Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:28 AM GMT

PDB ID	:	2QUI
Title	:	Crystal structures of human tryptophanyl-tRNA synthetase in complex with Tryptophanamide and ATP
Authors	:	Shen, N.; Ding, J.P.
Deposited on	:	2007-08-05
Resolution	:	2.40 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:

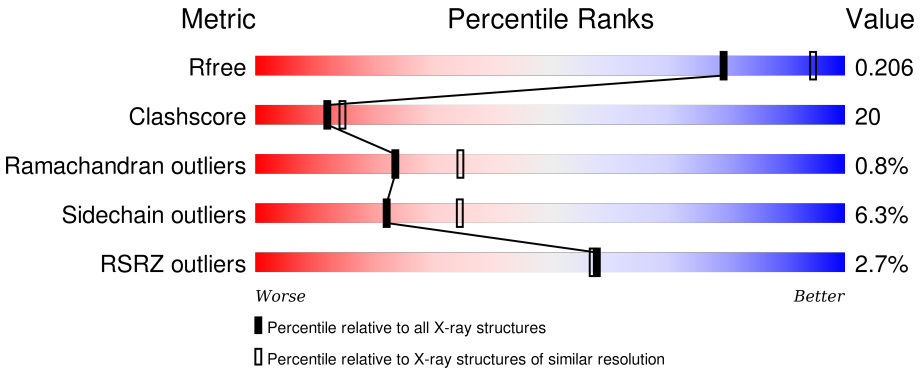
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	477	3% 54% 25% · 18%
1	B	477	% 49% 27% · 21%

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
4	ATP	A	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6469 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 Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3127	2005	525	582	15			
1	B	379	Total	C	N	O	S	0	0	0
			3054	1960	519	560	15			

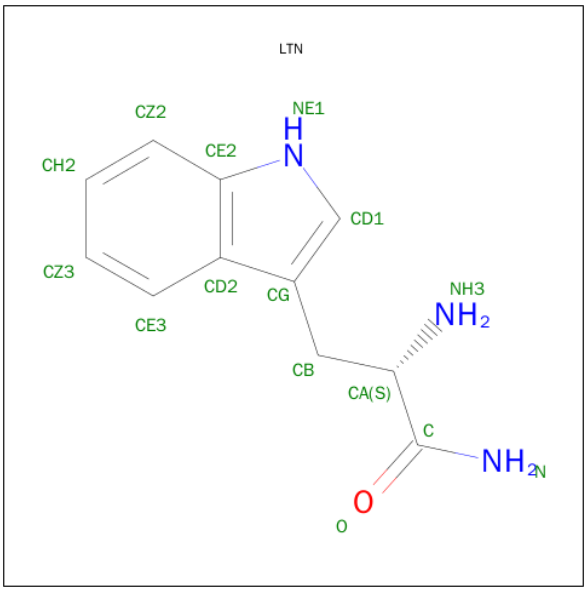
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	472	HIS	-	EXPRESSION TAG	UNP P23381
A	473	HIS	-	EXPRESSION TAG	UNP P23381
A	474	HIS	-	EXPRESSION TAG	UNP P23381
A	475	HIS	-	EXPRESSION TAG	UNP P23381
A	476	HIS	-	EXPRESSION TAG	UNP P23381
A	477	HIS	-	EXPRESSION TAG	UNP P23381
B	472	HIS	-	EXPRESSION TAG	UNP P23381
B	473	HIS	-	EXPRESSION TAG	UNP P23381
B	474	HIS	-	EXPRESSION TAG	UNP P23381
B	475	HIS	-	EXPRESSION TAG	UNP P23381
B	476	HIS	-	EXPRESSION TAG	UNP P23381
B	477	HIS	-	EXPRESSION TAG	UNP P23381

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

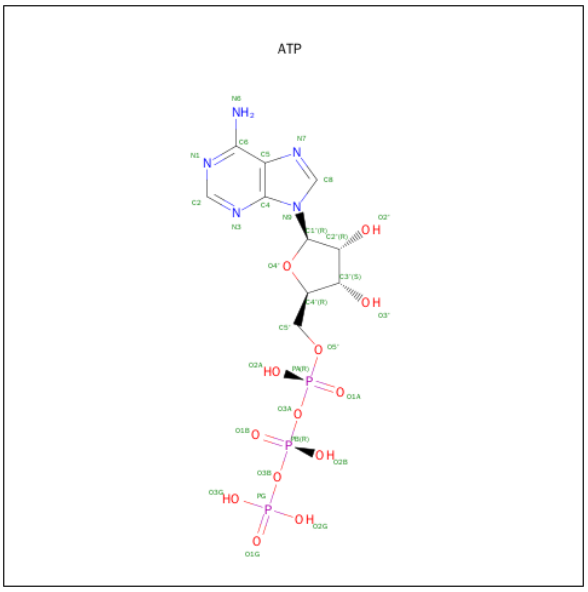
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is L-TRYPTOPHANAMIDE (three-letter code: LTN) (formula: $C_{11}H_{13}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	3	1		
3	B	1	Total	C	N	O	0	0
			15	11	3	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

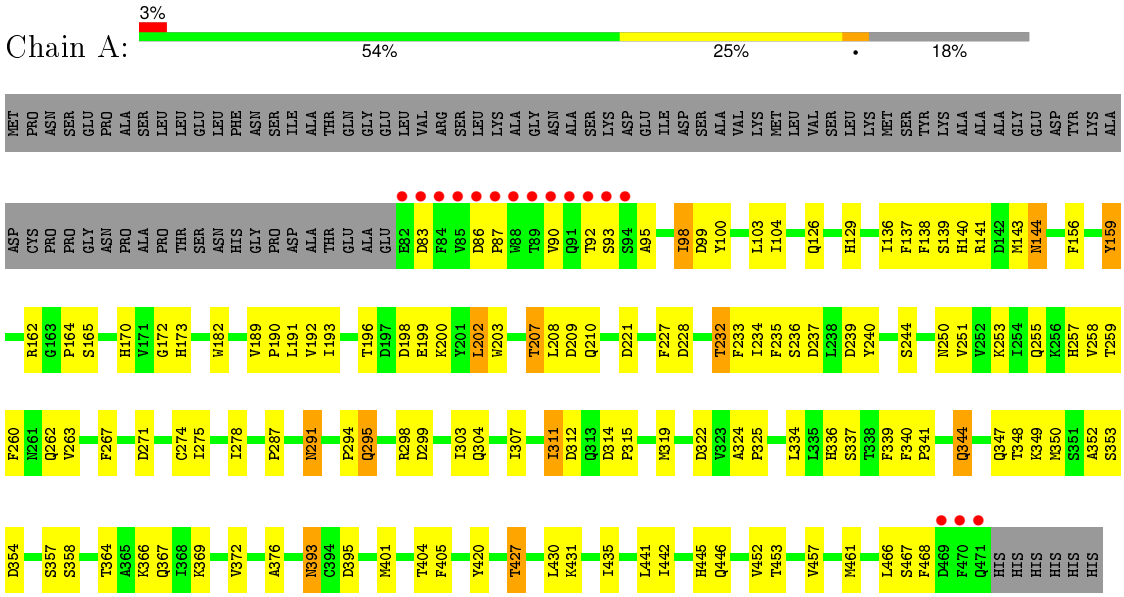
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	120	Total O 120 120	0	0
5	B	106	Total O 106 106	0	0

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.

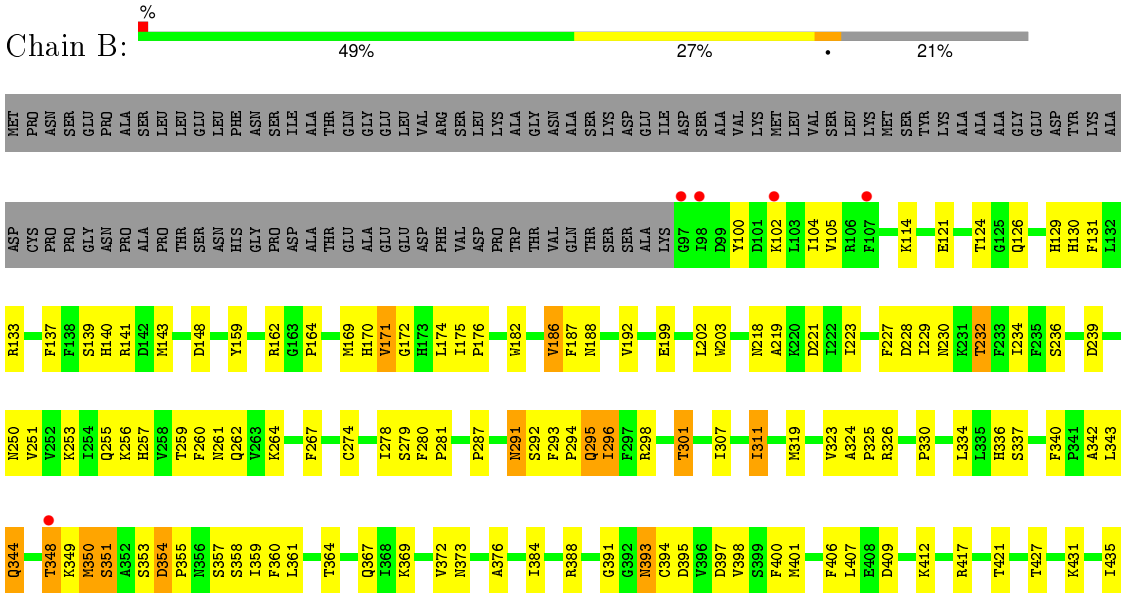
- Molecule 1: Tryptophanyl-tRNA synthetase

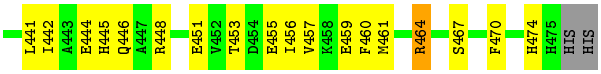
Chain A:



- Molecule 1: Tryptophanyl-tRNA synthetase

Chain B:




L441
T442
A443
E444
H445
Q446
A447
R448
E451
Y452
T453
D454
E455
I456
V457
K458
E459
F460
M461
R464
S467
F470
H474
H475
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	79.70Å 79.70Å 383.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.57 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.40) 95.1 (48.57-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.238 0.214 , 0.206	Depositor DCC
R_{free} test set	2405 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 47603 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6469	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: MG, LTN, ATP

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	0.38	0/3204	0.61	0/4331
1	B	0.39	0/3132	0.61	0/4230
All	All	0.38	0/6336	0.61	0/8561

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	3127	0	3049	123	0
1	B	3054	0	2978	126	0
2	A	1	0	0	0	0
3	A	15	0	11	1	0
3	B	15	0	11	1	0
4	A	31	0	12	10	0
5	A	120	0	0	8	0
5	B	106	0	0	4	0
All	All	6469	0	6061	244	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 20.

All (244) 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:250:ASN:HD21	1:B:291:ASN:ND2	1.59	0.98
1:A:207:THR:HG22	1:A:210:GLN:H	1.35	0.90
1:A:165:SER:HB2	4:A:502:ATP:O3G	1.73	0.88
1:A:250:ASN:HD21	1:A:291:ASN:ND2	1.73	0.87
1:A:344:GLN:HE22	1:A:357:SER:HA	1.40	0.87
1:A:98:ILE:HD11	1:A:103:LEU:HD22	1.61	0.83
1:B:250:ASN:HD21	1:B:291:ASN:HD21	1.27	0.80
1:A:227:PHE:HB3	1:A:232:THR:HG21	1.64	0.79
1:A:251:VAL:O	1:A:255:GLN:HG3	1.83	0.79
1:B:260:PHE:HE1	1:B:278:ILE:HD12	1.47	0.79
1:B:227:PHE:HB3	1:B:232:THR:HG21	1.65	0.78
1:A:250:ASN:HD21	1:A:291:ASN:HD21	1.30	0.78
1:B:409:ASP:OD2	1:B:412:LYS:HB2	1.85	0.77
1:B:293:PHE:HB3	1:B:296:ILE:HG23	1.65	0.77
1:B:129:HIS:HD2	1:B:131:PHE:H	1.30	0.77
1:A:141:ARG:HD2	1:A:334:LEU:HD12	1.65	0.76
1:A:92:THR:HG21	1:A:98:ILE:HA	1.67	0.76
1:B:372:VAL:HG12	1:B:431:LYS:HG3	1.66	0.76
1:B:293:PHE:HA	1:B:295:GLN:HE22	1.52	0.73
1:A:352:ALA:C	1:A:354:ASP:H	1.91	0.73
1:A:159:TYR:CZ	1:A:287:PRO:HG2	2.24	0.72
1:B:129:HIS:CD2	1:B:131:PHE:H	2.07	0.72
1:B:140:HIS:HD2	1:B:143:MET:H	1.35	0.72
1:A:307:ILE:HB	1:A:334:LEU:HD23	1.72	0.71
1:B:159:TYR:CZ	1:B:287:PRO:HG2	2.25	0.71
1:B:228:ASP:O	1:B:232:THR:HG23	1.91	0.70
1:A:364:THR:OG1	1:A:367:GLN:HG3	1.92	0.70
1:A:137:PHE:CZ	1:A:337:SER:HB3	2.27	0.69
1:A:228:ASP:O	1:A:232:THR:HG23	1.92	0.69
1:A:427:THR:HG21	5:A:597:HOH:O	1.92	0.69
1:B:455:GLU:CD	1:B:455:GLU:H	1.96	0.69
1:A:95:ALA:HA	1:A:347:GLN:HE21	1.56	0.69
1:B:393:ASN:C	1:B:393:ASN:HD22	1.97	0.68
1:A:253:LYS:O	1:A:257:HIS:HD2	1.78	0.66
1:A:376:ALA:HB3	1:A:431:LYS:HE2	1.78	0.66
1:B:324:ALA:HB3	1:B:325:PRO:HD3	1.77	0.66
1:B:307:ILE:HB	1:B:334:LEU:HD23	1.79	0.65
1:A:164:PRO:HG2	5:A:619:HOH:O	1.96	0.65
1:A:140:HIS:HD2	1:A:143:MET:H	1.45	0.65
1:B:137:PHE:CZ	1:B:337:SER:HB3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:HB3	1:B:261:ASN:ND2	2.12	0.64
1:A:466:LEU:O	1:A:468:PHE:N	2.30	0.64
1:A:202:LEU:HA	1:B:256:LYS:HD3	1.80	0.64
1:B:140:HIS:CD2	1:B:143:MET:H	2.15	0.64
1:A:344:GLN:HE22	1:A:357:SER:CA	2.11	0.63
1:B:234:ILE:O	1:B:461:MET:HA	1.98	0.63
1:B:253:LYS:O	1:B:257:HIS:HD2	1.81	0.62
1:B:376:ALA:HB3	1:B:431:LYS:HE2	1.81	0.62
1:B:259:THR:OG1	1:B:262:GLN:HG3	1.99	0.62
1:B:442:ILE:O	1:B:446:GLN:HG3	1.99	0.62
1:B:294:PRO:HD2	1:B:295:GLN:NE2	2.15	0.62
1:A:207:THR:CG2	1:A:210:GLN:H	2.11	0.61
1:A:207:THR:HG22	1:A:210:GLN:HG3	1.81	0.61
1:B:295:GLN:H	1:B:295:GLN:NE2	1.99	0.60
1:A:303:ILE:HD12	1:A:303:ILE:N	2.16	0.60
1:A:340:PHE:HB3	4:A:502:ATP:HN62	1.67	0.60
1:B:260:PHE:CE1	1:B:278:ILE:HD12	2.32	0.60
1:A:350:MET:HG3	1:A:358:SER:HB3	1.83	0.59
1:B:169:MET:HE1	1:B:218:ASN:HA	1.82	0.59
1:B:393:ASN:ND2	1:B:395:ASP:H	2.01	0.59
1:A:350:MET:CG	1:A:358:SER:HB3	2.32	0.59
1:B:359:ILE:HD12	1:B:359:ILE:N	2.18	0.59
1:A:372:VAL:HG12	1:A:431:LYS:HG3	1.85	0.58
1:A:86:ASP:HB2	1:A:87:PRO:HD2	1.85	0.58
1:B:350:MET:O	1:B:351:SER:HB2	2.04	0.58
1:B:124:THR:CG2	1:B:186:VAL:HG13	2.34	0.58
1:A:139:SER:HB3	1:A:336:HIS:HB2	1.86	0.57
1:B:311:ILE:HG23	1:B:336:HIS:HB3	1.86	0.57
1:B:174:LEU:HD11	1:B:361:LEU:HD11	1.86	0.57
1:A:259:THR:HG23	1:A:262:GLN:HE21	1.69	0.57
1:B:170:HIS:HD2	1:B:172:GLY:H	1.53	0.56
1:B:294:PRO:HD2	1:B:295:GLN:HE21	1.70	0.56
1:A:341:PRO:HA	5:A:551:HOH:O	2.05	0.55
1:B:121:GLU:HG3	1:B:126:GLN:O	2.06	0.55
1:B:169:MET:CE	1:B:218:ASN:HA	2.37	0.55
1:A:90:VAL:HG21	1:A:349:LYS:HD3	1.89	0.54
1:A:162:ARG:O	1:A:164:PRO:HD3	2.08	0.54
1:B:124:THR:HG21	1:B:186:VAL:CG1	2.37	0.54
1:A:442:ILE:O	1:A:446:GLN:HG3	2.06	0.54
1:A:258:VAL:HG11	1:A:319:MET:HE2	1.90	0.54
1:A:207:THR:HG23	1:A:209:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLU:HB2	1:B:280:PHE:CE1	2.43	0.53
1:A:366:LYS:HB2	5:A:546:HOH:O	2.08	0.53
1:B:293:PHE:HB3	1:B:296:ILE:CG2	2.35	0.53
1:A:98:ILE:CD1	1:A:103:LEU:HD22	2.34	0.53
1:A:350:MET:HB3	4:A:502:ATP:HN61	1.74	0.52
1:A:453:THR:O	1:A:457:VAL:HG23	2.08	0.52
1:B:393:ASN:HD22	1:B:394:CYS:N	2.07	0.52
1:B:171:VAL:HG22	1:B:406:PHE:CZ	2.44	0.52
1:B:221:ASP:OD2	1:B:445:HIS:HE1	1.92	0.52
1:A:401:MET:O	1:A:404:THR:HB	2.09	0.52
1:B:259:THR:H	1:B:262:GLN:NE2	2.08	0.52
1:B:139:SER:HB3	1:B:336:HIS:HB2	1.92	0.52
1:A:95:ALA:HA	1:A:347:GLN:NE2	2.24	0.52
1:B:343:LEU:HG	1:B:358:SER:HA	1.91	0.52
1:B:251:VAL:O	1:B:255:GLN:HG3	2.09	0.52
1:B:219:ALA:O	1:B:223:ILE:HG13	2.10	0.52
1:B:340:PHE:O	1:B:350:MET:HE2	2.10	0.51
1:A:136:ILE:HD11	1:A:404:THR:HG22	1.91	0.51
1:A:259:THR:H	1:A:262:GLN:NE2	2.09	0.51
1:B:393:ASN:C	1:B:393:ASN:ND2	2.62	0.51
1:A:234:ILE:O	1:A:461:MET:HA	2.10	0.51
1:B:170:HIS:HD2	1:B:172:GLY:N	2.08	0.51
1:A:228:ASP:O	1:A:232:THR:CG2	2.59	0.51
1:A:349:LYS:HA	5:A:551:HOH:O	2.11	0.51
4:A:502:ATP:H5'1	5:A:622:HOH:O	2.12	0.50
1:A:90:VAL:HG21	1:A:339:PHE:CE1	2.45	0.50
1:A:170:HIS:HD2	1:A:172:GLY:N	2.10	0.50
1:A:303:ILE:HD12	1:A:303:ILE:H	1.76	0.50
1:A:192:VAL:HG13	1:A:235:PHE:HE1	1.77	0.50
1:B:260:PHE:CE2	1:B:264:LYS:HD2	2.47	0.50
1:A:393:ASN:ND2	1:A:395:ASP:H	2.10	0.50
3:A:501:LTN:N	4:A:502:ATP:H4'	2.27	0.49
1:A:350:MET:HB3	4:A:502:ATP:N6	2.27	0.49
1:A:344:GLN:NE2	1:A:357:SER:HB2	2.26	0.49
1:A:87:PRO:HG3	1:A:315:PRO:HG2	1.94	0.49
1:A:452:VAL:CG2	1:A:452:VAL:O	2.60	0.49
1:B:355:PRO:HA	1:B:360:PHE:CE2	2.47	0.49
1:A:352:ALA:C	1:A:354:ASP:N	2.60	0.49
1:A:86:ASP:HB2	1:A:87:PRO:CD	2.43	0.49
1:B:364:THR:OG1	1:B:367:GLN:HG3	2.13	0.49
1:B:354:ASP:OD2	1:B:357:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:HG21	1:A:98:ILE:CA	2.38	0.49
1:B:296:ILE:HD12	1:B:296:ILE:O	2.13	0.49
1:A:259:THR:HA	1:B:274:CYS:HA	1.93	0.49
1:B:139:SER:OG	1:B:336:HIS:HD2	1.96	0.49
1:A:196:THR:HB	1:A:199:GLU:HB2	1.94	0.48
1:B:342:ALA:HA	1:B:350:MET:HG2	1.94	0.48
1:B:369:LYS:HA	1:B:435:ILE:HD13	1.94	0.48
1:B:358:SER:HB3	5:B:480:HOH:O	2.13	0.48
1:B:124:THR:HG21	1:B:186:VAL:HG13	1.96	0.48
1:B:102:LYS:O	1:B:105:VAL:HG12	2.14	0.48
1:B:464:ARG:NH1	5:B:509:HOH:O	2.46	0.48
1:A:86:ASP:OD2	1:A:86:ASP:N	2.46	0.48
1:B:250:ASN:ND2	1:B:291:ASN:HD21	2.03	0.47
1:A:324:ALA:N	1:A:325:PRO:HD2	2.29	0.47
1:A:221:ASP:OD1	1:A:445:HIS:HE1	1.97	0.47
1:B:398:VAL:HA	1:B:401:MET:HE3	1.95	0.47
1:A:87:PRO:HG2	1:A:267:PHE:HD2	1.80	0.47
1:A:198:ASP:O	1:A:202:LEU:HD22	2.14	0.47
1:A:100:TYR:O	1:A:104:ILE:HG13	2.14	0.47
1:A:312:ASP:OD2	4:A:502:ATP:O2'	2.31	0.46
1:B:441:LEU:HD22	1:B:442:ILE:HD12	1.97	0.46
1:A:87:PRO:HD3	1:A:315:PRO:HG3	1.98	0.46
1:B:267:PHE:HE1	1:B:319:MET:HE3	1.81	0.46
1:A:207:THR:CG2	1:A:210:GLN:HG3	2.46	0.46
1:A:137:PHE:CE2	1:A:337:SER:HB3	2.51	0.46
1:A:144:ASN:HB3	5:A:506:HOH:O	2.15	0.46
1:B:255:GLN:HE21	1:B:279:SER:HB2	1.80	0.46
1:B:448:ARG:HA	1:B:451:GLU:OE2	2.16	0.46
1:A:141:ARG:HB2	1:A:334:LEU:HB2	1.96	0.46
1:A:344:GLN:NE2	1:A:357:SER:CB	2.79	0.45
1:B:267:PHE:CE1	1:B:319:MET:HE3	2.51	0.45
1:B:391:GLY:HA3	1:B:421:THR:O	2.16	0.45
1:B:330:PRO:HD2	5:B:515:HOH:O	2.16	0.45
1:B:384:ILE:HG13	5:B:567:HOH:O	2.17	0.45
1:B:384:ILE:O	1:B:388:ARG:HG2	2.16	0.45
1:B:170:HIS:CD2	1:B:172:GLY:H	2.34	0.45
1:B:293:PHE:N	1:B:294:PRO:HD3	2.31	0.45
1:B:394:CYS:HB3	1:B:400:PHE:CD2	2.51	0.45
1:B:174:LEU:CD1	1:B:361:LEU:HD11	2.45	0.45
1:A:393:ASN:HD22	1:A:393:ASN:C	2.19	0.45
1:A:294:PRO:HG2	1:A:295:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASN:HD21	1:B:395:ASP:HB2	1.82	0.45
1:B:169:MET:CE	1:B:221:ASP:HB2	2.47	0.45
1:A:233:PHE:CZ	1:A:235:PHE:HB3	2.52	0.45
1:B:250:ASN:ND2	1:B:291:ASN:ND2	2.44	0.45
1:A:207:THR:HG23	1:A:209:ASP:N	2.30	0.45
1:A:352:ALA:O	1:A:354:ASP:N	2.49	0.45
1:A:441:LEU:C	1:A:441:LEU:HD23	2.37	0.45
1:B:453:THR:OG1	1:B:455:GLU:HG2	2.18	0.44
1:A:260:PHE:HA	1:A:263:VAL:HG22	1.99	0.44
1:A:274:CYS:HA	1:B:259:THR:HA	1.99	0.44
1:B:199:GLU:HB2	1:B:280:PHE:CZ	2.53	0.44
1:B:453:THR:H	1:B:456:ILE:HD12	1.83	0.44
1:B:141:ARG:HD2	1:B:334:LEU:HD12	1.99	0.44
1:A:100:TYR:HB3	1:A:138:PHE:CE2	2.52	0.44
1:A:126:GLN:HG2	5:A:514:HOH:O	2.17	0.44
1:A:311:ILE:HD13	1:A:311:ILE:O	2.17	0.44
1:A:140:HIS:CD2	1:A:143:MET:H	2.29	0.44
1:B:359:ILE:CD1	1:B:359:ILE:N	2.81	0.44
1:A:275:ILE:HG22	1:B:278:ILE:HG22	2.00	0.43
1:A:200:LYS:HD3	1:A:200:LYS:HA	1.77	0.43
1:B:124:THR:HB	1:B:186:VAL:HG13	1.99	0.43
1:B:298:ARG:HD2	1:B:470:PHE:O	2.18	0.43
1:A:141:ARG:NH1	1:A:314:ASP:OD2	2.51	0.43
1:B:294:PRO:CD	1:B:295:GLN:NE2	2.82	0.43
1:A:420:TYR:HE1	1:A:427:THR:HA	1.83	0.43
1:B:453:THR:OG1	1:B:456:ILE:HG13	2.18	0.43
1:A:348:THR:HG22	1:A:349:LYS:N	2.33	0.43
1:B:397:ASP:C	1:B:401:MET:HE2	2.38	0.43
1:A:92:THR:HG22	1:A:93:SER:N	2.34	0.43
1:A:267:PHE:HE1	1:A:319:MET:HE3	1.83	0.43
1:B:100:TYR:O	1:B:104:ILE:HG13	2.19	0.43
1:A:159:TYR:O	1:A:307:ILE:HG23	2.19	0.43
1:B:455:GLU:CD	1:B:455:GLU:N	2.70	0.42
1:A:129:HIS:HB2	1:A:182:TRP:CD2	2.54	0.42
1:B:175:ILE:HB	1:B:176:PRO:CD	2.49	0.42
1:B:229:ILE:HD11	1:B:459:GLU:HB3	2.00	0.42
1:A:83:ASP:OD2	1:A:99:ASP:N	2.43	0.42
1:B:373:ASN:HD22	1:B:431:LYS:HG2	1.83	0.42
1:B:159:TYR:CZ	3:B:478:LTN:HZ2	2.55	0.42
1:B:441:LEU:CD2	1:B:442:ILE:HD12	2.48	0.42
1:B:323:VAL:HG12	1:B:326:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:SER:OG	1:A:336:HIS:HD2	2.03	0.42
1:B:130:HIS:HB3	1:B:133:ARG:NH2	2.35	0.42
1:B:159:TYR:CE2	1:B:287:PRO:HG2	2.54	0.42
1:A:259:THR:OG1	1:A:262:GLN:HG3	2.20	0.42
1:A:348:THR:HG22	1:A:349:LYS:O	2.20	0.42
1:A:196:THR:HB	1:A:199:GLU:CB	2.49	0.42
1:B:348:THR:OG1	1:B:349:LYS:N	2.53	0.42
1:B:126:GLN:HG3	1:B:186:VAL:HG22	2.01	0.42
1:B:351:SER:C	1:B:353:SER:H	2.23	0.42
1:A:137:PHE:CE1	1:A:337:SER:HB3	2.54	0.42
1:A:334:LEU:HD13	1:A:336:HIS:HE1	1.85	0.41
1:A:191:LEU:HD21	1:A:193:ILE:HD11	2.01	0.41
1:A:271:ASP:HB3	1:B:261:ASN:HD21	1.85	0.41
1:B:344:GLN:H	1:B:344:GLN:CD	2.23	0.41
1:A:162:ARG:NH1	4:A:502:ATP:O1G	2.50	0.41
1:A:344:GLN:HE21	1:A:357:SER:HB2	1.85	0.41
1:B:186:VAL:HG12	1:B:187:PHE:CD1	2.55	0.41
1:A:198:ASP:OD2	1:A:237:ASP:HB3	2.19	0.41
1:A:340:PHE:HB3	4:A:502:ATP:N6	2.34	0.41
1:B:182:TRP:CZ2	1:B:186:VAL:HG21	2.55	0.41
1:B:280:PHE:N	1:B:281:PRO:CD	2.83	0.41
1:A:240:TYR:CZ	1:A:244:SER:HB2	2.56	0.41
1:B:417:ARG:HG2	1:B:417:ARG:HH11	1.86	0.41
1:A:278:ILE:CD1	1:B:260:PHE:HB2	2.50	0.41
1:B:259:THR:HG23	1:B:262:GLN:HE21	1.84	0.41
1:A:369:LYS:HG3	1:A:435:ILE:HD13	2.03	0.41
1:B:230:ASN:HB3	1:B:467:SER:OG	2.20	0.41
1:A:173:HIS:CE1	4:A:502:ATP:O2G	2.74	0.41
1:A:136:ILE:HD13	1:A:405:PHE:CD2	2.56	0.41
1:A:189:VAL:HB	1:A:190:PRO:HD2	2.02	0.41
1:B:457:VAL:HG12	1:B:461:MET:CE	2.51	0.40
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.95	0.40
1:A:156:PHE:HB2	1:A:304:GLN:HB3	2.03	0.40
1:B:301:THR:HG23	1:B:301:THR:O	2.21	0.40
1:A:344:GLN:NE2	1:A:357:SER:HA	2.22	0.40
1:B:229:ILE:HA	1:B:460:PHE:CE1	2.57	0.40
1:B:162:ARG:O	1:B:164:PRO:HD3	2.21	0.40
1:B:292:SER:C	1:B:294:PRO:HD3	2.41	0.40
1:B:129:HIS:HB2	1:B:182:TRP:CD2	2.56	0.40
1:B:169:MET:HE1	1:B:221:ASP:HB2	2.03	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	388/477 (81%)	366 (94%)	18 (5%)	4 (1%)	19 28
1	B	377/477 (79%)	359 (95%)	16 (4%)	2 (0%)	34 48
All	All	765/954 (80%)	725 (95%)	34 (4%)	6 (1%)	24 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	B	351	SER
1	A	298	ARG
1	A	353	SER
1	B	350	MET
1	A	299	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	340/416 (82%)	323 (95%)	17 (5%)	30 48
1	B	331/416 (80%)	306 (92%)	25 (8%)	16 25
All	All	671/832 (81%)	629 (94%)	42 (6%)	22 35

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	144	ASN
1	A	159	TYR
1	A	202	LEU
1	A	203	TRP
1	A	207	THR
1	A	232	THR
1	A	236	SER
1	A	239	ASP
1	A	291	ASN
1	A	295	GLN
1	A	311	ILE
1	A	322	ASP
1	A	344	GLN
1	A	393	ASN
1	A	427	THR
1	A	430	LEU
1	B	114	LYS
1	B	148	ASP
1	B	171	VAL
1	B	186	VAL
1	B	188	ASN
1	B	192	VAL
1	B	202	LEU
1	B	203	TRP
1	B	232	THR
1	B	236	SER
1	B	239	ASP
1	B	291	ASN
1	B	295	GLN
1	B	296	ILE
1	B	301	THR
1	B	311	ILE
1	B	344	GLN
1	B	348	THR
1	B	354	ASP
1	B	393	ASN
1	B	407	LEU
1	B	427	THR
1	B	444	GLU
1	B	464	ARG
1	B	474	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	257	HIS
1	A	262	GLN
1	A	291	ASN
1	A	295	GLN
1	A	336	HIS
1	A	344	GLN
1	A	347	GLN
1	A	393	ASN
1	A	445	HIS
1	B	129	HIS
1	B	140	HIS
1	B	145	GLN
1	B	170	HIS
1	B	188	ASN
1	B	255	GLN
1	B	257	HIS
1	B	261	ASN
1	B	262	GLN
1	B	291	ASN
1	B	295	GLN
1	B	304	GLN
1	B	336	HIS
1	B	344	GLN
1	B	356	ASN
1	B	373	ASN
1	B	393	ASN
1	B	445	HIS
1	B	471	GLN
1	B	474	HIS

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)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	LTN	A	501	-	15,16,16	3.04	8 (53%)	13,22,22	1.64	3 (23%)
4	ATP	A	502	-	24,33,33	1.03	1 (4%)	31,52,52	2.26	7 (22%)
3	LTN	B	478	-	15,16,16	3.10	8 (53%)	13,22,22	1.71	3 (23%)

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	LTN	A	501	-	-	0/6/8/8	0/2/2/2
4	ATP	A	502	-	-	0/18/38/38	0/3/3/3
3	LTN	B	478	-	-	0/6/8/8	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	478	LTN	C-N	-5.48	1.22	1.32
3	A	501	LTN	C-N	-5.43	1.22	1.32
3	A	501	LTN	CE2-NE1	-2.18	1.31	1.38
3	B	478	LTN	CD1-NE1	-2.14	1.32	1.36
3	B	478	LTN	CE2-NE1	-2.02	1.32	1.38
3	A	501	LTN	CD1-NE1	-2.02	1.32	1.36
3	A	501	LTN	CZ2-CE2	2.07	1.45	1.41
3	B	478	LTN	CZ2-CE2	2.13	1.45	1.41
4	A	502	ATP	O4'-C1'	2.43	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	478	LTN	CH2-CZ3	2.72	1.45	1.38
3	A	501	LTN	CH2-CZ3	2.77	1.45	1.38
3	A	501	LTN	CZ3-CE3	3.05	1.43	1.36
3	B	478	LTN	CZ3-CE3	3.22	1.44	1.36
3	A	501	LTN	CH2-CZ2	3.70	1.45	1.36
3	B	478	LTN	CH2-CZ2	3.88	1.45	1.36
3	A	501	LTN	O-C	7.92	1.38	1.23
3	B	478	LTN	O-C	8.09	1.38	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	ATP	N3-C2-N1	-9.37	121.72	128.89
4	A	502	ATP	PA-O3A-PB	-4.61	119.79	132.73
3	B	478	LTN	O-C-N	-3.74	117.53	123.08
3	A	501	LTN	O-C-N	-3.68	117.63	123.08
4	A	502	ATP	PB-O3B-PG	-3.56	120.74	132.67
3	B	478	LTN	CB-CG-CD1	-3.35	123.82	127.97
3	A	501	LTN	CB-CG-CD1	-2.81	124.49	127.97
4	A	502	ATP	C2'-C1'-N9	-2.72	110.14	114.29
4	A	502	ATP	C4'-O4'-C1'	-2.48	106.99	109.72
4	A	502	ATP	C4-C5-N7	-2.14	107.51	109.48
4	A	502	ATP	O4'-C1'-N9	2.13	112.57	108.10
3	B	478	LTN	CA-C-N	3.00	121.44	116.62
3	A	501	LTN	CA-C-N	3.15	121.69	116.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	LTN	1	0
4	A	502	ATP	10	0
3	B	478	LTN	1	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	390/477 (81%)	0.09	16 (4%) 41 42	33, 46, 93, 179	0
1	B	379/477 (79%)	-0.27	5 (1%) 79 79	33, 48, 69, 92	0
All	All	769/954 (80%)	-0.09	21 (2%) 58 57	33, 47, 80, 179	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	ASP	12.3
1	A	89	THR	10.4
1	A	88	TRP	10.2
1	A	92	THR	8.5
1	A	84	PHE	7.6
1	A	82	GLU	7.5
1	A	93	SER	6.9
1	A	85	VAL	6.6
1	A	90	VAL	6.4
1	A	470	PHE	5.8
1	A	87	PRO	5.2
1	A	471	GLN	4.7
1	A	91	GLN	4.3
1	A	83	ASP	3.6
1	B	98	ILE	3.5
1	B	97	GLY	3.3
1	A	94	SER	3.2
1	A	469	ASP	2.7
1	B	348	THR	2.5
1	B	107	PHE	2.5
1	B	102	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LTN	B	478	15/15	0.97	0.14	1.19	41,44,45,49	0
4	ATP	A	502	31/31	0.75	0.34	1.01	118,121,140,141	0
3	LTN	A	501	15/15	0.96	0.23	0.10	37,40,42,42	0
2	MG	A	500	1/1	0.84	0.22	-	74,74,74,74	0

6.5 Other polymers (i)

There are no such residues in this entry.