wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2021 – 12:46 am BST

PDB ID	:	6ZSM
Title	:	Crystal structure of rsGCaMP double mutant Ile80His/Val116Ile in the ON state (non-illuminated)
Authors	:	Janowski, R.; Fuenzalida-Werner, J.P.; Mishra, K.; Stiel, A.C.; Niessing, D.
Deposited on	:	2020-07-16
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

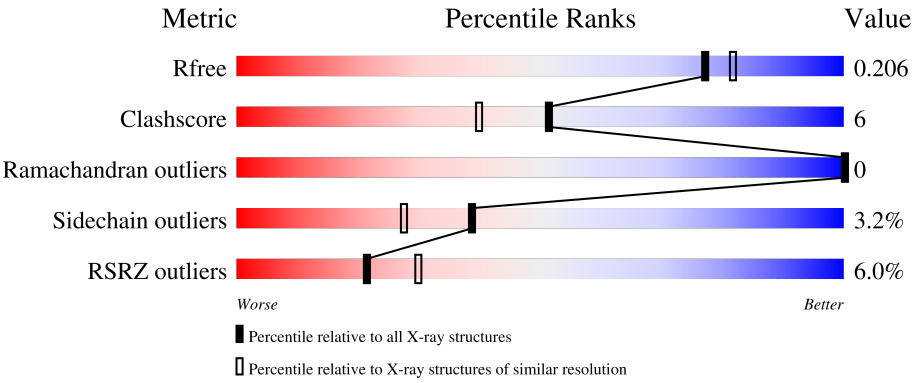
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	418	6% 80% 14% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3729 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,Green fluorescent protein,Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	9	2
			3218	2022	545	636	15			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	MET	-	initiating methionine	UNP P42212
A	37	VAL	-	expression tag	UNP P42212
A	38	ASP	-	expression tag	UNP P42212
A	39	SER	-	expression tag	UNP P42212
A	40	SER	-	expression tag	UNP P42212
A	41	ARG	-	expression tag	UNP P42212
A	42	ARG	-	expression tag	UNP P42212
A	43	LYS	-	expression tag	UNP P42212
A	44	TRP	-	expression tag	UNP P42212
A	45	ASN	-	expression tag	UNP P42212
A	46	LYS	-	expression tag	UNP P42212
A	47	THR	-	expression tag	UNP P42212
A	48	GLY	-	expression tag	UNP P42212
A	49	HIS	-	expression tag	UNP P42212
A	50	ALA	-	expression tag	UNP P42212
A	51	VAL	-	expression tag	UNP P42212
A	52	ARG	-	expression tag	UNP P42212
A	53	ALA	-	expression tag	UNP P42212
A	54	ILE	-	expression tag	UNP P42212
A	55	GLY	-	expression tag	UNP P42212
A	56	ARG	-	expression tag	UNP P42212
A	57	LEU	-	expression tag	UNP P42212
A	58	SER	-	expression tag	UNP P42212
A	59	SER	-	expression tag	UNP P42212
A	60	LEU	-	expression tag	UNP P42212
A	61	GLU	-	expression tag	UNP P42212
A	66	LYS	MET	conflict	UNP P42212

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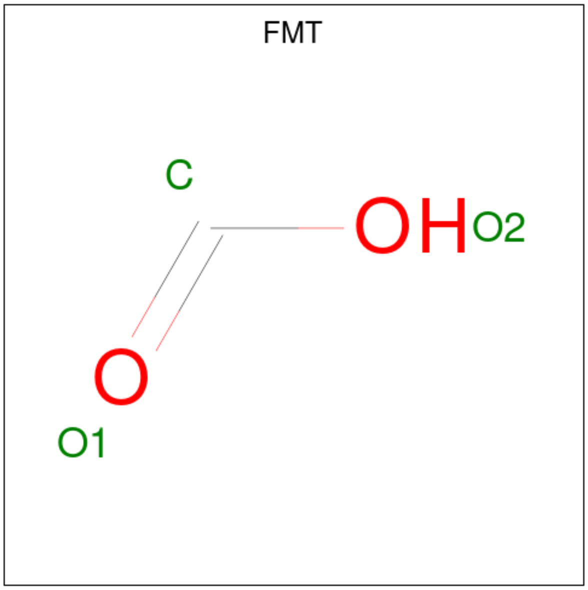
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	ALA	VAL	conflict	UNP P42212
A	80	HIS	ILE	conflict	UNP P42212
A	88	GLY	SER	conflict	UNP P42212
A	93	TYR	ASP	conflict	UNP P42212
A	116	ILE	THR	conflict	UNP P42212
A	119	LYS	ALA	conflict	UNP P42212
A	144	LEU	HIS	conflict	UNP P42212
A	152	GLY	-	linker	UNP P42212
A	153	GLY	-	linker	UNP P42212
A	154	THR	-	linker	UNP P42212
A	155	GLY	-	linker	UNP P42212
A	156	GLY	-	linker	UNP P42212
A	157	SER	-	linker	UNP P42212
A	158	MET	-	linker	UNP P42212
A	159	VAL	-	linker	UNP P42212
A	?	-	PHE	deletion	UNP P42212
A	?	-	SER	deletion	UNP P42212
A	222	LEU	TYR	conflict	UNP P42212
A	224	PIA	GLY	conflict	UNP P42212
A	227	LEU	GLN	conflict	UNP P42212
A	251	ILE	VAL	conflict	UNP P42212
A	373	THR	ILE	conflict	UNP K4DIE3
A	381	TYR	ASP	conflict	UNP K4DIE3
A	452	LEU	-	expression tag	UNP K4DIE3
A	453	GLU	-	expression tag	UNP K4DIE3
A	454	HIS	-	expression tag	UNP K4DIE3
A	455	HIS	-	expression tag	UNP K4DIE3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

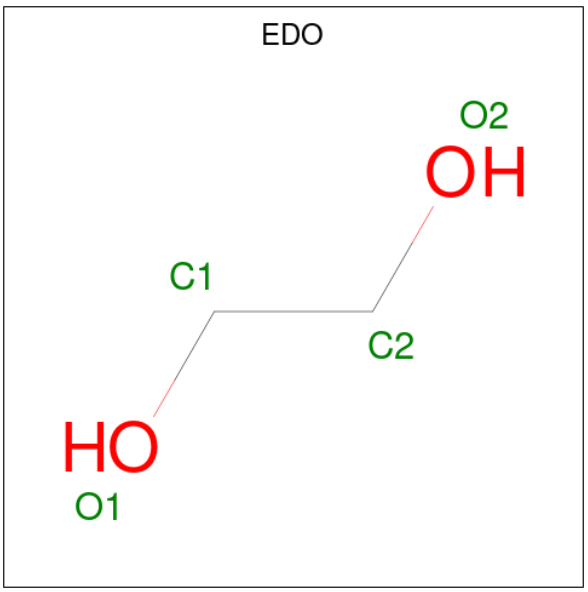
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	5	5	5	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

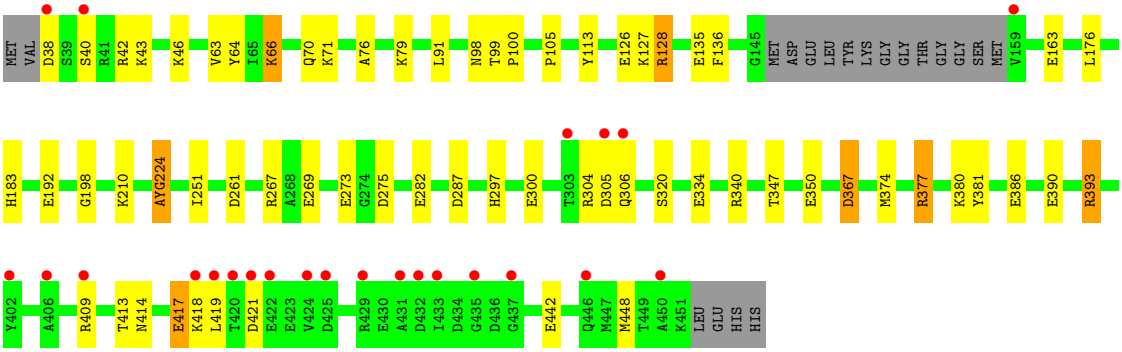
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	444	Total O 444 444	0	0

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,Green fluorescent protein,Calmodulin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.54Å 121.54Å 96.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.46 – 1.95 47.41 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.46-1.95) 100.0 (47.41-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.157 , 0.198 0.169 , 0.206	Depositor DCC
R_{free} test set	2665 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3729	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: CA, EDO, PIA, FMT

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	1.02	14/3278 (0.4%)	1.05	9/4413 (0.2%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269[A]	GLU	CD-OE2	8.73	1.35	1.25
1	A	269[B]	GLU	CD-OE2	8.73	1.35	1.25
1	A	287	ASP	CG-OD2	7.06	1.41	1.25
1	A	273	GLU	CD-OE2	6.53	1.32	1.25
1	A	192	GLU	CD-OE2	-6.29	1.18	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ASP	CB-CA-C	5.74	121.88	110.40
1	A	267	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	367	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	421	ASP	N-CA-CB	-5.25	101.16	110.60
1	A	377	ARG	CG-CD-NE	-5.19	100.90	111.80

There are no chirality outliers.

There are no planarity outliers.

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	3218	0	3138	36	0
2	A	5	0	0	0	0
3	A	42	0	14	0	0
4	A	20	0	30	3	0
5	A	444	0	0	9	0
All	All	3729	0	3182	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 36 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:275[A]:ASP:OD1	5:A:603:HOH:O	1.73	1.06
1:A:128[A]:ARG:HH21	1:A:128[A]:ARG:HG3	1.28	0.96
1:A:128[A]:ARG:NH1	5:A:604:HOH:O	2.14	0.80
1:A:43:LYS:HD3	1:A:419:LEU:HD11	1.66	0.77
1:A:380:LYS:NZ	1:A:381:TYR:OH	2.20	0.75

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	401/418 (96%)	391 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	351/358 (98%)	339 (97%)	12 (3%)	37 25

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	LYS
1	A	304	ARG
1	A	417	GLU
1	A	374	MET
1	A	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	183	HIS
1	A	297	HIS
1	A	344	GLN
1	A	410	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	PIA	A	224	1	21,21,22	4.60	5 (23%)	27,29,31	4.77	17 (62%)

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	PIA	A	224	1	-	0/8/27/28	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	PIA	CA2-C2	-15.22	1.33	1.48
1	A	224	PIA	CB2-CA2	12.87	1.45	1.35
1	A	224	PIA	CA2-N2	3.58	1.46	1.38
1	A	224	PIA	O2-C2	3.58	1.30	1.23
1	A	224	PIA	CD1-CG2	-2.37	1.34	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	PIA	O2-C2-CA2	11.43	137.38	130.96
1	A	224	PIA	C2-N3-C1	9.42	112.73	107.97
1	A	224	PIA	CA1-C1-N2	7.34	133.44	124.05
1	A	224	PIA	CE1-CD1-CG2	-7.13	111.96	121.25
1	A	224	PIA	CA1-C1-N3	-6.56	116.88	124.75

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	A	224	PIA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 5 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
3	FMT	A	518	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	519	-	0,2,2	-	-	0,1,1	-	-
4	EDO	A	520	-	3,3,3	0.34	0	2,2,2	0.55	0
3	FMT	A	511	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	515	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	517	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	506	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	509	-	0,2,2	-	-	0,1,1	-	-
4	EDO	A	522	-	3,3,3	0.44	0	2,2,2	0.39	0
3	FMT	A	513	-	0,2,2	-	-	0,1,1	-	-
4	EDO	A	521	-	3,3,3	0.26	0	2,2,2	0.54	0
4	EDO	A	523	-	3,3,3	0.16	0	2,2,2	0.20	0
3	FMT	A	510	-	0,2,2	-	-	0,1,1	-	-
4	EDO	A	524	-	3,3,3	0.49	0	2,2,2	0.61	0
3	FMT	A	508	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	516	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	512	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	514	-	0,2,2	-	-	0,1,1	-	-
3	FMT	A	507	-	0,2,2	-	-	0,1,1	-	-

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
4	EDO	A	524	-	-	1/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	A	521	-	-	1/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	521	EDO	O1-C1-C2-O2
4	A	522	EDO	O1-C1-C2-O2
4	A	524	EDO	O1-C1-C2-O2
4	A	523	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	521	EDO	2	0
4	A	524	EDO	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, 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	398/418 (95%)	0.21	24 (6%)	21	30	22, 33, 75, 161	8 (2%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	ILE	5.4
1	A	424	VAL	3.8
1	A	305	ASP	3.7
1	A	421	ASP	3.6
1	A	419	LEU	2.9

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	PIA	A	224	20/21	0.98	0.09	22,27,31,32	0

6.3 Carbohydrates

There are no monosaccharides 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. 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
3	FMT	A	511	3/3	0.75	0.32	74,74,81,83	0
3	FMT	A	515	3/3	0.79	0.32	75,75,81,84	0
3	FMT	A	513	3/3	0.84	0.27	52,52,66,71	0
3	FMT	A	507	3/3	0.84	0.15	43,43,58,59	0
4	EDO	A	523	4/4	0.86	0.27	62,64,65,68	0
3	FMT	A	512	3/3	0.87	0.18	59,59,59,71	0
3	FMT	A	509	3/3	0.88	0.22	52,52,65,67	0
4	EDO	A	524	4/4	0.88	0.15	44,47,48,53	0
3	FMT	A	516	3/3	0.89	0.23	57,57,69,71	0
4	EDO	A	522	4/4	0.89	0.24	44,45,45,49	0
3	FMT	A	514	3/3	0.89	0.17	66,66,68,71	0
3	FMT	A	510	3/3	0.89	0.32	52,52,61,65	0
3	FMT	A	517	3/3	0.90	0.21	71,71,74,74	0
3	FMT	A	518	3/3	0.91	0.12	48,48,58,63	0
3	FMT	A	506	3/3	0.91	0.12	51,51,58,62	0
4	EDO	A	521	4/4	0.92	0.21	57,59,62,64	0
2	CA	A	505	1/1	0.93	0.11	84,84,84,84	0
3	FMT	A	519	3/3	0.93	0.21	50,50,62,62	0
3	FMT	A	508	3/3	0.95	0.18	47,47,50,54	0
4	EDO	A	520	4/4	0.95	0.13	36,49,51,54	0
2	CA	A	501	1/1	0.97	0.07	44,44,44,44	0
2	CA	A	504	1/1	0.98	0.05	42,42,42,42	0
2	CA	A	503	1/1	1.00	0.11	29,29,29,29	0
2	CA	A	502	1/1	1.00	0.12	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.