



Full wwPDB X-ray Structure Validation Report

Apr 2, 2014 – 04:46 PM EDT

PDB ID : 3FD2
Title : Crystal structure of mMsoI/DNA complex with calcium
Authors : Li, H.; Monnat, R.J.
Deposited on : 2008-11-24
Resolution : 2.69 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

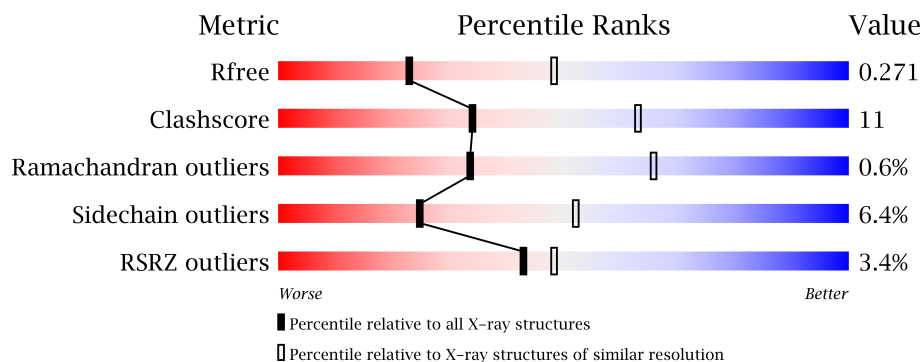
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.69 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	373	
2	B	24	
3	C	24	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3735 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA ENDONUCLEASE I-MSOI, linker, DNA ENDONUCLEASE I-MSOI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	0	0	0
			2720	1744	470	506			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	THR	-	SEE REMARK 999	UNP Q8WKW7
A	172	GLY	-	SEE REMARK 999	UNP Q8WKW7
A	173	SER	-	SEE REMARK 999	UNP Q8WKW7
A	174	GLY	-	SEE REMARK 999	UNP Q8WKW7
A	175	SER	-	SEE REMARK 999	UNP Q8WKW7
A	176	GLY	-	SEE REMARK 999	UNP Q8WKW7
A	177	SER	-	SEE REMARK 999	UNP Q8WKW7
A	178	LYS	-	SEE REMARK 999	UNP Q8WKW7
A	179	HIS	-	SEE REMARK 999	UNP Q8WKW7
A	180	PRO	-	SEE REMARK 999	UNP Q8WKW7
A	181	THR	-	SEE REMARK 999	UNP Q8WKW7
A	182	LEU	-	SEE REMARK 999	UNP Q8WKW7
A	183	THR	-	SEE REMARK 999	UNP Q8WKW7
A	184	LEU	-	SEE REMARK 999	UNP Q8WKW7
A	185	PRO	-	SEE REMARK 999	UNP Q8WKW7
A	186	THR	-	SEE REMARK 999	UNP Q8WKW7
A	187	THR	-	SEE REMARK 999	UNP Q8WKW7
A	188	THR	-	SEE REMARK 999	UNP Q8WKW7
A	189	SER	-	SEE REMARK 999	UNP Q8WKW7
A	190	GLN	-	SEE REMARK 999	UNP Q8WKW7
A	191	GLU	-	SEE REMARK 999	UNP Q8WKW7
A	192	ASN	-	SEE REMARK 999	UNP Q8WKW7
A	193	LEU	-	SEE REMARK 999	UNP Q8WKW7
A	194	PRO	-	SEE REMARK 999	UNP Q8WKW7
A	195	ASN	-	SEE REMARK 999	UNP Q8WKW7
A	196	GLY	-	SEE REMARK 999	UNP Q8WKW7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	SER	-	SEE REMARK 999	UNP Q8WKW7
A	198	GLY	-	SEE REMARK 999	UNP Q8WKW7
A	199	SER	-	SEE REMARK 999	UNP Q8WKW7
A	200	GLY	-	SEE REMARK 999	UNP Q8WKW7
A	201	SER	-	SEE REMARK 999	UNP Q8WKW7
A	202	GLY	-	SEE REMARK 999	UNP Q8WKW7
A	203	THR	-	SEE REMARK 999	UNP Q8WKW7

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*AP*GP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP*CP*AP*GP*TP*TP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	P	0	0	0
			493	234	96	140	23			

- Molecule 3 is a DNA chain called 5'-D(*CP*GP*GP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP*CP*GP*TP*TP*CP*TP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	24	Total	C	N	O	P	0	0	0
			485	232	86	144	23			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

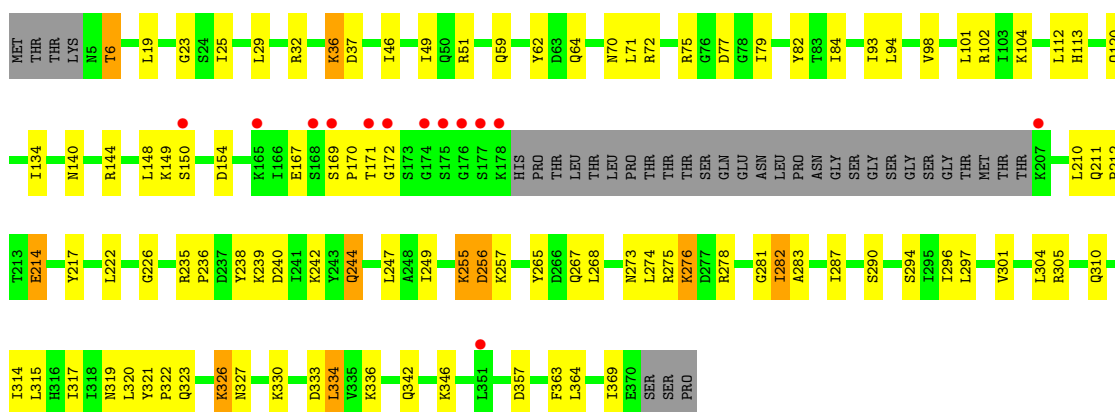
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	7	Total	O	0	0
			7	7		
5	C	8	Total	O	0	0
			8	8		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

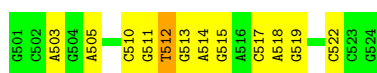
- Molecule 1: DNA ENDONUCLEASE I-MSOI, linker, DNA ENDONUCLEASE I-MSOI

Chain A: 



- Molecule 2: 5'-D(*GP*CP*AP*GP*AP*AP*CP*GP*TP*CP*GP*TP*GP*AP*GP*AP*CP*A P*GP*TP*TP*CP*CP*G)-3'

Chain B: 



- Molecule 3: 5'-D(*CP*GP*GP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*CP*GP*AP*CP*G P*TP*TP*CP*TP*GP*C)-3'

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.93Å 41.93Å 70.96Å 107.21° 95.43° 109.44°	Depositor
Resolution (Å)	50.00 – 2.69 30.54 – 2.69	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.69) 96.5 (30.54-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.281 0.212 , 0.271	Depositor DCC
R_{free} test set	546 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.2	EDS
Estimated twinning fraction	0.468 for k,h,-h-k-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 11406 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3735	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.43	3/2769 (0.1%)	0.55	1/3733 (0.0%)
2	B	0.67	0/554	1.27	5/854 (0.6%)
3	C	0.66	0/542	1.35	7/834 (0.8%)
All	All	0.51	3/3865 (0.1%)	0.86	13/5421 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	ASP	CG-OD2	7.51	1.42	1.25
1	A	154	ASP	CG-OD2	6.44	1.40	1.25
1	A	167	GLU	CD-OE1	5.61	1.31	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	512	DT	O4'-C1'-N1	7.25	113.08	108.00
3	C	562	DC	O4'-C1'-N1	7.03	112.92	108.00
3	C	553	DG	O4'-C1'-N9	6.33	112.43	108.00
2	B	522	DC	O4'-C1'-N1	6.15	112.30	108.00
3	C	570	DT	O4'-C1'-N1	6.12	112.29	108.00
3	C	556	DC	P-O3'-C3'	5.47	126.27	119.70
2	B	503	DA	O4'-C1'-N9	5.40	111.78	108.00
2	B	514	DA	C3'-C2'-C1'	-5.37	96.05	102.50
3	C	570	DT	C1'-O4'-C4'	-5.29	104.81	110.10
2	B	512	DT	C6-C5-C7	-5.16	119.80	122.90
3	C	569	DT	C6-C5-C7	-5.12	119.83	122.90
3	C	570	DT	C3'-C2'-C1'	-5.11	96.37	102.50
1	A	154	ASP	CB-CG-OD1	-5.04	113.77	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2720	0	2806	65	0
2	B	493	0	270	11	0
3	C	485	0	272	12	0
4	A	2	0	0	0	0
5	A	20	0	0	2	0
5	B	7	0	0	0	0
5	C	8	0	0	0	0
All	All	3735	0	3348	77	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (77) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:THR:HB	1:A:172:GLY:HA3	1.36	1.08
1:A:211:GLN:HE21	1:A:214:GLU:HG3	1.28	0.96
1:A:140:ASN:HD21	1:A:150:SER:H	1.21	0.89
1:A:171:THR:HB	1:A:172:GLY:CA	2.06	0.85
1:A:49:ILE:HD13	2:B:515:DG:H8	1.48	0.77
1:A:249:ILE:HD11	1:A:287:ILE:HD12	1.68	0.76
1:A:211:GLN:NE2	1:A:214:GLU:HG3	2.00	0.76
2:B:518:DA:H2"	2:B:519:DG:H5"	1.67	0.76
2:B:519:DG:H1	3:C:556:DC:H42	1.36	0.74
1:A:32:ARG:HH22	3:C:554:DA:H62	1.37	0.69
1:A:64:GLN:HE22	1:A:305:ARG:HH12	1.40	0.69
1:A:333:ASP:HA	1:A:336:LYS:HE3	1.76	0.68
1:A:222:LEU:HD23	1:A:304:LEU:HD21	1.77	0.66
1:A:265:TYR:CD1	1:A:274:LEU:HD11	2.33	0.63
1:A:46:ILE:HD11	1:A:84:ILE:HD12	1.82	0.62
1:A:98:VAL:HA	1:A:101:LEU:HD12	1.80	0.62
1:A:102:ARG:HH22	1:A:267:GLN:HE22	1.49	0.61
2:B:512:DT:H2"	2:B:513:DG:C8	2.37	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:ARG:HG2	1:A:282:ILE:O	2.03	0.58
1:A:287:ILE:HD13	1:A:296:ILE:HD13	1.87	0.56
1:A:19:LEU:HD23	1:A:101:LEU:HD21	1.87	0.56
1:A:235:ARG:HH21	1:A:244:GLN:NE2	2.03	0.56
1:A:326:LYS:H	1:A:326:LYS:HD2	1.70	0.56
1:A:113:HIS:HD2	1:A:134:ILE:HD13	1.71	0.56
3:C:562:DC:H2"	3:C:563:DA:C8	2.41	0.55
1:A:49:ILE:HD13	2:B:515:DG:C8	2.37	0.55
1:A:222:LEU:HD12	1:A:226:GLY:HA3	1.89	0.55
1:A:273:ASN:ND2	2:B:505:DA:H3'	2.22	0.55
1:A:51:ARG:HA	1:A:79:ILE:HD12	1.89	0.55
1:A:140:ASN:ND2	1:A:150:SER:H	1.97	0.54
1:A:363:PHE:HB3	1:A:369:ILE:HG12	1.90	0.54
1:A:238:TYR:HB2	1:A:242:LYS:HA	1.91	0.53
2:B:519:DG:H1	3:C:556:DC:N4	2.06	0.52
1:A:290:SER:O	1:A:294:SER:OG	2.22	0.50
1:A:320:LEU:HD12	1:A:334:LEU:HD12	1.93	0.50
2:B:510:DC:H42	3:C:565:DG:H1	1.58	0.50
1:A:211:GLN:HB2	1:A:212:PRO:HD2	1.92	0.49
2:B:518:DA:C2'	2:B:519:DG:H5"	2.41	0.49
1:A:32:ARG:HH22	3:C:554:DA:N6	2.09	0.48
1:A:323:GLN:HG2	5:A:382:HOH:O	2.13	0.48
1:A:210:LEU:HD11	1:A:268:LEU:HD23	1.95	0.47
1:A:36:LYS:HD2	1:A:37:ASP:HB2	1.96	0.47
1:A:171:THR:CB	1:A:172:GLY:CA	2.85	0.47
1:A:211:GLN:HE21	1:A:214:GLU:CG	2.13	0.46
1:A:36:LYS:HB3	1:A:36:LYS:NZ	2.29	0.46
1:A:297:LEU:O	1:A:301:VAL:HG23	2.16	0.46
3:C:551:DC:H2'	3:C:552:DG:C8	2.51	0.46
1:A:342:GLN:O	1:A:346:LYS:HE2	2.15	0.46
1:A:71:LEU:HD23	1:A:82:TYR:HB2	1.98	0.46
1:A:19:LEU:HD12	1:A:23:GLY:HA3	1.98	0.45
1:A:77:ASP:OD2	1:A:77:ASP:N	2.48	0.45
1:A:169:SER:HA	1:A:170:PRO:HD3	1.87	0.44
1:A:276:LYS:H	1:A:276:LYS:CD	2.30	0.44
1:A:255:LYS:HB3	1:A:281:GLY:O	2.18	0.44
1:A:265:TYR:CG	1:A:274:LEU:HD11	2.53	0.44
1:A:62:TYR:HD1	1:A:82:TYR:CE1	2.35	0.44
1:A:282:ILE:HD12	3:C:564:DC:H5	1.82	0.44
1:A:102:ARG:HD2	1:A:217:TYR:CZ	2.53	0.43
1:A:72:ARG:CZ	3:C:557:DT:H72	2.48	0.43
1:A:84:ILE:HD13	1:A:93:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:256:ASP:OD1	1:A:257:LYS:HG3	2.19	0.43
1:A:321:TYR:N	1:A:322:PRO:HD2	2.33	0.43
1:A:25:ILE:HD12	1:A:104:LYS:HB3	2.01	0.43
1:A:247:LEU:HD21	1:A:317:ILE:HG21	2.02	0.42
1:A:244:GLN:HE21	1:A:244:GLN:HB3	1.52	0.42
5:A:395:HOH:O	3:C:565:DG:H5'	2.19	0.42
1:A:72:ARG:CZ	1:A:75:ARG:HB2	2.50	0.42
1:A:94:LEU:O	1:A:98:VAL:HG23	2.20	0.42
2:B:517:DC:H2'	2:B:518:DA:C8	2.53	0.42
1:A:239:LYS:HG3	1:A:240:ASP:N	2.35	0.42
3:C:551:DC:H2'	3:C:552:DG:H8	1.85	0.42
1:A:310:GLN:O	1:A:314:ILE:HG12	2.20	0.41
1:A:275:ARG:O	1:A:283:ALA:HB1	2.20	0.41
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.98	0.41
1:A:144:ARG:HD3	3:C:563:DA:OP1	2.21	0.41
1:A:327:ASN:HD22	1:A:330:LYS:HD2	1.87	0.40
2:B:510:DC:H2''	2:B:511:DG:O5'	2.21	0.40

There are no symmetry-related clashes.

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	334/373 (90%)	305 (91%)	27 (8%)	2 (1%)	33	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	236	PRO

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	297/328 (90%)	278 (94%)	19 (6%)	25 52

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	29	LEU
1	A	36	LYS
1	A	59	GLN
1	A	70	ASN
1	A	120	GLN
1	A	148	LEU
1	A	149	LYS
1	A	214	GLU
1	A	244	GLN
1	A	255	LYS
1	A	256	ASP
1	A	276	LYS
1	A	282	ILE
1	A	315	LEU
1	A	319	ASN
1	A	326	LYS
1	A	334	LEU
1	A	364	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	109	ASN
1	A	113	HIS
1	A	122	GLN
1	A	140	ASN
1	A	211	GLN
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	267	GLN
1	A	273	ASN
1	A	327	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 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, 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	338/373 (90%)	0.16	13 (3%)	38	43	45, 52, 64, 76	0
2	B	24/24 (100%)	-0.20	0	100	100	64, 74, 92, 98	0
3	C	24/24 (100%)	-0.26	0	100	100	61, 79, 87, 90	0
All	All	386/421 (91%)	0.11	13 (3%)	43	48	45, 53, 79, 98	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	12.5
1	A	168	SER	8.0
1	A	172	GLY	7.8
1	A	177	SER	7.6
1	A	178	LYS	5.8
1	A	171	THR	4.7
1	A	175	SER	4.2
1	A	165	LYS	4.0
1	A	174	GLY	3.8
1	A	207	LYS	2.7
1	A	169	SER	2.6
1	A	351	LEU	2.5
1	A	150	SER	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	A	375	1/1	0.15	0.46	50,50,50,50	0
4	CA	A	374	1/1	0.09	-3.31	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.