Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:28 PM EDT

PDB ID	:	1M1D
Title	:	TETRAHYMENA GCN5 WITH BOUND BISUBSTRATE ANALOG INHIBITOR
Authors	:	Poux, A.N.; Cebrat, M.; Kim, C.M.; Cole, P.A.; Marmorstein, R.
Deposited on	:	2002-06-18
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

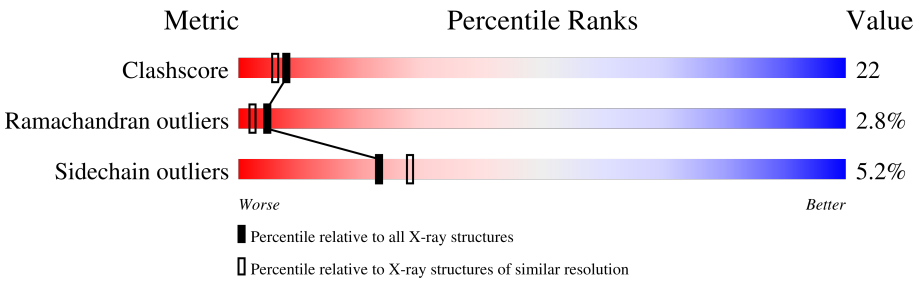
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	163	65% 33% •
1	C	163	63% 32% • ••
2	B	20	10% 5% 15% 70%
2	D	20	5% 95%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2965 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 TGCN5 HISTONE ACETYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	1369	885	238	237	9	0	0	0
1	C	162	1336	860	235	232	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	PHE	LEU	SEE REMARK 999	GB 1245146
A	210	ARG	ASN	SEE REMARK 999	GB 1245146
C	390	PHE	LEU	SEE REMARK 999	GB 1245146
C	510	ARG	ASN	SEE REMARK 999	GB 1245146

- Molecule 2 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	6	92	48	17	23	3	1	0	0	0
2	D	1	61	30	9	18	3	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	LYX	LYS	MODIFIED RESIDUE	UNP P02303
D	314	LYX	LYS	MODIFIED RESIDUE	UNP P02303

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	55	55	55	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	4	4	4	0	0
			Total	O		
3	C	46	46	46	0	0
			Total	O		
3	D	2	2	2	0	0

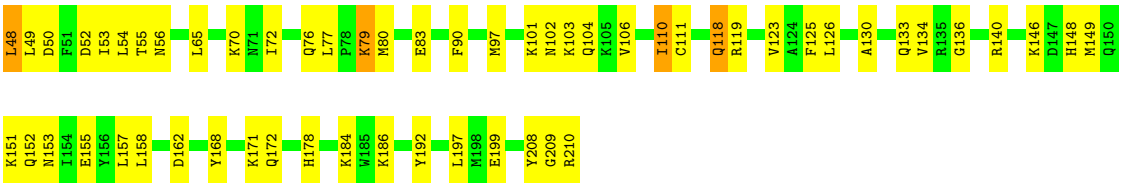
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

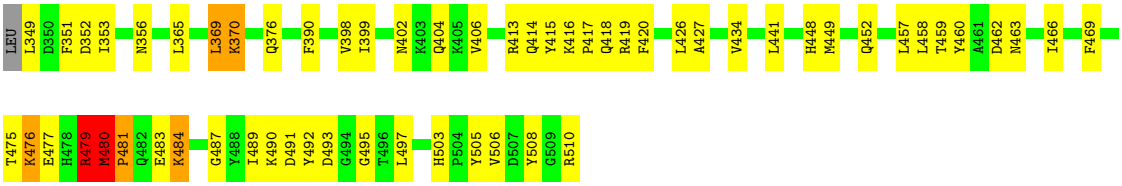
• Molecule 1: TGCN5 HISTONE ACETYL TRANSFERASE

Chain A:



• Molecule 1: TGCN5 HISTONE ACETYL TRANSFERASE

Chain C:

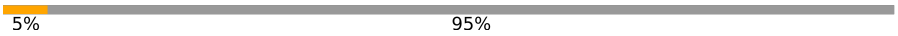


• Molecule 2: HISTONE H3

Chain B:

• Molecule 2: HISTONE H3

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.42Å 67.83Å 74.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2965	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.39	0/1402	0.59	0/1878
1	C	0.35	0/1365	0.61	1/1826 (0.1%)
2	B	2.20	1/30 (3.3%)	4.01	7/37 (18.9%)
All	All	0.43	1/2797 (0.0%)	0.71	8/3741 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	ALA	N-CA	-7.79	1.30	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	16	PRO	N-CA-C	12.18	143.78	112.10
2	B	16	PRO	CA-C-N	-9.23	96.90	117.20
2	B	16	PRO	C-N-CA	7.61	140.72	121.70
2	B	15	ALA	N-CA-C	7.23	130.53	111.00
2	B	15	ALA	C-N-CD	-6.67	105.94	120.60
1	C	481	PRO	N-CA-CB	5.65	110.08	103.30
2	B	16	PRO	CA-C-O	5.37	133.09	120.20
2	B	13	GLY	N-CA-C	-5.04	100.50	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	LYX	Mainchain
2	B	15	ALA	Mainchain

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	1369	0	1376	56	0
1	C	1336	0	1336	53	0
2	B	92	0	73	31	0
2	D	61	0	45	15	0
3	A	55	0	0	0	0
3	B	4	0	0	1	0
3	C	46	0	0	3	0
3	D	2	0	0	0	0
All	All	2965	0	2830	123	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 22.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CD2	2:B:16:PRO:HG2	1.52	1.37
1:A:162:ASP:OD2	2:B:16:PRO:HD2	1.48	1.12
1:A:77:LEU:HD23	2:B:16:PRO:HG2	1.11	1.09
1:A:77:LEU:HD23	2:B:16:PRO:CG	1.80	1.09
1:A:77:LEU:HD22	2:B:16:PRO:HG2	1.38	1.03
1:A:77:LEU:HA	2:B:16:PRO:HG3	1.42	1.00
1:A:133:GLN:OE1	2:B:17:ARG:HD2	1.63	0.98
1:C:503:HIS:HD2	1:C:505:TYR:H	1.16	0.92
3:C:643:HOH:O	2:D:314:LYX:HD3	1.68	0.91
2:B:14:LYX:H142	2:B:17:ARG:HG3	1.52	0.90
1:A:77:LEU:CD2	2:B:16:PRO:CG	2.45	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:OD1	1:A:90:PHE:HA	1.82	0.79
2:B:17:ARG:HB3	2:B:17:ARG:NH1	1.97	0.79
1:A:192:TYR:CD1	2:B:14:LYX:HE2	2.19	0.77
1:C:495:GLY:HA3	2:D:314:LYX:H	1.52	0.75
2:B:14:LYX:C14	2:B:17:ARG:HG3	2.18	0.73
1:C:484:LYS:N	1:C:484:LYS:HE2	2.04	0.72
1:A:79:LYS:HB2	2:B:15:ALA:HB3	1.70	0.72
1:C:417:PRO:HB2	1:C:418:GLN:NE2	2.06	0.71
1:A:192:TYR:HD1	2:B:14:LYX:HE2	1.55	0.70
1:A:125:PHE:HA	2:B:14:LYX:O33	1.91	0.70
2:D:314:LYX:S20	2:D:314:LYX:HE3	2.34	0.68
2:B:15:ALA:N	2:B:16:PRO:CD	2.55	0.68
2:B:15:ALA:N	2:B:16:PRO:HD3	2.07	0.68
1:C:460:TYR:HE1	1:C:489:ILE:HG22	1.57	0.68
3:C:643:HOH:O	2:D:314:LYX:CD	2.31	0.67
1:A:178:HIS:CE1	1:A:197:LEU:HD23	2.32	0.65
1:C:476:LYS:HD2	1:C:476:LYS:H	1.61	0.64
1:C:417:PRO:HB2	1:C:418:GLN:HE22	1.62	0.64
1:A:118:GLN:HE21	1:A:118:GLN:H	1.45	0.63
1:C:434:VAL:HA	2:D:314:LYX:O1	1.98	0.63
1:A:178:HIS:HA	1:A:199:GLU:OE2	1.99	0.63
1:C:462:ASP:O	1:C:466:ILE:HG13	1.99	0.63
1:A:192:TYR:CD1	2:B:14:LYX:CE	2.83	0.62
1:C:476:LYS:HD2	1:C:476:LYS:N	2.15	0.62
1:A:134:VAL:O	1:A:134:VAL:HG12	1.98	0.61
1:C:503:HIS:CD2	1:C:505:TYR:H	2.06	0.61
1:A:151:LYS:HE2	1:A:210:ARG:NH2	2.16	0.61
1:A:77:LEU:HD23	2:B:16:PRO:CB	2.29	0.60
1:C:489:ILE:HD12	1:C:489:ILE:N	2.17	0.60
2:B:15:ALA:H	2:B:16:PRO:HD3	1.67	0.59
1:C:426:LEU:HB3	2:D:314:LYX:H223	1.85	0.58
1:A:77:LEU:HA	2:B:16:PRO:CG	2.28	0.58
1:C:356:ASN:OD1	1:C:390:PHE:HA	2.04	0.57
1:C:469:PHE:HZ	2:D:314:LYX:C22	2.17	0.57
1:C:420:PHE:CZ	1:C:489:ILE:HD11	2.38	0.57
1:C:476:LYS:H	1:C:476:LYS:CD	2.13	0.57
1:C:376:GLN:HB3	2:D:314:LYX:H142	1.86	0.56
1:C:479:ARG:O	1:C:480:MET:HB2	2.05	0.56
1:C:459:THR:OG1	2:D:314:LYX:O33	2.24	0.55
1:A:48:LEU:C	1:A:49:LEU:HD22	2.27	0.55
1:A:110:ILE:C	1:A:110:ILE:HD13	2.27	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASP:OD1	2:B:15:ALA:O	2.25	0.55
1:A:83:GLU:H	1:A:83:GLU:CD	2.10	0.54
1:C:463:ASN:HA	1:C:466:ILE:CD1	2.37	0.54
1:C:495:GLY:CA	2:D:314:LYX:H	2.19	0.54
2:B:17:ARG:HB3	2:B:17:ARG:HH11	1.73	0.54
1:C:503:HIS:CG	1:C:506:VAL:HG23	2.43	0.53
1:A:126:LEU:HB3	2:B:14:LYX:H192	1.90	0.53
1:A:110:ILE:HD11	1:A:123:VAL:HG13	1.91	0.53
1:A:110:ILE:HD13	1:A:111:CYS:N	2.24	0.52
1:C:448:HIS:O	1:C:452:GLN:HG2	2.09	0.52
1:C:434:VAL:HG12	1:C:434:VAL:O	2.09	0.52
1:A:50:ASP:OD2	1:A:103:LYS:HE2	2.09	0.52
1:A:119:ARG:HH21	1:A:155:GLU:CD	2.13	0.52
1:C:483:GLU:O	1:C:484:LYS:HB2	2.09	0.52
1:C:495:GLY:HA3	2:D:314:LYX:N	2.23	0.52
1:A:48:LEU:HD13	1:A:102:ASN:HA	1.93	0.51
1:A:48:LEU:O	1:A:101:LYS:HA	2.09	0.51
1:C:484:LYS:HE2	1:C:484:LYS:CA	2.40	0.51
2:B:17:ARG:NH1	2:B:17:ARG:CB	2.73	0.50
1:C:483:GLU:O	1:C:484:LYS:CB	2.60	0.50
2:B:17:ARG:HH11	2:B:17:ARG:CB	2.25	0.50
1:C:352:ASP:OD1	1:C:353:ILE:N	2.46	0.48
1:A:76:GLN:OE1	2:B:17:ARG:HG2	2.13	0.48
1:C:399:ILE:HD11	1:C:441:LEU:HB2	1.97	0.47
1:C:449:MET:HG3	1:C:457:LEU:HD21	1.97	0.47
1:C:457:LEU:C	1:C:458:LEU:HD12	2.35	0.46
1:A:80:MET:SD	2:B:12:GLY:HA2	2.55	0.46
1:A:134:VAL:HA	2:B:14:LYX:O1	2.14	0.46
1:A:76:GLN:O	2:B:16:PRO:HB3	2.15	0.46
1:A:168:TYR:O	1:A:172:GLN:HG2	2.15	0.46
1:A:119:ARG:NH2	1:A:155:GLU:CD	2.69	0.46
1:C:484:LYS:HE2	1:C:484:LYS:HA	1.98	0.46
1:C:508:TYR:C	1:C:510:ARG:H	2.19	0.46
1:A:53:ILE:HD13	1:A:148:HIS:CE1	2.50	0.45
1:A:49:LEU:HD13	1:A:101:LYS:HG2	1.97	0.45
1:A:76:GLN:NE2	1:A:130:ALA:H	2.14	0.45
1:C:469:PHE:HZ	2:D:314:LYX:H223	1.80	0.45
1:A:118:GLN:HG2	1:A:184:LYS:HD2	1.98	0.45
1:C:418:GLN:CD	1:C:418:GLN:N	2.70	0.45
1:C:353:ILE:HD13	1:C:448:HIS:CE1	2.52	0.45
1:C:475:THR:OG1	1:C:477:GLU:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:PHE:HA	1:C:398:VAL:O	2.17	0.44
1:C:460:TYR:CE2	1:C:497:LEU:HB2	2.51	0.44
2:B:17:ARG:HB3	2:B:17:ARG:CZ	2.47	0.44
1:C:469:PHE:HZ	2:D:314:LYX:H221	1.83	0.43
1:A:119:ARG:HD2	1:A:153:ASN:O	2.19	0.43
1:A:118:GLN:CG	1:A:184:LYS:HD2	2.49	0.43
1:C:491:ASP:O	1:C:493:ASP:N	2.52	0.43
1:A:158:LEU:HD23	1:A:199:GLU:CB	2.49	0.43
1:A:118:GLN:HE21	1:A:118:GLN:N	2.13	0.42
1:C:370:LYS:HE3	1:C:370:LYS:HB3	1.76	0.42
2:D:314:LYX:H223	2:D:314:LYX:H191	1.78	0.42
1:A:136:GLY:O	1:A:140:ARG:HG3	2.19	0.42
1:A:186:LYS:HE2	1:A:186:LYS:HB2	1.90	0.42
1:A:171:LYS:HE3	3:B:658:HOH:O	2.19	0.42
1:A:54:LEU:HD21	1:A:65:LEU:HD13	2.01	0.42
1:C:414:GLN:OE1	1:C:416:LYS:NZ	2.49	0.42
1:C:369:LEU:HG	1:C:398:VAL:HG12	2.02	0.41
1:A:152:GLN:O	1:A:153:ASN:HB2	2.20	0.41
1:A:72:ILE:HD11	1:A:106:VAL:O	2.21	0.41
1:C:402:ASN:O	1:C:404:GLN:HG2	2.21	0.41
1:C:420:PHE:CE1	1:C:489:ILE:HD11	2.55	0.41
1:A:210:ARG:HG3	1:A:210:ARG:HH11	1.85	0.41
1:C:365:LEU:HD22	1:C:406:VAL:HG23	2.03	0.41
1:C:419:ARG:NH2	3:C:661:HOH:O	2.54	0.41
1:C:427:ALA:HA	2:D:314:LYX:O35	2.20	0.41
1:C:503:HIS:CD2	1:C:506:VAL:HG23	2.55	0.41
1:A:52:ASP:O	1:A:97:MET:HA	2.21	0.40
1:A:146:LYS:HD3	1:A:208:TYR:CE2	2.56	0.40
1:C:413:ARG:HD3	1:C:415:TYR:OH	2.21	0.40
1:A:149:MET:HG3	1:A:157:LEU:HD21	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	161/163 (99%)	155 (96%)	4 (2%)	2 (1%)	13	10
1	C	160/163 (98%)	143 (89%)	11 (7%)	6 (4%)	3	1
2	B	3/20 (15%)	0	2 (67%)	1 (33%)	0	0
All	All	324/346 (94%)	298 (92%)	17 (5%)	9 (3%)	5	2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	16	PRO
1	C	480	MET
1	C	481	PRO
1	C	484	LYS
1	C	492	TYR
1	C	479	ARG
1	A	104	GLN
1	A	209	GLY
1	C	487	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	146/146 (100%)	140 (96%)	6 (4%)	30	39
1	C	140/146 (96%)	133 (95%)	7 (5%)	24	30
2	B	2/14 (14%)	0	2 (100%)	0	0
All	All	288/306 (94%)	273 (95%)	15 (5%)	23	28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	THR
1	A	70	LYS
1	A	79	LYS
1	A	110	ILE
1	A	118	GLN
2	B	16	PRO
2	B	17	ARG
1	C	349	LEU
1	C	369	LEU
1	C	370	LYS
1	C	476	LYS
1	C	479	ARG
1	C	480	MET
1	C	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	118	GLN
1	A	131	ASN
1	A	148	HIS
1	A	163	ASN
1	A	178	HIS
1	C	362	ASN
1	C	433	GLN
1	C	503	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)

2 non-standard protein/DNA/RNA residues 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	LYX	D	314	-	52,63,64	2.66	14 (26%)	59,91,93	2.45	17 (28%)
2	LYX	B	14	2	52,63,64	2.80	15 (28%)	59,91,93	2.26	13 (22%)

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	LYX	D	314	-	-	14/60/81/83	0/3/3/3
2	LYX	B	14	2	-	16/60/81/83	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	LYX	O61-C50	9.86	1.54	1.41
2	D	314	LYX	O61-C50	9.68	1.54	1.41
2	B	14	LYX	C48-C42	-7.09	1.37	1.52
2	D	314	LYX	C48-C42	-6.95	1.37	1.52
2	B	14	LYX	P44-O43	6.12	1.70	1.59
2	D	314	LYX	P44-O43	5.98	1.70	1.59
2	B	14	LYX	CB-CA	-5.89	1.45	1.53
2	D	314	LYX	O35-C12	5.74	1.34	1.23
2	B	14	LYX	O35-C12	5.65	1.34	1.23
2	B	14	LYX	C19-S20	5.27	1.88	1.81
2	D	314	LYX	C19-S20	5.27	1.88	1.81
2	B	14	LYX	C57-N58	4.59	1.42	1.33
2	D	314	LYX	C57-N58	4.36	1.42	1.33
2	D	314	LYX	O61-C41	3.75	1.53	1.45
2	B	14	LYX	O61-C41	3.52	1.52	1.45
2	D	314	LYX	O34-C16	3.38	1.30	1.23
2	D	314	LYX	P44-O45	3.29	1.61	1.50
2	D	314	LYX	C57-N56	3.00	1.36	1.32
2	B	14	LYX	P44-O45	2.99	1.60	1.50
2	B	14	LYX	O34-C16	2.94	1.29	1.23
2	B	14	LYX	C57-N56	2.92	1.36	1.32
2	D	314	LYX	C59-C54	2.73	1.53	1.43
2	B	14	LYX	C55-N56	2.73	1.39	1.35
2	B	14	LYX	C59-C54	2.64	1.53	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	14	LYX	C18-N17	2.54	1.52	1.46
2	D	314	LYX	O11-C10	2.54	1.47	1.42
2	D	314	LYX	C55-N56	2.34	1.38	1.35
2	D	314	LYX	C8-C7	2.33	1.58	1.53
2	B	14	LYX	CG-CB	-2.14	1.43	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	314	LYX	C48-C42-C41	8.87	118.94	103.22
2	B	14	LYX	C48-C42-C41	8.56	118.40	103.22
2	B	14	LYX	O49-C48-C42	7.89	133.58	111.17
2	D	314	LYX	O49-C48-C42	7.84	133.44	111.17
2	D	314	LYX	O43-C42-C48	-7.24	85.44	111.68
2	B	14	LYX	O43-C42-C48	-6.81	87.02	111.68
2	D	314	LYX	C18-C19-S20	3.88	130.22	114.36
2	B	14	LYX	O43-C42-C41	3.74	123.60	110.08
2	D	314	LYX	CE-NZ-C23	3.61	129.03	122.59
2	D	314	LYX	O33-C23-NZ	-3.60	115.27	122.99
2	D	314	LYX	O43-C42-C41	3.52	122.81	110.08
2	B	14	LYX	CD-CG-CB	-3.51	101.20	113.62
2	D	314	LYX	C9-C7-C10	3.13	114.25	108.82
2	D	314	LYX	CD-CE-NZ	-3.09	103.37	112.21
2	B	14	LYX	N56-C57-N58	-2.79	124.31	128.68
2	D	314	LYX	O61-C41-C42	-2.75	98.97	104.87
2	D	314	LYX	C18-N17-C16	-2.75	117.73	122.84
2	B	14	LYX	C15-C16-N17	-2.72	111.84	116.42
2	D	314	LYX	N56-C57-N58	-2.68	124.50	128.68
2	B	14	LYX	C55-C54-N53	2.67	112.18	109.40
2	D	314	LYX	C55-C54-N53	2.61	112.12	109.40
2	B	14	LYX	C42-C48-C50	2.57	105.59	99.89
2	B	14	LYX	C9-C7-C10	2.55	113.25	108.82
2	D	314	LYX	C42-C48-C50	2.44	105.29	99.89
2	B	14	LYX	C19-C18-N17	-2.32	107.55	112.42
2	B	14	LYX	C57-N58-C59	2.19	122.50	118.75
2	D	314	LYX	O61-C41-C40	2.14	116.42	109.37
2	B	14	LYX	O61-C41-C42	-2.07	100.42	104.87
2	D	314	LYX	C57-N58-C59	2.02	122.21	118.75
2	D	314	LYX	C50-N51-C55	-2.01	123.11	126.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	14	LYX	O11-C10-C12-N13
2	B	14	LYX	S20-C21-C23-NZ
2	B	14	LYX	S20-C21-C23-O33
2	B	14	LYX	C22-C21-C23-NZ
2	B	14	LYX	C22-C21-C23-O33
2	B	14	LYX	C21-C23-NZ-CE
2	B	14	LYX	O33-C23-NZ-CE
2	B	14	LYX	N-CA-CB-CG
2	B	14	LYX	C-CA-CB-CG
2	B	14	LYX	C41-C42-O43-P44
2	D	314	LYX	S20-C21-C23-NZ
2	D	314	LYX	C21-C23-NZ-CE
2	D	314	LYX	O33-C23-NZ-CE
2	D	314	LYX	N-CA-CB-CG
2	D	314	LYX	C-CA-CB-CG
2	D	314	LYX	O-C-CA-CB
2	D	314	LYX	C41-C42-O43-P44
2	D	314	LYX	CG-CD-CE-NZ
2	B	14	LYX	O39-C40-C41-O61
2	D	314	LYX	C22-C21-C23-O33
2	D	314	LYX	N17-C18-C19-S20
2	B	14	LYX	O39-C40-C41-C42
2	D	314	LYX	C22-C21-C23-NZ
2	D	314	LYX	C23-C21-S20-C19
2	D	314	LYX	S20-C21-C23-O33
2	B	14	LYX	N17-C18-C19-S20
2	B	14	LYX	O11-C10-C12-O35
2	D	314	LYX	O11-C10-C12-O35
2	B	14	LYX	C41-C40-O39-P2
2	B	14	LYX	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	314	LYX	15	0
2	B	14	LYX	8	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.