



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:47 PM UTC

PDB ID : 3A4Y / pdb_00003a4y
Title : Crystal Structure of H61A mutant TTHA0252 from *Thermus thermophilus* HB8
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2009-07-22
Resolution : 2.50 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	:	4-5-2 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

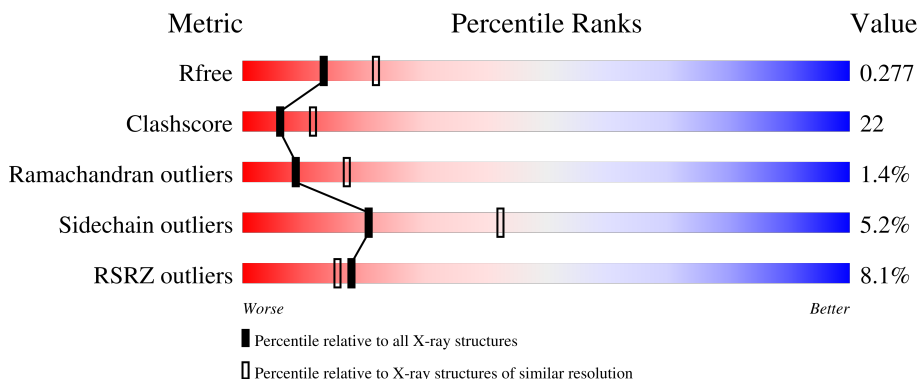
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13743 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.

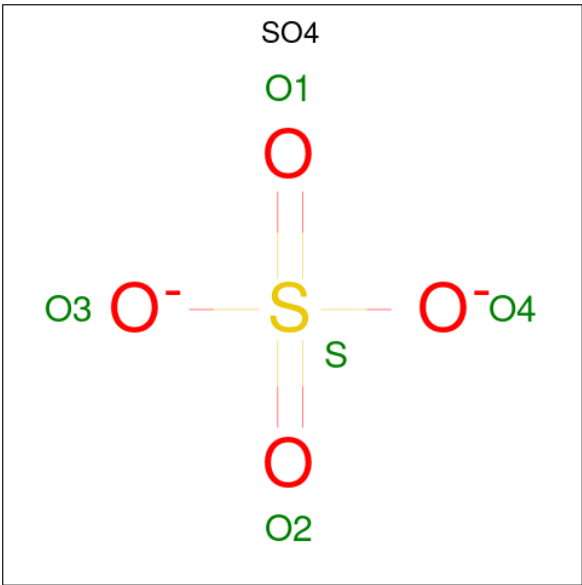
- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	HIS	engineered mutation	UNP Q5SLP1
B	61	ALA	HIS	engineered mutation	UNP Q5SLP1
C	61	ALA	HIS	engineered mutation	UNP Q5SLP1
D	61	ALA	HIS	engineered mutation	UNP Q5SLP1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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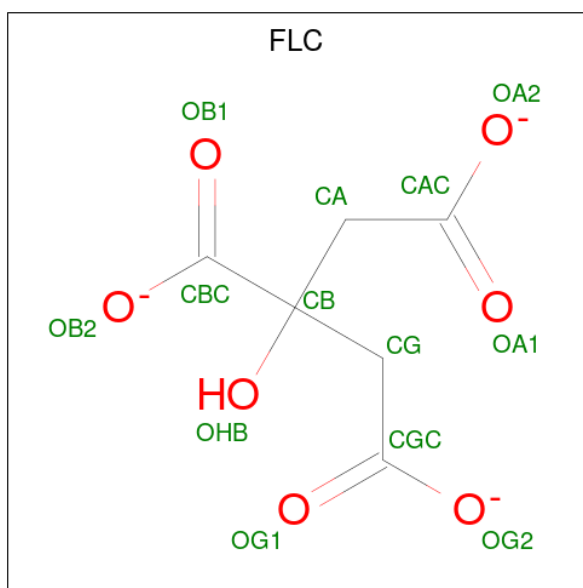
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

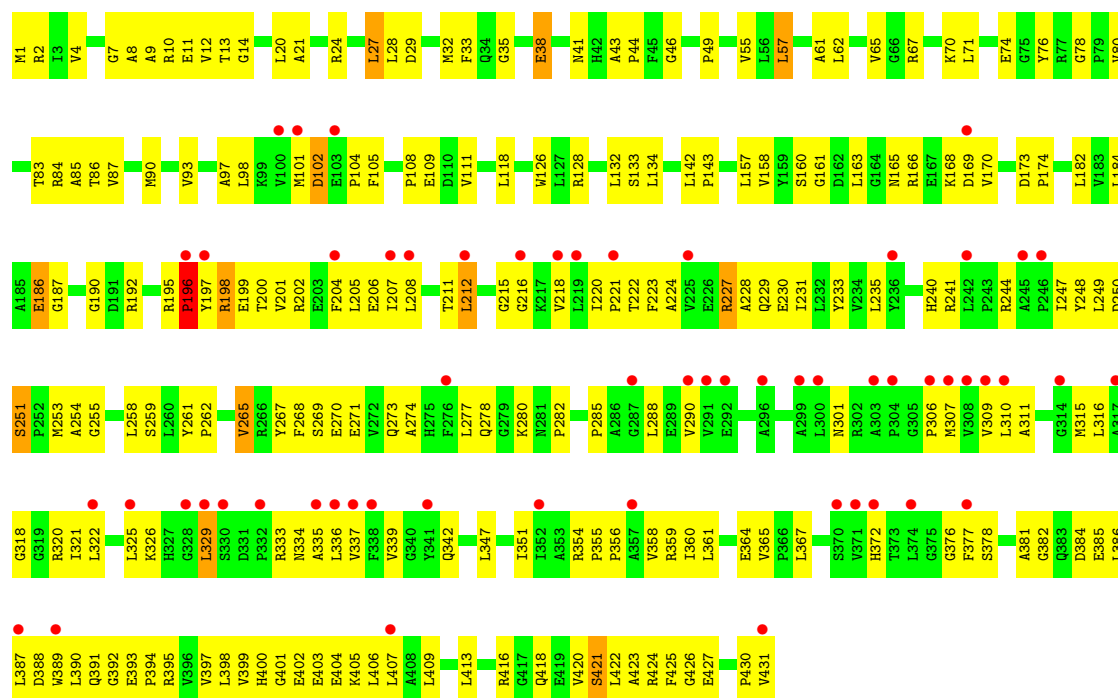
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	54	Total	O	0	0
			54	54		

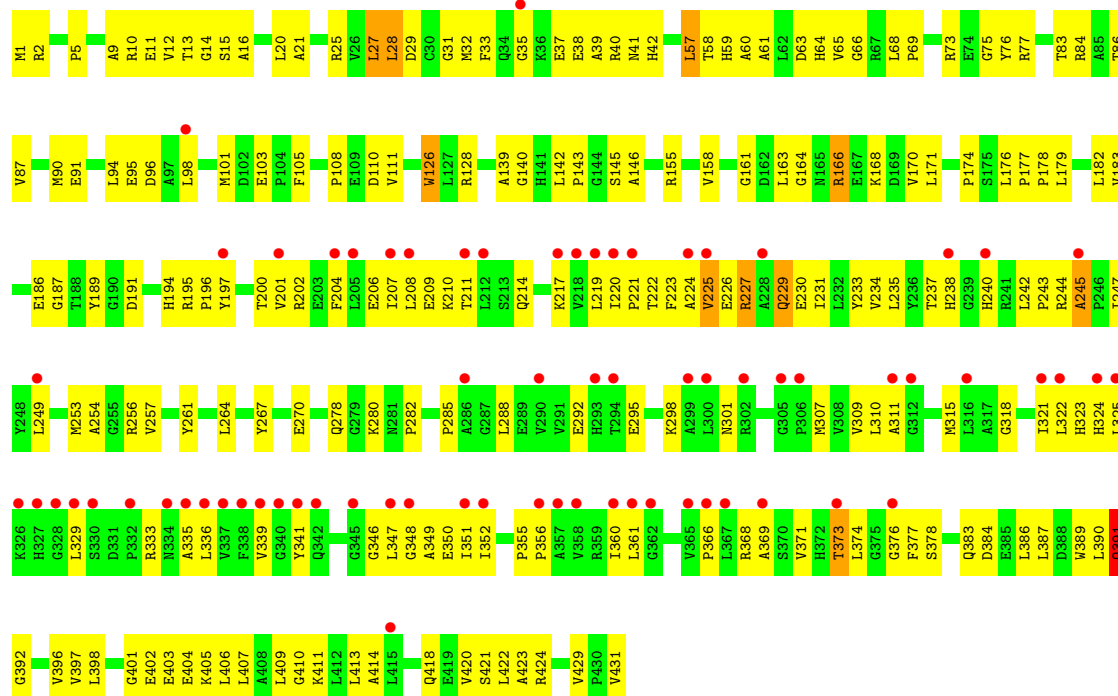
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	17	Total	O	0	0
			17	17		
5	D	15	Total	O	0	0
			15	15		



• Molecule 1: Ribonuclease TTHA0252



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.14Å 146.77Å 121.12Å 90.00° 109.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.50) 96.4 (50.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.282 0.235 , 0.277	Depositor DCC
R_{free} test set	8161 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13743	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: FLC, SO4, ZN

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	0.51	0/3401	0.99	15/4613 (0.3%)
1	B	0.48	0/3401	1.00	14/4613 (0.3%)
1	C	0.40	0/3401	0.92	8/4613 (0.2%)
1	D	0.38	0/3401	0.93	10/4613 (0.2%)
All	All	0.44	0/13604	0.96	47/18452 (0.3%)

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	VAL	N-CA-C	9.89	119.71	110.42
1	C	4	VAL	N-CA-C	8.66	116.12	107.55
1	B	60	ALA	N-CA-C	8.25	122.44	112.38
1	B	161	GLY	N-CA-C	-8.03	97.08	112.02
1	D	75	GLY	N-CA-C	7.82	124.00	114.69

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	3321	0	3349	121	0
1	B	3321	0	3349	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3321	0	3349	186	0
1	D	3321	0	3349	171	0
2	A	95	0	0	1	0
2	B	75	0	0	0	0
2	C	65	0	0	0	0
2	D	45	0	0	2	0
3	A	13	0	5	0	0
3	B	13	0	5	1	0
3	C	13	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	50	0	0	2	0
5	B	54	0	0	3	0
5	C	17	0	0	0	0
5	D	15	0	0	1	0
All	All	13743	0	13411	605	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 22.

The worst 5 of 605 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:37:GLU:HG3	1:B:40:ARG:HH11	1.11	1.09
1:C:391:GLN:HA	1:C:416:ARG:HH12	1.22	1.04
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.40	1.01
1:D:285:PRO:HD2	1:D:288:LEU:HD22	1.39	1.00
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.26	0.99

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	429/431 (100%)	402 (94%)	25 (6%)	2 (0%)	24	43
1	B	429/431 (100%)	393 (92%)	30 (7%)	6 (1%)	9	17
1	C	429/431 (100%)	376 (88%)	44 (10%)	9 (2%)	5	9
1	D	429/431 (100%)	384 (90%)	38 (9%)	7 (2%)	7	14
All	All	1716/1724 (100%)	1555 (91%)	137 (8%)	24 (1%)	9	17

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ASP
1	C	102	ASP
1	C	394	PRO
1	A	101	MET
1	B	225	VAL

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	341/341 (100%)	316 (93%)	25 (7%)	13	27
1	B	341/341 (100%)	317 (93%)	24 (7%)	14	29
1	C	341/341 (100%)	331 (97%)	10 (3%)	37	65
1	D	341/341 (100%)	329 (96%)	12 (4%)	32	58
All	All	1364/1364 (100%)	1293 (95%)	71 (5%)	21	42

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	320	ARG
1	D	27	LEU
1	D	227	ARG

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Mol	Chain	Res	Type
1	A	416	ARG
1	A	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	214	GLN
1	D	275	HIS
1	C	41	ASN
1	B	383	GLN
1	D	301	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 4 are monoatomic - leaving 59 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	$\# Z > 2$
2	SO4	D	432	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	434	-	4,4,4	1.06	0	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	443	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	439	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	444	-	4,4,4	1.07	0	6,6,6	0.55	0
2	SO4	D	435	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	440	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	441	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	D	436	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	A	448	-	4,4,4	1.11	0	6,6,6	0.57	0
2	SO4	B	435	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	B	442	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	B	446	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	443	-	4,4,4	1.04	0	6,6,6	0.64	0
2	SO4	B	438	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	B	439	-	4,4,4	1.04	0	6,6,6	0.57	0
2	SO4	B	433	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	B	436	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	A	442	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	A	447	-	4,4,4	1.08	0	6,6,6	0.55	0
2	SO4	C	444	-	4,4,4	1.05	0	6,6,6	0.59	0
2	SO4	A	449	-	4,4,4	1.08	0	6,6,6	0.60	0
2	SO4	C	435	-	4,4,4	1.04	0	6,6,6	0.61	0
2	SO4	B	434	-	4,4,4	1.06	0	6,6,6	0.57	0
3	FLC	C	445	-	12,12,12	1.63	5 (41%)	17,17,17	1.28	1 (5%)
2	SO4	A	445	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	440	-	4,4,4	1.08	0	6,6,6	0.54	0
2	SO4	B	445	-	4,4,4	1.07	0	6,6,6	0.60	0
2	SO4	A	450	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	D	438	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	D	433	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	A	435	-	4,4,4	1.07	0	6,6,6	0.62	0
2	SO4	B	443	-	4,4,4	1.03	0	6,6,6	0.60	0
3	FLC	B	447	-	12,12,12	1.67	5 (41%)	17,17,17	1.31	1 (5%)
3	FLC	A	451	-	12,12,12	1.59	3 (25%)	17,17,17	1.31	1 (5%)
2	SO4	A	439	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	B	432	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	444	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	440	-	4,4,4	1.10	0	6,6,6	0.55	0
2	SO4	B	441	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	434	-	4,4,4	1.05	0	6,6,6	0.57	0
2	SO4	D	434	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	433	-	4,4,4	1.09	0	6,6,6	0.61	0
2	SO4	C	437	-	4,4,4	1.08	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	436	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	438	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	B	437	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	D	437	-	4,4,4	1.08	0	6,6,6	0.58	0
2	SO4	C	432	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	A	446	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	439	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	C	433	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	432	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	438	-	4,4,4	1.08	0	6,6,6	0.59	0
2	SO4	C	440	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	C	436	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	A	437	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	442	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	441	-	4,4,4	1.04	0	6,6,6	0.58	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	FLC	B	447	-	-	0/16/16/16	-
3	FLC	A	451	-	-	0/16/16/16	-
3	FLC	C	445	-	-	0/16/16/16	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	451	FLC	OG2-CGC	-2.77	1.21	1.30
3	B	447	FLC	CG-CB	2.70	1.57	1.54
3	A	451	FLC	OA2-CAC	-2.65	1.22	1.30
3	C	445	FLC	OA2-CAC	-2.61	1.22	1.30
3	B	447	FLC	OA2-CAC	-2.55	1.22	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	451	FLC	OB2-CBC-CB	3.74	120.32	113.14
3	B	447	FLC	OB2-CBC-CB	3.67	120.19	113.14
3	C	445	FLC	OB2-CBC-CB	3.64	120.13	113.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	435	SO4	1	0
2	A	449	SO4	1	0
3	C	445	FLC	1	0
2	D	438	SO4	1	0
3	B	447	FLC	1	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	431/431 (100%)	-0.11	1 (0%) 91 89	22, 41, 63, 86	0
1	B	431/431 (100%)	0.14	9 (2%) 63 59	24, 43, 68, 87	0
1	C	431/431 (100%)	0.83	58 (13%) 7 5	28, 71, 111, 122	0
1	D	431/431 (100%)	0.91	71 (16%) 4 3	33, 67, 126, 131	0
All	All	1724/1724 (100%)	0.44	139 (8%) 18 15	22, 51, 115, 131	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	339	VAL	4.2
1	D	322	LEU	4.2
1	D	367	LEU	4.1
1	D	338	PHE	4.1
1	C	329	LEU	4.0

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	SO4	D	438	5/5	0.41	0.15	137,137,137,137	0
3	FLC	C	445	13/13	0.43	0.14	117,119,121,121	0
2	SO4	C	433	5/5	0.54	0.11	140,141,141,141	0
2	SO4	A	441	5/5	0.54	0.10	143,143,143,143	0
2	SO4	A	448	5/5	0.54	0.15	150,150,150,150	0
2	SO4	B	438	5/5	0.56	0.15	136,136,137,137	0
2	SO4	C	441	5/5	0.58	0.12	151,151,151,152	0
2	SO4	C	444	5/5	0.60	0.14	129,130,130,131	0
2	SO4	B	446	5/5	0.63	0.18	118,119,119,120	0
2	SO4	A	438	5/5	0.64	0.11	122,123,123,123	0
2	SO4	C	437	5/5	0.64	0.13	115,115,116,116	0
2	SO4	A	440	5/5	0.65	0.12	136,136,137,137	0
2	SO4	C	440	5/5	0.65	0.09	140,140,140,141	0
3	FLC	A	451	13/13	0.65	0.19	108,109,111,112	0
2	SO4	A	436	5/5	0.65	0.22	155,155,155,156	0
2	SO4	B	432	5/5	0.67	0.09	120,120,120,120	0
2	SO4	B	434	5/5	0.67	0.09	129,129,129,129	0
2	SO4	A	439	5/5	0.68	0.15	133,134,134,134	0
2	SO4	A	445	5/5	0.68	0.10	114,114,114,114	0
2	SO4	A	432	5/5	0.68	0.21	135,136,136,136	0
2	SO4	A	450	5/5	0.69	0.10	127,127,128,128	0
2	SO4	C	432	5/5	0.70	0.12	104,105,106,106	0
2	SO4	A	437	5/5	0.70	0.10	125,125,125,126	0
2	SO4	A	447	5/5	0.70	0.15	134,134,134,134	0
3	FLC	B	447	13/13	0.71	0.24	104,111,113,113	0
2	SO4	C	436	5/5	0.73	0.10	114,114,115,115	0
2	SO4	D	435	5/5	0.73	0.10	133,133,133,133	0
2	SO4	D	432	5/5	0.74	0.10	140,140,140,141	0
2	SO4	D	439	5/5	0.75	0.09	137,137,137,137	0
2	SO4	B	442	5/5	0.75	0.11	100,101,101,102	0
2	SO4	B	437	5/5	0.76	0.11	121,121,122,122	0
2	SO4	D	433	5/5	0.76	0.08	123,123,123,123	0
2	SO4	C	434	5/5	0.77	0.13	131,131,131,132	0
2	SO4	B	435	5/5	0.79	0.11	114,114,114,114	0
2	SO4	B	436	5/5	0.80	0.12	116,116,116,117	0
2	SO4	B	440	5/5	0.80	0.16	89,90,91,92	0
2	SO4	C	439	5/5	0.82	0.10	121,121,121,122	0
2	SO4	A	442	5/5	0.82	0.12	97,98,99,99	0
2	SO4	A	446	5/5	0.83	0.09	110,111,111,111	0
2	SO4	C	438	5/5	0.83	0.13	105,105,105,105	0
2	SO4	B	441	5/5	0.84	0.09	90,91,91,91	0
2	SO4	D	434	5/5	0.84	0.11	116,116,116,116	0
2	SO4	A	434	5/5	0.85	0.09	119,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	445	5/5	0.86	0.09	81,82,83,83	0
2	SO4	C	435	5/5	0.87	0.11	87,88,89,89	0
2	SO4	C	443	5/5	0.87	0.08	102,102,102,103	0
2	SO4	B	433	5/5	0.87	0.11	97,97,98,99	0
4	ZN	B	448	1/1	0.89	0.09	84,84,84,84	0
2	SO4	A	443	5/5	0.90	0.11	76,77,77,79	0
2	SO4	B	439	5/5	0.91	0.10	72,74,74,74	0
2	SO4	D	440	5/5	0.93	0.08	81,82,83,83	0
2	SO4	B	444	5/5	0.93	0.09	45,49,50,51	0
2	SO4	D	437	5/5	0.93	0.11	88,88,89,90	0
2	SO4	A	444	5/5	0.93	0.08	82,82,82,83	0
2	SO4	B	443	5/5	0.93	0.09	60,61,62,63	0
4	ZN	C	446	1/1	0.93	0.09	100,100,100,100	0
4	ZN	D	441	1/1	0.93	0.11	92,92,92,92	0
2	SO4	C	442	5/5	0.94	0.07	64,64,66,66	0
2	SO4	D	436	5/5	0.94	0.07	67,67,68,69	0
2	SO4	A	433	5/5	0.94	0.14	59,61,62,64	0
2	SO4	A	449	5/5	0.94	0.08	40,44,46,47	0
4	ZN	A	452	1/1	0.97	0.06	80,80,80,80	0
2	SO4	A	435	5/5	0.97	0.08	43,44,46,50	0

6.5 Other polymers

There are no such residues in this entry.