Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:00 pm BST

PDB ID	:	4ATV
Title	:	STRUCTURE OF A TRIPLE MUTANT OF THE NHAA DIMER, CRYSTALLISED AT LOW PH
Authors	:	Drew, D.; Lee, C.; Iwata, S.; Cameron, A.D.
Deposited on	:	2012-05-10
Resolution	:	3.50 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
https://www.wwpdb.org/validation/2017/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:

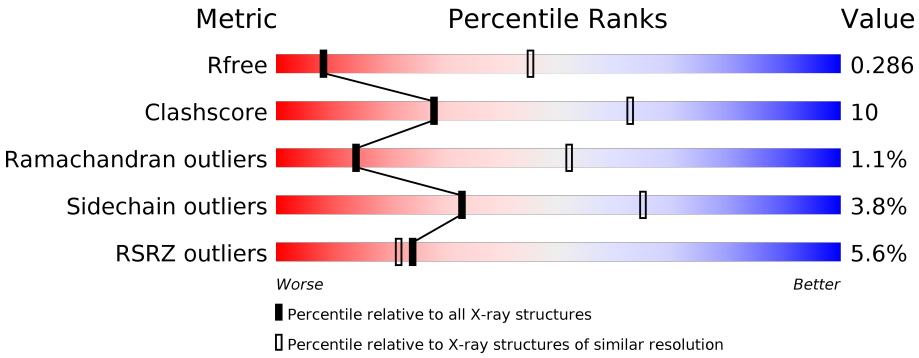
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	401	4% 68% 26% • 5%
1	B	401	4% 69% 23% • 7%
1	C	401	6% 68% 26% • 5%
1	D	401	7% 71% 21% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11331 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 NA(+)/H(+) ANTIPORTER NHAA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	Se	0	0	0
			2850	1892	464	480	3	11			
1	B	374	Total	C	N	O	S	Se	0	0	0
			2791	1853	454	470	3	11			
1	C	381	Total	C	N	O	S	Se	0	0	0
			2850	1892	464	480	3	11			
1	D	374	Total	C	N	O	S	Se	0	0	0
			2791	1853	454	470	3	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLU	-	expression tag	UNP P13738
A	390	PHE	-	expression tag	UNP P13738
A	391	ARG	-	expression tag	UNP P13738
A	392	VAL	-	expression tag	UNP P13738
A	393	PRO	-	expression tag	UNP P13738
A	394	GLY	-	expression tag	UNP P13738
A	395	SER	-	expression tag	UNP P13738
A	396	GLU	-	expression tag	UNP P13738
A	397	ASN	-	expression tag	UNP P13738
A	398	LEU	-	expression tag	UNP P13738
A	399	TYR	-	expression tag	UNP P13738
A	400	PHE	-	expression tag	UNP P13738
A	401	GLN	-	expression tag	UNP P13738
A	109	THR	ALA	engineered mutation	UNP P13738
A	277	GLY	GLN	engineered mutation	UNP P13738
A	296	MSE	LEU	engineered mutation	UNP P13738
B	389	GLU	-	expression tag	UNP P13738
B	390	PHE	-	expression tag	UNP P13738
B	391	ARG	-	expression tag	UNP P13738
B	392	VAL	-	expression tag	UNP P13738
B	393	PRO	-	expression tag	UNP P13738

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	GLY	-	expression tag	UNP P13738
B	395	SER	-	expression tag	UNP P13738
B	396	GLU	-	expression tag	UNP P13738
B	397	ASN	-	expression tag	UNP P13738
B	398	LEU	-	expression tag	UNP P13738
B	399	TYR	-	expression tag	UNP P13738
B	400	PHE	-	expression tag	UNP P13738
B	401	GLN	-	expression tag	UNP P13738
B	109	THR	ALA	engineered mutation	UNP P13738
B	277	GLY	GLN	engineered mutation	UNP P13738
B	296	MSE	LEU	engineered mutation	UNP P13738
C	389	GLU	-	expression tag	UNP P13738
C	390	PHE	-	expression tag	UNP P13738
C	391	ARG	-	expression tag	UNP P13738
C	392	VAL	-	expression tag	UNP P13738
C	393	PRO	-	expression tag	UNP P13738
C	394	GLY	-	expression tag	UNP P13738
C	395	SER	-	expression tag	UNP P13738
C	396	GLU	-	expression tag	UNP P13738
C	397	ASN	-	expression tag	UNP P13738
C	398	LEU	-	expression tag	UNP P13738
C	399	TYR	-	expression tag	UNP P13738
C	400	PHE	-	expression tag	UNP P13738
C	401	GLN	-	expression tag	UNP P13738
C	109	THR	ALA	engineered mutation	UNP P13738
C	277	GLY	GLN	engineered mutation	UNP P13738
C	296	MSE	LEU	engineered mutation	UNP P13738
D	389	GLU	-	expression tag	UNP P13738
D	390	PHE	-	expression tag	UNP P13738
D	391	ARG	-	expression tag	UNP P13738
D	392	VAL	-	expression tag	UNP P13738
D	393	PRO	-	expression tag	UNP P13738
D	394	GLY	-	expression tag	UNP P13738
D	395	SER	-	expression tag	UNP P13738
D	396	GLU	-	expression tag	UNP P13738
D	397	ASN	-	expression tag	UNP P13738
D	398	LEU	-	expression tag	UNP P13738
D	399	TYR	-	expression tag	UNP P13738
D	400	PHE	-	expression tag	UNP P13738
D	401	GLN	-	expression tag	UNP P13738
D	109	THR	ALA	engineered mutation	UNP P13738
D	277	GLY	GLN	engineered mutation	UNP P13738

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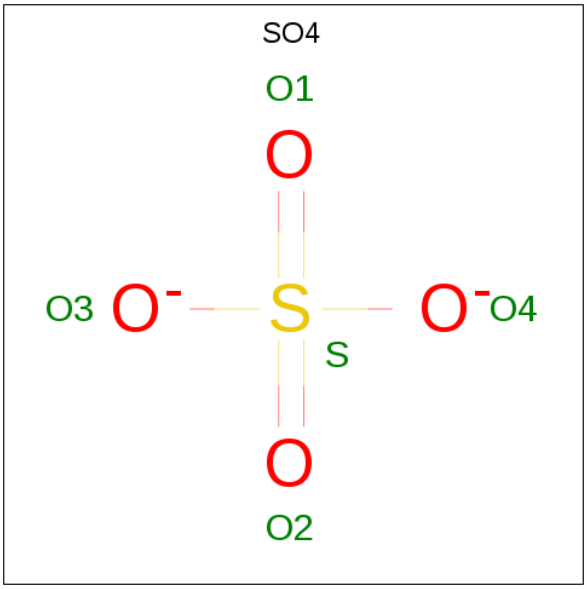
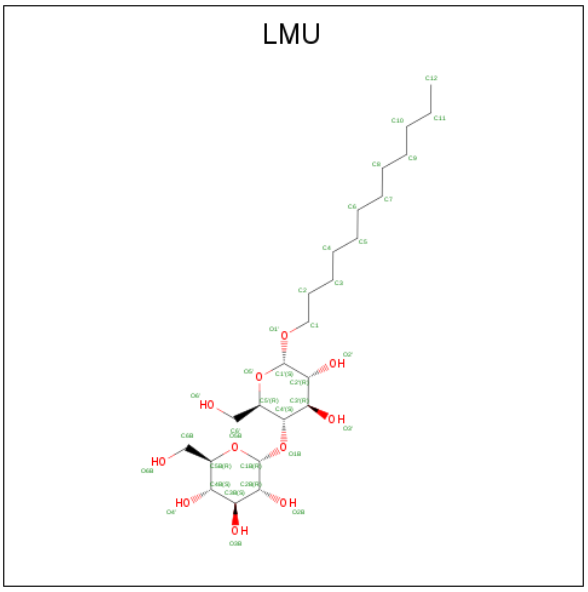
Chain	Residue	Modelled	Actual	Comment	Reference
D	296	MSE	LEU	engineered mutation	UNP P13738

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



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

- Molecule 3 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



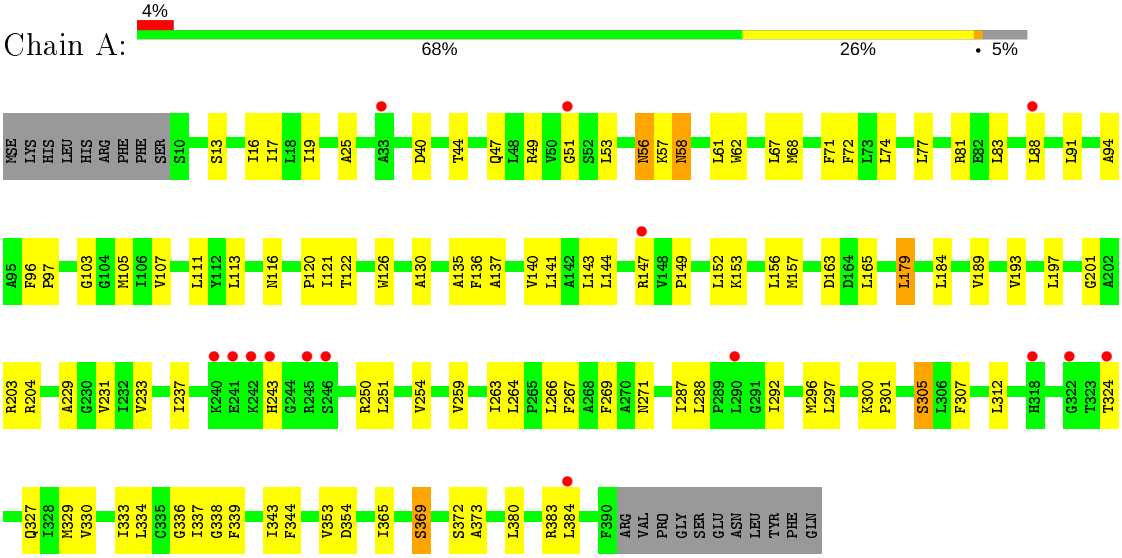
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	29	18	11	0	0

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 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.

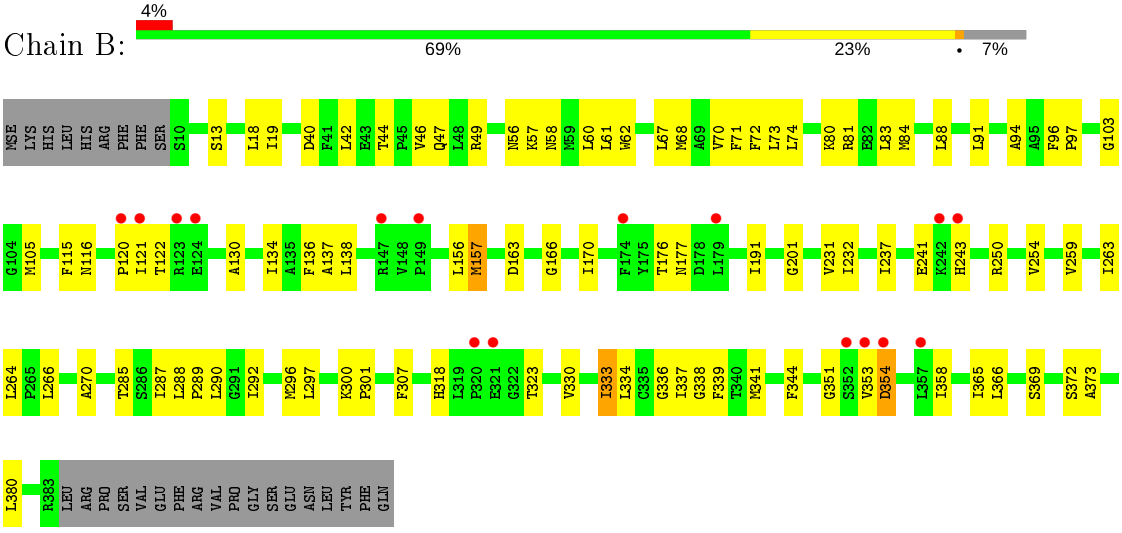
- Molecule 1: NA(+)/H(+) ANTIPORTER NHAA

Chain A:



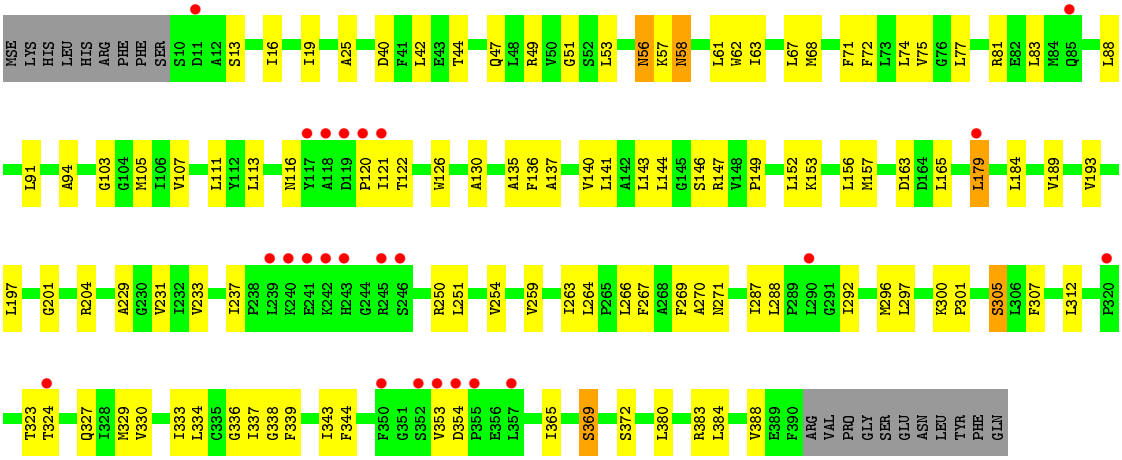
- Molecule 1: NA(+)/H(+) ANTIPORTER NHAA

Chain B:



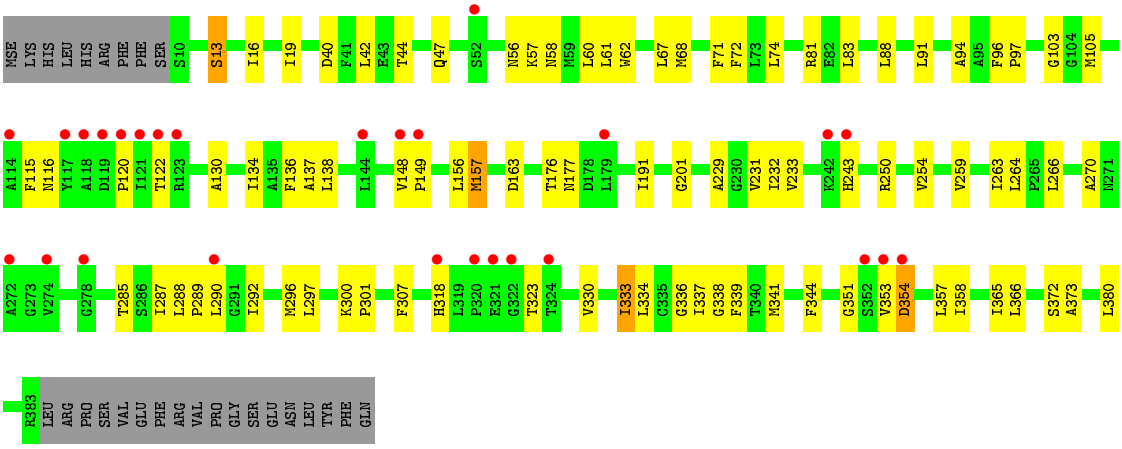
- Molecule 1: NA(+)/H(+) ANTIPORTER NHAA

Chain C:



- Molecule 1: NA(+)/H(+) ANTIPORTER NHAA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.76Å 99.40Å 140.23Å 90.00° 97.35° 90.00°	Depositor
Resolution (Å)	56.98 – 3.50 56.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (56.98-3.50) 94.5 (56.98-3.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.287 , 0.313 0.295 , 0.286	Depositor DCC
R_{free} test set	1894 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	158.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 112.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	11331	wwPDB-VP
Average B, all atoms (Å^2)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LMU

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	0.24	0/2900	0.45	0/3936
1	B	0.24	0/2839	0.45	0/3853
1	C	0.24	0/2900	0.46	0/3936
1	D	0.24	0/2839	0.45	0/3853
All	All	0.24	0/11478	0.45	0/15578

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

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	2850	0	3032	65	0
1	B	2791	0	2972	56	0
1	C	2850	0	3032	63	0
1	D	2791	0	2972	51	0
2	A	5	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
3	B	29	0	31	0	0
All	All	11331	0	12039	231	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 10.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ILE:HG13	1:A:365:ILE:HD11	1.58	0.86
1:C:343:ILE:HG13	1:C:365:ILE:HD11	1.57	0.85
1:D:330:VAL:HG11	1:D:380:LEU:HB2	1.72	0.71
1:B:330:VAL:HG11	1:B:380:LEU:HB2	1.73	0.69
1:C:47:GLN:HB3	1:C:56:ASN:HB3	1.76	0.68
1:A:74:LEU:HD13	1:A:259:VAL:HG11	1.77	0.67
1:B:259:VAL:HA	1:B:263:ILE:HB	1.77	0.66
1:D:259:VAL:HA	1:D:263:ILE:HB	1.77	0.66
1:A:137:ALA:HB1	1:A:156:LEU:HD21	1.78	0.66
1:A:47:GLN:HB3	1:A:56:ASN:HB3	1.76	0.66
1:C:147:ARG:HB3	1:C:384:LEU:HB3	1.77	0.65
1:C:74:LEU:HD13	1:C:259:VAL:HG11	1.78	0.65
1:C:137:ALA:HB1	1:C:156:LEU:HD21	1.79	0.64
1:A:57:LYS:HB2	1:A:62:TRP:CD1	2.33	0.63
1:A:147:ARG:HB3	1:A:384:LEU:HB3	1.81	0.63
1:C:57:LYS:HB2	1:C:62:TRP:CD1	2.34	0.63
1:B:351:GLY:HA2	1:B:358:ILE:HD11	1.82	0.62
1:C:136:PHE:HD2	1:C:337:ILE:HD12	1.65	0.62
1:C:40:ASP:O	1:C:44:THR:OG1	2.17	0.61
1:C:77:LEU:HD11	1:C:251:LEU:HD23	1.81	0.61
1:A:40:ASP:O	1:A:44:THR:OG1	2.19	0.61
1:D:351:GLY:HA2	1:D:358:ILE:HD11	1.83	0.61
1:A:77:LEU:HD11	1:A:251:LEU:HD23	1.81	0.61
1:C:163:ASP:OD2	1:C:300:LYS:NZ	2.34	0.60
1:A:136:PHE:HD2	1:A:337:ILE:HD12	1.64	0.60
1:B:74:LEU:HD13	1:B:259:VAL:HG11	1.83	0.60
1:D:74:LEU:HD13	1:D:259:VAL:HG11	1.84	0.60
1:A:71:PHE:HE2	1:A:264:LEU:HD11	1.67	0.59
1:D:137:ALA:HB1	1:D:156:LEU:HD21	1.84	0.59
1:A:163:ASP:OD2	1:A:300:LYS:NZ	2.35	0.59
1:A:330:VAL:HG11	1:A:380:LEU:HB2	1.83	0.59
1:B:71:PHE:HE2	1:B:264:LEU:HD11	1.68	0.59
1:D:40:ASP:O	1:D:44:THR:OG1	2.19	0.58
1:B:137:ALA:HB1	1:B:156:LEU:HD21	1.85	0.58
1:C:330:VAL:HG11	1:C:380:LEU:HB2	1.84	0.58
1:D:71:PHE:HE2	1:D:264:LEU:HD11	1.68	0.58
1:C:88:LEU:HD12	1:C:94:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HG23	1:A:353:VAL:HG11	1.86	0.58
1:A:88:LEU:HD12	1:A:94:ALA:HB1	1.86	0.57
1:C:71:PHE:HE2	1:C:264:LEU:HD11	1.68	0.57
1:D:88:LEU:HD12	1:D:94:ALA:HB1	1.85	0.57
1:B:88:LEU:HD12	1:B:94:ALA:HB1	1.85	0.56
1:B:72:PHE:HB3	1:B:231:VAL:HG23	1.87	0.56
1:B:334:LEU:O	1:B:337:ILE:HG12	2.06	0.56
1:D:72:PHE:HB3	1:D:231:VAL:HG23	1.86	0.56
1:A:259:VAL:HA	1:A:263:ILE:HB	1.87	0.56
1:D:334:LEU:O	1:D:337:ILE:HG12	2.06	0.56
1:C:259:VAL:HA	1:C:263:ILE:HB	1.87	0.55
1:B:40:ASP:O	1:B:44:THR:OG1	2.21	0.55
1:C:116:ASN:OD1	1:C:122:THR:OG1	2.25	0.55
1:B:105:MSE:HG3	1:B:130:ALA:HB1	1.89	0.55
1:B:301:PRO:HB3	1:B:333:ILE:HG12	1.89	0.55
1:B:57:LYS:HB2	1:B:62:TRP:CD1	2.43	0.54
1:C:121:ILE:HG23	1:C:353:VAL:HG11	1.88	0.54
1:D:116:ASN:OD1	1:D:122:THR:OG1	2.25	0.54
1:B:116:ASN:OD1	1:B:122:THR:OG1	2.26	0.54
1:C:271:ASN:HB3	1:C:343:ILE:HG21	1.89	0.54
1:B:138:LEU:HD11	1:B:157:MSE:HG3	1.89	0.54
1:D:301:PRO:HB3	1:D:333:ILE:HG12	1.88	0.54
1:D:105:MSE:HG3	1:D:130:ALA:HB1	1.90	0.54
1:D:138:LEU:HD11	1:D:157:MSE:HG3	1.89	0.54
1:C:91:LEU:HD12	1:C:91:LEU:H	1.74	0.53
1:A:105:MSE:HG3	1:A:130:ALA:HB1	1.90	0.53
1:A:271:ASN:HB3	1:A:343:ILE:HG21	1.89	0.53
1:C:105:MSE:HG3	1:C:130:ALA:HB1	1.90	0.53
1:D:57:LYS:HB2	1:D:62:TRP:CD1	2.43	0.53
1:A:72:PHE:HB3	1:A:231:VAL:HG23	1.91	0.53
1:C:122:THR:HB	1:C:288:LEU:HD11	1.91	0.53
1:A:292:ILE:HG21	1:A:365:ILE:HG22	1.91	0.52
1:A:91:LEU:H	1:A:91:LEU:HD12	1.73	0.52
1:A:116:ASN:OD1	1:A:122:THR:OG1	2.26	0.52
1:A:365:ILE:O	1:A:369:SER:HB2	2.10	0.52
1:C:365:ILE:O	1:C:369:SER:HB2	2.10	0.52
1:A:122:THR:HB	1:A:288:LEU:HD11	1.91	0.51
1:C:88:LEU:HA	1:C:94:ALA:HB2	1.92	0.51
1:C:292:ILE:HG21	1:C:365:ILE:HG22	1.91	0.51
1:B:163:ASP:OD2	1:B:300:LYS:NZ	2.44	0.51
1:D:163:ASP:OD2	1:D:300:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:HA	1:A:337:ILE:HD11	1.93	0.50
1:A:250:ARG:O	1:A:254:VAL:HG23	2.10	0.50
1:A:88:LEU:HA	1:A:94:ALA:HB2	1.92	0.50
1:C:179:LEU:HD23	1:C:184:LEU:HD21	1.94	0.50
1:A:67:LEU:HD11	1:A:266:LEU:HD23	1.94	0.50
1:C:250:ARG:O	1:C:254:VAL:HG23	2.11	0.49
1:A:179:LEU:HD23	1:A:184:LEU:HD21	1.94	0.49
1:A:144:LEU:HD13	1:A:384:LEU:HD11	1.93	0.49
1:A:47:GLN:HG3	1:B:49:ARG:HB2	1.94	0.49
1:C:72:PHE:HB3	1:C:231:VAL:HG23	1.92	0.49
1:C:305:SER:HB2	1:C:329:MSE:HG2	1.94	0.49
1:D:68:MSE:HG3	1:D:344:PHE:CE1	2.48	0.49
1:B:91:LEU:H	1:B:91:LEU:HD12	1.77	0.49
1:C:137:ALA:HA	1:C:337:ILE:HD11	1.94	0.49
1:D:47:GLN:HB3	1:D:56:ASN:HB3	1.95	0.49
1:B:47:GLN:HB3	1:B:56:ASN:HB3	1.94	0.49
1:C:25:ALA:HB2	1:C:269:PHE:HA	1.95	0.49
1:D:42:LEU:HD21	1:D:270:ALA:O	2.13	0.48
1:A:312:LEU:HD11	1:A:324:THR:HG21	1.95	0.48
1:A:25:ALA:HB2	1:A:269:PHE:HA	1.96	0.48
1:A:140:VAL:HA	1:A:143:LEU:HD12	1.96	0.48
1:C:144:LEU:HD13	1:C:384:LEU:HD11	1.95	0.48
1:A:305:SER:HB2	1:A:329:MSE:HG2	1.95	0.48
1:B:42:LEU:HG	1:B:60:LEU:HD13	1.95	0.48
1:D:91:LEU:HD12	1:D:91:LEU:H	1.79	0.48
1:D:287:ILE:HD12	1:D:288:LEU:HD12	1.96	0.48
1:B:68:MSE:HG3	1:B:344:PHE:CE1	2.49	0.47
1:C:296:MSE:HE3	1:C:338:GLY:H	1.79	0.47
1:D:42:LEU:HG	1:D:60:LEU:HD13	1.95	0.47
1:B:42:LEU:HD21	1:B:270:ALA:O	2.14	0.47
1:C:140:VAL:HA	1:C:143:LEU:HD12	1.95	0.47
1:A:296:MSE:HE3	1:A:338:GLY:H	1.79	0.47
1:A:83:LEU:HG	1:A:88:LEU:HD23	1.97	0.47
1:C:312:LEU:HD11	1:C:324:THR:HG21	1.96	0.47
1:D:337:ILE:HG21	1:D:373:ALA:HB2	1.96	0.47
1:A:193:VAL:O	1:A:197:LEU:HB2	2.15	0.47
1:B:137:ALA:HA	1:B:337:ILE:HD11	1.97	0.47
1:C:58:ASN:N	1:C:58:ASN:OD1	2.48	0.47
1:C:83:LEU:HG	1:C:88:LEU:HD23	1.96	0.47
1:A:165:LEU:HD11	1:A:231:VAL:HG11	1.97	0.47
1:C:165:LEU:HD11	1:C:231:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD11	1:C:266:LEU:HD23	1.95	0.47
1:D:296:MSE:HE3	1:D:338:GLY:H	1.79	0.47
1:B:287:ILE:HD12	1:B:288:LEU:HD12	1.96	0.47
1:D:292:ILE:HG21	1:D:365:ILE:HG22	1.97	0.46
1:C:193:VAL:O	1:C:197:LEU:HB2	2.15	0.46
1:B:296:MSE:HE3	1:B:338:GLY:H	1.80	0.46
1:B:297:LEU:HD13	1:B:372:SER:HB3	1.98	0.46
1:A:58:ASN:N	1:A:58:ASN:OD1	2.49	0.46
1:B:292:ILE:HG21	1:B:365:ILE:HG22	1.98	0.46
1:B:337:ILE:HG21	1:B:373:ALA:HB2	1.97	0.46
1:C:334:LEU:O	1:C:337:ILE:HG12	2.15	0.46
1:D:137:ALA:HA	1:D:337:ILE:HD11	1.97	0.46
1:C:13:SER:HA	1:C:16:ILE:HG12	1.98	0.46
1:A:334:LEU:O	1:A:337:ILE:HG12	2.17	0.45
1:A:113:LEU:HD21	1:A:126:TRP:HB3	1.99	0.45
1:A:13:SER:HA	1:A:16:ILE:HG12	1.98	0.45
1:D:297:LEU:HD13	1:D:372:SER:HB3	1.98	0.45
1:D:67:LEU:HD11	1:D:266:LEU:HD23	1.99	0.45
1:C:113:LEU:HD21	1:C:126:TRP:HB3	1.99	0.45
1:C:103:GLY:HA3	1:C:307:PHE:CG	2.53	0.44
1:C:233:VAL:O	1:C:237:ILE:HG13	2.18	0.44
1:B:67:LEU:HD11	1:B:266:LEU:HD23	1.98	0.44
1:B:96:PHE:HB3	1:B:97:PRO:HD3	1.99	0.44
1:C:107:VAL:O	1:C:111:LEU:HB2	2.17	0.44
1:A:68:MSE:HG3	1:A:344:PHE:CE1	2.53	0.44
1:A:49:ARG:HA	1:A:53:LEU:O	2.18	0.44
1:C:301:PRO:HB3	1:C:333:ILE:HG12	2.00	0.44
1:D:71:PHE:CZ	1:D:341:MSE:HE1	2.53	0.44
1:C:68:MSE:HG3	1:C:344:PHE:CE1	2.53	0.43
1:A:107:VAL:O	1:A:111:LEU:HB2	2.18	0.43
1:C:297:LEU:HD13	1:C:372:SER:HB3	2.00	0.43
1:D:148:VAL:HA	1:D:149:PRO:HD2	1.92	0.43
1:A:327:GLN:NE2	1:A:383:ARG:O	2.51	0.43
1:D:290:LEU:HA	1:D:290:LEU:HD12	1.86	0.43
1:D:96:PHE:HB3	1:D:97:PRO:HD3	2.00	0.43
1:A:16:ILE:HA	1:A:19:ILE:HG22	2.01	0.43
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.90	0.43
1:A:103:GLY:HA3	1:A:307:PHE:CG	2.53	0.43
1:A:297:LEU:HD13	1:A:372:SER:HB3	1.99	0.43
1:B:250:ARG:O	1:B:254:VAL:HG23	2.19	0.43
1:B:88:LEU:HA	1:B:94:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:VAL:O	1:A:237:ILE:HG13	2.18	0.43
1:B:243:HIS:CD2	1:B:243:HIS:H	2.37	0.43
1:A:49:ARG:O	1:B:46:VAL:HA	2.19	0.43
1:C:68:MSE:HE3	1:C:267:PHE:CD2	2.54	0.43
1:A:301:PRO:HB3	1:A:333:ILE:HG12	2.01	0.42
1:C:49:ARG:HA	1:C:53:LEU:O	2.18	0.42
1:D:88:LEU:HA	1:D:94:ALA:HB2	2.01	0.42
1:B:103:GLY:HA3	1:B:307:PHE:CG	2.54	0.42
1:B:290:LEU:HA	1:B:290:LEU:HD12	1.86	0.42
1:A:135:ALA:HB2	1:A:264:LEU:HD13	2.02	0.42
1:B:285:THR:HG23	1:B:290:LEU:HD22	2.01	0.42
1:A:141:LEU:HD23	1:A:153:LYS:HG2	2.01	0.42
1:A:300:LYS:HG3	1:A:336:GLY:HA2	2.01	0.42
1:B:288:LEU:HB2	1:B:289:PRO:HD3	2.02	0.42
1:C:16:ILE:HA	1:C:19:ILE:HG22	2.00	0.42
1:D:19:ILE:HD13	1:D:136:PHE:CE1	2.55	0.42
1:D:243:HIS:CD2	1:D:243:HIS:H	2.36	0.42
1:C:141:LEU:HD23	1:C:153:LYS:HG2	2.01	0.42
1:D:288:LEU:HB2	1:D:289:PRO:HD3	2.02	0.42
1:A:149:PRO:HG2	1:A:152:LEU:HB2	2.01	0.42
1:A:203:ARG:HD3	1:A:243:HIS:CG	2.55	0.42
1:D:353:VAL:HG12	1:D:354:ASP:HB2	2.02	0.42
1:B:353:VAL:HG12	1:B:354:ASP:HB2	2.02	0.41
1:D:103:GLY:HA3	1:D:307:PHE:CG	2.54	0.41
1:B:57:LYS:HB2	1:B:62:TRP:NE1	2.35	0.41
1:D:19:ILE:HD12	1:D:19:ILE:HA	1.84	0.41
1:D:229:ALA:O	1:D:233:VAL:HG23	2.19	0.41
1:D:300:LYS:HG3	1:D:336:GLY:HA2	2.02	0.41
1:A:229:ALA:O	1:A:233:VAL:HG23	2.21	0.41
1:D:13:SER:HA	1:D:16:ILE:HG12	2.02	0.41
1:B:71:PHE:CZ	1:B:341:MSE:HE1	2.55	0.41
1:C:323:THR:HG1	1:C:327:GLN:H	1.68	0.41
1:D:250:ARG:O	1:D:254:VAL:HG23	2.19	0.41
1:A:68:MSE:HE3	1:A:267:PHE:CD2	2.54	0.41
1:A:337:ILE:HG21	1:A:373:ALA:HB2	2.03	0.41
1:B:18:LEU:HD23	1:B:136:PHE:HD1	1.86	0.41
1:C:42:LEU:HD21	1:C:270:ALA:O	2.21	0.41
1:B:122:THR:HG21	1:B:288:LEU:HD11	2.02	0.41
1:B:191:ILE:HG12	1:B:232:ILE:HG21	2.03	0.41
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.91	0.41
1:B:365:ILE:O	1:B:369:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:VAL:O	1:B:73:LEU:HB3	2.20	0.41
1:C:300:LYS:HG3	1:C:336:GLY:HA2	2.02	0.41
1:A:19:ILE:HD13	1:A:136:PHE:CE1	2.56	0.41
1:A:96:PHE:HB3	1:A:97:PRO:HD3	2.03	0.41
1:B:300:LYS:HG3	1:B:336:GLY:HA2	2.02	0.41
1:C:149:PRO:HG2	1:C:152:LEU:HB2	2.02	0.41
1:D:285:THR:HG23	1:D:290:LEU:HD22	2.02	0.41
1:D:83:LEU:HG	1:D:88:LEU:HD23	2.02	0.41
1:B:83:LEU:HG	1:B:88:LEU:HD23	2.03	0.41
1:C:229:ALA:O	1:C:233:VAL:HG23	2.21	0.41
1:C:327:GLN:NE2	1:C:383:ARG:O	2.52	0.41
1:D:61:LEU:HD23	1:D:61:LEU:HA	1.83	0.41
1:A:16:ILE:HG13	1:A:17:ILE:N	2.36	0.41
1:B:121:ILE:HG23	1:B:353:VAL:HG11	2.04	0.41
1:A:189:VAL:O	1:A:193:VAL:HG23	2.22	0.40
1:B:241:GLU:HG3	1:C:146:SER:HB2	2.03	0.40
1:C:72:PHE:HA	1:C:75:VAL:HB	2.03	0.40
1:D:357:LEU:HD23	1:D:357:LEU:HA	1.89	0.40
1:B:80:LYS:NZ	1:B:237:ILE:O	2.52	0.40
1:B:84:MSE:HE3	1:C:388:VAL:O	2.22	0.40
1:D:122:THR:HG21	1:D:288:LEU:HD11	2.03	0.40
1:D:191:ILE:HG12	1:D:232:ILE:HG21	2.03	0.40
1:B:166:GLY:O	1:B:170:ILE:HG13	2.21	0.40
1:B:19:ILE:HD13	1:B:136:PHE:CE1	2.56	0.40
1:C:189:VAL:O	1:C:193:VAL:HG23	2.21	0.40
1:D:122:THR:CG2	1:D:288:LEU:HD11	2.51	0.40
1:D:57:LYS:HB2	1:D:62:TRP:NE1	2.36	0.40
1:B:122:THR:CG2	1:B:288:LEU:HD11	2.51	0.40
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.82	0.40
1:C:135:ALA:HB2	1:C:264:LEU:HD13	2.03	0.40

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	379/401 (94%)	348 (92%)	27 (7%)	4 (1%)	14	52
1	B	372/401 (93%)	344 (92%)	24 (6%)	4 (1%)	14	52
1	C	379/401 (94%)	349 (92%)	26 (7%)	4 (1%)	14	52
1	D	372/401 (93%)	343 (92%)	25 (7%)	4 (1%)	14	52
All	All	1502/1604 (94%)	1384 (92%)	102 (7%)	16 (1%)	14	52

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PHE
1	B	339	PHE
1	C	339	PHE
1	D	339	PHE
1	A	201	GLY
1	B	177	ASN
1	B	201	GLY
1	C	201	GLY
1	D	177	ASN
1	D	201	GLY
1	A	51	GLY
1	C	51	GLY
1	D	120	PRO
1	B	120	PRO
1	A	120	PRO
1	C	120	PRO

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	296/303 (98%)	286 (97%)	10 (3%)	37	68
1	B	289/303 (95%)	277 (96%)	12 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	296/303 (98%)	285 (96%)	11 (4%)	34 65
1	D	289/303 (95%)	277 (96%)	12 (4%)	30 63
All	All	1170/1212 (96%)	1125 (96%)	45 (4%)	33 65

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	58	ASN
1	A	81	ARG
1	A	157	MSE
1	A	179	LEU
1	A	204	ARG
1	A	287	ILE
1	A	305	SER
1	A	354	ASP
1	A	369	SER
1	B	13	SER
1	B	58	ASN
1	B	81	ARG
1	B	115	PHE
1	B	134	ILE
1	B	157	MSE
1	B	176	THR
1	B	318	HIS
1	B	323	THR
1	B	333	ILE
1	B	354	ASP
1	B	366	LEU
1	C	56	ASN
1	C	58	ASN
1	C	63	ILE
1	C	81	ARG
1	C	157	MSE
1	C	179	LEU
1	C	204	ARG
1	C	287	ILE
1	C	305	SER
1	C	354	ASP
1	C	369	SER
1	D	13	SER

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Mol	Chain	Res	Type
1	D	58	ASN
1	D	81	ARG
1	D	115	PHE
1	D	134	ILE
1	D	157	MSE
1	D	176	THR
1	D	318	HIS
1	D	323	THR
1	D	333	ILE
1	D	354	ASP
1	D	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	LMU	B	1384	-	30,30,36	1.45	6 (20%)	41,41,47	1.52	7 (17%)
2	SO4	A	1391	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	C	1391	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	B	1385	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	D	1384	-	4,4,4	0.11	0	6,6,6	0.25	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	LMU	B	1384	-	-	7/15/55/61	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1384	LMU	O5B-C1B	3.74	1.51	1.41
3	B	1384	LMU	C3'-C4'	-3.60	1.42	1.52
3	B	1384	LMU	C3'-C2'	-2.35	1.46	1.52
3	B	1384	LMU	C3B-C2B	-2.24	1.46	1.52
3	B	1384	LMU	O1B-C1B	-2.17	1.35	1.41
3	B	1384	LMU	O5'-C5'	2.17	1.49	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1384	LMU	O5'-C5'-C4'	3.95	118.08	109.75
3	B	1384	LMU	C1-O1'-C1'	3.70	119.98	113.84
3	B	1384	LMU	O5B-C5B-C4B	3.40	115.88	109.69
3	B	1384	LMU	C1'-O5'-C5'	3.00	119.58	113.69
3	B	1384	LMU	C3B-C4B-C5B	2.83	115.28	110.24
3	B	1384	LMU	O5'-C1'-C2'	2.40	115.42	110.35
3	B	1384	LMU	C6B-C5B-C4B	-2.15	107.97	113.00

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1384	LMU	O5'-C1'-O1'-C1
3	B	1384	LMU	O5'-C5'-C6'-O6'

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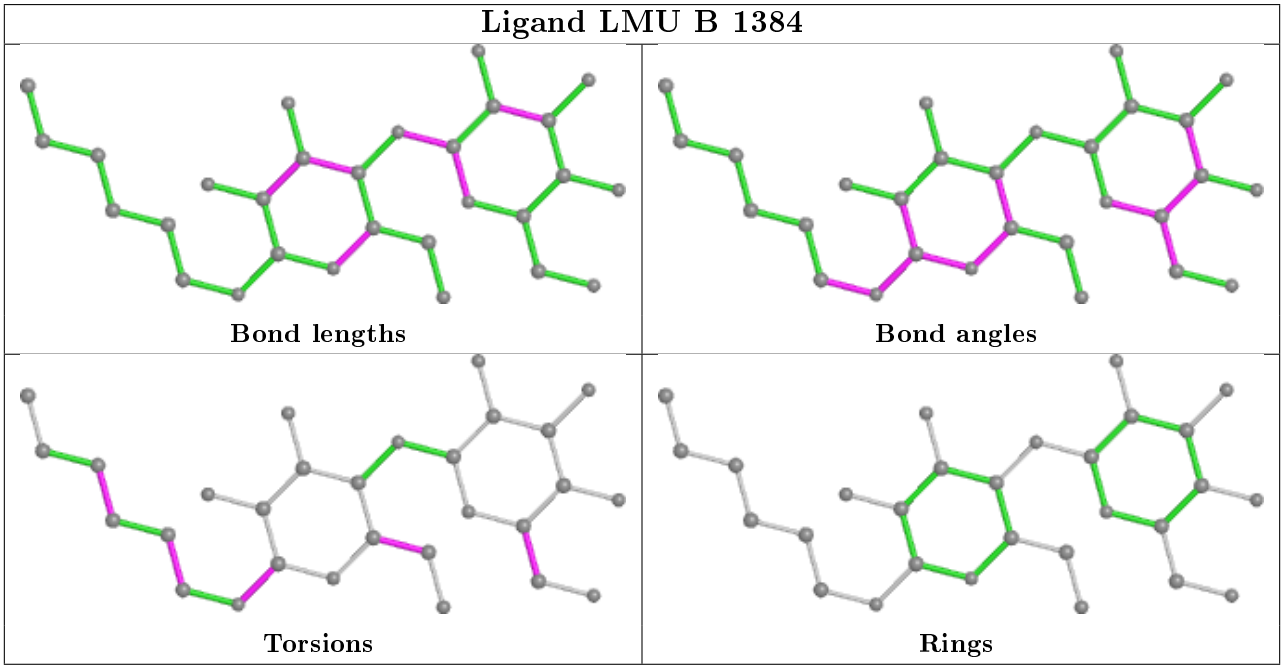
Mol	Chain	Res	Type	Atoms
3	B	1384	LMU	O1'-C1-C2-C3
3	B	1384	LMU	C4B-C5B-C6B-O6B
3	B	1384	LMU	C4'-C5'-C6'-O6'
3	B	1384	LMU	O5B-C5B-C6B-O6B
3	B	1384	LMU	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	370/401 (92%)	-0.22	15 (4%)	37	33	107, 172, 249, 390	0
1	B	363/401 (90%)	-0.11	16 (4%)	34	30	116, 173, 269, 398	0
1	C	370/401 (92%)	-0.04	24 (6%)	18	17	167, 235, 332, 397	0
1	D	363/401 (90%)	0.05	27 (7%)	14	14	139, 234, 322, 416	0
All	All	1466/1604 (91%)	-0.08	82 (5%)	24	22	107, 203, 304, 416	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	243	HIS	9.9
1	B	321	GLU	7.9
1	D	321	GLU	7.8
1	A	242	LYS	7.3
1	C	354	ASP	7.1
1	B	243	HIS	6.7
1	D	120	PRO	6.6
1	C	242	LYS	6.6
1	C	241	GLU	6.1
1	C	240	LYS	6.0
1	D	243	HIS	5.8
1	C	350	PHE	5.7
1	B	354	ASP	5.4
1	D	118	ALA	5.3
1	A	324	THR	5.3
1	D	149	PRO	5.2
1	A	241	GLU	5.1
1	B	242	LYS	5.1
1	D	354	ASP	4.8
1	D	242	LYS	4.8
1	B	120	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	121	ILE	4.4
1	B	147	ARG	4.2
1	D	122	THR	4.2
1	C	353	VAL	4.1
1	D	52	SER	4.1
1	D	324	THR	4.0
1	A	240	LYS	4.0
1	C	120	PRO	3.9
1	C	357	LEU	3.9
1	A	147	ARG	3.9
1	D	272	ALA	3.8
1	D	322	GLY	3.8
1	C	117	TYR	3.8
1	A	51	GLY	3.8
1	A	243	HIS	3.5
1	C	121	ILE	3.4
1	D	278	GLY	3.4
1	B	352	SER	3.3
1	C	245	ARG	3.3
1	D	123	ARG	3.2
1	D	144	LEU	3.2
1	D	114	ALA	3.1
1	C	85	GLN	3.1
1	A	384	LEU	3.1
1	D	119	ASP	3.0
1	A	33	ALA	3.0
1	D	320	PRO	3.0
1	A	246	SER	3.0
1	B	121	ILE	2.9
1	C	246	SER	2.9
1	D	318	HIS	2.9
1	A	245	ARG	2.8
1	B	149	PRO	2.8
1	A	88	LEU	2.8
1	D	353	VAL	2.8
1	B	320	PRO	2.7
1	C	179	LEU	2.7
1	C	118	ALA	2.7
1	D	117	TYR	2.6
1	C	352	SER	2.6
1	B	174	PHE	2.6
1	B	357	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	318	HIS	2.5
1	D	179	LEU	2.5
1	C	355	PRO	2.5
1	B	353	VAL	2.5
1	D	148	VAL	2.5
1	C	324	THR	2.5
1	D	274	VAL	2.4
1	A	290	LEU	2.4
1	D	352	SER	2.4
1	D	290	LEU	2.3
1	B	124	GLU	2.3
1	C	320	PRO	2.3
1	A	322	GLY	2.2
1	C	239	LEU	2.2
1	C	119	ASP	2.2
1	B	179	LEU	2.1
1	B	123	ARG	2.1
1	C	290	LEU	2.1
1	C	11	ASP	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. The B-factors column lists the minimum, median, 95^{th} 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	LMU	B	1384	29/35	0.75	0.35	206,206,206,206	0
2	SO4	B	1385	5/5	0.77	0.28	171,171,171,171	0
2	SO4	D	1384	5/5	0.78	0.26	200,200,200,200	0
2	SO4	C	1391	5/5	0.79	0.27	211,211,211,211	0

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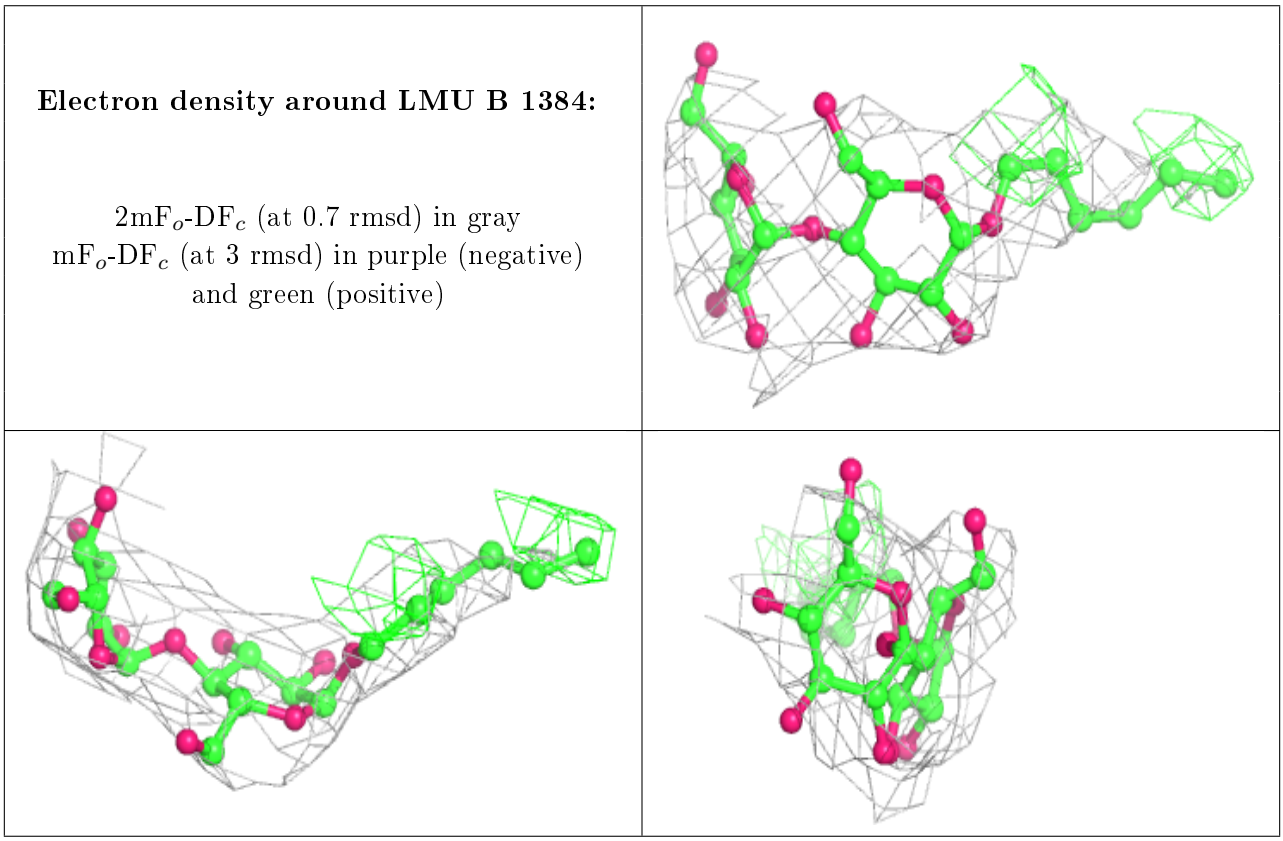
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1391	5/5	0.94	0.28	160,160,160,160	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMU B 1384:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.