W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2024 – 08:46 PM EST

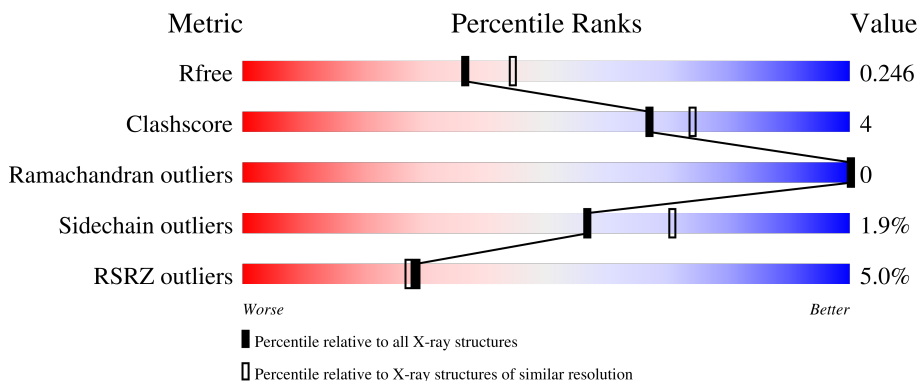|		
PDB ID	:	3H8D
Title	:	Crystal structure of Myosin VI in complex with Dab2 peptide
Authors	:	Yu, C.; Feng, W.; Wei, Z.; Zhang, M.
Deposited on	:	2009-04-29
Resolution	:	2.20 Å(reported)

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 2.20 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.9%
RSRZ outliers		5.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	141	2%: 73% / 12% / 15%
1	B	141	4%: 63% / 9% / • / 27%
1	C	141	4%: 77% / 9% / • / 13%
1	D	141	6%: 74% / 10% / 16%
2	E	48	4%: 73% / 6% / 21%

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Mol	Chain	Length	Quality of chain
2	F	48	73% · 23%
2	G	48	8% 73% 6% 21%
2	H	48	4% 71% 6% 23%

2　Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5371 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 Myosin-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	120	Total	C	N	O	S	0	1	0
			999	638	178	177	6			
1	B	103	Total	C	N	O	S	0	2	0
			868	556	155	153	4			
1	C	122	Total	C	N	O	S	0	1	0
			1027	654	187	179	7			
1	D	119	Total	C	N	O	S	0	2	0
			1005	639	186	174	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1135	GLY	-	expression tag	UNP Q64331
A	1136	SER	-	expression tag	UNP Q64331
A	1266	GLY	-	expression tag	UNP Q64331
A	1267	SER	-	expression tag	UNP Q64331
A	1268	SER	-	expression tag	UNP Q64331
A	1269	GLY	-	expression tag	UNP Q64331
A	1270	GLY	-	expression tag	UNP Q64331
A	1271	SER	-	expression tag	UNP Q64331
A	1272	LEU	-	expression tag	UNP Q64331
A	1273	VAL	-	expression tag	UNP Q64331
A	1274	PRO	-	expression tag	UNP Q64331
A	1275	ARG	-	expression tag	UNP Q64331
B	1135	GLY	-	expression tag	UNP Q64331
B	1136	SER	-	expression tag	UNP Q64331
B	1266	GLY	-	expression tag	UNP Q64331
B	1267	SER	-	expression tag	UNP Q64331
B	1268	SER	-	expression tag	UNP Q64331
B	1269	GLY	-	expression tag	UNP Q64331
B	1270	GLY	-	expression tag	UNP Q64331
B	1271	SER	-	expression tag	UNP Q64331
B	1272	LEU	-	expression tag	UNP Q64331

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1273	VAL	-	expression tag	UNP Q64331
B	1274	PRO	-	expression tag	UNP Q64331
B	1275	ARG	-	expression tag	UNP Q64331
C	1135	GLY	-	expression tag	UNP Q64331
C	1136	SER	-	expression tag	UNP Q64331
C	1266	GLY	-	expression tag	UNP Q64331
C	1267	SER	-	expression tag	UNP Q64331
C	1268	SER	-	expression tag	UNP Q64331
C	1269	GLY	-	expression tag	UNP Q64331
C	1270	GLY	-	expression tag	UNP Q64331
C	1271	SER	-	expression tag	UNP Q64331
C	1272	LEU	-	expression tag	UNP Q64331
C	1273	VAL	-	expression tag	UNP Q64331
C	1274	PRO	-	expression tag	UNP Q64331
C	1275	ARG	-	expression tag	UNP Q64331
D	1135	GLY	-	expression tag	UNP Q64331
D	1136	SER	-	expression tag	UNP Q64331
D	1266	GLY	-	expression tag	UNP Q64331
D	1267	SER	-	expression tag	UNP Q64331
D	1268	SER	-	expression tag	UNP Q64331
D	1269	GLY	-	expression tag	UNP Q64331
D	1270	GLY	-	expression tag	UNP Q64331
D	1271	SER	-	expression tag	UNP Q64331
D	1272	LEU	-	expression tag	UNP Q64331
D	1273	VAL	-	expression tag	UNP Q64331
D	1274	PRO	-	expression tag	UNP Q64331
D	1275	ARG	-	expression tag	UNP Q64331

- Molecule 2 is a protein called Disabled homolog 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	38	Total	C	N	O	0	0	0
			300	184	51	65			
2	F	37	Total	C	N	O	0	0	0
			294	181	50	63			
2	G	38	Total	C	N	O	0	0	0
			300	184	51	65			
2	H	37	Total	C	N	O	0	0	0
			294	181	50	63			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	664	GLY	-	expression tag	UNP O88797
E	665	SER	-	expression tag	UNP O88797
E	666	SER	-	expression tag	UNP O88797
E	667	SER	-	expression tag	UNP O88797
E	668	GLY	-	expression tag	UNP O88797
E	669	GLY	-	expression tag	UNP O88797
E	670	GLY	-	expression tag	UNP O88797
E	671	SER	-	expression tag	UNP O88797
E	672	SER	-	expression tag	UNP O88797
F	664	GLY	-	expression tag	UNP O88797
F	665	SER	-	expression tag	UNP O88797
F	666	SER	-	expression tag	UNP O88797
F	667	SER	-	expression tag	UNP O88797
F	668	GLY	-	expression tag	UNP O88797
F	669	GLY	-	expression tag	UNP O88797
F	670	GLY	-	expression tag	UNP O88797
F	671	SER	-	expression tag	UNP O88797
F	672	SER	-	expression tag	UNP O88797
G	664	GLY	-	expression tag	UNP O88797
G	665	SER	-	expression tag	UNP O88797
G	666	SER	-	expression tag	UNP O88797
G	667	SER	-	expression tag	UNP O88797
G	668	GLY	-	expression tag	UNP O88797
G	669	GLY	-	expression tag	UNP O88797
G	670	GLY	-	expression tag	UNP O88797
G	671	SER	-	expression tag	UNP O88797
G	672	SER	-	expression tag	UNP O88797
H	664	GLY	-	expression tag	UNP O88797
H	665	SER	-	expression tag	UNP O88797
H	666	SER	-	expression tag	UNP O88797
H	667	SER	-	expression tag	UNP O88797
H	668	GLY	-	expression tag	UNP O88797
H	669	GLY	-	expression tag	UNP O88797
H	670	GLY	-	expression tag	UNP O88797
H	671	SER	-	expression tag	UNP O88797
H	672	SER	-	expression tag	UNP O88797

- Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

SCN

S S⁻ C N N
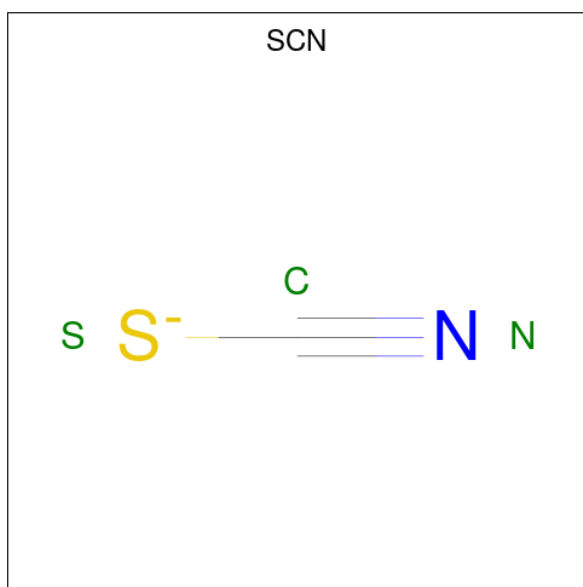
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 3	C 1	N 1	S 1	0	0
3	B	1	Total 3	C 1	N 1	S 1	0	0
3	C	1	Total 3	C 1	N 1	S 1	0	0

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).

DTT

O3 S4

HO SH

C3(R) C4

C1 C2(R)

HS OH

S1 O2
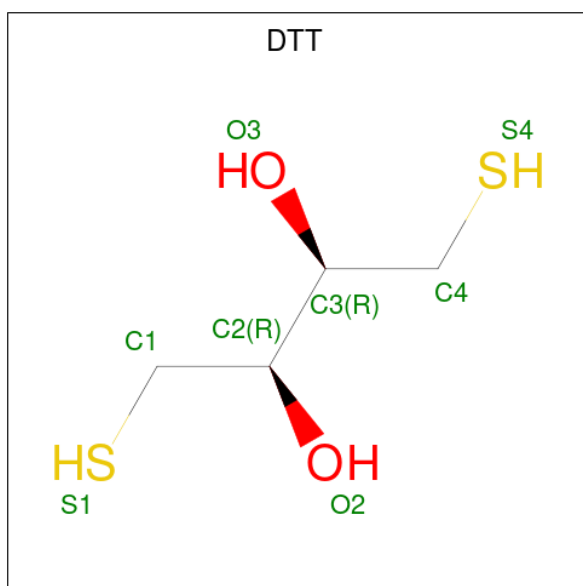
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total 8	C 4	O 2	S 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	51	Total 51	O 51	0	0
6	B	57	Total 57	O 57	0	0
6	C	37	Total 37	O 37	0	0
6	D	39	Total 39	O 39	0	0
6	E	17	Total 17	O 17	0	0
6	F	29	Total 29	O 29	0	0
6	G	20	Total 20	O 20	0	0
6	H	16	Total 16	O 16	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.
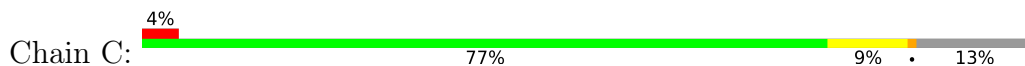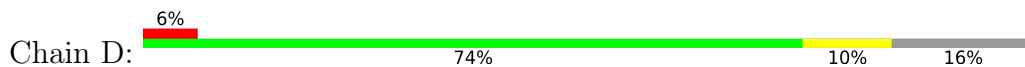
- Molecule 1: Myosin-VI
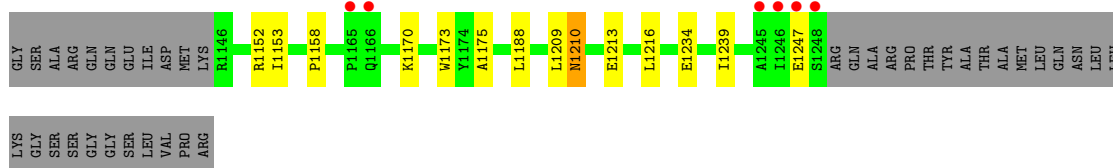
Chain A:

- Molecule 1: Myosin-VI

Chain B:

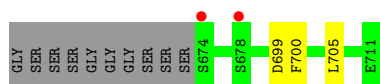- Molecule 1: Myosin-VI

Chain C:

- Molecule 1: Myosin-VI

Chain D:

- Molecule 2: Disabled homolog 2

Chain E:

• Molecule 2: Disabled homolog 2

Chain F:

• Molecule 2: Disabled homolog 2
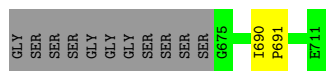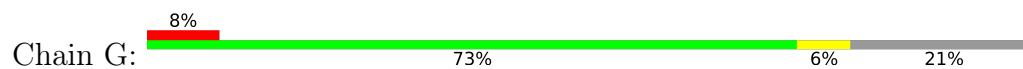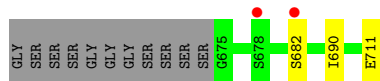
Chain G:

• Molecule 2: Disabled homolog 2

Chain H:
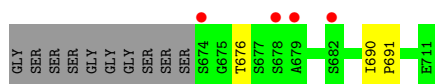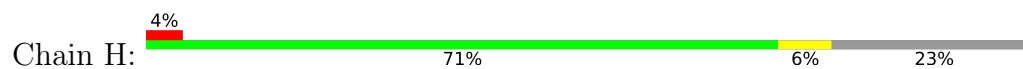
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.18Å 69.95Å 78.54Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.20) 96.7 (29.92-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.251 0.187 , 0.246	Depositor DCC
R_{free} test set	1833 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.3	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	0.95	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0863e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: CL, SCN, DTT

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	0.44	0/1029	0.55	0/1390
1	B	0.46	0/899	0.55	0/1213
1	C	0.45	0/1057	0.57	0/1425
1	D	0.43	0/1040	0.56	0/1402
2	E	0.47	0/306	0.50	0/412
2	F	0.51	0/300	0.55	0/404
2	G	0.44	0/306	0.53	0/412
2	H	0.46	0/300	0.53	0/404
All	All	0.45	0/5237	0.55	0/7062

There are no bond length outliers.

There are no bond angle outliers.

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	999	0	978	8	0
1	B	868	0	846	11	0
1	C	1027	0	1020	9	0
1	D	1005	0	994	9	0
2	E	300	0	266	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	294	0	261	3	0
2	G	300	0	266	2	0
2	H	294	0	261	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	C	8	0	10	0	0
5	H	1	0	0	0	0
6	A	51	0	0	0	0
6	B	57	0	0	1	0
6	C	37	0	0	0	0
6	D	39	0	0	0	0
6	E	17	0	0	0	0
6	F	29	0	0	0	0
6	G	20	0	0	0	0
6	H	16	0	0	0	0
All	All	5371	0	4902	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.

The worst 5 of 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:D:1209:LEU:HB3	1:D:1213:GLU:HG3	1.75	0.67
1:A:1209:LEU:HB3	1:A:1213:GLU:HG3	1.80	0.64
1:A:1153:ILE:HD11	1:A:1216:LEU:HD21	1.87	0.57
1:C:1192:LYS:HB2	1:C:1193:PRO:CD	2.36	0.56
1:B:1170:LYS:NZ	6:B:177:HOH:O	2.39	0.55

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	119/141 (84%)	118 (99%)	1 (1%)	0	100	100
1	B	103/141 (73%)	102 (99%)	1 (1%)	0	100	100
1	C	121/141 (86%)	118 (98%)	3 (2%)	0	100	100
1	D	119/141 (84%)	116 (98%)	3 (2%)	0	100	100
2	E	36/48 (75%)	35 (97%)	1 (3%)	0	100	100
2	F	35/48 (73%)	34 (97%)	1 (3%)	0	100	100
2	G	36/48 (75%)	35 (97%)	1 (3%)	0	100	100
2	H	35/48 (73%)	34 (97%)	1 (3%)	0	100	100
All	All	604/756 (80%)	592 (98%)	12 (2%)	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	103/120 (86%)	100 (97%)	3 (3%)	42	54
1	B	90/120 (75%)	88 (98%)	2 (2%)	52	65
1	C	107/120 (89%)	104 (97%)	3 (3%)	43	56
1	D	104/120 (87%)	103 (99%)	1 (1%)	76	86
2	E	34/40 (85%)	34 (100%)	0	100	100
2	F	33/40 (82%)	33 (100%)	0	100	100
2	G	34/40 (85%)	34 (100%)	0	100	100
2	H	33/40 (82%)	32 (97%)	1 (3%)	41	53
All	All	538/640 (84%)	528 (98%)	10 (2%)	57	71

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1227	ARG
1	D	1260	LEU
2	H	682	SER
1	B	1210	ASN
1	B	1247	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1210	ASN
1	D	1250	GLN
2	G	704	GLN
2	F	692	GLN
1	B	1210	ASN

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
3	SCN	C	1	-	1,2,2	2.15	1 (100%)	0,1,1	-	-
3	SCN	A	3	-	1,2,2	1.04	0	0,1,1	-	-
4	DTT	C	1276	-	7,7,7	0.59	0	4,8,8	0.91	0
3	SCN	B	2	-	1,2,2	1.68	0	0,1,1	-	-

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
4	DTT	C	1276	-	-	4/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	SCN	C-N	2.15	1.22	1.15

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1276	DTT	S1-C1-C2-O2
4	C	1276	DTT	S1-C1-C2-C3
4	C	1276	DTT	C2-C3-C4-S4
4	C	1276	DTT	O3-C3-C4-S4

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.

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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(Å²)	Q<0.9
1	A	120/141 (85%)	0.03	3 (2%)	57	55	15, 28, 50, 62	7 (5%)
1	B	103/141 (73%)	0.09	6 (5%)	23	22	15, 26, 47, 80	1 (0%)
1	C	122/141 (86%)	0.11	5 (4%)	37	35	17, 31, 52, 70	7 (5%)
1	D	119/141 (84%)	0.32	9 (7%)	13	12	18, 32, 59, 75	4 (3%)
2	E	38/48 (79%)	-0.03	2 (5%)	26	25	16, 30, 45, 56	0
2	F	37/48 (77%)	-0.20	0	100	100	17, 27, 41, 49	1 (2%)
2	G	38/48 (79%)	0.19	4 (10%)	6	5	20, 32, 55, 65	1 (2%)
2	H	37/48 (77%)	-0.04	2 (5%)	25	24	18, 34, 49, 53	0
All	All	614/756 (81%)	0.10	31 (5%)	28	27	15, 30, 52, 80	21 (3%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1146	ARG	5.7
1	B	1248	SER	5.0
1	D	1262	ASN	4.4
1	C	1143	ASP	4.2
2	H	678	SER	3.9

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
4	DTT	C	1276	8/8	0.90	0.15	55,61,65,67	0
5	CL	H	4	1/1	0.91	0.11	62,62,62,62	0
3	SCN	C	1	3/3	0.93	0.16	56,56,57,57	0
3	SCN	A	3	3/3	0.97	0.14	48,48,49,50	0
3	SCN	B	2	3/3	0.98	0.09	41,41,43,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.