



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:20 PM UTC

PDB ID : 4B30 / pdb_00004b30
Title : Structure of the mutant V44A of the fluorescent protein KillerRed
Authors : Carpentier, P.; de Rosny, E.
Deposited on : 2012-07-19
Resolution : 2.10 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

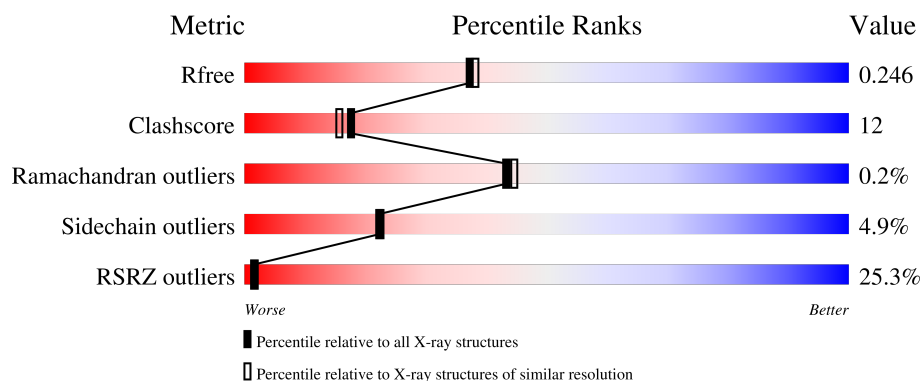
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	235	10% 74% 21% • •
2	B	235	38% 74% 20% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4164 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 KILLERRED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	227	1916	1210	332	358	16	0	17	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	VAL	engineered mutation	UNP Q2TCH5
A	65	CRQ	GLN	chromophore	UNP Q60I24
A	65	CRQ	TYR	chromophore	UNP Q60I24
A	65	CRQ	GLY	chromophore	UNP Q60I24

- Molecule 2 is a protein called KILLERRED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	229	1937	1219	335	365	18	0	19	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	ALA	VAL	engineered mutation	UNP Q2TCH5
B	65	CRQ	GLN	chromophore	UNP Q60I24
B	65	CRQ	TYR	chromophore	UNP Q60I24
B	65	CRQ	GLY	chromophore	UNP Q60I24

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cl	0	0
			5	5		
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

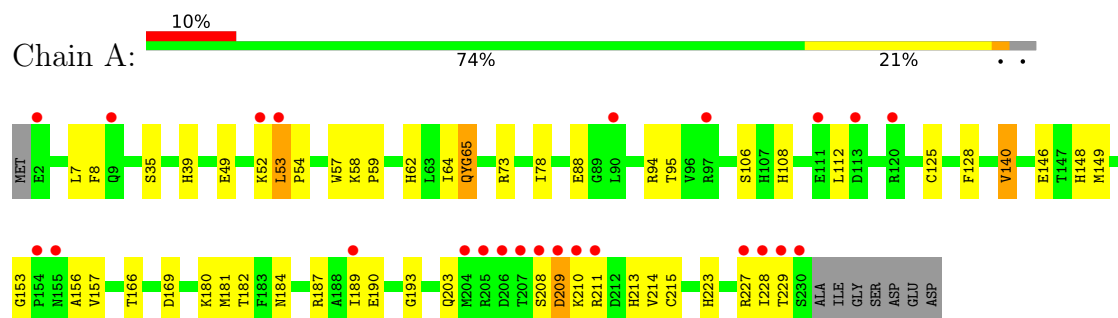
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	164	Total	O	0	0
			164	164		
7	B	96	Total	O	0	0
			96	96		

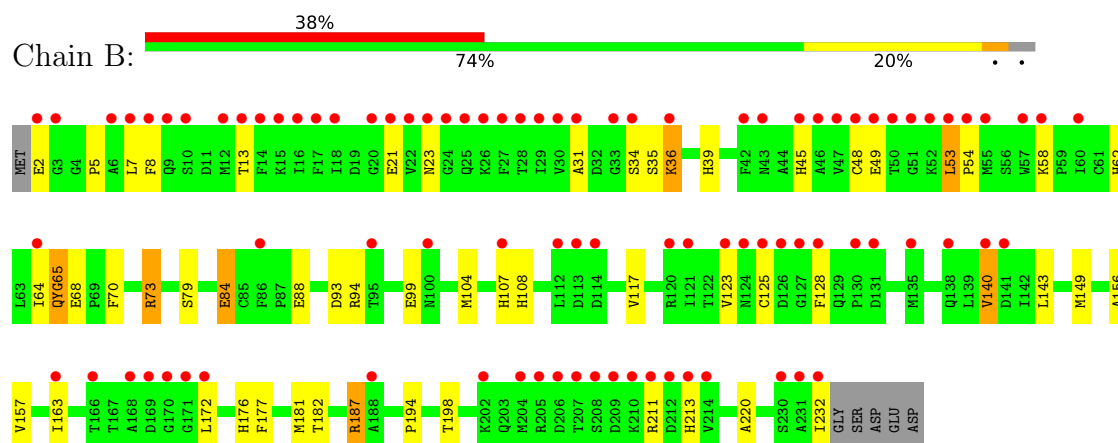
3 Residue-property plots [i](#)

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: KILLERRED



• Molecule 2: KILLERRED



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	134.31 Å 134.31 Å 76.22 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	116.32 – 2.10 116.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (116.32-2.10) 99.9 (116.32-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.165 , 0.199 0.222 , 0.246	Depositor DCC
R_{free} test set	2309 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: SO4, CL, CSO, CRQ, GOL, NA

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	1.07	3/1930 (0.2%)	0.96	2/2610 (0.1%)
2	B	0.91	0/1961	0.89	1/2653 (0.0%)
All	All	0.99	3/3891 (0.1%)	0.93	3/5263 (0.1%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	HIS	ND1-CE1	5.61	1.38	1.32
1	A	213	HIS	CG-CD2	5.23	1.41	1.35
1	A	148	HIS	CG-CD2	5.14	1.41	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	VAL	N-CA-C	7.30	117.81	111.90
1	A	153	GLY	CA-C-N	6.74	126.69	119.28
1	A	153	GLY	C-N-CA	6.74	126.69	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	SER	Peptide

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	1916	0	1826	48	1
2	B	1937	0	1830	44	0
3	A	5	0	0	0	0
4	A	5	0	0	0	0
4	B	3	0	0	1	0
5	A	2	0	0	0	0
6	A	24	0	32	4	0
6	B	12	0	16	4	0
7	A	164	0	0	9	2
7	B	96	0	0	8	0
All	All	4164	0	3704	95	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (95) 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:B:73[A]:ARG:HH11	2:B:73[A]:ARG:HG3	1.15	1.03
1:A:187[B]:ARG:NH1	1:A:189[B]:ILE:HG22	1.80	0.96
1:A:209:ASP:HB3	1:A:211:ARG:H	1.33	0.92
2:B:93:ASP:OD1	2:B:107[A]:HIS:HD2	1.51	0.91
2:B:73[A]:ARG:HH11	2:B:73[A]:ARG:CG	1.86	0.88
2:B:35:SER:OG	2:B:39:HIS:HD2	1.55	0.86
1:A:187[B]:ARG:NH1	1:A:189[B]:ILE:CG2	2.38	0.86
2:B:187[B]:ARG:NH2	7:B:2041:HOH:O	2.13	0.80
1:A:187[B]:ARG:HH12	1:A:189[B]:ILE:HG22	1.46	0.80
2:B:73[A]:ARG:NH1	7:B:2026:HOH:O	2.18	0.76
2:B:35:SER:OG	2:B:39:HIS:CD2	2.39	0.75
1:A:53[B]:LEU:HD12	1:A:54:PRO:HD2	1.69	0.74
2:B:88:GLU:OE2	2:B:187[B]:ARG:HD3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:O	7:A:2068:HOH:O	2.08	0.72
2:B:73[A]:ARG:HG3	2:B:73[A]:ARG:NH1	1.98	0.71
1:A:228:ILE:HG23	1:A:229:THR:HA	1.71	0.71
6:B:1235:GOL:H32	7:B:2089:HOH:O	1.90	0.70
2:B:88:GLU:OE2	2:B:187[A]:ARG:NH1	2.23	0.70
1:A:62:HIS:HD2	1:A:94:ARG:HH11	1.38	0.70
1:A:78:ILE:HA	6:A:1239:GOL:H31	1.74	0.69
2:B:93:ASP:OD1	2:B:107[A]:HIS:CD2	2.42	0.69
7:A:2150:HOH:O	2:B:232:ILE:O	2.11	0.69
2:B:99:GLU:OE2	2:B:176:HIS:HE1	1.76	0.68
1:A:187[B]:ARG:HH12	1:A:189[B]:ILE:CG2	2.06	0.67
4:B:1233:CL:CL	7:B:2088:HOH:O	2.51	0.66
2:B:84[A]:GLU:HA	2:B:84[A]:GLU:OE1	1.94	0.65
2:B:5:PRO:HD3	2:B:84[A]:GLU:OE1	1.98	0.64
2:B:62:HIS:HD2	2:B:94:ARG:HH11	1.46	0.63
1:A:149:MET:HE3	1:A:157[A]:VAL:HG11	1.80	0.63
6:B:1236:GOL:H12	7:B:2094:HOH:O	1.97	0.63
1:A:228:ILE:CG2	1:A:229:THR:HA	2.29	0.61
1:A:187[A]:ARG:HG2	7:A:2078:HOH:O	2.01	0.59
1:A:106:SER:OG	1:A:108:HIS:HE1	1.86	0.58
6:B:1236:GOL:C1	7:B:2094:HOH:O	2.51	0.58
1:A:35:SER:OG	1:A:39:HIS:HD2	1.87	0.58
2:B:53:LEU:HD22	2:B:54:PRO:HD2	1.87	0.56
1:A:73[B]:ARG:NE	7:A:2031:HOH:O	2.26	0.56
1:A:8:PHE:O	1:A:39:HIS:HE1	1.89	0.55
2:B:194:PRO:HD2	6:B:1236:GOL:H12	1.89	0.55
1:A:227:ARG:NH2	2:B:143:LEU:HD23	2.23	0.54
2:B:211:ARG:O	2:B:213:HIS:HD2	1.91	0.54
1:A:73[B]:ARG:NH2	7:A:2031:HOH:O	2.32	0.53
2:B:73[A]:ARG:CG	2:B:73[A]:ARG:NH1	2.55	0.53
1:A:57:TRP:CD2	1:A:214[A]:VAL:HG21	2.44	0.53
1:A:125:CYS:HB3	1:A:128:PHE:CE1	2.43	0.52
1:A:180:LYS:HD3	7:A:2082:HOH:O	2.09	0.52
1:A:52:LYS:NZ	7:A:2041:HOH:O	2.43	0.51
1:A:146:GLU:OE1	1:A:223:HIS:HE1	1.93	0.51
1:A:62:HIS:CD2	1:A:94:ARG:HH11	2.25	0.51
1:A:169[B]:ASP:OD1	1:A:169[B]:ASP:C	2.54	0.50
2:B:65:CRQ:HD2	2:B:65:CRQ:N2	2.27	0.50
2:B:31:ALA:HA	2:B:45:HIS:O	2.12	0.50
1:A:193:GLY:H	6:A:1239:GOL:H2	1.76	0.49
2:B:73[A]:ARG:CZ	7:B:2026:HOH:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:GLU:OE2	2:B:176:HIS:CE1	2.62	0.49
1:A:156:ALA:HB2	1:A:182[B]:THR:HG22	1.95	0.48
1:A:180:LYS:HE2	6:A:1242:GOL:H32	1.95	0.48
2:B:8:PHE:O	2:B:39:HIS:HE1	1.95	0.48
2:B:23:ASN:HA	7:B:2005:HOH:O	2.14	0.48
1:A:203:GLN:HG2	1:A:214[A]:VAL:CG1	2.44	0.47
2:B:48:CYS:O	2:B:211:ARG:HB3	2.14	0.47
1:A:95[A]:THR:HG23	7:A:2083:HOH:O	2.13	0.47
2:B:163[A]:ILE:HG13	2:B:163[A]:ILE:O	2.15	0.47
2:B:143:LEU:HD11	2:B:172:LEU:HD21	1.96	0.46
1:A:88:GLU:OE2	1:A:187[A]:ARG:HD3	2.15	0.46
1:A:140[A]:VAL:HG13	1:A:166:THR:OG1	2.15	0.46
2:B:125:CYS:HB3	2:B:128:PHE:CE1	2.50	0.46
2:B:156:ALA:HB2	2:B:182[B]:THR:HG22	1.97	0.46
2:B:62:HIS:CD2	2:B:94:ARG:HH11	2.30	0.46
1:A:157[B]:VAL:CG2	1:A:181:MET:HE3	2.47	0.45
1:A:187[B]:ARG:HH11	1:A:189[B]:ILE:HG22	1.75	0.45
2:B:70:PHE:CZ	2:B:117:VAL:HG11	2.52	0.45
1:A:193:GLY:H	6:A:1239:GOL:C2	2.29	0.44
1:A:35:SER:OG	1:A:39:HIS:CD2	2.69	0.44
1:A:149:MET:HE1	1:A:181:MET:CE	2.48	0.44
1:A:53[B]:LEU:CD1	1:A:54:PRO:HD2	2.44	0.44
2:B:64[A]:ILE:O	2:B:68[A]:GLU:OE1	2.35	0.43
1:A:157[B]:VAL:HG23	1:A:181:MET:HE3	2.00	0.43
1:A:203:GLN:HG2	1:A:214[A]:VAL:HG11	1.99	0.43
2:B:36:LYS:H	2:B:36:LYS:CE	2.31	0.42
2:B:49:GLU:HA	2:B:49:GLU:OE1	2.19	0.42
1:A:149:MET:HE1	1:A:181:MET:HE1	2.00	0.42
2:B:187[B]:ARG:H	2:B:187[B]:ARG:HG2	1.66	0.42
2:B:198:THR:O	2:B:220:ALA:HA	2.19	0.42
1:A:58:LYS:HB2	1:A:59:PRO:HD3	2.02	0.42
1:A:53[B]:LEU:HD12	1:A:54:PRO:CD	2.46	0.42
1:A:58:LYS:CB	1:A:59:PRO:HD3	2.49	0.42
2:B:13:THR:HA	2:B:34:SER:HA	2.01	0.42
2:B:149:MET:HE1	2:B:181:MET:HE1	2.03	0.41
1:A:65:CRQ:HD2	1:A:65:CRQ:N2	2.36	0.41
2:B:157[B]:VAL:CG2	2:B:181:MET:HE3	2.50	0.41
1:A:73[B]:ARG:CZ	7:A:2031:HOH:O	2.64	0.41
2:B:104:MET:HE3	2:B:123:VAL:HG21	2.03	0.41
2:B:149:MET:HE1	2:B:181:MET:CE	2.51	0.40
1:A:49:GLU:OE1	1:A:211:ARG:NH1	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2026:HOH:O	7:A:2158:HOH:O[2_544]	1.87	0.33
7:A:2026:HOH:O	7:A:2157:HOH:O[2_544]	2.01	0.19
1:A:73[A]:ARG:NH2	1:A:184:ASN:OD1[3_655]	2.11	0.09

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	234/235 (100%)	226 (97%)	7 (3%)	1 (0%)	30	28
2	B	239/235 (102%)	232 (97%)	7 (3%)	0	100	100
All	All	473/470 (101%)	458 (97%)	14 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ASP

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	208/199 (104%)	199 (96%)	9 (4%)	26	27
2	B	211/200 (106%)	194 (92%)	17 (8%)	11	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	419/399 (105%)	393 (94%)	26 (6%)	22	14

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	53[A]	LEU
1	A	53[B]	LEU
1	A	64[A]	ILE
1	A	64[B]	ILE
1	A	112	LEU
1	A	140[A]	VAL
1	A	140[B]	VAL
1	A	210	LYS
2	B	2	GLU
2	B	7	LEU
2	B	21	GLU
2	B	36	LYS
2	B	53	LEU
2	B	58	LYS
2	B	73[A]	ARG
2	B	73[B]	ARG
2	B	79[A]	SER
2	B	79[B]	SER
2	B	84[A]	GLU
2	B	84[B]	GLU
2	B	108	HIS
2	B	140	VAL
2	B	177	PHE
2	B	187[A]	ARG
2	B	187[B]	ARG

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	25	GLN
1	A	39	HIS
1	A	43	ASN
1	A	62	HIS
1	A	80	HIS
1	A	108	HIS

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Mol	Chain	Res	Type
1	A	124	ASN
1	A	203	GLN
2	B	39	HIS
2	B	43	ASN
2	B	62	HIS
2	B	80	HIS
2	B	155	ASN
2	B	176	HIS
2	B	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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	CRQ	B	65	2	25,25,26	3.03	11 (44%)	28,34,36	3.79	9 (32%)
2	CSO	B	116[B]	2	3,6,7	0.83	0	1,6,8	0.22	0
1	CSO	A	116[B]	1	3,6,7	0.65	0	1,6,8	1.00	0
1	CRQ	A	65	1	25,25,26	3.19	9 (36%)	28,34,36	3.51	9 (32%)
2	CSO	B	116[A]	2	3,6,7	0.89	0	1,6,8	0.65	0
1	CSO	A	215	1	3,6,7	0.58	0	1,6,8	2.24	1 (100%)
1	CSO	A	116[A]	1	3,6,7	0.68	0	1,6,8	1.27	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	CRQ	B	65	2	-	3/10/32/33	0/2/2/2
2	CSO	B	116[B]	2	-	1/1/5/7	-
1	CSO	A	116[B]	1	-	1/1/5/7	-
1	CRQ	A	65	1	-	3/10/32/33	0/2/2/2
2	CSO	B	116[A]	2	-	1/1/5/7	-
1	CSO	A	215	1	-	0/1/5/7	-
1	CSO	A	116[A]	1	-	0/1/5/7	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	CRQ	CA1-N1	10.52	1.51	1.27
2	B	65	CRQ	CA1-N1	8.20	1.45	1.27
2	B	65	CRQ	CB2-CA2	6.55	1.41	1.35
1	A	65	CRQ	CB2-CA2	6.50	1.41	1.35
1	A	65	CRQ	CE1-CZ	4.92	1.48	1.39
2	B	65	CRQ	CE2-CZ	4.92	1.48	1.39
1	A	65	CRQ	CA2-C2	-4.62	1.43	1.48
2	B	65	CRQ	CE1-CZ	4.47	1.47	1.39
1	A	65	CRQ	CE2-CZ	4.26	1.47	1.39
2	B	65	CRQ	CA2-C2	-3.89	1.44	1.48
2	B	65	CRQ	OH-CZ	-3.75	1.28	1.37
2	B	65	CRQ	CD1-CG2	3.20	1.45	1.39
2	B	65	CRQ	CD2-CG2	3.11	1.45	1.39
1	A	65	CRQ	CG2-CB2	-2.86	1.41	1.46
1	A	65	CRQ	OH-CZ	-2.50	1.31	1.37
2	B	65	CRQ	CG2-CB2	-2.47	1.42	1.46
2	B	65	CRQ	CA2-N2	2.42	1.43	1.38
1	A	65	CRQ	CD1-CG2	2.40	1.44	1.39
2	B	65	CRQ	C1-CA1	2.27	1.51	1.48
1	A	65	CRQ	CD2-CG2	2.04	1.43	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	CRQ	O2-C2-CA2	-10.25	124.48	131.02
2	B	65	CRQ	O2-C2-CA2	-10.20	124.51	131.02
2	B	65	CRQ	C2-CA2-N2	-9.39	102.22	108.95
2	B	65	CRQ	CA2-C2-N3	9.00	111.06	103.50
1	A	65	CRQ	CA2-C2-N3	8.81	110.90	103.50
2	B	65	CRQ	CG2-CB2-CA2	-8.34	119.96	129.87
1	A	65	CRQ	C2-CA2-N2	-8.00	103.22	108.95
1	A	65	CRQ	CG2-CB2-CA2	-6.52	122.12	129.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	CRQ	CA2-N2-C1	4.08	111.60	104.09
2	B	65	CRQ	CB2-CA2-N2	3.61	133.66	128.76
1	A	65	CRQ	CB2-CA2-N2	3.48	133.48	128.76
1	A	65	CRQ	CA2-N2-C1	3.44	110.42	104.09
2	B	65	CRQ	N3-C1-N2	-2.84	109.25	112.62
1	A	65	CRQ	C3-CA3-N3	2.80	118.79	112.43
2	B	65	CRQ	C3-CA3-N3	2.35	117.78	112.43
1	A	65	CRQ	N3-C1-N2	-2.24	109.96	112.62
1	A	215	CSO	CB-CA-C	-2.24	104.73	110.80
2	B	65	CRQ	O3-C3-CA3	-2.21	115.52	125.47
1	A	65	CRQ	O3-C3-CA3	-2.02	116.38	125.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	CRQ	N2-CA2-CB2-CG2
1	A	65	CRQ	C2-CA2-CB2-CG2
2	B	65	CRQ	N2-CA2-CB2-CG2
2	B	65	CRQ	C2-CA2-CB2-CG2
2	B	116[B]	CSO	N-CA-CB-SG
2	B	65	CRQ	CA1-CB1-CG1-CD3
1	A	65	CRQ	CA1-CB1-CG1-CD3
1	A	116[B]	CSO	N-CA-CB-SG
2	B	116[A]	CSO	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	65	CRQ	1	0
1	A	65	CRQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

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$
6	GOL	B	1236	-	5,5,5	0.62	0	5,5,5	0.88	0
6	GOL	A	1240	-	5,5,5	0.25	0	5,5,5	0.56	0
6	GOL	A	1242	-	5,5,5	0.34	0	5,5,5	0.32	0
6	GOL	A	1241	-	5,5,5	0.50	0	5,5,5	0.43	0
3	SO4	A	1231	5	4,4,4	0.23	0	6,6,6	0.07	0
6	GOL	A	1239	-	5,5,5	0.47	0	5,5,5	0.83	0
6	GOL	B	1235	-	5,5,5	0.11	0	5,5,5	0.68	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
6	GOL	B	1236	-	-	2/4/4/4	-
6	GOL	A	1241	-	-	2/4/4/4	-
6	GOL	A	1240	-	-	4/4/4/4	-
6	GOL	A	1242	-	-	4/4/4/4	-
6	GOL	A	1239	-	-	4/4/4/4	-
6	GOL	B	1235	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1239	GOL	C1-C2-C3-O3
6	A	1240	GOL	C1-C2-C3-O3
6	A	1241	GOL	O1-C1-C2-C3
6	B	1236	GOL	C1-C2-C3-O3
6	A	1241	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	1239	GOL	O1-C1-C2-C3
6	A	1240	GOL	O1-C1-C2-C3
6	A	1242	GOL	O1-C1-C2-C3
6	A	1242	GOL	C1-C2-C3-O3
6	A	1239	GOL	O1-C1-C2-O2
6	A	1242	GOL	O2-C2-C3-O3
6	B	1236	GOL	O2-C2-C3-O3
6	A	1239	GOL	O2-C2-C3-O3
6	A	1240	GOL	O1-C1-C2-O2
6	A	1240	GOL	O2-C2-C3-O3
6	A	1242	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1236	GOL	3	0
6	A	1242	GOL	1	0
6	A	1239	GOL	3	0
6	B	1235	GOL	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, 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	224/235 (95%)	0.84	24 (10%)	11 11	12, 28, 54, 91	16 (7%)
2	B	227/235 (96%)	1.68	90 (39%)	1 1	13, 42, 73, 120	19 (8%)
All	All	451/470 (95%)	1.26	114 (25%)	1 2	12, 33, 71, 120	35 (7%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	232	ILE	8.0
2	B	204	MET	6.7
1	A	230	SER	6.4
2	B	207	THR	6.1
1	A	229	THR	5.6
2	B	210	LYS	5.0
2	B	45	HIS	5.0
2	B	208	SER	4.9
1	A	205	ARG	4.8
2	B	188	ALA	4.5
1	A	204	MET	4.5
1	A	207	THR	4.5
1	A	209	ASP	4.5
2	B	52	LYS	4.5
1	A	210	LYS	4.4
2	B	205	ARG	4.3
1	A	97[A]	ARG	4.3
2	B	107[A]	HIS	4.3
2	B	51	GLY	4.3
2	B	206	ASP	4.2
2	B	57	TRP	4.2
2	B	213	HIS	4.2
1	A	211	ARG	4.0
2	B	141	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	168	ALA	3.9
1	A	228	ILE	3.7
2	B	212	ASP	3.7
2	B	209	ASP	3.7
2	B	24	GLY	3.7
2	B	27	PHE	3.7
2	B	166	THR	3.7
2	B	124	ASN	3.6
2	B	211	ARG	3.6
2	B	169	ASP	3.5
1	A	52	LYS	3.5
2	B	50	THR	3.5
2	B	128	PHE	3.4
2	B	48	CYS	3.4
1	A	208	SER	3.4
2	B	126	ASP	3.4
2	B	53	LEU	3.4
1	A	155	ASN	3.3
2	B	7	LEU	3.3
2	B	20	GLY	3.3
2	B	231	ALA	3.2
2	B	10	SER	3.2
2	B	2	GLU	3.2
2	B	230	SER	3.1
2	B	23	ASN	3.1
2	B	214	VAL	3.1
2	B	22	VAL	3.0
2	B	25	GLN	3.0
2	B	100	ASN	2.9
2	B	112	LEU	2.9
2	B	42	PHE	2.9
2	B	3	GLY	2.9
1	A	2	GLU	2.8
2	B	163[A]	ILE	2.8
2	B	113	ASP	2.8
2	B	18	ILE	2.8
2	B	6	ALA	2.8
2	B	13	THR	2.8
2	B	49	GLU	2.7
2	B	140	VAL	2.7
2	B	138	GLN	2.7
2	B	95[A]	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	54	PRO	2.7
2	B	131	ASP	2.6
2	B	14	PHE	2.6
2	B	127	GLY	2.6
2	B	172	LEU	2.6
1	A	206	ASP	2.6
2	B	29	ILE	2.5
2	B	135	MET	2.5
2	B	170	GLY	2.5
2	B	86	PHE	2.4
2	B	34	SER	2.4
2	B	12	MET	2.4
2	B	120	ARG	2.4
2	B	8	PHE	2.4
1	A	120	ARG	2.4
1	A	53[A]	LEU	2.3
1	A	111	GLU	2.3
2	B	64[A]	ILE	2.3
2	B	123	VAL	2.3
2	B	9	GLN	2.3
2	B	202	LYS	2.3
2	B	114	ASP	2.3
2	B	15	LYS	2.2
2	B	46	ALA	2.2
2	B	26	LYS	2.2
2	B	28[A]	THR	2.2
2	B	31	ALA	2.2
1	A	189[A]	ILE	2.2
2	B	17	PHE	2.2
2	B	21	GLU	2.2
1	A	154	PRO	2.1
2	B	60	ILE	2.1
2	B	47	VAL	2.1
2	B	33	GLY	2.1
2	B	130	PRO	2.1
2	B	121	ILE	2.1
2	B	55	MET	2.1
1	A	113	ASP	2.1
2	B	16	ILE	2.1
2	B	36	LYS	2.1
2	B	58	LYS	2.1
2	B	125	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	171	GLY	2.1
1	A	9	GLN	2.0
2	B	30	VAL	2.0
2	B	43	ASN	2.0
1	A	90	LEU	2.0
1	A	227	ARG	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(Å ²)	Q<0.9
1	CSO	A	215	7/8	0.87	0.12	28,29,55,60	0
2	CRQ	B	65	24/25	0.88	0.13	37,41,44,44	0
1	CSO	A	116[A]	7/8	0.90	0.10	26,28,29,30	7
1	CSO	A	116[B]	7/8	0.90	0.10	26,27,29,32	7
2	CSO	B	116[A]	7/8	0.90	0.14	40,44,47,50	7
2	CSO	B	116[B]	7/8	0.90	0.14	46,47,49,51	7
1	CRQ	A	65	24/25	0.93	0.09	23,27,31,31	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
4	CL	B	1237	1/1	0.49	0.35	84,84,84,84	1
3	SO4	A	1231	5/5	0.69	0.19	26,28,30,35	5
6	GOL	A	1239	6/6	0.72	0.27	41,57,69,74	0
6	GOL	A	1242	6/6	0.72	0.18	64,73,77,77	0
4	CL	A	1234	1/1	0.73	0.27	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	1235	1/1	0.74	0.30	71,71,71,71	0
6	GOL	A	1240	6/6	0.80	0.23	50,65,69,80	0
4	CL	A	1238	1/1	0.80	0.29	86,86,86,86	0
6	GOL	B	1236	6/6	0.83	0.21	42,56,57,61	0
6	GOL	B	1235	6/6	0.84	0.17	43,55,61,62	0
6	GOL	A	1241	6/6	0.85	0.21	35,66,71,78	0
5	NA	A	1237	1/1	0.88	0.16	40,40,40,40	0
4	CL	A	1233	1/1	0.90	0.16	69,69,69,69	0
5	NA	A	1236	1/1	0.90	0.09	35,35,35,35	0
4	CL	B	1234	1/1	0.90	0.19	61,61,61,61	0
4	CL	B	1233	1/1	0.94	0.15	59,59,59,59	0
4	CL	A	1232	1/1	0.95	0.10	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.