



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2016 – 06:22 AM EDT

PDB ID : 5I6C
Title : The structure of the eukaryotic purine/H⁺ symporter, UapA, in complex with Xanthine
Authors : Alguel, Y.; Amillis, S.; Leung, J.; Lambrinidis, G.; Capaldi, S.; Scull, N.J.; Craven, G.; Iwata, S.; Armstrong, A.; Mikros, E.; Dhalluin, G.; Cameron, A.D.; Byrne, B.
Deposited on : 2016-02-16
Resolution : 3.70 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
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) : rb-20027257

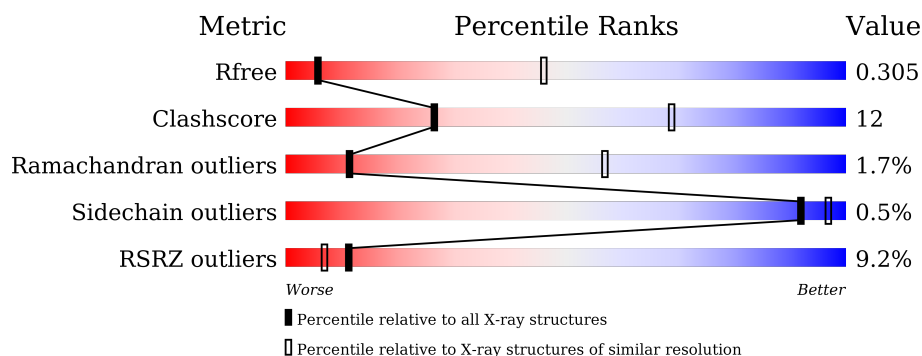
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	574	<div> <div>6%</div> <div>60% 22% • 16%</div> </div>
1	B	574	<div> <div>9%</div> <div>59% 21% • 18%</div> </div>

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
2	XAN	A	1001	-	-	-	X
2	XAN	B	1001	-	-	-	X
3	LMT	A	1002	-	-	-	X
3	LMT	A	1003	-	-	-	X
3	LMT	B	1002	-	-	-	X
3	LMT	B	1003	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7127 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.

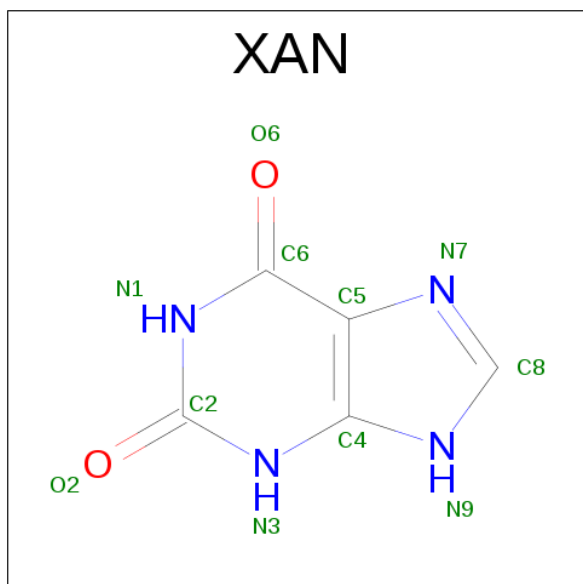
- Molecule 1 is a protein called Uric acid-xanthine permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3545	2319	565	626	35			
1	B	468	Total	C	N	O	S	0	0	0
			3434	2242	547	610	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	411	VAL	GLY	engineered mutation	UNP Q07307
B	411	VAL	GLY	engineered mutation	UNP Q07307

- Molecule 2 is XANTHINE (three-letter code: XAN) (formula: C₅H₄N₄O₂).



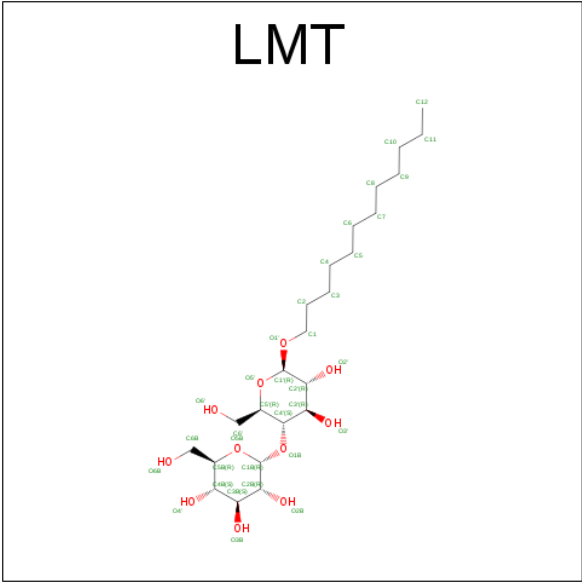
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	5	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			11	5	4	2		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).

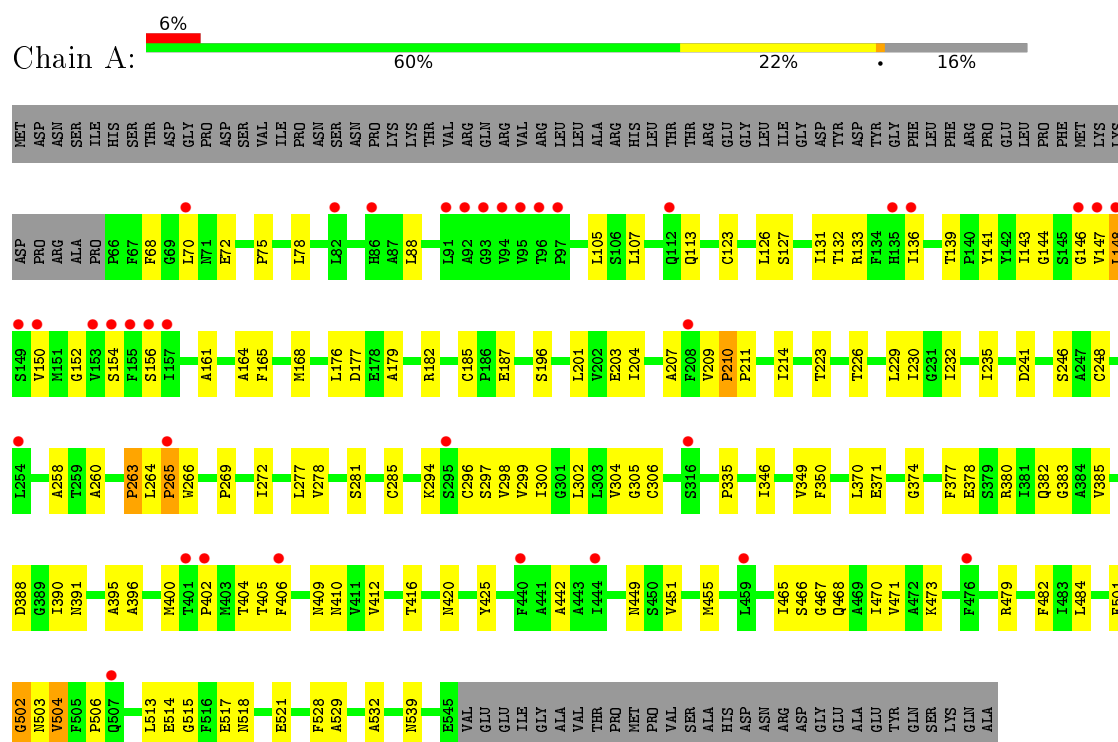


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			28	17	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			28	17	11		

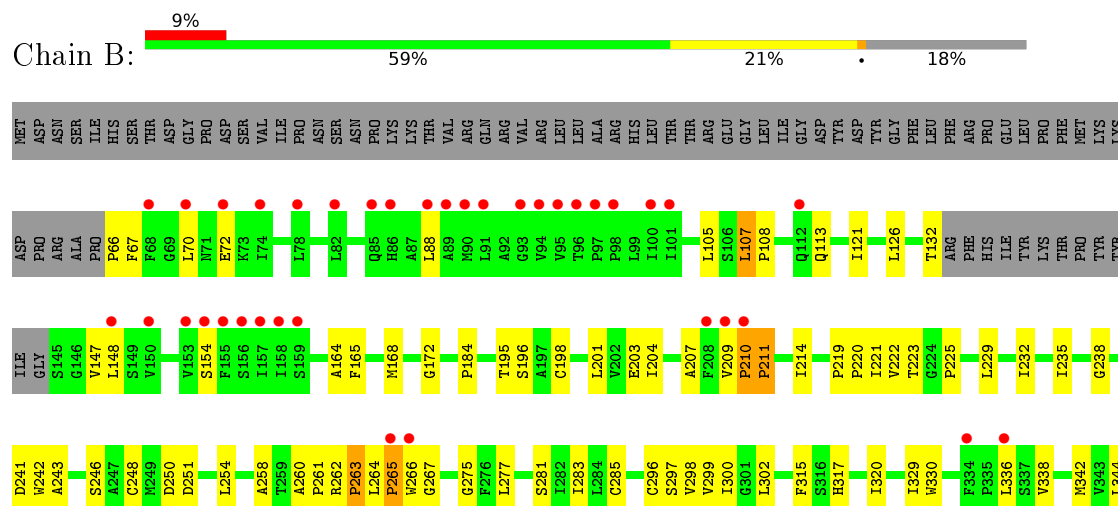
3 Residue-property plots

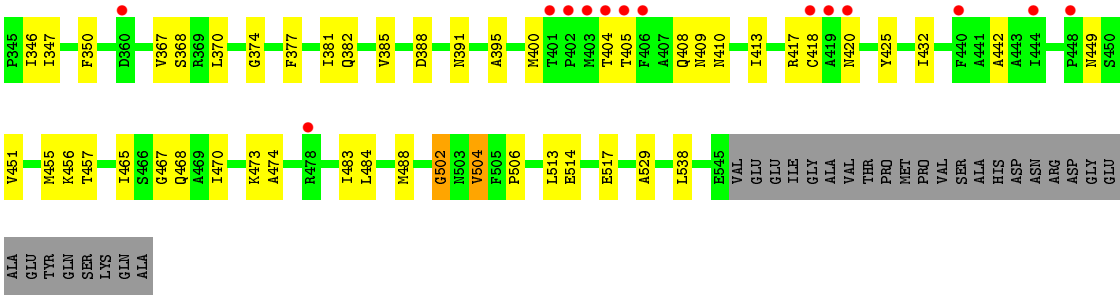
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Uric acid-xanthine permease



- Molecule 1: Uric acid-xanthine permease





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.09Å 173.83Å 82.39Å 90.00° 111.11° 90.00°	Depositor
Resolution (Å)	76.86 – 3.70 76.86 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (76.86-3.70) 97.7 (76.86-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.296 , 0.327 0.295 , 0.305	Depositor DCC
R_{free} test set	1938 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	128.3	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 71.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	7127	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

5.1 Standard geometry

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

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	0.35	0/3627	0.55	0/4949
1	B	0.34	0/3509	0.54	0/4787
All	All	0.34	0/7136	0.55	0/9736

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	3545	0	3646	91	0
1	B	3434	0	3537	89	0
2	A	11	0	4	3	0
2	B	11	0	4	2	0
3	A	63	0	72	5	0
3	B	63	0	73	4	0
All	All	7127	0	7336	176	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 12.

All (176) 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:223:THR:HG23	3:B:1002:LMT:H12	1.65	0.78
1:B:67:PHE:HA	1:B:417:ARG:HB3	1.67	0.76
1:A:223:THR:HG23	3:A:1002:LMT:H12	1.66	0.76
1:A:302:LEU:HD12	1:A:451:VAL:HG12	1.72	0.71
1:A:302:LEU:HB2	1:A:455:MET:HG3	1.74	0.70
1:A:502:GLY:HA2	1:A:506:PRO:HB3	1.74	0.70
1:A:260:ALA:HB3	1:A:263:PRO:HG3	1.74	0.69
1:A:529:ALA:HB1	3:A:1002:LMT:H122	1.74	0.69
1:B:502:GLY:HA2	1:B:506:PRO:HB3	1.74	0.69
1:A:72:GLU:O	1:A:420:ASN:ND2	2.25	0.68
1:B:201:LEU:HA	1:B:204:ILE:HG12	1.78	0.65
1:A:196:SER:HA	1:A:346:ILE:HG21	1.79	0.64
1:B:261:PRO:O	1:B:262:ARG:HG2	1.98	0.64
1:A:467:GLY:HA2	1:A:470:ILE:HD12	1.80	0.64
1:B:395:ALA:HB1	1:B:400:MET:HB2	1.81	0.63
1:B:260:ALA:HB3	1:B:263:PRO:HG3	1.81	0.62
1:A:504:VAL:HG11	1:A:513:LEU:HD23	1.82	0.62
1:B:121:ILE:HG23	1:B:432:ILE:HG23	1.82	0.61
1:B:113:GLN:HG2	1:B:442:ALA:HA	1.82	0.61
1:A:465:ILE:HD11	1:B:488:MET:HG3	1.84	0.60
1:B:126:LEU:HD13	1:B:391:ASN:HB3	1.81	0.60
1:B:88:LEU:O	1:B:299:VAL:HG21	2.02	0.60
1:B:105:LEU:HD22	1:B:165:PHE:CZ	2.37	0.59
1:A:187:GLU:HA	1:A:335:PRO:HG2	1.85	0.59
1:B:529:ALA:HB1	3:B:1002:LMT:H122	1.84	0.59
1:A:176:LEU:HD13	1:A:182:ARG:HA	1.84	0.59
1:B:164:ALA:O	1:B:168:MET:HG3	2.02	0.58
1:A:269:PRO:HA	1:A:272:ILE:HD12	1.85	0.58
1:B:66:PRO:N	1:B:417:ARG:HH11	2.01	0.58
1:B:504:VAL:HG11	1:B:513:LEU:HD23	1.85	0.58
1:B:302:LEU:HB2	1:B:455:MET:HG3	1.86	0.58
1:A:409:ASN:OD1	1:A:410:ASN:N	2.37	0.57
1:A:263:PRO:HB2	1:A:266:TRP:HB2	1.85	0.57
1:A:154:SER:HA	2:A:1001:XAN:C8	2.35	0.57
1:B:342:MET:O	1:B:346:ILE:HG12	2.05	0.57
1:A:164:ALA:O	1:A:168:MET:HG3	2.03	0.57
1:A:201:LEU:HA	1:A:204:ILE:HG12	1.86	0.57
1:B:473:LYS:NZ	3:B:1002:LMT:O2B	2.39	0.56
1:A:203:GLU:HB2	1:A:350:PHE:HB3	1.88	0.56
1:B:514:GLU:HA	1:B:517:GLU:HB3	1.88	0.56
1:B:302:LEU:HD12	1:B:451:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:SER:HA	1:B:346:ILE:HG21	1.87	0.55
1:B:70:LEU:HD22	1:B:147:VAL:HG23	1.88	0.55
1:A:70:LEU:HD22	1:A:147:VAL:HG23	1.87	0.55
1:B:132:THR:HB	1:B:425:TYR:OH	2.07	0.54
1:B:121:ILE:HA	1:B:432:ILE:HA	1.90	0.54
1:B:220:PRO:HG2	1:B:474:ALA:HB2	1.88	0.54
1:B:248:CYS:HB3	1:B:258:ALA:O	2.08	0.53
1:B:203:GLU:HB2	1:B:350:PHE:HB3	1.91	0.53
1:A:473:LYS:NZ	3:A:1002:LMT:O2B	2.41	0.53
1:A:88:LEU:O	1:A:299:VAL:HG21	2.08	0.53
1:B:207:ALA:O	1:B:382:GLN:NE2	2.29	0.53
1:A:468:GLN:NE2	1:B:468:GLN:HG3	2.24	0.52
1:B:222:VAL:O	1:B:225:PRO:HD2	2.09	0.51
1:A:229:LEU:HD12	1:A:232:ILE:HB	1.92	0.51
1:A:246:SER:O	1:A:264:LEU:HA	2.10	0.51
1:A:285:CYS:SG	1:A:297:SER:HA	2.50	0.51
1:B:72:GLU:O	1:B:420:ASN:ND2	2.43	0.51
1:A:278:VAL:HG21	1:A:451:VAL:HA	1.93	0.51
1:B:238:GLY:HA2	1:B:456:LYS:HE3	1.93	0.50
1:B:263:PRO:HB2	1:B:266:TRP:HB2	1.93	0.50
1:B:298:VAL:HG21	3:B:1003:LMT:H6'1	1.94	0.50
1:A:70:LEU:HD21	1:A:370:LEU:HD11	1.94	0.49
1:B:241:ASP:HB3	1:B:449:ASN:O	2.11	0.49
1:B:408:GLN:NE2	2:B:1001:XAN:O2	2.45	0.49
1:A:156:SER:OG	1:A:349:VAL:HG13	2.12	0.49
1:A:514:GLU:HA	1:A:517:GLU:HB3	1.94	0.49
1:B:484:LEU:O	1:B:488:MET:HG2	2.13	0.49
1:A:395:ALA:HB1	1:A:400:MET:HB2	1.94	0.48
1:A:371:GLU:HB2	1:A:380:ARG:HH22	1.78	0.48
1:B:243:ALA:O	1:B:267:GLY:HA3	2.14	0.48
1:A:264:LEU:HB2	1:A:265:PRO:HD3	1.95	0.48
1:A:136:ILE:HG13	1:A:143:ILE:HB	1.96	0.48
1:A:68:PHE:HB3	1:A:420:ASN:OD1	2.13	0.48
1:B:219:PRO:HG2	1:B:221:ILE:HG22	1.95	0.48
1:A:517:GLU:O	1:A:521:GLU:HG2	2.14	0.47
1:B:67:PHE:HZ	1:B:368:SER:HA	1.80	0.47
1:A:248:CYS:HB3	1:A:258:ALA:O	2.14	0.47
1:A:144:GLY:O	1:A:383:GLY:HA3	2.15	0.47
1:A:468:GLN:HG3	1:B:468:GLN:NE2	2.29	0.47
3:A:1002:LMT:H6E	3:A:1002:LMT:O2B	2.13	0.47
1:A:298:VAL:HG21	3:A:1003:LMT:H6'1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PRO:HA	1:B:223:THR:HB	1.96	0.47
1:A:210:PRO:O	1:A:214:ILE:HG13	2.14	0.47
1:A:154:SER:HA	2:A:1001:XAN:H8	1.97	0.47
1:B:296:CYS:O	1:B:300:ILE:N	2.35	0.47
1:B:329:ILE:HB	1:B:330:TRP:CE3	2.50	0.47
1:B:70:LEU:HD21	1:B:370:LEU:HD11	1.96	0.47
1:A:207:ALA:O	1:A:382:GLN:NE2	2.46	0.46
1:B:105:LEU:O	1:B:184:PRO:HA	2.14	0.46
1:B:107:LEU:H	1:B:108:PRO:CD	2.28	0.46
1:B:483:ILE:HG12	1:B:538:LEU:HB3	1.97	0.46
1:A:210:PRO:HG2	1:A:214:ILE:HD11	1.97	0.46
1:A:143:ILE:HG21	1:A:390:ILE:HD12	1.97	0.46
1:B:242:TRP:HZ3	1:B:457:THR:HG21	1.80	0.46
1:A:226:THR:HG23	1:A:528:PHE:HB2	1.97	0.46
1:A:294:LYS:C	1:A:296:CYS:H	2.19	0.46
1:A:176:LEU:HD12	1:A:177:ASP:H	1.80	0.46
1:B:246:SER:O	1:B:264:LEU:HA	2.16	0.46
1:A:132:THR:HB	1:A:425:TYR:OH	2.15	0.46
1:B:413:ILE:HG23	1:B:418:CYS:O	2.16	0.46
1:B:223:THR:HG22	1:B:470:ILE:HG21	1.97	0.46
1:B:70:LEU:HD11	1:B:370:LEU:HD11	1.97	0.46
1:A:306:CYS:HB2	1:A:451:VAL:HG11	1.97	0.45
1:A:501:PHE:O	1:A:503:ASN:N	2.50	0.45
1:B:467:GLY:HA2	1:B:470:ILE:HD12	1.97	0.45
1:B:242:TRP:CD1	1:B:275:GLY:HA3	2.51	0.45
1:B:126:LEU:HD22	1:B:391:ASN:OD1	2.16	0.45
1:B:385:VAL:O	1:B:388:ASP:HB3	2.17	0.45
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.65	0.45
1:A:230:ILE:HG12	1:A:528:PHE:CD2	2.52	0.45
1:A:277:LEU:O	1:A:281:SER:OG	2.17	0.45
1:A:482:PHE:HZ	1:B:283:ILE:HA	1.82	0.45
1:B:409:ASN:OD1	1:B:410:ASN:N	2.50	0.44
1:B:168:MET:HA	1:B:172:GLY:HA3	1.99	0.44
1:B:248:CYS:SG	1:B:263:PRO:HG2	2.57	0.44
1:A:154:SER:HA	2:A:1001:XAN:N9	2.33	0.44
1:A:113:GLN:HG2	1:A:442:ALA:HA	2.00	0.44
1:A:378:GLU:O	1:A:382:GLN:HG2	2.18	0.44
1:A:241:ASP:HB3	1:A:449:ASN:O	2.17	0.44
1:A:412:VAL:O	1:A:416:THR:N	2.51	0.44
1:B:154:SER:HB2	1:B:404:THR:HG22	1.99	0.44
1:A:404:THR:OG1	1:A:405:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:HB2	1:A:402:PRO:HG3	1.98	0.43
1:A:154:SER:HB2	1:A:404:THR:HG22	1.99	0.43
1:B:285:CYS:SG	1:B:297:SER:HA	2.57	0.43
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.85	0.43
1:A:133:ARG:NE	1:A:146:GLY:HA3	2.34	0.43
1:A:223:THR:HG22	1:A:470:ILE:HG21	2.00	0.43
1:B:277:LEU:O	1:B:281:SER:OG	2.19	0.43
1:A:278:VAL:HG22	1:A:305:GLY:HA3	1.99	0.43
1:B:264:LEU:HB2	1:B:265:PRO:HD3	2.01	0.43
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.81	0.43
1:A:161:ALA:HA	1:A:164:ALA:HB3	2.00	0.43
1:A:126:LEU:HB3	1:A:391:ASN:CG	2.39	0.43
1:A:300:ILE:O	1:A:304:VAL:HG23	2.19	0.43
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.89	0.43
1:A:75:PRO:O	1:A:78:LEU:N	2.52	0.43
1:B:210:PRO:HG2	1:B:214:ILE:HD11	2.00	0.43
1:A:479:ARG:NH2	1:A:539:ASN:O	2.51	0.42
1:B:229:LEU:HD12	1:B:229:LEU:HA	1.91	0.42
1:B:254:LEU:HD12	1:B:315:PHE:O	2.19	0.42
1:B:232:ILE:O	1:B:235:ILE:HG22	2.19	0.42
1:A:226:THR:OG1	1:A:532:ALA:HB2	2.20	0.42
1:B:210:PRO:N	1:B:211:PRO:HD3	2.35	0.42
1:B:381:ILE:O	1:B:385:VAL:HG23	2.19	0.42
1:A:127:SER:O	1:A:131:ILE:HG13	2.19	0.42
1:A:105:LEU:HD11	1:A:185:CYS:HB3	2.02	0.42
1:B:209:VAL:N	1:B:210:PRO:HD3	2.35	0.42
1:A:105:LEU:HD22	1:A:165:PHE:CZ	2.55	0.42
1:B:317:HIS:HA	1:B:320:ILE:HD12	2.02	0.42
1:A:385:VAL:O	1:A:388:ASP:HB3	2.19	0.42
1:B:344:LEU:HA	1:B:347:ILE:HD12	2.00	0.42
1:B:221:ILE:HA	1:B:221:ILE:HD12	1.88	0.41
1:B:250:ASP:OD1	1:B:251:ASP:N	2.44	0.41
1:B:261:PRO:C	1:B:263:PRO:HD3	2.40	0.41
1:B:456:LYS:HB2	1:B:456:LYS:HE3	1.81	0.41
1:A:396:ALA:HA	1:A:400:MET:O	2.21	0.41
1:A:150:VAL:HG12	1:A:406:PHE:HB2	2.02	0.41
1:A:467:GLY:O	1:A:471:VAL:HG23	2.20	0.41
1:B:210:PRO:O	1:B:214:ILE:HG13	2.21	0.41
1:A:374:GLY:O	1:A:377:PHE:HB3	2.21	0.41
1:B:154:SER:HA	2:B:1001:XAN:C8	2.51	0.41
1:B:195:THR:O	1:B:198:CYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:SG	1:A:152:GLY:HA2	2.60	0.41
1:A:515:GLY:O	1:A:518:ASN:HB2	2.21	0.41
1:B:336:LEU:O	1:B:338:VAL:HG23	2.21	0.41
1:A:377:PHE:O	1:A:380:ARG:HB2	2.21	0.40
1:A:468:GLN:O	1:A:471:VAL:HB	2.21	0.40
1:B:367:VAL:HG21	1:B:410:ASN:HB3	2.03	0.40
1:B:374:GLY:O	1:B:377:PHE:HB3	2.21	0.40
1:A:232:ILE:O	1:A:235:ILE:HG22	2.21	0.40
1:A:484:LEU:HB3	1:B:465:ILE:HD12	2.03	0.40
1:A:209:VAL:H	1:A:382:GLN:NE2	2.19	0.40
1:A:518:ASN:O	1:A:521:GLU:HB2	2.21	0.40
1:B:404:THR:OG1	1:B:405:THR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	478/574 (83%)	444 (93%)	25 (5%)	9 (2%)	10	55
1	B	464/574 (81%)	437 (94%)	20 (4%)	7 (2%)	13	59
All	All	942/1148 (82%)	881 (94%)	45 (5%)	16 (2%)	11	57

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PRO
1	B	210	PRO
1	B	148	LEU
1	A	139	THR
1	A	148	LEU
1	A	211	PRO

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Mol	Chain	Res	Type
1	A	263	PRO
1	A	265	PRO
1	A	502	GLY
1	B	211	PRO
1	B	263	PRO
1	B	265	PRO
1	A	179	ALA
1	B	107	LEU
1	A	107	LEU
1	B	502	GLY

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	382/464 (82%)	379 (99%)	3 (1%)	86	94
1	B	371/464 (80%)	370 (100%)	1 (0%)	94	98
All	All	753/928 (81%)	749 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	TYR
1	A	466	SER
1	A	504	VAL
1	B	504	VAL

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 ⓘ

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 ⓘ

6 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	XAN	A	1001	-	8,12,12	1.17	1 (12%)	5,17,17	3.57	4 (80%)
3	LMT	A	1002	-	36,36,36	1.18	5 (13%)	47,47,47	1.04	5 (10%)
3	LMT	A	1003	-	29,29,36	1.27	4 (13%)	40,40,47	0.95	1 (2%)
2	XAN	B	1001	-	8,12,12	1.26	1 (12%)	5,17,17	3.72	3 (60%)
3	LMT	B	1002	-	36,36,36	1.06	4 (11%)	47,47,47	1.10	4 (8%)
3	LMT	B	1003	-	29,29,36	1.27	5 (17%)	40,40,47	1.16	3 (7%)

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	XAN	A	1001	-	-	0/0/0/0	0/2/2/2
3	LMT	A	1002	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1003	-	-	0/14/54/61	0/2/2/2
2	XAN	B	1001	-	-	0/0/0/0	0/2/2/2
3	LMT	B	1002	-	-	0/21/61/61	0/2/2/2
3	LMT	B	1003	-	-	0/14/54/61	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	LMT	O3'-C3'	-2.76	1.36	1.43
3	A	1002	LMT	O3'-C3'	-2.72	1.36	1.43
3	A	1003	LMT	O2'-C2'	-2.71	1.36	1.43
3	B	1002	LMT	O3'-C3'	-2.62	1.36	1.43
3	B	1003	LMT	O3'-C3'	-2.61	1.36	1.43
2	A	1001	XAN	C5-C4	-2.53	1.34	1.40
3	A	1002	LMT	O3B-C3B	-2.37	1.37	1.43
2	B	1001	XAN	C5-C4	-2.34	1.35	1.40
3	A	1002	LMT	O2'-C2'	-2.34	1.37	1.43
3	B	1003	LMT	O2'-C2'	-2.30	1.37	1.43
3	A	1002	LMT	O4'-C4B	-2.26	1.37	1.43
3	B	1003	LMT	O4'-C4B	-2.21	1.37	1.43
3	A	1002	LMT	O2B-C2B	-2.18	1.37	1.43
3	B	1003	LMT	O3B-C3B	-2.13	1.37	1.43
3	B	1002	LMT	O2'-C2'	-2.12	1.38	1.43
3	B	1003	LMT	O2B-C2B	-2.12	1.38	1.43
3	A	1003	LMT	O2B-C2B	-2.11	1.38	1.43
3	B	1002	LMT	O4'-C4B	-2.09	1.38	1.43
3	B	1002	LMT	O3B-C3B	-2.09	1.38	1.43
3	A	1003	LMT	O4'-C4B	-2.06	1.38	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	XAN	N1-C2-N3	-4.85	119.52	127.69
2	A	1001	XAN	N1-C2-N3	-4.31	120.42	127.69
3	B	1003	LMT	C1'-O5'-C5'	-3.20	107.46	113.74
2	A	1001	XAN	C5-C6-N1	-3.03	119.56	123.52
3	B	1002	LMT	C3'-C4'-C5'	-2.81	104.42	110.85
3	A	1003	LMT	C3'-C4'-C5'	-2.57	104.98	110.85
2	B	1001	XAN	C5-C6-N1	-2.46	120.30	123.52
3	B	1003	LMT	C3'-C4'-C5'	-2.33	105.52	110.85
3	A	1002	LMT	C1'-O5'-C5'	-2.25	109.33	113.74
3	B	1002	LMT	C1'-O5'-C5'	-2.23	109.36	113.74
3	A	1002	LMT	C3'-C4'-C5'	-2.21	105.79	110.85
3	A	1002	LMT	C6B-C5B-C4B	-2.14	107.62	112.99
2	A	1001	XAN	C5-C4-N9	-2.01	107.56	111.12
3	B	1003	LMT	O1'-C1'-C2'	2.34	110.89	108.00
3	A	1002	LMT	O5B-C5B-C4B	2.43	114.30	109.67
3	A	1002	LMT	O1'-C1'-C2'	2.52	111.11	108.00
3	B	1002	LMT	O1'-C1'-C2'	2.95	111.64	108.00
3	B	1002	LMT	O5B-C5B-C4B	3.01	115.40	109.67
2	A	1001	XAN	C6-N1-C2	5.62	119.85	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1001	XAN	C6-N1-C2	5.93	120.10	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	XAN	3	0
3	A	1002	LMT	4	0
3	A	1003	LMT	1	0
2	B	1001	XAN	2	0
3	B	1002	LMT	3	0
3	B	1003	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	480/574 (83%)	0.29	36 (7%)	17 11	115, 146, 187, 212	0
1	B	468/574 (81%)	0.46	51 (10%)	7 5	127, 177, 223, 257	0
All	All	948/1148 (82%)	0.38	87 (9%)	11 7	115, 158, 212, 257	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	SER	8.0
1	B	156	SER	6.1
1	B	406	PHE	6.0
1	B	154	SER	5.8
1	B	402	PRO	5.5
1	A	93	GLY	5.3
1	A	148	LEU	5.3
1	B	94	VAL	5.0
1	B	404	THR	5.0
1	B	86	HIS	4.8
1	B	150	VAL	4.7
1	B	91	LEU	4.7
1	B	157	ILE	4.7
1	A	94	VAL	4.7
1	B	158	ILE	4.6
1	B	90	MET	4.6
1	B	100	ILE	4.6
1	A	92	ALA	4.6
1	A	96	THR	4.5
1	A	91	LEU	4.5
1	B	401	THR	4.4
1	A	86	HIS	4.2
1	B	208	PHE	4.2
1	B	155	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	265	PRO	4.1
1	A	95	VAL	4.0
1	B	70	LEU	3.8
1	B	403	MET	3.8
1	A	150	VAL	3.7
1	B	82	LEU	3.6
1	B	97	PRO	3.6
1	B	95	VAL	3.6
1	B	266	TRP	3.5
1	B	96	THR	3.3
1	B	88	LEU	3.3
1	A	440	PHE	3.3
1	B	98	PRO	3.2
1	A	153	VAL	3.2
1	B	209	VAL	3.1
1	B	112	GLN	3.0
1	B	405	THR	2.9
1	B	101	ILE	2.9
1	A	147	VAL	2.9
1	A	135	HIS	2.9
1	A	459	LEU	2.9
1	A	295	SER	2.8
1	B	85	GLN	2.8
1	A	476	PHE	2.8
1	B	153	VAL	2.8
1	A	136	ILE	2.7
1	B	74	ILE	2.6
1	A	112	GLN	2.6
1	B	418	CYS	2.6
1	B	68	PHE	2.6
1	B	360	ASP	2.6
1	A	154	SER	2.5
1	A	208	PHE	2.5
1	A	402	PRO	2.5
1	B	148	LEU	2.5
1	B	89	ALA	2.4
1	A	155	PHE	2.4
1	B	419	ALA	2.4
1	B	420	ASN	2.4
1	B	159	SER	2.4
1	A	70	LEU	2.4
1	A	507	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	157	ILE	2.3
1	A	146	GLY	2.3
1	B	444	ILE	2.3
1	A	444	ILE	2.3
1	A	156	SER	2.3
1	A	265	PRO	2.2
1	B	210	PRO	2.2
1	B	334	PHE	2.2
1	B	440	PHE	2.2
1	B	448	PRO	2.2
1	B	478	ARG	2.2
1	A	97	PRO	2.2
1	A	254	LEU	2.2
1	B	336	LEU	2.1
1	A	406	PHE	2.1
1	A	82	LEU	2.1
1	B	93	GLY	2.1
1	A	401	THR	2.1
1	B	72	GLU	2.1
1	B	78	LEU	2.1
1	A	316	SER	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, 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(Å ²)	Q<0.9
3	LMT	B	1002	35/35	0.77	1.22	8.23	160,195,206,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	LMT	A	1002	35/35	0.86	0.70	4.95	122,149,162,162	0
3	LMT	A	1003	28/35	0.91	0.76	1.34	115,142,162,169	0
3	LMT	B	1003	28/35	0.92	0.58	0.90	136,151,167,169	0
2	XAN	A	1001	11/11	0.90	0.52	0.01	119,119,129,129	0
2	XAN	B	1001	11/11	0.92	0.65	-0.13	158,160,161,162	0

6.5 Other polymers [i](#)

There are no such residues in this entry.