Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 07:31 AM EDT

PDB ID	:	4IX3
Title	:	Crystal structure of a Stt7 homolog from Micromonas algae
Authors	:	Guo, J.; Wei, X.; Li, M.; Pan, X.; Chang, W.; Liu, Z.
Deposited on	:	2013-01-24
Resolution	:	1.35 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
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
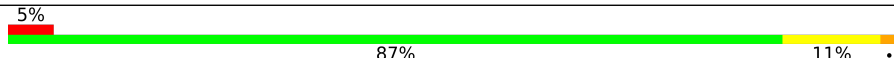*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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.
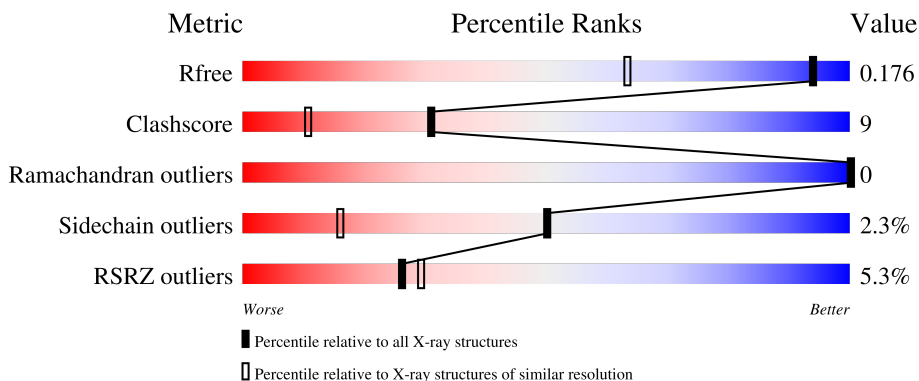
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	350	5% 88% ... 9% ..
1	B	350	5% 87% ... 11% .

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6175 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 MsStt7d protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	7	0
			2639	1659	464	496	20			
1	B	350	Total	C	N	O	S	0	4	0
			2656	1666	473	495	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ALA	-	expression tag	UNP C1EBN1
A	491	ALA	-	expression tag	UNP C1EBN1
A	492	ALA	-	expression tag	UNP C1EBN1
A	493	LEU	-	expression tag	UNP C1EBN1
A	494	GLU	-	expression tag	UNP C1EBN1
A	495	HIS	-	expression tag	UNP C1EBN1
A	496	HIS	-	expression tag	UNP C1EBN1
A	497	HIS	-	expression tag	UNP C1EBN1
A	498	HIS	-	expression tag	UNP C1EBN1
A	499	HIS	-	expression tag	UNP C1EBN1
A	500	HIS	-	expression tag	UNP C1EBN1
B	490	ALA	-	expression tag	UNP C1EBN1
B	491	ALA	-	expression tag	UNP C1EBN1
B	492	ALA	-	expression tag	UNP C1EBN1
B	493	LEU	-	expression tag	UNP C1EBN1
B	494	GLU	-	expression tag	UNP C1EBN1
B	495	HIS	-	expression tag	UNP C1EBN1
B	496	HIS	-	expression tag	UNP C1EBN1
B	497	HIS	-	expression tag	UNP C1EBN1
B	498	HIS	-	expression tag	UNP C1EBN1
B	499	HIS	-	expression tag	UNP C1EBN1
B	500	HIS	-	expression tag	UNP C1EBN1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	454	Total 454	O 454	0	0
3	B	422	Total 422	O 422	0	0

3 Residue-property plots ⓘ

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: MsStt7d protein
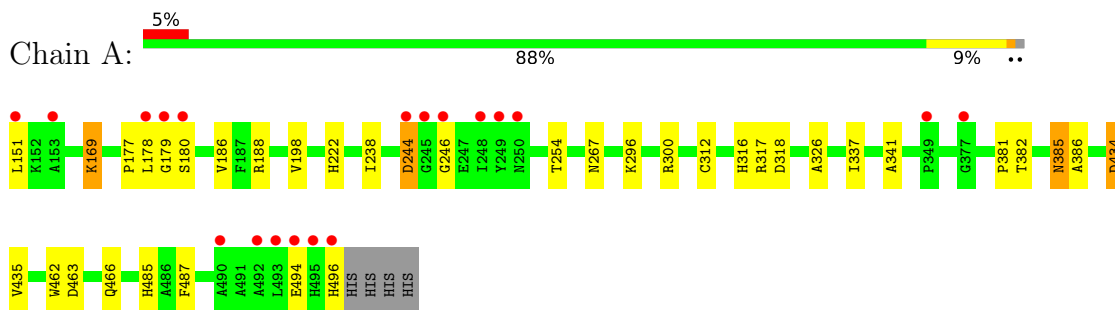
• Molecule 1: MsStt7d protein
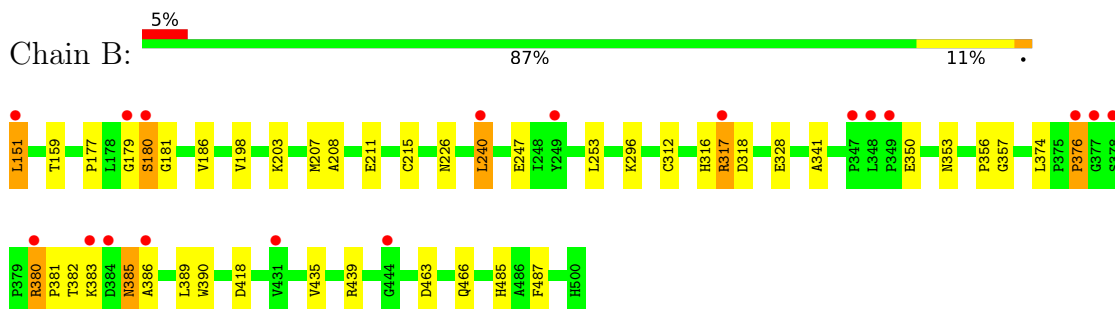
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.71Å 133.14Å 55.05Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	33.28 – 1.35 33.28 – 1.35	Depositor EDS
% Data completeness (in resolution range)	94.7 (33.28-1.35) 94.7 (33.28-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.133 , 0.174 0.137 , 0.176	Depositor DCC
R_{free} test set	7604 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	11.7	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6175	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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

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	0.66	0/2713	0.87	1/3673 (0.0%)
1	B	0.63	1/2725 (0.0%)	0.86	1/3689 (0.0%)
All	All	0.64	1/5438 (0.0%)	0.86	2/7362 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	TRP	CD2-CE2	5.62	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	418	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	434	ASP	CB-CG-OD1	5.27	123.04	118.30

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	2639	0	2617	37	0
1	B	2656	0	2612	59	0
2	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	454	0	0	8	0
3	B	422	0	0	16	0
All	All	6175	0	5229	96	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 9.

All (96) 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:B:485:HIS:HD2	1:B:487:PHE:H	1.09	1.00
1:A:485:HIS:HD2	1:A:487:PHE:H	1.16	0.92
1:B:385:ASN:O	1:B:389:LEU:CD1	2.20	0.90
1:B:376:PRO:CD	3:B:1096:HOH:O	2.22	0.87
1:B:385:ASN:O	1:B:389:LEU:HD13	1.73	0.86
1:B:316:HIS:HD2	1:B:318:ASP:H	1.23	0.86
1:A:267:ASN:HD21	1:A:326:ALA:H	1.25	0.84
1:A:296:LYS:HE2	3:A:815:HOH:O	1.77	0.84
1:B:159:THR:HG23	3:B:1068:HOH:O	1.76	0.84
1:A:316:HIS:HD2	1:A:318:ASP:H	1.24	0.84
1:A:169:LYS:HE3	3:A:1138:HOH:O	1.78	0.83
1:A:177:PRO:C	1:A:179:GLY:H	1.86	0.79
1:B:485:HIS:CD2	1:B:487:PHE:H	2.00	0.79
1:A:485:HIS:CD2	1:A:487:PHE:H	2.01	0.79
1:B:151:LEU:HD22	1:B:151:LEU:N	2.00	0.77
1:B:328:GLU:HG2	3:B:1120:HOH:O	1.89	0.72
1:B:328:GLU:CD	3:B:1107:HOH:O	2.29	0.71
1:B:376:PRO:CG	3:B:1096:HOH:O	2.36	0.69
1:A:186:VAL:CG1	1:A:198[B]:VAL:HG13	2.23	0.68
1:B:328:GLU:CG	3:B:1120:HOH:O	2.42	0.67
1:A:382:THR:H	1:A:385:ASN:HD21	1.42	0.66
1:A:382:THR:H	1:A:385:ASN:ND2	1.95	0.65
1:A:186:VAL:CG1	1:A:198[B]:VAL:CG1	2.75	0.64
1:B:151:LEU:N	1:B:151:LEU:CD2	2.61	0.64
1:B:385:ASN:CG	1:B:389:LEU:HD11	2.18	0.64
1:B:180:SER:CB	3:B:1100:HOH:O	2.45	0.64
1:A:296:LYS:CE	3:A:815:HOH:O	2.42	0.63
1:A:300:ARG:NH1	3:A:997:HOH:O	2.30	0.63
1:A:435:VAL:H	1:A:466:GLN:NE2	1.97	0.62
1:B:389:LEU:N	1:B:389:LEU:HD12	2.14	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:ASP:OD1	1:B:485:HIS:HE1	1.84	0.60
1:B:389:LEU:HD12	1:B:389:LEU:H	1.66	0.60
1:A:463:ASP:OD1	1:A:485:HIS:HE1	1.85	0.59
1:B:316:HIS:CD2	1:B:318:ASP:H	2.12	0.59
1:A:385:ASN:HD22	1:A:385:ASN:C	2.06	0.59
1:B:382:THR:H	1:B:385:ASN:ND2	2.00	0.59
1:B:296:LYS:HD2	3:B:1005:HOH:O	2.04	0.58
1:A:316:HIS:CD2	1:A:318:ASP:H	2.14	0.58
1:B:385:ASN:O	1:B:389:LEU:HD12	2.03	0.58
1:B:177:PRO:C	1:B:179:GLY:H	2.06	0.57
1:B:382:THR:H	1:B:385:ASN:HD21	1.52	0.57
1:B:435:VAL:H	1:B:466:GLN:NE2	2.01	0.57
1:A:494:GLU:OE1	1:A:496:HIS:NE2	2.38	0.56
1:B:385:ASN:HD22	1:B:385:ASN:C	2.08	0.56
1:B:385:ASN:HD22	1:B:386:ALA:N	2.04	0.56
1:A:246:GLY:O	1:A:254:THR:HG22	2.06	0.56
1:A:177:PRO:C	1:A:179:GLY:N	2.56	0.56
1:A:244:ASP:HB2	3:A:890:HOH:O	2.07	0.55
1:B:380:ARG:HD3	1:B:381:PRO:HD2	1.90	0.54
1:B:247:GLU:HG3	3:B:1105:HOH:O	2.08	0.54
3:A:1082:HOH:O	1:B:207:MET:HG2	2.06	0.54
1:A:222:HIS:HD2	3:A:732:HOH:O	1.90	0.54
1:B:186:VAL:CG1	1:B:198[A]:VAL:HG13	2.38	0.54
1:B:317:ARG:HD2	1:B:341:ALA:HB1	1.90	0.53
1:B:240:LEU:HD13	1:B:253:LEU:HB2	1.91	0.53
1:B:385:ASN:C	1:B:389:LEU:HD13	2.30	0.52
1:A:222:HIS:HE1	1:A:312:CYS:O	1.94	0.51
1:A:435:VAL:H	1:A:466:GLN:HE22	1.58	0.51
1:B:215[A]:CYS:SG	1:B:353:ASN:HB2	2.51	0.51
1:A:178:LEU:HD21	1:A:188:ARG:HG3	1.92	0.50
1:A:381:PRO:HA	1:A:385:ASN:HD21	1.76	0.50
1:B:208:ALA:HA	1:B:211:GLU:OE1	2.12	0.49
1:B:435:VAL:H	1:B:466:GLN:HE22	1.58	0.49
1:B:357:GLY:HA2	1:B:376:PRO:HD3	1.93	0.49
1:B:240:LEU:HD13	1:B:253:LEU:CB	2.43	0.49
1:A:267:ASN:HD21	1:A:326:ALA:N	2.03	0.48
1:B:317:ARG:NH2	3:B:882:HOH:O	2.46	0.48
1:B:181:GLY:HA2	3:B:1119:HOH:O	2.12	0.48
1:A:317[B]:ARG:HD2	1:A:341:ALA:O	2.13	0.48
1:B:316:HIS:HD2	1:B:318:ASP:N	2.03	0.48
1:B:203:LYS:NZ	3:B:852:HOH:O	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HD22	1:A:386:ALA:N	2.12	0.47
1:B:376:PRO:HD3	3:B:1096:HOH:O	2.01	0.47
1:B:385:ASN:CB	1:B:389:LEU:HD11	2.45	0.47
1:B:381:PRO:HA	1:B:385:ASN:HD21	1.81	0.46
1:A:434:ASP:HA	1:A:466:GLN:HE22	1.80	0.46
1:B:389:LEU:CD1	1:B:389:LEU:H	2.27	0.45
1:B:226:ASN:HB3	1:B:312[B]:CYS:SG	2.57	0.45
1:A:186:VAL:HG13	1:A:198[B]:VAL:CG1	2.47	0.44
1:B:439:ARG:NH2	3:B:939:HOH:O	2.29	0.44
1:B:350:GLU:HG2	1:B:383:LYS:NZ	2.33	0.44
1:B:180:SER:HB3	3:B:1100:HOH:O	2.12	0.44
1:A:316:HIS:HD2	1:A:318:ASP:N	2.04	0.43
1:A:300:ARG:HD3	3:A:1097:HOH:O	2.19	0.43
1:B:186:VAL:CG1	1:B:198[A]:VAL:CG1	2.97	0.42
1:A:316:HIS:HE1	1:A:337:ILE:O	2.02	0.42
1:B:385:ASN:ND2	1:B:385:ASN:C	2.72	0.42
1:B:385:ASN:HB2	1:B:389:LEU:HD11	2.02	0.42
1:B:328:GLU:CD	3:B:1120:HOH:O	2.57	0.41
1:B:240:LEU:CD1	1:B:253:LEU:HB2	2.49	0.41
1:B:177:PRO:C	1:B:179:GLY:N	2.70	0.41
1:B:316:HIS:O	1:B:317:ARG:CB	2.69	0.41
1:B:356:PRO:HA	1:B:374:LEU:HB2	2.02	0.40
1:A:385:ASN:ND2	1:A:385:ASN:C	2.73	0.40
1:A:435:VAL:HG13	1:A:462:TRP:CE3	2.57	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	351/350 (100%)	339 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	352/350 (101%)	345 (98%)	7 (2%)	0	100	100
All	All	703/700 (100%)	684 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	266/263 (101%)	261 (98%)	5 (2%)	57	23
1	B	267/263 (102%)	260 (97%)	7 (3%)	46	12
All	All	533/526 (101%)	521 (98%)	12 (2%)	50	16

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

Mol	Chain	Res	Type
1	A	151	LEU
1	A	169	LYS
1	A	180	SER
1	A	244	ASP
1	A	385	ASN
1	B	151	LEU
1	B	180	SER
1	B	240	LEU
1	B	317	ARG
1	B	376	PRO
1	B	380	ARG
1	B	385	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	267	ASN
1	A	316	HIS
1	A	323	ASN
1	A	385	ASN
1	A	409	GLN
1	A	436	ASN
1	A	466	GLN
1	A	485	HIS
1	B	250	ASN
1	B	316	HIS
1	B	385	ASN
1	B	409	GLN
1	B	466	GLN
1	B	485	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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.

No monomer is involved in short contacts.

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	346/350 (98%)	0.08	19 (5%)	25	27	8, 14, 38, 68	0
1	B	350/350 (100%)	0.05	18 (5%)	28	31	10, 17, 39, 55	0
All	All	696/700 (99%)	0.07	37 (5%)	26	29	8, 16, 39, 68	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	GLY	12.0
1	A	249	TYR	8.3
1	A	178	LEU	6.4
1	A	246	GLY	5.7
1	B	377	GLY	5.2
1	A	244	ASP	5.2
1	A	151	LEU	5.0
1	B	179	GLY	4.8
1	B	249	TYR	4.8
1	A	492	ALA	4.6
1	B	348	LEU	4.6
1	B	151	LEU	4.5
1	A	245	GLY	4.1
1	A	250	ASN	4.1
1	B	384	ASP	4.0
1	B	240	LEU	4.0
1	A	248	ILE	3.9
1	A	496	HIS	3.6
1	A	493	LEU	3.5
1	A	494	GLU	3.0
1	A	349	PRO	2.8
1	A	153	ALA	2.8
1	B	180	SER	2.7
1	A	495	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	490	ALA	2.5
1	B	383	LYS	2.5
1	B	444	GLY	2.4
1	B	347	PRO	2.3
1	B	349	PRO	2.3
1	A	180	SER	2.2
1	A	377	GLY	2.2
1	B	378	SER	2.2
1	B	380	ARG	2.2
1	B	376	PRO	2.1
1	B	386	ALA	2.1
1	B	431	VAL	2.0
1	B	317	ARG	2.0

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 monosaccharides 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, 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
2	MG	A	601	1/1	1.00	0.15	18,18,18,18	0
2	MG	A	602	1/1	1.00	0.06	10,10,10,10	0
2	MG	B	601	1/1	1.00	0.10	18,18,18,18	0
2	MG	B	602	1/1	1.00	0.23	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.