



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:37 AM UTC

PDB ID : 1NLM / pdb_00001nlm
Title : CRYSTAL STRUCTURE OF MURG:GLCNAC COMPLEX
Authors : Hu, Y.; Chen, L.; Ha, S.; Gross, B.; Falcone, B.; Walker, D.; Mokhtarzadeh, M.; Walker, S.
Deposited on : 2003-01-07
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

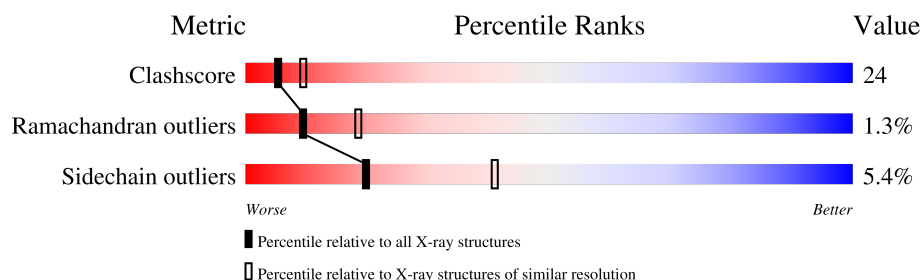
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	364	
1	B	364	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5478 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.

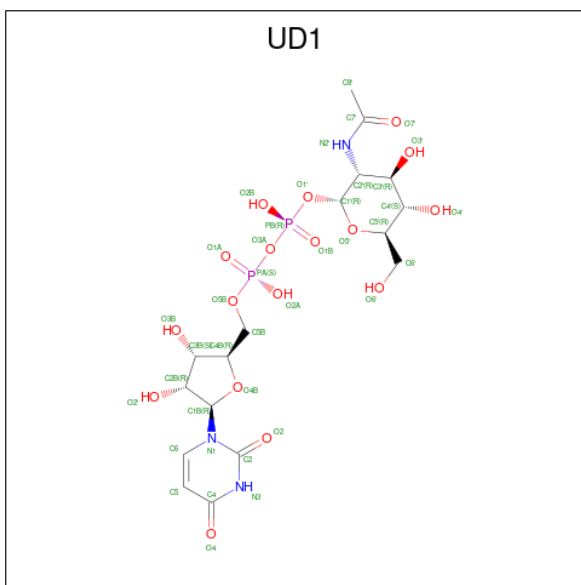
- Molecule 1 is a protein called UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2631	1671	483	466	11			
1	B	350	Total	C	N	O	S	0	0	0
			2631	1671	483	466	11			

There are 20 discrepancies between the modelled and reference sequences:

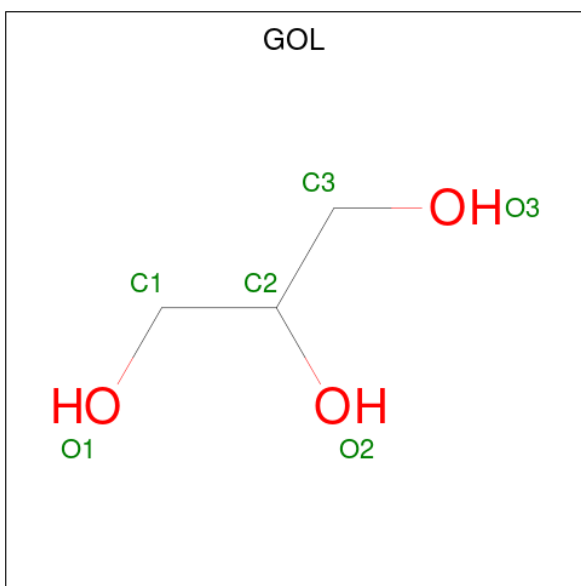
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P17443
A	2	MET	-	cloning artifact	UNP P17443
A	357	LEU	-	cloning artifact	UNP P17443
A	358	GLU	-	cloning artifact	UNP P17443
A	359	HIS	-	cloning artifact	UNP P17443
A	360	HIS	-	cloning artifact	UNP P17443
A	361	HIS	-	cloning artifact	UNP P17443
A	362	HIS	-	cloning artifact	UNP P17443
A	363	HIS	-	cloning artifact	UNP P17443
A	364	HIS	-	cloning artifact	UNP P17443
B	1	MET	-	cloning artifact	UNP P17443
B	2	MET	-	cloning artifact	UNP P17443
B	357	LEU	-	cloning artifact	UNP P17443
B	358	GLU	-	cloning artifact	UNP P17443
B	359	HIS	-	cloning artifact	UNP P17443
B	360	HIS	-	cloning artifact	UNP P17443
B	361	HIS	-	cloning artifact	UNP P17443
B	362	HIS	-	cloning artifact	UNP P17443
B	363	HIS	-	cloning artifact	UNP P17443
B	364	HIS	-	cloning artifact	UNP P17443

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 17	N 3	O 17	P 2	0	0
2	B	1	Total 39	C 17	N 3	O 17	P 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

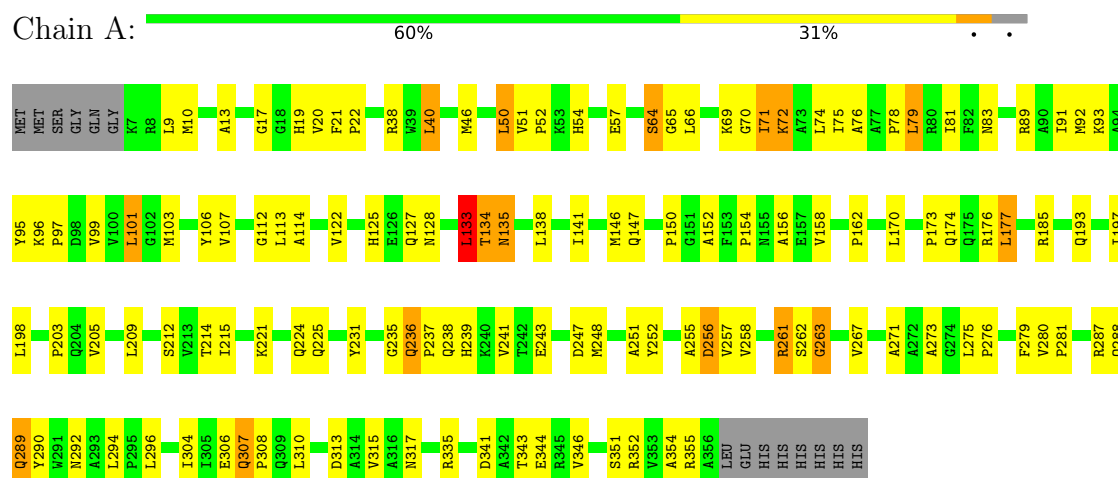
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	49	Total	O	0	0
			49	49		

3 Residue-property plots

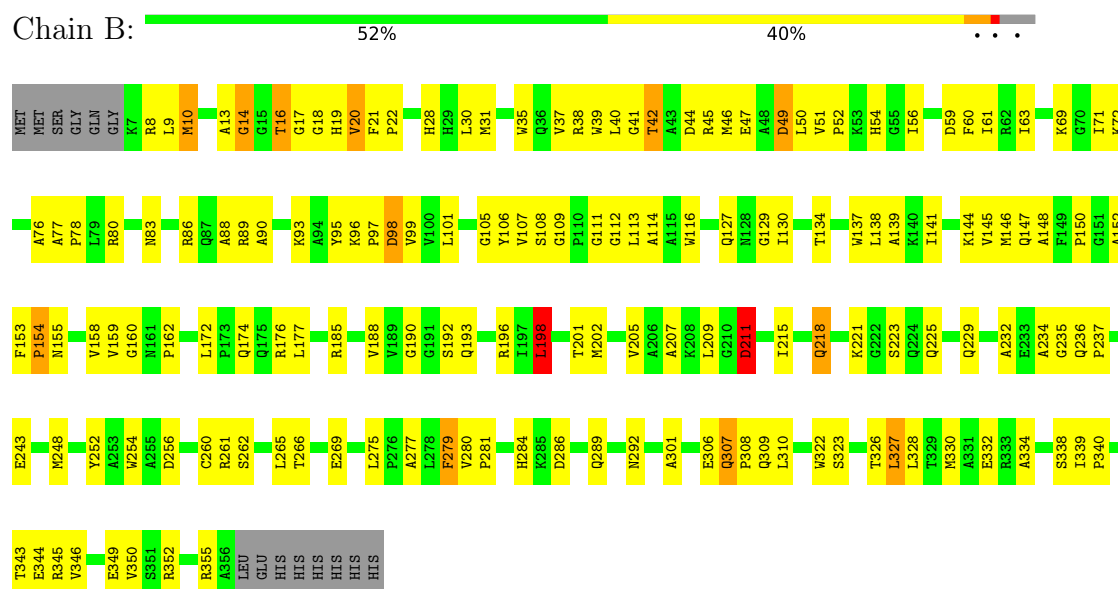
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase



- Molecule 1: UDP-N-acetylglucosamine--N-acetylmuramyl-(pentapeptide) pyrophosphoryl-undecaprenol N-acetylglucosamine transferase



4 Data and refinement statistics

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	66.70Å 83.65Å 146.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.50	Depositor
% Data completeness (in resolution range)	89.2 (19.96-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.226 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5478	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, UD1

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	0.47	0/2688	0.99	13/3653 (0.4%)
1	B	2.75	5/2688 (0.2%)	1.87	23/3653 (0.6%)
All	All	1.97	5/5376 (0.1%)	1.50	36/7306 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	LEU	CB-CG	-76.50	0.00	1.53
1	B	198	LEU	CA-CB	66.53	2.61	1.53
1	B	211	ASP	CB-CG	-60.64	0.00	1.52
1	B	211	ASP	CA-CB	59.88	2.54	1.53
1	B	279	PHE	CD1-CE1	46.99	2.79	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	PHE	CD1-CG-CD2	-79.07	0.00	118.60
1	B	279	PHE	CG-CD1-CE1	-35.22	60.82	120.70
1	B	279	PHE	CD1-CE1-CZ	-33.20	60.24	120.00
1	B	198	LEU	CB-CA-C	15.83	142.67	110.38
1	B	211	ASP	CB-CA-C	11.73	133.02	110.27
1	B	198	LEU	N-CA-CB	-10.64	93.91	110.30
1	A	263	GLY	N-CA-C	-7.70	102.69	112.54
1	B	256	ASP	N-CA-C	-7.53	104.23	113.50
1	B	339	ILE	CA-C-N	7.20	127.82	119.47
1	B	339	ILE	C-N-CA	7.20	127.82	119.47
1	B	215	ILE	N-CA-C	6.94	118.60	108.53
1	A	93	LYS	N-CA-C	-6.92	103.82	111.36
1	A	256	ASP	N-CA-C	-6.91	104.48	113.12
1	A	20	VAL	N-CA-C	6.91	117.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ALA	N-CA-C	6.90	120.23	110.50
1	A	215	ILE	N-CA-C	6.85	118.46	108.53
1	B	275	LEU	CA-C-N	6.48	126.24	119.76
1	B	275	LEU	C-N-CA	6.48	126.24	119.76
1	B	277	ALA	N-CA-C	6.30	118.99	109.23
1	B	20	VAL	N-CA-C	6.27	116.90	110.82
1	A	280	VAL	CA-C-N	6.11	126.14	119.90
1	A	280	VAL	C-N-CA	6.11	126.14	119.90
1	B	260	CYS	N-CA-C	6.10	116.61	108.38
1	B	334	ALA	N-CA-C	-6.01	104.65	111.14
1	B	37	VAL	N-CA-C	5.80	116.84	108.48
1	B	98	ASP	N-CA-C	-5.78	106.39	113.50
1	A	236	GLN	CA-C-N	5.54	125.21	119.56
1	A	236	GLN	C-N-CA	5.54	125.21	119.56
1	B	153	PHE	CA-C-N	5.32	126.49	119.84
1	B	153	PHE	C-N-CA	5.32	126.49	119.84
1	A	50	LEU	N-CA-C	5.26	116.82	111.14
1	B	280	VAL	CA-C-N	5.18	126.32	119.84
1	B	280	VAL	C-N-CA	5.18	126.32	119.84
1	A	128	ASN	N-CA-C	5.18	118.17	110.14
1	A	72	LYS	N-CA-C	-5.17	106.24	112.54
1	B	301	ALA	N-CA-C	-5.01	107.33	113.50

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	2631	0	2679	107	0
1	B	2631	0	2679	154	0
2	A	39	0	25	1	0
2	B	39	0	25	5	0
3	A	18	0	24	1	0
3	B	6	0	8	0	0
4	A	65	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	49	0	0	2	0
All	All	5478	0	5440	260	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 24.

All (260) 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:198:LEU:HD21	1:B:198:LEU:CG	1.51	1.38
1:B:198:LEU:CG	1:B:198:LEU:HD22	1.51	1.38
1:B:198:LEU:CG	1:B:198:LEU:HD23	1.51	1.38
1:B:198:LEU:CG	1:B:198:LEU:HD11	1.52	1.36
1:B:198:LEU:CG	1:B:198:LEU:HD12	1.52	1.36
1:B:198:LEU:CG	1:B:198:LEU:HD13	1.52	1.36
1:B:198:LEU:HD21	1:B:198:LEU:HB2	1.41	1.01
1:B:198:LEU:HD22	1:B:198:LEU:HB2	1.41	1.01
1:B:198:LEU:HD23	1:B:198:LEU:HB2	1.41	1.01
1:B:279:PHE:CE1	1:B:279:PHE:CG	2.44	0.93
1:A:69:LYS:HB3	1:A:74:LEU:HD21	1.50	0.92
1:A:125:HIS:HD2	1:A:127:GLN:HE21	1.16	0.90
1:A:79:LEU:HD12	1:A:79:LEU:H	1.36	0.89
1:B:14:GLY:HA3	1:B:105:GLY:HA3	1.54	0.89
1:B:129:GLY:H	1:B:292:ASN:ND2	1.69	0.88
1:B:31:MET:HE1	1:B:56:ILE:HD11	1.56	0.88
1:A:125:HIS:CD2	1:A:127:GLN:HE21	1.94	0.86
1:B:211:ASP:CB	1:B:211:ASP:CA	2.54	0.86
1:A:146:MET:HE1	1:A:346:VAL:HG13	1.58	0.85
1:B:198:LEU:HG	1:B:198:LEU:CA	2.08	0.84
1:A:236:GLN:HE21	1:A:238:GLN:HE22	1.27	0.83
1:A:236:GLN:NE2	1:A:238:GLN:HE22	1.77	0.82
1:B:211:ASP:CA	1:B:211:ASP:CG	2.54	0.80
1:B:198:LEU:CG	1:B:198:LEU:CA	2.61	0.78
1:B:198:LEU:CA	1:B:198:LEU:CB	2.61	0.77
1:A:95:TYR:HD2	1:A:97:PRO:HG3	1.49	0.76
1:B:190:GLY:H	1:B:218:GLN:HE22	1.34	0.75
1:B:129:GLY:H	1:B:292:ASN:HD21	1.32	0.75
1:B:207:ALA:HB2	1:B:234:ALA:HB1	1.69	0.74
1:B:19:HIS:HD2	1:B:127:GLN:NE2	1.88	0.72
1:A:235:GLY:C	1:A:237:PRO:HD3	2.14	0.72
1:A:17:GLY:N	1:A:46:MET:HE1	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:TRP:HB3	1:B:327:LEU:CD1	2.21	0.71
1:B:10:MET:HG3	1:B:97:PRO:HG3	1.73	0.71
1:B:190:GLY:H	1:B:218:GLN:NE2	1.89	0.70
1:A:69:LYS:HB3	1:A:74:LEU:CD2	2.22	0.70
1:A:307:GLN:HE21	1:A:307:GLN:N	1.90	0.70
1:B:28:HIS:HA	1:B:31:MET:HE3	1.75	0.69
1:A:221:LYS:HA	1:A:243:GLU:OE1	1.93	0.68
1:A:95:TYR:CD2	1:A:97:PRO:HG3	2.27	0.68
1:B:46:MET:HG3	1:B:47:GLU:N	2.08	0.68
1:B:192:SER:OG	2:B:402:UD1:H1'	1.94	0.68
1:B:14:GLY:CA	1:B:105:GLY:HA3	2.24	0.66
1:A:79:LEU:H	1:A:79:LEU:CD1	2.07	0.66
1:A:92:MET:HE1	1:A:114:ALA:HB3	1.77	0.66
1:B:144:LYS:HD2	1:B:145:VAL:H	1.61	0.66
1:B:225:GLN:CD	1:B:225:GLN:H	2.04	0.66
1:B:284:HIS:CD2	1:B:286:ASP:H	2.14	0.66
1:A:83:ASN:HB3	4:A:507:HOH:O	1.95	0.65
1:B:352:ARG:O	1:B:355:ARG:HG2	1.95	0.65
1:B:328:LEU:O	1:B:332:GLU:HG3	1.95	0.65
1:B:327:LEU:HD12	1:B:330:MET:HE3	1.79	0.65
1:A:306:GLU:HB2	1:A:308:PRO:HD2	1.77	0.64
1:B:10:MET:HE1	1:B:40:LEU:HB2	1.79	0.64
1:B:71:ILE:HG23	1:B:72:LYS:H	1.61	0.64
1:B:28:HIS:NE2	1:B:54:HIS:HD2	1.95	0.63
1:B:322:TRP:HB3	1:B:327:LEU:HD13	1.80	0.62
1:B:221:LYS:HD3	1:B:243:GLU:OE1	2.01	0.60
1:A:133:LEU:HD13	1:A:133:LEU:H	1.67	0.60
1:B:88:ALA:HB1	1:B:111:GLY:HA2	1.82	0.60
1:A:355:ARG:O	1:A:355:ARG:HG3	2.02	0.59
1:A:225:GLN:H	1:A:225:GLN:CD	2.11	0.59
1:B:38:ARG:HD2	1:B:59:ASP:OD2	2.02	0.59
1:B:9:LEU:HD12	1:B:10:MET:N	2.18	0.58
1:A:112:GLY:HA3	1:A:138:LEU:HD11	1.85	0.58
1:B:323:SER:OG	1:B:326:THR:HG23	2.03	0.58
1:B:188:VAL:HG21	1:B:202:MET:HG3	1.85	0.58
1:B:71:ILE:HG23	1:B:72:LYS:N	2.18	0.58
1:A:279:PHE:O	1:A:281:PRO:HD3	2.05	0.57
1:B:18:GLY:N	2:B:402:UD1:H6'1	2.20	0.57
1:A:89:ARG:CZ	1:B:78:PRO:HG2	2.34	0.57
1:B:83:ASN:O	1:B:86:ARG:HB2	2.04	0.57
1:A:146:MET:CE	1:A:346:VAL:HG13	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:MET:HG3	1:B:97:PRO:CG	2.33	0.56
1:A:176:ARG:NH2	1:A:273:ALA:O	2.38	0.56
1:A:147:GLN:NE2	1:A:156:ALA:HB3	2.21	0.56
1:A:236:GLN:HE21	1:A:238:GLN:NE2	2.02	0.55
1:B:306:GLU:HB3	1:B:308:PRO:HD2	1.88	0.55
1:B:31:MET:CE	1:B:56:ILE:HD11	2.35	0.55
1:B:113:LEU:HD21	1:B:137:TRP:HZ3	1.70	0.55
1:B:236:GLN:N	1:B:237:PRO:HD3	2.21	0.55
1:A:288:GLN:NE2	2:A:401:UD1:O3'	2.38	0.55
1:A:113:LEU:HD23	1:A:141:ILE:HD13	1.89	0.54
1:B:308:PRO:HB2	1:B:309:GLN:HE21	1.72	0.54
1:A:263:GLY:O	1:A:267:VAL:HG23	2.07	0.54
1:B:185:ARG:HD2	1:B:254:TRP:O	2.06	0.54
1:B:40:LEU:HG	1:B:107:VAL:HG11	1.90	0.54
1:B:177:LEU:HB2	1:B:328:LEU:HD13	1.89	0.54
1:B:211:ASP:CG	1:B:211:ASP:HB3	0.97	0.54
1:A:38:ARG:NH1	1:A:57:GLU:HB2	2.23	0.54
1:A:307:GLN:HE21	1:A:307:GLN:H	1.56	0.54
1:A:185:ARG:HG2	1:A:256:ASP:OD2	2.08	0.53
1:A:133:LEU:HD23	1:A:134:THR:HG23	1.90	0.53
1:B:176:ARG:HG3	1:B:176:ARG:HH11	1.74	0.53
1:B:207:ALA:HB2	1:B:234:ALA:CB	2.39	0.53
1:B:147:GLN:HE21	1:B:152:ALA:HB3	1.73	0.53
1:B:147:GLN:NE2	1:B:152:ALA:HB3	2.24	0.52
1:A:224:GLN:HG3	1:A:241:VAL:HG12	1.92	0.52
1:B:144:LYS:HD2	1:B:145:VAL:N	2.24	0.52
1:B:159:VAL:HG23	1:B:345:ARG:HB2	1.91	0.52
1:B:196:ARG:HH11	1:B:196:ARG:HG3	1.74	0.52
1:B:112:GLY:HA3	1:B:138:LEU:HD11	1.91	0.52
1:B:338:SER:C	1:B:340:PRO:HD3	2.35	0.52
1:A:92:MET:HG2	1:A:97:PRO:HG2	1.93	0.51
1:A:150:PRO:HG3	1:A:158:VAL:HG21	1.92	0.51
1:B:322:TRP:HB3	1:B:327:LEU:HD11	1.92	0.51
1:B:95:TYR:HD2	1:B:97:PRO:HG3	1.75	0.51
1:A:287:ARG:HB3	1:A:290:TYR:HB3	1.92	0.51
1:B:193:GLN:HA	1:B:193:GLN:NE2	2.26	0.51
1:B:76:ALA:C	1:B:78:PRO:HD3	2.36	0.51
1:A:74:LEU:HD22	1:A:74:LEU:N	2.25	0.51
1:A:173:PRO:O	1:A:177:LEU:HD22	2.11	0.51
1:B:89:ARG:HA	1:B:114:ALA:HB1	1.92	0.51
1:A:279:PHE:C	1:A:281:PRO:HD3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:N	1:B:172:LEU:HD22	2.26	0.50
1:A:236:GLN:N	1:A:237:PRO:HD3	2.26	0.50
1:A:176:ARG:HD2	4:A:542:HOH:O	2.11	0.50
1:B:201:THR:O	1:B:205:VAL:HG23	2.12	0.50
1:B:8:ARG:HG2	1:B:98:ASP:OD2	2.11	0.50
1:A:248:MET:HE3	1:A:251:ALA:HB3	1.94	0.50
1:A:261:ARG:HB3	1:A:289:GLN:NE2	2.27	0.49
1:A:262:SER:O	1:A:289:GLN:HG3	2.11	0.49
1:B:198:LEU:HG	1:B:198:LEU:N	2.27	0.49
1:A:310:LEU:HD13	1:A:310:LEU:C	2.38	0.49
1:B:159:VAL:HG22	1:B:159:VAL:O	2.13	0.49
1:B:40:LEU:HG	1:B:107:VAL:CG1	2.43	0.49
1:B:41:GLY:HA2	1:B:107:VAL:HG21	1.93	0.49
1:B:146:MET:SD	1:B:349:GLU:HG3	2.52	0.49
1:B:13:ALA:HB3	1:B:39:TRP:CZ2	2.48	0.49
1:A:205:VAL:HG21	1:A:315:VAL:CG1	2.43	0.49
1:B:198:LEU:HG	1:B:198:LEU:CB	0.97	0.49
1:B:205:VAL:HG12	1:B:209:LEU:CD1	2.43	0.48
1:B:20:VAL:HG21	1:B:46:MET:CE	2.43	0.48
1:B:147:GLN:HE22	1:B:152:ALA:H	1.60	0.48
1:A:17:GLY:H	1:A:46:MET:HE1	1.77	0.48
1:B:198:LEU:CG	1:B:198:LEU:HB2	0.97	0.48
1:A:22:PRO:HB2	1:A:103:MET:HE2	1.95	0.48
1:B:47:GLU:C	1:B:49:ASP:H	2.21	0.48
1:A:78:PRO:O	1:A:81:ILE:HG22	2.14	0.48
1:B:116:TRP:CD1	1:B:141:ILE:HB	2.48	0.48
1:B:50:LEU:HD11	1:B:54:HIS:HE1	1.79	0.48
1:B:225:GLN:CD	1:B:225:GLN:N	2.71	0.48
1:B:352:ARG:HG2	1:B:352:ARG:HH11	1.79	0.48
1:B:148:ALA:HA	1:B:160:GLY:CA	2.44	0.48
1:B:20:VAL:HG21	1:B:46:MET:SD	2.54	0.48
1:B:28:HIS:NE2	1:B:54:HIS:CD2	2.80	0.48
1:B:61:ILE:O	1:B:61:ILE:HG13	2.14	0.47
1:A:205:VAL:HG21	1:A:315:VAL:HG11	1.95	0.47
1:B:46:MET:HG3	1:B:47:GLU:H	1.76	0.47
1:B:51:VAL:HB	1:B:52:PRO:HD3	1.96	0.47
1:B:21:PHE:HB2	1:B:22:PRO:HD3	1.96	0.47
1:B:262:SER:HB2	1:B:289:GLN:HB3	1.96	0.47
1:A:352:ARG:NH1	1:A:355:ARG:NH1	2.62	0.47
1:B:17:GLY:HA3	2:B:402:UD1:O6'	2.15	0.47
1:B:346:VAL:O	1:B:350:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HA	1:A:214:THR:HG23	1.96	0.47
1:B:344:GLU:OE1	1:B:344:GLU:N	2.48	0.47
1:A:79:LEU:HD12	1:A:79:LEU:N	2.18	0.47
1:A:352:ARG:HH12	1:A:355:ARG:NH1	2.13	0.47
1:B:116:TRP:CB	1:B:141:ILE:HD12	2.44	0.47
1:A:19:HIS:HD2	1:A:127:GLN:OE1	1.97	0.46
1:A:225:GLN:CD	1:A:225:GLN:N	2.74	0.46
1:A:92:MET:HE1	1:A:114:ALA:CB	2.45	0.46
1:A:197:ILE:HG23	1:A:198:LEU:N	2.31	0.46
1:B:338:SER:O	1:B:340:PRO:HD3	2.15	0.46
1:B:355:ARG:O	1:B:355:ARG:HG3	2.16	0.46
1:A:133:LEU:N	1:A:133:LEU:HD22	2.30	0.46
1:A:173:PRO:O	1:A:174:GLN:C	2.59	0.46
1:B:20:VAL:HG23	1:B:21:PHE:N	2.31	0.46
1:A:306:GLU:CB	1:A:308:PRO:HD2	2.46	0.46
1:A:307:GLN:N	1:A:308:PRO:CD	2.79	0.46
1:B:211:ASP:CG	1:B:211:ASP:HB2	0.97	0.46
1:A:281:PRO:HG2	1:A:304:ILE:CG2	2.47	0.45
1:A:9:LEU:HD12	1:A:99:VAL:O	2.16	0.45
1:A:113:LEU:HD23	1:A:141:ILE:CD1	2.47	0.45
1:B:8:ARG:HD2	1:B:96:LYS:O	2.16	0.45
1:B:42:THR:C	1:B:60:PHE:HD2	2.24	0.45
1:B:69:LYS:HE3	1:B:80:ARG:HH21	1.81	0.45
1:A:13:ALA:HB2	1:A:103:MET:HB2	1.98	0.45
1:A:147:GLN:OE1	1:A:152:ALA:HB3	2.17	0.45
1:A:262:SER:C	1:A:289:GLN:HG3	2.42	0.45
1:B:159:VAL:HG21	1:B:346:VAL:HG23	1.99	0.45
1:A:271:ALA:HB2	1:A:296:LEU:HD21	1.98	0.45
1:A:70:GLY:C	1:A:72:LYS:H	2.25	0.45
1:B:185:ARG:HB3	1:B:254:TRP:CH2	2.51	0.45
1:B:159:VAL:HG23	1:B:345:ARG:CB	2.47	0.44
1:B:307:GLN:HB2	1:B:308:PRO:HD3	1.99	0.44
1:A:65:GLY:O	1:A:69:LYS:HE2	2.17	0.44
1:A:335:ARG:HG3	1:A:335:ARG:HH11	1.82	0.44
1:B:19:HIS:HD2	1:B:127:GLN:HE21	1.63	0.44
1:B:205:VAL:O	1:B:209:LEU:HG	2.17	0.44
1:A:174:GLN:NE2	1:A:174:GLN:HA	2.32	0.44
1:B:116:TRP:HB2	1:B:141:ILE:HD12	1.99	0.44
1:B:176:ARG:NH1	4:B:505:HOH:O	2.50	0.44
1:A:22:PRO:HB3	1:A:162:PRO:HD2	2.00	0.44
1:A:224:GLN:HB3	1:A:225:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:HA	4:B:548:HOH:O	2.16	0.44
1:A:40:LEU:C	1:A:40:LEU:CD2	2.91	0.44
1:B:159:VAL:CG2	1:B:345:ARG:HB2	2.48	0.44
1:B:308:PRO:HB2	1:B:309:GLN:NE2	2.33	0.43
1:A:267:VAL:HG11	1:A:292:ASN:O	2.17	0.43
1:B:44:ASP:O	1:B:45:ARG:NH1	2.49	0.43
1:B:248:MET:HG3	1:B:252:TYR:CE1	2.53	0.43
1:B:248:MET:HG2	2:B:402:UD1:O2'	2.17	0.43
1:B:61:ILE:HD11	1:B:107:VAL:HG13	2.00	0.43
1:B:198:LEU:HD11	1:B:198:LEU:HB3	0.64	0.43
1:B:198:LEU:HD12	1:B:198:LEU:HB3	0.64	0.43
1:B:198:LEU:HD13	1:B:198:LEU:HB3	0.64	0.43
1:A:307:GLN:HE21	1:A:307:GLN:CA	2.29	0.43
1:A:52:PRO:C	1:A:54:HIS:H	2.27	0.43
1:B:106:TYR:O	1:B:107:VAL:C	2.62	0.43
1:B:235:GLY:C	1:B:237:PRO:HD3	2.43	0.43
1:B:279:PHE:C	1:B:281:PRO:HD3	2.43	0.43
1:A:203:PRO:HA	1:A:231:TYR:CE1	2.54	0.43
1:A:101:LEU:HD11	1:A:103:MET:SD	2.58	0.43
1:B:205:VAL:HG12	1:B:209:LEU:HD12	2.00	0.43
1:A:50:LEU:O	1:A:54:HIS:HD2	2.02	0.42
1:A:106:TYR:HA	1:A:134:THR:HG21	2.01	0.42
1:A:257:VAL:HG22	1:A:258:VAL:N	2.35	0.42
1:B:229:GLN:O	1:B:232:ALA:HB3	2.19	0.42
1:B:310:LEU:HD13	1:B:310:LEU:C	2.44	0.42
1:A:10:MET:HE1	1:A:91:ILE:CG2	2.50	0.42
1:A:135:ASN:HD22	1:A:135:ASN:HA	1.62	0.42
1:B:352:ARG:HG2	1:B:352:ARG:NH1	2.33	0.42
1:B:51:VAL:HG12	1:B:56:ILE:HB	2.02	0.42
1:B:107:VAL:O	1:B:108:SER:C	2.63	0.42
1:B:137:TRP:C	1:B:139:ALA:N	2.77	0.42
1:A:351:SER:O	1:A:354:ALA:HB3	2.20	0.42
1:B:9:LEU:HD13	1:B:99:VAL:HG13	2.01	0.42
1:B:9:LEU:HD12	1:B:10:MET:H	1.84	0.42
1:B:22:PRO:HB3	1:B:162:PRO:HD2	2.02	0.42
1:B:265:LEU:O	1:B:269:GLU:HG3	2.19	0.42
1:B:307:GLN:HE21	1:B:307:GLN:HB3	1.67	0.42
1:A:71:ILE:O	1:A:75:ILE:HD13	2.20	0.41
1:A:313:ASP:O	1:A:317:ASN:HB2	2.19	0.41
1:B:109:GLY:N	1:B:134:THR:HG21	2.34	0.41
1:A:107:VAL:HG22	1:A:107:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HB3	1:A:212:SER:OG	2.20	0.41
1:A:352:ARG:NH1	1:A:355:ARG:CZ	2.83	0.41
1:B:89:ARG:CA	1:B:114:ALA:HB1	2.50	0.41
1:B:16:THR:O	1:B:20:VAL:HG22	2.19	0.41
1:A:72:LYS:O	1:A:76:ALA:HB2	2.21	0.41
1:A:252:TYR:O	1:A:275:LEU:HD11	2.21	0.41
1:A:341:ASP:HB2	1:A:344:GLU:HG2	2.03	0.41
1:A:162:PRO:HB3	1:A:343:THR:OG1	2.20	0.41
1:B:159:VAL:HG23	1:B:345:ARG:HD2	2.02	0.41
1:A:21:PHE:HB3	3:A:502:GOL:H11	2.03	0.41
1:A:64:SER:C	1:A:66:LEU:H	2.29	0.41
1:A:95:TYR:O	1:A:96:LYS:C	2.63	0.41
1:A:236:GLN:HB3	1:A:239:HIS:CD2	2.56	0.41
1:A:247:ASP:HA	4:A:538:HOH:O	2.21	0.41
1:B:150:PRO:HG3	1:B:158:VAL:HG21	2.01	0.41
1:B:343:THR:HB	1:B:344:GLU:OE1	2.21	0.41
1:A:51:VAL:HB	1:A:52:PRO:HD3	2.02	0.41
1:B:77:ALA:HB1	1:B:80:ARG:HG3	2.03	0.41
1:A:352:ARG:O	1:A:355:ARG:HG3	2.20	0.40
1:B:90:ALA:HA	1:B:93:LYS:HE2	2.03	0.40
1:A:275:LEU:HA	1:A:276:PRO:HD3	1.91	0.40
1:B:61:ILE:HG13	1:B:63:ILE:HG23	2.02	0.40
1:B:266:THR:OG1	2:B:402:UD1:H5'2	2.21	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	348/364 (96%)	328 (94%)	16 (5%)	4 (1%)	11	22
1	B	348/364 (96%)	317 (91%)	26 (8%)	5 (1%)	9	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	696/728 (96%)	645 (93%)	42 (6%)	9 (1%)	9	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	133	LEU
1	B	49	ASP
1	B	155	ASN
1	B	35	TRP
1	A	154	PRO
1	B	154	PRO
1	A	71	ILE
1	B	14	GLY

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	261/273 (96%)	247 (95%)	14 (5%)	20	41
1	B	261/273 (96%)	247 (95%)	14 (5%)	20	41
All	All	522/546 (96%)	494 (95%)	28 (5%)	20	41

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	79	LEU
1	A	101	LEU
1	A	122	VAL
1	A	133	LEU
1	A	134	THR
1	A	135	ASN
1	A	170	LEU
1	A	177	LEU

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Mol	Chain	Res	Type
1	A	193	GLN
1	A	261	ARG
1	A	289	GLN
1	A	294	LEU
1	A	307	GLN
1	B	10	MET
1	B	16	THR
1	B	30	LEU
1	B	42	THR
1	B	101	LEU
1	B	130	ILE
1	B	154	PRO
1	B	174	GLN
1	B	198	LEU
1	B	211	ASP
1	B	218	GLN
1	B	261	ARG
1	B	307	GLN
1	B	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	29	HIS
1	A	33	GLN
1	A	36	GLN
1	A	125	HIS
1	A	128	ASN
1	A	135	ASN
1	A	155	ASN
1	A	174	GLN
1	A	193	GLN
1	A	200	GLN
1	A	217	HIS
1	A	225	GLN
1	A	229	GLN
1	A	236	GLN
1	A	288	GLN
1	A	307	GLN
1	A	317	ASN
1	B	19	HIS

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Mol	Chain	Res	Type
1	B	54	HIS
1	B	128	ASN
1	B	135	ASN
1	B	147	GLN
1	B	174	GLN
1	B	193	GLN
1	B	200	GLN
1	B	218	GLN
1	B	283	GLN
1	B	288	GLN
1	B	292	ASN
1	B	309	GLN
1	B	317	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	UD1	B	402	-	40,41,41	1.87	2 (5%)	59,62,62	1.18	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	504	-	5,5,5	1.31	0	5,5,5	0.31	0
3	GOL	A	503	-	5,5,5	1.34	1 (20%)	5,5,5	0.41	0
3	GOL	A	502	-	5,5,5	1.27	1 (20%)	5,5,5	0.38	0
2	UD1	A	401	-	40,41,41	2.07	2 (5%)	59,62,62	1.08	4 (6%)
3	GOL	A	501	-	5,5,5	0.96	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UD1	B	402	-	-	6/26/63/63	0/3/3/3
3	GOL	B	504	-	-	3/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
2	UD1	A	401	-	-	6/26/63/63	0/3/3/3
3	GOL	A	501	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	UD1	PB-O3A	-9.01	1.49	1.59
2	A	401	UD1	PA-O3A	-8.80	1.50	1.59
2	B	402	UD1	PA-O3A	-8.40	1.50	1.59
2	B	402	UD1	PB-O3A	-7.58	1.51	1.59
3	A	503	GOL	C3-C2	2.10	1.59	1.51
3	A	502	GOL	C1-C2	2.05	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	UD1	O2B-PB-O3A	4.41	119.20	107.27
2	B	402	UD1	O2A-PA-O3A	4.32	118.95	107.27
2	A	401	UD1	O2A-PA-O3A	4.22	118.68	107.27
2	A	401	UD1	O2B-PB-O3A	4.00	118.09	107.27
2	B	402	UD1	O3A-PB-O1B	2.70	118.84	110.70
2	A	401	UD1	O3A-PB-O1B	2.64	118.63	110.70
2	A	401	UD1	O5'-C1'-O1'	-2.15	108.55	111.36
2	B	402	UD1	O5'-C1'-O1'	-2.08	108.64	111.36

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	UD1	C8'-C7'-N2'-C2'
2	A	401	UD1	O7'-C7'-N2'-C2'
2	A	401	UD1	O4B-C4B-C5B-O5B
2	B	402	UD1	C8'-C7'-N2'-C2'
3	A	501	GOL	O1-C1-C2-O2
3	A	501	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	B	504	GOL	O1-C1-C2-C3
2	B	402	UD1	O7'-C7'-N2'-C2'
2	A	401	UD1	C3B-C4B-C5B-O5B
3	A	502	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-O2
2	B	402	UD1	C3B-C4B-C5B-O5B
2	B	402	UD1	O4B-C4B-C5B-O5B
3	A	502	GOL	O2-C2-C3-O3
3	B	504	GOL	O2-C2-C3-O3
2	B	402	UD1	PB-O3A-PA-O2A
2	B	402	UD1	PB-O3A-PA-O1A
2	A	401	UD1	PB-O3A-PA-O1A
2	A	401	UD1	PB-O3A-PA-O2A

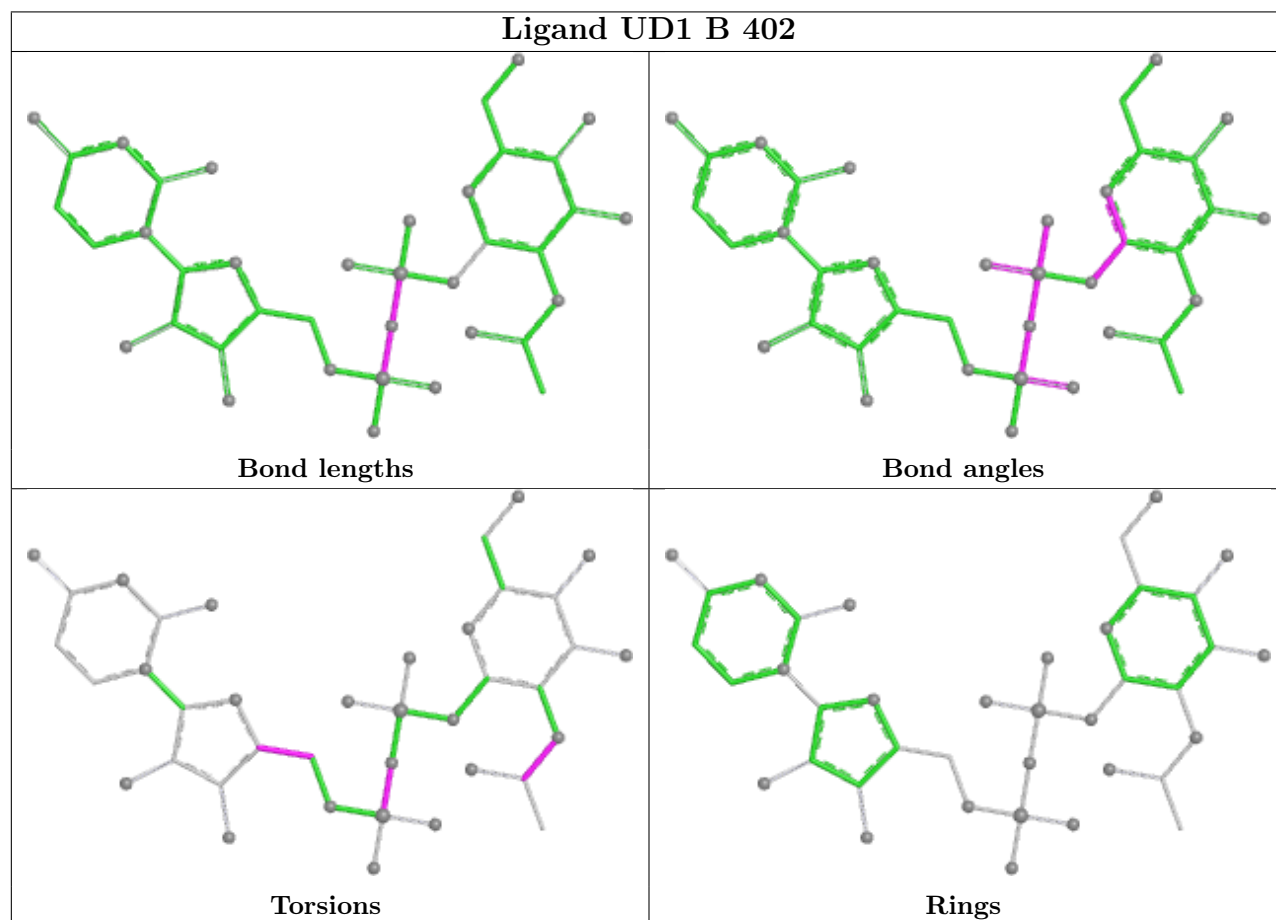
There are no ring outliers.

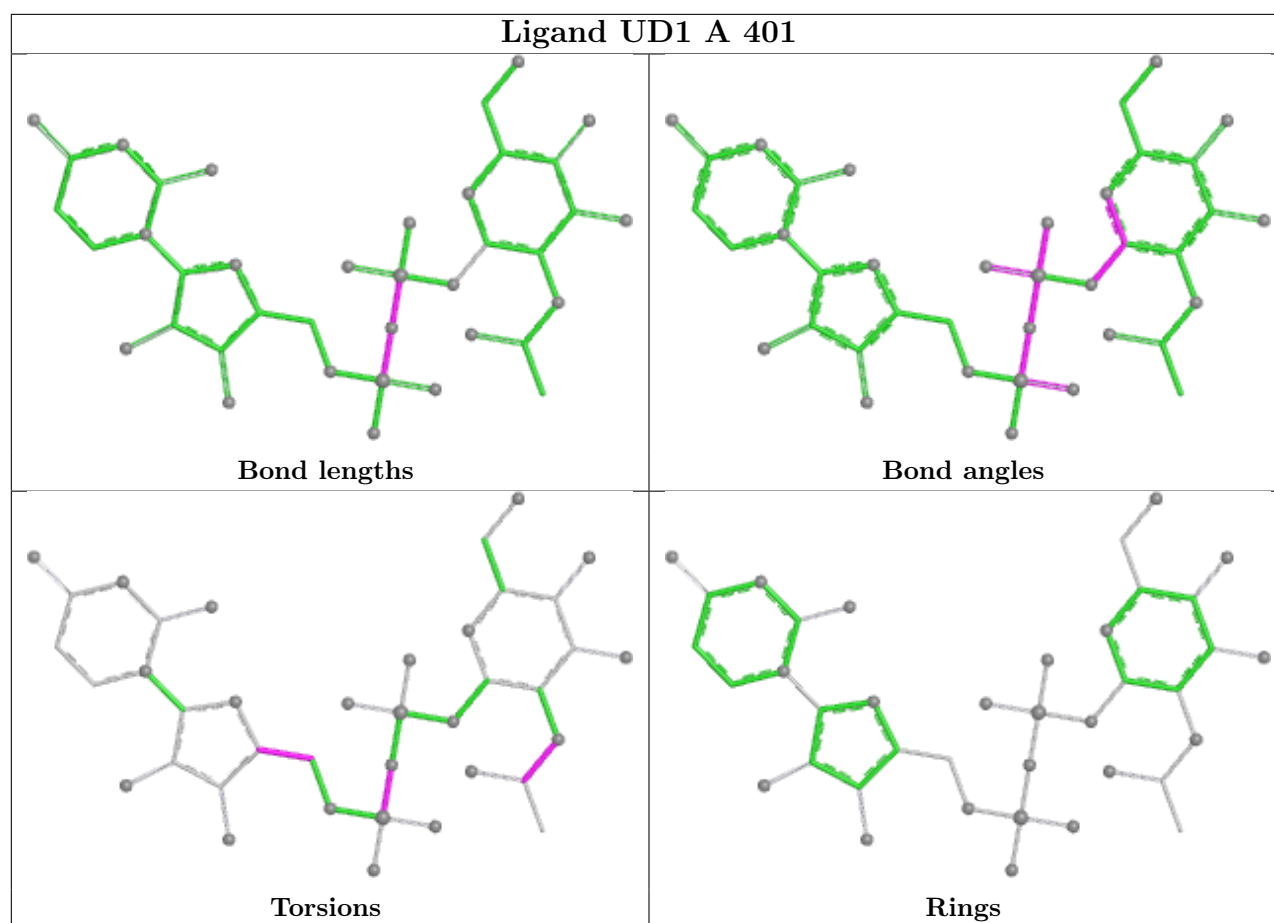
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	UD1	5	0
3	A	502	GOL	1	0
2	A	401	UD1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.