



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 11:43 PM EDT

PDB ID : 4AHT
Title : Parallel screening of a low molecular weight compound library: do differences in methodology affect hit identification
Authors : Wielens, J.; Heady, S.J.; Rhodes, D.I.; Mulder, R.J.; Dolezal, O.; Deadman, J.J.; Newman, J.; Chalmers, D.K.; Parker, M.W.; Peat, T.S.; Scanlon, M.J.
Deposited on : 2012-02-07
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 2.36.2
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) : 2.36.2

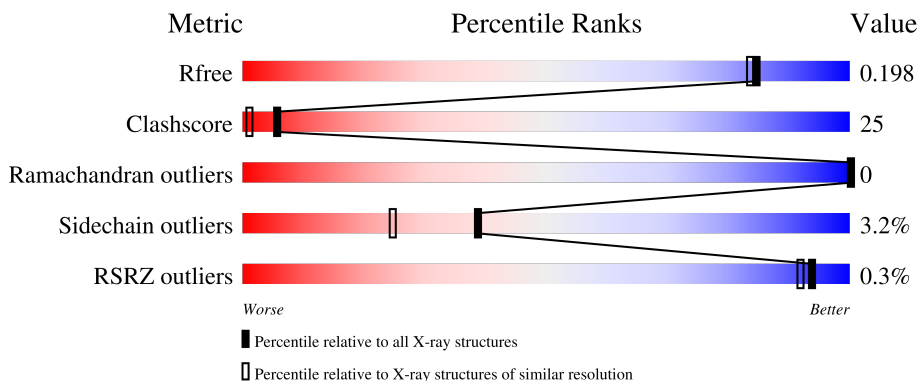
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	183	 59% 22% 17%
1	B	183	 55% 24% 18%

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	SO4	A	1211	-	-	X	-
3	EDO	A	1213	-	-	X	-
4	TAM	A	1215	-	X	X	-
4	TAM	B	1217	-	X	X	-
6	ACY	B	1215	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2782 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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	151	1253	808	211	230	4	0	15	0
1	B	150	1249	802	212	231	4	0	14	0

There are 46 discrepancies between the modelled and reference sequences:

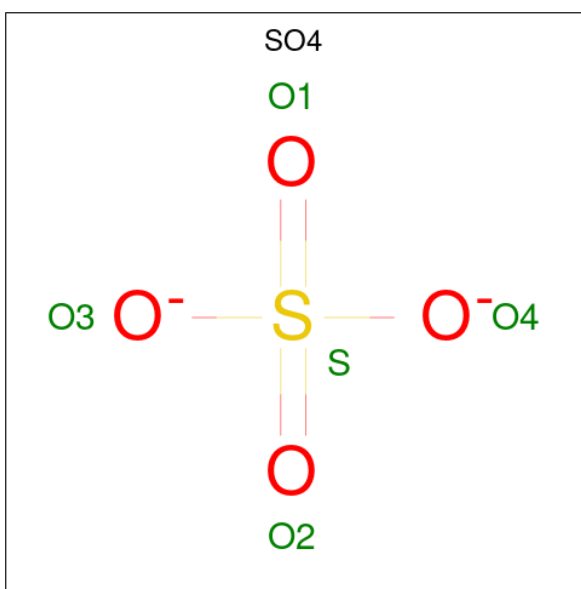
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P12497
A	31	GLY	-	expression tag	UNP P12497
A	32	SER	-	expression tag	UNP P12497
A	33	SER	-	expression tag	UNP P12497
A	34	HIS	-	expression tag	UNP P12497
A	35	HIS	-	expression tag	UNP P12497
A	36	HIS	-	expression tag	UNP P12497
A	37	HIS	-	expression tag	UNP P12497
A	38	HIS	-	expression tag	UNP P12497
A	39	HIS	-	expression tag	UNP P12497
A	40	SER	-	expression tag	UNP P12497
A	41	SER	-	expression tag	UNP P12497
A	42	GLY	-	expression tag	UNP P12497
A	43	LEU	-	expression tag	UNP P12497
A	44	VAL	-	expression tag	UNP P12497
A	45	PRO	-	expression tag	UNP P12497
A	46	ARG	-	expression tag	UNP P12497
A	47	GLY	-	expression tag	UNP P12497
A	48	SER	-	expression tag	UNP P12497
A	49	HIS	-	expression tag	UNP P12497
A	56	SER	CYS	engineered mutation	UNP P12497
A	139	ASP	PHE	engineered mutation	UNP P12497
A	185	HIS	PHE	engineered mutation	UNP P12497
B	30	MET	-	expression tag	UNP P12497
B	31	GLY	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	SER	-	expression tag	UNP P12497
B	33	SER	-	expression tag	UNP P12497
B	34	HIS	-	expression tag	UNP P12497
B	35	HIS	-	expression tag	UNP P12497
B	36	HIS	-	expression tag	UNP P12497
B	37	HIS	-	expression tag	UNP P12497
B	38	HIS	-	expression tag	UNP P12497
B	39	HIS	-	expression tag	UNP P12497
B	40	SER	-	expression tag	UNP P12497
B	41	SER	-	expression tag	UNP P12497
B	42	GLY	-	expression tag	UNP P12497
B	43	LEU	-	expression tag	UNP P12497
B	44	VAL	-	expression tag	UNP P12497
B	45	PRO	-	expression tag	UNP P12497
B	46	ARG	-	expression tag	UNP P12497
B	47	GLY	-	expression tag	UNP P12497
B	48	SER	-	expression tag	UNP P12497
B	49	HIS	-	expression tag	UNP P12497
B	56	SER	CYS	engineered mutation	UNP P12497
B	139	ASP	PHE	engineered mutation	UNP P12497
B	185	HIS	PHE	engineered mutation	UNP P12497

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



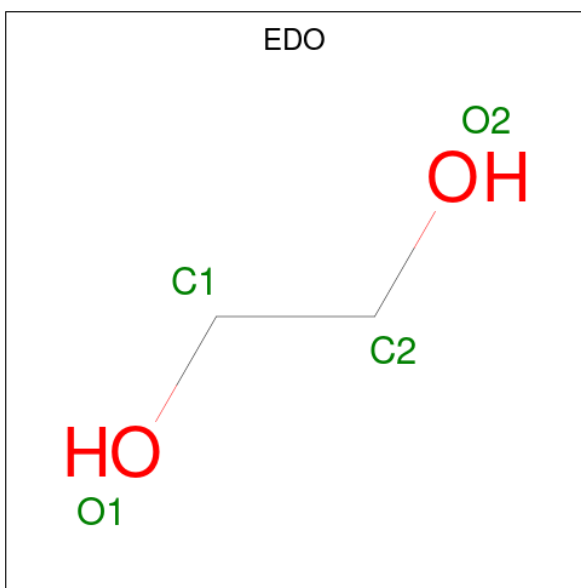
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

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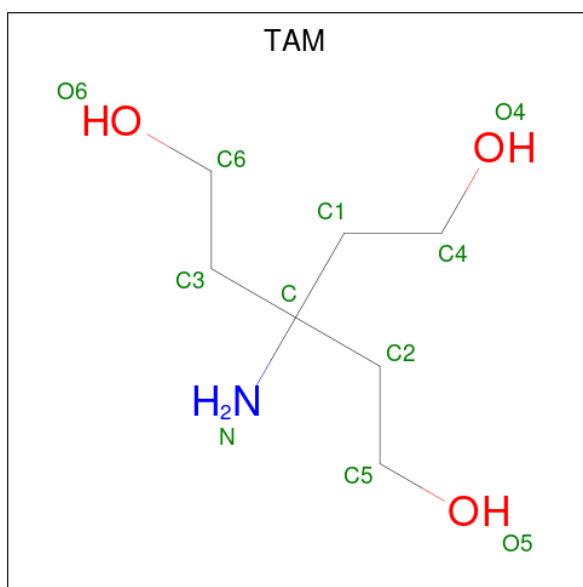
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



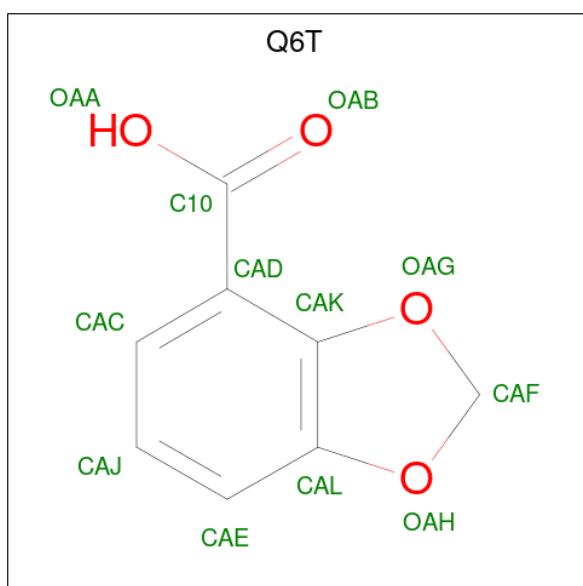
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C₇H₁₇NO₃).



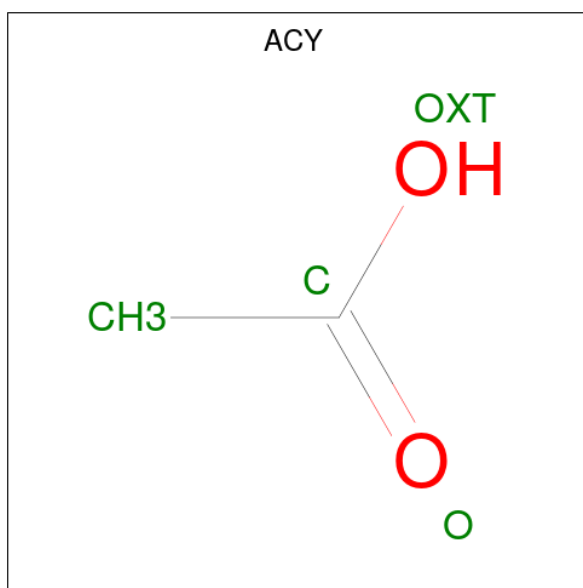
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	11	7	1	3	0	0
4	B	1	11	7	1	3	0	0

- Molecule 5 is 1,3-benzodioxole-4-carboxylic acid (three-letter code: Q6T) (formula: C₈H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	12	8	4	0	0
5	B	1	12	8	4	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			4	2 2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	103	Total	O	0	0
			103	103		
7	B	75	Total	O	0	0
			75	75		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	70.74Å 70.74Å 66.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.31 – 1.80 45.09 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (61.31-1.80) 94.7 (45.09-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.198 0.159 , 0.198	Depositor DCC
R_{free} test set	1643 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l 0.488 for h,-h-k,-l 0.020 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2782	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Q6T, ACY, EDO, TAM, 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	1.18	3/1313 (0.2%)	1.06	1/1780 (0.1%)
1	B	1.22	4/1303 (0.3%)	1.07	2/1766 (0.1%)
All	All	1.20	7/2616 (0.3%)	1.06	3/3546 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	TRP	CD2-CE2	7.42	1.50	1.41
1	A	83	TYR	CE2-CZ	6.37	1.46	1.38
1	B	61	TRP	CD2-CE2	5.75	1.48	1.41
1	A	131	TRP	CD2-CE2	5.72	1.48	1.41
1	B	61	TRP	CG-CD1	5.65	1.44	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	154	MET	CG-SD-CE	5.77	109.43	100.20
1	A	116	ASP	CB-CG-OD1	5.59	123.33	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1253	0	1303	64	0
1	B	1249	0	1288	59	0
2	A	15	0	0	3	0
2	B	25	0	0	1	0
3	A	8	0	12	11	0
3	B	4	0	6	0	0
4	A	11	0	17	7	0
4	B	11	0	17	8	0
5	A	12	0	5	2	0
5	B	12	0	5	2	0
6	B	4	0	3	28	0
7	A	103	0	0	13	0
7	B	75	0	0	7	0
All	All	2782	0	2656	134	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 25.

The worst 5 of 134 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:62[B]:GLN:NE2	1:B:151[B]:ILE:HD11	1.41	1.35
1:A:103[B]:LYS:NZ	6:B:1215:ACY:OXT	1.60	1.34
1:B:103[B]:LYS:NZ	6:B:1215:ACY:OXT	1.62	1.32
1:A:103[B]:LYS:CE	6:B:1215:ACY:H1	1.61	1.30
1:A:62[B]:GLN:NE2	1:A:151[B]:ILE:HD11	1.49	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	162/183 (88%)	161 (99%)	1 (1%)	0	100	100
1	B	160/183 (87%)	159 (99%)	1 (1%)	0	100	100
All	All	322/366 (88%)	320 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	139/150 (93%)	137 (99%)	2 (1%)	67	59
1	B	138/150 (92%)	132 (96%)	6 (4%)	29	14
All	All	277/300 (92%)	269 (97%)	8 (3%)	39	29

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	209	GLN
1	B	188	LYS
1	B	153	SER
1	B	148	GLN
1	B	166	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	HIS
1	B	171	HIS
1	B	146	GLN
1	A	209	GLN
1	B	148	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	EDO	A	1213	-	3,3,3	0.65	0	2,2,2	1.73	1 (50%)
2	SO4	B	1213	-	4,4,4	0.34	0	6,6,6	1.06	0
4	TAM	A	1215	-	10,10,10	1.49	3 (30%)	12,12,12	4.42	8 (66%)
5	Q6T	A	1216	-	13,13,13	0.93	0	18,18,18	2.21	5 (27%)
5	Q6T	B	1218	-	13,13,13	1.00	1 (7%)	18,18,18	1.82	6 (33%)
2	SO4	B	1211	-	4,4,4	0.55	0	6,6,6	1.31	0
2	SO4	A	1210	-	4,4,4	0.24	0	6,6,6	1.11	0
6	ACY	B	1215	-	3,3,3	0.79	0	3,3,3	0.87	0
3	EDO	A	1214	-	3,3,3	0.35	0	2,2,2	1.09	0
3	EDO	B	1216	-	3,3,3	0.50	0	2,2,2	0.55	0
4	TAM	B	1217	-	10,10,10	1.49	2 (20%)	12,12,12	4.51	6 (50%)
2	SO4	B	1212	-	4,4,4	0.56	0	6,6,6	0.75	0
2	SO4	A	1212	-	4,4,4	0.48	0	6,6,6	1.14	0
2	SO4	B	1214	-	4,4,4	0.86	0	6,6,6	1.55	2 (33%)
2	SO4	B	1210	-	4,4,4	0.30	0	6,6,6	1.05	0
2	SO4	A	1211	-	4,4,4	0.31	0	6,6,6	0.67	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	EDO	A	1213	-	-	0/1/1/1	-
4	TAM	A	1215	-	-	5/12/12/12	-
5	Q6T	A	1216	-	-	0/4/10/10	0/2/2/2
5	Q6T	B	1218	-	-	0/4/10/10	0/2/2/2
3	EDO	A	1214	-	-	1/1/1/1	-
3	EDO	B	1216	-	-	0/1/1/1	-
4	TAM	B	1217	-	-	9/12/12/12	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1215	TAM	C1-C4	2.50	1.56	1.52
4	B	1217	TAM	C3-C	-2.50	1.50	1.53
4	B	1217	TAM	C1-C4	2.36	1.56	1.52
4	A	1215	TAM	C1-C	-2.12	1.50	1.53
5	B	1218	Q6T	OAH-CAL	2.08	1.41	1.38

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1217	TAM	C6-C3-C	-11.17	102.80	115.97
4	A	1215	TAM	C6-C3-C	-10.26	103.87	115.97
4	B	1217	TAM	C3-C-N	-6.95	90.77	108.22
4	A	1215	TAM	C3-C-N	-6.82	91.10	108.22
5	A	1216	Q6T	CAF-OAH-CAL	-5.07	98.53	105.32

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1215	TAM	C1-C-C3-C6
4	A	1215	TAM	C2-C-C3-C6
4	A	1215	TAM	N-C-C3-C6
4	A	1215	TAM	C-C2-C5-O5
4	A	1215	TAM	C-C3-C6-O6

There are no ring outliers.

8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1213	EDO	11	0
4	A	1215	TAM	7	0
5	A	1216	Q6T	2	0
5	B	1218	Q6T	2	0
6	B	1215	ACY	28	0
4	B	1217	TAM	8	0
2	B	1214	SO4	1	0
2	A	1211	SO4	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	151/183 (82%)	-0.69	0 100 100	10, 17, 44, 66	14 (9%)
1	B	150/183 (81%)	-0.66	1 (0%) 87 86	10, 18, 43, 57	13 (8%)
All	All	301/366 (82%)	-0.67	1 (0%) 94 92	10, 17, 44, 66	27 (8%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	TYR	2.4

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 monosaccharides 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(Å ²)	Q<0.9
6	ACY	B	1215	4/4	0.76	0.29	29,31,34,38	4
4	TAM	A	1215	11/11	0.91	0.13	27,33,45,47	0
4	TAM	B	1217	11/11	0.91	0.13	27,35,47,51	0
2	SO4	B	1214	5/5	0.91	0.12	28,29,39,45	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	Q6T	A	1216	12/12	0.92	0.18	38,40,47,49	0
3	EDO	A	1213	4/4	0.93	0.08	29,32,35,41	0
5	Q6T	B	1218	12/12	0.94	0.15	31,38,46,47	0
3	EDO	A	1214	4/4	0.95	0.13	38,39,40,58	0
2	SO4	A	1211	5/5	0.96	0.07	33,41,49,52	5
2	SO4	B	1212	5/5	0.96	0.07	39,48,56,58	5
3	EDO	B	1216	4/4	0.97	0.07	27,35,41,41	0
2	SO4	B	1211	5/5	0.97	0.07	30,41,46,47	5
2	SO4	B	1213	5/5	0.98	0.10	29,35,37,40	5
2	SO4	A	1212	5/5	0.98	0.09	28,35,36,38	5
2	SO4	A	1210	5/5	0.99	0.10	26,28,31,36	5
2	SO4	B	1210	5/5	0.99	0.09	23,26,34,34	5

6.5 Other polymers [i](#)

There are no such residues in this entry.