



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:53 PM UTC

PDB ID : 1XMZ / pdb_00001xmz
Title : Crystal structure of the dark state of kindling fluorescent protein kfp from anemonia sulcata
Authors : Quillin, M.L.; Anstrom, D.M.; Shu, X.; O'Leary, S.; Kallio, K.; Chudakov, D.M.; Remington, S.J.
Deposited on : 2004-10-04
Resolution : 1.38 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

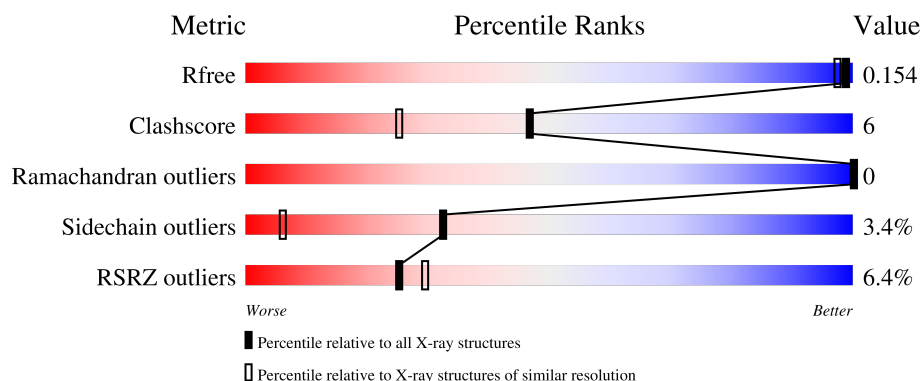
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.38 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	74	4% 65% 15% 19%
1	B	74	5% 78% 11% 9%
2	C	168	8% 80% 17% ..
2	D	168	5% 82% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4295 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 GFP-like non-fluorescent chromoprotein FP595 chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	S	0	10	1
			500	324	76	95	5			
1	B	67	Total	C	N	O	S	0	6	1
			534	341	88	100	5			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q9GZ28
A	-9	ARG	-	expression tag	UNP Q9GZ28
A	-8	GLY	-	expression tag	UNP Q9GZ28
A	-7	SER	-	expression tag	UNP Q9GZ28
A	-6	HIS	-	expression tag	UNP Q9GZ28
A	-5	HIS	-	expression tag	UNP Q9GZ28
A	-4	HIS	-	expression tag	UNP Q9GZ28
A	-3	HIS	-	expression tag	UNP Q9GZ28
A	-2	HIS	-	expression tag	UNP Q9GZ28
A	-1	HIS	-	expression tag	UNP Q9GZ28
A	0	GLY	-	expression tag	UNP Q9GZ28
A	1	SER	-	expression tag	UNP Q9GZ28
A	63	NH2	-	cloning artifact	UNP Q9GZ28
B	-10	MET	-	initiating methionine	UNP Q9GZ28
B	-9	ARG	-	expression tag	UNP Q9GZ28
B	-8	GLY	-	expression tag	UNP Q9GZ28
B	-7	SER	-	expression tag	UNP Q9GZ28
B	-6	HIS	-	expression tag	UNP Q9GZ28
B	-5	HIS	-	expression tag	UNP Q9GZ28
B	-4	HIS	-	expression tag	UNP Q9GZ28
B	-3	HIS	-	expression tag	UNP Q9GZ28
B	-2	HIS	-	expression tag	UNP Q9GZ28
B	-1	HIS	-	expression tag	UNP Q9GZ28
B	0	GLY	-	expression tag	UNP Q9GZ28
B	1	SER	-	expression tag	UNP Q9GZ28

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	63	NH2	-	cloning artifact	UNP Q9GZ28

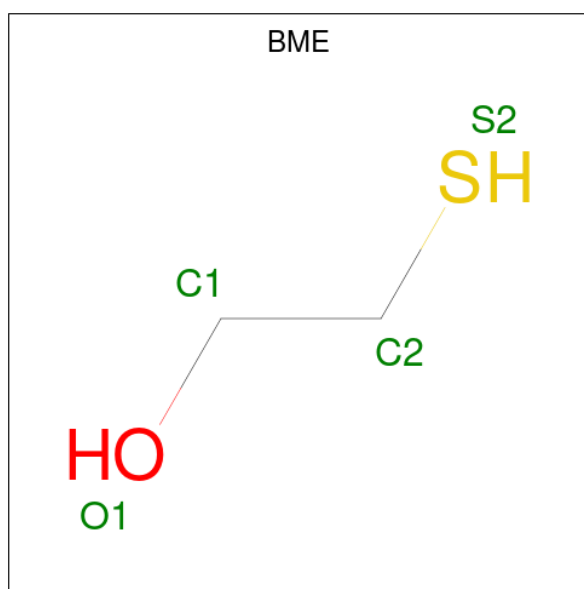
- Molecule 2 is a protein called GFP-like non-fluorescent chromoprotein FP595 chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	166	Total	C	N	O	S	0	12	0
			1385	886	235	254	10			
2	D	166	Total	C	N	O	S	0	13	0
			1385	886	234	255	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	65	CRK	MET	chromophore	UNP Q9GZ28
C	65	CRK	TYR	chromophore	UNP Q9GZ28
C	65	CRK	GLY	chromophore	UNP Q9GZ28
C	143	GLY	ALA	engineered mutation	UNP Q9GZ28
D	65	CRK	MET	chromophore	UNP Q9GZ28
D	65	CRK	TYR	chromophore	UNP Q9GZ28
D	65	CRK	GLY	chromophore	UNP Q9GZ28
D	143	GLY	ALA	engineered mutation	UNP Q9GZ28

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O S 4 2 1 1	0	0
3	C	1	Total C O S 4 2 1 1	0	0
3	C	1	Total C O S 4 2 1 1	0	0
3	C	1	Total C O S 4 2 1 1	0	0
3	D	1	Total C O S 4 2 1 1	0	0
3	D	1	Total C O S 4 2 1 1	0	0
3	D	1	Total C O S 4 2 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	230	Total O 230 230	0	2
4	D	233	Total O 233 233	0	3

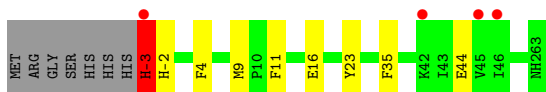
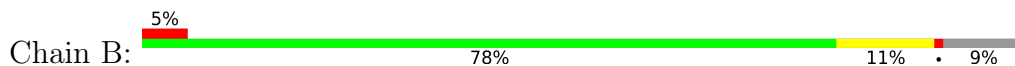
3 Residue-property plots [i](#)

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.

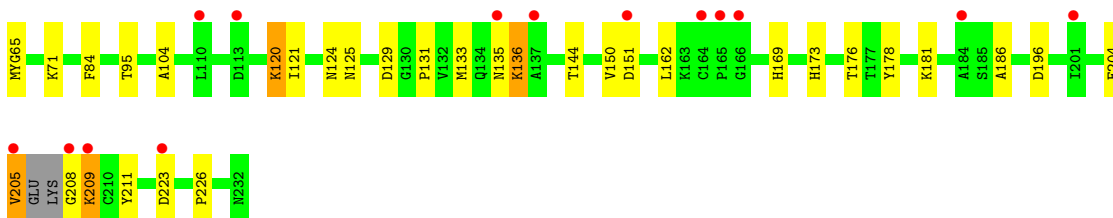
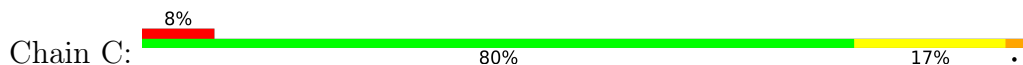
- Molecule 1: GFP-like non-fluorescent chromoprotein FP595 chain 1



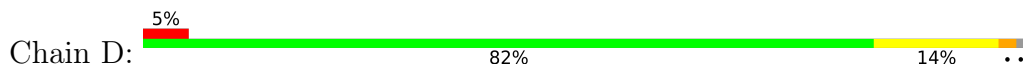
- Molecule 1: GFP-like non-fluorescent chromoprotein FP595 chain 1



- Molecule 2: GFP-like non-fluorescent chromoprotein FP595 chain 2



- Molecule 2: GFP-like non-fluorescent chromoprotein FP595 chain 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.52Å 125.40Å 92.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.38 50.00 – 1.38	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-1.38) 95.5 (50.00-1.38)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.35 (at 1.38Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.139 , 0.191 0.147 , 0.154	Depositor DCC
R_{free} test set	4307 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.014 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4295	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: NH2, CRK, BME

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	0.75	0/551	1.28	2/740 (0.3%)
1	B	0.71	0/574	1.72	6/772 (0.8%)
2	C	0.74	0/1450	1.47	14/1951 (0.7%)
2	D	0.76	0/1453	1.39	10/1957 (0.5%)
All	All	0.74	0/4028	1.46	32/5420 (0.6%)

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

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

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	-3	HIS	CA-C-N	20.16	161.24	122.53
1	B	-3	HIS	C-N-CA	20.16	161.24	122.53
2	D	151	ASP	CA-CB-CG	14.21	126.81	112.60
2	D	232	ASN	CA-CB-CG	9.70	122.30	112.60
2	C	150	VAL	CA-C-N	9.58	139.84	121.54
2	C	150	VAL	C-N-CA	9.58	139.84	121.54
1	B	-3	HIS	CA-CB-CG	8.92	122.72	113.80
2	C	129	ASP	CA-CB-CG	8.84	121.44	112.60
2	C	223	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	11	PHE	CA-CB-CG	7.88	121.67	113.80
1	B	4	PHE	CA-CB-CG	-7.77	106.03	113.80
2	D	195	GLU	CB-CG-CD	7.33	125.06	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	151	ASP	CA-C-N	7.01	135.14	121.41
2	C	151	ASP	C-N-CA	7.01	135.14	121.41
2	C	84	PHE	CA-CB-CG	-6.81	106.99	113.80
2	D	223[A]	ASP	CA-CB-CG	6.78	119.38	112.60
2	D	223[B]	ASP	CA-CB-CG	6.78	119.38	112.60
2	C	125	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	B	11	PHE	CA-CB-CG	6.04	119.84	113.80
2	C	186	ALA	CA-C-O	5.99	126.53	119.28
2	D	125	ASN	CA-CB-CG	5.83	118.43	112.60
2	C	151	ASP	CA-CB-CG	-5.79	106.81	112.60
2	D	151	ASP	O-C-N	-5.67	114.97	122.40
2	C	135	ASN	CA-CB-CG	-5.63	106.97	112.60
2	D	135	ASN	OD1-CG-ND2	-5.60	117.00	122.60
2	C	205	VAL	CA-C-O	-5.57	111.33	120.80
2	D	209	LYS	CA-C-O	-5.52	112.18	118.47
1	B	35	PHE	CA-CB-CG	-5.40	108.40	113.80
2	C	173	HIS	CA-CB-CG	5.40	119.20	113.80
2	D	125	ASN	CB-CG-ND2	5.28	124.31	116.40
1	A	4	PHE	O-C-N	-5.22	114.65	123.00
2	C	226	PRO	CB-CA-C	-5.18	104.16	110.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	-3	HIS	Peptide

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	500	0	488	9	0
1	B	534	0	507	4	0
2	C	1385	0	1336	15	0
2	D	1385	0	1332	16	0
3	C	16	0	20	5	0
3	D	12	0	15	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	230	0	0	8	0
4	D	233	0	0	6	0
All	All	4295	0	3698	43	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 6.

All (43) 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)
2:C:131:PRO:HG3	3:C:252:BME:H22	1.52	0.91
2:D:95[A]:THR:HG21	4:D:335:HOH:O	1.85	0.76
2:D:114:CYS:HB2	3:D:251:BME:H12	1.71	0.72
2:C:144[A]:THR:HG22	2:C:196:ASP:OD1	1.93	0.68
2:D:144[A]:THR:HG22	2:D:196:ASP:OD1	1.92	0.67
2:C:133:MET:HE1	4:C:417:HOH:O	1.94	0.67
3:C:252:BME:H12	4:C:407:HOH:O	1.96	0.66
2:D:204:GLU:HB3	2:D:211[A]:TYR:CE2	2.32	0.64
1:B:44[B]:GLU:HG2	4:D:377:HOH:O	2.00	0.60
1:A:5:LEU:HA	1:A:9[A]:MET:CE	2.38	0.54
2:C:95[A]:THR:HG21	4:C:335:HOH:O	2.08	0.53
2:C:208:GLY:HA2	2:C:211[B]:TYR:OH	2.09	0.53
1:A:25[A]:LYS:HE3	4:C:457:HOH:O	2.11	0.49
1:A:13[A]:THR:HG21	1:A:62:CYS:O	2.13	0.49
1:A:5:LEU:HD22	1:A:9[A]:MET:SD	2.53	0.48
2:C:162:LEU:O	2:C:169:HIS:HA	2.14	0.48
2:C:204:GLU:HG3	2:C:211[A]:TYR:CE2	2.48	0.48
2:D:175:HIS:HE1	4:D:316:HOH:O	1.97	0.47
2:C:205:VAL:O	2:C:209:LYS:NZ	2.49	0.46
2:D:150[B]:VAL:HG11	2:D:155[B]:ARG:HG3	1.98	0.45
1:A:42[B]:LYS:NZ	3:C:253:BME:O1	2.49	0.45
2:D:114:CYS:CB	3:D:251:BME:H12	2.43	0.45
1:A:12:LYS:NZ	4:C:475:HOH:O	2.50	0.45
1:A:36[B]:GLU:HG3	4:C:386:HOH:O	2.16	0.45
2:C:131:PRO:CG	3:C:252:BME:H22	2.35	0.45
1:B:9[B]:MET:SD	2:D:115:LEU:HD11	2.56	0.44
2:D:155[A]:ARG:NH1	4:D:471:HOH:O	2.50	0.44
1:B:16[B]:GLU:OE1	1:B:23:TYR:OH	2.35	0.44
2:D:152:GLY:N	4:D:485:HOH:O	2.48	0.44
2:C:104:ALA:HB2	2:C:121[B]:ILE:HD13	2.00	0.43
1:A:44:GLU:CD	3:C:253:BME:H21	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:LYS:NZ	4:C:477:HOH:O	2.50	0.42
1:A:58:LEU:HD22	2:C:121[A]:ILE:CD1	2.50	0.42
2:C:120[A]:LYS:HE3	4:D:370:HOH:O	2.18	0.42
2:C:71[A]:LYS:NZ	4:C:405:HOH:O	2.50	0.42
2:D:150[B]:VAL:CG1	2:D:155[B]:ARG:HG3	2.50	0.42
2:D:95[A]:THR:HG22	2:D:101:PHE:CE2	2.55	0.41
2:D:162:LEU:O	2:D:169:HIS:HA	2.20	0.41
2:D:203:GLU:HG3	2:D:204:GLU:N	2.35	0.41
2:C:176:THR:HG21	2:C:178:TYR:CZ	2.56	0.41
2:D:65:CRK:O2	2:D:65:CRK:HD2	2.21	0.41
2:D:84:PHE:O	2:D:182:LYS:NZ	2.54	0.41
1:B:-3:HIS:ND1	1:B:-2:HIS:N	2.68	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	68/74 (92%)	68 (100%)	0	0	100	100
1	B	71/74 (96%)	70 (99%)	1 (1%)	0	100	100
2	C	173/168 (103%)	167 (96%)	6 (4%)	0	100	100
2	D	174/168 (104%)	171 (98%)	3 (2%)	0	100	100
All	All	486/484 (100%)	476 (98%)	10 (2%)	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	60/61 (98%)	59 (98%)	1 (2%)	53	21
1	B	61/61 (100%)	60 (98%)	1 (2%)	55	22
2	C	150/140 (107%)	143 (95%)	7 (5%)	23	3
2	D	151/140 (108%)	145 (96%)	6 (4%)	28	4
All	All	422/402 (105%)	407 (96%)	15 (4%)	32	5

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
2	C	120[A]	LYS
2	C	120[B]	LYS
2	C	124	ASN
2	C	136	LYS
2	C	181[A]	LYS
2	C	181[B]	LYS
2	C	209	LYS
1	B	-3	HIS
2	D	124	ASN
2	D	202	MET
2	D	203	GLU
2	D	204	GLU
2	D	209	LYS
2	D	229	LEU

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

Mol	Chain	Res	Type
2	C	124	ASN
2	C	134	GLN
2	C	175	HIS
2	D	124	ASN
2	D	157	GLN
2	D	232	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
2	CRK	D	65	2	24,24,25	2.08	9 (37%)	29,32,34	3.90	12 (41%)
2	CRK	C	65	2	24,24,25	2.16	8 (33%)	29,32,34	4.46	14 (48%)

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	CRK	D	65	2	-	4/14/31/32	0/2/2/2
2	CRK	C	65	2	-	5/14/31/32	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	65	CRK	CG2-CB2	-5.16	1.37	1.46
2	C	65	CRK	OH-CZ	-4.57	1.26	1.37
2	D	65	CRK	OH-CZ	-4.28	1.27	1.37
2	D	65	CRK	CE1-CZ	4.27	1.47	1.39
2	C	65	CRK	CE1-CZ	4.00	1.46	1.39
2	D	65	CRK	CG2-CB2	-3.81	1.39	1.46
2	C	65	CRK	CE2-CZ	3.59	1.45	1.39
2	D	65	CRK	C1-N3	3.06	1.43	1.38
2	D	65	CRK	CE2-CZ	2.96	1.44	1.39
2	C	65	CRK	CD2-CG2	2.94	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	65	CRK	CA3-N3	-2.88	1.41	1.47
2	D	65	CRK	CD1-CG2	2.36	1.44	1.39
2	D	65	CRK	CD2-CG2	2.28	1.44	1.39
2	C	65	CRK	CA3-N3	-2.25	1.43	1.47
2	C	65	CRK	CA1-C1	-2.23	1.45	1.47
2	D	65	CRK	O1-CA1	2.14	1.27	1.23
2	C	65	CRK	O1-CA1	2.05	1.27	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	65	CRK	CB2-CA2-N2	-11.50	113.15	128.76
2	D	65	CRK	O2-C2-CA2	10.43	137.68	131.02
2	C	65	CRK	CA1-C1-N3	-9.98	117.62	124.88
2	D	65	CRK	CB2-CA2-N2	-9.73	115.55	128.76
2	C	65	CRK	CG2-CB2-CA2	9.56	141.23	129.87
2	D	65	CRK	CA1-C1-N3	-9.52	117.95	124.88
2	C	65	CRK	CB2-CA2-C2	8.40	132.54	122.36
2	D	65	CRK	CB2-CA2-C2	7.88	131.91	122.36
2	C	65	CRK	O2-C2-CA2	7.72	135.95	131.02
2	C	65	CRK	C2-CA2-N2	6.77	113.80	108.95
2	D	65	CRK	C2-CA2-N2	4.40	112.11	108.95
2	C	65	CRK	N3-C1-N2	3.53	116.81	112.62
2	C	65	CRK	CA3-N3-C1	3.52	135.33	128.39
2	D	65	CRK	CG2-CB2-CA2	3.43	133.94	129.87
2	D	65	CRK	CA1-C1-N2	3.42	126.56	123.79
2	C	65	CRK	CB-CA1-C1	2.80	118.67	115.78
2	C	65	CRK	CA3-N3-C2	-2.76	117.60	123.67
2	D	65	CRK	CE1-CZ-CE2	-2.67	115.53	119.77
2	C	65	CRK	CE1-CZ-CE2	-2.63	115.58	119.77
2	C	65	CRK	CA2-C2-N3	-2.41	101.48	103.50
2	D	65	CRK	O2-C2-N3	-2.39	119.33	124.31
2	D	65	CRK	N3-C1-N2	2.31	115.37	112.62
2	D	65	CRK	CD2-CE2-CZ	2.29	122.30	119.88
2	C	65	CRK	CD1-CE1-CZ	2.15	122.15	119.88
2	C	65	CRK	CA1-C1-N2	2.13	125.52	123.79
2	D	65	CRK	CA3-N3-C1	2.10	132.53	128.39

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	65	CRK	O1-CA1-CB-CG
2	D	65	CRK	O1-CA1-CB-CG
2	C	65	CRK	C2-CA2-CB2-CG2
2	D	65	CRK	C2-CA2-CB2-CG2
2	C	65	CRK	N2-CA2-CB2-CG2
2	D	65	CRK	N2-CA2-CB2-CG2
2	C	65	CRK	CB-CG-SD-CE
2	D	65	CRK	CB-CG-SD-CE
2	C	65	CRK	C1-CA1-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	65	CRK	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
3	BME	D	250	2	3,3,3	0.46	0	2,2,2	0.53	0
3	BME	C	252	2	3,3,3	0.37	0	2,2,2	0.51	0
3	BME	D	251	2	3,3,3	0.51	0	2,2,2	0.64	0
3	BME	C	253	2	3,3,3	0.36	0	2,2,2	0.86	0
3	BME	D	252	2	3,3,3	0.51	0	2,2,2	1.66	1 (50%)
3	BME	C	250	2	3,3,3	0.28	0	2,2,2	0.42	0
3	BME	C	251	2	3,3,3	0.53	0	2,2,2	0.15	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
3	BME	D	250	2	-	0/1/1/1	-
3	BME	C	252	2	-	0/1/1/1	-
3	BME	D	251	2	-	1/1/1/1	-
3	BME	C	253	2	-	0/1/1/1	-
3	BME	D	252	2	-	1/1/1/1	-
3	BME	C	250	2	-	0/1/1/1	-
3	BME	C	251	2	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	252	BME	O1-C1-C2	-2.35	101.64	110.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	251	BME	O1-C1-C2-S2
3	D	252	BME	O1-C1-C2-S2
3	D	251	BME	O1-C1-C2-S2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	252	BME	3	0
3	D	251	BME	2	0
3	C	253	BME	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	59/74 (79%)	0.59	3 (5%) 33 38	13, 22, 32, 51	10 (16%)
1	B	66/74 (89%)	0.51	4 (6%) 27 31	12, 20, 30, 65	6 (9%)
2	C	165/168 (98%)	0.54	14 (8%) 16 19	8, 19, 37, 47	12 (7%)
2	D	165/168 (98%)	0.20	8 (4%) 35 41	8, 15, 33, 57	13 (7%)
All	All	455/484 (94%)	0.42	29 (6%) 25 29	8, 19, 35, 65	41 (9%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	151	ASP	5.5
2	C	165	PRO	5.5
2	C	151	ASP	5.4
1	A	4	PHE	5.2
1	B	-3	HIS	4.9
2	C	166	GLY	4.7
2	C	205	VAL	4.7
2	C	164	CYS	4.5
2	C	184	ALA	4.1
2	C	135	ASN	4.1
2	D	229	LEU	4.0
2	D	205	VAL	3.5
1	A	5	LEU	3.4
2	C	113	ASP	3.2
2	C	110	LEU	3.0
2	D	184	ALA	2.9
2	C	209	LYS	2.5
2	D	203	GLU	2.5
2	D	201	ILE	2.4
2	D	208	GLY	2.4
1	B	46	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	201	ILE	2.3
2	D	137	ALA	2.3
2	C	223	ASP	2.2
2	C	137	ALA	2.2
2	C	208	GLY	2.2
1	B	42	LYS	2.1
1	B	45	VAL	2.1
1	A	51	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CRK	C	65	23/24	0.97	0.07	13,16,20,24	0
2	CRK	D	65	23/24	0.98	0.06	12,15,17,22	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BME	D	252	4/4	0.88	0.16	23,28,32,39	0
3	BME	C	252	4/4	0.89	0.17	60,92,92,93	0
3	BME	C	253	4/4	0.95	0.12	41,54,57,57	0
3	BME	C	251	4/4	0.96	0.11	29,47,47,54	0
3	BME	D	251	4/4	0.98	0.10	22,34,36,45	0
3	BME	C	250	4/4	0.98	0.07	18,18,20,33	0
3	BME	D	250	4/4	0.99	0.06	14,15,18,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.