wwPDB X-ray Structure Validation Summary Report (i)

Mar 14, 2026 – 08:21 PM UTC

PDB ID	:	5PI8 / pdb_00005pi8
Title	:	PanDDA analysis group deposition – Crystal Structure of JMJD2D after initial refinement with no ligand modelled (structure 21)
Authors	:	Pearce, N.M.; Krojer, T.; Talon, R.; Bradley, A.R.; Fairhead, M.; Sethi, R.; Wright, N.; MacLean, E.; Collins, P.; Brandao-Neto, J.; Douangamath, A.; Renjie, Z.; Dias, A.; Vollmar, M.; Ng, J.; Szykowska, A.; Burgess-Brown, N.; Brennan, P.E.; Cox, O.; Oppermann, U.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; von Delft, F.
Deposited on	:	2017-02-07
Resolution	:	1.27 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:

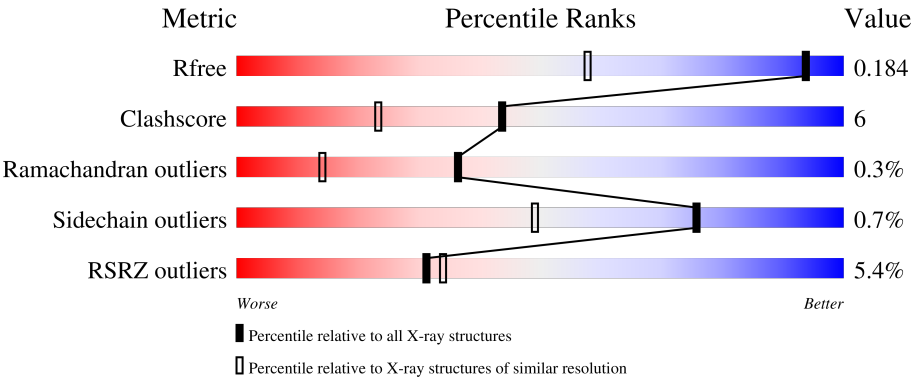
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.27 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	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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	364	5% 77% 13% • 9%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3384 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 Lysine-specific demethylase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	2	27	0
			2882	1852	493	519	18			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q6B0I6
A	-20	HIS	-	expression tag	UNP Q6B0I6
A	-19	HIS	-	expression tag	UNP Q6B0I6
A	-18	HIS	-	expression tag	UNP Q6B0I6
A	-17	HIS	-	expression tag	UNP Q6B0I6
A	-16	HIS	-	expression tag	UNP Q6B0I6
A	-15	HIS	-	expression tag	UNP Q6B0I6
A	-14	SER	-	expression tag	UNP Q6B0I6
A	-13	SER	-	expression tag	UNP Q6B0I6
A	-12	GLY	-	expression tag	UNP Q6B0I6
A	-11	VAL	-	expression tag	UNP Q6B0I6
A	-10	ASP	-	expression tag	UNP Q6B0I6
A	-9	LEU	-	expression tag	UNP Q6B0I6
A	-8	GLY	-	expression tag	UNP Q6B0I6
A	-7	THR	-	expression tag	UNP Q6B0I6
A	-6	GLU	-	expression tag	UNP Q6B0I6
A	-5	ASN	-	expression tag	UNP Q6B0I6
A	-4	LEU	-	expression tag	UNP Q6B0I6
A	-3	TYR	-	expression tag	UNP Q6B0I6
A	-2	PHE	-	expression tag	UNP Q6B0I6
A	-1	GLN	-	expression tag	UNP Q6B0I6
A	0	SER	-	expression tag	UNP Q6B0I6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

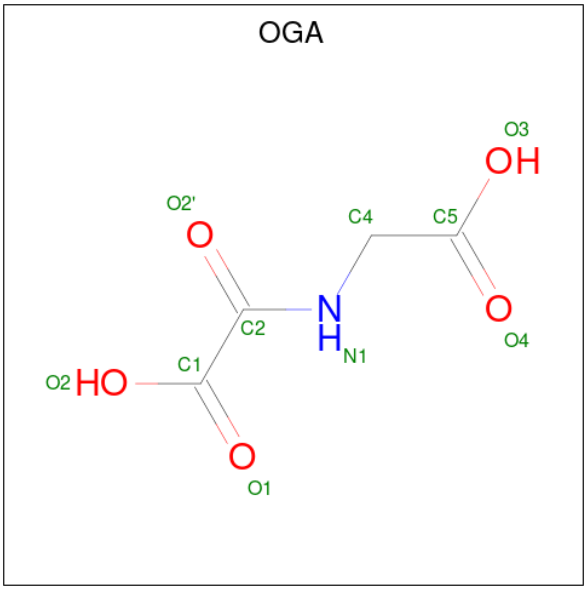
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

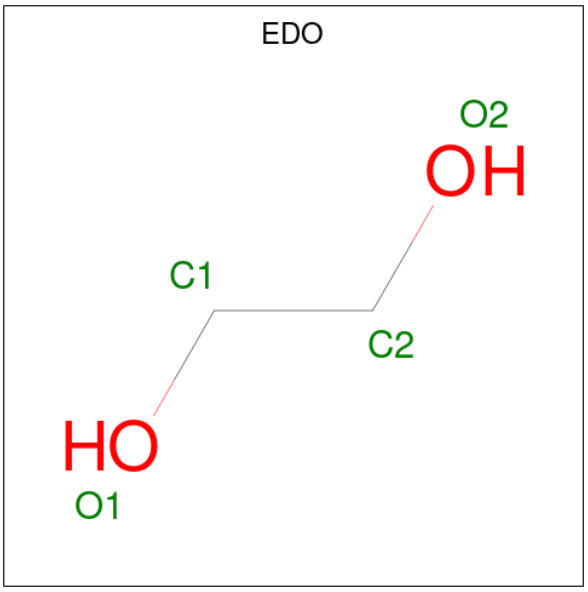
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is N-OXALYLGLYCINE (CCD ID: OGA) (formula: $C_4H_5NO_5$).



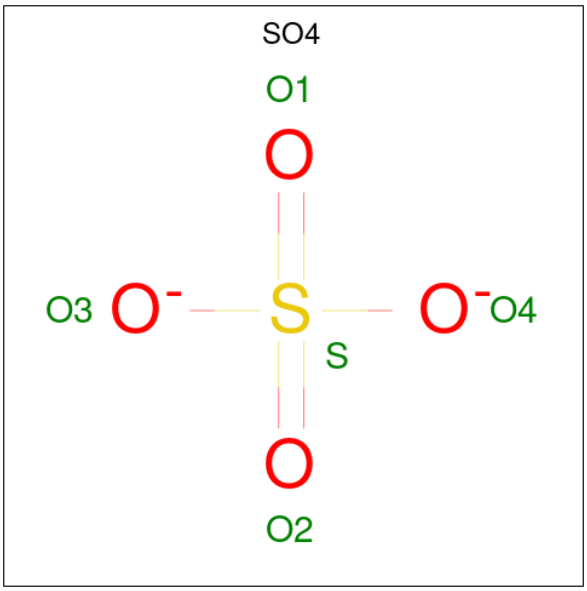
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 10 4 1 5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

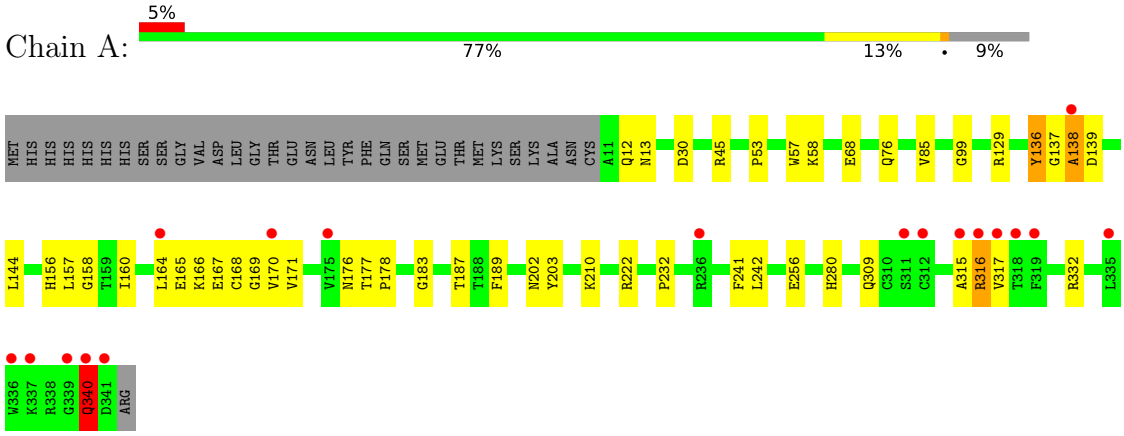
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	441	Total O 442 442	0	8

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: Lysine-specific demethylase 4D



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	71.45Å 71.45Å 150.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 1.27 29.41 – 1.27	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.41-1.27) 95.9 (29.41-1.27)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.27Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.157 , 0.176 0.166 , 0.184	Depositor DCC
R_{free} test set	5097 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.4	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	3384	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: MG, OGA, EDO, SO4, ZN, NI

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	1.73	34/2985 (1.1%)	1.43	10/4043 (0.2%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLN	CG-CD	12.17	1.82	1.52
1	A	53	PRO	CA-C	8.14	1.56	1.51
1	A	177	THR	C-O	-7.60	1.16	1.24
1	A	309	GLN	N-CA	-7.49	1.36	1.46
1	A	138	ALA	CA-C	-7.38	1.43	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	GLN	CG-CD-NE2	-25.04	78.84	116.40
1	A	340	GLN	CG-CD-OE1	17.73	156.26	120.80
1	A	340	GLN	CA-CB-CG	8.93	131.95	114.10
1	A	53	PRO	O-C-N	8.30	125.13	121.31
1	A	340	GLN	CB-CG-CD	-6.91	100.86	112.60

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	2882	0	2746	35	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	3	1	0
6	A	32	0	47	5	0
7	A	15	0	0	0	0
8	A	442	0	0	4	2
All	All	3384	0	2796	35	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 6.

The worst 5 of 35 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:136[B]:TYR:CE2	1:A:138:ALA:HB2	2.02	0.95
1:A:242:LEU:HB2	6:A:407:EDO:H22	1.58	0.84
1:A:168[B]:CYS:SG	1:A:170:VAL:HG12	2.18	0.82
1:A:136[A]:TYR:CD2	1:A:187[A]:THR:HG23	2.20	0.76
1:A:176[B]:ASN:HB3	8:A:608:HOH:O	1.84	0.76

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)
8:A:537:HOH:O	8:A:829:HOH:O[3_544]	2.06	0.14
8:A:510:HOH:O	8:A:674:HOH:O[7_555]	2.17	0.03

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	356/364 (98%)	349 (98%)	6 (2%)	1 (0%)	36 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ARG

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	301/312 (96%)	299 (99%)	2 (1%)	76 49

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	340	GLN

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	12	GLN
1	A	65	ASN
1	A	106	ASN
1	A	128	ASN
1	A	340	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
7	SO4	A	414	-	4,4,4	0.75	0	6,6,6	0.93	0
6	EDO	A	409	-	3,3,3	0.84	0	2,2,2	1.00	0
6	EDO	A	412	-	3,3,3	0.90	0	2,2,2	1.29	0
5	OGA	A	404	3	9,9,9	2.47	3 (33%)	8,11,11	1.31	1 (12%)
6	EDO	A	405	-	3,3,3	0.97	0	2,2,2	0.07	0
7	SO4	A	415	-	4,4,4	0.49	0	6,6,6	0.81	0
6	EDO	A	407	-	3,3,3	0.77	0	2,2,2	2.14	1 (50%)
6	EDO	A	406	-	3,3,3	0.30	0	2,2,2	0.75	0
6	EDO	A	411	-	3,3,3	0.49	0	2,2,2	0.33	0
6	EDO	A	408	-	3,3,3	0.64	0	2,2,2	0.31	0
6	EDO	A	410	-	3,3,3	0.61	0	2,2,2	0.42	0
7	SO4	A	413	-	4,4,4	0.50	0	6,6,6	0.50	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
6	EDO	A	409	-	-	1/1/1/1	-
6	EDO	A	412	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OGA	A	404	3	-	0/8/9/9	-
6	EDO	A	405	-	-	0/1/1/1	-
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	A	406	-	-	1/1/1/1	-
6	EDO	A	411	-	-	0/1/1/1	-
6	EDO	A	408	-	-	1/1/1/1	-
6	EDO	A	410	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	OGA	C2-C1	-5.44	1.47	1.54
5	A	404	OGA	O2'-C2	3.61	1.30	1.23
5	A	404	OGA	C2-N1	-2.22	1.29	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	404	OGA	O2'-C2-C1	-2.92	117.51	121.36
6	A	407	EDO	O2-C2-C1	2.88	134.31	112.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	EDO	O1-C1-C2-O2
6	A	409	EDO	O1-C1-C2-O2
6	A	407	EDO	O1-C1-C2-O2
6	A	406	EDO	O1-C1-C2-O2
6	A	412	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	OGA	1	0
6	A	407	EDO	2	0
6	A	408	EDO	1	0
6	A	410	EDO	2	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	331/364 (90%)	0.09	18 (5%) 31 34	5, 12, 26, 71	28 (8%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236[A]	ARG	6.0
1	A	317	VAL	5.7
1	A	319[A]	PHE	5.2
1	A	341	ASP	3.9
1	A	318	THR	3.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides 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
6	EDO	A	412	4/4	0.84	0.14	28,29,33,39	0
6	EDO	A	410	4/4	0.85	0.17	28,29,30,33	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	411	4/4	0.86	0.13	27,27,28,28	1
6	EDO	A	409	4/4	0.87	0.12	22,23,24,29	2
6	EDO	A	408	4/4	0.87	0.13	26,32,34,37	1
7	SO4	A	415	5/5	0.87	0.11	39,39,41,49	4
6	EDO	A	406	4/4	0.89	0.12	25,32,35,35	0
6	EDO	A	407	4/4	0.89	0.14	22,30,30,31	3
7	SO4	A	414	5/5	0.90	0.10	20,23,28,28	4
7	SO4	A	413	5/5	0.90	0.10	28,32,34,36	5
6	EDO	A	405	4/4	0.93	0.10	18,20,21,23	1
5	OGA	A	404	10/10	0.95	0.07	11,13,16,16	10
2	ZN	A	401	1/1	0.95	0.06	15,15,15,15	0
4	MG	A	403	1/1	0.98	0.10	21,21,21,21	0
3	NI	A	402	1/1	1.00	0.04	10,10,10,10	1

6.5 Other polymers (i)

There are no such residues in this entry.