



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2023 – 06:03 am GMT

PDB ID : 2V0T
Title : The A178L mutation in the C-terminal hinge of the flexible loop-6 of triosephosphate isomerase (TIM) induces a more closed conformation of this hinge region in dimeric and monomeric TIM
Authors : Alahuhta, M.; Casteleijn, M.G.; Neubauer, P.; Wierenga, R.K.
Deposited on : 2007-05-18
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, 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

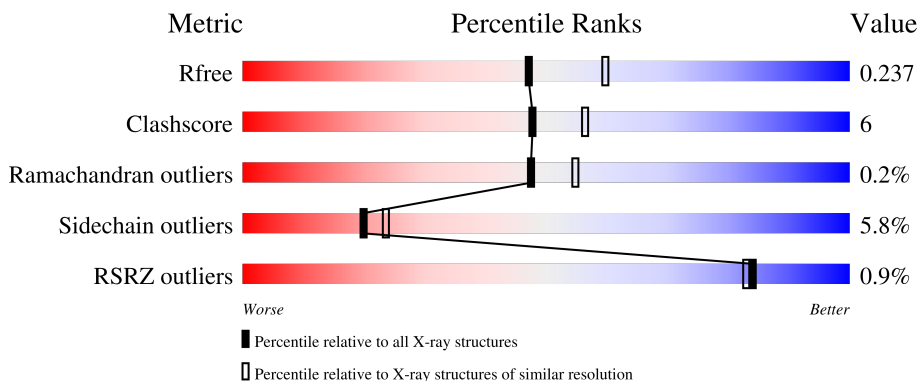
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	250	
1	B	250	
1	C	250	
1	D	250	
1	E	250	

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Mol	Chain	Length	Quality of chain
1	F	250	 82% 12% ..
1	G	250	 82% 15% ..
1	H	250	 2% 85% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16444 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 TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	Total 1849	C 1177	N 324	O 343	S 5	0	0	0
1	B	249	Total 1886	C 1200	N 331	O 350	S 5	0	0	0
1	C	242	Total 1851	C 1177	N 324	O 345	S 5	0	1	0
1	D	249	Total 1886	C 1200	N 331	O 350	S 5	0	0	0
1	E	244	Total 1853	C 1180	N 325	O 343	S 5	0	0	0
1	F	242	Total 1842	C 1172	N 323	O 342	S 5	0	0	0
1	G	249	Total 1886	C 1200	N 331	O 350	S 5	0	0	0
1	H	242	Total 1842	C 1172	N 323	O 342	S 5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

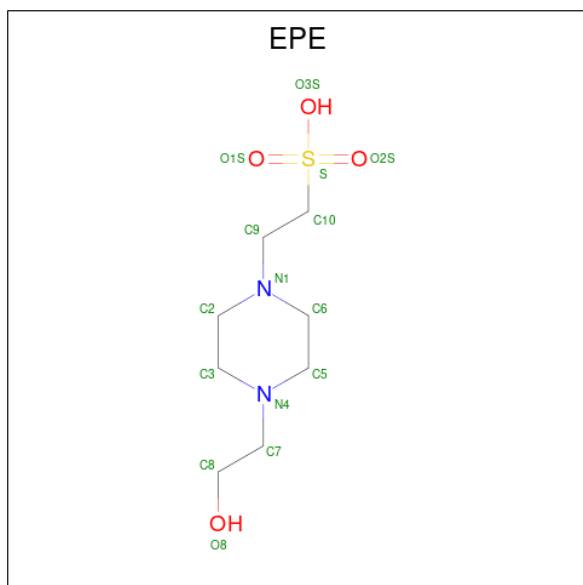
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LEU	ALA	engineered mutation	UNP P04789
B	178	LEU	ALA	engineered mutation	UNP P04789
C	178	LEU	ALA	engineered mutation	UNP P04789
D	178	LEU	ALA	engineered mutation	UNP P04789
E	178	LEU	ALA	engineered mutation	UNP P04789
F	178	LEU	ALA	engineered mutation	UNP P04789
G	178	LEU	ALA	engineered mutation	UNP P04789
H	178	LEU	ALA	engineered mutation	UNP P04789

- Molecule 2 is SULFATE ION (three-letter code: 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	B	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	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	C	1	15	8	2	4	1	0	0
3	D	1	15	8	2	4	1	0	0

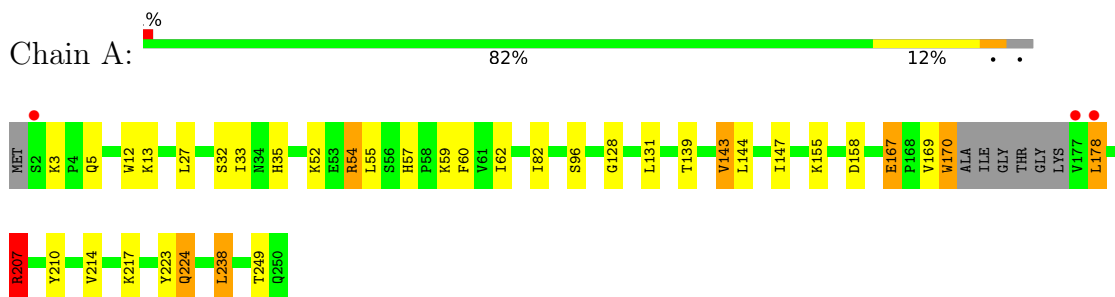
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	196	Total	O	0	0
			196	196		
4	C	202	Total	O	0	0
			202	202		
4	D	214	Total	O	0	0
			214	214		
4	E	206	Total	O	0	0
			206	206		
4	F	187	Total	O	0	0
			187	187		
4	G	126	Total	O	0	0
			126	126		
4	H	132	Total	O	0	0
			132	132		

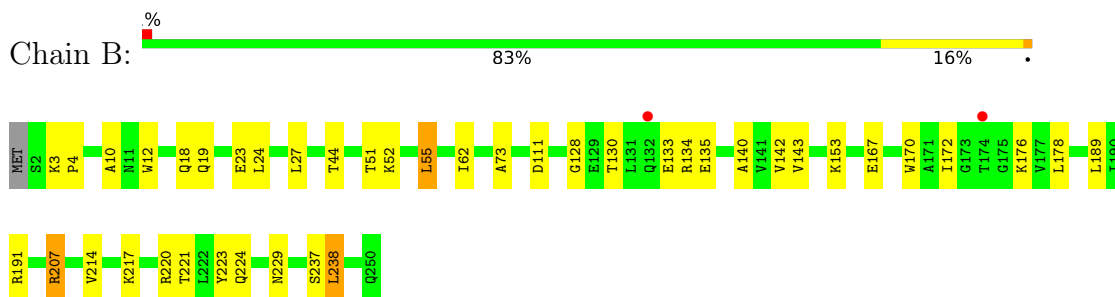
3 Residue-property plots [i](#)

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.

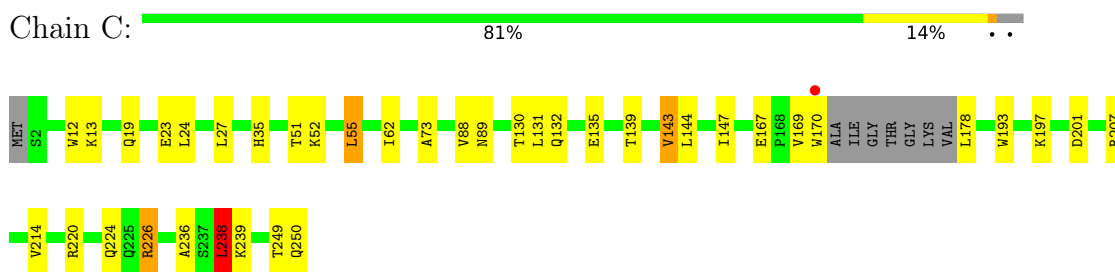
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL



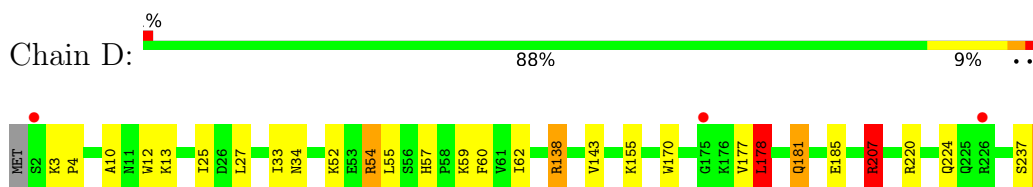
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL




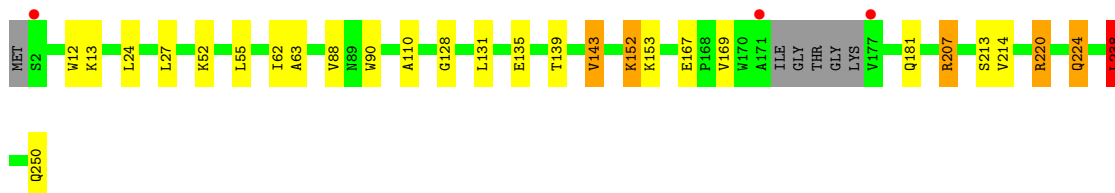
- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL




- Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL




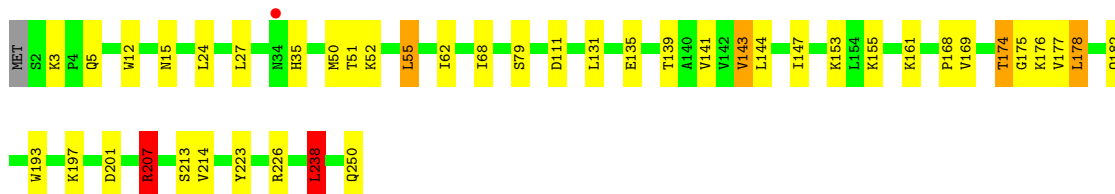
● Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL

Chain E:  86% 9% ..


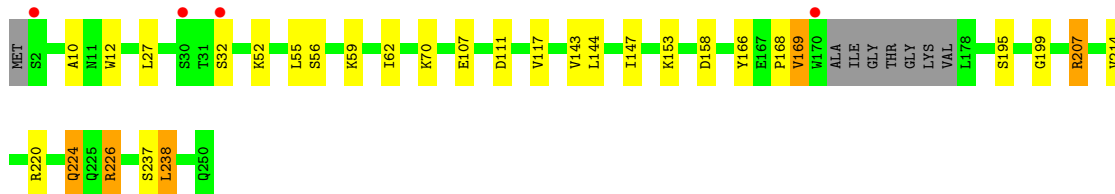
● Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL

Chain F:  82% 12% ..

● Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL

Chain G:  82% 15% ..

● Molecule 1: TRIOSEPHOSPHATE ISOMERASE GLYCOSOMAL

Chain H:  85% 10% ..

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.69Å 79.25Å 174.00Å 90.00° 99.22° 90.00°	Depositor
Resolution (Å)	19.81 – 2.20 19.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.81-2.20) 98.8 (19.81-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.21Å)	Xtrriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.178 , 0.238 0.178 , 0.237	Depositor DCC
R_{free} test set	5153 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtrriage
Anisotropy	0.498	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16444	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: SO4, EPE

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	0.69	0/1882	0.80	2/2551 (0.1%)
1	B	0.68	0/1920	0.77	2/2603 (0.1%)
1	C	0.75	0/1884	0.87	4/2553 (0.2%)
1	D	0.69	0/1920	0.76	4/2603 (0.2%)
1	E	0.70	0/1886	0.80	3/2558 (0.1%)
1	F	0.69	0/1875	0.77	4/2541 (0.2%)
1	G	0.62	0/1920	0.73	3/2603 (0.1%)
1	H	0.62	0/1875	0.70	2/2541 (0.1%)
All	All	0.68	0/15162	0.78	24/20553 (0.1%)

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	F	0	1

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	ARG	NE-CZ-NH1	-16.49	112.06	120.30
1	C	207	ARG	NE-CZ-NH2	14.34	127.47	120.30
1	A	207	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	E	207	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	B	207	ARG	NE-CZ-NH2	-9.97	115.31	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	169	VAL	Peptide

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	1849	0	1880	20	0
1	B	1886	0	1923	25	0
1	C	1851	0	1876	29	0
1	D	1886	0	1923	15	0
1	E	1853	0	1885	22	0
1	F	1842	0	1871	27	0
1	G	1886	0	1923	27	0
1	H	1842	0	1871	24	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	C	15	0	17	0	0
3	D	15	0	17	0	0
4	A	206	0	0	2	0
4	B	196	0	0	2	0
4	C	202	0	0	2	0
4	D	214	0	0	2	0
4	E	206	0	0	3	0
4	F	187	0	0	4	0
4	G	126	0	0	5	0
4	H	132	0	0	1	0
All	All	16444	0	15186	184	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 6.

The worst 5 of 184 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:C:89:ASN:HB2	4:C:2097:HOH:O	1.52	1.10
1:E:153:LYS:HE2	4:E:2143:HOH:O	1.63	0.96
1:H:226:ARG:HH21	1:H:226:ARG:HG2	1.31	0.96
1:F:226:ARG:HG2	1:F:226:ARG:HH21	1.29	0.95
1:E:220:ARG:HG2	1:E:220:ARG:HH21	1.36	0.90

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	239/250 (96%)	235 (98%)	4 (2%)	0	100	100
1	B	247/250 (99%)	240 (97%)	7 (3%)	0	100	100
1	C	239/250 (96%)	236 (99%)	2 (1%)	1 (0%)	34	37
1	D	247/250 (99%)	243 (98%)	4 (2%)	0	100	100
1	E	240/250 (96%)	233 (97%)	7 (3%)	0	100	100
1	F	238/250 (95%)	233 (98%)	4 (2%)	1 (0%)	34	37
1	G	247/250 (99%)	240 (97%)	7 (3%)	0	100	100
1	H	238/250 (95%)	228 (96%)	9 (4%)	1 (0%)	34	37
All	All	1935/2000 (97%)	1888 (98%)	44 (2%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	169	VAL
1	H	169	VAL
1	C	13	LYS

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	194/198 (98%)	181 (93%)	13 (7%)	16	18
1	B	197/198 (100%)	185 (94%)	12 (6%)	18	21
1	C	194/198 (98%)	184 (95%)	10 (5%)	23	28
1	D	197/198 (100%)	186 (94%)	11 (6%)	21	25
1	E	194/198 (98%)	181 (93%)	13 (7%)	16	18
1	F	193/198 (98%)	182 (94%)	11 (6%)	20	24
1	G	197/198 (100%)	186 (94%)	11 (6%)	21	25
1	H	193/198 (98%)	183 (95%)	10 (5%)	23	28
All	All	1559/1584 (98%)	1468 (94%)	91 (6%)	20	23

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	238	LEU
1	G	27	LEU
1	F	19	GLN
1	F	207	ARG
1	G	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	19	GLN
1	H	250	GLN
1	F	19	GLN
1	G	224	GLN
1	E	224	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	C	1252	-	15,15,15	1.51	1 (6%)	18,20,20	2.48	6 (33%)
3	EPE	D	1252	-	15,15,15	1.03	1 (6%)	18,20,20	1.76	2 (11%)
2	SO4	A	1252	-	4,4,4	0.22	0	6,6,6	0.48	0
2	SO4	C	1251	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	E	1252	-	4,4,4	0.29	0	6,6,6	0.65	0
2	SO4	F	1251	-	4,4,4	0.15	0	6,6,6	0.36	0
2	SO4	D	1251	-	4,4,4	0.09	0	6,6,6	0.42	0
2	SO4	G	1251	-	4,4,4	0.14	0	6,6,6	0.60	0
2	SO4	E	1251	-	4,4,4	0.14	0	6,6,6	0.52	0
2	SO4	B	1251	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	A	1251	-	4,4,4	0.21	0	6,6,6	0.43	0
2	SO4	H	1251	-	4,4,4	0.15	0	6,6,6	0.27	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	EPE	D	1252	-	-	5/9/19/19	0/1/1/1
3	EPE	C	1252	-	-	5/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1252	EPE	C10-S	5.39	1.85	1.77
3	D	1252	EPE	C10-S	3.29	1.82	1.77

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1252	EPE	O1S-S-C10	-5.67	100.09	106.92
3	C	1252	EPE	O2S-S-C10	-5.01	100.88	106.92
3	D	1252	EPE	O1S-S-C10	-4.38	101.64	106.92
3	C	1252	EPE	O3S-S-C10	-3.80	99.62	105.77
3	D	1252	EPE	O2S-S-C10	-3.63	102.55	106.92

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1252	EPE	C8-C7-N4-C3
3	C	1252	EPE	C9-C10-S-O2S
3	C	1252	EPE	C9-C10-S-O3S
3	D	1252	EPE	C10-C9-N1-C6
3	C	1252	EPE	N4-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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	243/250 (97%)	-0.34	3 (1%) 79 77	6, 12, 21, 32	0
1	B	249/250 (99%)	-0.35	2 (0%) 86 85	6, 12, 28, 39	0
1	C	242/250 (96%)	-0.37	1 (0%) 92 91	8, 12, 20, 45	0
1	D	249/250 (99%)	-0.34	3 (1%) 79 77	6, 12, 19, 27	0
1	E	244/250 (97%)	-0.35	3 (1%) 79 77	6, 13, 21, 29	0
1	F	242/250 (96%)	-0.39	1 (0%) 92 91	6, 12, 19, 34	0
1	G	249/250 (99%)	-0.15	1 (0%) 92 91	8, 13, 18, 28	0
1	H	242/250 (96%)	-0.20	4 (1%) 70 68	7, 13, 20, 34	0
All	All	1960/2000 (98%)	-0.31	18 (0%) 84 83	6, 12, 21, 45	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	TRP	4.5
1	F	170	TRP	3.8
1	A	177	VAL	3.5
1	H	170	TRP	3.0
1	B	132	GLN	2.8

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
3	EPE	D	1252	15/15	0.93	0.27	38,45,52,53	0
2	SO4	G	1251	5/5	0.95	0.21	40,42,42,44	0
2	SO4	E	1252	5/5	0.95	0.18	25,27,32,32	0
2	SO4	A	1252	5/5	0.96	0.27	34,37,37,38	0
2	SO4	H	1251	5/5	0.97	0.16	39,41,42,42	0
3	EPE	C	1252	15/15	0.97	0.15	9,16,25,30	0
2	SO4	E	1251	5/5	0.97	0.20	35,36,37,37	0
2	SO4	A	1251	5/5	0.98	0.11	29,30,31,31	0
2	SO4	B	1251	5/5	0.98	0.13	23,24,25,25	0
2	SO4	C	1251	5/5	0.98	0.16	21,21,23,24	0
2	SO4	D	1251	5/5	0.99	0.17	16,16,19,19	0
2	SO4	F	1251	5/5	0.99	0.13	34,34,34,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.