



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:26 AM UTC

PDB ID : 4GOB / pdb_00004gob
Title : Low pH Crystal Structure of a reconstructed Kaede-type Red Fluorescent Protein, Least Evolved Ancestor (LEA)
Authors : Kim, H.; Grunkemeyer, T.J.; Chen, L.; Fromme, R.; Wachter, R.M.
Deposited on : 2012-08-19
Resolution : 1.53 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

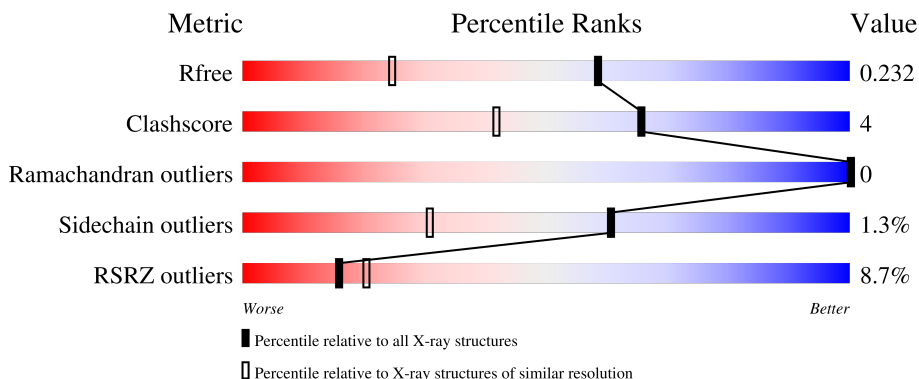
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	228	4% 84% 10% • 5%
1	B	228	3% 86% 8% • •
1	C	228	4% 84% 10% • 5%
1	D	228	23% 80% 13% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7504 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 Kaede-type Fluorescent Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	7	0
			1818	1162	305	340	11			
1	B	218	Total	C	N	O	S	2	4	0
			1802	1152	303	336	11			
1	C	217	Total	C	N	O	S	0	7	0
			1816	1161	304	337	14			
1	D	217	Total	C	N	O	S	0	1	0
			1774	1137	301	325	11			

- Molecule 2 is water.

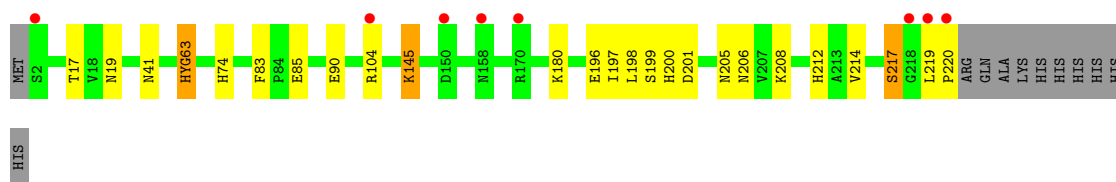
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	81	Total	O	0	0
			81	81		
2	C	71	Total	O	0	0
			71	71		
2	D	28	Total	O	0	0
			28	28		

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: Kaede-type Fluorescent Protein

Chain A: 



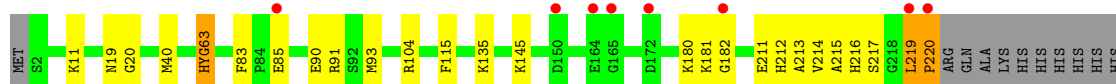
• Molecule 1: Kaede-type Fluorescent Protein

Chain B: 



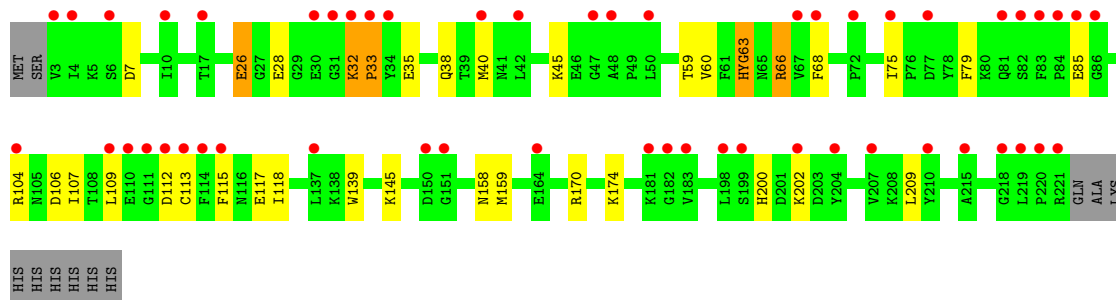
• Molecule 1: Kaede-type Fluorescent Protein

Chain C: 



• Molecule 1: Kaede-type Fluorescent Protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.44Å 100.79Å 120.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.98 – 1.53 33.98 – 1.53	Depositor EDS
% Data completeness (in resolution range)	94.1 (33.98-1.53) 94.1 (33.98-1.53)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.175 , 0.231 (Not available) , 0.232	Depositor DCC
R_{free} test set	7485 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	1.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CR8

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	1.05	8/1839 (0.4%)	0.89	1/2478 (0.0%)
1	B	0.99	11/1823 (0.6%)	0.83	0/2458
1	C	0.90	6/1837 (0.3%)	0.85	1/2475 (0.0%)
1	D	1.23	15/1795 (0.8%)	1.00	4/2419 (0.2%)
All	All	1.05	40/7294 (0.5%)	0.89	6/9830 (0.1%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	28	GLU	C-O	-8.98	1.13	1.24
1	D	106	ASP	C-O	-8.58	1.13	1.24
1	C	213	ALA	C-O	-8.47	1.13	1.23
1	C	214	VAL	C-O	-8.37	1.15	1.24
1	B	214	VAL	C-O	-7.68	1.16	1.24
1	B	216	HIS	CG-ND1	-7.59	1.29	1.38
1	C	216	HIS	CG-ND1	-7.41	1.30	1.38
1	D	107	ILE	C-O	-7.07	1.16	1.24
1	B	216	HIS	CD2-NE2	-6.90	1.30	1.37
1	D	75	ILE	C-O	-6.80	1.16	1.24
1	B	213	ALA	C-O	-6.79	1.15	1.23
1	C	216	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	212	HIS	CG-ND1	-6.61	1.30	1.38
1	D	200	HIS	CG-ND1	-6.50	1.31	1.38
1	A	200	HIS	CG-ND1	-6.35	1.31	1.38
1	B	219	LEU	C-O	-6.34	1.16	1.24
1	D	59	THR	C-O	-6.23	1.15	1.24
1	D	117	GLU	C-O	-6.22	1.16	1.24
1	A	206	ASN	C-O	-6.19	1.17	1.23
1	D	79	PHE	N-CA	-6.15	1.38	1.46
1	D	32	LYS	C-O	-6.05	1.19	1.25
1	B	222	GLN	C-O	-6.03	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	115	PHE	CA-C	5.93	1.59	1.52
1	D	200	HIS	CD2-NE2	-5.81	1.31	1.37
1	B	215	ALA	C-O	-5.78	1.16	1.23
1	B	221	ARG	CZ-NH2	-5.75	1.25	1.33
1	B	212	HIS	C-O	-5.71	1.17	1.24
1	A	217	SER	C-O	-5.66	1.16	1.24
1	A	201	ASP	C-O	-5.65	1.17	1.23
1	A	197	ILE	C-O	-5.63	1.17	1.23
1	A	214	VAL	C-O	-5.62	1.18	1.24
1	A	205	ASN	C-O	-5.39	1.17	1.24
1	D	60	VAL	C-O	-5.35	1.16	1.24
1	D	26	GLU	C-O	-5.34	1.17	1.23
1	D	115	PHE	C-O	-5.30	1.17	1.24
1	D	66	ARG	C-O	-5.18	1.17	1.24
1	C	217	SER	C-O	-5.17	1.17	1.24
1	C	215	ALA	C-O	-5.09	1.17	1.23
1	B	217	SER	C-O	-5.09	1.17	1.23
1	A	199	SER	C-O	-5.04	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	GLN	N-CA-C	6.18	117.92	108.52
1	D	35	GLU	N-CA-C	-5.57	106.48	113.72
1	A	83	PHE	CB-CA-C	5.31	116.73	108.61
1	D	118	ILE	N-CA-C	5.28	115.56	108.17
1	D	33	PRO	N-CA-C	5.21	120.92	113.47
1	C	83	PHE	CB-CA-C	5.14	116.47	108.61

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	1818	0	1737	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1802	0	1722	13	0
1	C	1816	0	1736	13	0
1	D	1774	0	1708	18	0
2	A	114	0	0	2	0
2	B	81	0	0	0	0
2	C	71	0	0	1	0
2	D	28	0	0	1	0
All	All	7504	0	6903	53	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 4.

All (53) 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:D:158:ASN:HB3	1:D:170:ARG:HH12	1.41	0.85
1:D:158:ASN:HB3	1:D:170:ARG:NH1	1.92	0.84
1:A:219:LEU:HA	1:A:220:PRO:C	2.11	0.75
1:C:219:LEU:HA	1:C:220:PRO:C	2.10	0.75
1:B:11:LYS:HG2	1:B:113:CYS:SG	2.32	0.69
1:A:212:HIS:HD2	1:B:220:PRO:O	1.79	0.64
1:B:181:LYS:HE2	1:B:182:GLY:H	1.62	0.64
1:A:74:HIS:HD2	2:A:412:HOH:O	1.81	0.62
1:A:145[B]:LYS:N	1:A:145[B]:LYS:HD3	2.14	0.61
1:A:41:ASN:HD21	1:A:208:LYS:NZ	2.00	0.60
1:A:198:LEU:CD2	1:B:221:ARG:HH21	2.16	0.58
1:A:19:ASN:HA	1:C:90:GLU:OE2	2.03	0.58
1:D:109:LEU:HD12	1:D:113:CYS:O	2.04	0.57
1:A:17[B]:THR:OG1	1:C:104:ARG:NH2	2.38	0.57
1:D:158:ASN:HB3	1:D:170:ARG:CZ	2.35	0.56
1:A:85[A]:GLU:O	1:A:180:LYS:HE2	2.05	0.56
1:A:41:ASN:HD21	1:A:208:LYS:HZ3	1.52	0.56
1:D:33:PRO:HD3	1:D:68:PHE:CE2	2.41	0.55
1:C:85:GLU:HB2	2:C:352:HOH:O	2.06	0.55
1:D:158:ASN:CB	1:D:170:ARG:HH12	2.16	0.55
1:A:85[B]:GLU:O	1:A:180:LYS:HE2	2.07	0.54
1:A:90:GLU:OE2	1:C:19:ASN:HA	2.08	0.53
1:D:33:PRO:HD3	1:D:68:PHE:HE2	1.75	0.52
1:D:112:ASP:C	1:D:112:ASP:OD2	2.51	0.52
1:B:145:LYS:HG3	1:B:190:PHE:CE2	2.45	0.52
1:C:181:LYS:HG2	1:C:182:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HD2	1:C:93[B]:MET:HE2	1.92	0.51
1:D:139:TRP:CE3	1:D:159:MET:HE3	2.47	0.50
1:D:7:ASP:OD1	1:D:32:LYS:HE2	2.11	0.50
1:D:40:MET:HB2	1:D:63:CR8:H10	1.95	0.48
1:C:11:LYS:HD3	1:C:115:PHE:CE1	2.50	0.47
1:A:74:HIS:HE1	1:A:217:SER:OG	1.98	0.46
1:C:219:LEU:CA	1:C:220:PRO:C	2.87	0.46
1:A:196:GLU:OE1	1:B:221:ARG:CZ	2.63	0.46
1:D:158:ASN:HB3	1:D:170:ARG:NH2	2.30	0.46
1:A:63:CR8:H10	2:A:413:HOH:O	2.16	0.46
1:A:145[B]:LYS:HE3	1:B:158:ASN:HB2	1.98	0.45
1:C:181:LYS:HG2	1:C:182:GLY:H	1.82	0.45
1:A:196:GLU:OE1	1:B:221:ARG:NH2	2.50	0.45
1:B:20:GLY:H	1:D:104[A]:ARG:HH11	1.65	0.45
1:B:40:MET:HB2	1:B:63:CR8:H10	1.99	0.45
1:A:104[A]:ARG:HH11	1:C:20:GLY:H	1.65	0.44
1:D:174:LYS:HE3	2:D:324:HOH:O	2.17	0.44
1:D:66:ARG:HB2	1:D:66:ARG:CZ	2.48	0.44
1:A:90:GLU:HG2	1:A:104[A]:ARG:HG2	1.99	0.43
1:C:40:MET:HB2	1:C:63:CR8:H10	2.01	0.42
1:D:63:CR8:H23	1:D:209:LEU:HG	2.02	0.42
1:B:145:LYS:HG3	1:B:190:PHE:CD2	2.54	0.42
1:D:202:LYS:HA	1:D:202:LYS:HD3	1.60	0.41
1:D:26:GLU:OE1	1:D:45:LYS:HE3	2.20	0.41
1:B:63:CR8:H23	1:B:211:GLU:HB2	2.03	0.41
1:B:9:LYS:C	1:B:10:ILE:HG13	2.46	0.41
1:C:211:GLU:HG2	1:C:212:HIS:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/228 (96%)	219 (100%)	0	0	100	100
1	B	217/228 (95%)	217 (100%)	0	0	100	100
1	C	219/228 (96%)	216 (99%)	3 (1%)	0	100	100
1	D	213/228 (93%)	211 (99%)	2 (1%)	0	100	100
All	All	868/912 (95%)	863 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	195/198 (98%)	193 (99%)	2 (1%)	68	42
1	B	193/198 (98%)	191 (99%)	2 (1%)	68	42
1	C	195/198 (98%)	190 (97%)	5 (3%)	40	11
1	D	189/198 (96%)	187 (99%)	2 (1%)	65	38
All	All	772/792 (98%)	761 (99%)	11 (1%)	61	29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145[A]	LYS
1	A	145[B]	LYS
1	B	145	LYS
1	B	181	LYS
1	C	135	LYS
1	C	145	LYS
1	C	180	LYS
1	C	219	LEU
1	C	220	PRO
1	D	85	GLU
1	D	145	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	41	ASN
1	A	74	HIS
1	A	81	GLN
1	A	212	HIS
1	B	38	GLN
1	B	74	HIS
1	B	212	HIS
1	C	38	GLN
1	C	74	HIS
1	C	81	GLN
1	C	212	HIS
1	D	38	GLN
1	D	41	ASN
1	D	74	HIS
1	D	81	GLN

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	CR8	A	63	1	25,27,28	1.72	6 (24%)	24,37,39	2.07	7 (29%)
1	CR8	B	63	1	25,27,28	1.53	5 (20%)	24,37,39	1.65	6 (25%)
1	CR8	C	63	1	25,27,28	1.34	5 (20%)	24,37,39	1.97	8 (33%)
1	CR8	D	63	1	25,27,28	2.06	7 (28%)	24,37,39	2.06	8 (33%)

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	CR8	A	63	1	-	4/12/25/26	0/3/3/3
1	CR8	B	63	1	-	4/12/25/26	0/3/3/3
1	CR8	C	63	1	-	5/12/25/26	0/3/3/3
1	CR8	D	63	1	-	4/12/25/26	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	CR8	C20-C21	4.37	1.56	1.49
1	A	63	CR8	C1-N3	4.05	1.44	1.37
1	D	63	CR8	O2-C2	-4.01	1.18	1.31
1	D	63	CR8	CA3-N3	-3.80	1.40	1.47
1	D	63	CR8	C4-C11	-3.69	1.36	1.46
1	B	63	CR8	C1-N3	3.16	1.42	1.37
1	A	63	CR8	C6-C12	3.07	1.42	1.35
1	A	63	CR8	C4-C11	-3.05	1.38	1.46
1	C	63	CR8	C1-N3	3.05	1.42	1.37
1	D	63	CR8	C1-N2	-2.96	1.27	1.32
1	D	63	CR8	C21-N22	-2.84	1.32	1.37
1	A	63	CR8	CA3-N3	-2.79	1.42	1.47
1	B	63	CR8	C12-C11	-2.64	1.39	1.46
1	B	63	CR8	C4-C11	-2.50	1.39	1.46
1	C	63	CR8	C12-C11	-2.44	1.39	1.46
1	B	63	CR8	C6-C12	2.38	1.41	1.35
1	A	63	CR8	C12-C11	-2.23	1.40	1.46
1	C	63	CR8	O2-C2	-2.21	1.24	1.31
1	D	63	CR8	C12-C11	-2.20	1.40	1.46
1	B	63	CR8	C23-N11	-2.18	1.33	1.37
1	C	63	CR8	C4-C11	-2.14	1.40	1.46
1	C	63	CR8	C6-C12	2.13	1.40	1.35
1	A	63	CR8	O2-C2	-2.10	1.24	1.31

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	CR8	C3-CA3-N3	5.49	124.91	112.43
1	A	63	CR8	C3-CA3-N3	4.86	123.48	112.43
1	A	63	CR8	N3-C1-N2	4.54	115.06	111.48
1	D	63	CR8	N3-C1-N2	4.52	115.05	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	CR8	C12-C6-C7	-3.77	118.54	122.10
1	C	63	CR8	N3-C1-N2	3.57	114.30	111.48
1	C	63	CR8	C8-CA2-C2	-3.26	122.65	129.19
1	C	63	CR8	CA1-C1-N3	-3.26	120.60	124.84
1	D	63	CR8	C8-CA2-C2	-3.14	122.89	129.19
1	B	63	CR8	C8-CA2-C2	-3.02	123.14	129.19
1	B	63	CR8	CA1-C1-N3	-3.01	120.92	124.84
1	B	63	CR8	CA2-N2-C1	2.90	108.07	105.80
1	A	63	CR8	C8-CA2-C2	-2.79	123.59	129.19
1	C	63	CR8	C12-C6-C7	-2.77	119.48	122.10
1	B	63	CR8	C12-C6-C7	-2.64	119.60	122.10
1	C	63	CR8	C3-CA3-N3	2.55	118.24	112.43
1	A	63	CR8	C20-C21-N22	2.55	130.09	123.22
1	B	63	CR8	C20-C21-N22	2.48	129.89	123.22
1	B	63	CR8	C3-CA3-N3	2.46	118.03	112.43
1	D	63	CR8	C10-N22-C21	2.45	111.09	107.91
1	A	63	CR8	CA1-C1-N3	-2.42	121.69	124.84
1	D	63	CR8	N22-C10-N11	-2.35	106.65	111.00
1	D	63	CR8	C4-C5-C7	-2.29	119.93	122.10
1	C	63	CR8	C1-N3-C2	-2.20	105.06	107.83
1	C	63	CR8	C4-C11-C12	2.14	120.66	116.67
1	D	63	CR8	C23-N11-C10	2.04	109.94	105.94
1	D	63	CR8	C21-C23-N11	-2.03	106.09	109.73
1	A	63	CR8	C1-N3-C2	-2.03	105.28	107.83
1	C	63	CR8	N22-C10-N11	-2.02	107.26	111.00

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	CR8	C3-CA3-N3-C2
1	A	63	CR8	CA1-C20-C21-N22
1	A	63	CR8	CA1-C20-C21-C23
1	B	63	CR8	C3-CA3-N3-C2
1	B	63	CR8	C3-CA3-N3-C1
1	B	63	CR8	CA1-C20-C21-N22
1	B	63	CR8	CA1-C20-C21-C23
1	C	63	CR8	C3-CA3-N3-C2
1	C	63	CR8	C3-CA3-N3-C1
1	C	63	CR8	CA1-C20-C21-N22
1	C	63	CR8	CA1-C20-C21-C23
1	D	63	CR8	CA1-C20-C21-N22

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Mol	Chain	Res	Type	Atoms
1	D	63	CR8	CA1-C20-C21-C23
1	C	63	CR8	C21-C20-CA1-N1
1	D	63	CR8	C3-CA3-N3-C2
1	A	63	CR8	C3-CA3-N3-C1
1	D	63	CR8	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	CR8	1	0
1	B	63	CR8	2	0
1	C	63	CR8	1	0
1	D	63	CR8	2	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	216/228 (94%)	0.09	8 (3%)	45	54	7, 15, 25, 54	7 (3%)
1	B	217/228 (95%)	0.21	7 (3%)	50	59	9, 18, 34, 43	6 (2%)
1	C	216/228 (94%)	0.33	8 (3%)	45	54	8, 19, 34, 59	7 (3%)
1	D	216/228 (94%)	1.27	52 (24%)	2	2	16, 35, 54, 60	1 (0%)
All	All	865/912 (94%)	0.47	75 (8%)	16	20	7, 20, 46, 60	21 (2%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	PRO	6.6
1	B	222	GLN	5.5
1	D	3	VAL	5.0
1	C	220	PRO	4.8
1	A	220	PRO	4.7
1	D	82	SER	4.1
1	D	199	SER	4.1
1	D	34	TYR	3.9
1	C	219	LEU	3.9
1	D	198	LEU	3.6
1	D	83	PHE	3.6
1	D	221	ARG	3.5
1	D	109	LEU	3.5
1	D	40	MET	3.5
1	D	33	PRO	3.5
1	B	3	VAL	3.5
1	D	113	CYS	3.4
1	D	207	VAL	3.4
1	B	181	LYS	3.4
1	D	48	ALA	3.4
1	D	4	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	204	TYR	3.3
1	D	17	THR	3.2
1	D	10	ILE	3.2
1	D	181	LYS	3.1
1	C	165	GLY	3.0
1	D	202	LYS	2.8
1	D	6	SER	2.8
1	A	150	ASP	2.8
1	D	42	LEU	2.8
1	D	215	ALA	2.8
1	D	86	GLY	2.8
1	D	182	GLY	2.7
1	A	2	SER	2.7
1	D	67	VAL	2.7
1	D	218	GLY	2.7
1	B	150	ASP	2.7
1	D	81	GLN	2.7
1	D	111	GLY	2.7
1	C	85	GLU	2.7
1	C	150	ASP	2.6
1	D	84	PRO	2.6
1	D	137	LEU	2.5
1	A	158	ASN	2.5
1	D	150	ASP	2.5
1	D	104[A]	ARG	2.5
1	A	219	LEU	2.4
1	D	115	PHE	2.4
1	C	164	GLU	2.4
1	C	182	GLY	2.4
1	D	75	ILE	2.4
1	A	104[A]	ARG	2.4
1	D	30	GLU	2.3
1	A	218	GLY	2.3
1	D	77	ASP	2.3
1	D	32	LYS	2.3
1	D	112	ASP	2.3
1	D	210	TYR	2.3
1	D	114	PHE	2.2
1	D	72	PRO	2.2
1	D	164	GLU	2.2
1	D	85	GLU	2.2
1	D	151	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	170	ARG	2.1
1	D	47	GLY	2.1
1	D	50	LEU	2.1
1	B	113	CYS	2.1
1	C	172	ASP	2.1
1	D	31	GLY	2.1
1	D	183	VAL	2.1
1	D	110	GLU	2.1
1	D	68	PHE	2.0
1	B	164	GLU	2.0
1	B	202	LYS	2.0
1	D	219	LEU	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($\text{\AA}^2$)	Q<0.9
1	CR8	D	63	25/26	0.93	0.10	26,29,39,44	0
1	CR8	C	63	25/26	0.95	0.07	13,16,18,20	0
1	CR8	B	63	25/26	0.95	0.08	13,14,19,20	0
1	CR8	A	63	25/26	0.96	0.06	10,13,15,17	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.