

wwPDB X-ray Structure Validation Summary Report (i)

Nov 5, 2023 – 12:16 PM EST

PDB ID : 4LJB

Title : Structure of a photobleached state of IrisFP under high intensity laser-light Authors : Duan, C.; Adam, V.; Byrdin, M.; Ridard, J.; Kieffer-Jacquinod, S.; Morlot,

C.; Arcizet, D.; Demachy, I.; Bourgeois, D.

2013-07-04 Deposited on

Resolution 1.90 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 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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.36

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

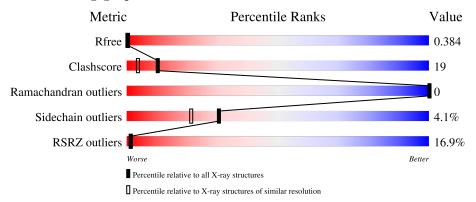
Validation Pipeline (wwPDB-VP) 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.90 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\mathring{A}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 cha	ain
1	A	227	9% 74%	23% • •
1	В	227	64%	30%
1	С	227	70%	26%
1	D	227	19%	28%

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	SO4	В	302	-	-	X	-
2	SO4	В	303	-	-	X	-
2	SO4	С	303	-	-	-	X
3	SO3	A	304	-	-	-	X
3	SO3	В	304	-	-	-	X
3	SO3	C	304	_	_	-	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7520 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 to red photoconvertible GPF-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Λ	221	Total	С	N	О	S	0	0	0	
1	A	221	1778	1133	305	329	11	0	U	U	
1	В	220	Total	С	N	О	S	0	0	0	
1	Ъ	220	1767	1127	304	326	10	0	0	U	
1	С	223	Total	С	N	О	S	0	1	0	
1		223	1807	1150	313	333	11	0	1	0	
1	D	221	Total	С	N	О	S	0	0	0	
1		221	1778	1133	305	329	11			U	

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q5S6Z9
A	-4	HIS	-	expression tag	UNP Q5S6Z9
A	-3	HIS	-	expression tag	UNP Q5S6Z9
A	-2	HIS	-	expression tag	UNP Q5S6Z9
A	-1	HIS	-	expression tag	UNP Q5S6Z9
A	0	HIS	-	expression tag	UNP Q5S6Z9
A	64	CR8	HIS	chromophore	UNP Q5S6Z9
A	64	CR8	TYR	chromophore	UNP Q5S6Z9
A	64	CR8	GLY	chromophore	UNP Q5S6Z9
A	173	SER	PHE	engineered mutation	UNP Q5S6Z9
A	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
В	-5	HIS	-	expression tag	UNP Q5S6Z9
В	-4	HIS	-	expression tag	UNP Q5S6Z9
В	-3	HIS	-	expression tag	UNP Q5S6Z9
В	-2	HIS	-	expression tag	UNP Q5S6Z9
В	-1	HIS	-	expression tag	UNP Q5S6Z9
В	0	HIS	-	expression tag	UNP Q5S6Z9
В	64	CR8	HIS	chromophore	UNP Q5S6Z9
В	64	CR8	TYR	chromophore	UNP Q5S6Z9
В	64	CR8	GLY	chromophore	UNP Q5S6Z9
В	173	SER	PHE	engineered mutation	UNP Q5S6Z9

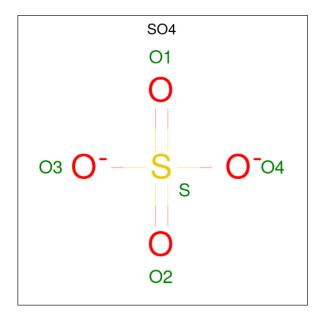
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Chain	Residue	Modelled	Actual	Comment	Reference
В	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
С	-5	HIS	-	expression tag	UNP Q5S6Z9
С	-4	HIS	-	expression tag	UNP Q5S6Z9
С	-3	HIS	-	expression tag	UNP Q5S6Z9
С	-2	HIS	-	expression tag	UNP Q5S6Z9
С	-1	HIS	-	expression tag	UNP Q5S6Z9
С	0	HIS	-	expression tag	UNP Q5S6Z9
С	64	CR8	HIS	chromophore	UNP Q5S6Z9
С	64	CR8	TYR	chromophore	UNP Q5S6Z9
С	64	CR8	GLY	chromophore	UNP Q5S6Z9
С	173	SER	PHE	engineered mutation	UNP Q5S6Z9
С	191	LEU	PHE	engineered mutation	UNP Q5S6Z9
D	-5	HIS	-	expression tag	UNP Q5S6Z9
D	-4	HIS	-	expression tag	UNP Q5S6Z9
D	-3	HIS	-	expression tag	UNP Q5S6Z9
D	-2	HIS	-	expression tag	UNP Q5S6Z9
D	-1	HIS	-	expression tag	UNP Q5S6Z9
D	0	HIS	_	expression tag	UNP Q5S6Z9
D	64	CR8	HIS	chromophore	UNP Q5S6Z9
D	64	CR8	TYR	chromophore	UNP Q5S6Z9
D	64	CR8	GLY	chromophore	UNP Q5S6Z9
D	173	SER	PHE	engineered mutation	UNP Q5S6Z9
D	191	LEU	PHE	engineered mutation	UNP Q5S6Z9

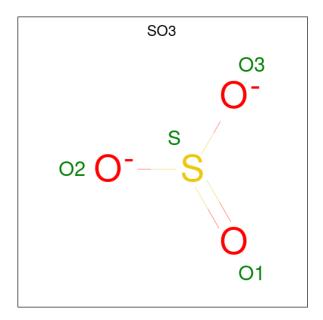
 \bullet Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

 \bullet Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O_3S).





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

• Molecule 4 is water.

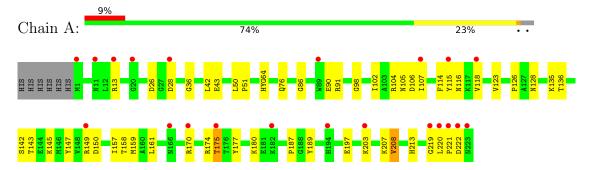
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	105	Total O 105 105	0	0
4	В	72	Total O 72 72	0	0
4	С	68	Total O 68 68	0	0
4	D	68	Total O 68 68	0	0



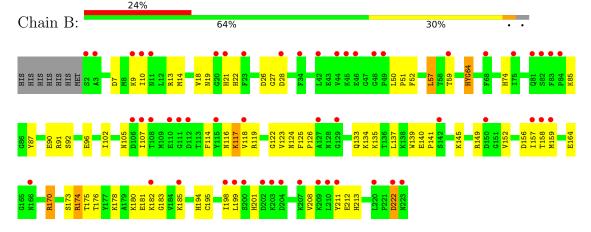
3 Residue-property plots (i)

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.

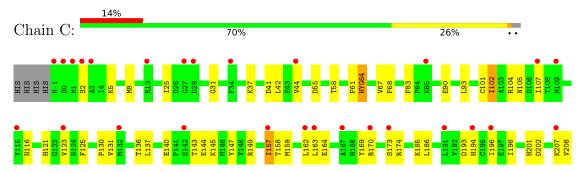
• Molecule 1: Green to red photoconvertible GPF-like protein EosFP



• Molecule 1: Green to red photoconvertible GPF-like protein EosFP



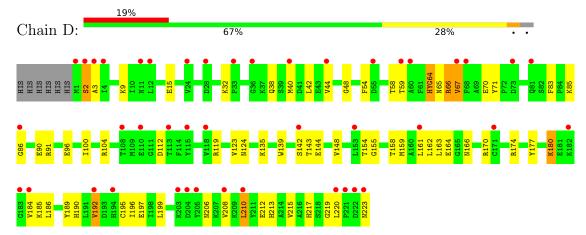
• Molecule 1: Green to red photoconvertible GPF-like protein EosFP







• Molecule 1: Green to red photoconvertible GPF-like protein EosFP





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	86.10Å 96.42Å 140.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.01 - 1.90	Depositor
resolution (A)	10.01 - 1.90	EDS
% Data completeness	85.9 (10.01-1.90)	Depositor
(in resolution range)	85.9 (10.01-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	1.37 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
P. P.	0.339 , 0.384	Depositor
R, R_{free}	0.339 , 0.384	DCC
R_{free} test set	3938 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	1.649	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.46, 55.6	EDS
L-test for twinning ²	$< L >=0.56, < L^2>=0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7520	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SO3, SO4, CR8

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	Bo	nd lengths	Bond	\mathbf{angles}
MIOI	Mol Chain		# Z > 5	RMSZ	# Z > 5
1	A	0.47	0/1798	0.67	0/2424
1	В	0.44	0/1787	0.63	0/2410
1	С	0.43	0/1829	0.64	0/2466
1	D	0.48	1/1798 (0.1%)	0.65	0/2424
All	All	0.46	$1/7212 \ (0.0\%)$	0.65	0/9724

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
1	D	2	SER	C-N	-5.34	1.21	1.34

There are no bond angle outliers.

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	1778	0	1703	52	0
1	В	1767	0	1689	96	0
1	С	1807	0	1724	59	0
1	D	1778	0	1703	90	0
2	A	20	0	0	2	0
2	В	15	0	0	5	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
2	С	20	0	0	0	0
2	D	10	0	0	0	0
3	A	4	0	0	1	0
3	В	4	0	0	0	0
3	С	4	0	0	0	0
4	A	105	0	0	5	0
4	В	72	0	0	5	0
4	С	68	0	0	4	0
4	D	68	0	0	14	0
All	All	7520	0	6819	264	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 19.

The worst 5 of 264 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:D:210:LEU:HD12	1:D:210:LEU:H	1.07	1.17
1:B:174:ARG:HH21	1:B:174:ARG:CG	1.66	1.08
1:A:158:THR:O	1:B:145:LYS:HE3	1.52	1.07
1:D:139:TRP:CE2	1:D:161:LEU:HD21	1.92	1.05
1:B:170:ARG:HH21	1:B:170:ARG:CG	1.68	1.04

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	Perce	ntiles	
1	A	$216/227 \ (95\%)$	215 (100%)	1 (0%)	0	100	100
1	В	215/227 (95%)	213 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured Allowed		Outliers	Perce	ntiles
1	C	$219/227 \ (96\%)$	213 (97%)	6 (3%)	0	100	100
1	D	$216/227\ (95\%)$	214 (99%)	2 (1%)	0	100	100
All	All	866/908 (95%)	855 (99%)	11 (1%)	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	188/195~(96%)	184 (98%)	4 (2%)	53 48
1	В	186/195~(95%)	175 (94%)	11 (6%)	19 10
1	С	191/195 (98%)	185 (97%)	6 (3%)	40 32
1	D	188/195 (96%)	178 (95%)	10 (5%)	22 13
All	All	753/780 (96%)	722 (96%)	31 (4%)	30 21

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	222	ASP
1	D	184	VAL
1	С	123	VAL
1	D	196	ILE
1	D	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	В	124	ASN
1	D	22	HIS
1	D	223	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)

4 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		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CR8	D	64	1	20,27,28	1.84	6 (30%)	17,37,39	2.06	8 (47%)
1	CR8	С	64	1	20,27,28	1.92	6 (30%)	17,37,39	1.33	2 (11%)
1	CR8	A	64	1	20,27,28	1.94	7 (35%)	17,37,39	1.40	3 (17%)
1	CR8	В	64	1	20,27,28	1.81	5 (25%)	17,37,39	1.83	6 (35%)

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	CR8	D	64	1	-	5/8/25/26	0/3/3/3
1	CR8	С	64	1	-	6/8/25/26	0/3/3/3
1	CR8	A	64	1	-	8/8/25/26	0/3/3/3
1	CR8	В	64	1	-	6/8/25/26	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	С	64	CR8	C8-C7	5.40	1.49	1.36
1	A	64	CR8	C8-C7	5.26	1.49	1.36
1	В	64	CR8	C8-C7	4.76	1.47	1.36
1	D	64	CR8	C8-C7	4.53	1.47	1.36
1	D	64	CR8	C12-C11	-3.47	1.38	1.45



The worst 5	of	19	bond	angle	outliers	are	listed	below:
THE WOLDE	, 01	10	Olia	WII SIC	Outiloid	COL	iibuca	DOIOW.

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	D	64	CR8	C4-C5-C7	-4.64	118.01	121.95
1	В	64	CR8	C12-C6-C7	-4.00	118.55	121.95
1	С	64	CR8	O3-C3-CA3	-3.36	116.76	126.32
1	D	64	CR8	C3-CA3-N3	-3.04	107.32	111.92
1	A	64	CR8	O3-C3-CA3	-2.99	117.82	126.32

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	64	CR8	C5-C7-C8-CA2
1	A	64	CR8	C6-C7-C8-CA2
1	A	64	CR8	C7-C8-CA2-C2
1	A	64	CR8	C7-C8-CA2-N2
1	A	64	CR8	CA1-C20-C21-N22

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	64	CR8	4	0
1	С	64	CR8	1	0
1	В	64	CR8	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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).



Mal	Т	Clasia	Dan	Link	В	ond leng	$_{ m gths}$	Bond angles		
Mol	Type	Chain	Res		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	SO3	A	304	-	1,3,3	0.75	0	0,3,3	-	-
3	SO3	С	304	-	1,3,3	0.56	0	0,3,3	-	-
2	SO4	С	301	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	D	302	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	A	305	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	С	305	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	С	303	-	4,4,4	0.56	0	6,6,6	0.78	0
2	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	A	301	-	4,4,4	0.32	0	6,6,6	0.05	0
2	SO4	С	302	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	В	301	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	В	303	-	4,4,4	0.55	0	6,6,6	0.47	0
3	SO3	В	304	-	1,3,3	0.56	0	0,3,3	-	-
2	SO4	D	301	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	В	302	-	4,4,4	0.32	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	SO3	1	0
2	A	305	SO4	1	0
2	A	301	SO4	1	0
2	В	303	SO4	2	0
2	В	302	SO4	3	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, 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		2	$OWAB(A^2)$	Q<0.9
1	A	220/227~(96%)	0.96	21 (9%)	8	9	12, 19, 33, 88	0
1	В	219/227 (96%)	1.51	54 (24%)	0	0	16, 30, 51, 72	0
1	С	222/227 (97%)	1.21	31 (13%)	2	2	12, 24, 42, 107	0
1	D	220/227 (96%)	1.51	43 (19%)	1	1	15, 26, 40, 101	0
All	All	881/908 (97%)	1.30	149 (16%)	1	1	12, 24, 46, 107	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	18.2
1	D	2	SER	12.8
1	D	222	ASP	8.0
1	В	2	SER	7.5
1	С	223	ASN	7.3

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, 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	CR8	В	64	25/26	0.64	0.33	39,48,59,63	0
1	CR8	D	64	25/26	0.71	0.30	21,43,54,55	0
1	CR8	A	64	25/26	0.76	0.26	13,26,52,59	0
1	CR8	С	64	25/26	0.81	0.21	21,30,44,47	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	$\operatorname{B-factors}({ m \AA}^2)$	Q<0.9
3	SO3	С	304	4/4	0.02	0.69	116,118,118,118	0
2	SO4	С	305	5/5	0.46	0.37	86,89,90,90	0
2	SO4	A	302	5/5	0.49	0.35	70,70,70,71	5
2	SO4	С	303	5/5	0.57	0.55	22,27,27,28	5
3	SO3	A	304	4/4	0.59	0.53	11,13,16,18	4
2	SO4	A	305	5/5	0.62	0.37	93,94,95,95	0
2	SO4	A	303	5/5	0.68	0.39	29,30,33,36	5
2	SO4	В	301	5/5	0.72	0.33	78,80,80,81	0
2	SO4	A	301	5/5	0.74	0.25	81,82,82,83	0
2	SO4	В	303	5/5	0.75	0.27	47,48,49,49	5
2	SO4	С	301	5/5	0.75	0.31	99,99,100,101	0
2	SO4	D	301	5/5	0.77	0.22	86,87,87,89	0
3	SO3	В	304	4/4	0.79	0.43	36,36,36,38	4
2	SO4	В	302	5/5	0.79	0.28	97,97,97,98	0
2	SO4	С	302	5/5	0.81	0.27	46,47,47,48	5
2	SO4	D	302	5/5	0.88	0.22	29,36,37,38	5

6.5 Other polymers (i)

There are no such residues in this entry.

