Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:35 AM GMT

PDB ID	:	2XMN
Title	:	HIGH RESOLUTION SNAPSHOTS OF DEFINED TOLC OPEN STATES PRESENT AN IRIS-LIKE MOVEMENT OF PERIPLASMIC ENTRANCE HELICES
Authors	:	Pei, X.Y.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on	:	2010-07-28
Resolution	:	2.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

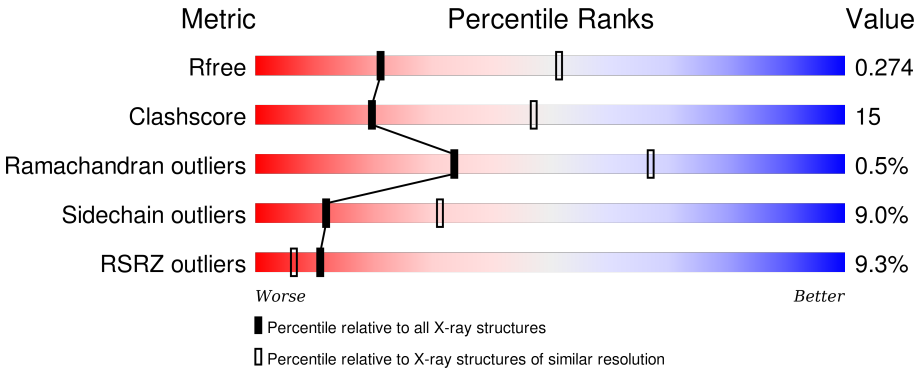
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 <=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	428	9% 66% 30% ·
1	B	428	6% 68% 27% ·
1	C	428	13% 66% 30% ·

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	B	1429	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9944 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 OUTER MEMBRANE PROTEIN TOLC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3290	2028	580	677	5			
1	B	428	Total	C	N	O	S	0	0	0
			3296	2032	582	677	5			
1	C	428	Total	C	N	O	S	0	0	0
			3300	2035	583	677	5			

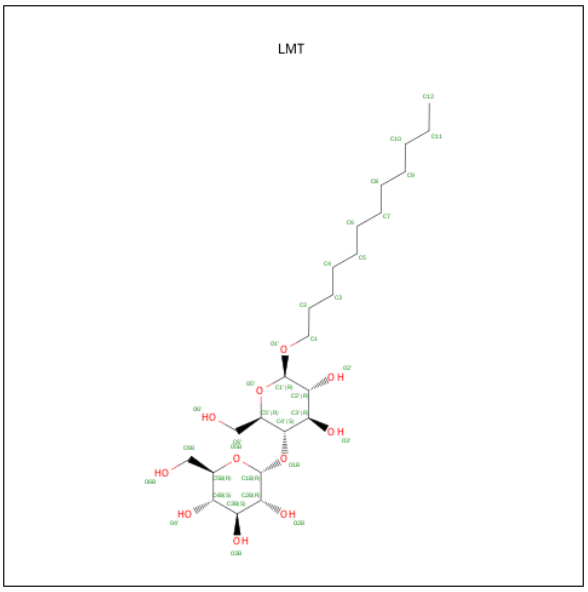
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	LEU	VAL	SEE REMARK 999	UNP P02930
A	362	PHE	TYR	ENGINEERED MUTATION	UNP P02930
A	367	SER	ARG	ENGINEERED MUTATION	UNP P02930
B	169	LEU	VAL	SEE REMARK 999	UNP P02930
B	362	PHE	TYR	ENGINEERED MUTATION	UNP P02930
B	367	SER	ARG	ENGINEERED MUTATION	UNP P02930
C	169	LEU	VAL	SEE REMARK 999	UNP P02930
C	362	PHE	TYR	ENGINEERED MUTATION	UNP P02930
C	367	SER	ARG	ENGINEERED MUTATION	UNP P02930

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 35 24 11	0	0

- Molecule 4 is water.

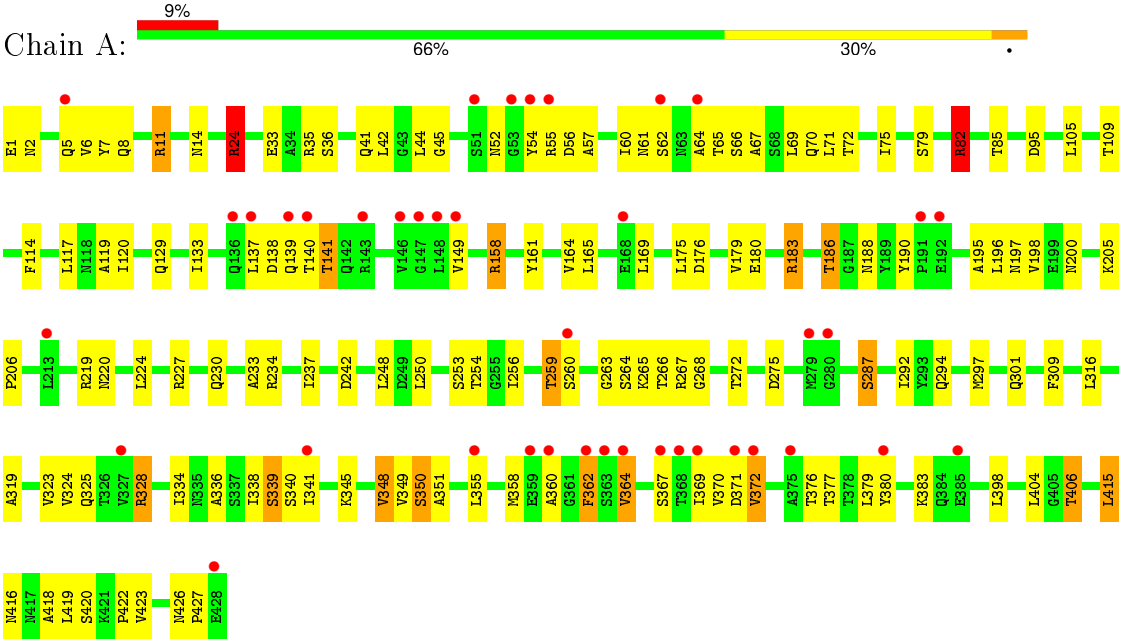
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	8	Total O 8 8	0	0
4	C	3	Total O 3 3	0	0

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.

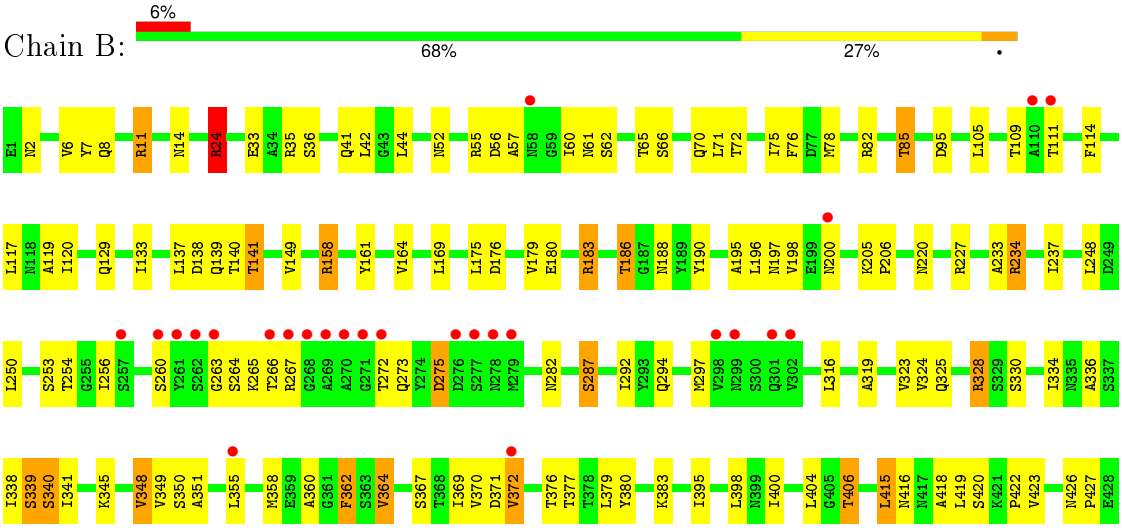
- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain A:



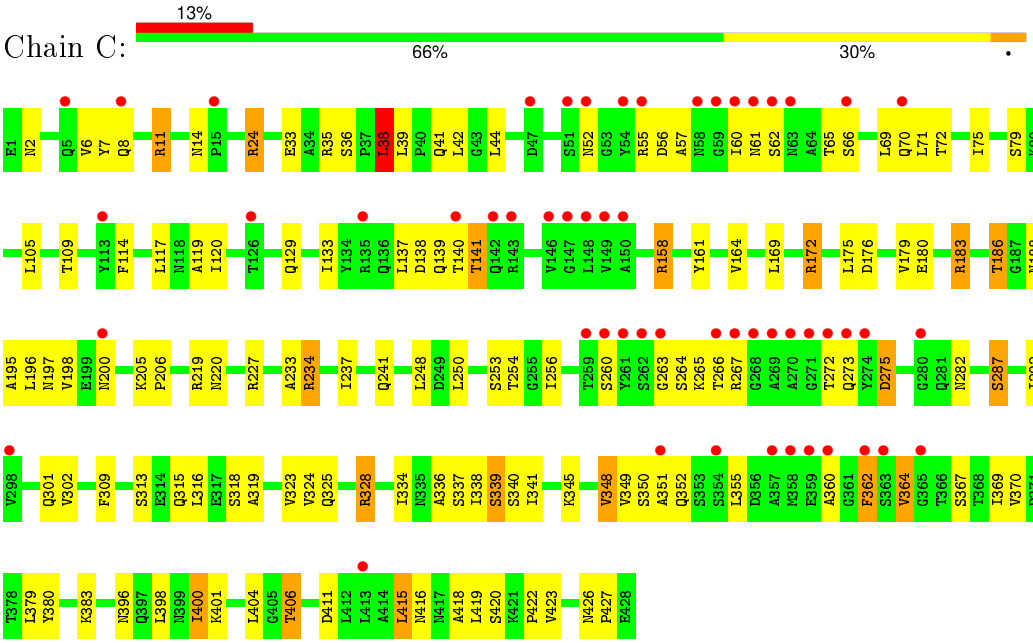
- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain B:



- Molecule 1: OUTER MEMBRANE PROTEIN TOLC

Chain C:


13%
66%
30%
E1 N2 Q5 V6 Y7 Q8 R11 N14 P15 R24 E33 A34 R35 S36 P37 I38 L39 P40 Q41 L42 G43 L44 D47 S51 N52 G53 Y54 R55 D56 A57 N58 G59 I60 N61 S62 N63 A64 T65 S66 L69 Q70 L71 T72 I75 S79 K80 W81 R82 T85
L105 T109 Y113 F114 L117 N118 A119 I120 T126 Q129 I133 Y134 R135 Q136 L137 D138 Q139 T140 T141 Q142 R143 V146 G147 L148 V149 A150 R158 Y161 V164 L169 R172 L175 D176 V179 E180 R183 T186 G187 N188 Y189 Y190 A194
A195 L196 N197 V198 E199 N200 K205 P206 R219 N220 R227 A233 R234 I237 Q241 L248 D249 L250 S253 T254 G255 I256 T259 S260 Y261 S262 G263 S264 K265 T266 R267 G268 A269 A270 G271 T272 Q273 Y274 D275 G280 Q281 N282 S287 I292 Y293 Q294 M297
V298 Q301 V302 F309 S313 E314 Q315 L316 E317 S318 A319 V323 V324 Q325 R328 I334 N335 A336 S337 I338 S339 S340 I341 K345 V348 V349 S350 A351 Q352 S353 S354 L355 D356 A357 M358 E359 A360 G361 F362 S363 V364 G365 T366 S367 T368 I369 V370 D371 V372 T376 T377
T378 L379 Y380 K383 N396 Q397 L398 N399 I400 K401 L404 G405 T406 D411 L412 L413 A414 L415 N416 N417 A418 L419 S420 K421 P422 V423 N426 P427 E428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	134.12Å 135.52Å 136.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.94 – 2.85 29.37 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.4 (16.94-2.85) 93.6 (29.37-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.85 (at 2.85Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.271 , 0.309 0.273 , 0.274	Depositor DCC
R_{free} test set	2689 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	1.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.6	EDS
Estimated twinning fraction	0.010 for -h,l,k 0.000 for -l,-k,-h 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	5 of 54834 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9944	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: LMT, CL

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	0.43	0/3331	0.97	20/4525 (0.4%)
1	B	0.54	0/3337	0.77	17/4533 (0.4%)
1	C	0.47	0/3341	0.97	20/4537 (0.4%)
All	All	0.48	0/10009	0.91	57/13595 (0.4%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	ARG	NE-CZ-NH1	-17.69	111.46	120.30
1	C	24	ARG	NE-CZ-NH1	-17.20	111.70	120.30
1	A	234	ARG	NE-CZ-NH2	17.05	128.83	120.30
1	A	234	ARG	NE-CZ-NH1	-16.70	111.95	120.30
1	C	24	ARG	NE-CZ-NH2	16.25	128.43	120.30
1	C	267	ARG	NE-CZ-NH1	-16.06	112.27	120.30
1	A	328	ARG	NE-CZ-NH2	15.97	128.29	120.30
1	A	11	ARG	NE-CZ-NH1	-15.84	112.38	120.30
1	C	35	ARG	NE-CZ-NH2	-15.75	112.42	120.30
1	C	267	ARG	NE-CZ-NH2	15.45	128.02	120.30
1	A	11	ARG	NE-CZ-NH2	15.32	127.96	120.30
1	C	158	ARG	NE-CZ-NH1	-14.90	112.85	120.30
1	C	158	ARG	NE-CZ-NH2	14.63	127.61	120.30
1	C	35	ARG	NE-CZ-NH1	14.24	127.42	120.30
1	A	82	ARG	NE-CZ-NH1	-13.92	113.34	120.30
1	A	82	ARG	NE-CZ-NH2	12.96	126.78	120.30
1	B	328	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	24	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	267	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	35	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	A	234	ARG	CD-NE-CZ	8.81	135.93	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	328	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	35	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	267	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	234	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	C	24	ARG	CD-NE-CZ	8.24	135.14	123.60
1	B	35	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	A	267	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	158	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	267	ARG	CD-NE-CZ	7.94	134.71	123.60
1	A	158	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	234	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	C	11	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	C	234	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	158	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	24	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	11	ARG	CD-NE-CZ	7.56	134.18	123.60
1	B	82	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	328	ARG	CD-NE-CZ	7.53	134.14	123.60
1	B	35	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	A	24	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	11	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	11	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	C	158	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	158	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	234	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	82	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	C	11	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	35	ARG	CD-NE-CZ	6.85	133.19	123.60
1	B	82	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	328	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	24	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	328	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	267	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	82	ARG	CD-NE-CZ	5.54	131.36	123.60
1	C	38	LEU	CB-CG-CD1	5.21	119.86	111.00
1	B	234	ARG	CD-NE-CZ	5.21	130.89	123.60

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	3290	0	3223	109	0
1	B	3296	0	3237	106	0
1	C	3300	0	3248	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	B	35	0	44	4	0
4	A	9	0	0	1	0
4	B	8	0	0	0	0
4	C	3	0	0	0	0
All	All	9944	0	9752	294	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 15.

All (294) 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:B:183:ARG:HH11	1:B:183:ARG:HG3	1.30	0.95
1:C:183:ARG:HH11	1:C:183:ARG:HG3	1.37	0.89
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.36	0.88
1:B:183:ARG:HH11	1:B:183:ARG:CG	1.93	0.82
1:A:2:ASN:HD22	1:A:416:ASN:HD21	1.29	0.79
1:C:2:ASN:HD22	1:C:416:ASN:HD21	1.30	0.76
1:C:183:ARG:HH11	1:C:183:ARG:CG	1.99	0.75
1:A:183:ARG:HH11	1:A:183:ARG:CG	1.99	0.75
1:C:205:LYS:HG2	1:C:206:PRO:HD2	1.70	0.74
1:A:319:ALA:O	1:A:323:VAL:HG23	1.87	0.74
1:A:169:LEU:HD11	1:B:339:SER:OG	1.87	0.74
1:A:2:ASN:ND2	1:A:416:ASN:HD21	1.86	0.73
1:B:319:ALA:O	1:B:323:VAL:HG23	1.88	0.73
1:C:254:THR:HG23	1:C:254:THR:O	1.89	0.73
1:C:319:ALA:O	1:C:323:VAL:HG23	1.88	0.72
1:B:2:ASN:ND2	1:B:416:ASN:HD21	1.87	0.72
1:B:2:ASN:HD22	1:B:416:ASN:HD21	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASN:ND2	1:C:416:ASN:HD21	1.87	0.71
1:A:292:ILE:HB	1:C:42:LEU:O	1.90	0.70
1:B:254:THR:HG23	1:B:254:THR:O	1.92	0.69
1:B:2:ASN:O	1:B:6:VAL:HG23	1.92	0.69
1:A:254:THR:O	1:A:254:THR:HG23	1.93	0.68
1:A:339:SER:OG	1:C:169:LEU:HD11	1.94	0.67
1:B:169:LEU:HD11	1:C:339:SER:OG	1.94	0.67
1:A:294:GLN:HG2	1:C:41:GLN:NE2	2.11	0.66
1:C:55:ARG:C	1:C:57:ALA:H	1.99	0.66
1:A:41:GLN:NE2	1:B:294:GLN:HG2	2.10	0.66
3:B:1429:LMT:O6'	3:B:1429:LMT:O5B	2.16	0.64
1:A:186:THR:HG23	1:A:188:ASN:H	1.63	0.64
1:A:2:ASN:HB2	1:A:416:ASN:OD1	1.97	0.63
1:A:2:ASN:O	1:A:6:VAL:HG23	1.99	0.63
1:B:41:GLN:NE2	1:C:294:GLN:HG2	2.14	0.63
1:B:220:ASN:ND2	1:B:323:VAL:HG22	2.14	0.62
1:C:117:LEU:HD13	1:C:195:ALA:HA	1.82	0.62
1:B:117:LEU:HD13	1:B:195:ALA:HA	1.82	0.62
1:A:220:ASN:ND2	1:A:323:VAL:HG22	2.15	0.62
1:A:380:TYR:HA	1:A:383:LYS:HB2	1.82	0.62
1:A:328:ARG:HD2	1:C:180:GLU:OE2	2.00	0.61
1:B:169:LEU:HD11	1:C:339:SER:CB	2.29	0.61
1:A:197:ASN:ND2	1:A:200:ASN:HB2	2.16	0.61
1:B:186:THR:HG23	1:B:188:ASN:H	1.66	0.61
1:C:334:ILE:O	1:C:338:ILE:HG13	2.01	0.61
1:B:119:ALA:HB1	1:B:175:LEU:HA	1.82	0.61
1:C:2:ASN:O	1:C:6:VAL:HG23	2.00	0.60
1:B:75:ILE:HD12	1:B:250:LEU:HB2	1.83	0.60
1:C:205:LYS:CG	1:C:206:PRO:HD2	2.31	0.60
1:B:137:LEU:HA	1:B:140:THR:HG22	1.83	0.60
1:C:2:ASN:HB2	1:C:416:ASN:OD1	2.02	0.60
1:A:44:LEU:HB2	1:B:292:ILE:HD11	1.84	0.59
1:A:205:LYS:HG2	1:A:206:PRO:HD2	1.84	0.59
1:B:55:ARG:C	1:B:57:ALA:H	2.04	0.59
1:C:172:ARG:CZ	1:C:172:ARG:HB2	2.32	0.59
1:C:197:ASN:ND2	1:C:200:ASN:HB2	2.17	0.59
1:A:369:ILE:O	1:A:372:VAL:HG12	2.02	0.59
1:C:55:ARG:O	1:C:57:ALA:N	2.35	0.59
1:A:55:ARG:C	1:A:57:ALA:H	2.06	0.59
1:C:220:ASN:ND2	1:C:323:VAL:HG22	2.18	0.59
1:A:75:ILE:HD12	1:A:250:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LYS:HG2	1:B:206:PRO:HD2	1.84	0.59
1:C:137:LEU:HA	1:C:140:THR:HG22	1.85	0.59
1:B:120:ILE:HG21	1:B:423:VAL:HG11	1.85	0.58
1:B:369:ILE:O	1:B:372:VAL:HG12	2.03	0.58
1:C:369:ILE:O	1:C:372:VAL:HG12	2.03	0.58
1:B:334:ILE:O	1:B:338:ILE:HG13	2.03	0.58
3:B:1429:LMT:O6'	3:B:1429:LMT:O6B	2.21	0.58
1:A:120:ILE:HG21	1:A:423:VAL:HG11	1.85	0.58
1:B:140:THR:HB	1:B:369:ILE:HD12	1.86	0.58
1:C:120:ILE:HG21	1:C:423:VAL:HG11	1.84	0.58
1:C:75:ILE:HD12	1:C:250:LEU:HB2	1.84	0.58
1:A:292:ILE:HD11	1:C:44:LEU:HB2	1.86	0.58
1:A:140:THR:HB	1:A:369:ILE:HD12	1.86	0.58
1:C:341:ILE:O	1:C:345:LYS:HB2	2.04	0.57
1:B:24:ARG:HD3	1:B:95:ASP:OD1	2.04	0.57
1:C:380:TYR:HA	1:C:383:LYS:HB2	1.87	0.57
1:B:180:GLU:HA	1:B:180:GLU:OE1	2.03	0.57
1:A:169:LEU:HD11	1:B:339:SER:CB	2.35	0.57
1:B:220:ASN:HD22	1:B:323:VAL:HG22	1.70	0.57
1:A:334:ILE:O	1:A:338:ILE:HG13	2.03	0.57
1:B:114:PHE:HZ	1:B:415:LEU:CD2	2.18	0.57
1:B:380:TYR:HA	1:B:383:LYS:HB2	1.86	0.56
1:C:404:LEU:HB3	1:C:406:THR:HG23	1.86	0.56
1:B:2:ASN:HB2	1:B:416:ASN:OD1	2.05	0.56
1:B:186:THR:CG2	1:B:188:ASN:H	2.18	0.56
1:A:117:LEU:HD13	1:A:195:ALA:HA	1.87	0.56
1:A:119:ALA:HB1	1:A:175:LEU:HA	1.86	0.56
1:A:137:LEU:HA	1:A:140:THR:HG22	1.88	0.56
1:B:169:LEU:HD21	1:C:339:SER:HB3	1.87	0.56
1:B:404:LEU:HB3	1:B:406:THR:HG23	1.88	0.56
1:C:140:THR:HB	1:C:369:ILE:HD12	1.87	0.55
1:A:186:THR:CG2	1:A:188:ASN:H	2.19	0.55
1:B:85:THR:OG1	3:B:1429:LMT:H6'1	2.06	0.55
1:C:180:GLU:HA	1:C:180:GLU:OE1	2.06	0.55
1:C:119:ALA:HB1	1:C:175:LEU:HA	1.88	0.55
1:B:186:THR:HG21	1:B:190:TYR:HE2	1.71	0.55
1:B:117:LEU:CD1	1:B:195:ALA:HA	2.36	0.55
1:B:197:ASN:ND2	1:B:200:ASN:HB2	2.20	0.55
1:A:36:SER:OG	1:B:297:MET:HB2	2.07	0.55
1:A:24:ARG:HD3	1:A:95:ASP:OD1	2.07	0.55
1:B:180:GLU:OE2	1:C:328:ARG:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PHE:HZ	1:A:415:LEU:CD2	2.19	0.55
1:A:351:ALA:HB1	1:A:379:LEU:HA	1.89	0.55
1:C:117:LEU:CD1	1:C:195:ALA:HA	2.37	0.55
1:A:227:ARG:HG2	1:A:316:LEU:HD11	1.89	0.55
1:B:330:SER:OG	1:B:400:ILE:HG13	2.06	0.55
1:A:297:MET:HB2	1:C:36:SER:OG	2.07	0.54
1:B:36:SER:OG	1:C:297:MET:HB2	2.08	0.54
1:A:180:GLU:HA	1:A:180:GLU:OE1	2.07	0.54
1:C:186:THR:HG23	1:C:188:ASN:H	1.72	0.54
1:B:355:LEU:HD11	1:B:376:THR:OG1	2.08	0.54
1:B:227:ARG:HG2	1:B:316:LEU:HD11	1.89	0.54
3:B:1429:LMT:H6'	3:B:1429:LMT:H6B	1.55	0.54
1:C:114:PHE:HZ	1:C:415:LEU:CD2	2.21	0.54
1:A:220:ASN:HD22	1:A:323:VAL:CG2	2.21	0.54
1:B:336:ALA:O	1:B:340:SER:HB2	2.07	0.54
1:B:220:ASN:HD22	1:B:323:VAL:CG2	2.21	0.54
1:A:82:ARG:HD2	1:A:242:ASP:OD2	2.08	0.54
1:B:8:GLN:HE21	1:B:11:ARG:HH22	1.54	0.54
1:A:42:LEU:O	1:B:292:ILE:HB	2.08	0.53
1:C:172:ARG:HB2	1:C:172:ARG:NH1	2.23	0.53
1:B:351:ALA:HB1	1:B:379:LEU:HA	1.90	0.53
1:A:404:LEU:HB3	1:A:406:THR:HG23	1.89	0.53
1:A:140:THR:CB	1:A:369:ILE:HD12	2.39	0.53
1:A:341:ILE:O	1:A:345:LYS:HB2	2.07	0.53
1:A:426:ASN:N	1:A:427:PRO:HD3	2.24	0.53
1:A:220:ASN:HD22	1:A:323:VAL:HG22	1.72	0.53
1:C:227:ARG:HG2	1:C:316:LEU:HD11	1.90	0.53
1:A:117:LEU:CD1	1:A:195:ALA:HA	2.39	0.53
1:B:205:LYS:CG	1:B:206:PRO:HD2	2.39	0.52
1:C:140:THR:CB	1:C:369:ILE:HD12	2.39	0.52
1:B:426:ASN:N	1:B:427:PRO:HD3	2.25	0.52
1:B:341:ILE:O	1:B:345:LYS:HB2	2.09	0.52
1:C:75:ILE:CD1	1:C:250:LEU:HB2	2.40	0.52
1:B:140:THR:CB	1:B:369:ILE:HD12	2.39	0.52
1:A:75:ILE:CD1	1:A:250:LEU:HB2	2.39	0.52
1:C:351:ALA:HB1	1:C:379:LEU:HA	1.90	0.52
1:C:8:GLN:HE21	1:C:11:ARG:HH22	1.57	0.52
1:A:328:ARG:CD	1:C:180:GLU:OE2	2.57	0.52
1:B:55:ARG:O	1:B:57:ALA:N	2.43	0.52
1:B:42:LEU:O	1:C:292:ILE:HB	2.10	0.52
1:A:205:LYS:CG	1:A:206:PRO:HD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASN:ND2	1:A:105:LEU:HD13	2.24	0.52
1:C:186:THR:CG2	1:C:188:ASN:H	2.22	0.52
1:B:75:ILE:CD1	1:B:250:LEU:HB2	2.40	0.52
1:A:339:SER:CB	1:C:169:LEU:HD11	2.39	0.51
1:C:220:ASN:HD22	1:C:323:VAL:HG22	1.74	0.51
1:A:66:SER:HA	1:A:256:ILE:O	2.10	0.51
1:C:233:ALA:O	1:C:237:ILE:HG13	2.09	0.51
1:C:254:THR:CG2	1:C:254:THR:O	2.57	0.51
1:A:180:GLU:OE2	1:B:328:ARG:HD3	2.10	0.51
1:B:358:MET:SD	1:B:371:ASP:HB3	2.51	0.51
1:A:129:GLN:O	1:A:133:ILE:HG13	2.10	0.51
1:B:254:THR:CG2	1:B:254:THR:O	2.59	0.51
1:A:254:THR:O	1:A:254:THR:CG2	2.59	0.51
1:A:233:ALA:O	1:A:237:ILE:HG13	2.11	0.50
1:C:220:ASN:HD22	1:C:323:VAL:CG2	2.24	0.50
1:B:176:ASP:O	1:B:179:VAL:HG22	2.11	0.50
1:C:362:PHE:HA	1:C:367:SER:O	2.12	0.50
1:B:60:ILE:C	1:B:61:ASN:HD22	2.14	0.50
1:A:60:ILE:C	1:A:61:ASN:HD22	2.15	0.49
1:A:360:ALA:O	1:A:364:VAL:HG23	2.12	0.49
1:C:183:ARG:NH1	1:C:183:ARG:HG3	2.17	0.49
1:A:186:THR:HG21	1:A:190:TYR:HE2	1.77	0.49
1:A:362:PHE:HA	1:A:367:SER:O	2.13	0.49
1:A:161:TYR:O	1:A:164:VAL:HG12	2.13	0.49
1:C:14:ASN:ND2	1:C:105:LEU:HD13	2.28	0.49
1:C:336:ALA:O	1:C:340:SER:HB2	2.13	0.49
1:C:55:ARG:C	1:C:57:ALA:N	2.64	0.48
1:C:355:LEU:HD11	1:C:376:THR:OG1	2.12	0.48
1:A:355:LEU:HD11	1:A:376:THR:OG1	2.14	0.48
1:C:186:THR:HG21	1:C:190:TYR:HE2	1.78	0.48
1:C:66:SER:HA	1:C:256:ILE:O	2.14	0.48
1:C:315:GLN:O	1:C:318:SER:HB2	2.13	0.48
1:A:44:LEU:HD12	1:A:69:LEU:HD12	1.95	0.48
1:B:169:LEU:HD11	1:C:339:SER:HB3	1.94	0.48
1:B:324:VAL:HG12	1:B:325:GLN:N	2.29	0.48
1:C:60:ILE:C	1:C:61:ASN:HD22	2.16	0.48
1:A:336:ALA:O	1:A:340:SER:HB2	2.14	0.47
1:A:54:TYR:HE2	1:B:282:ASN:OD1	1.96	0.47
1:C:263:GLY:O	1:C:266:THR:HG22	2.15	0.47
1:A:196:LEU:HD12	1:A:418:ALA:O	2.14	0.47
1:B:183:ARG:NH1	1:B:183:ARG:HG3	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ASN:H	1:B:419:LEU:HA	1.79	0.47
1:B:420:SER:O	1:B:422:PRO:HD3	2.14	0.47
1:C:426:ASN:N	1:C:427:PRO:HD3	2.29	0.47
1:C:7:TYR:HA	1:C:109:THR:HG21	1.96	0.47
1:C:420:SER:O	1:C:422:PRO:HD3	2.15	0.47
1:C:197:ASN:H	1:C:419:LEU:HA	1.80	0.47
1:B:55:ARG:C	1:B:57:ALA:N	2.68	0.47
1:A:7:TYR:HA	1:A:109:THR:HG21	1.97	0.46
1:A:141:THR:HG23	1:A:141:THR:O	2.15	0.46
1:B:362:PHE:HA	1:B:367:SER:O	2.14	0.46
1:A:55:ARG:O	1:A:57:ALA:N	2.48	0.46
1:B:196:LEU:HD12	1:B:418:ALA:O	2.15	0.46
1:C:360:ALA:O	1:C:364:VAL:HG23	2.15	0.46
1:B:419:LEU:C	1:B:419:LEU:HD12	2.36	0.46
1:C:141:THR:HG23	1:C:141:THR:O	2.15	0.46
1:A:264:SER:C	1:A:266:THR:H	2.19	0.46
1:B:141:THR:HG23	1:B:141:THR:O	2.14	0.46
1:A:248:LEU:HD12	1:A:287:SER:O	2.16	0.46
1:B:360:ALA:O	1:B:364:VAL:HG23	2.16	0.46
1:B:7:TYR:HA	1:B:109:THR:HG21	1.96	0.46
1:A:263:GLY:O	1:A:266:THR:HG22	2.14	0.46
1:B:370:VAL:O	1:B:370:VAL:HG12	2.15	0.46
1:A:419:LEU:O	1:A:419:LEU:HD12	2.16	0.46
1:B:248:LEU:HD12	1:B:287:SER:O	2.15	0.46
1:A:324:VAL:HG12	1:A:325:GLN:N	2.31	0.45
1:B:129:GLN:O	1:B:133:ILE:HG13	2.16	0.45
1:C:396:ASN:O	1:C:400:ILE:HG12	2.15	0.45
1:A:419:LEU:C	1:A:419:LEU:HD12	2.37	0.45
1:C:161:TYR:O	1:C:164:VAL:HG12	2.16	0.45
1:B:263:GLY:O	1:B:266:THR:HG22	2.16	0.45
1:A:183:ARG:NH1	1:A:183:ARG:HG3	2.15	0.45
1:B:14:ASN:ND2	1:B:105:LEU:HD13	2.30	0.45
1:A:370:VAL:O	1:A:370:VAL:HG12	2.15	0.45
1:C:129:GLN:O	1:C:133:ILE:HG13	2.17	0.45
1:B:419:LEU:HD12	1:B:419:LEU:O	2.16	0.45
1:B:161:TYR:O	1:B:164:VAL:HG12	2.17	0.45
1:A:6:VAL:HG13	1:A:190:TYR:CZ	2.52	0.45
1:A:169:LEU:HD21	1:B:339:SER:HB3	1.97	0.45
1:C:196:LEU:HD12	1:C:418:ALA:O	2.16	0.45
1:B:137:LEU:HA	1:B:140:THR:CG2	2.47	0.44
1:C:401:LYS:HE3	1:C:411:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:C	1:A:57:ALA:N	2.70	0.44
1:C:264:SER:C	1:C:266:THR:H	2.19	0.44
1:B:169:LEU:CD2	1:C:339:SER:HB3	2.48	0.44
1:A:45:GLY:O	1:A:67:ALA:HA	2.17	0.44
1:B:233:ALA:O	1:B:237:ILE:HG13	2.18	0.44
1:C:241:GLN:HG3	1:C:302:VAL:HG22	1.99	0.44
1:B:345:LYS:O	1:B:348:VAL:HG12	2.17	0.43
1:A:8:GLN:HE21	1:A:11:ARG:HH22	1.66	0.43
1:A:358:MET:SD	1:A:371:ASP:HB3	2.58	0.43
1:C:44:LEU:HD12	1:C:69:LEU:HD12	2.00	0.43
1:A:237:ILE:HD11	1:A:309:PHE:HB2	1.99	0.43
1:A:52:ASN:C	1:A:52:ASN:OD1	2.57	0.43
1:A:272:THR:HG23	1:A:272:THR:O	2.19	0.43
1:A:197:ASN:H	1:A:419:LEU:HA	1.82	0.43
1:B:139:GLN:OE1	1:B:362:PHE:HE1	2.02	0.43
1:C:297:MET:CE	1:C:301:GLN:HE22	2.32	0.43
1:B:111:THR:HA	1:B:395:ILE:HD11	2.01	0.43
1:A:339:SER:HB3	1:C:169:LEU:HD21	1.99	0.43
1:C:313:SER:O	1:C:316:LEU:HB3	2.19	0.43
1:B:273:GLN:C	1:B:275:ASP:H	2.22	0.43
1:C:272:THR:HG23	1:C:272:THR:O	2.19	0.43
1:B:66:SER:HA	1:B:256:ILE:O	2.19	0.43
1:A:230:GLN:OE1	1:A:316:LEU:HD22	2.19	0.42
1:B:264:SER:C	1:B:266:THR:H	2.22	0.42
1:C:370:VAL:O	1:C:370:VAL:HG12	2.20	0.42
1:C:38:LEU:HD21	1:C:81:TRP:CD2	2.54	0.42
1:A:44:LEU:HB2	1:B:292:ILE:CD1	2.49	0.42
1:B:52:ASN:HB3	1:C:282:ASN:HB2	2.01	0.42
1:B:348:VAL:CG1	1:B:349:VAL:N	2.83	0.42
1:C:139:GLN:OE1	1:C:362:PHE:HE1	2.03	0.42
1:A:348:VAL:CG1	1:A:349:VAL:N	2.82	0.42
1:A:219:ARG:HE	1:A:219:ARG:HB3	1.67	0.42
1:B:44:LEU:HB2	1:C:292:ILE:HD11	2.01	0.42
1:A:297:MET:CE	1:A:301:GLN:HE22	2.33	0.42
1:B:8:GLN:HE21	1:B:11:ARG:NH2	2.17	0.42
1:C:176:ASP:O	1:C:179:VAL:HG22	2.20	0.42
1:B:272:THR:O	1:B:272:THR:HG23	2.19	0.42
1:A:129:GLN:HG2	1:A:164:VAL:HG21	2.02	0.41
1:B:137:LEU:CA	1:B:140:THR:HG22	2.50	0.41
1:A:1:GLU:HB3	1:A:5:GLN:HB2	2.03	0.41
1:A:195:ALA:O	1:A:419:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:VAL:CG1	1:C:349:VAL:N	2.83	0.41
1:C:219:ARG:HE	1:C:219:ARG:HB3	1.59	0.41
1:B:183:ARG:NH1	1:B:183:ARG:CG	2.63	0.41
1:B:195:ALA:O	1:B:419:LEU:HB2	2.20	0.41
1:A:250:LEU:C	1:A:250:LEU:HD23	2.41	0.41
1:C:273:GLN:C	1:C:275:ASP:H	2.24	0.41
1:A:268:GLY:N	4:A:2006:HOH:O	2.53	0.41
1:C:6:VAL:HG13	1:C:190:TYR:CZ	2.56	0.41
1:A:169:LEU:CD2	1:B:339:SER:HB3	2.50	0.41
1:B:250:LEU:HD23	1:B:250:LEU:C	2.40	0.41
1:A:161:TYR:CE2	1:A:165:LEU:HD11	2.56	0.41
1:A:176:ASP:O	1:A:179:VAL:HG22	2.20	0.41
1:C:248:LEU:HD12	1:C:287:SER:O	2.21	0.41
1:C:297:MET:HE2	1:C:301:GLN:HE22	1.85	0.41
1:A:139:GLN:OE1	1:A:362:PHE:HE1	2.04	0.41
1:A:224:LEU:O	1:A:224:LEU:HD12	2.21	0.41
1:C:52:ASN:C	1:C:52:ASN:OD1	2.58	0.41
1:C:237:ILE:HD11	1:C:309:PHE:HB2	2.03	0.41
1:C:39:LEU:HD12	1:C:39:LEU:N	2.36	0.41
1:A:420:SER:O	1:A:422:PRO:HD3	2.20	0.41
1:C:352:GLN:HA	1:C:379:LEU:HD13	2.02	0.41
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.92	0.41
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.81	0.41
1:B:76:PHE:HE2	1:B:78:MET:CE	2.33	0.41
1:A:349:VAL:HG12	1:A:350:SER:N	2.36	0.40
1:C:337:SER:O	1:C:341:ILE:HG13	2.21	0.40
1:C:324:VAL:HG12	1:C:325:GLN:N	2.36	0.40
1:C:205:LYS:HG2	1:C:206:PRO:CD	2.46	0.40
1:B:60:ILE:C	1:B:61:ASN:ND2	2.75	0.40
1:C:137:LEU:CA	1:C:140:THR:HG22	2.52	0.40
1:A:64:ALA:HB2	1:A:259:THR:HG23	2.04	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	426/428 (100%)	390 (92%)	34 (8%)	2 (0%)	34	67
1	B	426/428 (100%)	386 (91%)	38 (9%)	2 (0%)	34	67
1	C	426/428 (100%)	385 (90%)	38 (9%)	3 (1%)	26	59
All	All	1278/1284 (100%)	1161 (91%)	110 (9%)	7 (0%)	34	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	B	56	ASP
1	C	56	ASP
1	A	265	LYS
1	C	265	LYS
1	B	265	LYS
1	C	194	ALA

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	355/358 (99%)	323 (91%)	32 (9%)	12	31
1	B	357/358 (100%)	326 (91%)	31 (9%)	13	33
1	C	358/358 (100%)	325 (91%)	33 (9%)	11	30
All	All	1070/1074 (100%)	974 (91%)	96 (9%)	12	31

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	33	GLU
1	A	62	SER

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Mol	Chain	Res	Type
1	A	65	THR
1	A	70	GLN
1	A	71	LEU
1	A	72	THR
1	A	79	SER
1	A	82	ARG
1	A	85	THR
1	A	138	ASP
1	A	141	THR
1	A	149	VAL
1	A	158	ARG
1	A	183	ARG
1	A	186	THR
1	A	198	VAL
1	A	253	SER
1	A	259	THR
1	A	260	SER
1	A	275	ASP
1	A	287	SER
1	A	339	SER
1	A	348	VAL
1	A	350	SER
1	A	362	PHE
1	A	364	VAL
1	A	372	VAL
1	A	377	THR
1	A	398	LEU
1	A	406	THR
1	A	415	LEU
1	B	24	ARG
1	B	33	GLU
1	B	62	SER
1	B	65	THR
1	B	70	GLN
1	B	71	LEU
1	B	72	THR
1	B	85	THR
1	B	138	ASP
1	B	141	THR
1	B	149	VAL
1	B	158	ARG
1	B	183	ARG

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Mol	Chain	Res	Type
1	B	186	THR
1	B	198	VAL
1	B	234	ARG
1	B	253	SER
1	B	260	SER
1	B	275	ASP
1	B	287	SER
1	B	339	SER
1	B	340	SER
1	B	348	VAL
1	B	350	SER
1	B	362	PHE
1	B	364	VAL
1	B	372	VAL
1	B	377	THR
1	B	398	LEU
1	B	406	THR
1	B	415	LEU
1	C	24	ARG
1	C	33	GLU
1	C	38	LEU
1	C	62	SER
1	C	65	THR
1	C	70	GLN
1	C	71	LEU
1	C	72	THR
1	C	79	SER
1	C	85	THR
1	C	138	ASP
1	C	141	THR
1	C	158	ARG
1	C	172	ARG
1	C	183	ARG
1	C	186	THR
1	C	198	VAL
1	C	234	ARG
1	C	253	SER
1	C	260	SER
1	C	275	ASP
1	C	287	SER
1	C	339	SER
1	C	348	VAL

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Mol	Chain	Res	Type
1	C	350	SER
1	C	362	PHE
1	C	364	VAL
1	C	372	VAL
1	C	377	THR
1	C	398	LEU
1	C	400	ILE
1	C	406	THR
1	C	415	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	8	GLN
1	A	14	ASN
1	A	32	ASN
1	A	41	GLN
1	A	61	ASN
1	A	103	GLN
1	A	142	GLN
1	A	210	ASN
1	A	220	ASN
1	A	230	GLN
1	A	244	HIS
1	A	301	GLN
1	A	304	GLN
1	A	342	ASN
1	A	397	GLN
1	A	399	ASN
1	B	2	ASN
1	B	8	GLN
1	B	14	ASN
1	B	32	ASN
1	B	41	GLN
1	B	61	ASN
1	B	103	GLN
1	B	142	GLN
1	B	210	ASN
1	B	220	ASN
1	B	230	GLN
1	B	244	HIS

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Mol	Chain	Res	Type
1	B	301	GLN
1	B	304	GLN
1	B	342	ASN
1	B	399	ASN
1	C	8	GLN
1	C	14	ASN
1	C	32	ASN
1	C	41	GLN
1	C	61	ASN
1	C	103	GLN
1	C	142	GLN
1	C	210	ASN
1	C	220	ASN
1	C	230	GLN
1	C	244	HIS
1	C	301	GLN
1	C	342	ASN
1	C	397	GLN
1	C	399	ASN
1	C	416	ASN

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

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	LMT	B	1429	-	36,36,36	2.72	13 (36%)	47,47,47	2.10	13 (27%)

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	LMT	B	1429	-	-	0/21/61/61	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1429	LMT	C3B-C2B	-8.86	1.29	1.52
3	B	1429	LMT	O4'-C4B	-5.65	1.29	1.43
3	B	1429	LMT	O1B-C1B	-5.39	1.27	1.41
3	B	1429	LMT	C3'-C4'	-2.91	1.44	1.52
3	B	1429	LMT	O3'-C3'	2.40	1.48	1.43
3	B	1429	LMT	C6B-C5B	2.46	1.60	1.51
3	B	1429	LMT	O1'-C1'	2.62	1.44	1.40
3	B	1429	LMT	O3B-C3B	2.71	1.49	1.43
3	B	1429	LMT	C1'-C2'	2.83	1.61	1.52
3	B	1429	LMT	O5'-C5'	3.49	1.53	1.44
3	B	1429	LMT	O2B-C2B	3.86	1.52	1.43
3	B	1429	LMT	C4B-C3B	4.45	1.64	1.52
3	B	1429	LMT	C4B-C5B	4.90	1.63	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1429	LMT	C6'-C5'-C4'	-4.71	99.53	113.25
3	B	1429	LMT	C1B-O1B-C4'	-4.09	107.33	118.01
3	B	1429	LMT	O1B-C1B-C2B	2.14	113.30	108.10
3	B	1429	LMT	O1'-C1-C2	2.30	119.03	109.88
3	B	1429	LMT	O1B-C4'-C3'	2.62	113.92	107.17
3	B	1429	LMT	C3'-C4'-C5'	2.94	117.48	110.84
3	B	1429	LMT	O5'-C1'-C2'	3.26	116.96	110.28
3	B	1429	LMT	O1'-C1'-C2'	3.47	112.42	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1429	LMT	C1-O1'-C1'	3.56	120.17	113.94
3	B	1429	LMT	O5B-C1B-C2B	4.20	118.89	110.28
3	B	1429	LMT	C1B-O5B-C5B	4.31	122.12	113.75
3	B	1429	LMT	C1'-C2'-C3'	4.40	118.64	109.97
3	B	1429	LMT	O5'-C5'-C4'	4.51	119.27	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1429	LMT	4	0

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	428/428 (100%)	0.59	40 (9%) 11 6	58, 106, 180, 254	0
1	B	428/428 (100%)	0.39	26 (6%) 25 18	56, 79, 138, 238	0
1	C	428/428 (100%)	0.59	54 (12%) 5 3	52, 89, 188, 259	0
All	All	1284/1284 (100%)	0.52	120 (9%) 11 6	52, 90, 174, 259	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	THR	10.9
1	A	139	GLN	8.1
1	C	148	LEU	6.9
1	C	140	THR	6.9
1	B	270	ALA	6.8
1	A	362	PHE	6.3
1	C	142	GLN	6.2
1	C	363	SER	6.1
1	B	267	ARG	5.9
1	A	136	GLN	5.8
1	A	54	TYR	5.8
1	B	200	ASN	5.7
1	C	150	ALA	5.5
1	C	362	PHE	5.4
1	A	148	LEU	5.0
1	A	363	SER	4.9
1	B	278	ASN	4.9
1	A	149	VAL	4.9
1	B	269	ALA	4.9
1	B	268	GLY	4.7
1	A	367	SER	4.7
1	A	55	ARG	4.6
1	A	428	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	372	VAL	4.5
1	C	146	VAL	4.5
1	C	365	GLY	4.5
1	C	269	ALA	4.3
1	C	266	THR	4.2
1	C	61	ASN	4.0
1	A	146	VAL	4.0
1	C	263	GLY	3.9
1	C	270	ALA	3.7
1	B	279	MET	3.6
1	B	262	SER	3.6
1	A	168	GLU	3.6
1	B	263	GLY	3.6
1	A	137	LEU	3.5
1	A	62	SER	3.5
1	C	262	SER	3.5
1	C	58	ASN	3.4
1	C	274	TYR	3.4
1	A	147	GLY	3.3
1	B	266	THR	3.3
1	C	268	GLY	3.3
1	C	135	ARG	3.3
1	C	267	ARG	3.2
1	B	302	VAL	3.2
1	C	62	SER	3.2
1	A	280	GLY	3.1
1	C	63	ASN	3.1
1	C	351	ALA	3.1
1	A	5	GLN	3.1
1	C	280	GLY	3.0
1	C	271	GLY	3.0
1	C	143	ARG	3.0
1	C	147	GLY	3.0
1	C	272	THR	3.0
1	C	259	THR	3.0
1	A	53	GLY	2.9
1	A	143	ARG	2.9
1	B	277	SER	2.9
1	A	364	VAL	2.9
1	B	298	VAL	2.8
1	A	368	THR	2.8
1	B	301	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	359	GLU	2.8
1	C	52	ASN	2.8
1	C	113	TYR	2.8
1	C	60	ILE	2.8
1	C	298	VAL	2.7
1	C	357	ALA	2.7
1	A	327	VAL	2.7
1	A	380	TYR	2.7
1	A	279	MET	2.7
1	C	47	ASP	2.6
1	B	276	ASP	2.6
1	B	271	GLY	2.6
1	C	358	MET	2.6
1	C	54	TYR	2.6
1	A	371	ASP	2.5
1	B	110	ALA	2.5
1	A	191	PRO	2.5
1	A	385	GLU	2.5
1	C	70	GLN	2.4
1	C	359	GLU	2.4
1	B	272	THR	2.4
1	C	126	THR	2.4
1	B	261	TYR	2.4
1	C	5	GLN	2.4
1	C	260	SER	2.4
1	C	15	PRO	2.4
1	C	59	GLY	2.3
1	A	355	LEU	2.3
1	C	413	LEU	2.3
1	A	51	SER	2.3
1	A	213	LEU	2.3
1	B	111	THR	2.3
1	B	58	ASN	2.3
1	B	257	SER	2.2
1	A	341	ILE	2.2
1	A	260	SER	2.2
1	B	260	SER	2.2
1	C	200	ASN	2.2
1	C	261	TYR	2.2
1	A	375	ALA	2.2
1	B	372	VAL	2.2
1	C	8	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	354	SER	2.2
1	C	66	SER	2.1
1	B	355	LEU	2.1
1	C	149	VAL	2.1
1	A	192	GLU	2.1
1	C	360	ALA	2.1
1	C	55	ARG	2.1
1	A	360	ALA	2.1
1	C	51	SER	2.1
1	C	273	GLN	2.1
1	B	299	ASN	2.0
1	A	369	ILE	2.0
1	A	64	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
3	LMT	B	1429	35/35	0.76	0.28	3.24	95,129,165,195	0
2	CL	B	1430	1/1	0.95	0.26	-0.30	25,25,25,25	0
2	CL	A	1429	1/1	0.89	0.21	-0.45	25,25,25,25	0
2	CL	C	1429	1/1	0.93	0.11	-1.38	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.