Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2024 – 10:11 am BST

PDB ID	:	9GLE
Title	:	Jumonji domain-containing protein 2A with crystallization epitope mutations A91T:T93S
Authors	:	Fairhead, M.; Strain-Damerell, C.; Ye, M.; Mackinnon, S.R.; Pinkas, D.; MacLean, E.M.; Koekemoer, L.; Damerell, D.; Krojer, T.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Yue, W.; Burgess-Brown, N.; Marsden, B.; von Delft, F.; Structural Genomics Consortium (SGC)
Deposited on	:	2024-08-27
Resolution	:	1.88 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:

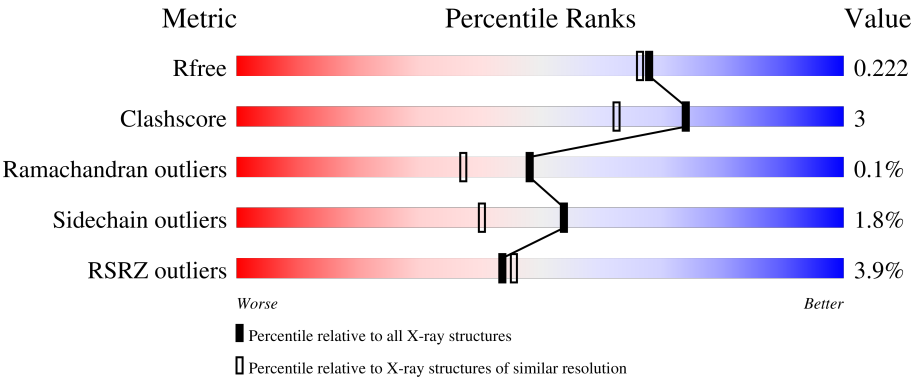
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.88 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}	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	360	4% 87% 7%
1	B	360	3% 89% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11239 atoms, of which 5155 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 4A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	345	Total	C	H	N	O	S	0	11	0
			5466	1834	2633	472	511	16			
1	B	341	Total	C	H	N	O	S	0	8	0
			5250	1782	2498	452	502	16			

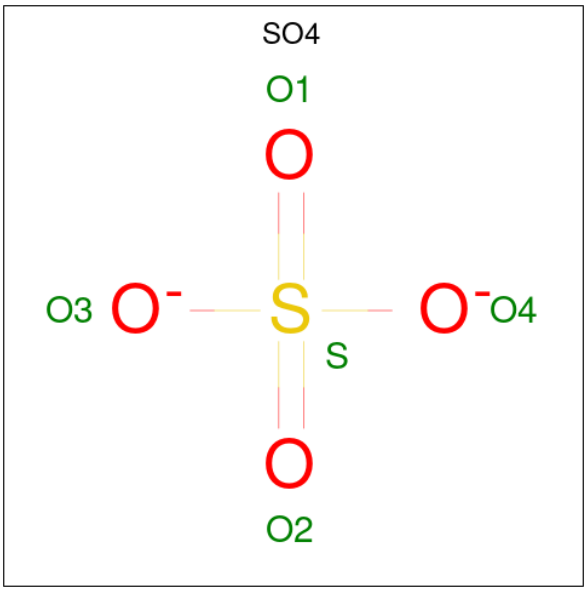
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O75164
A	92	THR	ALA	engineered mutation	UNP O75164
A	94	SER	THR	engineered mutation	UNP O75164
B	1	SER	-	expression tag	UNP O75164
B	92	THR	ALA	engineered mutation	UNP O75164
B	94	SER	THR	engineered mutation	UNP O75164

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		

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

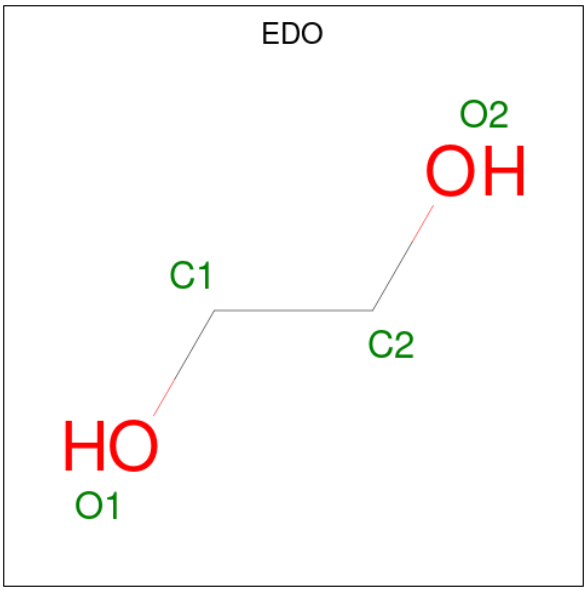


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 8 2 4 2	0	0
5	A	1	Total C H O 8 2 4 2	0	0
5	A	1	Total C H O 8 2 4 2	0	0
5	A	1	Total C H O 8 2 4 2	0	0
5	A	1	Total C H O 8 2 4 2	0	0
5	B	1	Total C H O 8 2 4 2	0	0

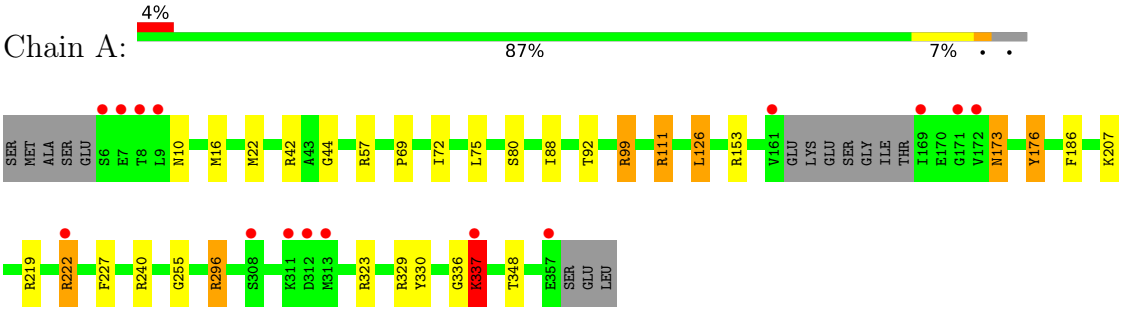
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	254	Total O 254 254	0	0
6	B	192	Total O 192 192	0	0

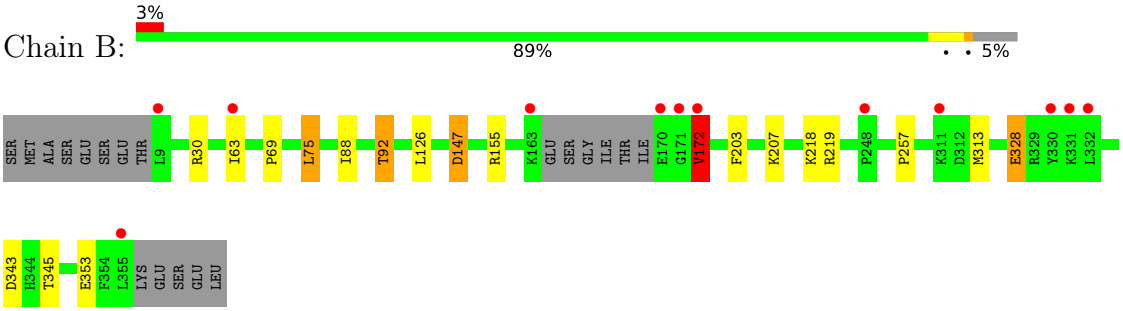
3 Residue-property plots (i)

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: Lysine-specific demethylase 4A



• Molecule 1: Lysine-specific demethylase 4A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.70Å 90.78Å 90.67Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	40.45 – 1.88 40.45 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.45-1.88) 99.4 (40.45-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.77)	Depositor
R, R_{free}	0.185 , 0.222 0.185 , 0.222	Depositor DCC
R_{free} test set	3667 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11239	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: SO4, EDO, NI, ZN

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	0.67	0/2957	1.13	18/4017 (0.4%)
1	B	0.63	0/2872	1.01	2/3909 (0.1%)
All	All	0.65	0/5829	1.07	20/7926 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ARG	NE-CZ-NH2	-18.13	111.23	120.30
1	A	99	ARG	NE-CZ-NH1	17.83	129.22	120.30
1	A	176	TYR	CB-CG-CD1	8.22	125.93	121.00
1	A	176	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	240	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	111	ARG	CD-NE-CZ	6.64	132.90	123.60
1	A	111	ARG	CG-CD-NE	6.61	125.69	111.80
1	A	240	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	176	TYR	CA-CB-CG	5.57	123.98	113.40
1	A	22[A]	MET	CG-SD-CE	-5.57	91.29	100.20
1	A	22[B]	MET	CG-SD-CE	-5.57	91.29	100.20
1	A	337	LYS	CD-CE-NZ	-5.51	99.03	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	A	57	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	328	GLU	CB-CA-C	-5.24	99.92	110.40
1	B	92	THR	CA-C-N	5.22	128.68	117.20
1	A	42	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	222[A]	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	222[B]	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	99	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	155[A]	ARG	Sidechain

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	2833	2633	2652	18	3
1	B	2752	2498	2530	15	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	0	0	0
3	B	10	0	0	2	3
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	20	30	0	0
5	B	4	4	6	0	0
6	A	254	0	0	4	0
6	B	192	0	0	4	0
All	All	6084	5155	5218	33	6

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 3.

All (33) 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:207:LYS:HE2	6:A:520:HOH:O	1.62	0.97
1:B:207:LYS:HE2	6:B:509:HOH:O	1.80	0.82
1:B:218:LYS:HB2	3:B:403:SO4:O2	1.85	0.76
1:B:75:LEU:HD13	1:B:88:ILE:HG13	1.83	0.60
1:A:336:GLY:C	1:A:337:LYS:HG3	2.25	0.56
1:A:72:ILE:HD11	6:A:616:HOH:O	2.04	0.56
1:B:63:ILE:HD13	1:B:203:PHE:CE2	2.43	0.54
1:A:222[A]:ARG:HG2	1:A:222[A]:ARG:HH11	1.74	0.53
1:B:147:ASP:OD1	6:B:501:HOH:O	2.19	0.52
1:B:30[A]:ARG:NH1	1:B:353:GLU:OE2	2.44	0.51
1:B:172:VAL:HA	6:B:607:HOH:O	2.11	0.50
1:B:126:LEU:H	1:B:126:LEU:HD23	1.78	0.49
1:B:63:ILE:HD13	1:B:203:PHE:HE2	1.79	0.47
1:B:218:LYS:CB	3:B:403:SO4:O2	2.62	0.47
1:A:173[A]:ASN:HD22	1:A:173[A]:ASN:HA	1.51	0.46
1:A:126[A]:LEU:N	1:A:126[A]:LEU:HD23	2.31	0.46
1:A:126[A]:LEU:HD23	1:A:126[A]:LEU:H	1.80	0.46
1:A:219:ARG:NH1	1:A:255:GLY:O	2.50	0.45
1:B:343:ASP:OD1	1:B:345:THR:OG1	2.28	0.44
1:B:126:LEU:HD23	1:B:126:LEU:N	2.32	0.44
1:A:80:SER:N	6:A:509:HOH:O	2.52	0.43
1:A:126[A]:LEU:H	1:A:126[A]:LEU:CD2	2.31	0.43
1:A:296:ARG:HB2	1:A:348:THR:HA	2.00	0.43
1:A:10:ASN:HB2	1:A:16:MET:HE1	1.99	0.43
1:A:323:ARG:HG3	1:A:330:TYR:CE1	2.54	0.43
1:B:69:PRO:HA	1:B:92:THR:HG23	1.99	0.43
1:B:313:MET:HE3	6:B:567:HOH:O	2.19	0.42
1:A:75[A]:LEU:HD22	1:A:88:ILE:HD11	2.01	0.42
1:A:44:GLY:HA3	6:A:615:HOH:O	2.21	0.41
1:B:219:ARG:NH2	1:B:257:PRO:HD3	2.36	0.41
1:A:186:PHE:CE1	1:A:207:LYS:HD3	2.56	0.41
1:A:69:PRO:HA	1:A:92:THR:HG23	2.02	0.40

All (6) 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)
3:B:403:SO4:O3	3:B:403:SO4:O3[2_655]	1.05	1.15
1:A:337:LYS:NZ	1:B:92:THR:O[2_555]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:403:SO4:O1	3:B:403:SO4:O1[2_655]	1.75	0.45
3:B:403:SO4:S	3:B:403:SO4:O3[2_655]	1.96	0.24
1:A:337:LYS:HZ3	1:B:92:THR:O[2_555]	1.37	0.23
1:A:337:LYS:HZ2	1:B:92:THR:O[2_555]	1.41	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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	352/360 (98%)	347 (99%)	5 (1%)	0	100 100
1	B	345/360 (96%)	337 (98%)	7 (2%)	1 (0%)	37 26
All	All	697/720 (97%)	684 (98%)	12 (2%)	1 (0%)	48 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	VAL

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	298/317 (94%)	290 (97%)	8 (3%)	40 24
1	B	284/317 (90%)	280 (99%)	4 (1%)	62 52
All	All	582/634 (92%)	570 (98%)	12 (2%)	54 34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	126[A]	LEU
1	A	126[B]	LEU
1	A	173[A]	ASN
1	A	173[B]	ASN
1	A	176	TYR
1	A	296	ARG
1	A	337	LYS
1	B	75	LEU
1	B	147	ASP
1	B	172	VAL
1	B	328	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	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, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.58	0
5	EDO	A	407	-	3,3,3	0.14	0	2,2,2	0.50	0
5	EDO	B	405	-	3,3,3	0.58	0	2,2,2	0.91	0
5	EDO	A	410	-	3,3,3	0.33	0	2,2,2	0.43	0
3	SO4	B	402	-	4,4,4	0.29	0	6,6,6	0.13	0
5	EDO	A	409	-	3,3,3	0.33	0	2,2,2	0.15	0
5	EDO	A	406	-	3,3,3	0.16	0	2,2,2	0.05	0
3	SO4	B	403	-	4,4,4	0.28	0	6,6,6	0.59	0
3	SO4	A	404	-	4,4,4	0.46	0	6,6,6	0.36	0
3	SO4	A	402	-	4,4,4	0.53	0	6,6,6	0.22	0
3	SO4	A	403	-	4,4,4	0.37	0	6,6,6	0.13	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
5	EDO	A	408	-	-	1/1/1/1	-
5	EDO	A	407	-	-	1/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	A	410	-	-	0/1/1/1	-
5	EDO	A	409	-	-	1/1/1/1	-
5	EDO	A	406	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	409	EDO	O1-C1-C2-O2
5	A	408	EDO	O1-C1-C2-O2
5	A	407	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	SO4	2	3

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	345/360 (95%)	-0.10	15 (4%)	40	42	16, 34, 64, 89	6 (1%)
1	B	341/360 (94%)	0.30	12 (3%)	47	50	16, 39, 69, 88	4 (1%)
All	All	686/720 (95%)	0.10	27 (3%)	44	46	16, 37, 68, 89	10 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	GLY	5.4
1	A	169	ILE	4.5
1	B	163	LYS	4.4
1	B	9	LEU	4.3
1	B	170	GLU	3.3
1	A	337	LYS	3.2
1	A	308	SER	3.1
1	B	63	ILE	3.1
1	A	171	GLY	3.1
1	B	172	VAL	3.0
1	B	355	LEU	3.0
1	A	312	ASP	3.0
1	A	9	LEU	2.9
1	A	7	GLU	2.8
1	A	311	LYS	2.8
1	A	357	GLU	2.7
1	A	161	VAL	2.5
1	A	313	MET	2.5
1	B	330	TYR	2.4
1	A	222[A]	ARG	2.4
1	B	331	LYS	2.3
1	B	311	LYS	2.2
1	A	172	VAL	2.2
1	A	8	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	248	PRO	2.1
1	A	6	SER	2.1
1	B	332	LEU	2.1

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

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

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	B-factors(Å^2)	Q<0.9
5	EDO	B	405	4/4	0.83	0.19	60,64,64,67	0
5	EDO	A	408	4/4	0.86	0.12	55,57,59,67	0
3	SO4	B	402	5/5	0.87	0.09	56,65,74,83	0
5	EDO	A	406	4/4	0.90	0.14	38,55,57,62	0
5	EDO	A	409	4/4	0.91	0.15	45,54,55,57	0
3	SO4	A	404	5/5	0.92	0.09	52,57,65,80	0
5	EDO	A	407	4/4	0.93	0.10	45,47,54,56	0
5	EDO	A	410	4/4	0.93	0.10	49,55,58,60	0
3	SO4	B	403	5/5	0.93	0.17	51,61,89,95	1
3	SO4	A	403	5/5	0.94	0.06	54,58,74,79	0
3	SO4	A	402	5/5	0.98	0.05	46,48,51,53	0
4	ZN	A	405	1/1	0.98	0.04	38,38,38,38	0
4	ZN	B	404	1/1	0.99	0.02	39,39,39,39	0
2	NI	B	401	1/1	1.00	0.02	31,31,31,31	0
2	NI	A	401	1/1	1.00	0.04	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.