



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:27 AM GMT

PDB ID : 2F0X
Title : Crystal structure and function of human thioesterase superfamily member 2(THEM2)
Authors : Cheng, Z.; Song, F.; Shan, X.; Wang, Y.; Wei, Z.; Gong, W.
Deposited on : 2005-11-14
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

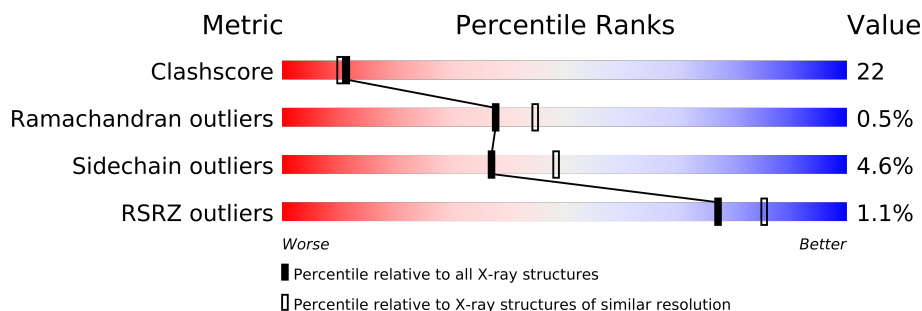
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	148	
1	B	148	
1	C	148	
1	D	148	
1	E	148	
1	F	148	
1	G	148	
1	H	148	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	1008	-	X
2	SO4	C	1012	-	X
2	SO4	C	1020	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	E	1018	-	X
2	SO4	E	1019	-	X
2	SO4	F	1014	-	X
2	SO4	G	1010	-	X
2	SO4	H	1013	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8460 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Thioesterase superfamily member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	Se	0	1	0
			986	615	170	193	2	6			
1	B	136	Total	C	N	O	S	Se	0	1	0
			998	622	177	191	2	6			
1	C	136	Total	C	N	O	S	Se	0	1	0
			1006	627	178	193	2	6			
1	D	135	Total	C	N	O	S	Se	0	1	0
			982	613	171	190	2	6			
1	E	135	Total	C	N	O	S	Se	0	1	0
			971	608	168	187	2	6			
1	F	136	Total	C	N	O	S	Se	0	1	0
			1002	624	177	193	2	6			
1	G	136	Total	C	N	O	S	Se	0	1	0
			992	619	173	192	2	6			
1	H	135	Total	C	N	O	S	Se	0	1	0
			977	612	169	188	2	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
A	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
A	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
A	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
A	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
B	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
B	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
B	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
B	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
C	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
C	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
C	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
C	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
D	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
D	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
D	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3

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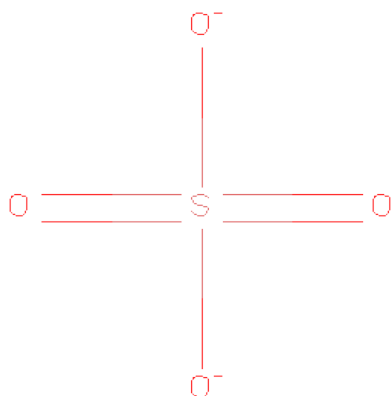
Chain	Residue	Modelled	Actual	Comment	Reference
D	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
D	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
E	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
E	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
E	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
E	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
F	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
F	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
F	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
F	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
G	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
G	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
G	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
G	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
G	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
G	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
G	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
G	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
G	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	4	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	15	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	42	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	70	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	86	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	91	MSE	MET	MODIFIED RESIDUE	UNP Q9NPJ3
H	141	LEU	-	EXPRESSION TAG	UNP Q9NPJ3
H	142	GLU	-	EXPRESSION TAG	UNP Q9NPJ3
H	143	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	144	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	145	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	146	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	147	HIS	-	EXPRESSION TAG	UNP Q9NPJ3
H	148	HIS	-	EXPRESSION TAG	UNP Q9NPJ3

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



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

- Molecule 3 is water.

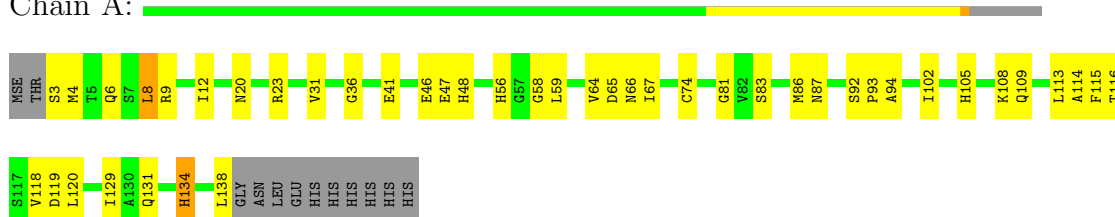
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total 56	O 56	0	0
3	B	57	Total 57	O 57	0	0
3	C	61	Total 61	O 61	0	0
3	D	59	Total 59	O 59	0	0
3	E	45	Total 45	O 45	0	0
3	F	71	Total 71	O 71	0	0
3	G	51	Total 51	O 51	0	0
3	H	46	Total 46	O 46	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

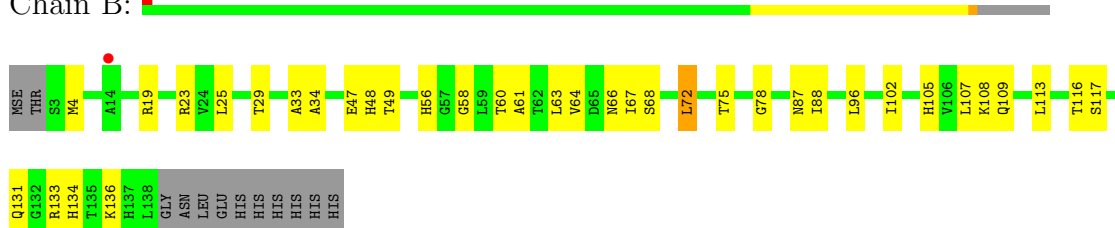
- Molecule 1: Thioesterase superfamily member 2

Chain A:



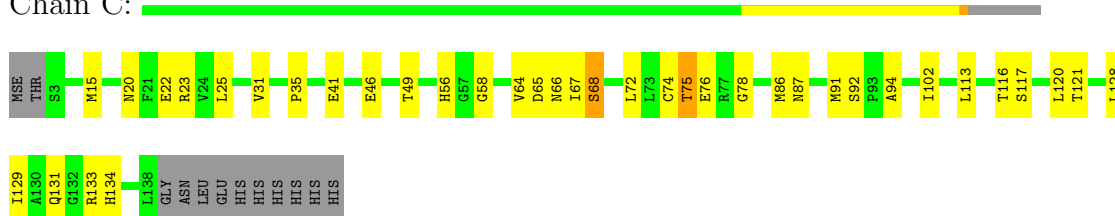
- Molecule 1: Thioesterase superfamily member 2

Chain B:



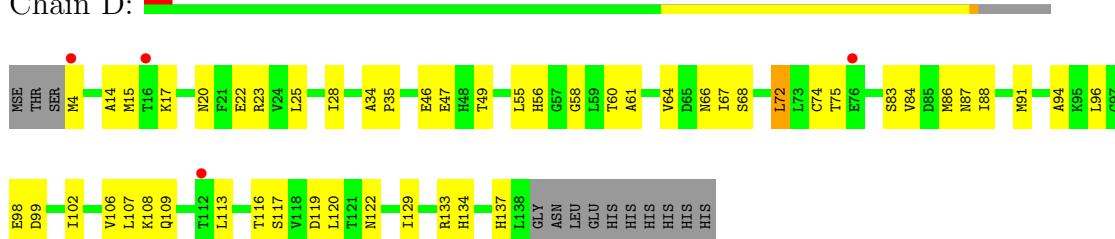
- Molecule 1: Thioesterase superfamily member 2

Chain C:



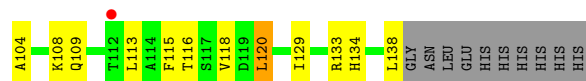
- Molecule 1: Thioesterase superfamily member 2

Chain D:



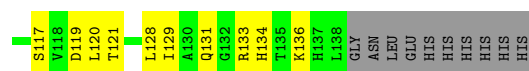
- Molecule 1: Thioesterase superfamily member 2

Chain E:



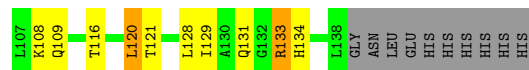
- Molecule 1: Thioesterase superfamily member 2

Chain F:



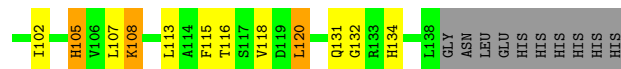
- Molecule 1: Thioesterase superfamily member 2

Chain G:



- Molecule 1: Thioesterase superfamily member 2

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.94Å 122.08Å 90.98Å 90.00° 123.90° 90.00°	Depositor
Resolution (Å)	47.47 – 2.30 47.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.47-2.30) 97.2 (47.47-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.247 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52679 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8460	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	2/994 (0.2%)	0.65	0/1340
1	B	0.32	0/1006	0.65	0/1353
1	C	0.34	0/1014	0.67	0/1362
1	D	0.39	1/991 (0.1%)	0.65	0/1337
1	E	0.32	0/980	0.64	0/1324
1	F	0.32	0/1010	0.67	0/1358
1	G	0.32	0/1000	0.67	0/1346
1	H	0.41	1/986 (0.1%)	0.63	0/1330
All	All	0.36	4/7981 (0.1%)	0.65	0/10750

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	118	VAL	C-N	8.29	1.53	1.34
1	A	118	VAL	C-N	7.45	1.51	1.34
1	A	119	ASP	C-N	6.79	1.49	1.34
1	D	119	ASP	C-N	6.42	1.48	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	986	0	994	39	0
1	B	998	0	1023	56	0
1	C	1006	0	1038	59	0
1	D	982	0	994	52	0
1	E	971	0	976	60	0
1	F	1002	0	1027	51	0
1	G	992	0	1010	64	0
1	H	977	0	986	50	0
2	A	10	0	0	0	0
2	B	15	0	0	1	0
2	C	20	0	0	0	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	1	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
3	A	56	0	0	3	0
3	B	57	0	0	3	0
3	C	61	0	0	3	0
3	D	59	0	0	4	0
3	E	45	0	0	0	0
3	F	71	0	0	4	0
3	G	51	0	0	4	0
3	H	46	0	0	3	0
All	All	8460	0	8048	357	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

The worst 5 of 357 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:56:HIS:HD2	1:E:58:GLY:H	1.09	1.01
1:B:131:GLN:HE22	1:C:133:ARG:HH11	1.01	0.98
1:B:56:HIS:HD2	1:B:58:GLY:H	1.07	0.97
1:H:56:HIS:HD2	1:H:58:GLY:H	1.06	0.94
1:G:56:HIS:CD2	1:G:58:GLY:H	1.88	0.92

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	135/148 (91%)	132 (98%)	3 (2%)	0	100	100
1	B	135/148 (91%)	130 (96%)	5 (4%)	0	100	100
1	C	135/148 (91%)	133 (98%)	2 (2%)	0	100	100
1	D	134/148 (90%)	132 (98%)	2 (2%)	0	100	100
1	E	134/148 (90%)	128 (96%)	4 (3%)	2 (2%)	15	13
1	F	135/148 (91%)	131 (97%)	4 (3%)	0	100	100
1	G	135/148 (91%)	130 (96%)	3 (2%)	2 (2%)	15	13
1	H	134/148 (90%)	123 (92%)	10 (8%)	1 (1%)	30	34
All	All	1077/1184 (91%)	1039 (96%)	33 (3%)	5 (0%)	38	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	20	ASN
1	E	20	ASN
1	E	18	ALA
1	H	26	GLY
1	G	35	PRO

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	106/116 (91%)	102 (96%)	4 (4%)	44	59
1	B	108/116 (93%)	104 (96%)	4 (4%)	45	60
1	C	110/116 (95%)	106 (96%)	4 (4%)	47	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	105/116 (90%)	101 (96%)	4 (4%)	44	59
1	E	102/116 (88%)	98 (96%)	4 (4%)	43	57
1	F	109/116 (94%)	102 (94%)	7 (6%)	25	31
1	G	107/116 (92%)	102 (95%)	5 (5%)	36	47
1	H	103/116 (89%)	96 (93%)	7 (7%)	22	28
All	All	850/928 (92%)	811 (95%)	39 (5%)	37	48

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	96	LEU
1	F	19	ARG
1	H	108	LYS
1	E	113	LEU
1	E	120	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	109	GLN
1	E	105	HIS
1	H	56	HIS
1	E	56	HIS
1	E	109	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry

20 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
2	SO4	A	1002	-	4,4,4	0.31	0	6,6,6	0.06	0
2	SO4	A	1011	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	1003	-	4,4,4	0.20	0	6,6,6	0.07	0
2	SO4	B	1007	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	B	1008	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	C	1001	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	C	1009	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	1012	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	C	1020	-	4,4,4	0.27	0	6,6,6	0.12	0
2	SO4	D	1015	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	D	1016	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	E	1017	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	E	1018	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	E	1019	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	F	1005	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	F	1014	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	G	1006	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	G	1010	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	H	1004	-	4,4,4	0.29	0	6,6,6	0.09	0
2	SO4	H	1013	-	4,4,4	0.24	0	6,6,6	0.09	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
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1011	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1008	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1009	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1012	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1020	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1015	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1016	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1017	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1018	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1019	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1014	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1010	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1013	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.

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	136/148 (91%)	-0.23	0 100 100	15, 28, 46, 65	0
1	B	136/148 (91%)	-0.06	1 (0%) 84 91	18, 29, 48, 64	0
1	C	136/148 (91%)	-0.17	0 100 100	14, 27, 39, 59	0
1	D	135/148 (91%)	-0.07	4 (2%) 48 58	15, 27, 53, 58	0
1	E	135/148 (91%)	-0.07	2 (1%) 70 78	18, 32, 53, 62	0
1	F	136/148 (91%)	-0.11	1 (0%) 84 91	16, 28, 41, 57	0
1	G	136/148 (91%)	0.05	0 100 100	14, 32, 47, 49	0
1	H	135/148 (91%)	0.02	4 (2%) 48 58	20, 32, 54, 69	0
All	All	1085/1184 (91%)	-0.08	12 (1%) 77 85	14, 30, 49, 69	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	16	THR	3.9
1	H	4	MSE	3.2
1	D	4	MSE	2.8
1	H	17	LYS	2.7
1	D	16	THR	2.4

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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	C	1020	5/5	0.29	9.19	99,100,100,100	0
2	SO4	H	1013	5/5	0.25	8.40	84,84,85,86	0
2	SO4	C	1012	5/5	0.18	4.38	97,97,98,98	0
2	SO4	G	1010	5/5	0.27	3.06	89,89,89,89	0
2	SO4	B	1008	5/5	0.14	2.59	71,71,71,71	0
2	SO4	F	1014	5/5	0.17	2.48	84,85,85,85	0
2	SO4	E	1018	5/5	0.34	2.47	99,100,100,100	0
2	SO4	E	1019	5/5	0.21	2.38	91,92,92,92	0
2	SO4	A	1011	5/5	0.16	1.65	99,100,100,100	0
2	SO4	D	1015	5/5	0.22	1.08	86,87,87,88	0
2	SO4	G	1006	5/5	0.13	1.01	80,80,81,81	0
2	SO4	E	1017	5/5	0.13	0.65	73,74,74,74	0
2	SO4	H	1004	5/5	0.14	0.03	70,70,71,71	0
2	SO4	C	1001	5/5	0.12	-0.21	47,47,49,49	0
2	SO4	D	1016	5/5	0.12	-0.62	70,70,71,71	0
2	SO4	B	1003	5/5	0.11	-0.65	62,63,63,64	0
2	SO4	C	1009	5/5	0.14	-0.87	80,80,80,81	0
2	SO4	A	1002	5/5	0.07	-1.86	46,46,46,47	0
2	SO4	F	1005	5/5	0.07	-1.98	41,42,43,44	0
2	SO4	B	1007	5/5	0.12	-2.42	82,83,83,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.