



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7A40 / pdb_00007a40
Title : Nucleotide-free OSM-3 kinesin motor domain
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Deposited on : 2020-08-19
Resolution : 2.30 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

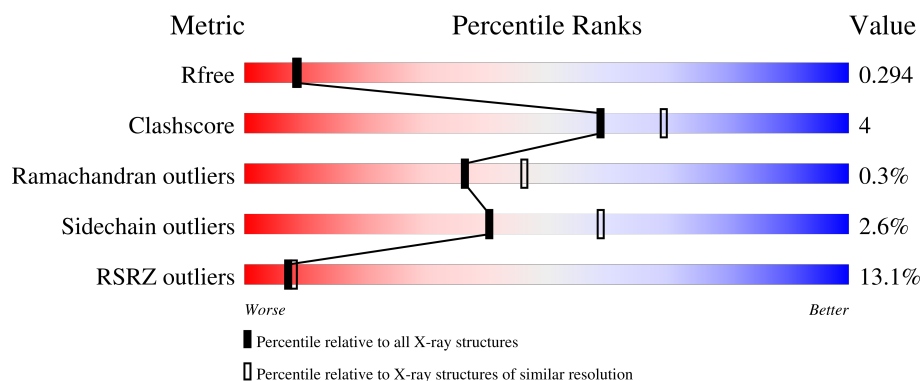
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	346	 13% 79% 11% 10%
1	B	346	 11% 80% 11% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4633 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 Osmotic avoidance abnormal protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2276	1413	390	461	12			
1	B	315	Total	C	N	O	S	0	0	0
			2270	1411	394	453	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P46873
A	1	ALA	-	expression tag	UNP P46873
A	338	LEU	-	expression tag	UNP P46873
A	339	GLU	-	expression tag	UNP P46873
A	340	HIS	-	expression tag	UNP P46873
A	341	HIS	-	expression tag	UNP P46873
A	342	HIS	-	expression tag	UNP P46873
A	343	HIS	-	expression tag	UNP P46873
A	344	HIS	-	expression tag	UNP P46873
A	345	HIS	-	expression tag	UNP P46873
B	0	MET	-	initiating methionine	UNP P46873
B	1	ALA	-	expression tag	UNP P46873
B	338	LEU	-	expression tag	UNP P46873
B	339	GLU	-	expression tag	UNP P46873
B	340	HIS	-	expression tag	UNP P46873
B	341	HIS	-	expression tag	UNP P46873
B	342	HIS	-	expression tag	UNP P46873
B	343	HIS	-	expression tag	UNP P46873
B	344	HIS	-	expression tag	UNP P46873
B	345	HIS	-	expression tag	UNP P46873

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total 31	O 31	0	0
4	B	34	Total 34	O 34	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.77Å 155.18Å 63.72Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	47.59 – 2.30 47.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.59-2.30) 99.6 (47.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.225 , 0.254 (Not available) , 0.294	Depositor DCC
R_{free} test set	1740 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4633	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.77	0/2310	1.11	5/3145 (0.2%)
1	B	0.77	0/2304	1.11	1/3137 (0.0%)
All	All	0.77	0/4614	1.11	6/6282 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASN	CA-CB-CG	6.86	119.46	112.60
1	A	129	PHE	N-CA-C	6.17	119.54	109.24
1	A	231	VAL	N-CA-C	5.71	116.32	107.99
1	B	32	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	118	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	67	ILE	N-CA-C	5.53	116.32	111.56

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	2276	0	2100	23	0
1	B	2270	0	2092	16	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	31	0	0	0	0
4	B	34	0	0	0	0
All	All	4633	0	4208	39	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 4.

All (39) 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:23:THR:HG21	1:A:307:SER:HB2	1.30	1.10
1:A:23:THR:CG2	1:A:307:SER:HB2	2.04	0.86
1:A:84:PHE:HB3	1:A:231:VAL:HB	1.65	0.78
1:A:0:MET:HA	1:A:332:THR:HG22	1.73	0.69
1:A:110:ILE:HG12	1:A:230:LEU:HD13	1.75	0.69
1:A:84:PHE:CB	1:A:231:VAL:HB	2.25	0.65
1:A:130:LEU:HD21	1:A:132:HIS:NE2	2.12	0.65
1:A:71:LEU:HD22	1:A:299:ILE:HD12	1.81	0.62
1:A:270:VAL:HG21	1:A:323:ARG:HG2	1.81	0.61
1:B:97:MET:HA	1:B:109:VAL:HG22	1.85	0.59
1:B:255:ILE:HG13	1:B:256:ASN:H	1.69	0.58
1:A:6:ARG:HD3	1:A:67:ILE:HD12	1.86	0.56
1:B:72:VAL:HB	1:B:116:HIS:CE1	2.40	0.56
1:B:71:LEU:HD22	1:B:299:ILE:HD12	1.89	0.54
1:A:38:LEU:HD23	1:A:315:LEU:HD13	1.92	0.51
1:B:6:ARG:HE	2:B:401:GOL:H31	1.76	0.51
1:B:257:LEU:HA	1:B:260:SER:HB2	1.94	0.50
1:A:207:HIS:HE1	1:A:259:LEU:HG	1.78	0.49
1:A:305:SER:OG	1:A:310:ASN:ND2	2.43	0.48
1:A:222:SER:HB3	1:A:337:PRO:HA	1.94	0.48
1:A:15:ASN:O	1:A:16:GLN:C	2.56	0.47
1:A:118:PHE:HE2	1:A:181:CYS:SG	2.38	0.47
1:B:84:PHE:CB	1:B:231:VAL:HB	2.45	0.47
1:B:95:PHE:O	1:B:99:GLY:HA2	2.15	0.47
1:B:6:ARG:HE	2:B:401:GOL:C3	2.28	0.46
1:A:12:ARG:HH12	1:A:15:ASN:ND2	2.14	0.45
1:A:136:LEU:HD11	1:A:209:ILE:HD12	1.98	0.45
1:A:130:LEU:CD2	1:A:132:HIS:NE2	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ARG:HD2	1:A:67:ILE:HG23	2.01	0.43
1:A:12:ARG:NH1	1:A:15:ASN:HD22	2.16	0.42
1:A:336:ASP:HA	1:A:337:PRO:HD3	1.92	0.42
1:B:336:ASP:HA	1:B:337:PRO:HD3	1.86	0.42
1:B:14:PHE:HD1	1:B:18:GLU:HB3	1.84	0.42
1:B:333:ILE:HG22	1:B:335:GLU:HB2	2.02	0.42
1:B:266:ILE:HG23	1:B:327:ILE:HD11	2.01	0.42
1:B:7:VAL:HG11	1:B:321:ALA:HB1	2.02	0.42
1:B:71:LEU:HD11	1:B:297:LYS:HB2	2.01	0.41
1:B:9:VAL:HG22	1:B:302:ALA:HB3	2.03	0.41
1:A:5:VAL:HG22	1:A:298:THR:HB	2.04	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	305/346 (88%)	295 (97%)	9 (3%)	1 (0%)	36	46
1	B	307/346 (89%)	294 (96%)	12 (4%)	1 (0%)	36	46
All	All	612/692 (88%)	589 (96%)	21 (3%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	SER
1	A	168	ALA

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	233/295 (79%)	228 (98%)	5 (2%)	47	66
1	B	228/295 (77%)	221 (97%)	7 (3%)	35	52
All	All	461/590 (78%)	449 (97%)	12 (3%)	40	59

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

Mol	Chain	Res	Type
1	A	109	VAL
1	A	124	THR
1	A	151	ASN
1	A	255	ILE
1	A	257	LEU
1	B	62	GLN
1	B	101	GLU
1	B	124	THR
1	B	153	GLN
1	B	259	LEU
1	B	274	SER
1	B	276	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	37	ASN
1	A	39	ASN
1	A	88	GLN
1	A	264	ASN
1	A	310	ASN
1	B	74	ASN
1	B	151	ASN
1	B	193	HIS

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](#)

4 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	$\# Z > 2$
3	SO4	B	402	-	4,4,4	0.40	0	6,6,6	0.61	0
3	SO4	A	402	-	4,4,4	0.56	0	6,6,6	0.59	0
2	GOL	A	401	-	5,5,5	0.10	0	5,5,5	0.21	0
2	GOL	B	401	-	5,5,5	0.17	0	5,5,5	0.36	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	GOL	A	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	GOL	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, 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	313/346 (90%)	0.99	45 (14%) 6 7	44, 80, 140, 169	0
1	B	315/346 (91%)	0.91	37 (11%) 9 10	52, 83, 132, 152	0
All	All	628/692 (90%)	0.95	82 (13%) 7 8	44, 82, 138, 169	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	PRO	5.3
1	A	185	MET	4.8
1	B	258	SER	4.5
1	B	257	LEU	4.4
1	A	67	ILE	3.7
1	B	255	ILE	3.6
1	B	200	ASN	3.3
1	B	159	GLU	3.3
1	A	165	VAL	3.3
1	B	135	TYR	3.3
1	B	221	GLY	3.1
1	B	202	ASP	3.1
1	B	195	GLY	3.1
1	B	146	LEU	3.1
1	B	199	MET	3.1
1	B	103	ILE	3.0
1	A	131	VAL	3.0
1	A	133	CYS	3.0
1	B	192	ARG	3.0
1	A	166	TYR	2.9
1	A	38	LEU	2.9
1	A	194	VAL	2.9
1	A	193	HIS	2.8
1	A	189	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	2.8
1	B	232	ASP	2.8
1	A	255	ILE	2.7
1	A	239	GLN	2.7
1	A	0	MET	2.7
1	B	45	ALA	2.7
1	A	195	GLY	2.7
1	B	38	LEU	2.7
1	A	320	TYR	2.7
1	A	124	THR	2.7
1	B	256	ASN	2.7
1	A	157	ILE	2.7
1	B	1	ALA	2.6
1	B	254	LYS	2.6
1	A	315	LEU	2.6
1	A	48	PHE	2.6
1	A	169	GLY	2.6
1	B	203	SER	2.6
1	A	176	HIS	2.6
1	A	168	ALA	2.5
1	B	164	GLY	2.5
1	A	156	GLU	2.5
1	B	320	TYR	2.5
1	A	272	GLY	2.5
1	A	84	PHE	2.5
1	A	130	LEU	2.5
1	A	338	LEU	2.4
1	B	157	ILE	2.4
1	A	146	LEU	2.4
1	B	194	VAL	2.4
1	B	277	ILE	2.4
1	B	204	SER	2.4
1	A	138	ILE	2.4
1	A	183	GLU	2.4
1	A	135	TYR	2.3
1	A	192	ARG	2.3
1	B	189	PHE	2.3
1	A	1	ALA	2.3
1	B	208	SER	2.3
1	A	45	ALA	2.3
1	A	170	LEU	2.2
1	A	34	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	167	VAL	2.2
1	A	284	LEU	2.2
1	B	147	LEU	2.2
1	B	214	VAL	2.2
1	A	63	ILE	2.1
1	A	32	ASN	2.1
1	A	31	PRO	2.1
1	A	50	PHE	2.1
1	A	203	SER	2.0
1	A	47	ASP	2.0
1	B	337	PRO	2.0
1	B	36	VAL	2.0
1	B	172	MET	2.0
1	A	113	ALA	2.0
1	B	136	LEU	2.0
1	B	336	ASP	2.0

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 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($\text{\AA}^2$)	Q<0.9
2	GOL	A	401	6/6	0.82	0.19	89,90,90,90	0
2	GOL	B	401	6/6	0.82	0.16	73,73,74,74	0
3	SO4	B	402	5/5	0.85	0.11	66,66,66,67	0
3	SO4	A	402	5/5	0.93	0.08	59,59,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.