Full wwPDB X-ray Structure Validation Report (i)

Nov 30, 2023 – 09:03 AM EST

PDB ID	:	4EN1
Title	:	The 1.62A 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 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 (i) 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 (1)) were used in the production of this report:

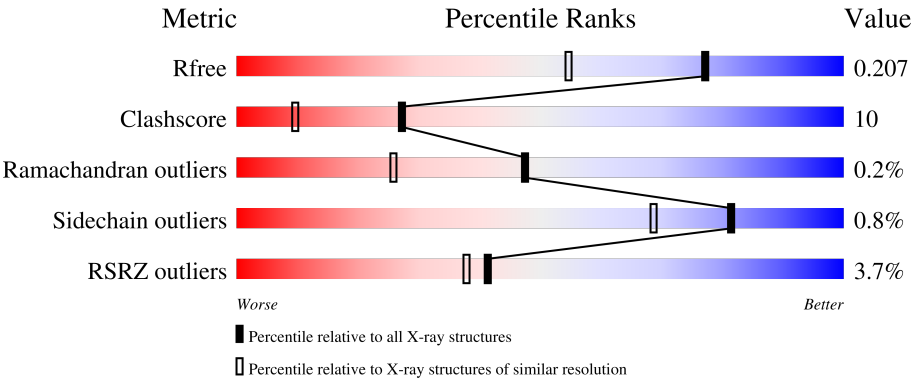
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (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 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 <=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	264	3%, 77%, 12%, 11%
1	B	264	3%, 77%, 8%, 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	306	-	-	X	-
3	PEG	A	306	-	-	-	X
4	ACT	A	307	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4184 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 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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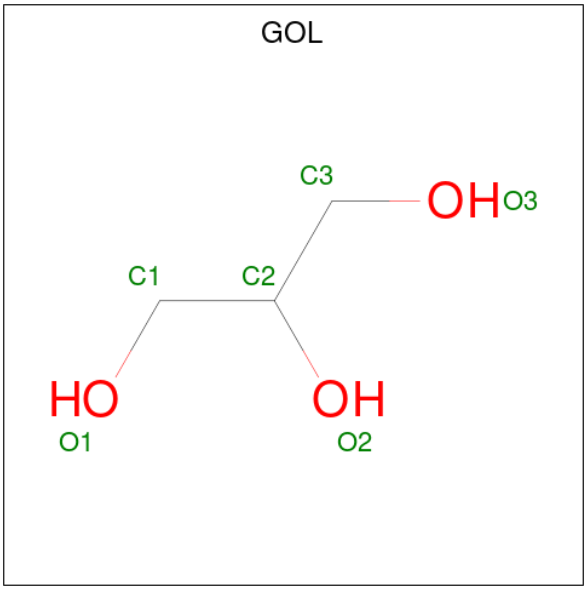
Chain	Residue	Modelled	Actual	Comment	Reference
B	147	HIS	SER	engineered mutation	UNP P42212
B	148	GLY	HIS	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	166	GLY	LYS	engineered mutation	UNP P42212
B	167	LEU	ILE	engineered mutation	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: $C_3H_8O_3$).



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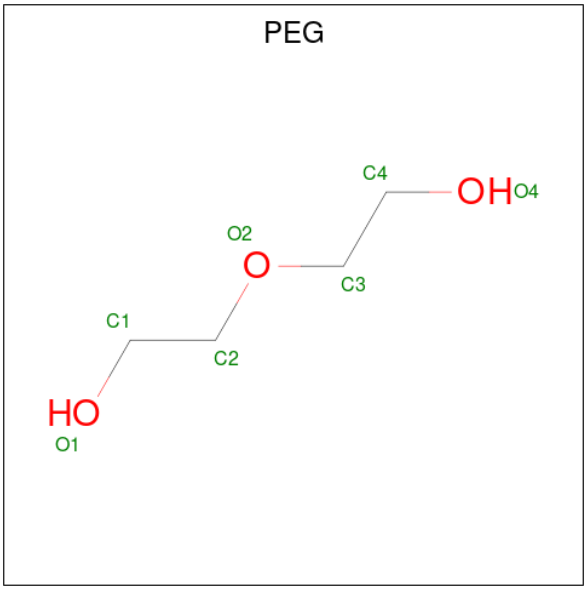
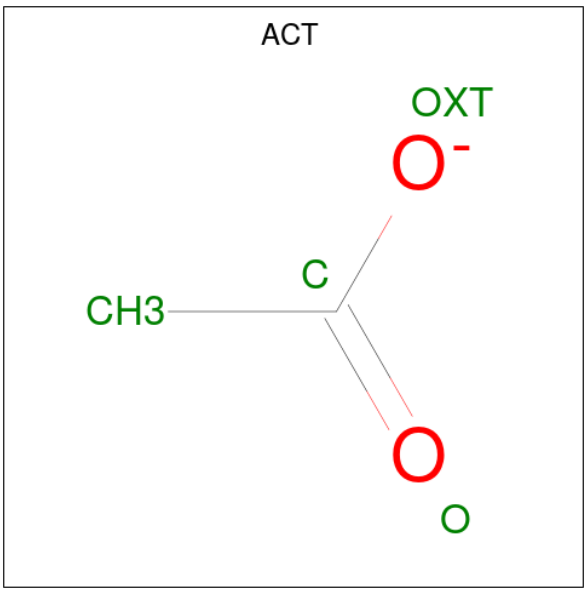
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



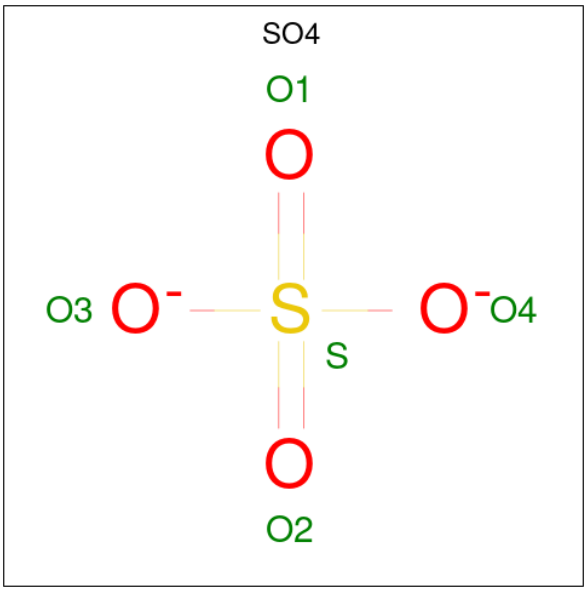
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- 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 4 2 2	0	0

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



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

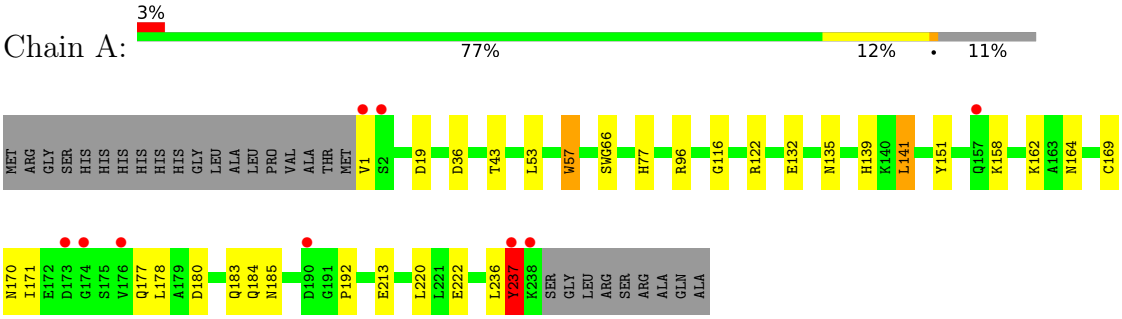
- Molecule 6 is water.

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

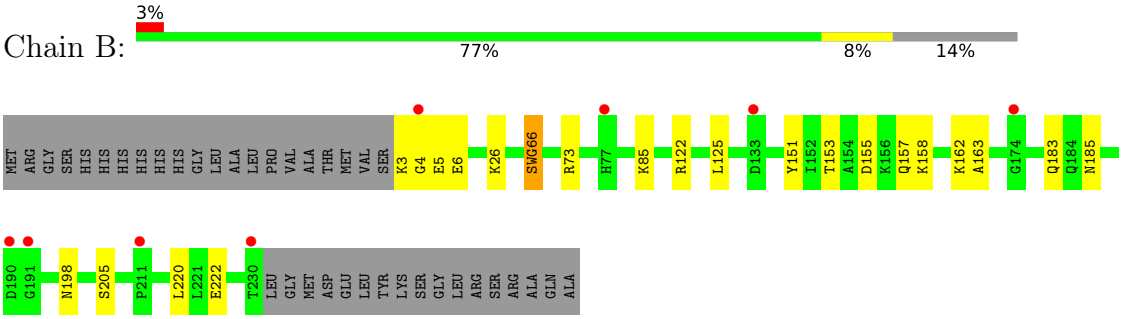
3 Residue-property plots (i)

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: Green fluorescent protein



• Molecule 1: Green fluorescent protein



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.28 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.178 , 0.205 0.179 , 0.207	Depositor DCC
R_{free} test set	4196 reflections (4.99%)	wwPDB-VP
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 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, SWG, ACT, PEG

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(^{o})	Ideal(^{o})
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 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	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

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 10.

All (77) 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: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	Interatomic distance (Å)	Clash overlap (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:139:HIS:HE1	6:A:441:HOH:O	1.87	0.58
1:A:141:LEU:HD23	1:A:171:ILE:HD13	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:CD	2:A:303:GOL:H31	2.35	0.46
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:HD1	1:B:66:SWG:N2	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:53:LEU:HD22	1:A:57:TRP:CE2	2.55	0.41
1:A:116:GLY:H	2:A:305:GOL:C3	2.30	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:125:LEU:C	1:B:125:LEU:HD23	2.41	0.41
1:B:205:SER:HB3	1:B:220[A]:LEU:HD11	2.03	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	241/264 (91%)	236 (98%)	4 (2%)	1 (0%)	34 15
1	B	230/264 (87%)	227 (99%)	3 (1%)	0	100 100
All	All	471/528 (89%)	463 (98%)	7 (2%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	TYR

5.3.2 Protein sidechains (i)

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%)	76 60
1	B	201/223 (90%)	200 (100%)	1 (0%)	88 80
All	All	410/446 (92%)	407 (99%)	3 (1%)	81 72

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	24,25,26	1.89	4 (16%)	29,35,37	2.29	10 (34%)
1	SWG	B	66	1	24,25,26	1.84	7 (29%)	29,35,37	2.72	12 (41%)

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	-	0/7/29/30	0/3/3/3
1	SWG	B	66	1	-	0/7/29/30	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	SWG	CA2-C2	-5.26	1.43	1.48
1	A	66	SWG	CB2-CA2	4.36	1.38	1.35
1	B	66	SWG	CA2-C2	-4.22	1.44	1.48
1	B	66	SWG	C1-N2	3.07	1.36	1.32
1	A	66	SWG	CD2-CE2	-3.02	1.34	1.42
1	B	66	SWG	CB2-CA2	2.94	1.37	1.35
1	B	66	SWG	CZ3-CE3	2.77	1.43	1.36
1	B	66	SWG	CD1-NE1	2.58	1.41	1.36
1	B	66	SWG	CD2-CE2	-2.50	1.35	1.42
1	B	66	SWG	CG-CB2	2.47	1.52	1.46
1	A	66	SWG	CZ3-CE3	2.07	1.41	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	SWG	CH2-CZ2-CE2	-5.46	112.23	120.08
1	B	66	SWG	CZ2-CE2-CD2	5.33	130.51	120.76
1	A	66	SWG	CZ2-CE2-CD2	5.12	130.13	120.76
1	A	66	SWG	CG-CB2-CA2	-4.96	121.19	130.81
1	A	66	SWG	CH2-CZ2-CE2	-4.65	113.39	120.08
1	B	66	SWG	CG-CB2-CA2	-4.65	121.79	130.81
1	B	66	SWG	CB2-CA2-C2	4.64	127.81	122.28
1	B	66	SWG	CZ3-CE3-CD2	-4.38	114.82	120.89
1	B	66	SWG	O2-C2-CA2	-3.81	128.82	130.96
1	B	66	SWG	CB2-CA2-N2	-3.79	123.57	128.83
1	A	66	SWG	C2-N3-C1	3.76	109.87	107.97
1	B	66	SWG	CH2-CZ3-CE3	3.60	125.49	120.44
1	B	66	SWG	CA2-C2-N3	3.50	105.02	103.37
1	B	66	SWG	O3-C3-CA3	-3.16	116.86	126.39
1	A	66	SWG	CB2-CA2-C2	2.89	125.73	122.28
1	A	66	SWG	CA2-N2-C1	2.76	107.81	105.77
1	B	66	SWG	CZ2-CE2-NE1	-2.76	123.17	130.80
1	A	66	SWG	CZ2-CE2-NE1	-2.32	124.37	130.80
1	A	66	SWG	CE3-CD2-CE2	-2.32	115.09	118.17
1	A	66	SWG	O3-C3-CA3	-2.30	119.45	126.39
1	A	66	SWG	N3-C1-N2	-2.24	109.90	111.45
1	B	66	SWG	CA1-C1-N3	-2.03	122.20	124.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	SWG	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	304	-	5,5,5	0.47	0	5,5,5	0.55	0
2	GOL	B	306	-	5,5,5	0.73	0	5,5,5	1.43	2 (40%)
3	PEG	A	306	-	6,6,6	0.57	0	5,5,5	0.33	0
2	GOL	A	305	-	5,5,5	0.48	0	5,5,5	0.68	0
2	GOL	B	302	-	5,5,5	0.54	0	5,5,5	0.75	0
2	GOL	A	309	-	5,5,5	0.70	0	5,5,5	0.89	0
5	SO4	B	303	-	4,4,4	0.40	0	6,6,6	0.84	0
2	GOL	B	301	-	5,5,5	0.42	0	5,5,5	0.55	0
2	GOL	A	303	-	5,5,5	0.50	0	5,5,5	0.49	0
2	GOL	A	304	-	5,5,5	0.42	0	5,5,5	1.18	0
3	PEG	B	305	-	6,6,6	0.45	0	5,5,5	0.47	0
3	PEG	A	308	-	6,6,6	0.57	0	5,5,5	2.29	2 (40%)
2	GOL	A	302	-	5,5,5	0.31	0	5,5,5	1.36	1 (20%)
2	GOL	A	301	-	5,5,5	0.27	0	5,5,5	0.54	0
4	ACT	A	307	-	3,3,3	0.66	0	3,3,3	1.28	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	GOL	B	304	-	-	0/4/4/4	-
2	GOL	B	306	-	-	2/4/4/4	-
3	PEG	A	306	-	-	2/4/4/4	-
2	GOL	A	305	-	-	2/4/4/4	-
2	GOL	B	302	-	-	3/4/4/4	-
2	GOL	A	309	-	-	4/4/4/4	-
2	GOL	B	301	-	-	4/4/4/4	-
2	GOL	A	303	-	-	2/4/4/4	-
2	GOL	A	304	-	-	2/4/4/4	-
3	PEG	B	305	-	-	3/4/4/4	-
3	PEG	A	308	-	-	2/4/4/4	-
2	GOL	A	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	301	-	-	1/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	308	PEG	C3-O2-C2	3.93	130.32	113.29
2	A	302	GOL	O1-C1-C2	-2.59	97.79	110.20
3	A	308	PEG	O1-C1-C2	2.20	124.59	111.81
2	B	306	GOL	O2-C2-C1	-2.10	99.87	109.12
2	B	306	GOL	O3-C3-C2	2.02	119.88	110.20

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	GOL	O1-C1-C2-C3
2	A	305	GOL	O1-C1-C2-C3
2	A	309	GOL	O1-C1-C2-O2
2	A	309	GOL	O1-C1-C2-C3
2	A	309	GOL	C1-C2-C3-O3
2	A	309	GOL	O2-C2-C3-O3
2	B	301	GOL	O1-C1-C2-C3
2	B	301	GOL	C1-C2-C3-O3
2	B	302	GOL	O1-C1-C2-C3
2	B	306	GOL	O1-C1-C2-C3
2	A	305	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-O2
3	B	305	PEG	O1-C1-C2-O2
2	A	304	GOL	C1-C2-C3-O3
2	A	302	GOL	O2-C2-C3-O3
2	A	303	GOL	O1-C1-C2-O2
2	A	304	GOL	O2-C2-C3-O3
2	B	301	GOL	O2-C2-C3-O3
2	B	302	GOL	O1-C1-C2-O2
3	A	306	PEG	O2-C3-C4-O4
2	B	302	GOL	O2-C2-C3-O3
2	B	306	GOL	O1-C1-C2-O2
3	A	306	PEG	C4-C3-O2-C2
3	B	305	PEG	C1-C2-O2-C3
2	A	302	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	308	PEG	C1-C2-O2-C3
3	A	308	PEG	O2-C3-C4-O4
2	A	301	GOL	O1-C1-C2-C3
3	B	305	PEG	O2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	304	GOL	1	0
2	B	306	GOL	6	0
3	A	306	PEG	2	0
2	A	305	GOL	2	0
2	A	309	GOL	3	0
2	B	301	GOL	1	0
2	A	303	GOL	2	0
2	A	301	GOL	1	0
4	A	307	ACT	3	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, 95^{th} 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	235/264 (89%)	-0.30	9 (3%)	40	37	11, 17, 36, 67	2 (0%)
1	B	225/264 (85%)	-0.23	8 (3%)	42	39	12, 19, 38, 60	0
All	All	460/528 (87%)	-0.27	17 (3%)	41	38	11, 18, 38, 67	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	10.4
1	A	238	LYS	5.8
1	B	230	THR	4.9
1	A	237	TYR	4.2
1	B	190	ASP	3.5
1	B	191	GLY	3.3
1	B	174	GLY	3.2
1	A	173	ASP	2.8
1	B	211	PRO	2.7
1	A	174	GLY	2.5
1	A	190	ASP	2.3
1	B	133	ASP	2.2
1	A	2	SER	2.2
1	B	4	GLY	2.2
1	A	157	GLN	2.1
1	A	176	VAL	2.0
1	B	77	HIS	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. The B-factors column lists the minimum, median, 95^{th} 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	SWG	A	66	23/24	0.98	0.08	10,12,13,14	0
1	SWG	B	66	23/24	0.98	0.09	12,14,16,16	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	GOL	B	304	6/6	0.54	0.19	57,58,61,63	0
2	GOL	B	301	6/6	0.65	0.23	48,51,56,56	0
2	GOL	B	302	6/6	0.66	0.21	47,53,54,56	0
3	PEG	B	305	7/7	0.66	0.34	48,70,81,83	0
3	PEG	A	306	7/7	0.71	0.41	42,46,69,69	0
2	GOL	A	309	6/6	0.80	0.16	36,46,50,52	0
2	GOL	A	304	6/6	0.81	0.14	36,40,40,43	0
2	GOL	A	303	6/6	0.83	0.26	31,37,43,43	0
3	PEG	A	308	7/7	0.83	0.31	13,15,18,20	7
2	GOL	B	306	6/6	0.83	0.16	31,42,48,52	0
2	GOL	A	305	6/6	0.85	0.26	34,45,50,51	0
2	GOL	A	302	6/6	0.90	0.13	32,40,41,42	0
2	GOL	A	301	6/6	0.90	0.12	31,34,34,38	0
5	SO4	B	303	5/5	0.93	0.11	24,25,29,31	5
4	ACT	A	307	4/4	0.95	0.10	21,23,29,33	0

6.5 Other polymers (i)

There are no such residues in this entry.