wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 10:20 PM EDT

PDB ID	:	3IE0
Title	:	Crystal Structure of S378Y 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	:	2.73 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 (i) 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 (i)) were used in the production of this report:

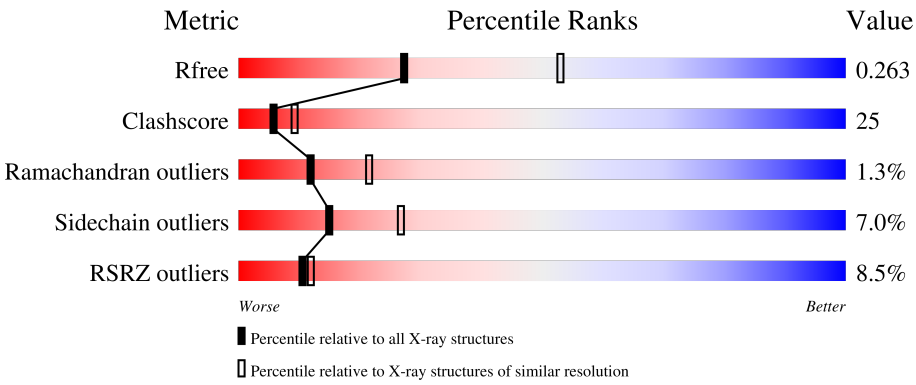
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	431	2%, 67%, 29%, •
1	B	431	%, 58%, 38%, •
1	C	431	11%, 50%, 45%, 5%
1	D	431	20%, 49%, 48%, •

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	B	433	-	-	X	X
2	SO4	B	437	-	-	-	X
2	SO4	B	446	-	-	X	X
2	SO4	B	448	-	-	X	X
2	SO4	C	441	-	-	-	X
2	SO4	D	433	-	-	X	-
2	SO4	D	434	-	-	-	X
3	FLC	A	453	-	-	-	X
3	FLC	B	451	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13790 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.

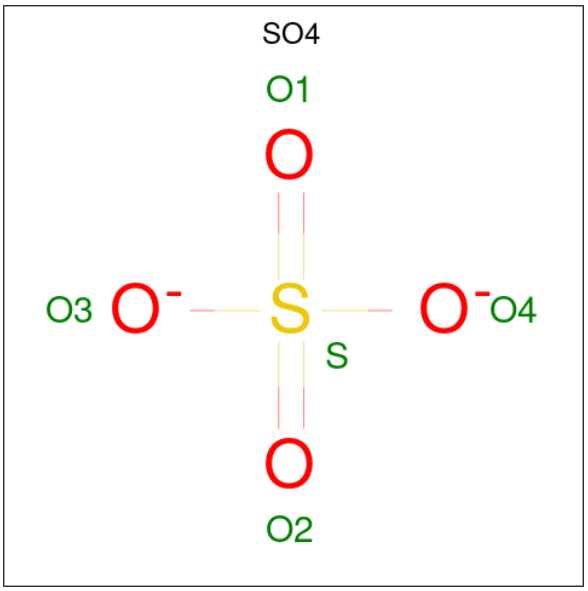
- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	431	3332	2133	597	594	8	0	0	0
1	B	431	3332	2133	597	594	8	0	0	0
1	C	431	3332	2133	597	594	8	0	0	0
1	D	431	3332	2133	597	594	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	TYR	SER	engineered mutation	UNP Q5SLP1
B	378	TYR	SER	engineered mutation	UNP Q5SLP1
C	378	TYR	SER	engineered mutation	UNP Q5SLP1
D	378	TYR	SER	engineered mutation	UNP Q5SLP1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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

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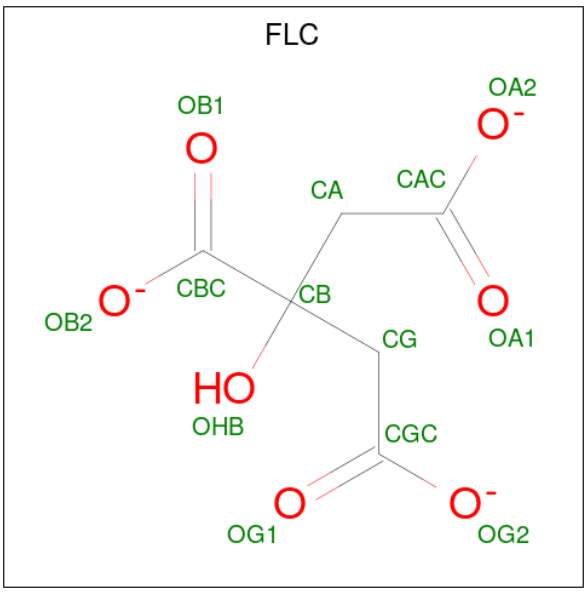
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0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

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	2	2	2	0	0
			Total	Zn		
4	B	2	2	2	0	0
			Total	Zn		
4	C	2	2	2	0	0
			Total	Zn		
4	D	2	2	2	0	0

- Molecule 5 is water.

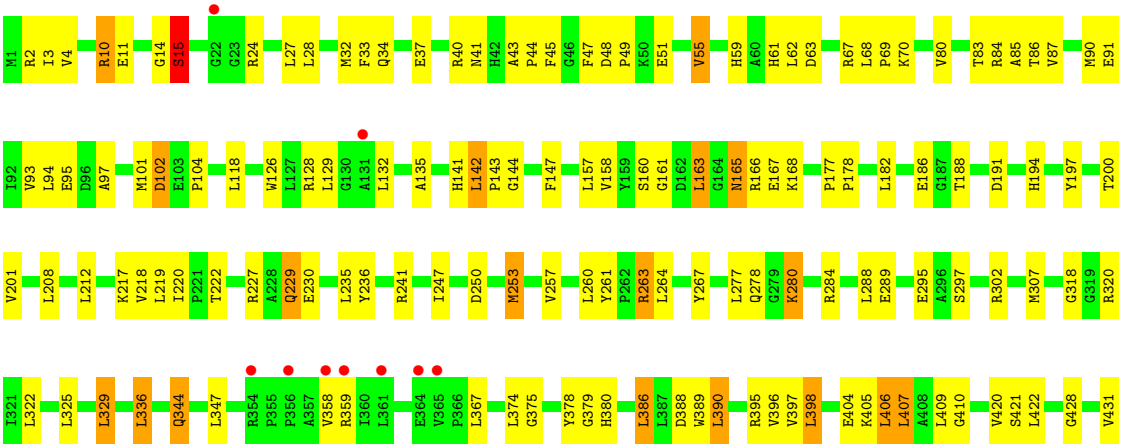
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	26	26	26	0	0
			Total	O		
5	B	33	33	33	0	0
			Total	O		
5	C	9	9	9	0	0
			Total	O		
5	D	12	12	12	0	0

3 Residue-property plots (i)

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.

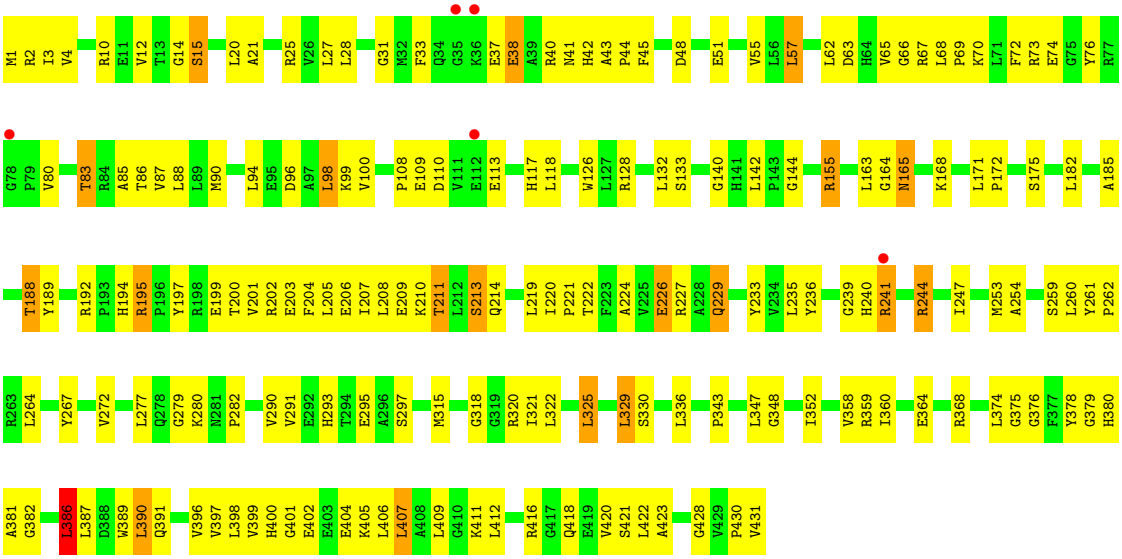
- Molecule 1: Ribonuclease TTHA0252

Chain A:



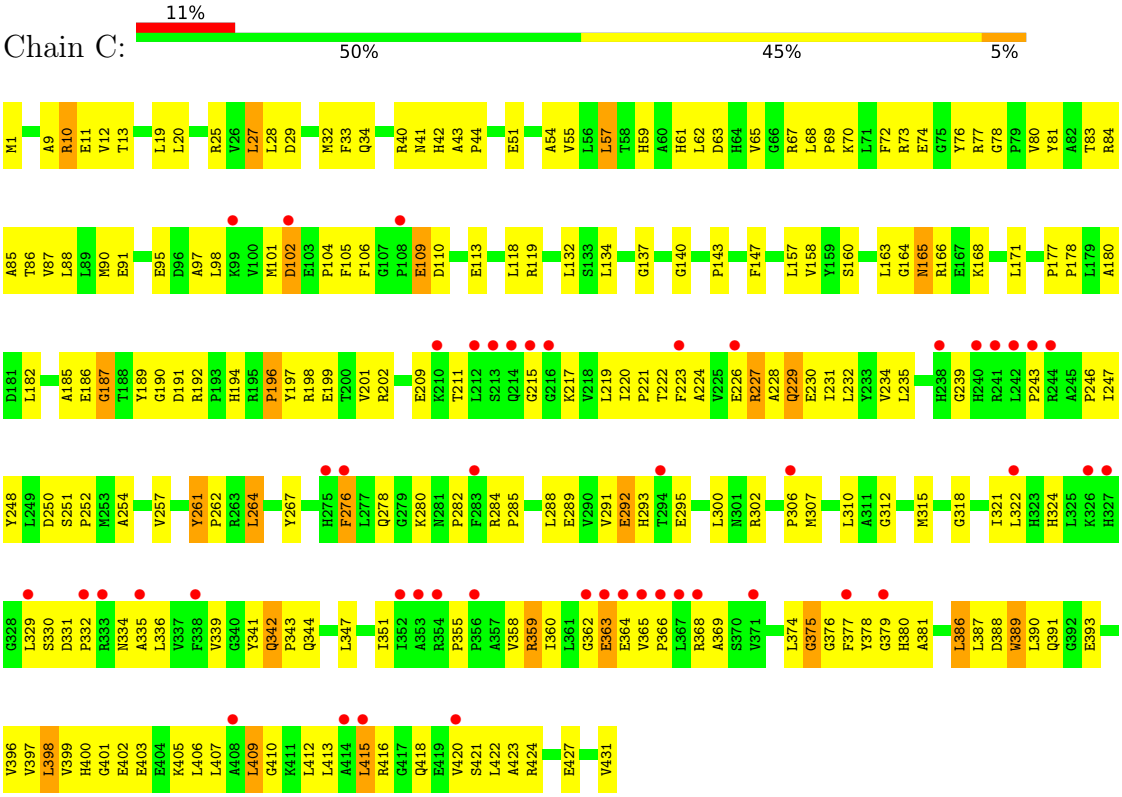
- Molecule 1: Ribonuclease TTHA0252

Chain B:



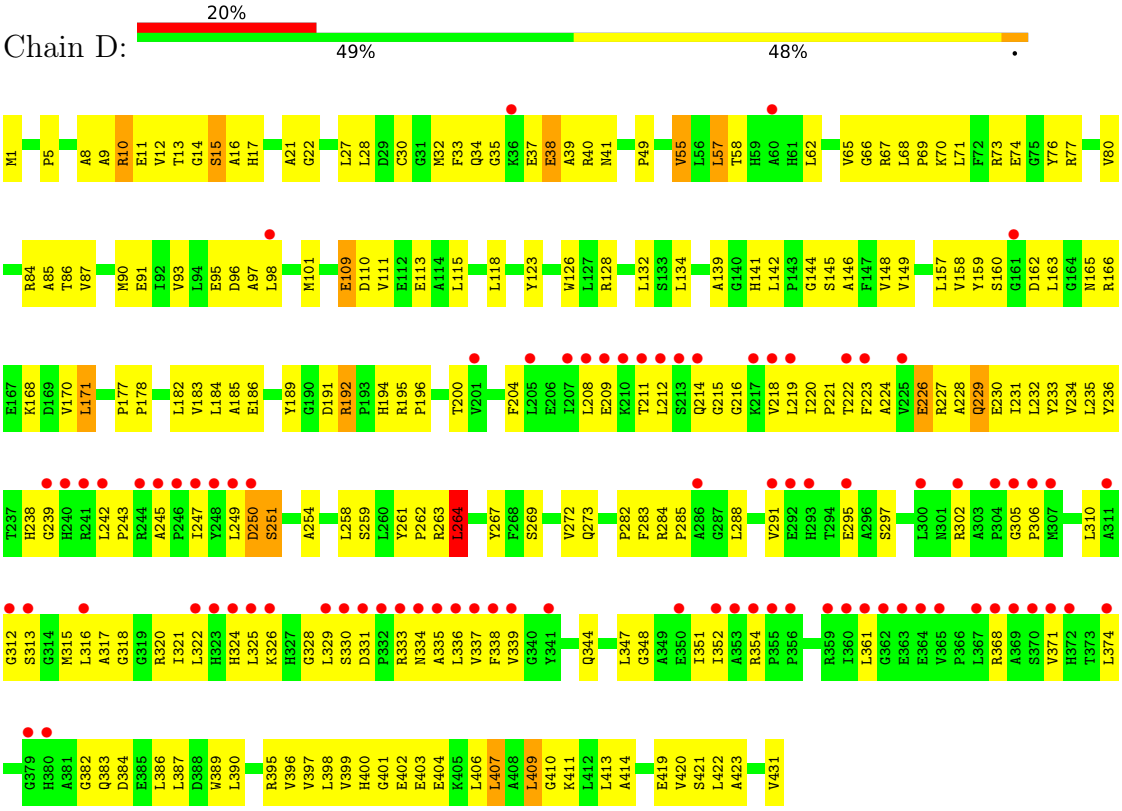
- Molecule 1: Ribonuclease TTHA0252

Chain C:



- Molecule 1: Ribonuclease TTHA0252

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.18Å 146.12Å 121.00Å 90.00° 109.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.73 41.86 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.73) 96.1 (41.86-2.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.48 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.272 0.213 , 0.263	Depositor DCC
R_{free} test set	6258 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13790	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, ZN, 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	0.41	0/3414	0.68	2/4631 (0.0%)
1	B	0.39	0/3414	0.69	2/4631 (0.0%)
1	C	0.32	0/3414	0.59	0/4631
1	D	0.31	0/3414	0.58	0/4631
All	All	0.36	0/13656	0.64	4/18524 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	379	GLY	N-CA-C	7.17	131.03	113.10
1	B	379	GLY	N-CA-C	6.04	128.19	113.10
1	B	386	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	161	GLY	N-CA-C	-5.29	99.86	113.10

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	3332	0	3355	121	0
1	B	3332	0	3355	162	0
1	C	3332	0	3355	208	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3332	0	3355	205	0
2	A	100	0	0	2	0
2	B	95	0	0	9	0
2	C	95	0	0	1	0
2	D	45	0	0	4	0
3	A	26	0	10	2	0
3	B	13	0	5	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	26	0	0	1	0
5	B	33	0	0	2	0
5	C	9	0	0	0	0
5	D	12	0	0	1	0
All	All	13790	0	13435	689	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 689 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:A:263:ARG:HH21	1:A:263:ARG:HB3	1.00	1.14
1:C:73:ARG:HH21	1:C:106:PHE:HA	1.23	1.03
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.40	1.02
1:D:13:THR:CG2	1:D:33:PHE:HA	1.91	1.00
1:B:430:PRO:HG3	2:B:446:SO4:O3	1.62	0.98

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%)	400 (93%)	28 (6%)	1 (0%)	47	69
1	B	429/431 (100%)	387 (90%)	36 (8%)	6 (1%)	11	20
1	C	429/431 (100%)	370 (86%)	54 (13%)	5 (1%)	13	24
1	D	429/431 (100%)	376 (88%)	43 (10%)	10 (2%)	6	10
All	All	1716/1724 (100%)	1533 (89%)	161 (9%)	22 (1%)	12	21

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	HIS
1	B	38	GLU
1	B	188	THR
1	B	241	ARG
1	C	375	GLY

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	342/342 (100%)	314 (92%)	28 (8%)	11	21
1	B	342/342 (100%)	313 (92%)	29 (8%)	10	20
1	C	342/342 (100%)	319 (93%)	23 (7%)	16	29
1	D	342/342 (100%)	326 (95%)	16 (5%)	26	45
All	All	1368/1368 (100%)	1272 (93%)	96 (7%)	15	27

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	10	ARG
1	C	342	GLN
1	C	57	LEU
1	C	261	TYR
1	C	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	194	HIS
1	D	214	GLN
1	D	301	ASN
1	B	383	GLN
1	B	165	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 8 are monoatomic - leaving 70 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	B	449	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	C	444	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	C	438	-	4,4,4	1.04	0	6,6,6	0.66	0
2	SO4	A	436	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	A	448	-	4,4,4	1.01	0	6,6,6	0.67	0
2	SO4	C	439	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	C	437	-	4,4,4	1.05	0	6,6,6	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	D	438	-	4,4,4	0.98	0	6,6,6	0.69	0
2	SO4	B	443	-	4,4,4	1.04	0	6,6,6	0.68	0
2	SO4	A	445	-	4,4,4	0.99	0	6,6,6	0.66	0
2	SO4	C	442	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	A	438	-	4,4,4	1.02	0	6,6,6	0.63	0
2	SO4	B	439	-	4,4,4	0.93	0	6,6,6	0.72	0
2	SO4	C	445	-	4,4,4	1.01	0	6,6,6	0.64	0
2	SO4	C	446	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	D	436	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	B	448	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	D	440	-	4,4,4	1.04	0	6,6,6	0.64	0
2	SO4	A	441	-	4,4,4	0.98	0	6,6,6	0.70	0
2	SO4	A	437	-	4,4,4	1.05	0	6,6,6	0.64	0
2	SO4	A	450	-	4,4,4	0.99	0	6,6,6	0.67	0
2	SO4	B	445	-	4,4,4	1.00	0	6,6,6	0.65	0
2	SO4	D	432	-	4,4,4	1.01	0	6,6,6	0.67	0
2	SO4	C	432	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	C	436	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	A	434	-	4,4,4	1.00	0	6,6,6	0.65	0
2	SO4	C	433	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	A	439	-	4,4,4	1.00	0	6,6,6	0.64	0
2	SO4	A	432	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	C	434	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	B	440	-	4,4,4	1.04	0	6,6,6	0.61	0
2	SO4	B	435	-	4,4,4	1.00	0	6,6,6	0.69	0
2	SO4	A	446	-	4,4,4	1.01	0	6,6,6	0.64	0
2	SO4	A	449	-	4,4,4	1.04	0	6,6,6	0.61	0
2	SO4	D	439	-	4,4,4	1.04	0	6,6,6	0.69	0
2	SO4	A	451	-	4,4,4	1.03	0	6,6,6	0.71	0
2	SO4	C	449	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	D	437	-	4,4,4	1.03	0	6,6,6	0.62	0
2	SO4	B	446	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	D	434	-	4,4,4	1.05	0	6,6,6	0.65	0
2	SO4	B	444	-	4,4,4	1.02	0	6,6,6	0.66	0
3	FLC	B	451	-	12,12,12	2.26	5 (41%)	17,17,17	1.25	1 (5%)
2	SO4	B	438	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	A	433	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	C	448	-	4,4,4	1.05	0	6,6,6	0.66	0
2	SO4	A	442	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	B	437	-	4,4,4	1.00	0	6,6,6	0.68	0
3	FLC	A	452	-	12,12,12	1.63	4 (33%)	17,17,17	1.44	1 (5%)
2	SO4	C	447	-	4,4,4	1.00	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	435	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	B	436	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	D	433	-	4,4,4	1.03	0	6,6,6	0.71	0
3	FLC	A	453	-	12,12,12	1.69	6 (50%)	17,17,17	1.42	1 (5%)
2	SO4	C	443	-	4,4,4	1.03	0	6,6,6	0.62	0
2	SO4	C	441	-	4,4,4	1.01	0	6,6,6	0.67	0
2	SO4	A	447	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	B	441	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	D	435	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	C	440	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	B	442	-	4,4,4	1.01	0	6,6,6	0.64	0
2	SO4	B	432	-	4,4,4	1.00	0	6,6,6	0.68	0
2	SO4	B	450	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	B	433	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	B	434	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	A	440	-	4,4,4	1.00	0	6,6,6	0.64	0
2	SO4	A	444	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	A	443	-	4,4,4	1.01	0	6,6,6	0.67	0
2	SO4	C	450	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	B	447	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	C	435	-	4,4,4	1.02	0	6,6,6	0.68	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	451	-	-	0/16/16/16	-
3	FLC	A	453	-	-	0/16/16/16	-
3	FLC	A	452	-	-	0/16/16/16	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	451	FLC	CB-CBC	-5.57	1.47	1.53
3	A	452	FLC	CA-CB	2.62	1.57	1.53
3	A	452	FLC	OA2-CAC	-2.59	1.22	1.30
3	B	451	FLC	OG2-CGC	-2.56	1.22	1.30
3	B	451	FLC	CA-CB	2.49	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	452	FLC	OB2-CBC-CB	4.33	120.56	113.05
3	A	453	FLC	OB2-CBC-CB	4.22	120.38	113.05
3	B	451	FLC	OB2-CBC-CB	2.94	118.16	113.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	448	SO4	1	0
2	B	448	SO4	2	0
2	A	441	SO4	1	0
2	C	434	SO4	1	0
2	B	446	SO4	2	0
3	B	451	FLC	4	0
2	B	437	SO4	1	0
3	A	452	FLC	1	0
2	D	433	SO4	4	0
3	A	453	FLC	1	0
2	B	441	SO4	1	0
2	B	433	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	431/431 (100%)	-0.10	9 (2%)	63	70	22, 40, 63, 89	0
1	B	431/431 (100%)	-0.05	5 (1%)	79	83	22, 43, 74, 93	0
1	C	431/431 (100%)	0.62	48 (11%)	5	5	26, 72, 125, 136	0
1	D	431/431 (100%)	0.95	85 (19%)	1	1	34, 75, 147, 153	0
All	All	1724/1724 (100%)	0.36	147 (8%)	10	12	22, 51, 129, 153	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	216	GLY	6.5
1	D	218	VAL	6.1
1	D	212	LEU	5.8
1	D	242	LEU	5.6
1	D	360	ILE	5.4

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
2	SO4	B	436	5/5	0.53	0.32	148,148,149,149	0
2	SO4	D	436	5/5	0.53	0.32	170,170,170,170	0
2	SO4	C	445	5/5	0.56	0.33	162,162,163,163	0
4	ZN	A	455	1/1	0.57	0.15	88,88,88,88	0
2	SO4	A	435	5/5	0.65	0.34	142,142,143,143	0
2	SO4	B	448	5/5	0.66	0.58	178,178,178,178	0
2	SO4	B	437	5/5	0.68	0.45	169,169,170,170	0
2	SO4	D	434	5/5	0.68	0.48	163,163,164,164	0
2	SO4	B	450	5/5	0.71	0.30	137,137,138,138	0
2	SO4	A	442	5/5	0.72	0.30	141,141,141,142	0
3	FLC	A	453	13/13	0.72	0.41	122,123,124,124	0
2	SO4	C	438	5/5	0.72	0.24	138,138,139,139	0
2	SO4	D	433	5/5	0.75	0.38	156,157,158,158	0
2	SO4	B	442	5/5	0.77	0.25	121,122,123,123	0
2	SO4	A	443	5/5	0.77	0.20	123,124,124,124	0
2	SO4	C	441	5/5	0.77	0.46	147,147,147,147	0
2	SO4	A	437	5/5	0.78	0.28	148,148,149,149	0
2	SO4	B	446	5/5	0.78	0.57	154,154,155,155	0
2	SO4	C	442	5/5	0.78	0.28	139,140,140,140	0
2	SO4	B	433	5/5	0.79	0.55	171,171,171,171	0
3	FLC	A	452	13/13	0.79	0.38	108,111,112,112	0
2	SO4	C	434	5/5	0.80	0.51	146,146,147,147	0
2	SO4	C	437	5/5	0.80	0.19	133,134,134,134	0
2	SO4	A	438	5/5	0.80	0.36	130,130,131,131	0
4	ZN	C	451	1/1	0.80	0.10	82,82,82,82	0
2	SO4	D	435	5/5	0.81	0.24	126,127,127,127	0
2	SO4	A	450	5/5	0.81	0.29	145,145,145,145	0
2	SO4	C	447	5/5	0.81	0.17	153,154,154,154	0
2	SO4	A	436	5/5	0.84	0.32	131,131,131,131	0
4	ZN	D	442	1/1	0.84	0.21	121,121,121,121	0
2	SO4	A	433	5/5	0.85	0.23	121,121,122,122	0
2	SO4	A	434	5/5	0.85	0.21	117,117,117,118	0
2	SO4	A	444	5/5	0.85	0.26	111,111,111,111	0
2	SO4	A	446	5/5	0.86	0.17	113,114,114,114	0
2	SO4	B	434	5/5	0.86	0.23	136,136,136,137	0
2	SO4	B	444	5/5	0.87	0.16	124,124,124,124	0
4	ZN	B	452	1/1	0.87	0.13	74,74,74,74	0
2	SO4	D	437	5/5	0.89	0.21	109,110,110,110	0
2	SO4	D	438	5/5	0.89	0.15	110,110,111,111	0
2	SO4	A	448	5/5	0.89	0.35	135,135,136,136	0
4	ZN	C	452	1/1	0.89	0.18	125,125,125,125	0
2	SO4	B	441	5/5	0.89	0.32	117,118,119,119	0
2	SO4	C	432	5/5	0.90	0.18	131,131,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	446	5/5	0.90	0.29	119,120,120,120	0
3	FLC	B	451	13/13	0.90	0.33	68,70,79,80	0
2	SO4	A	447	5/5	0.90	0.20	125,126,126,126	0
2	SO4	C	443	5/5	0.91	0.11	102,102,103,103	0
2	SO4	C	433	5/5	0.91	0.38	141,141,141,141	0
2	SO4	A	445	5/5	0.92	0.21	101,102,103,103	0
2	SO4	C	448	5/5	0.92	0.17	97,97,98,98	0
2	SO4	C	449	5/5	0.92	0.10	114,114,114,115	0
2	SO4	C	450	5/5	0.92	0.34	116,116,116,116	0
2	SO4	B	445	5/5	0.92	0.24	114,115,115,115	0
2	SO4	B	435	5/5	0.92	0.19	101,101,102,103	0
2	SO4	C	439	5/5	0.93	0.11	105,105,105,105	0
2	SO4	C	436	5/5	0.93	0.45	139,139,139,139	0
4	ZN	B	453	1/1	0.93	0.09	88,88,88,88	0
2	SO4	B	438	5/5	0.93	0.24	110,110,111,111	0
2	SO4	B	449	5/5	0.93	0.17	98,98,99,99	0
4	ZN	D	441	1/1	0.93	0.20	98,98,98,98	0
2	SO4	C	444	5/5	0.93	0.24	118,118,118,118	0
2	SO4	B	440	5/5	0.94	0.18	81,81,82,83	0
2	SO4	A	432	5/5	0.94	0.22	103,103,104,104	0
2	SO4	B	447	5/5	0.94	0.22	121,121,121,121	0
2	SO4	D	440	5/5	0.95	0.25	85,85,85,86	0
2	SO4	C	440	5/5	0.96	0.15	87,87,88,88	0
2	SO4	B	443	5/5	0.96	0.15	57,59,60,61	0
2	SO4	B	432	5/5	0.96	0.09	76,77,79,79	0
2	SO4	D	432	5/5	0.96	0.19	80,80,81,82	0
4	ZN	A	454	1/1	0.96	0.08	72,72,72,72	0
2	SO4	A	439	5/5	0.96	0.24	91,92,92,93	0
2	SO4	A	440	5/5	0.97	0.12	81,81,82,82	0
2	SO4	A	449	5/5	0.97	0.18	48,49,52,53	0
2	SO4	B	439	5/5	0.97	0.17	45,45,49,49	0
2	SO4	A	451	5/5	0.98	0.11	56,58,60,62	0
2	SO4	C	435	5/5	0.98	0.09	71,72,73,73	0
2	SO4	A	441	5/5	0.98	0.13	43,45,48,49	0
2	SO4	D	439	5/5	0.98	0.10	67,67,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.