.74	0	2,2,2	0.91	0
2	EDO	C	1228	-	3,3,3	0.42	0	2,2,2	0.10	0
2	EDO	F	1228	-	3,3,3	0.55	0	2,2,2	0.30	0
2	EDO	E	1226	-	3,3,3	0.38	0	2,2,2	0.64	0
2	EDO	H	1227	-	3,3,3	0.39	0	2,2,2	0.28	0

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	EDO	D	1228	-	-	0/1/1/1	-
2	EDO	H	1226	-	-	1/1/1/1	-
2	EDO	G	1226	-	-	0/1/1/1	-
2	EDO	A	1226	-	-	1/1/1/1	-
2	EDO	H	1228	-	-	0/1/1/1	-
2	EDO	A	1228	-	-	1/1/1/1	-
2	EDO	E	1227	-	-	1/1/1/1	-
2	EDO	F	1229	-	-	1/1/1/1	-
2	EDO	B	1227	-	-	0/1/1/1	-
2	EDO	C	1227	-	-	1/1/1/1	-
2	EDO	D	1226	-	-	0/1/1/1	-
2	EDO	C	1229	-	-	1/1/1/1	-
2	EDO	G	1227	-	-	0/1/1/1	-
2	EDO	A	1227	-	-	0/1/1/1	-
2	EDO	C	1226	-	-	0/1/1/1	-
2	EDO	D	1227	-	-	1/1/1/1	-
2	EDO	F	1227	-	-	0/1/1/1	-
2	EDO	F	1226	-	-	1/1/1/1	-
2	EDO	B	1226	-	-	0/1/1/1	-
2	EDO	H	1229	-	-	0/1/1/1	-
2	EDO	B	1228	-	-	1/1/1/1	-
2	EDO	H	1230	-	-	0/1/1/1	-
2	EDO	B	1229	-	-	1/1/1/1	-
2	EDO	C	1228	-	-	0/1/1/1	-
2	EDO	F	1228	-	-	0/1/1/1	-
2	EDO	E	1226	-	-	0/1/1/1	-
2	EDO	H	1227	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1227	EDO	O1-C1-C2-O2
2	B	1228	EDO	O1-C1-C2-O2
2	B	1229	EDO	O1-C1-C2-O2
2	C	1229	EDO	O1-C1-C2-O2
2	H	1226	EDO	O1-C1-C2-O2
2	E	1227	EDO	O1-C1-C2-O2
2	D	1227	EDO	O1-C1-C2-O2
2	F	1229	EDO	O1-C1-C2-O2
2	A	1226	EDO	O1-C1-C2-O2
2	A	1228	EDO	O1-C1-C2-O2
2	H	1227	EDO	O1-C1-C2-O2
2	F	1226	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1226	EDO	1	0
2	F	1229	EDO	1	0
2	D	1226	EDO	1	0

## 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	A	216/223 (96%)	-0.21	2 (0%) 84 85	3, 7, 15, 23	0
1	B	216/223 (96%)	-0.15	3 (1%) 75 76	4, 7, 15, 23	0
1	C	216/223 (96%)	-0.18	2 (0%) 84 85	4, 8, 16, 23	0
1	D	216/223 (96%)	-0.22	5 (2%) 60 60	4, 7, 15, 24	0
1	E	216/223 (96%)	-0.19	2 (0%) 84 85	4, 7, 14, 23	0
1	F	216/223 (96%)	-0.22	0 100 100	4, 7, 15, 21	0
1	G	216/223 (96%)	-0.16	5 (2%) 60 60	5, 8, 15, 24	0
1	H	216/223 (96%)	-0.21	1 (0%) 91 91	4, 8, 16, 22	0
All	All	1728/1784 (96%)	-0.19	20 (1%) 79 79	3, 7, 15, 24	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	LEU	4.1
1	D	225	LEU	4.0
1	E	225	LEU	3.9
1	G	225	LEU	3.5
1	B	169	ASP	3.4
1	D	169	ASP	3.3
1	G	169	ASP	3.3
1	C	7	VAL	2.9
1	B	7	VAL	2.6
1	E	169	ASP	2.6
1	C	115	ASP	2.6
1	G	7	VAL	2.5
1	H	225	LEU	2.4
1	D	7	VAL	2.2
1	D	132	ASP	2.2
1	D	170	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	114	GLN	2.1
1	A	7	VAL	2.1
1	G	115	ASP	2.1
1	A	225	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRQ	F	66[A]	24/25	0.95	0.11	6,10,15,19	24
1	CRQ	F	66[B]	24/25	0.95	0.11	6,10,16,19	24
1	CRQ	H	66[A]	24/25	0.95	0.10	6,11,14,19	24
1	CRQ	H	66[B]	24/25	0.95	0.10	6,11,15,19	24
1	CRQ	D	66[A]	24/25	0.96	0.10	6,8,14,16	24
1	CRQ	D	66[B]	24/25	0.96	0.10	6,8,15,16	24
1	CRQ	E	66[A]	24/25	0.96	0.11	6,9,14,15	24
1	CRQ	E	66[B]	24/25	0.96	0.11	6,9,14,15	24
1	CRQ	A	66[A]	24/25	0.96	0.10	7,9,13,14	24
1	CRQ	A	66[B]	24/25	0.96	0.10	6,9,14,15	24
1	CRQ	G	66[A]	24/25	0.96	0.11	5,9,15,17	24
1	CRQ	G	66[B]	24/25	0.96	0.11	5,9,16,17	24
1	CRQ	C	66[A]	24/25	0.96	0.10	6,9,15,18	24
1	CRQ	C	66[B]	24/25	0.96	0.10	6,9,15,18	24
1	CRQ	B	66[A]	24/25	0.97	0.11	5,9,17,18	24
1	CRQ	B	66[B]	24/25	0.97	0.11	5,9,17,18	24

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	1229	4/4	0.61	0.20	21,22,22,26	0
2	EDO	H	1228	4/4	0.73	0.18	23,24,25,26	0
2	EDO	B	1228	4/4	0.85	0.18	15,18,18,20	0
2	EDO	H	1230	4/4	0.85	0.13	18,19,20,27	0
2	EDO	D	1226	4/4	0.86	0.14	20,22,23,25	0
2	EDO	F	1228	4/4	0.87	0.12	16,19,19,25	0
2	EDO	H	1226	4/4	0.87	0.12	18,20,21,25	0
2	EDO	A	1227	4/4	0.87	0.14	18,20,22,26	0
2	EDO	A	1226	4/4	0.87	0.15	22,23,24,25	0
2	EDO	C	1226	4/4	0.88	0.12	17,18,23,25	0
2	EDO	C	1229	4/4	0.88	0.12	18,21,21,23	0
2	EDO	H	1229	4/4	0.88	0.14	19,20,21,23	0
2	EDO	G	1227	4/4	0.88	0.13	19,22,23,23	0
2	EDO	E	1226	4/4	0.89	0.11	24,25,25,25	0
2	EDO	E	1227	4/4	0.89	0.11	15,18,22,24	0
2	EDO	H	1227	4/4	0.89	0.12	20,20,21,24	0
2	EDO	F	1227	4/4	0.89	0.15	21,23,24,26	0
2	EDO	A	1228	4/4	0.89	0.13	17,17,19,24	0
2	EDO	F	1229	4/4	0.89	0.11	16,20,21,22	0
2	EDO	F	1226	4/4	0.90	0.12	19,19,19,20	0
2	EDO	C	1228	4/4	0.90	0.11	18,20,21,23	0
2	EDO	B	1226	4/4	0.91	0.10	15,18,19,20	0
2	EDO	B	1227	4/4	0.91	0.11	17,19,20,23	0
2	EDO	D	1227	4/4	0.92	0.09	19,20,22,24	0
2	EDO	G	1226	4/4	0.92	0.12	21,21,22,23	0
2	EDO	D	1228	4/4	0.94	0.09	20,22,22,22	0
2	EDO	C	1227	4/4	0.95	0.10	17,17,17,24	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.