



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 09:06 AM UTC

PDB ID : 6ZJY / pdb_00006zjy
EMDB ID : EMD-11238
Title : Respiratory complex I from Thermus thermophilus, NAD⁺ dataset, minor state
Authors : Kaszuba, K.; Tambalo, M.; Gallagher, G.T.; Sazanov, L.A.
Deposited on : 2020-06-29
Resolution : 5.50 Å(reported)
Based on initial model : 6Y11

This is a wwPDB EM 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/EMValidationReportHelp>
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:

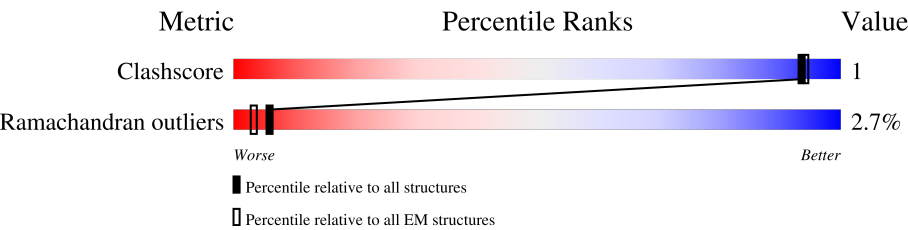
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	438	86%13%.
2	2	181	87%10%..
3	3	783	79%16%..
4	4	409	81%12%6%
5	5	207	84%11%5%
6	6	181	77%14%.8%
7	9	182	79%17%..
8	7	129	80%18%..
9	A	119	90%8%..
10	J	176	82%9%.9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	K	95	 92% 8%
12	L	606	 92% 8%
13	M	469	 88% 11%
14	N	427	 91% 9%
15	H	365	 85% 11% ..

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
16	SF4	1	501	-	-	X	-
16	SF4	3	803	-	-	X	-
16	SF4	9	202	-	-	X	-

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 22855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	437	Total	C	N	O	0	0
			2136	1262	437	437		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	178	Total	C	N	O	0	0
			875	519	178	178		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	754	Total	C	N	O	0	0
			3714	2206	754	754		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	384	Total	C	N	O	0	0
			1890	1122	384	384		

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	196	Total	C	N	O	0	0
			961	569	196	196		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	6	166	Total	C	N	O	0	0
			818	486	166	166		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	9	180	Total	C	N	O	0	0
			885	525	180	180		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	7	127	Total	C	N	O	0	0
			628	374	127	127		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	A	117	Total	C	N	O	0	0
			570	336	117	117		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	160	Total	C	N	O	0	0
			783	463	160	160		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total	C	N	O	0	0
			467	277	95	95		

- Molecule 12 is a protein called NADH-quinone oxidoreductase subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	605	Total	C	N	O	0	0
			2955	1745	605	605		

- Molecule 13 is a protein called NADH-quinone oxidoreductase subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	467	Total	C	N	O	0	0
			2276	1342	467	467		

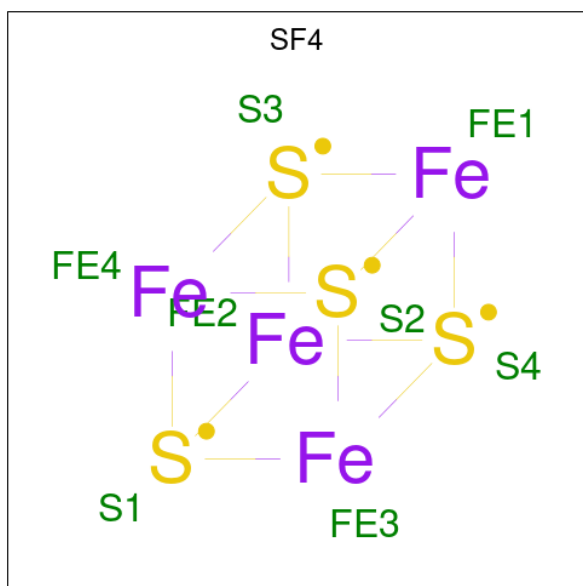
- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	427	Total	C	N	O	0	0
			2092	1238	427	427		

- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	353	Total	C	N	O	0	0
			1741	1035	353	353		

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
16	1	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	6	1	Total	Fe	S	0
			8	4	4	
16	9	1	Total	Fe	S	0
			8	4	4	
16	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

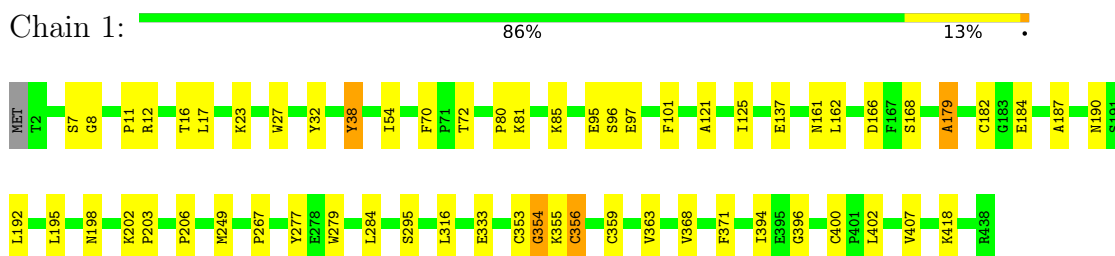


Mol	Chain	Residues	Atoms			AltConf
17	2	1	Total	Fe	S	0
			4	2	2	
17	3	1	Total	Fe	S	0
			4	2	2	

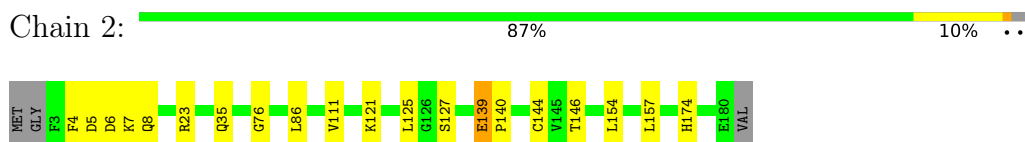
3 Residue-property plots

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. 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. 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.

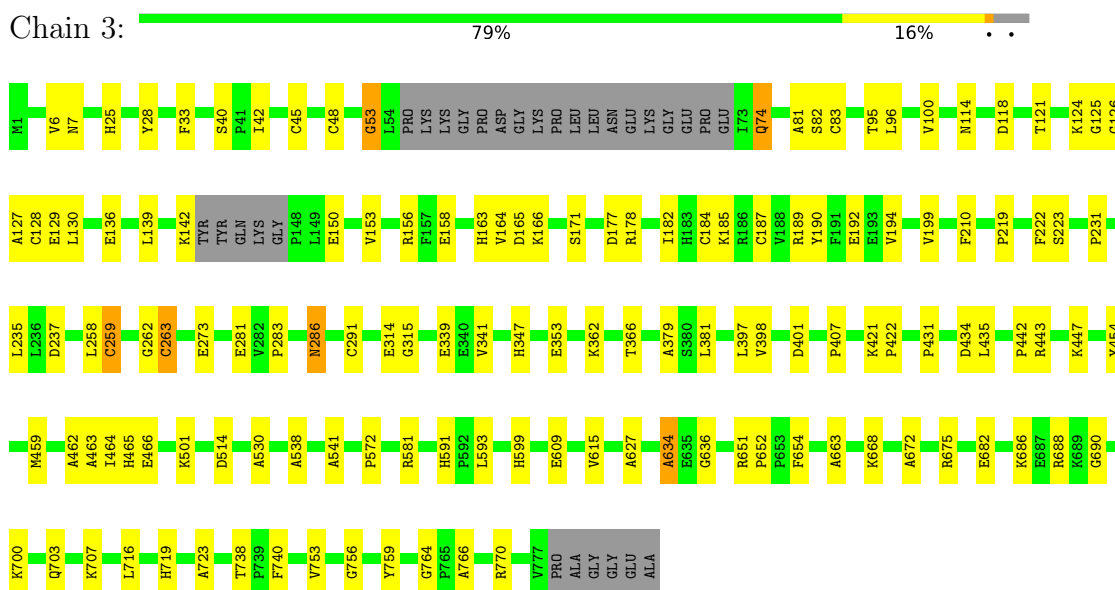
- Molecule 1: NADH-quinone oxidoreductase subunit 1



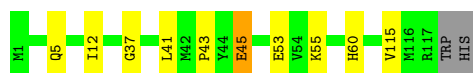
- Molecule 2: NADH-quinone oxidoreductase subunit 2



- Molecule 3: NADH-quinone oxidoreductase subunit 3



- Molecule 4: NADH-quinone oxidoreductase subunit 4



- Molecule 10: NADH-quinone oxidoreductase subunit 10

Chain J: 82% 9% 9%



- Molecule 11: NADH-quinone oxidoreductase subunit 11

Chain K: 92% 8%



- Molecule 12: NADH-quinone oxidoreductase subunit 12

Chain L: 92% 8%



- Molecule 13: NADH-quinone oxidoreductase subunit 13

Chain M: 88% 11%



- Molecule 14: NADH-quinone oxidoreductase subunit 14

Chain N: 91% 9%



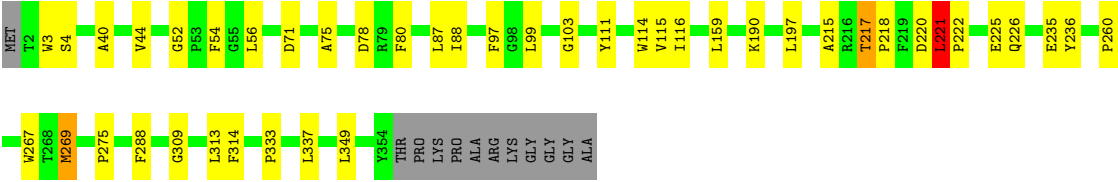
- Molecule 15: NADH-quinone oxidoreductase subunit 8

Chain H:

85%

11%

••



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES

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	1	1.80	10/2135 (0.5%)	1.92	50/2958 (1.7%)
2	2	1.75	1/874 (0.1%)	1.96	23/1213 (1.9%)
3	3	1.83	23/3711 (0.6%)	1.92	101/5157 (2.0%)
4	4	1.89	11/1889 (0.6%)	1.93	42/2625 (1.6%)
5	5	1.79	2/960 (0.2%)	1.89	24/1331 (1.8%)
6	6	1.95	6/817 (0.7%)	1.94	22/1135 (1.9%)
7	9	1.92	10/884 (1.1%)	1.94	26/1227 (2.1%)
8	7	1.91	4/627 (0.6%)	1.93	22/872 (2.5%)
9	A	1.62	0/569	1.81	10/786 (1.3%)
10	J	1.81	1/782 (0.1%)	1.89	18/1083 (1.7%)
11	K	1.76	0/466	1.79	7/646 (1.1%)
12	L	1.66	4/2954 (0.1%)	1.92	60/4092 (1.5%)
13	M	1.76	7/2275 (0.3%)	1.88	36/3148 (1.1%)
14	N	1.79	6/2091 (0.3%)	1.76	32/2900 (1.1%)
15	H	1.85	8/1740 (0.5%)	1.87	29/2420 (1.2%)
All	All	1.80	93/22774 (0.4%)	1.90	502/31593 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
2	2	0	1
4	4	0	3
6	6	0	1
7	9	0	4
9	A	0	1
10	J	0	1
11	K	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	1
14	N	0	1
15	H	0	2
All	All	0	19

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	9	99	ILE	CA-C	-8.66	1.41	1.53
3	3	74	GLN	CA-C	-7.22	1.46	1.53
3	3	222	PHE	CA-C	-6.95	1.44	1.52
3	3	466	GLU	CA-C	-6.20	1.45	1.52
4	4	213	ILE	CA-C	-6.00	1.46	1.52

The worst 5 of 502 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	156	ARG	N-CA-C	-11.22	101.83	114.62
1	1	356	CYS	CA-C-N	10.56	136.60	120.97
1	1	356	CYS	C-N-CA	10.56	136.60	120.97
6	6	66	GLU	N-CA-C	-10.50	100.77	114.31
4	4	213	ILE	N-CA-C	-10.30	102.95	111.81

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	166	ASP	Peptide
1	1	203	PRO	Peptide
1	1	396	GLY	Peptide
2	2	139	GLU	Peptide
4	4	36	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2136	0	989	7	0
2	2	875	0	398	0	0
3	3	3714	0	1785	16	0
4	4	1890	0	833	2	0
5	5	961	0	427	1	0
6	6	818	0	388	2	0
7	9	885	0	406	9	0
8	7	628	0	300	1	0
9	A	570	0	280	0	0
10	J	783	0	409	0	0
11	K	467	0	248	0	0
12	L	2955	0	1499	0	0
13	M	2276	0	1200	2	0
14	N	2092	0	1120	1	0
15	H	1741	0	818	3	0
16	1	8	0	0	6	0
16	3	24	0	0	7	0
16	6	8	0	0	1	0
16	9	16	0	0	8	0
17	2	4	0	0	0	0
17	3	4	0	0	0	0
All	All	22855	0	11100	43	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 1.

The worst 5 of 43 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)
3:3:262:GLY:N	16:3:803:SF4:S2	2.05	1.26
1:1:355:LYS:N	16:1:501:SF4:S3	2.36	0.97
3:3:262:GLY:CA	16:3:803:SF4:S2	2.52	0.96
1:1:354:GLY:C	16:1:501:SF4:S3	2.49	0.96
1:1:356:CYS:O	16:1:501:SF4:S3	2.27	0.91

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 PDB entries followed by that with respect to all EM entries.

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	1	435/438 (99%)	387 (89%)	38 (9%)	10 (2%)	5	27
2	2	176/181 (97%)	160 (91%)	13 (7%)	3 (2%)	7	35
3	3	748/783 (96%)	650 (87%)	73 (10%)	25 (3%)	3	20
4	4	382/409 (93%)	339 (89%)	30 (8%)	13 (3%)	3	20
5	5	194/207 (94%)	173 (89%)	15 (8%)	6 (3%)	3	21
6	6	164/181 (91%)	134 (82%)	25 (15%)	5 (3%)	3	22
7	9	178/182 (98%)	155 (87%)	18 (10%)	5 (3%)	4	24
8	7	125/129 (97%)	109 (87%)	12 (10%)	4 (3%)	3	21
9	A	115/119 (97%)	104 (90%)	8 (7%)	3 (3%)	4	25
10	J	158/176 (90%)	133 (84%)	23 (15%)	2 (1%)	9	41
11	K	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	5	28
12	L	603/606 (100%)	540 (90%)	55 (9%)	8 (1%)	9	41
13	M	465/469 (99%)	408 (88%)	41 (9%)	16 (3%)	3	20
14	N	425/427 (100%)	378 (89%)	40 (9%)	7 (2%)	7	37
15	H	351/365 (96%)	306 (87%)	31 (9%)	14 (4%)	2	18
All	All	4612/4767 (97%)	4061 (88%)	428 (9%)	123 (3%)	6	25

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	101	PHE
1	1	179	ALA
3	3	165	ASP
3	3	263	CYS
3	3	634	ALA

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

9 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	$\# Z > 2$
16	SF4	1	501	1	0,12,12	-	-	-		
17	FES	2	201	-	0,4,4	-	-	-		
17	FES	3	804	-	0,4,4	-	-	-		
16	SF4	9	201	7	0,12,12	-	-	-		
16	SF4	6	201	-	0,12,12	-	-	-		
16	SF4	3	802	3	0,12,12	-	-	-		
16	SF4	9	202	7	0,12,12	-	-	-		
16	SF4	3	801	-	0,12,12	-	-	-		
16	SF4	3	803	-	0,12,12	-	-	-		

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
16	SF4	1	501	1	-	-	0/6/5/5
17	FES	2	201	-	-	-	0/1/1/1
17	FES	3	804	-	-	-	0/1/1/1
16	SF4	9	201	7	-	-	0/6/5/5
16	SF4	6	201	-	-	-	0/6/5/5
16	SF4	3	802	3	-	-	0/6/5/5
16	SF4	9	202	7	-	-	0/6/5/5
16	SF4	3	801	-	-	-	0/6/5/5
16	SF4	3	803	-	-	-	0/6/5/5

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 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	501	SF4	6	0
16	6	201	SF4	1	0
16	9	202	SF4	8	0
16	3	801	SF4	1	0
16	3	803	SF4	6	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-11238. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.