Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 04:45 AM EDT

PDB ID	:	4KAG
Title	:	Crystal structure analysis of a single amino acid deletion mutation in EGFP
Authors	:	Arpino, J.A.J.; Rizkallah, P.J.
Deposited on	:	2013-04-22
Resolution	:	1.12 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 (i)) were used in the production of this report:

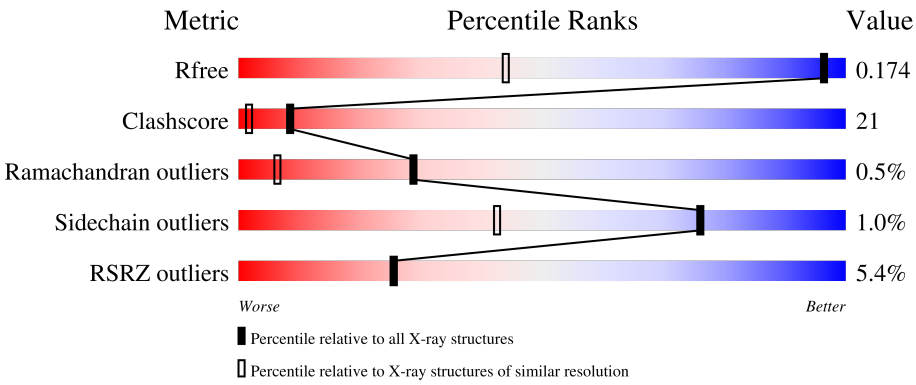
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.12 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	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

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 <=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	236	5%; 68%; 23%; 5%; 5%

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	EDO	A	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	302	-	-	X	-
2	EDO	A	303	-	-	X	-
2	EDO	A	307	-	-	X	-
2	EDO	A	321	-	X	X	-
4	TRS	A	319	-	-	X	X
4	TRS	A	320	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2444 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.

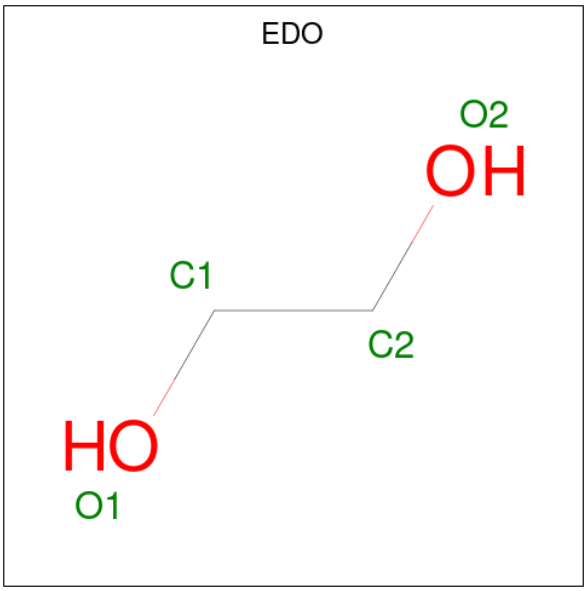
- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	2066	1308	348	402	8	0	31	0

There are 7 discrepancies between the modelled and reference sequences:

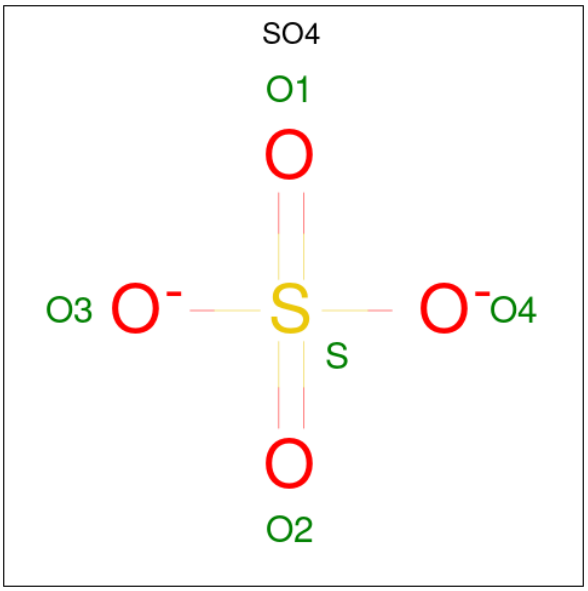
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	insertion	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	?	-	ASP	deletion	UNP P42212
A	231	LEU	HIS	conflict	UNP P42212

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



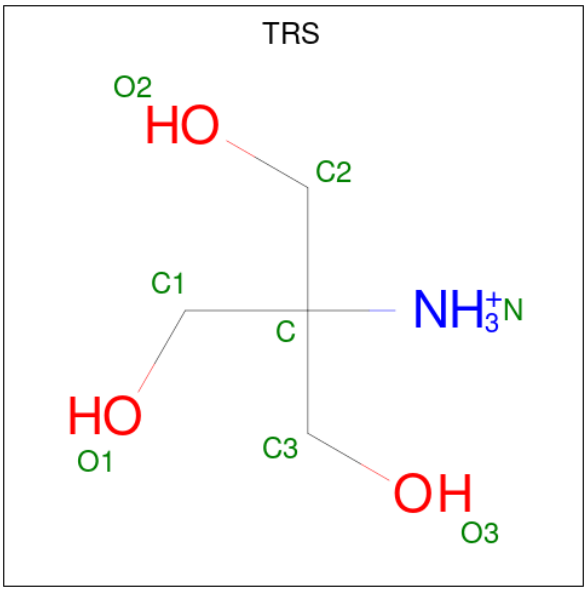
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0
2	A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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

- Molecule 5 is water.

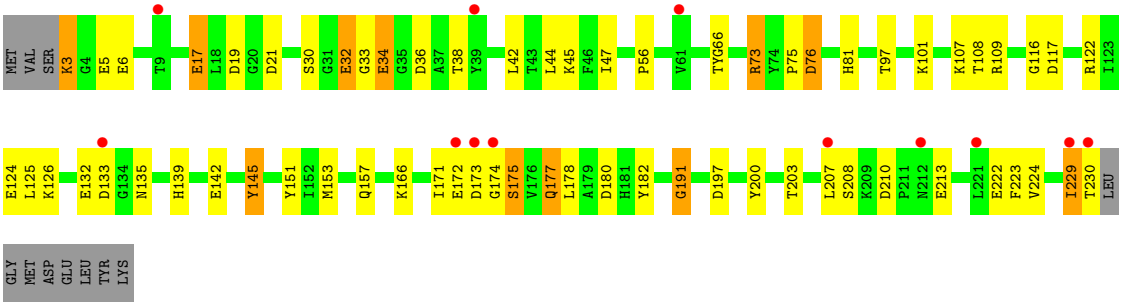
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	280	280	280	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	57.14Å 57.14Å 135.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.94 – 1.12 39.94 – 1.12	Depositor EDS
% Data completeness (in resolution range)	96.1 (39.94-1.12) 96.1 (39.94-1.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.161 0.153 , 0.174	Depositor DCC
R_{free} test set	4723 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	2444	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, TRS, CRO, SO4

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	1.45	16/2086 (0.8%)	1.24	16/2817 (0.6%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	GLU	CD-OE1	-6.55	1.18	1.25
1	A	17	GLU	CD-OE1	6.40	1.32	1.25
1	A	34	GLU	CB-CG	-6.32	1.40	1.52
1	A	200	TYR	CE2-CZ	-6.14	1.30	1.38
1	A	151	TYR	CD1-CE1	5.77	1.48	1.39
1	A	177	GLN	CD-NE2	-5.72	1.18	1.32
1	A	151	TYR	CE1-CZ	-5.64	1.31	1.38
1	A	133	ASP	CB-CG	5.62	1.63	1.51
1	A	6	GLU	CG-CD	5.58	1.60	1.51
1	A	200	TYR	CZ-OH	5.43	1.47	1.37
1	A	200	TYR	CE1-CZ	-5.39	1.31	1.38
1	A	191	GLY	C-O	5.38	1.32	1.23
1	A	182	TYR	CE1-CZ	-5.36	1.31	1.38
1	A	122[A]	ARG	CZ-NH2	-5.35	1.26	1.33
1	A	122[B]	ARG	CZ-NH2	-5.35	1.26	1.33
1	A	32	GLU	CB-CG	-5.27	1.42	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	ASP	CB-CG-OD1	10.91	128.12	118.30
1	A	109	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	73[A]	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	73[B]	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	73[A]	ARG	NE-CZ-NH2	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73[B]	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	21	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	210	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	197	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	A	229	ILE	CA-CB-CG1	-5.62	100.32	111.00
1	A	76	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	175	SER	N-CA-CB	-5.44	102.33	110.50
1	A	145	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	A	132[A]	GLU	CA-C-O	-5.22	109.14	120.10
1	A	132[B]	GLU	CA-C-O	-5.22	109.14	120.10
1	A	145	TYR	CB-CG-CD2	5.06	124.04	121.00

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	2066	0	1994	83	1
2	A	64	0	93	43	0
3	A	10	0	0	1	0
4	A	24	0	36	15	0
5	A	280	0	0	15	2
All	All	2444	0	2123	90	2

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 21.

All (90) 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:157:GLN:OE1	4:A:320:TRS:O1	1.59	1.17
1:A:81[B]:HIS:CE1	2:A:302:EDO:H22	1.86	1.11
1:A:180[B]:ASP:OD1	2:A:312:EDO:C2	1.99	1.09
1:A:180[B]:ASP:OD1	2:A:312:EDO:H21	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81[B]:HIS:HE1	2:A:302:EDO:H11	1.22	1.03
1:A:107:LYS:NZ	2:A:307:EDO:H21	1.74	1.02
1:A:81[B]:HIS:CE1	2:A:302:EDO:H11	1.94	1.01
1:A:229:ILE:O	5:A:670:HOH:O	1.81	0.98
1:A:222[B]:GLU:OE1	5:A:669:HOH:O	1.87	0.93
4:A:320:TRS:O2	4:A:320:TRS:O3	1.79	0.93
1:A:180[B]:ASP:OD1	2:A:312:EDO:H22	1.70	0.92
1:A:81[B]:HIS:CE1	2:A:302:EDO:C2	2.55	0.90
1:A:76:ASP:H	2:A:303:EDO:H21	1.37	0.88
1:A:108:THR:HA	4:A:319:TRS:N	1.90	0.86
1:A:81[B]:HIS:CE1	2:A:302:EDO:C1	2.60	0.83
1:A:3:LYS:HG3	1:A:5:GLU:HG2	1.61	0.82
1:A:107:LYS:HZ2	2:A:307:EDO:H21	1.42	0.81
1:A:139:HIS:ND1	2:A:321:EDO:O2	2.14	0.80
1:A:171[A]:ILE:HG22	1:A:173[A]:ASP:H	1.47	0.80
3:A:316:SO4:O2	5:A:465:HOH:O	2.00	0.79
1:A:107:LYS:HZ1	2:A:307:EDO:H21	1.48	0.75
1:A:81[B]:HIS:HE1	2:A:302:EDO:C1	1.99	0.75
1:A:73[B]:ARG:NH1	2:A:303:EDO:O2	2.22	0.71
1:A:36:ASP:OD1	5:A:639:HOH:O	2.08	0.71
1:A:180[B]:ASP:OD2	2:A:306:EDO:O1	2.09	0.69
1:A:38[A]:THR:HG23	5:A:639:HOH:O	1.92	0.68
1:A:81[B]:HIS:ND1	2:A:302:EDO:H22	2.08	0.67
1:A:166[B]:LYS:HB2	1:A:166[B]:LYS:HZ3	1.60	0.65
1:A:108:THR:CA	4:A:319:TRS:N	2.59	0.64
1:A:107:LYS:O	4:A:319:TRS:N	2.25	0.64
1:A:76:ASP:H	2:A:303:EDO:C2	2.10	0.62
1:A:213:GLU:O	2:A:314:EDO:H11	1.99	0.62
1:A:139:HIS:HD1	2:A:321:EDO:C2	2.12	0.61
1:A:108:THR:CA	4:A:319:TRS:HN2	2.13	0.61
1:A:126:LYS:HB3	4:A:319:TRS:H21	1.83	0.61
2:A:321:EDO:H11	5:A:679:HOH:O	2.00	0.60
1:A:73[A]:ARG:NH1	5:A:672:HOH:O	2.33	0.60
1:A:191:GLY:O	2:A:313:EDO:H22	2.01	0.59
1:A:76:ASP:N	2:A:303:EDO:H21	2.14	0.59
1:A:178:LEU:H	2:A:301:EDO:C1	2.16	0.58
1:A:101:LYS:HB2	2:A:304:EDO:H12	1.85	0.58
1:A:229:ILE:HG23	1:A:230:THR:HA	1.85	0.57
2:A:321:EDO:H21	5:A:424:HOH:O	2.04	0.57
1:A:135:ASN:HD22	1:A:177:GLN:HE21	1.53	0.55
1:A:177:GLN:HA	2:A:301:EDO:H12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171[A]:ILE:HD12	1:A:175:SER:OG	2.07	0.54
1:A:171[B]:ILE:HD11	1:A:177:GLN:HB2	1.88	0.54
1:A:171[A]:ILE:CD1	1:A:175:SER:OG	2.55	0.54
2:A:315:EDO:H22	5:A:510:HOH:O	2.08	0.53
1:A:101:LYS:HB3	2:A:301:EDO:H11	1.90	0.53
1:A:208[B]:SER:OG	5:A:671:HOH:O	2.16	0.52
1:A:108:THR:O	2:A:307:EDO:H11	2.10	0.51
1:A:172[B]:GLU:CG	5:A:647:HOH:O	2.59	0.51
1:A:171[B]:ILE:HD11	1:A:177:GLN:CB	2.41	0.51
4:A:319:TRS:O3	4:A:319:TRS:O2	2.29	0.50
1:A:166[B]:LYS:HB2	1:A:166[B]:LYS:NZ	2.27	0.50
1:A:107:LYS:NZ	2:A:307:EDO:C2	2.63	0.49
1:A:126:LYS:CB	4:A:319:TRS:H21	2.42	0.49
1:A:42[B]:LEU:HD12	1:A:42[B]:LEU:C	2.33	0.49
1:A:56:PRO:HA	2:A:321:EDO:H22	1.95	0.49
1:A:17:GLU:HB3	2:A:308:EDO:H22	1.95	0.48
1:A:75:PRO:HB3	2:A:303:EDO:H11	1.96	0.48
1:A:116:GLY:HA3	2:A:310:EDO:H22	1.95	0.48
1:A:173[B]:ASP:O	1:A:175:SER:N	2.40	0.48
2:A:303:EDO:H12	5:A:428:HOH:O	2.13	0.47
1:A:19[A]:ASP:O	4:A:318:TRS:N	2.45	0.47
1:A:180[B]:ASP:HB2	2:A:304:EDO:H11	1.96	0.47
1:A:3:LYS:CG	1:A:5:GLU:HG2	2.40	0.47
1:A:19[B]:ASP:O	4:A:318:TRS:N	2.46	0.46
1:A:145:TYR:HB2	1:A:207[A]:LEU:HD13	1.98	0.46
1:A:178:LEU:H	2:A:301:EDO:H11	1.79	0.46
1:A:34:GLU:HG3	2:A:305:EDO:H12	1.98	0.45
1:A:45:LYS:HE2	1:A:47:ILE:HD11	1.99	0.45
1:A:30[A]:SER:OG	2:A:308:EDO:H11	2.16	0.45
1:A:124:GLU:HB2	4:A:319:TRS:H31	1.98	0.45
1:A:75:PRO:HB3	2:A:303:EDO:C1	2.48	0.44
1:A:76:ASP:H	2:A:303:EDO:H12	1.83	0.44
1:A:203[A]:THR:HG23	1:A:224:VAL:HG22	1.99	0.44
1:A:30[B]:SER:O	1:A:30[B]:SER:OG	2.36	0.43
1:A:36:ASP:HB2	2:A:305:EDO:H11	2.00	0.43
1:A:33:GLY:HA3	1:A:44:LEU:HD23	2.01	0.43
1:A:172[B]:GLU:HG2	5:A:647:HOH:O	2.19	0.42
1:A:108:THR:HA	4:A:319:TRS:HN1	1.77	0.42
1:A:172[B]:GLU:HG3	5:A:647:HOH:O	2.20	0.42
1:A:107:LYS:HB3	1:A:107:LYS:HE3	1.28	0.41
1:A:97[B]:THR:O	1:A:97[B]:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153[A]:MET:HE3	5:A:563:HOH:O	2.21	0.41
1:A:125:LEU:N	4:A:318:TRS:N	2.70	0.40
1:A:124:GLU:CB	4:A:319:TRS:H31	2.51	0.40
1:A:42[B]:LEU:HD13	1:A:44:LEU:CD1	2.51	0.40

All (2) 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)
5:A:450:HOH:O	5:A:634:HOH:O[4_465]	1.68	0.52
1:A:223[B]:PHE:CE2	5:A:598:HOH:O[4_465]	1.81	0.39

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	254/236 (108%)	249 (98%)	3 (1%)	2 (1%)	19 3

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174[A]	GLY
1	A	174[B]	GLY

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	229/206 (111%)	227 (99%)	2 (1%)	78 47

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	32	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	177	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CRO	A	66	1	23,23,24	2.42	6 (26%)	30,32,34	2.06	8 (26%)

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	CRO	A	66	1	-	0/12/31/32	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CB2-CA2	7.48	1.41	1.35
1	A	66	CRO	CA2-C2	-7.07	1.41	1.48
1	A	66	CRO	C2-N3	-2.74	1.33	1.39
1	A	66	CRO	C1-N3	-2.52	1.32	1.37
1	A	66	CRO	CG2-CB2	-2.14	1.42	1.46
1	A	66	CRO	CA1-C1	2.08	1.54	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CRO	CA2-C2-N3	6.00	106.21	103.37
1	A	66	CRO	C2-CA2-N2	-3.83	106.25	108.93
1	A	66	CRO	CA2-N2-C1	3.76	108.54	105.77
1	A	66	CRO	O2-C2-CA2	-3.44	129.03	130.96
1	A	66	CRO	O3-C3-CA3	-3.21	116.69	126.39
1	A	66	CRO	C2-N3-C1	3.01	109.49	107.97
1	A	66	CRO	N3-C1-N2	-2.81	109.51	111.45
1	A	66	CRO	CB2-CA2-N2	2.16	131.82	128.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	SO4	A	316	-	4,4,4	1.89	1 (25%)	6,6,6	0.95	0
2	EDO	A	304	-	3,3,3	1.26	0	2,2,2	1.83	1 (50%)
2	EDO	A	313	-	3,3,3	1.20	0	2,2,2	1.59	1 (50%)
2	EDO	A	310	-	3,3,3	0.70	0	2,2,2	0.61	0
2	EDO	A	309	-	3,3,3	0.76	0	2,2,2	1.27	0
4	TRS	A	318	-	7,7,7	0.89	0	9,9,9	1.42	2 (22%)
2	EDO	A	306	-	3,3,3	0.97	0	2,2,2	0.48	0
2	EDO	A	308	-	3,3,3	1.47	0	2,2,2	0.12	0
2	EDO	A	314	-	3,3,3	1.85	2 (66%)	2,2,2	1.53	0
2	EDO	A	315	-	3,3,3	0.87	0	2,2,2	1.24	0
2	EDO	A	321	-	3,3,3	3.24	2 (66%)	2,2,2	2.29	1 (50%)
4	TRS	A	320	-	7,7,7	1.63	2 (28%)	9,9,9	2.60	5 (55%)
2	EDO	A	307	-	3,3,3	0.41	0	2,2,2	0.91	0
2	EDO	A	311	-	3,3,3	0.57	0	2,2,2	0.45	0
2	EDO	A	302	-	3,3,3	1.07	0	2,2,2	0.36	0
3	SO4	A	317	-	4,4,4	1.07	0	6,6,6	0.74	0
2	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.75	0
2	EDO	A	312	-	3,3,3	1.11	0	2,2,2	0.40	0
4	TRS	A	319	-	7,7,7	0.62	0	9,9,9	1.22	1 (11%)
2	EDO	A	303	-	3,3,3	0.46	0	2,2,2	1.06	0
2	EDO	A	301	-	3,3,3	1.24	0	2,2,2	1.91	1 (50%)

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	EDO	A	304	-	-	1/1/1/1	-
2	EDO	A	313	-	-	1/1/1/1	-
2	EDO	A	310	-	-	1/1/1/1	-
2	EDO	A	309	-	-	1/1/1/1	-
4	TRS	A	318	-	-	7/9/9/9	-
2	EDO	A	306	-	-	0/1/1/1	-
2	EDO	A	308	-	-	1/1/1/1	-
2	EDO	A	314	-	-	0/1/1/1	-
2	EDO	A	315	-	-	1/1/1/1	-
2	EDO	A	321	-	-	0/1/1/1	-
4	TRS	A	320	-	-	9/9/9/9	-
2	EDO	A	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	311	-	-	1/1/1/1	-
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	A	305	-	-	1/1/1/1	-
2	EDO	A	312	-	-	0/1/1/1	-
4	TRS	A	319	-	-	5/9/9/9	-
2	EDO	A	303	-	-	1/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	321	EDO	O1-C1	-4.92	1.16	1.42
4	A	320	TRS	C3-C	-3.14	1.43	1.53
3	A	316	SO4	O1-S	-3.08	1.29	1.46
4	A	320	TRS	C-N	-2.50	1.41	1.49
2	A	314	EDO	C2-C1	2.24	1.63	1.48
2	A	314	EDO	O2-C2	2.24	1.53	1.42
2	A	321	EDO	O2-C2	-2.22	1.30	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	320	TRS	C1-C-N	4.14	120.33	107.98
4	A	320	TRS	O1-C1-C	3.90	123.36	111.00
4	A	320	TRS	C2-C-N	-3.35	97.99	107.98
4	A	318	TRS	O2-C2-C	-3.05	101.33	111.00
2	A	321	EDO	O1-C1-C2	2.99	133.45	111.91
4	A	320	TRS	O3-C3-C	-2.90	101.80	111.00
4	A	320	TRS	O2-C2-C	-2.67	102.55	111.00
2	A	301	EDO	O2-C2-C1	2.43	129.37	111.91
4	A	319	TRS	O1-C1-C	-2.42	103.34	111.00
4	A	318	TRS	C3-C-C1	2.29	117.92	110.81
2	A	304	EDO	O2-C2-C1	2.25	128.10	111.91
2	A	313	EDO	O2-C2-C1	-2.24	95.76	111.91

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	318	TRS	N-C-C3-O3
4	A	319	TRS	C2-C-C1-O1

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Mol	Chain	Res	Type	Atoms
4	A	319	TRS	C3-C-C1-O1
4	A	319	TRS	N-C-C1-O1
4	A	319	TRS	N-C-C2-O2
4	A	320	TRS	C2-C-C1-O1
4	A	320	TRS	C3-C-C1-O1
4	A	320	TRS	C1-C-C2-O2
4	A	320	TRS	C3-C-C2-O2
4	A	320	TRS	N-C-C2-O2
2	A	305	EDO	O1-C1-C2-O2
2	A	302	EDO	O1-C1-C2-O2
2	A	303	EDO	O1-C1-C2-O2
2	A	307	EDO	O1-C1-C2-O2
2	A	308	EDO	O1-C1-C2-O2
4	A	318	TRS	C3-C-C1-O1
4	A	318	TRS	C1-C-C3-O3
2	A	315	EDO	O1-C1-C2-O2
4	A	318	TRS	N-C-C1-O1
4	A	318	TRS	N-C-C2-O2
4	A	320	TRS	N-C-C1-O1
4	A	320	TRS	N-C-C3-O3
2	A	309	EDO	O1-C1-C2-O2
2	A	304	EDO	O1-C1-C2-O2
2	A	310	EDO	O1-C1-C2-O2
2	A	313	EDO	O1-C1-C2-O2
4	A	318	TRS	C2-C-C1-O1
4	A	320	TRS	C2-C-C3-O3
2	A	311	EDO	O1-C1-C2-O2
4	A	318	TRS	C3-C-C2-O2
4	A	319	TRS	C3-C-C2-O2
4	A	320	TRS	C1-C-C3-O3

There are no ring outliers.

18 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	316	SO4	1	0
2	A	304	EDO	2	0
2	A	313	EDO	1	0
2	A	310	EDO	1	0
4	A	318	TRS	3	0
2	A	306	EDO	1	0
2	A	308	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	314	EDO	1	0
2	A	315	EDO	1	0
2	A	321	EDO	5	0
4	A	320	TRS	2	0
2	A	307	EDO	5	0
2	A	302	EDO	7	0
2	A	305	EDO	2	0
2	A	312	EDO	3	0
4	A	319	TRS	10	0
2	A	303	EDO	8	0
2	A	301	EDO	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	224/236 (94%)	0.33	12 (5%)	25	25	8, 11, 22, 72	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	7.3
1	A	173[A]	ASP	5.2
1	A	229	ILE	4.0
1	A	133	ASP	3.2
1	A	174[A]	GLY	2.6
1	A	39	TYR	2.4
1	A	207[A]	LEU	2.3
1	A	9	THR	2.3
1	A	212	ASN	2.1
1	A	61	VAL	2.1
1	A	172[A]	GLU	2.1
1	A	221[A]	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CRO	A	66	22/23	0.95	0.10	8,9,12,13	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, 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	TRS	A	319	8/8	0.65	0.48	22,25,29,34	8
2	EDO	A	308	4/4	0.74	0.16	22,24,31,40	0
4	TRS	A	320	8/8	0.74	0.34	23,25,35,38	8
2	EDO	A	302	4/4	0.76	0.20	36,38,40,45	0
2	EDO	A	314	4/4	0.77	0.24	31,31,31,35	0
2	EDO	A	313	4/4	0.79	0.21	24,30,33,36	0
2	EDO	A	304	4/4	0.80	0.25	27,32,37,43	0
4	TRS	A	318	8/8	0.83	0.32	31,33,44,44	8
2	EDO	A	312	4/4	0.84	0.17	26,30,32,35	0
3	SO4	A	316	5/5	0.86	0.21	13,13,20,23	5
2	EDO	A	311	4/4	0.86	0.11	50,53,53,55	0
2	EDO	A	301	4/4	0.87	0.24	15,29,32,35	0
2	EDO	A	307	4/4	0.89	0.27	21,34,38,42	0
2	EDO	A	303	4/4	0.89	0.10	30,33,34,38	0
3	SO4	A	317	5/5	0.90	0.27	26,72,84,92	0
2	EDO	A	309	4/4	0.90	0.12	25,27,27,40	0
2	EDO	A	315	4/4	0.91	0.14	27,30,40,51	0
2	EDO	A	305	4/4	0.91	0.20	22,30,31,34	0
2	EDO	A	310	4/4	0.91	0.20	27,34,41,41	0
2	EDO	A	306	4/4	0.92	0.14	23,23,24,26	0
2	EDO	A	321	4/4	0.96	0.19	10,15,15,39	0

6.5 Other polymers (i)

There are no such residues in this entry.