



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:35 PM GMT

PDB ID : 4EN1
Title : The 1.62Å structure of a FRET-optimized Cerulean Fluorescent Protein
Authors : Watkins, J.L.
Deposited on : 2012-04-12
Resolution : 1.62 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

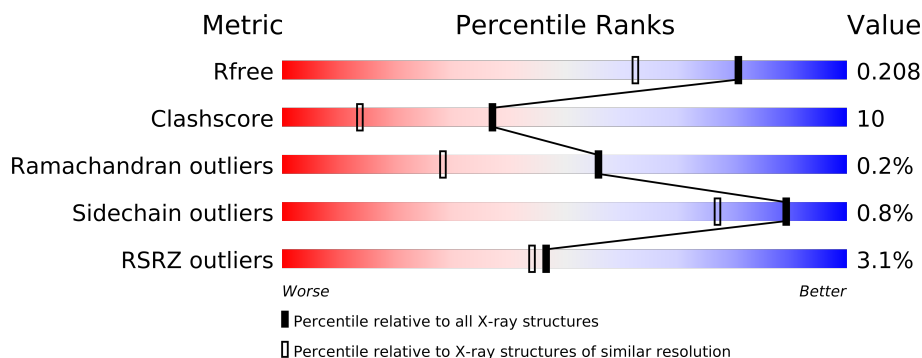
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.62 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}	66092	2327 (1.64-1.60)
Clashscore	79885	2723 (1.64-1.60)
Ramachandran outliers	78287	2639 (1.64-1.60)
Sidechain outliers	78261	2638 (1.64-1.60)
RSRZ outliers	66119	2327 (1.64-1.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	302	-	X
2	GOL	A	303	-	X
2	GOL	A	304	-	X
2	GOL	A	305	-	X
2	GOL	A	309	-	X
2	GOL	B	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	B	302	-	X
2	GOL	B	306	-	X
3	PEG	A	306	-	X
3	PEG	A	308	-	X
3	PEG	B	305	-	X
4	ACT	A	307	-	X
5	SO4	B	303	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4184 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	10	0
			1909	1219	311	372	7			
1	B	226	Total	C	N	O	S	0	9	0
			1835	1173	301	355	6			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	INITIATING METHIONINE	UNP P42212
A	-17	ARG	-	EXPRESSION TAG	UNP P42212
A	-16	GLY	-	EXPRESSION TAG	UNP P42212
A	-15	SER	-	EXPRESSION TAG	UNP P42212
A	-14	HIS	-	EXPRESSION TAG	UNP P42212
A	-13	HIS	-	EXPRESSION TAG	UNP P42212
A	-12	HIS	-	EXPRESSION TAG	UNP P42212
A	-11	HIS	-	EXPRESSION TAG	UNP P42212
A	-10	HIS	-	EXPRESSION TAG	UNP P42212
A	-9	HIS	-	EXPRESSION TAG	UNP P42212
A	-8	GLY	-	EXPRESSION TAG	UNP P42212
A	-7	LEU	-	EXPRESSION TAG	UNP P42212
A	-6	ALA	-	EXPRESSION TAG	UNP P42212
A	-5	LEU	-	EXPRESSION TAG	UNP P42212
A	-4	PRO	-	EXPRESSION TAG	UNP P42212
A	-3	VAL	-	EXPRESSION TAG	UNP P42212
A	-2	ALA	-	EXPRESSION TAG	UNP P42212
A	-1	THR	-	EXPRESSION TAG	UNP P42212
A	0	MET	-	EXPRESSION TAG	UNP P42212
A	1	VAL	-	EXPRESSION TAG	UNP P42212
A	64	LEU	TYR	ENGINEERED MUTATION	UNP P42212
A	72	ALA	SER	ENGINEERED MUTATION	UNP P42212
A	145	ALA	TYR	ENGINEERED MUTATION	UNP P42212
A	146	ILE	ASN	ENGINEERED MUTATION	UNP P42212
A	147	HIS	SER	ENGINEERED MUTATION	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	HIS	ENGINEERED MUTATION	UNP P42212
A	153	THR	MET	ENGINEERED MUTATION	UNP P42212
A	163	ALA	VAL	ENGINEERED MUTATION	UNP P42212
A	166	GLY	LYS	ENGINEERED MUTATION	UNP P42212
A	167	LEU	ILE	ENGINEERED MUTATION	UNP P42212
A	168	ASN	ARG	ENGINEERED MUTATION	UNP P42212
A	169	CYS	HIS	ENGINEERED MUTATION	UNP P42212
A	206	LYS	ALA	ENGINEERED MUTATION	UNP P42212
A	231	LEU	HIS	ENGINEERED MUTATION	UNP P42212
A	239	SER	-	EXPRESSION TAG	UNP P42212
A	240	GLY	-	EXPRESSION TAG	UNP P42212
A	241	LEU	-	EXPRESSION TAG	UNP P42212
A	242	ARG	-	EXPRESSION TAG	UNP P42212
A	243	SER	-	EXPRESSION TAG	UNP P42212
A	244	ARG	-	EXPRESSION TAG	UNP P42212
A	245	ALA	-	EXPRESSION TAG	UNP P42212
A	246	GLN	-	EXPRESSION TAG	UNP P42212
A	247	ALA	-	EXPRESSION TAG	UNP P42212
B	-18	MET	-	INITIATING METHIONINE	UNP P42212
B	-17	ARG	-	EXPRESSION TAG	UNP P42212
B	-16	GLY	-	EXPRESSION TAG	UNP P42212
B	-15	SER	-	EXPRESSION TAG	UNP P42212
B	-14	HIS	-	EXPRESSION TAG	UNP P42212
B	-13	HIS	-	EXPRESSION TAG	UNP P42212
B	-12	HIS	-	EXPRESSION TAG	UNP P42212
B	-11	HIS	-	EXPRESSION TAG	UNP P42212
B	-10	HIS	-	EXPRESSION TAG	UNP P42212
B	-9	HIS	-	EXPRESSION TAG	UNP P42212
B	-8	GLY	-	EXPRESSION TAG	UNP P42212
B	-7	LEU	-	EXPRESSION TAG	UNP P42212
B	-6	ALA	-	EXPRESSION TAG	UNP P42212
B	-5	LEU	-	EXPRESSION TAG	UNP P42212
B	-4	PRO	-	EXPRESSION TAG	UNP P42212
B	-3	VAL	-	EXPRESSION TAG	UNP P42212
B	-2	ALA	-	EXPRESSION TAG	UNP P42212
B	-1	THR	-	EXPRESSION TAG	UNP P42212
B	0	MET	-	EXPRESSION TAG	UNP P42212
B	1	VAL	-	EXPRESSION TAG	UNP P42212
B	64	LEU	TYR	ENGINEERED MUTATION	UNP P42212
B	72	ALA	SER	ENGINEERED MUTATION	UNP P42212
B	145	ALA	TYR	ENGINEERED MUTATION	UNP P42212
B	146	ILE	ASN	ENGINEERED MUTATION	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	147	HIS	SER	ENGINEERED MUTATION	UNP P42212
B	148	GLY	HIS	ENGINEERED MUTATION	UNP P42212
B	153	THR	MET	ENGINEERED MUTATION	UNP P42212
B	163	ALA	VAL	ENGINEERED MUTATION	UNP P42212
B	166	GLY	LYS	ENGINEERED MUTATION	UNP P42212
B	167	LEU	ILE	ENGINEERED MUTATION	UNP P42212
B	168	ASN	ARG	ENGINEERED MUTATION	UNP P42212
B	169	CYS	HIS	ENGINEERED MUTATION	UNP P42212
B	206	LYS	ALA	ENGINEERED MUTATION	UNP P42212
B	231	LEU	HIS	ENGINEERED MUTATION	UNP P42212
B	239	SER	-	EXPRESSION TAG	UNP P42212
B	240	GLY	-	EXPRESSION TAG	UNP P42212
B	241	LEU	-	EXPRESSION TAG	UNP P42212
B	242	ARG	-	EXPRESSION TAG	UNP P42212
B	243	SER	-	EXPRESSION TAG	UNP P42212
B	244	ARG	-	EXPRESSION TAG	UNP P42212
B	245	ALA	-	EXPRESSION TAG	UNP P42212
B	246	GLN	-	EXPRESSION TAG	UNP P42212
B	247	ALA	-	EXPRESSION TAG	UNP P42212

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



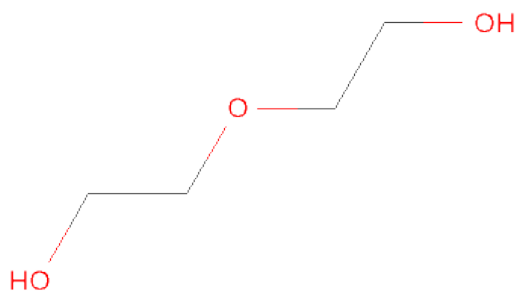
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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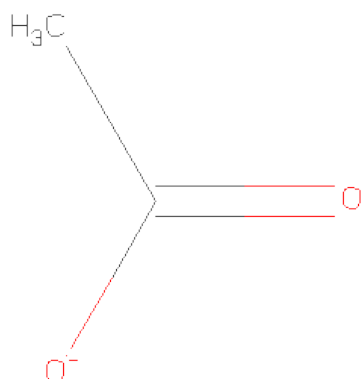
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



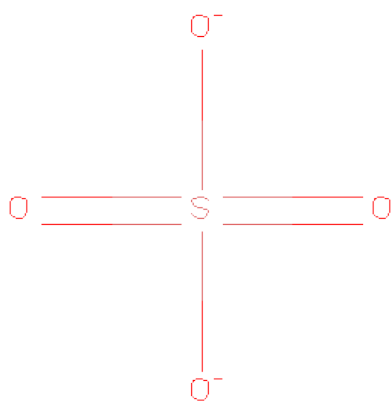
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

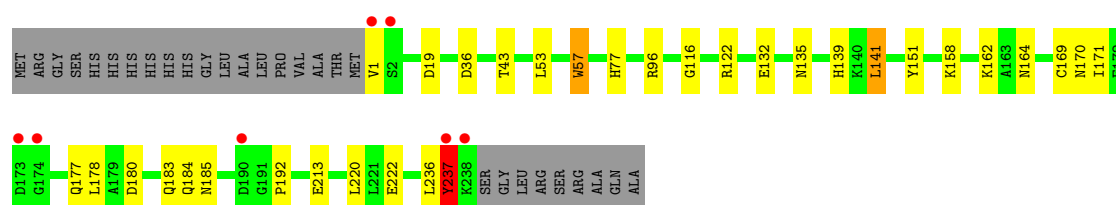
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	199	Total 199	O 199	0	0
6	B	151	Total 151	O 151	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

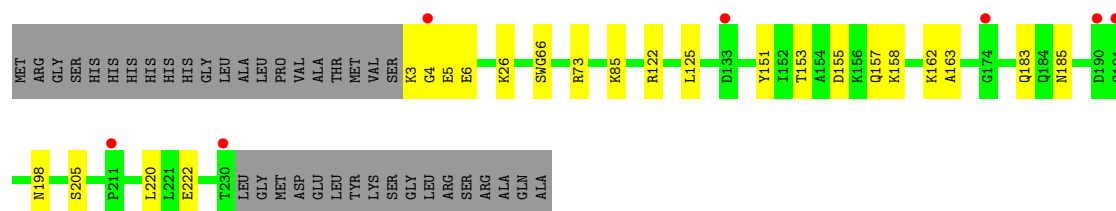
- Molecule 1: Green fluorescent protein

Chain A: 



- Molecule 1: Green fluorescent protein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.41Å 88.73Å 94.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 1.62 29.98 – 1.62	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.98-1.62) 98.3 (29.98-1.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.205 0.180 , 0.208	Depositor DCC
R_{free} test set	4196 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 84091 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4184	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, SO4, SWG, ACT

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	0.89	1/1954 (0.1%)	1.03	8/2644 (0.3%)
1	B	0.89	0/1877	0.95	2/2538 (0.1%)
All	All	0.89	1/3831 (0.0%)	0.99	10/5182 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	TRP	CD2-CE2	5.06	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19[A]	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	A	19[B]	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	A	19[A]	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	19[B]	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	122	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	96	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	122	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	180	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	141	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	26	LYS	CD-CE-NZ	5.25	123.79	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1909	0	1860	52	0
1	B	1835	0	1799	21	0
2	A	36	0	48	8	0
2	B	24	0	32	8	0
3	A	14	0	20	2	0
3	B	7	0	10	0	0
4	A	4	0	3	3	0
5	B	5	0	0	0	0
6	A	199	0	0	13	0
6	B	151	0	0	4	0
All	All	4184	0	3772	77	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (77) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:VAL:CG1	1:A:192:PRO:HG3	1.48	1.44
1:A:1:VAL:HG12	1:A:192:PRO:CG	1.61	1.30
1:A:1:VAL:CG1	1:A:192:PRO:CG	2.20	1.09
1:A:158:LYS:HE2	1:A:184[B]:GLN:NE2	1.72	1.03
1:A:1:VAL:HG12	1:A:192:PRO:HG3	1.03	1.02
1:A:158:LYS:HE2	1:A:184[B]:GLN:HE22	1.30	0.95
1:A:158:LYS:CE	1:A:184[B]:GLN:HE22	1.80	0.94
1:A:1:VAL:HG11	1:A:192:PRO:CB	1.97	0.93
1:A:158:LYS:CE	1:A:184[B]:GLN:NE2	2.33	0.92
1:A:183:GLN:HE21	1:A:185:ASN:HD21	1.23	0.86
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.20	0.86
1:A:171:ILE:HD11	1:A:177:GLN:HB2	1.58	0.85
1:A:132:GLU:H	3:A:306:PEG:H31	1.39	0.85
1:A:184[B]:GLN:HG3	6:A:500:HOH:O	1.76	0.84
1:A:1:VAL:HG11	1:A:192:PRO:HG3	1.60	0.82
1:A:1:VAL:CG1	1:A:192:PRO:CB	2.59	0.80
1:A:141:LEU:CD2	1:A:171:ILE:HD13	2.14	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:HIS:HD2	6:A:547:HOH:O	1.69	0.76
1:A:158:LYS:HE2	1:A:184[B]:GLN:CD	2.08	0.73
4:A:307:ACT:H1	6:A:578:HOH:O	1.89	0.72
1:A:1:VAL:HG11	1:A:192:PRO:HB3	1.70	0.71
1:B:157:GLN:HB2	2:B:306:GOL:H31	1.72	0.71
1:A:162:LYS:HG2	1:A:184[A]:GLN:HG2	1.73	0.71
1:A:43[B]:THR:HG23	6:A:520:HOH:O	1.90	0.71
2:A:309:GOL:H32	6:A:595:HOH:O	1.92	0.69
1:A:1:VAL:HG12	1:A:192:PRO:HG2	1.72	0.69
1:A:1:VAL:HG11	1:A:192:PRO:CG	2.08	0.69
1:B:153[B]:THR:HG23	1:B:198:ASN:OD1	1.95	0.67
1:A:116:GLY:H	2:A:305:GOL:H32	1.60	0.66
1:A:164[A]:ASN:ND2	2:A:309:GOL:O3	2.26	0.66
4:A:307:ACT:H3	6:A:447:HOH:O	1.94	0.65
1:A:213:GLU:OE1	2:A:303:GOL:H31	1.97	0.64
2:B:306:GOL:H11	6:B:460:HOH:O	1.99	0.62
1:A:178:LEU:HD21	1:B:158:LYS:CE	2.29	0.62
1:A:132:GLU:H	3:A:306:PEG:C3	2.11	0.61
1:B:3:LYS:CB	6:B:539:HOH:O	2.47	0.61
1:A:141:LEU:CD2	1:A:171:ILE:CD1	2.79	0.60
1:B:220[A]:LEU:HG	1:B:222[A]:GLU:HG3	1.83	0.60
1:A:184[B]:GLN:CG	6:A:500:HOH:O	2.43	0.60
1:A:141:LEU:HD23	1:A:171:ILE:HD13	1.85	0.58
1:A:139:HIS:HE1	6:A:441:HOH:O	1.87	0.58
1:A:220:LEU:HG	1:A:222[A]:GLU:HG3	1.84	0.57
1:A:236:LEU:O	1:A:237:TYR:HB2	2.05	0.56
1:A:141:LEU:HD22	1:A:171:ILE:HD13	1.88	0.55
1:A:178:LEU:HD21	1:B:158:LYS:HE3	1.87	0.55
1:A:164[B]:ASN:HB2	6:A:532:HOH:O	2.06	0.55
1:A:184[A]:GLN:OE1	2:A:301:GOL:O2	2.25	0.54
2:A:309:GOL:H2	6:B:547:HOH:O	2.08	0.52
6:A:477:HOH:O	1:B:153[B]:THR:HG21	2.09	0.51
1:B:157:GLN:HB2	2:B:306:GOL:C3	2.39	0.50
1:A:158:LYS:HE2	1:A:184[B]:GLN:OE1	2.12	0.49
1:B:220[A]:LEU:HD21	1:B:222[A]:GLU:CD	2.33	0.49
1:A:158:LYS:HE3	1:A:184[B]:GLN:NE2	2.21	0.49
1:A:36:ASP:OD1	6:A:531:HOH:O	2.20	0.49
1:A:77:HIS:HE1	6:A:505:HOH:O	1.96	0.48
1:A:178:LEU:HD21	1:B:158:LYS:HE2	1.95	0.47
1:B:220[A]:LEU:HG	1:B:222[A]:GLU:CG	2.44	0.47
1:B:73:ARG:HH12	2:B:301:GOL:H12	1.80	0.47
1:A:213:GLU:CD	2:A:303:GOL:H31	2.35	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:220:LEU:HD21	1:A:222[A]:GLU:CD	2.37	0.45
4:A:307:ACT:C	6:A:565:HOH:O	2.65	0.44
2:B:306:GOL:C1	6:B:460:HOH:O	2.63	0.44
1:B:66:SWG:N2	1:B:66:SWG:HD1	2.34	0.42
1:B:151:TYR:O	1:B:163:ALA:HA	2.20	0.42
1:B:5:GLU:HB3	2:B:304:GOL:O2	2.20	0.42
1:A:135:ASN:HD22	1:A:177:GLN:HE21	1.68	0.42
1:A:151:TYR:OH	2:B:306:GOL:H2	2.20	0.42
1:A:169:CYS:HB2	1:A:177:GLN:HB3	2.02	0.41
1:B:157:GLN:HB2	2:B:306:GOL:H12	2.02	0.41
1:B:155:ASP:OD2	1:B:162:LYS:HE3	2.20	0.41
1:A:116:GLY:H	2:A:305:GOL:C3	2.30	0.41
1:A:53:LEU:HD22	1:A:57:TRP:CE2	2.55	0.41
1:B:4:GLY:HA3	1:B:85:LYS:O	2.20	0.41
1:A:158:LYS:NZ	1:A:184[B]:GLN:HE22	2.19	0.41
1:B:205:SER:HB3	1:B:220[A]:LEU:HD11	2.03	0.41
1:B:125:LEU:C	1:B:125:LEU:HD23	2.41	0.41
1:A:135:ASN:HD22	1:A:177:GLN:NE2	2.18	0.41

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	241/264 (91%)	236 (98%)	4 (2%)	1 (0%)	43	17
1	B	230/264 (87%)	227 (99%)	3 (1%)	0	100	100
All	All	471/528 (89%)	463 (98%)	7 (2%)	1 (0%)	56	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	TYR

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	209/223 (94%)	207 (99%)	2 (1%)	85	69
1	B	201/223 (90%)	200 (100%)	1 (0%)	94	86
All	All	410/446 (92%)	407 (99%)	3 (1%)	89	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	237	TYR
1	B	6	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	139	HIS
1	A	177	GLN
1	A	185	ASN
1	B	139	HIS
1	B	164	ASN
1	B	170	ASN
1	B	185	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
1	SWG	A	66	1	25,25,26	5.68	7 (28%)	33,35,37	2.30	10 (30%)
1	SWG	B	66	1	25,25,26	4.79	11 (44%)	33,35,37	2.39	13 (39%)

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	SWG	A	66	1	-	0/10/29/30	0/1/3/3
1	SWG	B	66	1	-	0/10/29/30	0/1/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	SWG	O3-C3	23.14	1.27	1.11
1	B	66	SWG	O3-C3	18.14	1.23	1.11
1	A	66	SWG	CD1-CG	-13.23	1.31	1.39
1	B	66	SWG	CD1-CG	-11.87	1.32	1.39
1	A	66	SWG	CB2-CA2	5.34	1.38	1.35
1	A	66	SWG	CA2-C2	-4.67	1.43	1.48
1	B	66	SWG	CA3-N3	-4.46	1.43	1.47
1	A	66	SWG	CD2-CE2	-3.88	1.34	1.41
1	B	66	SWG	CA2-C2	-3.72	1.44	1.48
1	B	66	SWG	CB2-CA2	3.63	1.37	1.35
1	B	66	SWG	CD2-CE2	-3.08	1.35	1.41
1	B	66	SWG	CZ3-CE3	2.78	1.43	1.36
1	B	66	SWG	C1-N2	2.72	1.36	1.32
1	B	66	SWG	CA3-C3	-2.61	1.44	1.48
1	B	66	SWG	CD1-NE1	2.56	1.41	1.37
1	B	66	SWG	CG-CB2	2.36	1.52	1.47
1	A	66	SWG	CB1-CA1	2.32	1.57	1.52
1	A	66	SWG	CZ3-CE3	2.09	1.41	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	SWG	CZ2-CE2-CD2	6.18	130.51	120.96
1	A	66	SWG	CZ2-CE2-CD2	5.93	130.13	120.96
1	A	66	SWG	CA3-N3-C2	-5.33	120.15	123.46
1	A	66	SWG	CG-CD2-CE2	5.18	111.27	107.82
1	A	66	SWG	CG-CB2-CA2	-4.80	121.19	130.52
1	B	66	SWG	CG-CB2-CA2	-4.49	121.79	130.52
1	B	66	SWG	CZ3-CE3-CD2	-4.16	114.82	120.88
1	B	66	SWG	CG-CD2-CE2	3.71	110.30	107.82
1	B	66	SWG	O2-C2-CA2	-3.69	128.82	130.96
1	B	66	SWG	CB2-CA2-C2	3.48	127.81	122.46
1	B	66	SWG	CH2-CZ3-CE3	3.43	125.49	120.47
1	B	66	SWG	CH2-CZ2-CE2	-3.38	112.23	118.88
1	A	66	SWG	CE3-CD2-CE2	-2.82	115.09	119.08
1	A	66	SWG	CH2-CZ2-CE2	-2.79	113.39	118.88
1	B	66	SWG	CA2-C2-N3	2.78	105.02	103.44
1	B	66	SWG	CB2-CA2-N2	-2.72	123.57	128.59
1	A	66	SWG	CA2-N2-C1	2.51	107.81	105.79
1	B	66	SWG	C1-CA1-N1	-2.50	102.66	108.47
1	B	66	SWG	CZ2-CE2-NE1	-2.44	123.17	132.00
1	B	66	SWG	CA1-C1-N3	-2.28	122.20	124.54
1	A	66	SWG	N3-C1-N2	-2.19	109.90	111.51
1	A	66	SWG	CB2-CA2-C2	2.12	125.73	122.46
1	A	66	SWG	CZ2-CE2-NE1	-2.11	124.37	132.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	301	-	5,5,5	0.24	0	5,5,5	0.44	0
2	GOL	A	302	-	5,5,5	0.36	0	5,5,5	1.25	1 (20%)
2	GOL	A	303	-	5,5,5	0.41	0	5,5,5	0.49	0
2	GOL	A	304	-	5,5,5	0.37	0	5,5,5	1.14	0
2	GOL	A	305	-	5,5,5	0.43	0	5,5,5	0.69	0
3	PEG	A	306	-	6,6,6	0.57	0	5,5,5	0.33	0
4	ACT	A	307	-	1,3,3	0.86	0	0,3,3	0.00	-
3	PEG	A	308	-	6,6,6	0.56	0	5,5,5	2.18	1 (20%)
2	GOL	A	309	-	5,5,5	0.63	0	5,5,5	0.96	0
2	GOL	B	301	-	5,5,5	0.34	0	5,5,5	0.63	0
2	GOL	B	302	-	5,5,5	0.47	0	5,5,5	0.73	0
5	SO4	B	303	-	4,4,4	0.64	0	6,6,6	1.04	0
2	GOL	B	304	-	5,5,5	0.40	0	5,5,5	0.58	0
3	PEG	B	305	-	6,6,6	0.44	0	5,5,5	0.45	0
2	GOL	B	306	-	5,5,5	0.73	0	5,5,5	1.37	1 (20%)

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	GOL	A	301	-	-	0/4/4/4	0/0/0/0
2	GOL	A	302	-	-	0/4/4/4	0/0/0/0
2	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	GOL	A	304	-	-	0/4/4/4	0/0/0/0
2	GOL	A	305	-	-	0/4/4/4	0/0/0/0
3	PEG	A	306	-	-	0/4/4/4	0/0/0/0
4	ACT	A	307	-	-	0/0/0/0	0/0/0/0
3	PEG	A	308	-	-	0/4/4/4	0/0/0/0
2	GOL	A	309	-	-	0/4/4/4	0/0/0/0
2	GOL	B	301	-	-	0/4/4/4	0/0/0/0
2	GOL	B	302	-	-	0/4/4/4	0/0/0/0
5	SO4	B	303	-	-	0/0/0/0	0/0/0/0
2	GOL	B	304	-	-	0/4/4/4	0/0/0/0
3	PEG	B	305	-	-	0/4/4/4	0/0/0/0
2	GOL	B	306	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	308	PEG	C3-O2-C2	3.85	130.32	113.38
2	A	302	GOL	O1-C1-C2	-2.44	97.79	109.71
2	B	306	GOL	O3-C3-C2	2.08	119.88	109.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	236/264 (89%)	-0.30	7 (2%)	48 46	11, 17, 37, 67	2 (0%)
1	B	226/264 (85%)	-0.25	7 (3%)	47 44	12, 19, 38, 60	0
All	All	462/528 (87%)	-0.28	14 (3%)	47 46	11, 18, 38, 67	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	10.0
1	A	238	LYS	5.6
1	A	237	TYR	4.3
1	B	230	THR	4.3
1	B	190	ASP	3.2
1	B	191	GLY	2.7
1	A	173	ASP	2.5
1	B	211	PRO	2.5
1	A	174	GLY	2.3
1	B	174	GLY	2.3
1	A	190	ASP	2.2
1	A	2	SER	2.0
1	B	4	GLY	2.0
1	B	133	ASP	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	SWG	B	66	23/24	0.09	0.75	12,14,16,16	0
1	SWG	A	66	23/24	0.08	-0.14	10,12,13,14	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PEG	B	305	7/7	0.30	21.61	48,70,81,83	0
3	PEG	A	308	7/7	0.28	12.54	13,15,18,20	7
2	GOL	A	305	6/6	0.24	11.47	34,45,50,51	0
2	GOL	B	302	6/6	0.20	9.02	47,53,54,56	0
4	ACT	A	307	4/4	0.10	8.89	21,23,29,33	0
3	PEG	A	306	7/7	0.38	6.27	42,46,69,69	0
2	GOL	A	303	6/6	0.23	5.23	31,37,43,43	0
2	GOL	A	309	6/6	0.15	3.23	36,46,50,52	0
5	SO4	B	303	5/5	0.10	2.99	24,25,29,31	5
2	GOL	A	302	6/6	0.13	2.98	32,40,41,42	0
2	GOL	A	304	6/6	0.14	2.64	36,40,40,43	0
2	GOL	B	306	6/6	0.17	2.39	31,42,48,52	0
2	GOL	B	301	6/6	0.24	2.38	48,51,56,56	0
2	GOL	A	301	6/6	0.13	1.83	31,34,34,38	0
2	GOL	B	304	6/6	0.20	1.19	57,58,61,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.