



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:45 pm GMT

PDB ID : 2FIM
Title : Structure of the C-terminal domain of Human Tubby-like protein 1
Authors : Hallberg, B.M.; Ogg, D.; Arrowsmith, C.; Berglund, H.; Edwards, A.; Ehn, M.; Flodin, S.; Graslund, S.; Hammarstrom, M.; Hogbom, M.; Holmberg-Schiavone, L.; Kotenyova, T.; Kursula, P.; Nilsson-Ehle, P.; Nordlund, P.; Nyman, T.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Persson, C.
Deposited on : 2005-12-29
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

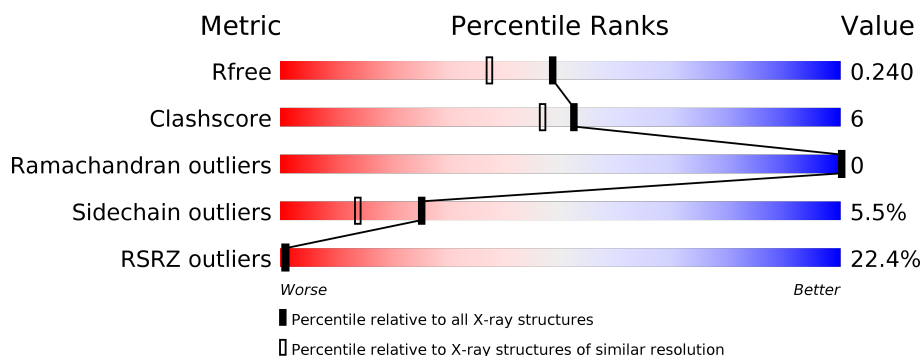
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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. 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	276	
1	B	276	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3DP	A	1003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3841 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 Tubby related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1813	1148	333	328	4			
1	B	232	Total	C	N	O	S	0	0	0
			1870	1187	344	335	4			

There are 46 discrepancies between the modelled and reference sequences:

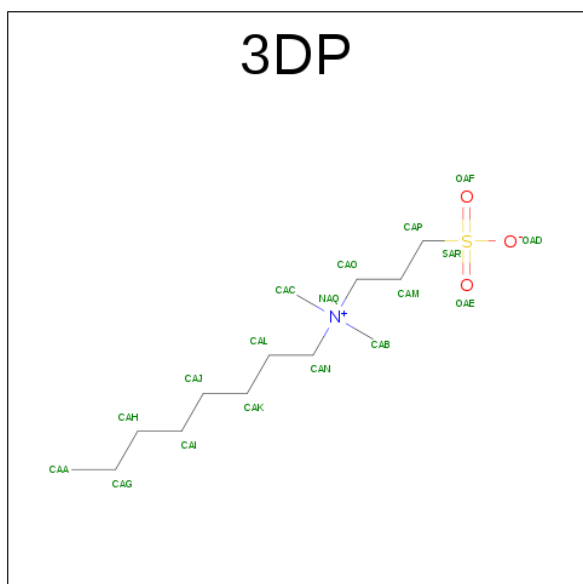
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	EXPRESSION TAG	UNP O00294
A	215	HIS	-	EXPRESSION TAG	UNP O00294
A	216	HIS	-	EXPRESSION TAG	UNP O00294
A	217	HIS	-	EXPRESSION TAG	UNP O00294
A	218	HIS	-	EXPRESSION TAG	UNP O00294
A	219	HIS	-	EXPRESSION TAG	UNP O00294
A	220	HIS	-	EXPRESSION TAG	UNP O00294
A	221	SER	-	EXPRESSION TAG	UNP O00294
A	222	SER	-	EXPRESSION TAG	UNP O00294
A	223	GLY	-	EXPRESSION TAG	UNP O00294
A	224	VAL	-	EXPRESSION TAG	UNP O00294
A	225	ASP	-	EXPRESSION TAG	UNP O00294
A	226	LEU	-	EXPRESSION TAG	UNP O00294
A	227	GLY	-	EXPRESSION TAG	UNP O00294
A	228	THR	-	EXPRESSION TAG	UNP O00294
A	229	GLU	-	EXPRESSION TAG	UNP O00294
A	230	ASN	-	EXPRESSION TAG	UNP O00294
A	231	LEU	-	EXPRESSION TAG	UNP O00294
A	232	TYR	-	EXPRESSION TAG	UNP O00294
A	233	PHE	-	EXPRESSION TAG	UNP O00294
A	234	GLN	-	EXPRESSION TAG	UNP O00294
A	235	SER	-	EXPRESSION TAG	UNP O00294
A	236	MET	-	EXPRESSION TAG	UNP O00294
B	214	MET	-	EXPRESSION TAG	UNP O00294
B	215	HIS	-	EXPRESSION TAG	UNP O00294

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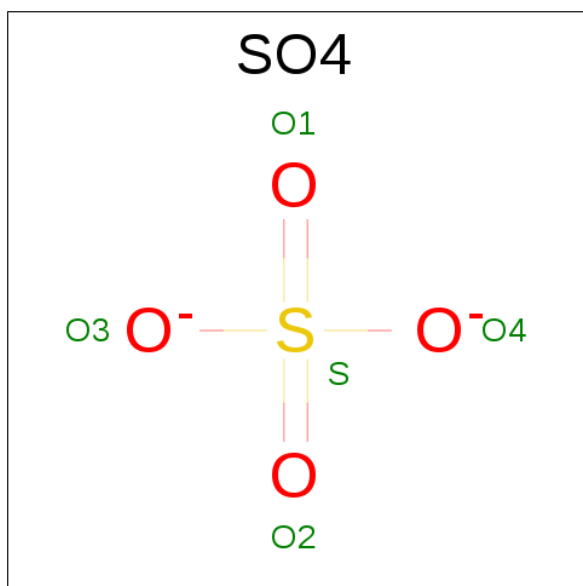
Chain	Residue	Modelled	Actual	Comment	Reference
B	216	HIS	-	EXPRESSION TAG	UNP O00294
B	217	HIS	-	EXPRESSION TAG	UNP O00294
B	218	HIS	-	EXPRESSION TAG	UNP O00294
B	219	HIS	-	EXPRESSION TAG	UNP O00294
B	220	HIS	-	EXPRESSION TAG	UNP O00294
B	221	SER	-	EXPRESSION TAG	UNP O00294
B	222	SER	-	EXPRESSION TAG	UNP O00294
B	223	GLY	-	EXPRESSION TAG	UNP O00294
B	224	VAL	-	EXPRESSION TAG	UNP O00294
B	225	ASP	-	EXPRESSION TAG	UNP O00294
B	226	LEU	-	EXPRESSION TAG	UNP O00294
B	227	GLY	-	EXPRESSION TAG	UNP O00294
B	228	THR	-	EXPRESSION TAG	UNP O00294
B	229	GLU	-	EXPRESSION TAG	UNP O00294
B	230	ASN	-	EXPRESSION TAG	UNP O00294
B	231	LEU	-	EXPRESSION TAG	UNP O00294
B	232	TYR	-	EXPRESSION TAG	UNP O00294
B	233	PHE	-	EXPRESSION TAG	UNP O00294
B	234	GLN	-	EXPRESSION TAG	UNP O00294
B	235	SER	-	EXPRESSION TAG	UNP O00294
B	236	MET	-	EXPRESSION TAG	UNP O00294

- Molecule 2 is 3-(N,N-DIMETHYLOCTYLAMMONIO)PROPANESULFONATE (three-letter code: 3DP) (formula: $C_{13}H_{29}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	13	1	3	1		

- Molecule 3 is SULFATE ION (three-letter code: 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	52	Total	O	0	0
			52	52		
4	B	78	Total	O	0	0
			78	78		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.96Å 85.15Å 58.79Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	19.89 – 1.90 19.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.89-1.90) 99.7 (19.74-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.235 0.206 , 0.240	Depositor DCC
R_{free} test set	2228 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.007 for l,k,-h 0.037 for h,-k,-l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3841	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: 3DP, SO4

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	0.95	0/1850	0.96	8/2501 (0.3%)
1	B	0.95	1/1910 (0.1%)	0.91	2/2582 (0.1%)
All	All	0.95	1/3760 (0.0%)	0.93	10/5083 (0.2%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	CYS	CB-SG	-5.15	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	287	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	330	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	367	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	255	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	466	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	259	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	391	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	302	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	255	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	482	PHE	Peptide

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	1813	0	1814	23	0
1	B	1870	0	1880	23	0
2	A	18	0	29	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	52	0	0	1	0
4	B	78	0	0	4	0
All	All	3841	0	3723	47	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 6.

All (47) 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:277:THR:HB	4:B:1028:HOH:O	1.76	0.85
1:B:416:ASN:HD22	1:B:417:ASP:N	1.74	0.83
1:A:336:GLN:HE22	1:A:388:ASN:HA	1.47	0.80
1:B:277:THR:HG23	1:B:280:LYS:H	1.47	0.78
1:A:367:ARG:HH11	1:A:367:ARG:HG2	1.50	0.75
1:A:425:ASN:ND2	1:A:427:GLN:H	1.84	0.75
1:A:425:ASN:HD22	1:A:427:GLN:H	1.39	0.71
1:A:367:ARG:HG3	4:A:1027:HOH:O	1.90	0.70
1:A:367:ARG:CG	1:A:367:ARG:HH11	2.03	0.70
1:B:416:ASN:C	1:B:416:ASN:HD22	1.95	0.69
1:A:416:ASN:HD22	1:A:419:SER:H	1.40	0.67
2:A:1003:3DP:HAC2	1:B:322:LEU:O	1.96	0.65
1:A:277:THR:HG23	1:A:279:LYS:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:HD21	1:A:418:ASP:HB3	1.63	0.64
1:B:396:ARG:HD2	1:B:405:LEU:HD11	1.85	0.58
1:B:261:LYS:NZ	4:B:1014:HOH:O	2.29	0.57
1:A:279:LYS:O	1:A:279:LYS:HD2	2.04	0.56
1:B:275:LEU:HD22	1:B:281:VAL:CG1	2.37	0.54
1:B:367:ARG:HD2	4:B:1010:HOH:O	2.09	0.52
1:A:342:ASN:HD21	1:A:344:ALA:HB3	1.73	0.52
1:A:278:GLU:N	1:A:278:GLU:CD	2.65	0.50
1:A:291:ARG:O	1:A:291:ARG:HG2	2.11	0.50
2:A:1003:3DP:HAC3	4:B:1019:HOH:O	2.12	0.49
1:A:416:ASN:ND2	1:A:418:ASP:HB3	2.27	0.49
1:A:279:LYS:O	1:A:279:LYS:CD	2.61	0.49
1:A:278:GLU:H	1:A:278:GLU:CD	2.15	0.48
1:B:275:LEU:HD13	1:B:283:LEU:HD11	1.96	0.47
1:B:298:LEU:HD11	1:B:313:PHE:CD1	2.49	0.47
1:B:451:LEU:HD11	1:B:463:LEU:HD11	1.96	0.46
1:A:367:ARG:CG	1:A:367:ARG:NH1	2.71	0.46
1:B:416:ASN:C	1:B:416:ASN:ND2	2.67	0.46
1:A:425:ASN:HD22	1:A:425:ASN:C	2.18	0.46
1:B:296:ASN:HD21	1:B:316:LYS:HE3	1.80	0.46
1:B:277:THR:HG21	1:B:279:LYS:HE3	1.98	0.46
1:B:259:ASP:OD1	1:B:261:LYS:HG2	2.15	0.46
1:B:397:TRP:O	1:B:400:LYS:HD3	2.16	0.46
1:B:277:THR:HG21	1:B:279:LYS:CE	2.46	0.45
1:B:277:THR:OG1	1:B:278:GLU:N	2.46	0.45
1:B:279:LYS:H	1:B:279:LYS:HD3	1.82	0.45
1:A:397:TRP:O	1:A:400:LYS:HE2	2.20	0.42
1:A:258:ARG:CZ	1:A:260:LYS:HE3	2.50	0.42
1:A:467:TYR:CD1	1:A:468:PRO:HA	2.56	0.41
1:A:277:THR:HG23	1:A:279:LYS:HD2	2.01	0.41
1:B:277:THR:HG21	1:B:279:LYS:CD	2.51	0.41
1:B:314:ILE:O	1:B:314:ILE:HG13	2.21	0.41
1:B:278:GLU:CD	1:B:278:GLU:N	2.73	0.41
1:A:259:ASP:OD1	1:A:259:ASP:O	2.39	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	216/276 (78%)	211 (98%)	5 (2%)	0	100	100
1	B	226/276 (82%)	218 (96%)	8 (4%)	0	100	100
All	All	442/552 (80%)	429 (97%)	13 (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	197/239 (82%)	188 (95%)	9 (5%)	31	20
1	B	202/239 (84%)	189 (94%)	13 (6%)	20	10
All	All	399/478 (84%)	377 (94%)	22 (6%)	25	14

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	A	278	GLU
1	A	279	LYS
1	A	280	LYS
1	A	367	ARG
1	A	398	GLN
1	A	417	ASP
1	A	425	ASN

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Mol	Chain	Res	Type
1	A	483	ASP
1	B	239	ARG
1	B	250	ARG
1	B	275	LEU
1	B	278	GLU
1	B	279	LYS
1	B	280	LYS
1	B	314	ILE
1	B	336	GLN
1	B	387	ARG
1	B	416	ASN
1	B	417	ASP
1	B	418	ASP
1	B	419	SER

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

Mol	Chain	Res	Type
1	A	336	GLN
1	A	342	ASN
1	A	398	GLN
1	A	416	ASN
1	A	425	ASN
1	B	248	GLN
1	B	296	ASN
1	B	336	GLN
1	B	416	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	A	1001	-	4,4,4	0.28	0	6,6,6	0.54	0
2	3DP	A	1003	-	17,17,17	1.33	3 (17%)	20,22,22	1.69	5 (25%)
3	SO4	B	1002	-	4,4,4	0.23	0	6,6,6	0.27	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
3	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	3DP	A	1003	-	-	0/17/17/17	0/0/0/0
3	SO4	B	1002	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	3DP	CAO-NAQ	-2.65	1.46	1.52
2	A	1003	3DP	CAN-NAQ	-2.48	1.47	1.52
2	A	1003	3DP	CAP-SAR	3.07	1.82	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	3DP	CAM-CAO-NAQ	-2.94	108.97	115.34
2	A	1003	3DP	CAL-CAN-NAQ	-2.70	109.48	115.34
2	A	1003	3DP	OAD-SAR-CAP	2.27	108.85	106.06
2	A	1003	3DP	OAE-SAR-CAP	3.65	109.92	106.79
2	A	1003	3DP	OAF-SAR-CAP	3.97	110.20	106.79

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	A	1003	3DP	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	224/276 (81%)	1.22	51 (22%)  	30, 35, 41, 52	0
1	B	232/276 (84%)	1.35	51 (21%)  	28, 35, 41, 50	0
All	All	456/552 (82%)	1.29	102 (22%)  	28, 35, 41, 52	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	VAL	7.6
1	B	417	ASP	7.1
1	A	291	ARG	6.1
1	B	390	SER	5.8
1	B	278	GLU	5.8
1	B	339	TYR	5.7
1	A	435	VAL	5.6
1	B	418	ASP	5.3
1	B	360	LEU	5.2
1	B	273	LEU	5.1
1	A	259	ASP	5.0
1	B	415	TRP	4.7
1	A	483	ASP	4.7
1	B	403	GLU	4.6
1	A	353	VAL	4.4
1	B	290	LYS	4.4
1	B	291	ARG	4.4
1	A	268	TYR	4.4
1	B	284	LEU	4.1
1	A	290	LYS	4.0
1	A	293	LYS	3.9
1	A	292	SER	3.9
1	B	277	THR	3.9
1	B	423	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	339	TYR	3.8
1	A	403	GLU	3.8
1	B	256	LEU	3.8
1	B	294	THR	3.7
1	A	418	ASP	3.6
1	B	393	LEU	3.6
1	B	419	SER	3.5
1	A	240	GLU	3.5
1	B	483	ASP	3.4
1	A	356	GLU	3.2
1	A	367	ARG	3.2
1	A	277	THR	3.2
1	A	404	SER	3.1
1	A	398	GLN	3.1
1	B	313	PHE	3.1
1	B	475	PHE	3.1
1	B	250	ARG	3.0
1	A	260	LYS	3.0
1	A	453	PHE	2.9
1	B	240	GLU	2.9
1	A	438	PHE	2.9
1	A	278	GLU	2.9
1	A	393	LEU	2.9
1	B	254	CYS	2.9
1	B	414	VAL	2.8
1	A	352	ALA	2.8
1	B	389	ALA	2.8
1	B	283	LEU	2.8
1	A	370	VAL	2.7
1	B	257	THR	2.7
1	B	469	LEU	2.7
1	A	372	ILE	2.7
1	A	371	ILE	2.6
1	B	371	ILE	2.6
1	A	289	ARG	2.6
1	B	268	TYR	2.6
1	B	416	ASN	2.6
1	B	272	PHE	2.5
1	A	312	ASN	2.5
1	B	262	GLY	2.5
1	B	402	LEU	2.5
1	A	450	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	350	LEU	2.5
1	A	378	GLU	2.5
1	A	477	ILE	2.4
1	B	422	TYR	2.4
1	B	372	ILE	2.4
1	A	478	ALA	2.4
1	A	458	GLU	2.4
1	B	350	LEU	2.4
1	B	289	ARG	2.3
1	A	273	LEU	2.3
1	A	294	THR	2.3
1	B	279	LYS	2.3
1	A	462	THR	2.3
1	A	256	LEU	2.3
1	B	261	LYS	2.3
1	A	344	ALA	2.2
1	B	435	VAL	2.2
1	A	390	SER	2.2
1	B	337	ARG	2.2
1	A	327	THR	2.2
1	B	463	LEU	2.2
1	B	478	ALA	2.2
1	B	351	ALA	2.1
1	A	354	ILE	2.1
1	B	299	ILE	2.1
1	A	402	LEU	2.1
1	A	408	LEU	2.1
1	A	430	VAL	2.1
1	A	280	LYS	2.1
1	A	440	ILE	2.1
1	B	353	VAL	2.0
1	B	354	ILE	2.0
1	A	431	THR	2.0
1	B	462	THR	2.0
1	A	284	LEU	2.0
1	A	451	LEU	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 [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	3DP	A	1003	18/18	0.79	0.25	2.87	38,68,76,77	0
3	SO4	A	1001	5/5	0.94	0.39	-	60,63,65,68	0
3	SO4	B	1002	5/5	0.95	0.26	-	74,75,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.