



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:36 PM UTC

PDB ID : 1G7K / pdb_00001g7k
Title : CRYSTAL STRUCTURE OF DSRED, A RED FLUORESCENT PROTEIN FROM DISCOSOMA SP. RED
Authors : Yarbrough, D.; Wachter, R.M.; Kallio, K.; Matz, M.V.; Remington, S.J.
Deposited on : 2000-11-10
Resolution : 2.00 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

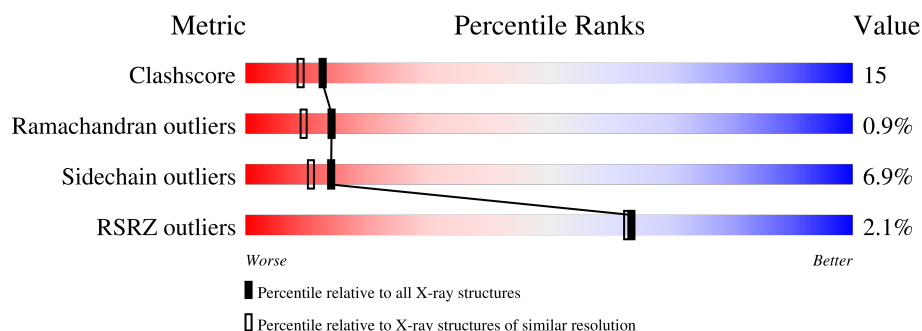
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	234	2% 68% 21% . 7%
1	B	234	2% 66% 23% . 7%
1	C	234	% 66% 22% . 7%
1	D	234	3% 67% 21% . 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7586 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 FLUORESCENT PROTEIN FP583.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			
1	B	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			
1	C	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			
1	D	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	insertion	UNP Q9U6Y8
A	-9	ARG	-	insertion	UNP Q9U6Y8
A	-8	GLY	-	insertion	UNP Q9U6Y8
A	-7	SER	-	insertion	UNP Q9U6Y8
A	-6	HIS	-	insertion	UNP Q9U6Y8
A	-5	HIS	-	insertion	UNP Q9U6Y8
A	-4	HIS	-	insertion	UNP Q9U6Y8
A	-3	HIS	-	insertion	UNP Q9U6Y8
A	-2	HIS	-	insertion	UNP Q9U6Y8
A	-1	HIS	-	insertion	UNP Q9U6Y8
A	0	GLY	-	insertion	UNP Q9U6Y8
A	1	SER	-	insertion	UNP Q9U6Y8
A	66	CRQ	GLN	chromophore	UNP Q9U6Y8
A	66	CRQ	TYR	chromophore	UNP Q9U6Y8
A	66	CRQ	GLY	chromophore	UNP Q9U6Y8
B	-10	MSE	-	insertion	UNP Q9U6Y8
B	-9	ARG	-	insertion	UNP Q9U6Y8
B	-8	GLY	-	insertion	UNP Q9U6Y8
B	-7	SER	-	insertion	UNP Q9U6Y8
B	-6	HIS	-	insertion	UNP Q9U6Y8
B	-5	HIS	-	insertion	UNP Q9U6Y8

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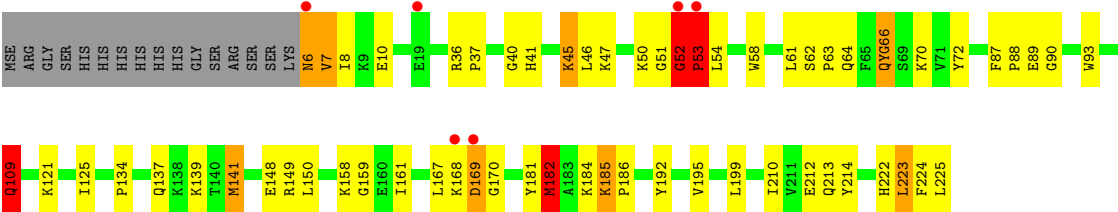
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	insertion	UNP Q9U6Y8
B	-3	HIS	-	insertion	UNP Q9U6Y8
B	-2	HIS	-	insertion	UNP Q9U6Y8
B	-1	HIS	-	insertion	UNP Q9U6Y8
B	0	GLY	-	insertion	UNP Q9U6Y8
B	1	SER	-	insertion	UNP Q9U6Y8
B	66	CRQ	GLN	chromophore	UNP Q9U6Y8
B	66	CRQ	TYR	chromophore	UNP Q9U6Y8
B	66	CRQ	GLY	chromophore	UNP Q9U6Y8
C	-10	MSE	-	insertion	UNP Q9U6Y8
C	-9	ARG	-	insertion	UNP Q9U6Y8
C	-8	GLY	-	insertion	UNP Q9U6Y8
C	-7	SER	-	insertion	UNP Q9U6Y8
C	-6	HIS	-	insertion	UNP Q9U6Y8
C	-5	HIS	-	insertion	UNP Q9U6Y8
C	-4	HIS	-	insertion	UNP Q9U6Y8
C	-3	HIS	-	insertion	UNP Q9U6Y8
C	-2	HIS	-	insertion	UNP Q9U6Y8
C	-1	HIS	-	insertion	UNP Q9U6Y8
C	0	GLY	-	insertion	UNP Q9U6Y8
C	1	SER	-	insertion	UNP Q9U6Y8
C	66	CRQ	GLN	chromophore	UNP Q9U6Y8
C	66	CRQ	TYR	chromophore	UNP Q9U6Y8
C	66	CRQ	GLY	chromophore	UNP Q9U6Y8
D	-10	MSE	-	insertion	UNP Q9U6Y8
D	-9	ARG	-	insertion	UNP Q9U6Y8
D	-8	GLY	-	insertion	UNP Q9U6Y8
D	-7	SER	-	insertion	UNP Q9U6Y8
D	-6	HIS	-	insertion	UNP Q9U6Y8
D	-5	HIS	-	insertion	UNP Q9U6Y8
D	-4	HIS	-	insertion	UNP Q9U6Y8
D	-3	HIS	-	insertion	UNP Q9U6Y8
D	-2	HIS	-	insertion	UNP Q9U6Y8
D	-1	HIS	-	insertion	UNP Q9U6Y8
D	0	GLY	-	insertion	UNP Q9U6Y8
D	1	SER	-	insertion	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	96	Total 96	O 96	0	0
2	B	116	Total 116	O 116	0	0
2	C	100	Total 100	O 100	0	0
2	D	106	Total 106	O 106	0	0

● Molecule 1: FLUORESCENT PROTEIN FP583



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.37Å 112.27Å 70.69Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.00) 95.1 (30.00-2.00)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	36.12 (at 1.99Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.162 , 0.249 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	1.29	1/1815 (0.1%)	1.43	10/2435 (0.4%)
1	B	1.27	1/1815 (0.1%)	1.42	8/2435 (0.3%)
1	C	1.26	2/1815 (0.1%)	1.23	6/2435 (0.2%)
1	D	1.26	2/1815 (0.1%)	1.30	4/2435 (0.2%)
All	All	1.27	6/7260 (0.1%)	1.35	28/9740 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	182	MSE	CA-C	-6.29	1.45	1.52
1	B	53	PRO	N-CA	-6.06	1.39	1.47
1	D	169	ASP	CG-OD2	5.36	1.35	1.25
1	A	212	GLU	CD-OE2	5.33	1.35	1.25
1	C	102	GLY	C-N	-5.30	1.28	1.33
1	D	54	LEU	CA-C	-5.06	1.47	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLY	CA-C-N	19.89	144.71	119.84
1	A	52	GLY	C-N-CA	19.89	144.71	119.84
1	B	52	GLY	CA-C-N	19.02	143.62	119.84
1	B	52	GLY	C-N-CA	19.02	143.62	119.84
1	A	52	GLY	C-N-CD	-17.63	52.72	125.00
1	D	52	GLY	C-N-CD	-17.35	53.85	125.00
1	B	52	GLY	C-N-CD	-16.23	58.44	125.00
1	A	52	GLY	O-C-N	11.30	133.07	121.77
1	B	52	GLY	O-C-N	11.00	132.77	121.77
1	A	53	PRO	N-CA-CB	10.20	113.96	103.25
1	B	53	PRO	N-CA-CB	9.17	112.88	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	PHE	CA-CB-CG	7.10	120.90	113.80
1	B	182	MSE	CG-SE-CE	-6.03	85.67	98.92
1	B	124	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	53	PRO	N-CA-C	-5.83	100.45	112.47
1	A	182	MSE	CG-SE-CE	-5.82	86.12	98.92
1	D	109	GLN	N-CA-C	5.73	117.89	109.24
1	D	182	MSE	CG-SE-CE	-5.54	86.73	98.92
1	C	87	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	188	GLN	N-CA-C	5.42	117.56	109.59
1	A	53	PRO	CA-N-CD	-5.39	104.46	112.00
1	C	19	GLU	CA-C-N	-5.29	115.88	121.48
1	C	19	GLU	C-N-CA	-5.29	115.88	121.48
1	A	87	PHE	CA-CB-CG	-5.26	108.54	113.80
1	C	7	VAL	N-CA-CB	5.25	120.43	111.50
1	C	6	ASN	CA-C-N	5.10	130.88	121.70
1	C	6	ASN	C-N-CA	5.10	130.88	121.70
1	D	53	PRO	N-CA-CB	5.07	108.57	103.25

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	1792	0	1744	49	0
1	B	1792	0	1744	61	0
1	C	1792	0	1744	49	0
1	D	1792	0	1744	64	0
2	A	96	0	0	6	0
2	B	116	0	0	6	0
2	C	100	0	0	1	0
2	D	106	0	0	2	0
All	All	7586	0	6976	215	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 15.

All (215) 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:6:ASN:HA	1:C:7:VAL:HB	1.42	1.00
1:B:141:MSE:HE3	1:B:168:LYS:HG2	1.46	0.95
1:D:141:MSE:HE3	1:D:168:LYS:HG2	1.50	0.94
1:D:148:GLU:HB3	1:D:195:VAL:HG23	1.51	0.92
1:B:17:ARG:HH12	1:B:19:GLU:HG3	1.35	0.92
1:D:150:LEU:HD11	1:D:195:VAL:HG22	1.52	0.91
1:B:45:LYS:HE2	1:B:47:LYS:HZ1	1.33	0.90
1:B:45:LYS:HE2	1:B:47:LYS:NZ	1.87	0.88
1:C:45:LYS:HE2	1:C:47:LYS:HE3	1.60	0.83
1:B:132:ASP:HA	1:B:137:GLN:HE21	1.45	0.81
1:C:134:PRO:HA	1:C:139:LYS:HG2	1.62	0.81
1:B:17:ARG:NH1	1:B:19:GLU:HG3	1.96	0.80
1:A:158:LYS:HE2	1:A:180:ILE:HD12	1.64	0.80
1:B:45:LYS:HE2	1:B:47:LYS:CE	2.11	0.80
1:A:45:LYS:CD	1:A:212:GLU:HG3	2.12	0.79
1:C:36:ARG:HG3	1:C:41:HIS:CE1	2.20	0.77
1:C:82:TYR:CD1	1:C:187:VAL:HG22	2.20	0.77
1:A:16:VAL:C	1:A:17:ARG:HD2	2.10	0.76
1:B:45:LYS:HE2	1:B:47:LYS:HE3	1.66	0.76
1:B:181:TYR:C	1:B:182:MSE:HG3	2.11	0.74
1:D:134:PRO:HA	1:D:139:LYS:HE3	1.69	0.73
1:D:150:LEU:HD11	1:D:195:VAL:CG2	2.20	0.72
1:D:150:LEU:CD1	1:D:195:VAL:HG22	2.19	0.72
1:A:181:TYR:C	1:A:182:MSE:HG3	2.14	0.71
1:B:9:LYS:HE3	2:B:294:HOH:O	1.90	0.71
1:C:45:LYS:CE	1:C:47:LYS:HE3	2.20	0.71
1:C:181:TYR:C	1:C:182:MSE:HG3	2.14	0.71
1:A:6:ASN:ND2	1:A:9:LYS:HG3	2.06	0.71
1:B:58:TRP:HE1	1:B:213:GLN:HE21	1.39	0.70
1:D:148:GLU:HB3	1:D:195:VAL:CG2	2.21	0.70
1:A:16:VAL:N	1:A:17:ARG:HH11	1.89	0.70
1:D:137:GLN:HB2	1:D:139:LYS:HE2	1.72	0.70
1:D:109:GLN:HB2	1:D:121:LYS:O	1.91	0.70
1:A:45:LYS:HD3	1:A:212:GLU:HG3	1.73	0.69
1:D:47:LYS:HD3	1:D:210:ILE:HG12	1.76	0.67
1:B:17:ARG:HD3	2:B:313:HOH:O	1.95	0.67
1:B:132:ASP:HA	1:B:137:GLN:NE2	2.10	0.66
1:B:17:ARG:HH11	1:B:17:ARG:HG2	1.58	0.66
1:B:216:ARG:HG2	1:D:224:PHE:CE2	2.31	0.66
1:C:134:PRO:HB3	1:C:139:LYS:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:N	1:A:17:ARG:NH1	2.44	0.65
1:A:121:LYS:NZ	2:A:276:HOH:O	2.29	0.65
1:A:6:ASN:HD21	1:A:9:LYS:HG3	1.62	0.65
1:B:76:PRO:HG2	1:B:79:ILE:HD12	1.79	0.65
1:D:89:GLU:OE1	1:D:185:LYS:HD3	1.95	0.65
1:D:222:HIS:HB3	1:D:225:LEU:HG	1.78	0.65
1:C:17:ARG:NH1	1:C:30:GLU:OE1	2.30	0.64
1:D:149:ARG:HD3	1:D:192:TYR:CZ	2.32	0.64
1:D:181:TYR:C	1:D:182:MSE:HG3	2.18	0.64
1:A:6:ASN:O	1:A:7:VAL:HG13	1.97	0.64
1:D:141:MSE:HE3	1:D:168:LYS:CG	2.28	0.64
1:B:17:ARG:HH12	1:B:19:GLU:CG	2.10	0.63
1:C:36:ARG:HG3	1:C:41:HIS:HE1	1.64	0.63
1:B:216:ARG:HD2	1:B:218:GLU:OE2	1.99	0.62
1:C:106:THR:HG23	1:D:125:ILE:CG2	2.29	0.62
1:D:40:GLY:HA2	1:D:72:TYR:O	1.99	0.62
1:B:141:MSE:HE3	1:B:168:LYS:CG	2.26	0.62
1:B:144:GLU:OE2	1:B:172:HIS:HE1	1.83	0.62
1:B:58:TRP:HE1	1:B:213:GLN:NE2	1.97	0.62
1:A:16:VAL:H	1:A:17:ARG:NH1	1.97	0.62
1:A:58:TRP:HE1	1:A:213:GLN:HE21	1.48	0.61
1:A:52:GLY:HA3	2:A:288:HOH:O	1.99	0.61
1:D:148:GLU:OE1	1:D:195:VAL:HG21	1.99	0.61
1:D:87:PHE:HB3	1:D:88:PRO:HA	1.83	0.60
1:C:94:GLU:HG3	1:C:180:ILE:HD13	1.83	0.60
1:A:134:PRO:HA	1:A:139:LYS:HD2	1.84	0.60
1:C:89:GLU:OE1	1:C:185:LYS:NZ	2.29	0.60
1:B:141:MSE:CE	1:B:168:LYS:HG2	2.28	0.60
1:C:134:PRO:HA	1:C:139:LYS:CG	2.31	0.60
1:A:17:ARG:HG3	1:A:30:GLU:HG2	1.84	0.60
1:A:58:TRP:HE1	1:A:213:GLN:NE2	2.00	0.59
1:D:141:MSE:SE	1:D:168:LYS:HA	2.52	0.59
1:A:45:LYS:HD2	1:A:212:GLU:HG3	1.83	0.59
1:C:62:SER:OG	1:C:63:PRO:HD3	2.01	0.59
1:B:79:ILE:HG12	2:B:331:HOH:O	2.03	0.58
1:B:47:LYS:HG3	1:B:210:ILE:HG12	1.85	0.58
1:D:141:MSE:CE	1:D:168:LYS:HG2	2.30	0.58
1:B:75:HIS:HE1	1:B:193:TYR:OH	1.85	0.58
1:B:123:LYS:NZ	2:B:313:HOH:O	2.28	0.57
1:C:58:TRP:HE1	1:C:213:GLN:NE2	2.02	0.57
1:B:149:ARG:HD3	1:B:192:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:HIS:HD2	2:D:281:HOH:O	1.88	0.57
1:C:58:TRP:HE1	1:C:213:GLN:HE21	1.52	0.56
1:B:66:CRQ:HE1	1:B:199:LEU:HB2	1.88	0.56
1:B:122:VAL:C	1:B:123:LYS:HD2	2.31	0.56
1:D:66:CRQ:HE1	1:D:199:LEU:HB2	1.88	0.56
1:A:158:LYS:HE2	1:A:180:ILE:CD1	2.32	0.56
1:C:199:LEU:C	1:C:199:LEU:HD23	2.31	0.55
1:B:90:GLY:C	1:B:184:LYS:HD2	2.32	0.55
1:A:114:GLN:HG3	1:A:119:ILE:HG13	1.88	0.55
1:D:6:ASN:O	1:D:7:VAL:HG22	2.07	0.54
1:A:149:ARG:HD3	1:A:192:TYR:CZ	2.43	0.54
1:B:216:ARG:HG3	1:B:217:THR:N	2.21	0.54
1:C:92:LYS:NZ	1:C:110:ASP:OD1	2.40	0.54
1:D:6:ASN:C	1:D:8:ILE:H	2.14	0.54
1:C:17:ARG:HG2	1:C:30:GLU:HG2	1.90	0.54
1:D:45:LYS:HD3	1:D:212:GLU:OE1	2.08	0.54
1:A:47:LYS:HG2	1:A:210:ILE:HG12	1.90	0.53
1:C:149:ARG:HD3	1:C:192:TYR:CZ	2.43	0.53
1:A:43:THR:HG22	1:A:214:TYR:HD1	1.73	0.53
1:B:119:ILE:HG21	1:B:121:LYS:HZ1	1.73	0.53
1:D:70:LYS:HE2	2:D:270:HOH:O	2.08	0.53
1:C:40:GLY:HA2	1:C:72:TYR:O	2.07	0.53
1:B:18:MSE:HE3	1:B:65:PHE:CE2	2.43	0.53
1:D:62:SER:OG	1:D:63:PRO:HD3	2.09	0.53
1:B:6:ASN:ND2	1:B:8:ILE:H	2.07	0.53
1:D:45:LYS:HD3	1:D:212:GLU:CD	2.34	0.53
1:C:89:GLU:H	1:C:89:GLU:CD	2.17	0.53
1:B:45:LYS:CE	1:B:47:LYS:HE3	2.37	0.52
1:D:89:GLU:CD	1:D:89:GLU:H	2.17	0.52
1:A:54:LEU:O	1:A:138:LYS:NZ	2.31	0.52
1:A:28:GLU:HB2	1:A:50:LYS:HG3	1.92	0.52
1:A:180:ILE:HD11	1:B:128:ASN:OD1	2.10	0.52
1:D:45:LYS:HB2	1:D:212:GLU:HG2	1.92	0.52
1:A:16:VAL:O	1:A:17:ARG:NH1	2.44	0.51
1:D:134:PRO:CA	1:D:139:LYS:HE3	2.40	0.51
1:C:6:ASN:CA	1:C:7:VAL:HB	2.29	0.51
1:A:16:VAL:C	1:A:17:ARG:HH11	2.19	0.51
1:A:149:ARG:HD2	1:A:149:ARG:C	2.35	0.51
1:D:93:TRP:CE2	1:D:109:GLN:HG3	2.46	0.50
1:D:149:ARG:HD3	1:D:192:TYR:CE1	2.46	0.50
1:A:178:LYS:NZ	2:A:265:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LEU:C	1:B:199:LEU:HD23	2.37	0.50
1:A:128:ASN:OD1	1:B:158:LYS:NZ	2.44	0.50
1:B:70:LYS:HD2	1:B:73:VAL:CG2	2.42	0.50
1:B:141:MSE:HE3	1:B:168:LYS:HA	1.93	0.50
1:A:14:PHE:HB3	1:A:118:PHE:HB2	1.93	0.49
1:D:51:GLY:O	1:D:52:GLY:O	2.29	0.49
1:C:70:LYS:HE2	2:C:269:HOH:O	2.12	0.49
1:B:17:ARG:HH11	1:B:17:ARG:CG	2.22	0.49
1:D:52:GLY:O	1:D:53:PRO:O	2.29	0.49
1:B:121:LYS:HE2	2:B:227:HOH:O	2.12	0.49
1:C:6:ASN:OD1	1:C:8:ILE:O	2.30	0.49
1:C:167:LEU:HD11	1:C:173:TYR:HB2	1.95	0.49
1:D:90:GLY:C	1:D:184:LYS:HD2	2.38	0.48
1:D:148:GLU:HG2	1:D:150:LEU:CD1	2.44	0.48
1:C:6:ASN:OD1	1:C:8:ILE:HB	2.14	0.48
1:D:148:GLU:HB2	1:D:161:ILE:HG12	1.94	0.48
1:A:6:ASN:HD21	1:A:9:LYS:CG	2.25	0.48
1:C:36:ARG:HB2	1:C:39:GLU:HB2	1.96	0.48
1:D:93:TRP:CE2	1:D:109:GLN:CG	2.97	0.47
1:A:17:ARG:NH1	1:A:31:GLY:O	2.40	0.47
1:C:106:THR:HG23	1:D:125:ILE:HG21	1.96	0.47
1:A:36:ARG:HE	1:A:39:GLU:CD	2.23	0.47
1:C:204:HIS:HD2	1:C:205:ASN:O	1.97	0.47
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.73	0.47
1:D:62:SER:HA	1:D:213:GLN:HE22	1.80	0.47
1:B:119:ILE:HG21	1:B:121:LYS:NZ	2.30	0.46
1:C:138:LYS:O	1:C:168:LYS:NZ	2.48	0.46
1:D:45:LYS:HB2	1:D:212:GLU:CG	2.45	0.46
1:A:41:HIS:HD2	2:A:242:HOH:O	1.97	0.46
1:B:91:PHE:N	1:B:184:LYS:HD2	2.31	0.46
1:D:46:LEU:N	1:D:46:LEU:HD22	2.29	0.46
1:D:37:PRO:HA	1:D:72:TYR:HA	1.98	0.46
1:D:199:LEU:C	1:D:199:LEU:HD23	2.41	0.46
1:C:106:THR:CG2	1:D:125:ILE:HB	2.45	0.46
1:A:137:GLN:HB2	1:A:139:LYS:HD2	1.98	0.46
1:A:52:GLY:HA3	2:A:263:HOH:O	2.16	0.45
1:A:153:ARG:CG	1:A:154:ASP:N	2.79	0.45
1:C:59:ASP:HB3	1:C:165:LEU:HD21	1.98	0.45
1:D:93:TRP:NE1	1:D:109:GLN:CG	2.79	0.45
1:B:62:SER:OG	1:B:63:PRO:HD3	2.16	0.45
1:B:149:ARG:HD3	1:B:192:TYR:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASP:O	1:B:217:THR:HA	2.16	0.45
1:C:52:GLY:HA2	1:C:53:PRO:C	2.42	0.45
1:A:105:VAL:HG22	1:A:126:GLY:HA2	1.98	0.45
1:C:66:CRQ:HE1	1:C:199:LEU:HB2	1.98	0.44
1:D:137:GLN:CB	1:D:139:LYS:HE2	2.44	0.44
1:A:17:ARG:HD2	1:A:17:ARG:N	2.32	0.44
1:B:17:ARG:NH1	1:B:17:ARG:CG	2.79	0.44
1:B:157:LEU:C	1:B:158:LYS:HG2	2.40	0.44
1:C:134:PRO:HA	1:C:139:LYS:HE2	1.99	0.44
1:B:94:GLU:HG2	1:B:108:THR:HA	2.00	0.44
1:A:36:ARG:NE	1:A:39:GLU:OE1	2.45	0.44
1:A:134:PRO:HA	1:A:139:LYS:CD	2.46	0.44
1:A:94:GLU:HG2	1:A:108:THR:HA	2.00	0.44
1:B:71:VAL:HG12	2:B:255:HOH:O	2.18	0.44
1:D:66:CRQ:NE1	1:D:213:GLN:OE1	2.50	0.44
1:B:62:SER:HA	1:B:213:GLN:HE22	1.83	0.43
1:D:10:GLU:O	1:D:36:ARG:HD2	2.18	0.43
1:D:58:TRP:HE1	1:D:213:GLN:HE21	1.66	0.43
1:C:25:HIS:HE1	1:C:51:GLY:O	2.01	0.43
1:D:41:HIS:ND1	1:D:214:TYR:OH	2.39	0.43
1:B:6:ASN:HD21	1:B:8:ILE:HB	1.83	0.43
1:D:149:ARG:O	1:D:159:GLY:HA2	2.19	0.42
1:D:141:MSE:HE2	1:D:141:MSE:HB3	1.85	0.42
1:B:114:GLN:N	1:B:119:ILE:CD1	2.82	0.42
1:D:6:ASN:C	1:D:8:ILE:N	2.78	0.42
1:D:45:LYS:HD3	1:D:212:GLU:CG	2.49	0.42
1:B:19:GLU:HB2	1:B:123:LYS:HE3	2.01	0.42
1:B:87:PHE:HB3	1:B:88:PRO:HA	2.01	0.42
1:A:71:VAL:HG22	1:A:71:VAL:O	2.20	0.42
1:B:71:VAL:O	1:B:71:VAL:HG22	2.19	0.42
1:D:61:LEU:O	1:D:64:GLN:HG2	2.19	0.42
1:C:106:THR:CG2	1:D:125:ILE:CG2	2.98	0.42
1:A:199:LEU:HD23	1:A:199:LEU:C	2.45	0.41
1:A:62:SER:OG	1:A:63:PRO:HD3	2.20	0.41
1:B:149:ARG:C	1:B:149:ARG:HD2	2.45	0.41
1:A:114:GLN:CG	1:A:119:ILE:HG13	2.49	0.41
1:C:167:LEU:HD12	1:C:167:LEU:HA	1.76	0.41
1:C:47:LYS:HG3	1:C:210:ILE:HG12	2.02	0.41
1:C:166:LYS:HB2	1:C:166:LYS:HE3	1.89	0.41
1:A:70:LYS:HE3	2:A:237:HOH:O	2.20	0.41
1:C:76:PRO:HG2	1:C:79:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASN:OD1	1:D:158:LYS:NZ	2.50	0.41
1:C:141:MSE:SE	1:C:168:LYS:HG3	2.71	0.41
1:D:52:GLY:O	1:D:53:PRO:C	2.63	0.41
1:D:89:GLU:CD	1:D:89:GLU:N	2.79	0.41
1:D:168:LYS:C	1:D:170:GLY:H	2.29	0.40
1:B:46:LEU:O	1:B:47:LYS:HD2	2.21	0.40
1:C:143:TRP:CZ3	1:C:165:LEU:HG	2.56	0.40
1:C:17:ARG:CG	1:C:30:GLU:HG2	2.51	0.40
1:B:47:LYS:HE3	1:B:210:ILE:HG23	2.03	0.40
1:C:99:PHE:HD2	1:C:173:TYR:CE2	2.39	0.40
1:C:149:ARG:HD2	1:C:149:ARG:C	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/234 (91%)	208 (98%)	3 (1%)	2 (1%)	14	9
1	B	213/234 (91%)	206 (97%)	6 (3%)	1 (0%)	24	21
1	C	213/234 (91%)	208 (98%)	4 (2%)	1 (0%)	24	21
1	D	213/234 (91%)	205 (96%)	4 (2%)	4 (2%)	6	3
All	All	852/936 (91%)	827 (97%)	17 (2%)	8 (1%)	14	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	53	PRO
1	B	53	PRO
1	C	7	VAL

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Mol	Chain	Res	Type
1	D	52	GLY
1	D	53	PRO
1	D	7	VAL
1	D	186	PRO

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	192/198 (97%)	182 (95%)	10 (5%)	21	18
1	B	192/198 (97%)	176 (92%)	16 (8%)	10	7
1	C	192/198 (97%)	174 (91%)	18 (9%)	8	5
1	D	192/198 (97%)	182 (95%)	10 (5%)	21	18
All	All	768/792 (97%)	714 (93%)	54 (7%)	14	10

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	70	LYS
1	A	121	LYS
1	A	161	ILE
1	A	167	LEU
1	A	180	ILE
1	A	182	MSE
1	A	203	SER
1	A	212	GLU
1	A	223	LEU
1	B	9	LYS
1	B	10	GLU
1	B	32	GLU
1	B	46	LEU
1	B	47	LYS
1	B	50	LYS
1	B	117	CYS

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Mol	Chain	Res	Type
1	B	121	LYS
1	B	123	LYS
1	B	139	LYS
1	B	141	MSE
1	B	161	ILE
1	B	178	LYS
1	B	182	MSE
1	B	188	GLN
1	B	216	ARG
1	C	6	ASN
1	C	17	ARG
1	C	26	GLU
1	C	47	LYS
1	C	69[A]	SER
1	C	69[B]	SER
1	C	106	THR
1	C	121	LYS
1	C	139	LYS
1	C	141	MSE
1	C	161	ILE
1	C	167	LEU
1	C	168	LYS
1	C	182	MSE
1	C	187	VAL
1	C	203	SER
1	C	206	GLU
1	C	223	LEU
1	D	6	ASN
1	D	45	LYS
1	D	50	LYS
1	D	109	GLN
1	D	141	MSE
1	D	167	LEU
1	D	169	ASP
1	D	182	MSE
1	D	185	LYS
1	D	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN

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Mol	Chain	Res	Type
1	A	41	HIS
1	A	213	GLN
1	B	6	ASN
1	B	25	HIS
1	B	75	HIS
1	B	137	GLN
1	B	172	HIS
1	B	213	GLN
1	C	25	HIS
1	C	41	HIS
1	C	204	HIS
1	C	213	GLN
1	D	6	ASN
1	D	25	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	C	66	1	25,25,26	2.71	10 (40%)	28,34,36	1.60	6 (21%)
1	CRQ	D	66	1	25,25,26	3.51	10 (40%)	28,34,36	1.73	7 (25%)
1	CRQ	B	66	1	25,25,26	3.68	10 (40%)	28,34,36	1.87	7 (25%)
1	CRQ	A	66	1	25,25,26	3.92	9 (36%)	28,34,36	1.59	5 (17%)

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	C	66	1	-	3/10/32/33	0/2/2/2
1	CRQ	D	66	1	-	2/10/32/33	0/2/2/2
1	CRQ	B	66	1	-	2/10/32/33	0/2/2/2
1	CRQ	A	66	1	-	2/10/32/33	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRQ	C1-CA1	-15.70	1.25	1.48
1	B	66	CRQ	CA1-N1	-13.87	0.96	1.27
1	D	66	CRQ	CA1-N1	-13.44	0.97	1.27
1	C	66	CRQ	C1-CA1	6.75	1.57	1.48
1	B	66	CRQ	OH-CZ	-5.15	1.25	1.37
1	C	66	CRQ	OH-CZ	-4.94	1.25	1.37
1	A	66	CRQ	CE1-CZ	4.90	1.48	1.39
1	A	66	CRQ	CG2-CB2	-4.68	1.38	1.46
1	C	66	CRQ	C1-N3	4.66	1.45	1.38
1	B	66	CRQ	CB2-CA2	4.58	1.39	1.35
1	D	66	CRQ	OH-CZ	-4.51	1.26	1.37
1	A	66	CRQ	C1-N3	4.51	1.45	1.38
1	D	66	CRQ	CB2-CA2	4.47	1.39	1.35
1	C	66	CRQ	CB2-CA2	4.40	1.39	1.35
1	B	66	CRQ	CE1-CZ	4.33	1.47	1.39
1	D	66	CRQ	CE1-CZ	4.28	1.47	1.39
1	A	66	CRQ	OH-CZ	-4.26	1.27	1.37
1	B	66	CRQ	CE2-CZ	4.12	1.46	1.39
1	D	66	CRQ	CE2-CZ	4.08	1.46	1.39
1	C	66	CRQ	CG2-CB2	-4.03	1.39	1.46
1	C	66	CRQ	CE1-CZ	3.76	1.46	1.39
1	B	66	CRQ	C1-N3	3.74	1.44	1.38
1	A	66	CRQ	CE2-CZ	3.74	1.46	1.39
1	B	66	CRQ	CG2-CB2	-3.72	1.40	1.46
1	D	66	CRQ	CG2-CB2	-3.27	1.40	1.46
1	D	66	CRQ	CD1-CG2	2.99	1.45	1.39
1	A	66	CRQ	CB1-CA1	2.99	1.58	1.50
1	D	66	CRQ	C1-N3	2.94	1.43	1.38
1	C	66	CRQ	CA1-N1	-2.71	1.21	1.27
1	B	66	CRQ	CB1-CA1	2.70	1.57	1.50
1	D	66	CRQ	C1-CA1	-2.52	1.44	1.48
1	D	66	CRQ	CD2-CG2	2.51	1.44	1.39
1	B	66	CRQ	CD2-CG2	2.51	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRQ	CD2-CG2	2.44	1.44	1.39
1	A	66	CRQ	CA3-N3	-2.41	1.42	1.47
1	B	66	CRQ	CD1-CG2	2.40	1.44	1.39
1	C	66	CRQ	CE2-CZ	2.37	1.43	1.39
1	C	66	CRQ	CE2-CD2	-2.28	1.35	1.38
1	C	66	CRQ	CB1-CA1	2.25	1.56	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRQ	CG2-CB2-CA2	6.12	137.14	129.87
1	C	66	CRQ	CG2-CB2-CA2	4.95	135.75	129.87
1	D	66	CRQ	CG2-CB2-CA2	4.83	135.61	129.87
1	A	66	CRQ	CG1-CB1-CA1	-4.44	100.04	113.51
1	D	66	CRQ	CG1-CB1-CA1	-3.35	103.35	113.51
1	B	66	CRQ	CA2-C2-N3	3.24	106.22	103.50
1	A	66	CRQ	CE2-CZ-CE1	-3.23	114.63	119.77
1	A	66	CRQ	CG2-CB2-CA2	3.22	133.69	129.87
1	D	66	CRQ	CE2-CZ-CE1	-3.06	114.90	119.77
1	C	66	CRQ	CE2-CZ-CE1	-2.90	115.16	119.77
1	B	66	CRQ	CE2-CZ-CE1	-2.86	115.21	119.77
1	D	66	CRQ	CD2-CE2-CZ	2.64	122.67	119.88
1	B	66	CRQ	CB2-CA2-C2	-2.63	119.17	122.36
1	C	66	CRQ	CB2-CA2-C2	-2.55	119.27	122.36
1	B	66	CRQ	CB2-CA2-N2	2.49	132.14	128.76
1	B	66	CRQ	CG1-CB1-CA1	-2.49	105.97	113.51
1	B	66	CRQ	CD2-CE2-CZ	2.39	122.41	119.88
1	D	66	CRQ	CB2-CA2-C2	-2.34	119.52	122.36
1	D	66	CRQ	CB2-CA2-N2	2.27	131.84	128.76
1	C	66	CRQ	CB2-CA2-N2	2.24	131.80	128.76
1	C	66	CRQ	CD1-CE1-CZ	2.16	122.17	119.88
1	A	66	CRQ	CD1-CE1-CZ	2.10	122.10	119.88
1	A	66	CRQ	CB2-CA2-C2	-2.08	119.84	122.36
1	D	66	CRQ	CA2-C2-N3	2.08	105.25	103.50
1	C	66	CRQ	CA2-C2-N3	2.04	105.21	103.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRQ	C1-CA1-CB1-CG1
1	C	66	CRQ	C1-CA1-CB1-CG1

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Mol	Chain	Res	Type	Atoms
1	D	66	CRQ	C1-CA1-CB1-CG1
1	B	66	CRQ	OE1-CD3-CG1-CB1
1	C	66	CRQ	NE1-CD3-CG1-CB1
1	C	66	CRQ	OE1-CD3-CG1-CB1
1	D	66	CRQ	NE1-CD3-CG1-CB1
1	B	66	CRQ	NE1-CD3-CG1-CB1
1	A	66	CRQ	NE1-CD3-CG1-CB1

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	CRQ	1	0
1	D	66	CRQ	2	0
1	B	66	CRQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	211/234 (90%)	-0.24	5 (2%) 59 59	8, 14, 37, 89	1 (0%)
1	B	211/234 (90%)	-0.30	5 (2%) 59 59	7, 13, 32, 63	1 (0%)
1	C	211/234 (90%)	-0.18	2 (0%) 81 80	9, 16, 36, 67	1 (0%)
1	D	211/234 (90%)	-0.20	6 (2%) 55 54	9, 15, 37, 81	1 (0%)
All	All	844/936 (90%)	-0.23	18 (2%) 63 63	7, 15, 37, 89	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	6.7
1	D	52	GLY	5.7
1	C	6	ASN	5.0
1	D	6	ASN	4.5
1	B	6	ASN	4.2
1	D	169	ASP	3.6
1	B	169	ASP	2.9
1	B	206	GLU	2.7
1	A	17	ARG	2.5
1	D	53	PRO	2.5
1	A	53	PRO	2.4
1	A	114	GLN	2.3
1	C	168	LYS	2.2
1	B	170	GLY	2.2
1	A	52	GLY	2.2
1	D	168	LYS	2.1
1	B	53	PRO	2.1
1	D	19	GLU	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, 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	66	24/25	0.94	0.08	8,19,27,35	0
1	CRQ	D	66	24/25	0.94	0.08	11,17,23,33	0
1	CRQ	A	66	24/25	0.95	0.08	6,19,26,27	0
1	CRQ	B	66	24/25	0.96	0.07	6,14,20,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.