



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:11 AM GMT

PDB ID : 2PNO
Title : Crystal structure of human leukotriene C4 synthase
Authors : Ago, H.; Kanaoka, Y.; Irikura, D.; Lam, B.K.; Shimamura, T.; Austen, K.F.; Miyano, M.
Deposited on : 2007-04-24
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

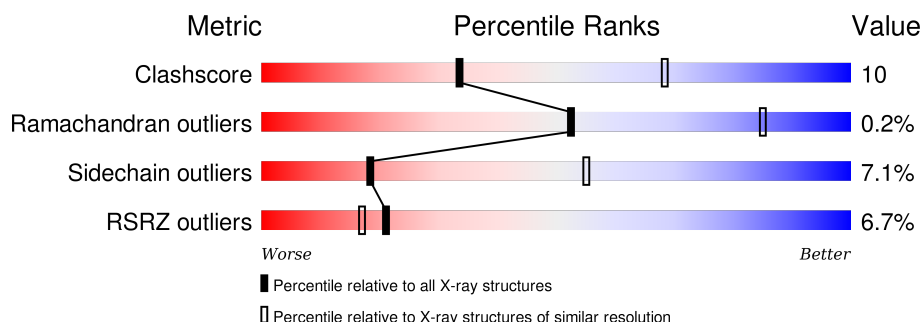
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	156	<div> <div>4%</div> <div>76%</div> <div>16%</div> <div>6%</div> </div>
1	B	156	<div> <div>3%</div> <div>77%</div> <div>14%</div> <div>6%</div> </div>
1	C	156	<div> <div>9%</div> <div>74%</div> <div>17%</div> <div>6%</div> </div>
1	D	156	<div> <div>10%</div> <div>65%</div> <div>26%</div> <div>6%</div> </div>
1	E	156	<div> <div>3%</div> <div>72%</div> <div>19%</div> <div>6%</div> </div>
1	F	156	<div> <div>2%</div> <div>68%</div> <div>24%</div> <div>6%</div> </div>
1	G	156	<div> <div>4%</div> <div>74%</div> <div>18%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	156	
1	I	156	
1	J	156	
1	K	156	
1	L	156	

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
3	LMT	A	215	-	-	-	X
3	LMT	A	228	-	-	-	X
3	LMT	A	229	-	-	-	X
3	LMT	A	256	-	-	-	X
3	LMT	B	213	-	-	-	X
3	LMT	B	218	-	-	-	X
3	LMT	B	227	-	-	-	X
3	LMT	B	242	-	-	-	X
3	LMT	C	214	-	-	-	X
3	LMT	C	216	-	-	-	X
3	LMT	C	237	-	-	-	X
3	LMT	D	220	-	-	-	X
3	LMT	D	238	-	-	-	X
3	LMT	D	247	-	-	-	X
3	LMT	E	230	-	-	-	X
3	LMT	E	231	-	-	-	X
3	LMT	E	232	-	-	-	X
3	LMT	E	243	-	-	-	X
3	LMT	E	249	-	-	-	X
3	LMT	E	263	-	-	-	X
3	LMT	E	268	-	-	-	X
3	LMT	F	219	-	-	-	X
3	LMT	F	233	-	-	-	X
3	LMT	F	241	-	-	-	X
3	LMT	F	248	-	-	-	X
3	LMT	G	235	-	-	-	X
3	LMT	G	251	-	-	-	X
3	LMT	G	264	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMT	H	234	-	-	-	X
3	LMT	I	240	-	-	-	X
3	LMT	I	252	-	-	-	X
3	LMT	I	258	-	-	-	X
3	LMT	J	239	-	-	-	X
3	LMT	J	253	-	-	-	X
3	LMT	K	225	-	-	-	X
3	LMT	L	226	-	-	-	X
3	LMT	L	254	-	-	-	X
3	LMT	L	265	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14603 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 Leukotriene C4 synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1115	743	189	181	2			
1	B	146	Total	C	N	O	S	0	1	0
			1129	757	189	181	2			
1	C	146	Total	C	N	O	S	0	0	0
			1129	750	195	182	2			
1	D	146	Total	C	N	O	S	0	1	0
			1123	754	186	181	2			
1	E	146	Total	C	N	O	S	0	1	0
			1131	758	189	182	2			
1	F	146	Total	C	N	O	S	0	1	0
			1121	753	186	180	2			
1	G	146	Total	C	N	O	S	0	1	0
			1102	742	177	181	2			
1	H	146	Total	C	N	O	S	0	1	0
			1122	752	186	182	2			
1	I	146	Total	C	N	O	S	0	1	0
			1123	754	186	181	2			
1	J	146	Total	C	N	O	S	0	1	0
			1110	746	180	182	2			
1	K	146	Total	C	N	O	S	0	1	0
			1114	748	183	181	2			
1	L	146	Total	C	N	O	S	0	1	0
			1114	745	186	181	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	HIS	-	EXPRESSION TAG	UNP Q16873
A	152	HIS	-	EXPRESSION TAG	UNP Q16873
A	153	HIS	-	EXPRESSION TAG	UNP Q16873
A	154	HIS	-	EXPRESSION TAG	UNP Q16873
A	155	HIS	-	EXPRESSION TAG	UNP Q16873

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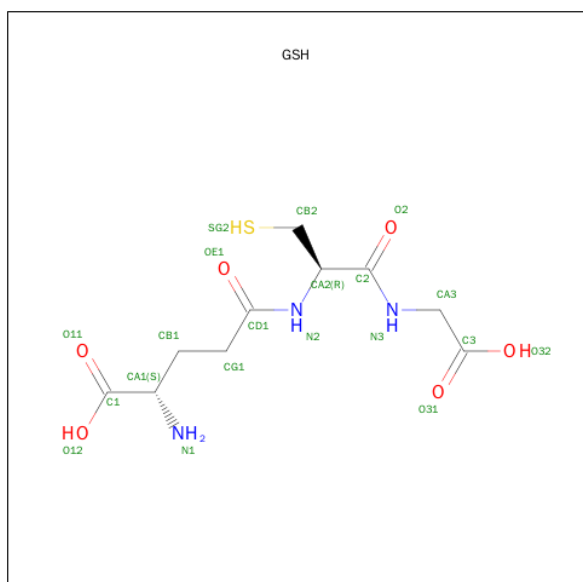
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	HIS	-	EXPRESSION TAG	UNP Q16873
B	151	HIS	-	EXPRESSION TAG	UNP Q16873
B	152	HIS	-	EXPRESSION TAG	UNP Q16873
B	153	HIS	-	EXPRESSION TAG	UNP Q16873
B	154	HIS	-	EXPRESSION TAG	UNP Q16873
B	155	HIS	-	EXPRESSION TAG	UNP Q16873
B	156	HIS	-	EXPRESSION TAG	UNP Q16873
C	151	HIS	-	EXPRESSION TAG	UNP Q16873
C	152	HIS	-	EXPRESSION TAG	UNP Q16873
C	153	HIS	-	EXPRESSION TAG	UNP Q16873
C	154	HIS	-	EXPRESSION TAG	UNP Q16873
C	155	HIS	-	EXPRESSION TAG	UNP Q16873
C	156	HIS	-	EXPRESSION TAG	UNP Q16873
D	151	HIS	-	EXPRESSION TAG	UNP Q16873
D	152	HIS	-	EXPRESSION TAG	UNP Q16873
D	153	HIS	-	EXPRESSION TAG	UNP Q16873
D	154	HIS	-	EXPRESSION TAG	UNP Q16873
D	155	HIS	-	EXPRESSION TAG	UNP Q16873
D	156	HIS	-	EXPRESSION TAG	UNP Q16873
E	151	HIS	-	EXPRESSION TAG	UNP Q16873
E	152	HIS	-	EXPRESSION TAG	UNP Q16873
E	153	HIS	-	EXPRESSION TAG	UNP Q16873
E	154	HIS	-	EXPRESSION TAG	UNP Q16873
E	155	HIS	-	EXPRESSION TAG	UNP Q16873
E	156	HIS	-	EXPRESSION TAG	UNP Q16873
F	151	HIS	-	EXPRESSION TAG	UNP Q16873
F	152	HIS	-	EXPRESSION TAG	UNP Q16873
F	153	HIS	-	EXPRESSION TAG	UNP Q16873
F	154	HIS	-	EXPRESSION TAG	UNP Q16873
F	155	HIS	-	EXPRESSION TAG	UNP Q16873
F	156	HIS	-	EXPRESSION TAG	UNP Q16873
G	151	HIS	-	EXPRESSION TAG	UNP Q16873
G	152	HIS	-	EXPRESSION TAG	UNP Q16873
G	153	HIS	-	EXPRESSION TAG	UNP Q16873
G	154	HIS	-	EXPRESSION TAG	UNP Q16873
G	155	HIS	-	EXPRESSION TAG	UNP Q16873
G	156	HIS	-	EXPRESSION TAG	UNP Q16873
H	151	HIS	-	EXPRESSION TAG	UNP Q16873
H	152	HIS	-	EXPRESSION TAG	UNP Q16873
H	153	HIS	-	EXPRESSION TAG	UNP Q16873
H	154	HIS	-	EXPRESSION TAG	UNP Q16873
H	155	HIS	-	EXPRESSION TAG	UNP Q16873

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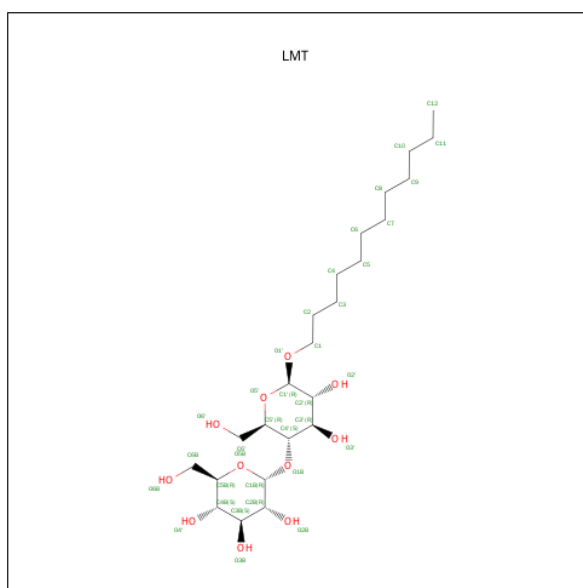
Chain	Residue	Modelled	Actual	Comment	Reference
H	156	HIS	-	EXPRESSION TAG	UNP Q16873
I	151	HIS	-	EXPRESSION TAG	UNP Q16873
I	152	HIS	-	EXPRESSION TAG	UNP Q16873
I	153	HIS	-	EXPRESSION TAG	UNP Q16873
I	154	HIS	-	EXPRESSION TAG	UNP Q16873
I	155	HIS	-	EXPRESSION TAG	UNP Q16873
I	156	HIS	-	EXPRESSION TAG	UNP Q16873
J	151	HIS	-	EXPRESSION TAG	UNP Q16873
J	152	HIS	-	EXPRESSION TAG	UNP Q16873
J	153	HIS	-	EXPRESSION TAG	UNP Q16873
J	154	HIS	-	EXPRESSION TAG	UNP Q16873
J	155	HIS	-	EXPRESSION TAG	UNP Q16873
J	156	HIS	-	EXPRESSION TAG	UNP Q16873
K	151	HIS	-	EXPRESSION TAG	UNP Q16873
K	152	HIS	-	EXPRESSION TAG	UNP Q16873
K	153	HIS	-	EXPRESSION TAG	UNP Q16873
K	154	HIS	-	EXPRESSION TAG	UNP Q16873
K	155	HIS	-	EXPRESSION TAG	UNP Q16873
K	156	HIS	-	EXPRESSION TAG	UNP Q16873
L	151	HIS	-	EXPRESSION TAG	UNP Q16873
L	152	HIS	-	EXPRESSION TAG	UNP Q16873
L	153	HIS	-	EXPRESSION TAG	UNP Q16873
L	154	HIS	-	EXPRESSION TAG	UNP Q16873
L	155	HIS	-	EXPRESSION TAG	UNP Q16873
L	156	HIS	-	EXPRESSION TAG	UNP Q16873

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	G	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	H	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	I	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	J	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	K	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	L	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 23 18 5	0	0
3	C	1	Total C O 35 24 11	0	0
3	A	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0
3	A	1	Total C 7 7	0	0
3	B	1	Total C O 23 18 5	0	0
3	F	1	Total C 9 9	0	0
3	D	1	Total C 9 9	0	0
3	E	1	Total C 10 10	0	0
3	G	1	Total C 9 9	0	0
3	L	1	Total C 9 9	0	0
3	K	1	Total C 7 7	0	0
3	K	1	Total C O 23 18 5	0	0
3	L	1	Total C 9 9	0	0
3	B	1	Total C O 23 18 5	0	0
3	A	1	Total C O 23 18 5	0	0
3	A	1	Total C 9 9	0	0
3	E	1	Total C O 35 24 11	0	0
3	E	1	Total C O 23 18 5	0	0
3	E	1	Total C 6 6	0	0
3	F	1	Total C O 23 18 5	0	0
3	H	1	Total C O 23 18 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			23	18	5		
3	B	1	Total	C	O	0	0
			18	13	5		
3	C	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	J	1	Total	C	O	0	0
			35	24	11		
3	I	1	Total	C	O	0	0
			18	13	5		
3	F	1	Total	C	O	0	0
			18	13	5		
3	B	1	Total	C		0	0
			12	12			
3	E	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C		0	0
			9	9			
3	A	1	Total	C		0	0
			9	9			
3	C	1	Total	C		0	0
			9	9			
3	D	1	Total	C		0	0
			9	9			
3	F	1	Total	C		0	0
			9	9			
3	E	1	Total	C		0	0
			9	9			
3	H	1	Total	C		0	0
			9	9			
3	G	1	Total	C		0	0
			9	9			
3	I	1	Total	C		0	0
			9	9			
3	J	1	Total	C		0	0
			9	9			
3	L	1	Total	C		0	0
			9	9			
3	L	1	Total	C		0	0
			9	9			

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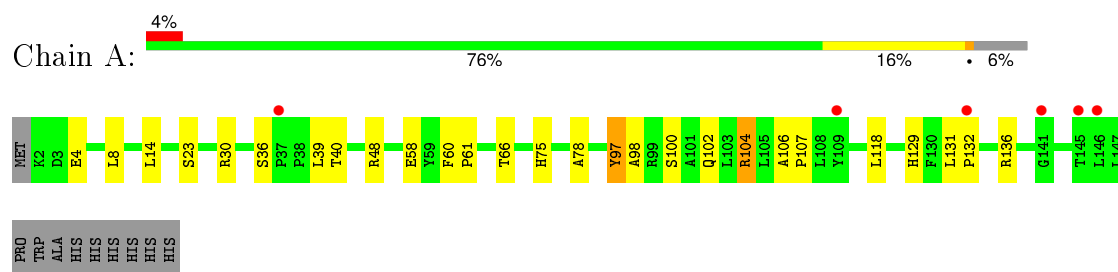
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 18 13 5	0	0
3	I	1	Total C 9 9	0	0
3	I	1	Total C 9 9	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 9 9	0	0
3	C	1	Total C 9 9	0	0
3	A	1	Total C 9 9	0	0
3	E	1	Total C 9 9	0	0
3	G	1	Total C 9 9	0	0
3	L	1	Total C 7 7	0	0
3	E	1	Total C 9 9	0	0
3	G	1	Total C 9 9	0	0
3	E	1	Total C O 35 24 11	0	0
3	E	1	Total C O 35 24 11	0	0

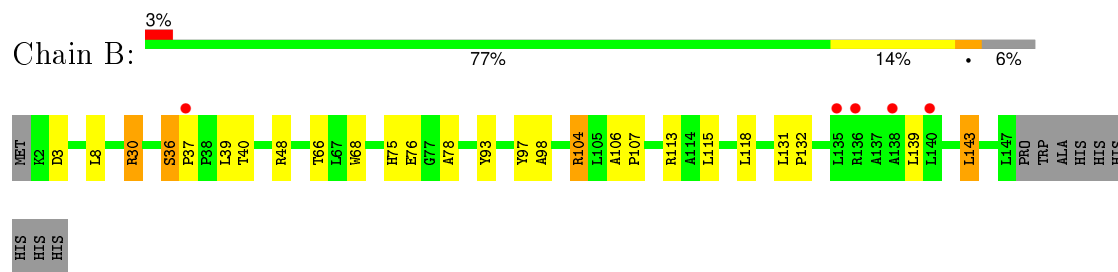
3 Residue-property plots [i](#)

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.

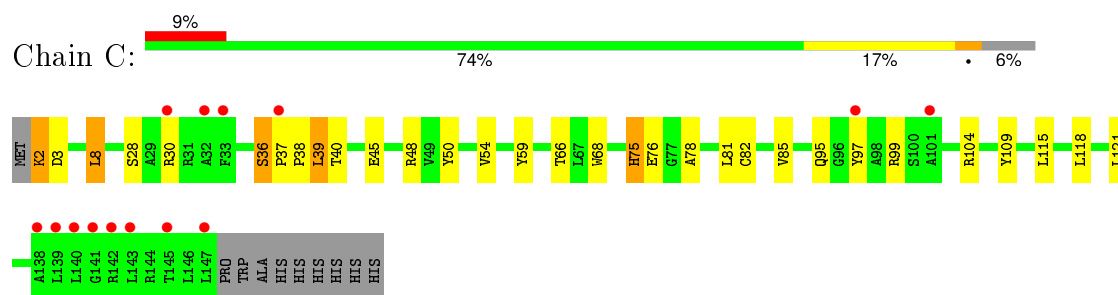
- Molecule 1: Leukotriene C4 synthase



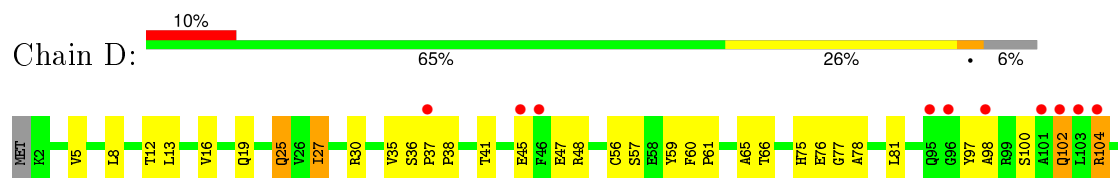
- Molecule 1: Leukotriene C4 synthase



- Molecule 1: Leukotriene C4 synthase

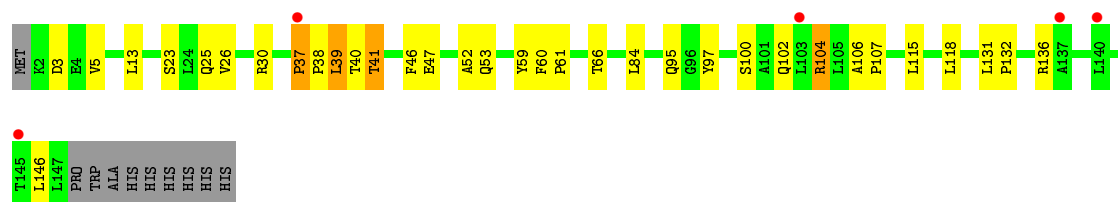


- Molecule 1: Leukotriene C4 synthase

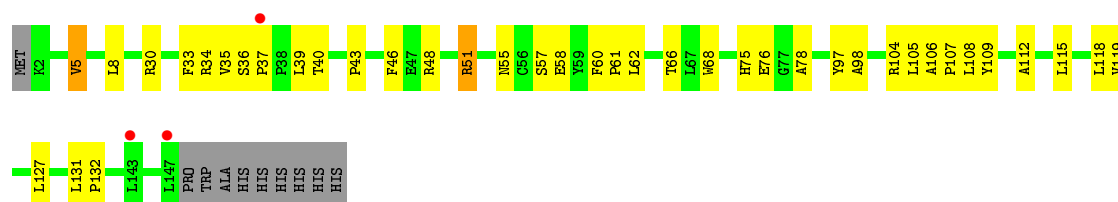




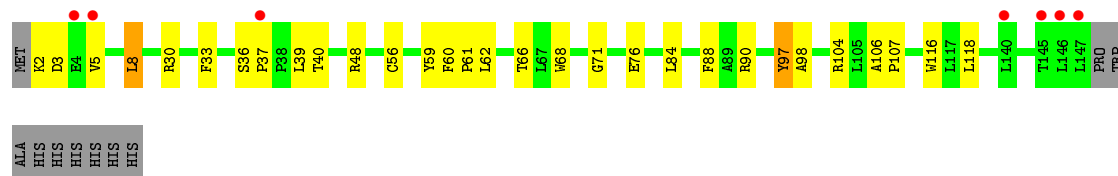
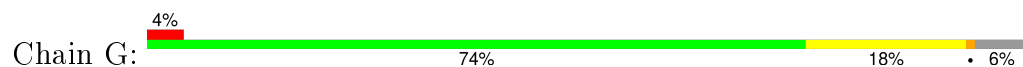
- Molecule 1: Leukotriene C4 synthase



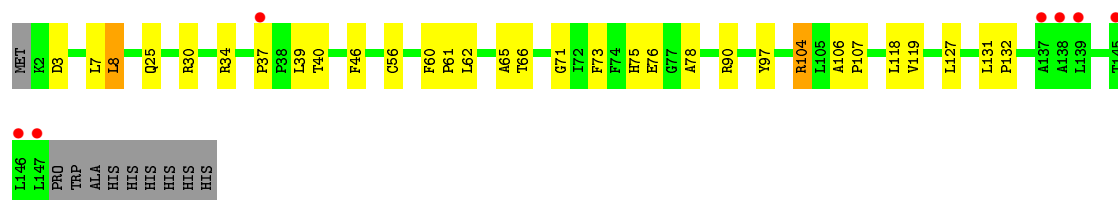
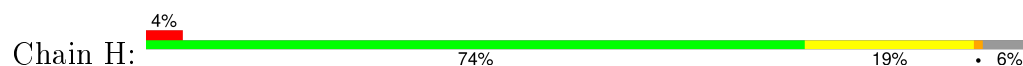
- Molecule 1: Leukotriene C4 synthase



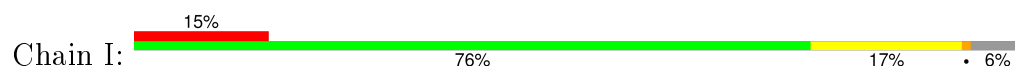
- Molecule 1: Leukotriene C4 synthase

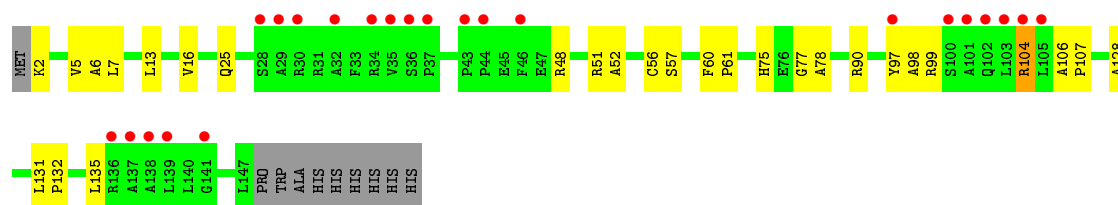


- Molecule 1: Leukotriene C4 synthase

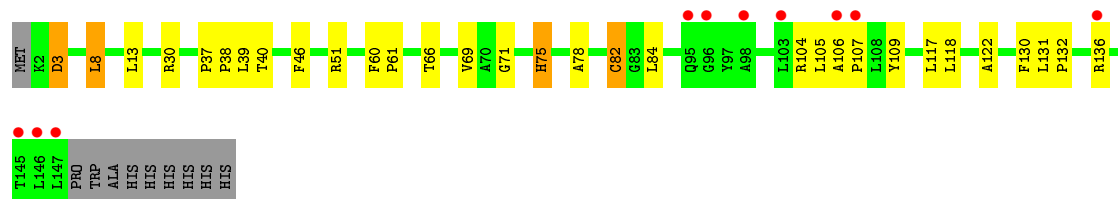
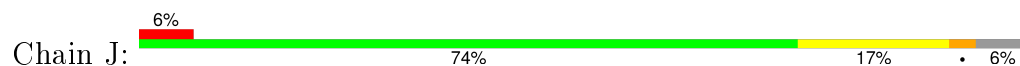


- Molecule 1: Leukotriene C4 synthase

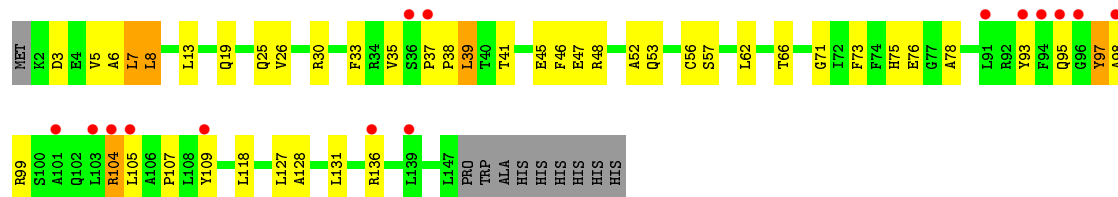




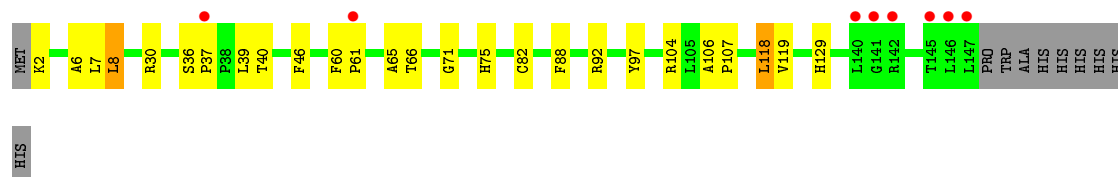
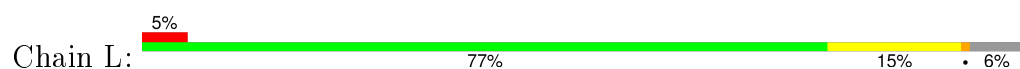
- Molecule 1: Leukotriene C4 synthase



- Molecule 1: Leukotriene C4 synthase



- Molecule 1: Leukotriene C4 synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.50 Å 293.90 Å 206.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 48.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.30) 100.0 (48.98-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 3.33 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.255 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54055 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14603	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GSH, LMT

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	0.34	0/1144	0.46	0/1563
1	B	0.35	0/1162	0.47	0/1587
1	C	0.33	0/1158	0.46	0/1580
1	D	0.35	0/1156	0.47	0/1580
1	E	0.34	0/1164	0.45	0/1590
1	F	0.34	0/1154	0.45	0/1578
1	G	0.31	0/1135	0.44	0/1555
1	H	0.33	0/1155	0.45	0/1579
1	I	0.33	0/1156	0.46	0/1580
1	J	0.35	0/1143	0.46	0/1565
1	K	0.35	0/1147	0.47	0/1569
1	L	0.33	0/1147	0.45	0/1568
All	All	0.34	0/13821	0.46	0/18894

There are no bond length outliers.

There are no bond angle outliers.

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	1115	0	1139	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1129	0	1166	26	0
1	C	1129	0	1166	24	0
1	D	1123	0	1155	37	0
1	E	1131	0	1171	29	0
1	F	1121	0	1156	35	1
1	G	1102	0	1113	22	1
1	H	1122	0	1151	24	0
1	I	1123	0	1155	20	0
1	J	1110	0	1129	27	0
1	K	1114	0	1135	40	0
1	L	1114	0	1128	22	0
2	A	20	0	15	2	0
2	B	20	0	15	1	0
2	C	20	0	15	1	0
2	D	20	0	15	0	0
2	E	20	0	15	0	0
2	F	20	0	15	2	0
2	G	20	0	15	0	0
2	H	20	0	15	1	0
2	I	20	0	15	1	0
2	J	20	0	15	2	0
2	K	20	0	15	0	0
2	L	20	0	15	2	0
3	A	119	0	182	3	0
3	B	117	0	180	3	0
3	C	123	0	172	8	0
3	D	53	0	80	6	0
3	E	206	0	299	11	0
3	F	59	0	89	4	0
3	G	59	0	102	3	0
3	H	32	0	51	0	0
3	I	45	0	72	5	0
3	J	44	0	63	1	0
3	K	30	0	47	0	0
3	L	43	0	81	1	0
All	All	14603	0	15362	304	1

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 10.

All (304) 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:E:30:ARG:NH1	1:E:37:PRO:HA	1.73	1.04
1:B:75:HIS:HD2	1:B:78:ALA:H	1.12	0.96
1:K:75:HIS:HD2	1:K:78:ALA:H	1.05	0.96
1:H:66:THR:CG2	1:H:118:LEU:HB3	1.95	0.95
1:A:75:HIS:HD2	1:A:78:ALA:H	1.18	0.91
1:E:30:ARG:HH12	1:E:37:PRO:HA	1.32	0.90
1:J:75:HIS:HD2	1:J:78:ALA:H	1.17	0.89
2:C:203:GSH:HSG	3:C:216:LMT:H6'	1.19	0.88
1:G:66:THR:CG2	1:G:118:LEU:HB3	2.04	0.88
1:H:75:HIS:HD2	1:H:78:ALA:H	1.14	0.88
1:D:75:HIS:HD2	1:D:78:ALA:H	1.16	0.87
1:K:66:THR:CG2	1:K:118:LEU:HB3	2.05	0.86
1:A:104:ARG:NH2	1:B:37:PRO:HG2	1.92	0.85
1:J:3:ASP:HB3	1:L:129:HIS:HE1	1.42	0.85
1:B:66:THR:CG2	1:B:118:LEU:HB3	2.05	0.85
1:K:75:HIS:CD2	1:K:78:ALA:H	1.93	0.85
1:F:66:THR:HG22	1:F:118:LEU:HB3	1.58	0.84
1:K:104:ARG:HH22	1:L:37:PRO:HG3	1.40	0.83
1:F:66:THR:CG2	1:F:118:LEU:HB3	2.09	0.82
1:B:113:ARG:HH12	3:B:218:LMT:H6D	1.44	0.81
1:I:128:ALA:HB2	3:I:258:LMT:H62	1.63	0.81
1:H:75:HIS:CD2	1:H:78:ALA:H	1.98	0.80
1:H:66:THR:HG21	1:H:118:LEU:HB3	1.61	0.80
1:J:30:ARG:NH2	1:J:39:LEU:O	2.14	0.80
1:F:106:ALA:HB3	1:F:107:PRO:HD3	1.64	0.79
1:F:75:HIS:HD2	1:F:78:ALA:H	1.31	0.79
1:D:25:GLN:HA	1:D:25:GLN:HE21	1.46	0.78
1:B:75:HIS:CD2	1:B:78:ALA:H	2.02	0.76
1:J:75:HIS:CD2	1:J:78:ALA:H	2.01	0.76
1:K:66:THR:HG22	1:K:118:LEU:HB3	1.68	0.76
1:J:106:ALA:HB3	1:J:107:PRO:HD3	1.68	0.75
1:H:66:THR:HG22	1:H:118:LEU:HB3	1.69	0.74
1:A:75:HIS:CD2	1:A:78:ALA:H	2.03	0.74
1:F:51:ARG:HG3	2:F:206:GSH:O32	1.86	0.74
1:B:66:THR:HG22	1:B:118:LEU:HB3	1.69	0.74
1:D:37:PRO:HG2	1:D:38:PRO:HD3	1.68	0.74
1:H:106:ALA:HB3	1:H:107:PRO:HD3	1.68	0.73
1:J:66:THR:HG22	1:J:118:LEU:HB3	1.70	0.73
3:A:244:LMT:H62	3:A:245:LMT:H61	1.70	0.73
1:G:37:PRO:HB3	1:I:104:ARG:NH1	2.04	0.73
1:B:30:ARG:NH2	1:B:39:LEU:O	2.22	0.72
1:J:66:THR:CG2	1:J:118:LEU:HB3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LYS:N	1:C:2:LYS:HE3	2.06	0.71
1:E:106:ALA:HB3	1:E:107:PRO:HD3	1.73	0.70
1:D:75:HIS:CD2	1:D:78:ALA:H	2.05	0.70
1:I:52:ALA:HB2	1:I:97:TYR:HD2	1.56	0.69
1:E:66:THR:HG22	1:E:118:LEU:HB3	1.75	0.69
1:C:75:HIS:HD2	1:C:78:ALA:H	1.41	0.69
1:A:30:ARG:NH2	1:A:39:LEU:O	2.26	0.69
1:K:75:HIS:HD2	1:K:78:ALA:N	1.86	0.68
1:F:75:HIS:CD2	1:F:78:ALA:H	2.10	0.68
1:B:75:HIS:HD2	1:B:78:ALA:N	1.90	0.68
1:E:104:ARG:NH2	1:F:37:PRO:HG2	2.09	0.68
1:C:48:ARG:NH1	1:C:99:ARG:O	2.26	0.68
1:D:97:TYR:HB2	1:D:104:ARG:HB3	1.76	0.68
1:E:41:THR:HG22	1:E:47:GLU:OE2	1.94	0.68
1:C:75:HIS:CD2	1:C:78:ALA:H	2.12	0.67
1:A:48:ARG:NH1	1:A:98:ALA:O	2.27	0.67
1:E:66:THR:CG2	1:E:118:LEU:HB3	2.24	0.67
1:K:104:ARG:HH22	1:L:37:PRO:CG	2.08	0.67
1:B:48:ARG:NH1	1:B:98:ALA:O	2.28	0.66
1:H:75:HIS:HD2	1:H:78:ALA:N	1.92	0.66
1:A:66:THR:HG22	1:A:118:LEU:HB3	1.78	0.66
1:A:66:THR:CG2	1:A:118:LEU:HB3	2.27	0.65
1:K:25:GLN:HA	1:K:25:GLN:OE1	1.97	0.65
1:D:75:HIS:HD2	1:D:78:ALA:N	1.91	0.64
1:C:66:THR:CG2	1:C:118:LEU:HB3	2.28	0.64
1:F:5:VAL:HG22	1:F:68:TRP:CZ3	2.32	0.64
1:I:106:ALA:HB3	1:I:107:PRO:HD3	1.79	0.63
1:D:119:VAL:HG13	1:E:13:LEU:HD11	1.80	0.63
1:K:66:THR:HG21	1:K:118:LEU:HB3	1.82	0.62
1:J:8:LEU:HD21	1:J:71:GLY:HA3	1.81	0.62
1:E:52:ALA:HB2	1:E:97:TYR:HD2	1.65	0.61
1:L:106:ALA:HB3	1:L:107:PRO:HD3	1.82	0.61
1:D:25:GLN:NE2	1:D:25:GLN:HA	2.15	0.61
1:A:75:HIS:HD2	1:A:78:ALA:N	1.95	0.61
1:D:41:THR:OG1	1:D:47:GLU:OE2	2.06	0.61
1:B:106:ALA:HB3	1:B:107:PRO:HD3	1.83	0.60
3:I:240:LMT:H62	1:K:128:ALA:HB2	1.81	0.60
1:H:104:ARG:NH1	2:H:208:GSH:SG2	2.74	0.60
1:B:8:LEU:HD13	1:B:76:GLU:HG3	1.82	0.60
1:D:27:ILE:HD11	2:F:206:GSH:HB22	1.83	0.60
1:L:66:THR:CG2	1:L:118:LEU:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:ARG:NH1	1:G:98:ALA:O	2.36	0.59
1:G:104:ARG:HH21	1:H:37:PRO:HG3	1.68	0.59
1:H:30:ARG:HG3	1:H:46:PHE:HE1	1.66	0.59
1:A:106:ALA:HB3	1:A:107:PRO:HD3	1.85	0.59
1:K:104:ARG:HD2	1:K:104:ARG:C	2.24	0.58
1:F:60:PHE:HB3	1:F:61:PRO:HD3	1.85	0.58
1:E:25:GLN:NE2	3:E:243:LMT:O4'	2.36	0.58
1:D:116:TRP:CE2	3:D:220:LMT:H121	2.38	0.58
1:G:59:TYR:HE2	3:G:222:LMT:H91	1.69	0.58
1:A:58:GLU:OE2	2:A:201:GSH:N1	2.36	0.58
1:G:66:THR:HG21	1:G:118:LEU:HB3	1.87	0.57
1:I:75:HIS:CD2	1:I:78:ALA:H	2.21	0.57
1:C:37:PRO:HG2	1:C:38:PRO:HD3	1.85	0.57
1:K:104:ARG:NH2	1:L:37:PRO:HG3	2.17	0.57
1:E:52:ALA:HB2	1:E:97:TYR:CD2	2.40	0.57
1:J:130:PHE:HE1	1:K:6:ALA:HB1	1.68	0.56
1:C:59:TYR:HE2	3:C:216:LMT:H91	1.71	0.56
1:C:66:THR:HG22	1:C:118:LEU:HB3	1.87	0.56
1:K:8:LEU:HD13	1:K:76:GLU:HG2	1.86	0.56
1:D:66:THR:CG2	1:D:118:LEU:HB3	2.36	0.56
1:A:60:PHE:HB3	1:A:61:PRO:HD3	1.88	0.56
1:L:66:THR:HG22	1:L:118:LEU:HB3	1.88	0.55
1:A:97:TYR:HB2	1:A:104:ARG:HB3	1.88	0.55
1:K:104:ARG:NH2	1:L:37:PRO:CG	2.69	0.55
1:D:8:LEU:HG	1:D:76:GLU:HG3	1.89	0.55
2:J:210:GSH:HB12	1:K:26:VAL:HG11	1.89	0.55
1:D:59:TYR:HE2	3:D:220:LMT:H91	1.72	0.55
1:D:48:ARG:NH1	1:D:98:ALA:O	2.40	0.54
1:A:129:HIS:HE1	1:B:3:ASP:HB2	1.72	0.54
1:K:19:GLN:HE22	1:K:56:CYS:HB3	1.72	0.54
1:E:30:ARG:NH2	1:E:39:LEU:O	2.40	0.54
1:I:131:LEU:N	1:I:132:PRO:HD2	2.23	0.54
1:B:131:LEU:N	1:B:132:PRO:HD2	2.23	0.54
1:H:65:ALA:HA	3:I:252:LMT:H112	1.90	0.54
1:I:48:ARG:NH1	1:I:98:ALA:O	2.41	0.54
1:J:75:HIS:HD2	1:J:78:ALA:N	1.97	0.54
1:C:66:THR:HG21	1:C:118:LEU:HB3	1.91	0.53
1:J:60:PHE:HB3	1:J:61:PRO:HD3	1.90	0.53
1:E:95:GLN:HE22	3:E:268:LMT:C1	2.21	0.53
1:A:104:ARG:HH22	1:B:37:PRO:HG2	1.72	0.53
2:A:201:GSH:O12	1:B:30:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:127:LEU:HD22	1:K:131:LEU:HD22	1.91	0.53
1:K:30:ARG:HG2	1:K:35:VAL:O	2.09	0.53
1:H:25:GLN:NE2	1:H:25:GLN:HA	2.24	0.53
1:B:66:THR:HG21	1:B:118:LEU:HB3	1.89	0.53
1:F:115:LEU:O	1:F:119:VAL:HG23	2.08	0.53
1:J:69:VAL:HG12	1:J:122:ALA:HB1	1.90	0.52
1:E:30:ARG:HG2	1:E:46:PHE:HE1	1.73	0.52
1:E:95:GLN:HE22	3:E:268:LMT:H11	1.73	0.52
1:B:93:TYR:OH	2:B:202:GSH:O2	2.24	0.52
1:K:105:LEU:O	1:K:109:TYR:CD1	2.62	0.52
1:I:128:ALA:CB	3:I:258:LMT:H62	2.36	0.52
1:C:30:ARG:NH2	1:C:39:LEU:O	2.42	0.52
1:F:30:ARG:HG2	1:F:35:VAL:O	2.10	0.51
1:C:109:TYR:CE2	3:C:216:LMT:H31	2.45	0.51
1:K:48:ARG:NH1	1:K:98:ALA:O	2.43	0.51
1:G:66:THR:HG22	1:G:118:LEU:HB3	1.88	0.51
1:C:75:HIS:HD2	1:C:78:ALA:N	2.07	0.51
1:F:5:VAL:HG22	1:F:68:TRP:HZ3	1.73	0.51
1:I:75:HIS:HD2	1:I:78:ALA:H	1.57	0.51
1:I:48:ARG:NH1	1:I:99:ARG:O	2.43	0.51
1:J:3:ASP:CB	1:L:129:HIS:HE1	2.18	0.51
3:A:244:LMT:H101	1:B:68:TRP:CE2	2.44	0.51
1:D:66:THR:HG22	1:D:118:LEU:HB3	1.92	0.51
1:K:73:PHE:CZ	1:L:6:ALA:HA	2.45	0.51
1:J:3:ASP:HB3	1:L:129:HIS:CE1	2.33	0.51
1:F:33:PHE:HD1	1:F:46:PHE:HB2	1.75	0.51
1:F:66:THR:HG21	1:F:118:LEU:HB3	1.90	0.51
1:F:5:VAL:CG2	1:F:68:TRP:HZ3	2.24	0.51
1:I:56:CYS:HA	1:I:90:ARG:NH1	2.26	0.50
1:D:104:ARG:NH2	1:E:37:PRO:HG3	2.26	0.50
1:C:115:LEU:HD23	3:C:216:LMT:H112	1.93	0.50
1:J:30:ARG:HG2	1:J:46:PHE:CE1	2.46	0.50
1:C:95:GLN:HE22	3:C:214:LMT:H1'	1.76	0.50
1:J:131:LEU:N	1:J:132:PRO:HD2	2.27	0.50
1:F:30:ARG:NH2	1:F:39:LEU:O	2.45	0.49
1:L:30:ARG:HH21	1:L:37:PRO:HA	1.75	0.49
1:F:30:ARG:HG3	1:F:46:PHE:CE1	2.47	0.49
1:K:8:LEU:HD21	1:K:71:GLY:HA3	1.93	0.49
1:F:127:LEU:HD22	1:F:131:LEU:HD22	1.94	0.49
1:J:30:ARG:HG2	1:J:46:PHE:HE1	1.77	0.49
1:F:48:ARG:NH1	1:F:98:ALA:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ARG:HE	1:K:37:PRO:HA	1.77	0.49
1:B:139:LEU:O	1:B:143:LEU:HB2	2.13	0.49
3:D:247:LMT:H101	3:E:249:LMT:H101	1.95	0.49
1:G:8:LEU:HD21	1:G:71:GLY:HA3	1.93	0.48
1:G:30:ARG:NH2	1:G:39:LEU:O	2.46	0.48
1:B:113:ARG:HH12	3:B:218:LMT:C6'	2.19	0.48
1:E:59:TYR:HE2	3:E:221:LMT:H91	1.77	0.48
1:D:13:LEU:HD11	1:F:119:VAL:HG13	1.95	0.48
1:K:33:PHE:CE2	1:K:45:GLU:HB2	2.49	0.48
1:F:112:ALA:HB2	3:F:219:LMT:H71	1.96	0.48
1:J:37:PRO:HG2	1:J:38:PRO:HD3	1.96	0.47
1:K:41:THR:OG1	1:K:47:GLU:OE2	2.22	0.47
1:D:97:TYR:CB	1:D:104:ARG:HB3	2.43	0.47
3:E:249:LMT:H52	3:F:248:LMT:H62	1.97	0.47
1:F:30:ARG:HE	1:F:37:PRO:HA	1.80	0.47
1:D:65:ALA:HA	3:E:249:LMT:H122	1.96	0.47
3:J:239:LMT:H6D	3:J:239:LMT:H5B	1.95	0.47
1:L:88[B]:PHE:CE2	1:L:92:ARG:HD2	2.49	0.46
1:A:131:LEU:N	1:A:132:PRO:HD2	2.30	0.46
1:J:51:ARG:HB3	2:J:210:GSH:O32	2.16	0.46
1:E:84:LEU:HD11	3:E:231:LMT:H102	1.98	0.46
1:D:16:VAL:HG13	1:F:62:LEU:HD22	1.97	0.46
1:G:84:LEU:O	1:G:88[A]:PHE:HD1	1.98	0.46
1:F:33:PHE:HB3	1:F:43:PRO:HG2	1.97	0.46
1:J:30:ARG:NH1	2:L:212:GSH:O11	2.49	0.46
1:F:30:ARG:HG3	1:F:46:PHE:HE1	1.81	0.46
1:C:45:GLU:HA	1:C:48:ARG:HH21	1.80	0.46
1:A:100:SER:C	1:A:102:GLN:H	2.17	0.46
1:C:81:LEU:HD22	1:D:143:LEU:HD22	1.97	0.46
1:D:37:PRO:CG	1:D:38:PRO:HD3	2.41	0.46
1:F:108:LEU:HD21	3:F:219:LMT:H61	1.98	0.46
1:H:131:LEU:N	1:H:132:PRO:HD2	2.31	0.46
1:K:30:ARG:NH2	1:K:39:LEU:O	2.49	0.46
1:F:131:LEU:N	1:F:132:PRO:HD2	2.31	0.46
1:A:14:LEU:HD13	3:A:228:LMT:H121	1.98	0.45
1:H:30:ARG:HG3	1:H:46:PHE:CE1	2.50	0.45
1:F:115:LEU:HD23	3:F:219:LMT:H112	1.99	0.45
1:A:66:THR:HG21	1:A:118:LEU:HB3	1.99	0.45
1:E:26:VAL:O	1:E:30:ARG:HG3	2.16	0.45
3:I:258:LMT:H52	1:K:136:ARG:HB2	1.97	0.45
1:L:8:LEU:HD21	1:L:71:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:SER:CB	1:C:37:PRO:HD2	2.46	0.45
1:C:8:LEU:HD13	1:C:76:GLU:HG3	1.98	0.45
1:C:121:LEU:HD21	1:D:135:LEU:HD21	1.97	0.45
1:J:30:ARG:NH1	2:L:212:GSH:O12	2.50	0.45
3:C:214:LMT:O3'	3:C:214:LMT:H1B	2.16	0.45
1:G:5:VAL:HB	1:G:68:TRP:HZ3	1.82	0.45
1:G:106:ALA:HB3	1:G:107:PRO:CD	2.47	0.45
1:J:13:LEU:HD11	1:L:119:VAL:HG13	1.99	0.45
1:E:52:ALA:CB	1:E:97:TYR:HD2	2.29	0.45
1:D:59:TYR:CE2	3:D:220:LMT:H91	2.51	0.45
1:E:115:LEU:HD23	3:E:221:LMT:H112	1.99	0.45
1:L:60:PHE:HB3	1:L:61:PRO:HD3	1.99	0.45
3:C:216:LMT:H3'	3:C:216:LMT:H1B	1.69	0.45
1:G:116:TRP:CD2	3:G:222:LMT:H121	2.52	0.45
1:D:12:THR:O	1:D:16:VAL:HG23	2.17	0.44
1:D:60:PHE:HB3	1:D:61:PRO:HD3	1.98	0.44
1:D:117:LEU:O	1:D:121:LEU:HG	2.17	0.44
1:F:36:SER:HA	1:F:37:PRO:HD3	1.82	0.44
1:K:37:PRO:HG2	1:K:38:PRO:HD3	1.99	0.44
1:C:50:TYR:O	1:C:54:VAL:HG23	2.16	0.44
1:E:60:PHE:HB3	1:E:61:PRO:HD3	1.99	0.44
1:K:52:ALA:HB2	1:K:97:TYR:CD2	2.52	0.44
1:I:51:ARG:HB3	2:I:209:GSH:O32	2.17	0.44
1:I:75:HIS:HD2	1:I:77:GLY:N	2.16	0.44
1:D:19:GLN:HE22	1:D:56:CYS:HB3	1.82	0.44
3:C:237:LMT:H62	3:D:238:LMT:H61	2.00	0.44
1:D:77:GLY:O	1:D:81:LEU:HG	2.17	0.44
1:F:55:ASN:HA	1:F:58:GLU:OE2	2.17	0.44
1:E:66:THR:HG21	1:E:118:LEU:HB3	1.98	0.44
1:D:102:GLN:HE21	1:D:102:GLN:HB3	1.60	0.44
1:E:97:TYR:HB2	1:E:104:ARG:HB3	1.99	0.43
1:G:8:LEU:HD13	1:G:76:GLU:HG2	1.99	0.43
1:L:36:SER:O	1:L:39:LEU:HB2	2.18	0.43
1:G:104:ARG:NH2	1:H:37:PRO:HB3	2.33	0.43
1:C:8:LEU:HD23	1:C:68:TRP:CE3	2.54	0.43
1:H:60:PHE:HB3	1:H:61:PRO:HD3	2.00	0.43
1:K:104:ARG:HH12	1:L:37:PRO:HB3	1.83	0.43
1:G:116:TRP:CE2	3:G:222:LMT:H121	2.53	0.43
1:G:56:CYS:SG	1:G:90:ARG:HD2	2.59	0.43
1:G:97:TYR:CD1	1:G:104:ARG:HD3	2.53	0.43
1:H:56:CYS:SG	1:H:90:ARG:HD2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:CYS:HB3	1:C:118:LEU:HG	2.01	0.43
1:A:129:HIS:HE1	1:B:3:ASP:CB	2.30	0.42
1:K:95:GLN:O	1:K:99:ARG:HG3	2.19	0.42
1:H:119:VAL:HG13	1:I:13:LEU:HD11	2.00	0.42
1:K:48:ARG:HD2	1:K:97:TYR:O	2.18	0.42
1:D:100:SER:C	1:D:102:GLN:H	2.21	0.42
1:A:104:ARG:NH2	1:B:37:PRO:CG	2.74	0.42
1:K:45:GLU:HG3	1:K:48:ARG:HH22	1.84	0.42
1:D:30:ARG:HG2	1:D:35:VAL:O	2.20	0.42
1:G:8:LEU:HD23	1:G:68:TRP:CE3	2.55	0.42
1:B:115:LEU:HD23	3:B:218:LMT:H112	2.00	0.42
1:G:37:PRO:HB3	1:I:104:ARG:HH12	1.81	0.42
1:F:5:VAL:CG2	1:F:68:TRP:CZ3	3.01	0.42
1:G:37:PRO:HB3	1:I:104:ARG:CZ	2.49	0.42
1:H:30:ARG:NH2	1:H:39:LEU:O	2.53	0.42
1:J:105:LEU:O	1:J:109:TYR:CD1	2.73	0.42
1:F:51:ARG:HD2	1:F:51:ARG:HA	1.45	0.42
1:L:66:THR:HG21	1:L:118:LEU:HB3	2.01	0.42
1:E:95:GLN:NE2	3:E:268:LMT:H11	2.33	0.42
1:B:8:LEU:HD23	1:B:68:TRP:CE3	2.55	0.41
1:C:81:LEU:O	1:C:85:VAL:HG23	2.20	0.41
1:B:36:SER:HA	1:B:37:PRO:HD3	1.82	0.41
1:E:25:GLN:NE2	1:E:25:GLN:HA	2.35	0.41
1:D:45:GLU:HG3	1:D:48:ARG:HH22	1.85	0.41
1:J:66:THR:HG21	1:J:118:LEU:HB3	2.02	0.41
1:F:33:PHE:CD1	1:F:46:PHE:HB2	2.55	0.41
1:B:104:ARG:HH21	1:C:37:PRO:HG3	1.84	0.41
1:K:33:PHE:CZ	1:K:45:GLU:HB2	2.55	0.41
1:K:13:LEU:HD12	1:K:13:LEU:HA	1.87	0.41
1:A:36:SER:O	1:A:39:LEU:HB2	2.20	0.41
3:E:268:LMT:H62	3:E:268:LMT:H92	1.84	0.41
1:J:82:CYS:SG	1:J:117:LEU:HD23	2.60	0.41
1:H:8:LEU:HD21	1:H:71:GLY:HA3	2.02	0.41
1:F:8:LEU:HG	1:F:76:GLU:HG3	2.02	0.41
1:E:37:PRO:HB2	1:E:38:PRO:HD3	2.02	0.41
1:J:130:PHE:CE1	1:K:6:ALA:HB1	2.52	0.41
1:E:131:LEU:N	1:E:132:PRO:HD2	2.36	0.41
1:H:62:LEU:HD22	1:I:16:VAL:HG13	2.02	0.41
1:L:30:ARG:HG3	1:L:46:PHE:HE1	1.86	0.41
1:D:66:THR:HG21	1:D:118:LEU:HB3	2.01	0.41
1:E:100:SER:C	1:E:102:GLN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:LEU:HB2	1:K:76:GLU:OE2	2.21	0.41
1:D:124:LEU:HD22	3:D:238:LMT:H62	2.02	0.41
1:L:65:ALA:HA	3:L:254:LMT:H112	2.02	0.41
1:G:60:PHE:HB3	1:G:61:PRO:HD3	2.02	0.41
1:I:25:GLN:HE21	1:I:25:GLN:HA	1.85	0.41
1:H:75:HIS:CD2	1:H:78:ALA:N	2.75	0.40
1:H:73:PHE:CZ	1:I:6:ALA:HA	2.56	0.40
1:I:60:PHE:HB3	1:I:61:PRO:HD3	2.03	0.40
1:L:36:SER:HA	1:L:37:PRO:HD3	1.91	0.40
1:A:100:SER:C	1:A:102:GLN:N	2.75	0.40
1:K:93:TYR:HA	1:K:107:PRO:HG2	2.03	0.40
1:D:131:LEU:HB3	1:D:132:PRO:HD3	2.03	0.40
1:K:30:ARG:NH1	1:K:46:PHE:HZ	2.19	0.40
1:H:8:LEU:HD13	1:H:76:GLU:HG3	2.02	0.40
1:J:84:LEU:HA	1:J:84:LEU:HD23	1.97	0.40
1:F:105:LEU:O	1:F:109:TYR:CD1	2.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ARG:NH1	1:G:33:PHE:O[8_545]	2.12	0.08

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	144/156 (92%)	137 (95%)	7 (5%)	0	100	100
1	B	145/156 (93%)	136 (94%)	9 (6%)	0	100	100
1	C	144/156 (92%)	138 (96%)	5 (4%)	1 (1%)	26	66
1	D	145/156 (93%)	140 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	145/156 (93%)	137 (94%)	7 (5%)	1 (1%)	26	66
1	F	145/156 (93%)	139 (96%)	6 (4%)	0	100	100
1	G	145/156 (93%)	138 (95%)	7 (5%)	0	100	100
1	H	145/156 (93%)	138 (95%)	7 (5%)	0	100	100
1	I	145/156 (93%)	138 (95%)	7 (5%)	0	100	100
1	J	145/156 (93%)	138 (95%)	6 (4%)	1 (1%)	26	66
1	K	145/156 (93%)	137 (94%)	8 (6%)	0	100	100
1	L	145/156 (93%)	139 (96%)	5 (3%)	1 (1%)	26	66
All	All	1738/1872 (93%)	1655 (95%)	79 (4%)	4 (0%)	52	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	75	HIS
1	C	75	HIS
1	E	37	PRO
1	J	75	HIS

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	105/120 (88%)	98 (93%)	7 (7%)	20	58
1	B	108/120 (90%)	102 (94%)	6 (6%)	26	65
1	C	108/120 (90%)	99 (92%)	9 (8%)	14	47
1	D	107/120 (89%)	100 (94%)	7 (6%)	21	59
1	E	109/120 (91%)	99 (91%)	10 (9%)	11	40
1	F	107/120 (89%)	101 (94%)	6 (6%)	26	65
1	G	103/120 (86%)	96 (93%)	7 (7%)	20	57
1	H	107/120 (89%)	99 (92%)	8 (8%)	17	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	107/120 (89%)	101 (94%)	6 (6%)	26	65
1	J	105/120 (88%)	99 (94%)	6 (6%)	25	65
1	K	105/120 (88%)	95 (90%)	10 (10%)	11	38
1	L	104/120 (87%)	96 (92%)	8 (8%)	16	51
All	All	1275/1440 (88%)	1185 (93%)	90 (7%)	18	55

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	8	LEU
1	A	23	SER
1	A	40	THR
1	A	97	TYR
1	A	104	ARG
1	A	136	ARG
1	B	30	ARG
1	B	36	SER
1	B	40	THR
1	B	97	TYR
1	B	104	ARG
1	B	143	LEU
1	C	2	LYS
1	C	3	ASP
1	C	8	LEU
1	C	28	SER
1	C	36	SER
1	C	39	LEU
1	C	40	THR
1	C	97	TYR
1	C	104	ARG
1	D	5	VAL
1	D	25	GLN
1	D	27	ILE
1	D	36	SER
1	D	57	SER
1	D	102	GLN
1	D	104	ARG
1	E	3	ASP
1	E	5	VAL
1	E	23	SER

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Mol	Chain	Res	Type
1	E	39	LEU
1	E	40	THR
1	E	41	THR
1	E	53	GLN
1	E	104	ARG
1	E	136	ARG
1	E	146	LEU
1	F	5	VAL
1	F	40	THR
1	F	51	ARG
1	F	57	SER
1	F	97	TYR
1	F	104	ARG
1	G	2	LYS
1	G	3	ASP
1	G	8	LEU
1	G	36	SER
1	G	40	THR
1	G	62	LEU
1	G	97	TYR
1	H	3	ASP
1	H	7	LEU
1	H	8	LEU
1	H	34	ARG
1	H	40	THR
1	H	97	TYR
1	H	104	ARG
1	H	127	LEU
1	I	2	LYS
1	I	5	VAL
1	I	7	LEU
1	I	57	SER
1	I	104	ARG
1	I	135	LEU
1	J	3	ASP
1	J	8	LEU
1	J	40	THR
1	J	82	CYS
1	J	104	ARG
1	J	136	ARG
1	K	3	ASP
1	K	5	VAL

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Mol	Chain	Res	Type
1	K	7	LEU
1	K	8	LEU
1	K	39	LEU
1	K	53	GLN
1	K	57	SER
1	K	62	LEU
1	K	97	TYR
1	K	104	ARG
1	L	2	LYS
1	L	7	LEU
1	L	8	LEU
1	L	40	THR
1	L	82	CYS
1	L	97	TYR
1	L	104	ARG
1	L	118	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	75	HIS
1	A	129	HIS
1	B	75	HIS
1	B	129	HIS
1	C	75	HIS
1	C	95	GLN
1	D	19	GLN
1	D	25	GLN
1	D	75	HIS
1	D	102	GLN
1	D	129	HIS
1	E	25	GLN
1	E	95	GLN
1	E	129	HIS
1	F	75	HIS
1	H	19	GLN
1	H	25	GLN
1	H	75	HIS
1	H	129	HIS
1	I	75	HIS
1	I	129	HIS

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Mol	Chain	Res	Type
1	J	75	HIS
1	J	129	HIS
1	K	19	GLN
1	K	53	GLN
1	K	75	HIS
1	L	129	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

69 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	GSH	A	201	-	13,19,19	3.47	2 (15%)	15,24,24	1.02	2 (13%)
3	LMT	A	215	-	36,36,36	0.49	0	47,47,47	0.67	0
3	LMT	A	217	-	6,6,36	0.31	0	5,5,47	0.36	0
3	LMT	A	228	-	23,23,36	0.53	0	27,27,47	0.64	0
3	LMT	A	229	-	8,8,36	0.26	0	7,7,47	0.49	0
3	LMT	A	244	-	8,8,36	0.28	0	7,7,47	0.44	0
3	LMT	A	245	-	8,8,36	0.29	0	7,7,47	0.42	0
3	LMT	A	256	-	18,18,36	0.62	0	22,22,47	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	A	262	-	8,8,36	0.30	0	7,7,47	0.45	0
2	GSH	B	202	-	13,19,19	3.47	2 (15%)	15,24,24	1.27	2 (13%)
3	LMT	B	213	-	23,23,36	0.56	0	27,27,47	0.89	2 (7%)
3	LMT	B	218	-	23,23,36	0.59	0	27,27,47	1.14	3 (11%)
3	LMT	B	227	-	23,23,36	0.58	1 (4%)	27,27,47	0.97	2 (7%)
3	LMT	B	236	-	18,18,36	0.68	1 (5%)	22,22,47	1.29	2 (9%)
3	LMT	B	242	-	11,11,36	0.28	0	10,10,47	0.49	0
3	LMT	B	259	-	8,8,36	0.26	0	7,7,47	0.48	0
3	LMT	B	260	-	8,8,36	0.29	0	7,7,47	0.41	0
2	GSH	C	203	-	13,19,19	3.48	2 (15%)	15,24,24	0.97	2 (13%)
3	LMT	C	214	-	36,36,36	0.50	0	47,47,47	0.85	1 (2%)
3	LMT	C	216	-	36,36,36	0.49	0	47,47,47	0.81	1 (2%)
3	LMT	C	237	-	36,36,36	0.47	0	47,47,47	0.75	0
3	LMT	C	246	-	8,8,36	0.26	0	7,7,47	0.45	0
3	LMT	C	261	-	8,8,36	0.33	0	7,7,47	0.48	0
2	GSH	D	204	-	13,19,19	3.50	2 (15%)	15,24,24	1.27	2 (13%)
3	LMT	D	220	-	8,8,36	0.28	0	7,7,47	0.39	0
3	LMT	D	238	-	36,36,36	0.44	0	47,47,47	0.75	0
3	LMT	D	247	-	8,8,36	0.27	0	7,7,47	0.43	0
2	GSH	E	205	-	13,19,19	3.46	2 (15%)	15,24,24	0.96	1 (6%)
3	LMT	E	221	-	9,9,36	0.23	0	8,8,47	0.53	0
3	LMT	E	230	-	36,36,36	0.51	0	47,47,47	1.04	3 (6%)
3	LMT	E	231	-	23,23,36	0.56	0	27,27,47	0.89	1 (3%)
3	LMT	E	232	-	5,5,36	0.29	0	4,4,47	0.31	0
3	LMT	E	243	-	36,36,36	0.44	0	47,47,47	0.61	0
3	LMT	E	249	-	8,8,36	0.28	0	7,7,47	0.46	0
3	LMT	E	263	-	8,8,36	0.31	0	7,7,47	0.34	0
3	LMT	E	266	-	8,8,36	0.29	0	7,7,47	0.40	0
3	LMT	E	268	-	36,36,36	0.52	1 (2%)	47,47,47	0.86	1 (2%)
3	LMT	E	269	-	36,36,36	0.48	0	47,47,47	0.72	0
2	GSH	F	206	-	13,19,19	3.53	2 (15%)	15,24,24	1.31	2 (13%)
3	LMT	F	219	-	8,8,36	0.29	0	7,7,47	0.41	0
3	LMT	F	233	-	23,23,36	0.59	1 (4%)	27,27,47	0.86	1 (3%)
3	LMT	F	241	-	18,18,36	0.65	0	22,22,47	1.32	4 (18%)
3	LMT	F	248	-	8,8,36	0.26	0	7,7,47	0.47	0
2	GSH	G	207	-	13,19,19	3.46	2 (15%)	15,24,24	1.14	2 (13%)
3	LMT	G	222	-	8,8,36	0.24	0	7,7,47	0.54	0
3	LMT	G	235	-	23,23,36	0.51	0	27,27,47	0.69	0
3	LMT	G	251	-	8,8,36	0.29	0	7,7,47	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	G	264	-	8,8,36	0.29	0	7,7,47	0.43	0
3	LMT	G	267	-	8,8,36	0.30	0	7,7,47	0.41	0
2	GSH	H	208	-	13,19,19	3.51	2 (15%)	15,24,24	1.19	1 (6%)
3	LMT	H	234	-	23,23,36	0.56	0	27,27,47	0.96	1 (3%)
3	LMT	H	250	-	8,8,36	0.28	0	7,7,47	0.41	0
2	GSH	I	209	-	13,19,19	3.53	2 (15%)	15,24,24	1.16	1 (6%)
3	LMT	I	240	-	18,18,36	0.60	0	22,22,47	0.93	2 (9%)
3	LMT	I	252	-	8,8,36	0.27	0	7,7,47	0.46	0
3	LMT	I	257	-	8,8,36	0.28	0	7,7,47	0.44	0
3	LMT	I	258	-	8,8,36	0.29	0	7,7,47	0.42	0
2	GSH	J	210	-	13,19,19	3.55	2 (15%)	15,24,24	1.07	1 (6%)
3	LMT	J	239	-	36,36,36	0.44	0	47,47,47	0.79	0
3	LMT	J	253	-	8,8,36	0.25	0	7,7,47	0.50	0
2	GSH	K	211	-	13,19,19	3.50	2 (15%)	15,24,24	1.38	2 (13%)
3	LMT	K	224	-	6,6,36	0.30	0	5,5,47	0.35	0
3	LMT	K	225	-	23,23,36	0.56	0	27,27,47	0.97	1 (3%)
2	GSH	L	212	-	13,19,19	3.56	2 (15%)	15,24,24	1.08	2 (13%)
3	LMT	L	223	-	8,8,36	0.25	0	7,7,47	0.48	0
3	LMT	L	226	-	8,8,36	0.28	0	7,7,47	0.45	0
3	LMT	L	254	-	8,8,36	0.25	0	7,7,47	0.52	0
3	LMT	L	255	-	8,8,36	0.26	0	7,7,47	0.46	0
3	LMT	L	265	-	6,6,36	0.32	0	5,5,47	0.34	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	GSH	A	201	-	-	0/18/24/24	0/0/0/0
3	LMT	A	215	-	-	0/21/61/61	0/2/2/2
3	LMT	A	217	-	-	0/4/4/61	0/0/0/2
3	LMT	A	228	-	-	0/15/31/61	0/1/1/2
3	LMT	A	229	-	-	0/6/6/61	0/0/0/2
3	LMT	A	244	-	-	0/6/6/61	0/0/0/2
3	LMT	A	245	-	-	0/6/6/61	0/0/0/2
3	LMT	A	256	-	-	0/10/26/61	0/1/1/2
3	LMT	A	262	-	-	0/6/6/61	0/0/0/2
2	GSH	B	202	-	-	0/18/24/24	0/0/0/0
3	LMT	B	213	-	-	0/15/31/61	0/1/1/2
3	LMT	B	218	-	-	0/15/31/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	B	227	-	-	0/15/31/61	0/1/1/2
3	LMT	B	236	-	-	0/10/26/61	0/1/1/2
3	LMT	B	242	-	-	0/9/9/61	0/0/0/2
3	LMT	B	259	-	-	0/6/6/61	0/0/0/2
3	LMT	B	260	-	-	0/6/6/61	0/0/0/2
2	GSH	C	203	-	-	0/18/24/24	0/0/0/0
3	LMT	C	214	-	-	0/21/61/61	0/2/2/2
3	LMT	C	216	-	-	0/21/61/61	0/2/2/2
3	LMT	C	237	-	-	0/21/61/61	0/2/2/2
3	LMT	C	246	-	-	0/6/6/61	0/0/0/2
3	LMT	C	261	-	-	0/6/6/61	0/0/0/2
2	GSH	D	204	-	-	0/18/24/24	0/0/0/0
3	LMT	D	220	-	-	0/6/6/61	0/0/0/2
3	LMT	D	238	-	-	0/21/61/61	0/2/2/2
3	LMT	D	247	-	-	0/6/6/61	0/0/0/2
2	GSH	E	205	-	-	0/18/24/24	0/0/0/0
3	LMT	E	221	-	-	0/7/7/61	0/0/0/2
3	LMT	E	230	-	-	0/21/61/61	0/2/2/2
3	LMT	E	231	-	-	0/15/31/61	0/1/1/2
3	LMT	E	232	-	-	0/3/3/61	0/0/0/2
3	LMT	E	243	-	-	0/21/61/61	0/2/2/2
3	LMT	E	249	-	-	0/6/6/61	0/0/0/2
3	LMT	E	263	-	-	0/6/6/61	0/0/0/2
3	LMT	E	266	-	-	0/6/6/61	0/0/0/2
3	LMT	E	268	-	-	0/21/61/61	0/2/2/2
3	LMT	E	269	-	-	0/21/61/61	0/2/2/2
2	GSH	F	206	-	-	0/18/24/24	0/0/0/0
3	LMT	F	219	-	-	0/6/6/61	0/0/0/2
3	LMT	F	233	-	-	0/15/31/61	0/1/1/2
3	LMT	F	241	-	-	0/10/26/61	0/1/1/2
3	LMT	F	248	-	-	0/6/6/61	0/0/0/2
2	GSH	G	207	-	-	0/18/24/24	0/0/0/0
3	LMT	G	222	-	-	0/6/6/61	0/0/0/2
3	LMT	G	235	-	-	0/15/31/61	0/1/1/2
3	LMT	G	251	-	-	0/6/6/61	0/0/0/2
3	LMT	G	264	-	-	0/6/6/61	0/0/0/2
3	LMT	G	267	-	-	0/6/6/61	0/0/0/2
2	GSH	H	208	-	-	0/18/24/24	0/0/0/0
3	LMT	H	234	-	-	0/15/31/61	0/1/1/2
3	LMT	H	250	-	-	0/6/6/61	0/0/0/2
2	GSH	I	209	-	-	0/18/24/24	0/0/0/0
3	LMT	I	240	-	-	0/10/26/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	I	252	-	-	0/6/6/61	0/0/0/2
3	LMT	I	257	-	-	0/6/6/61	0/0/0/2
3	LMT	I	258	-	-	0/6/6/61	0/0/0/2
2	GSH	J	210	-	-	0/18/24/24	0/0/0/0
3	LMT	J	239	-	-	0/21/61/61	0/2/2/2
3	LMT	J	253	-	-	0/6/6/61	0/0/0/2
2	GSH	K	211	-	-	0/18/24/24	0/0/0/0
3	LMT	K	224	-	-	0/4/4/61	0/0/0/2
3	LMT	K	225	-	-	0/15/31/61	0/1/1/2
2	GSH	L	212	-	-	0/18/24/24	0/0/0/0
3	LMT	L	223	-	-	0/6/6/61	0/0/0/2
3	LMT	L	226	-	-	0/6/6/61	0/0/0/2
3	LMT	L	254	-	-	0/6/6/61	0/0/0/2
3	LMT	L	255	-	-	0/6/6/61	0/0/0/2
3	LMT	L	265	-	-	0/4/4/61	0/0/0/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	227	LMT	O1'-C1'	2.02	1.43	1.40
3	F	233	LMT	O1'-C1'	2.06	1.43	1.40
3	E	268	LMT	O1'-C1'	2.10	1.43	1.40
3	B	236	LMT	O1'-C1'	2.22	1.44	1.40
2	D	204	GSH	OE1-CD1	8.19	1.40	1.23
2	C	203	GSH	OE1-CD1	8.31	1.40	1.23
2	B	202	GSH	OE1-CD1	8.35	1.40	1.23
2	E	205	GSH	OE1-CD1	8.48	1.41	1.23
2	H	208	GSH	OE1-CD1	8.48	1.41	1.23
2	K	211	GSH	OE1-CD1	8.53	1.41	1.23
2	F	206	GSH	OE1-CD1	8.57	1.41	1.23
2	L	212	GSH	OE1-CD1	8.60	1.41	1.23
2	G	207	GSH	OE1-CD1	8.60	1.41	1.23
2	A	201	GSH	OE1-CD1	8.69	1.41	1.23
2	I	209	GSH	OE1-CD1	8.70	1.41	1.23
2	J	210	GSH	OE1-CD1	8.74	1.41	1.23
2	A	201	GSH	O2-C2	8.76	1.40	1.23
2	G	207	GSH	O2-C2	8.90	1.40	1.23
2	E	205	GSH	O2-C2	9.05	1.41	1.23
2	K	211	GSH	O2-C2	9.15	1.41	1.23
2	B	202	GSH	O2-C2	9.16	1.41	1.23
2	I	209	GSH	O2-C2	9.21	1.41	1.23
2	H	208	GSH	O2-C2	9.21	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	210	GSH	O2-C2	9.22	1.41	1.23
2	C	203	GSH	O2-C2	9.24	1.41	1.23
2	F	206	GSH	O2-C2	9.25	1.41	1.23
2	L	212	GSH	O2-C2	9.36	1.41	1.23
2	D	204	GSH	O2-C2	9.46	1.41	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	211	GSH	CA2-CB2-SG2	-4.07	109.15	114.16
2	F	206	GSH	CA2-CB2-SG2	-3.68	109.64	114.16
2	D	204	GSH	CA2-CB2-SG2	-3.58	109.76	114.16
2	I	209	GSH	CA2-CB2-SG2	-3.53	109.82	114.16
2	H	208	GSH	CA2-CB2-SG2	-3.50	109.86	114.16
2	B	202	GSH	CB2-CA2-N2	-3.38	106.65	111.40
2	B	202	GSH	CA2-CB2-SG2	-3.04	110.42	114.16
3	F	241	LMT	C1'-O5'-C5'	-3.01	110.12	113.15
2	J	210	GSH	CA2-CB2-SG2	-2.95	110.53	114.16
2	L	212	GSH	CA2-CB2-SG2	-2.90	110.59	114.16
2	G	207	GSH	CA2-CB2-SG2	-2.90	110.60	114.16
2	F	206	GSH	CB2-CA2-N2	-2.88	107.36	111.40
3	B	218	LMT	C1'-O5'-C5'	-2.61	110.52	113.15
2	E	205	GSH	CA2-CB2-SG2	-2.60	110.96	114.16
2	G	207	GSH	CB2-CA2-N2	-2.55	107.81	111.40
2	A	201	GSH	CB2-CA2-N2	-2.52	107.86	111.40
2	C	203	GSH	CA2-CB2-SG2	-2.51	111.07	114.16
2	A	201	GSH	CA2-CB2-SG2	-2.42	111.19	114.16
2	K	211	GSH	CB2-CA2-N2	-2.28	108.20	111.40
2	D	204	GSH	CB2-CA2-N2	-2.27	108.21	111.40
2	L	212	GSH	CB2-CA2-N2	-2.18	108.33	111.40
2	C	203	GSH	CB2-CA2-N2	-2.18	108.33	111.40
3	B	227	LMT	O1'-C1'-C2'	2.02	110.59	108.04
3	F	241	LMT	C4'-C3'-C2'	2.07	113.38	110.56
3	B	218	LMT	O5'-C5'-C6'	2.13	109.23	106.62
3	C	214	LMT	C2'-C3'-C4'	2.15	114.31	109.60
3	E	268	LMT	C1'-C2'-C3'	2.22	114.35	109.97
3	E	230	LMT	O1'-C1'-C2'	2.35	111.01	108.04
3	I	240	LMT	O1'-C1'-C2'	2.40	111.07	108.04
3	I	240	LMT	O5'-C5'-C6'	2.41	109.56	106.62
3	E	231	LMT	O5'-C5'-C6'	2.47	109.64	106.62
3	C	216	LMT	O1B-C4'-C3'	2.50	113.63	107.17
3	B	213	LMT	O1'-C1'-C2'	2.52	111.23	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	241	LMT	O1'-C1'-C2'	2.54	111.25	108.04
3	E	230	LMT	O5B-C1B-C2B	2.70	115.82	110.28
3	F	241	LMT	O5'-C5'-C6'	2.97	110.25	106.62
3	F	233	LMT	O5'-C5'-C6'	3.00	110.29	106.62
3	B	213	LMT	O5'-C5'-C6'	3.01	110.31	106.62
3	E	230	LMT	C1B-C2B-C3B	3.08	116.05	109.97
3	B	236	LMT	O1'-C1'-C2'	3.10	111.95	108.04
3	B	227	LMT	O5'-C5'-C6'	3.41	110.79	106.62
3	K	225	LMT	O5'-C5'-C6'	3.47	110.87	106.62
3	H	234	LMT	O5'-C5'-C6'	3.62	111.05	106.62
3	B	218	LMT	O1'-C1'-C2'	3.66	112.66	108.04
3	B	236	LMT	O5'-C5'-C6'	4.14	111.69	106.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	GSH	2	0
3	A	228	LMT	1	0
3	A	244	LMT	2	0
3	A	245	LMT	1	0
2	B	202	GSH	1	0
3	B	218	LMT	3	0
2	C	203	GSH	1	0
3	C	214	LMT	2	0
3	C	216	LMT	5	0
3	C	237	LMT	1	0
3	D	220	LMT	3	0
3	D	238	LMT	2	0
3	D	247	LMT	1	0
3	E	221	LMT	2	0
3	E	231	LMT	1	0
3	E	243	LMT	1	0
3	E	249	LMT	3	0
3	E	268	LMT	4	0
2	F	206	GSH	2	0
3	F	219	LMT	3	0
3	F	248	LMT	1	0
3	G	222	LMT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	208	GSH	1	0
2	I	209	GSH	1	0
3	I	240	LMT	1	0
3	I	252	LMT	1	0
3	I	258	LMT	3	0
2	J	210	GSH	2	0
3	J	239	LMT	1	0
2	L	212	GSH	2	0
3	L	254	LMT	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

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	146/156 (93%)	0.20	6 (4%) 41 34	51, 67, 94, 119	0
1	B	146/156 (93%)	0.15	5 (3%) 49 42	51, 67, 95, 119	0
1	C	146/156 (93%)	0.38	14 (9%) 10 9	51, 67, 93, 119	0
1	D	146/156 (93%)	0.39	15 (10%) 9 7	52, 67, 93, 119	0
1	E	146/156 (93%)	0.15	5 (3%) 49 42	51, 67, 93, 118	0
1	F	146/156 (93%)	0.13	3 (2%) 67 60	51, 67, 94, 118	0
1	G	146/156 (93%)	0.04	7 (4%) 34 28	51, 67, 96, 119	0
1	H	146/156 (93%)	0.06	7 (4%) 34 28	52, 67, 94, 119	0
1	I	146/156 (93%)	0.49	23 (15%) 3 2	52, 67, 94, 119	0
1	J	146/156 (93%)	0.19	10 (6%) 20 17	52, 67, 94, 119	0
1	K	146/156 (93%)	0.32	15 (10%) 9 7	52, 67, 94, 119	0
1	L	146/156 (93%)	0.23	8 (5%) 29 23	52, 67, 93, 119	0
All	All	1752/1872 (93%)	0.23	118 (6%) 21 17	51, 67, 97, 119	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	147	LEU	8.4
1	D	147	LEU	6.2
1	L	145	THR	5.5
1	G	147	LEU	5.4
1	D	145	THR	5.0
1	L	146	LEU	4.8
1	A	37	PRO	4.7
1	F	147	LEU	3.9
1	J	146	LEU	3.8
1	C	145	THR	3.8
1	K	37	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	103	LEU	3.6
1	I	138	ALA	3.6
1	I	37	PRO	3.6
1	D	102	GLN	3.5
1	C	142	ARG	3.5
1	C	101	ALA	3.4
1	D	37	PRO	3.4
1	C	33	PHE	3.3
1	J	103	LEU	3.3
1	C	141	GLY	3.3
1	J	107	PRO	3.3
1	I	103	LEU	3.3
1	C	138	ALA	3.2
1	G	146	LEU	3.2
1	G	4	GLU	3.2
1	L	140	LEU	3.2
1	C	143	LEU	3.1
1	D	146	LEU	3.1
1	I	46	PHE	3.1
1	J	96	GLY	3.1
1	F	143	LEU	3.1
1	G	145	THR	3.1
1	G	140	LEU	3.0
1	I	100	SER	3.0
1	D	95	GLN	3.0
1	I	29	ALA	3.0
1	I	34	ARG	3.0
1	C	147	LEU	3.0
1	B	37	PRO	3.0
1	H	145	THR	3.0
1	I	32	ALA	3.0
1	H	138	ALA	2.9
1	A	132	PRO	2.9
1	J	95	GLN	2.9
1	K	94	PHE	2.9
1	I	36	SER	2.9
1	K	96	GLY	2.8
1	K	103	LEU	2.8
1	H	147	LEU	2.8
1	I	97	TYR	2.8
1	C	37	PRO	2.8
1	K	91	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	145	THR	2.7
1	C	32	ALA	2.7
1	K	93	TYR	2.7
1	I	30	ARG	2.7
1	I	139	LEU	2.6
1	D	144	ARG	2.6
1	D	98	ALA	2.6
1	I	102	GLN	2.6
1	I	136	ARG	2.6
1	K	109	TYR	2.6
1	I	35	VAL	2.6
1	I	141	GLY	2.5
1	B	135	LEU	2.5
1	H	137	ALA	2.5
1	K	95	GLN	2.5
1	K	98	ALA	2.5
1	D	143	LEU	2.5
1	J	147	LEU	2.5
1	H	146	LEU	2.5
1	D	101	ALA	2.5
1	A	141	GLY	2.5
1	B	138	ALA	2.4
1	D	104	ARG	2.4
1	D	46	PHE	2.4
1	E	137	ALA	2.4
1	I	137	ALA	2.4
1	K	36	SER	2.4
1	A	146	LEU	2.4
1	J	98	ALA	2.4
1	L	141	GLY	2.3
1	K	105	LEU	2.3
1	C	140	LEU	2.3
1	I	101	ALA	2.3
1	B	136	ARG	2.3
1	K	136	ARG	2.3
1	D	45	GLU	2.3
1	L	37	PRO	2.3
1	I	28	SER	2.3
1	G	37	PRO	2.2
1	L	61	PRO	2.2
1	G	5	VAL	2.2
1	I	43	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	101	ALA	2.2
1	E	37	PRO	2.2
1	I	104	ARG	2.2
1	K	139	LEU	2.2
1	C	30	ARG	2.2
1	E	103	LEU	2.2
1	F	37	PRO	2.2
1	B	140	LEU	2.1
1	E	140	LEU	2.1
1	C	139	LEU	2.1
1	D	96	GLY	2.1
1	A	109	TYR	2.1
1	A	145	THR	2.1
1	I	44	PRO	2.1
1	J	106	ALA	2.1
1	H	139	LEU	2.0
1	I	105	LEU	2.0
1	E	145	THR	2.0
1	H	37	PRO	2.0
1	L	142	ARG	2.0
1	K	104	ARG	2.0
1	C	97	TYR	2.0
1	J	136	ARG	2.0

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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LMT	I	252	9/35	0.77	0.39	9.83	79,81,85,85	0
3	LMT	A	228	23/35	0.78	0.39	7.66	78,104,118,119	0
3	LMT	B	213	23/35	0.79	0.41	7.66	96,112,119,120	0
3	LMT	L	265	7/35	0.78	0.41	6.51	52,57,62,62	0
3	LMT	B	242	12/35	0.78	0.41	6.07	72,77,87,87	0
3	LMT	D	220	9/35	0.91	0.46	5.98	49,56,62,62	0
3	LMT	J	239	35/35	0.74	0.54	5.70	117,138,148,150	0
3	LMT	E	249	9/35	0.83	0.37	5.44	56,65,75,77	0
3	LMT	E	230	35/35	0.62	0.49	5.26	88,147,154,154	0
3	LMT	E	243	35/35	0.81	0.31	5.26	94,109,113,114	0
3	LMT	D	247	9/35	0.86	0.31	4.78	65,73,74,75	0
3	LMT	A	229	9/35	0.88	0.42	4.51	77,78,80,80	0
3	LMT	C	237	35/35	0.72	0.45	4.38	100,125,136,136	0
3	LMT	H	234	23/35	0.58	0.55	4.27	97,124,139,139	0
3	LMT	F	233	23/35	0.56	0.56	4.26	73,112,131,132	0
3	LMT	J	253	9/35	0.81	0.37	4.25	106,107,108,108	0
3	LMT	B	227	23/35	0.63	0.51	4.18	67,109,127,127	0
3	LMT	E	268	35/35	0.67	0.37	4.13	54,139,155,156	0
3	LMT	F	241	18/35	0.74	0.62	4.06	83,110,113,114	0
3	LMT	I	240	18/35	0.75	0.87	3.95	99,121,123,124	0
3	LMT	A	256	18/35	0.65	0.71	3.93	92,111,114,114	0
3	LMT	L	254	9/35	0.81	0.39	3.80	99,99,101,101	0
3	LMT	A	215	35/35	0.70	0.38	3.76	76,105,113,113	0
3	LMT	E	232	6/35	0.87	0.38	3.55	59,62,63,64	0
3	LMT	D	238	35/35	0.72	0.47	3.39	106,133,145,145	0
3	LMT	L	226	9/35	0.64	0.71	3.38	90,94,99,100	0
3	LMT	E	231	23/35	0.59	0.48	3.36	84,124,138,139	0
3	LMT	E	263	9/35	0.64	0.50	3.26	75,77,80,80	0
3	LMT	F	248	9/35	0.86	0.32	3.21	66,69,80,81	0
3	LMT	K	225	23/35	0.67	0.45	3.19	79,111,129,132	0
3	LMT	C	214	35/35	0.42	0.54	3.06	100,130,142,142	0
3	LMT	G	264	9/35	0.82	0.35	2.94	65,68,70,70	0
3	LMT	G	251	9/35	0.58	0.60	2.79	82,85,92,92	0
3	LMT	B	218	23/35	0.75	0.42	2.61	68,106,117,118	0
3	LMT	F	219	9/35	0.92	0.28	2.08	68,74,77,77	0
3	LMT	G	235	23/35	0.74	0.52	1.95	82,108,127,127	0
3	LMT	I	258	9/35	0.83	0.54	1.88	66,69,71,72	0
3	LMT	K	224	7/35	0.86	0.31	1.86	81,83,84,84	0
3	LMT	C	261	9/35	0.88	0.27	1.72	46,53,62,63	0
3	LMT	A	244	9/35	0.92	0.32	1.45	53,60,64,64	0
3	LMT	G	222	9/35	0.97	0.27	1.41	55,56,59,59	0
3	LMT	L	255	9/35	0.85	0.30	1.31	85,89,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LMT	C	216	35/35	0.71	0.44	1.09	52,122,137,139	0
3	LMT	E	221	10/35	0.96	0.26	0.98	64,70,71,72	0
3	LMT	A	217	7/35	0.84	0.32	0.83	62,64,67,68	0
3	LMT	I	257	9/35	0.84	0.27	0.49	79,83,85,85	0
3	LMT	B	236	18/35	0.79	0.38	0.24	62,99,103,105	0
3	LMT	L	223	9/35	0.93	0.22	0.23	64,67,69,70	0
2	GSH	I	209	20/20	0.91	0.32	0.20	56,61,65,69	0
3	LMT	A	245	9/35	0.93	0.23	-0.05	53,59,64,64	0
2	GSH	C	203	20/20	0.96	0.28	-0.09	56,61,65,69	0
3	LMT	C	246	9/35	0.91	0.25	-0.22	66,73,82,82	0
2	GSH	H	208	20/20	0.94	0.23	-0.40	56,61,65,69	0
2	GSH	A	201	20/20	0.96	0.25	-0.51	55,61,65,69	0
2	GSH	E	205	20/20	0.94	0.22	-0.53	55,61,65,69	0
2	GSH	L	212	20/20	0.96	0.21	-0.56	56,61,65,69	0
2	GSH	D	204	20/20	0.91	0.25	-0.57	56,61,65,69	0
2	GSH	K	211	20/20	0.92	0.20	-0.64	56,61,65,70	0
2	GSH	G	207	20/20	0.96	0.18	-0.69	56,61,65,69	0
2	GSH	J	210	20/20	0.91	0.20	-0.69	56,61,65,70	0
2	GSH	B	202	20/20	0.95	0.22	-0.97	56,61,65,69	0
2	GSH	F	206	20/20	0.97	0.16	-0.99	56,61,65,69	0
3	LMT	B	259	9/35	0.82	0.39	-	114,115,116,116	0
3	LMT	E	269	35/35	0.13	0.60	-	139,180,186,187	0
3	LMT	H	250	9/35	0.55	0.58	-	80,82,84,84	0
3	LMT	A	262	9/35	0.70	0.49	-	74,81,85,85	0
3	LMT	G	267	9/35	0.71	0.53	-	71,72,75,75	0
3	LMT	B	260	9/35	0.66	0.43	-	108,111,112,112	0
3	LMT	E	266	9/35	0.44	0.41	-	102,107,109,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.