



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 8Q6W / pdb_00008q6w
Title : LSSmOrange - Directionality of Optical Properties of Fluorescent Proteins
Authors : Myskova, J.; Brynda, J.; Lazar, J.
Deposited on : 2023-08-15
Resolution : 1.43 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

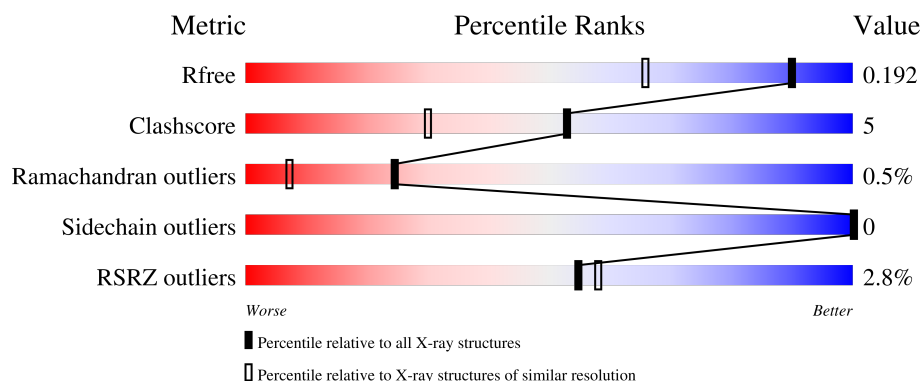
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

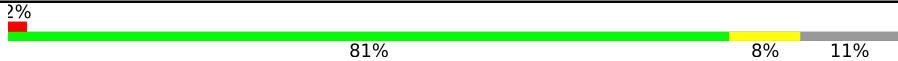
The reported resolution of this entry is 1.43 Å.

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}	180053	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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 $\leq 5\%$. 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	242	

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
3	ACT	A	303	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 1973 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 mOrange.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	4	0
			1763	1129	291	336	7			

There are 19 discrepancies between the modelled and reference sequences:

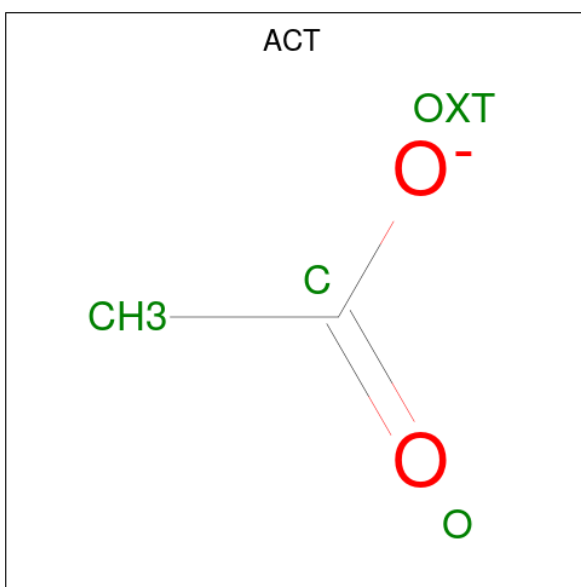
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP D0VWW2
A	-12	HIS	-	expression tag	UNP D0VWW2
A	-11	HIS	-	expression tag	UNP D0VWW2
A	-10	HIS	-	expression tag	UNP D0VWW2
A	-9	HIS	-	expression tag	UNP D0VWW2
A	-8	HIS	-	expression tag	UNP D0VWW2
A	-7	GLY	-	expression tag	UNP D0VWW2
A	-6	ARG	-	expression tag	UNP D0VWW2
A	-5	SER	-	expression tag	UNP D0VWW2
A	44	VAL	ALA	conflict	UNP D0VWW2
A	66	OFM	PHE	conflict	UNP D0VWW2
A	?	-	GLY	deletion	UNP D0VWW2
A	?	-	TYR	deletion	UNP D0VWW2
A	?	-	GLY	deletion	UNP D0VWW2
A	83	LEU	PHE	conflict	UNP D0VWW2
A	143	MET	TRP	conflict	UNP D0VWW2
A	161	ASP	ILE	conflict	UNP D0VWW2
A	163	LEU	MET	conflict	UNP D0VWW2
A	196	ASP	GLY	conflict	UNP D0VWW2

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



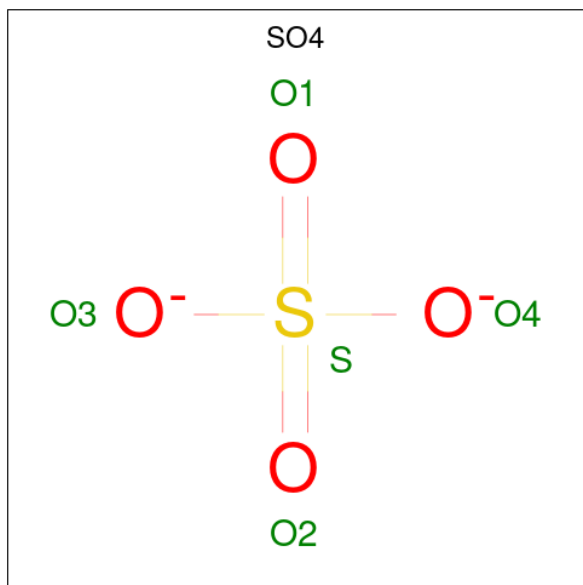
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

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

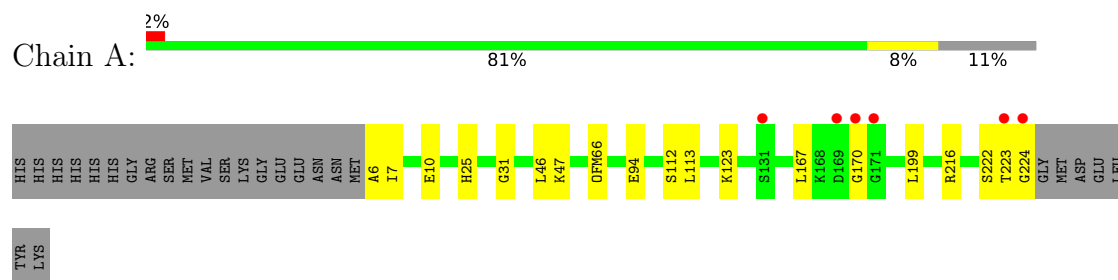
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		

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: mOrange



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	68.09Å 68.09Å 41.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.04 – 1.43 34.04 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.04-1.43) 99.9 (34.04-1.43)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.134 , 0.181 0.139 , 0.192	Depositor DCC
R_{free} test set	1966 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.026 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	1973	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: OFM, PG4, ACT, SO4, 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	1.04	2/1780 (0.1%)	1.09	2/2392 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	LEU	C-O	5.46	1.30	1.23
1	A	25	HIS	CE1-NE2	5.16	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	SER	CA-C-N	5.22	127.23	120.44
1	A	222	SER	C-N-CA	5.22	127.23	120.44

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	1763	0	1736	17	0
2	A	36	0	49	5	0
3	A	4	0	3	2	0
4	A	7	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
6	A	148	0	0	5	0
All	All	1973	0	1798	18	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 5.

All (18) 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:223:THR:C	1:A:224:GLY:N	2.01	1.18
1:A:10[B]:GLU:OE1	6:A:401:HOH:O	1.81	0.95
1:A:94:GLU:HG3	6:A:534:HOH:O	1.70	0.91
1:A:6:ALA:N	6:A:403:HOH:O	2.06	0.87
1:A:10[A]:GLU:OE1	6:A:402:HOH:O	1.97	0.81
1:A:123:LYS:HG3	3:A:303:ACT:H2	1.61	0.80
1:A:123:LYS:HG3	3:A:303:ACT:CH3	2.26	0.65
1:A:47:LYS:HZ1	2:A:301:PG4:H22	1.67	0.60
1:A:7:ILE:HG12	1:A:113:LEU:HD21	1.86	0.56
1:A:223:THR:CA	1:A:224:GLY:N	2.70	0.55
1:A:216:ARG:HB2	2:A:302:PG4:H41	1.96	0.47
1:A:112:SER:HB2	6:A:405:HOH:O	2.15	0.46
1:A:47:LYS:HG2	2:A:301:PG4:H51	1.99	0.45
1:A:7:ILE:HG12	1:A:113:LEU:CD2	2.48	0.43
2:A:302:PG4:H42	2:A:302:PG4:H21	1.84	0.42
1:A:47:LYS:NZ	2:A:301:PG4:H41	2.36	0.41
1:A:31:GLY:HA3	1:A:46:LEU:HD23	2.02	0.40

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	214/242 (88%)	208 (97%)	5 (2%)	1 (0%)	24 7

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	188/207 (91%)	188 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	OFM	A	66	1	32,36,37	3.24	6 (18%)	35,52,54	2.16	8 (22%)

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	OFM	A	66	1	-	1/12/51/52	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	OFM	CB2-CA2	12.72	1.47	1.35
1	A	66	OFM	CA2-C2	-10.79	1.36	1.48
1	A	66	OFM	O2-C2	3.78	1.30	1.23
1	A	66	OFM	C2-N3	-3.47	1.32	1.40
1	A	66	OFM	O0-C0	2.57	1.41	1.38
1	A	66	OFM	CE1-CD1	2.56	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	OFM	CA2-C2-N3	8.29	110.47	103.50
1	A	66	OFM	O2-C2-CA2	-4.62	128.07	131.02
1	A	66	OFM	CE1-CD1-CG2	-3.23	117.05	121.22
1	A	66	OFM	CZ0-CEX-CDX	-2.48	117.17	120.24
1	A	66	OFM	CZ0-CEY-CDY	2.48	123.29	120.24
1	A	66	OFM	O0-C0-OG1	-2.44	108.78	111.47
1	A	66	OFM	C3-CA3-N3	2.35	117.79	112.43
1	A	66	OFM	CD2-CG2-CB2	-2.14	113.88	121.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	OFM	N2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 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	$\# Z > 2$
5	SO4	A	308	-	4,4,4	0.41	0	6,6,6	0.12	0
5	SO4	A	307	-	4,4,4	0.45	0	6,6,6	0.25	0
2	PG4	A	301	-	12,12,12	0.42	0	11,11,11	0.84	0
2	PG4	A	302	-	12,12,12	0.42	0	11,11,11	0.52	0
4	PEG	A	304	-	6,6,6	0.17	0	5,5,5	0.23	0
2	PG4	A	305	-	9,9,12	0.26	0	8,8,11	0.25	0
5	SO4	A	306	-	4,4,4	0.31	0	6,6,6	0.22	0
3	ACT	A	303	-	3,3,3	0.89	0	3,3,3	0.94	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	PG4	A	302	-	-	6/10/10/10	-
2	PG4	A	301	-	-	6/10/10/10	-
4	PEG	A	304	-	-	3/4/4/4	-
2	PG4	A	305	-	-	0/7/7/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PG4	O3-C5-C6-O4
2	A	301	PG4	O2-C3-C4-O3
2	A	301	PG4	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	301	PG4	O4-C7-C8-O5
2	A	302	PG4	O4-C7-C8-O5
2	A	302	PG4	O1-C1-C2-O2
2	A	302	PG4	C6-C5-O3-C4
2	A	301	PG4	C6-C5-O3-C4
2	A	302	PG4	O3-C5-C6-O4
2	A	301	PG4	C4-C3-O2-C2
2	A	302	PG4	C8-C7-O4-C6
4	A	304	PEG	C4-C3-O2-C2
4	A	304	PEG	C1-C2-O2-C3
4	A	304	PEG	O2-C3-C4-O4
2	A	302	PG4	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PG4	3	0
2	A	302	PG4	2	0
3	A	303	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	223:THR	C	224:GLY	N	2.01

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	215/242 (88%)	-0.20	6 (2%) 55 58	10, 20, 38, 73	4 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	5.7
1	A	224	GLY	4.1
1	A	223	THR	3.8
1	A	169	ASP	2.3
1	A	171	GLY	2.1
1	A	131	SER	2.1

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	OFM	A	66	33/34	0.98	0.05	14,17,21,22	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	PEG	A	304	7/7	0.79	0.18	44,45,47,52	1
5	SO4	A	308	5/5	0.84	0.13	34,38,44,44	1
2	PG4	A	301	13/13	0.86	0.17	29,36,47,50	0
2	PG4	A	302	13/13	0.90	0.14	20,38,46,69	0
2	PG4	A	305	10/13	0.91	0.09	23,24,28,30	0
5	SO4	A	307	5/5	0.91	0.10	31,32,38,38	1
3	ACT	A	303	4/4	0.91	0.13	40,41,43,47	0
5	SO4	A	306	5/5	0.95	0.07	36,37,40,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.