



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:29 PM UTC

PDB ID : 1L9N / pdb_0000119n
Title : Three-dimensional structure of the human transglutaminase 3 enzyme: binding of calcium ions change structure for activation
Authors : Ahvazi, B.
Deposited on : 2002-03-26
Resolution : 2.10 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

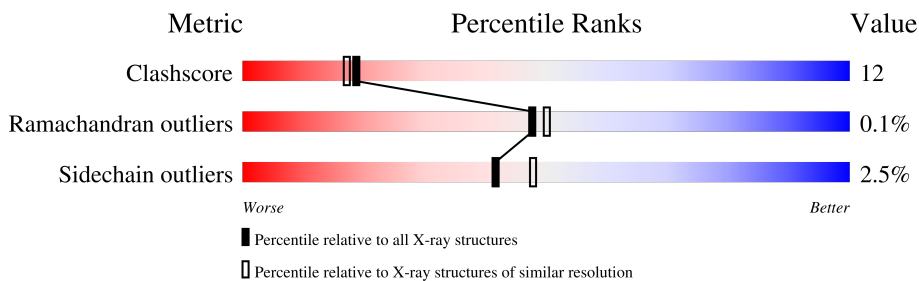
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	692	 71%24% . .
1	B	692	 74%22% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11561 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.

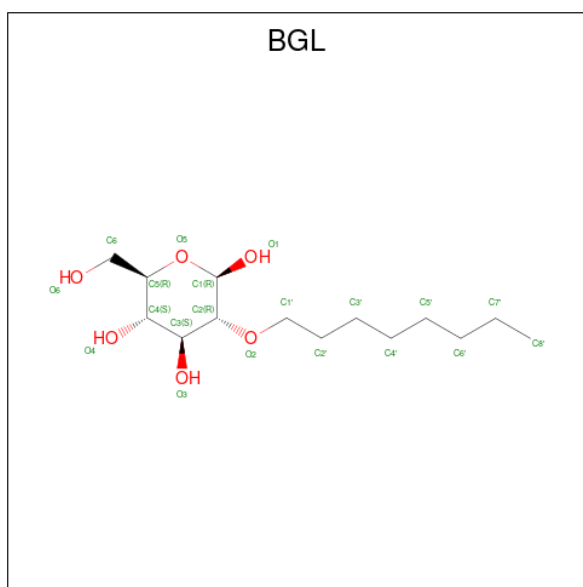
- Molecule 1 is a protein called Protein-glutamine glutamyltransferase E3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	0	0
			5250	3313	913	1001	23			
1	B	673	Total	C	N	O	S	0	0	0
			5250	3313	913	1001	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ASP	ASN	SEE REMARK 999	UNP Q08188
A	264	LEU	PHE	engineered mutation	UNP Q08188
A	561	ARG	LYS	SEE REMARK 999	UNP Q08188
A	653	ARG	GLY	SEE REMARK 999	UNP Q08188
B	250	ASP	ASN	SEE REMARK 999	UNP Q08188
B	264	LEU	PHE	engineered mutation	UNP Q08188
B	561	ARG	LYS	SEE REMARK 999	UNP Q08188
B	653	ARG	GLY	SEE REMARK 999	UNP Q08188

- Molecule 2 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	3	Total	Ca	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	511	Total	O	0	0
			511	511		

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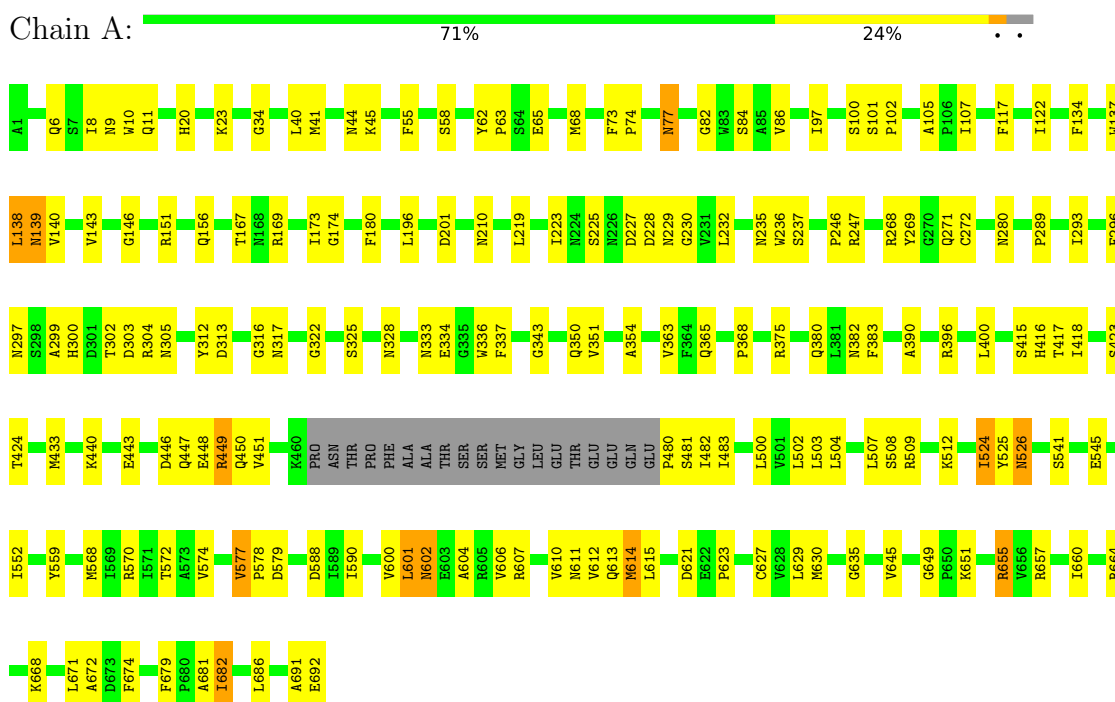
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	502	Total	O	0	0
			502	502		

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.

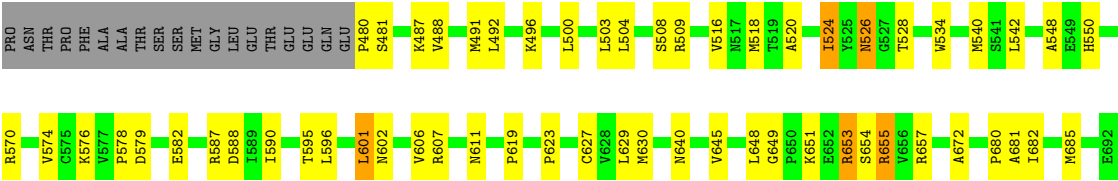
Note EDS was not executed.

• Molecule 1: Protein-glutamine glutamyltransferase E3



• Molecule 1: Protein-glutamine glutamyltransferase E3





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.49Å 116.54Å 60.77Å 93.23° 92.99° 89.51°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11561	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: CA, CL, BGL

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	0/5360	0.89	12/7270 (0.2%)
1	B	0.37	0/5360	0.90	16/7270 (0.2%)
All	All	0.36	0/10720	0.89	28/14540 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	VAL	N-CA-C	9.67	119.51	110.42
1	B	343	GLY	CA-C-N	8.00	127.72	119.56
1	B	343	GLY	C-N-CA	8.00	127.72	119.56
1	A	272	CYS	N-CA-C	7.83	120.50	111.11
1	B	272	CYS	N-CA-C	7.71	120.36	111.11
1	A	232	LEU	N-CA-C	6.90	120.48	109.24
1	B	232	LEU	N-CA-C	6.76	120.85	109.76
1	A	423	SER	N-CA-C	6.56	120.22	109.85
1	B	681	ALA	N-CA-C	6.27	119.90	111.24
1	B	423	SER	N-CA-C	6.23	119.34	109.50
1	A	524	ILE	N-CA-C	-6.04	99.61	108.97
1	A	681	ALA	N-CA-C	6.02	119.54	111.24
1	B	524	ILE	N-CA-C	-6.01	99.62	109.12
1	A	146	GLY	N-CA-C	5.82	120.22	112.77
1	A	682	ILE	N-CA-C	-5.82	101.21	108.89
1	A	210	ASN	N-CA-C	-5.71	105.97	113.17
1	B	146	GLY	N-CA-C	5.70	121.01	113.37
1	B	318	PRO	N-CA-C	-5.61	102.46	111.38
1	A	343	GLY	CA-C-N	5.57	125.24	119.56
1	A	343	GLY	C-N-CA	5.57	125.24	119.56
1	B	682	ILE	N-CA-C	-5.54	101.57	108.89
1	B	210	ASN	N-CA-C	-5.53	106.20	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	ILE	N-CA-C	5.37	116.04	108.36
1	B	516	VAL	N-CA-C	5.26	115.16	107.37
1	B	311	TYR	N-CA-C	5.23	117.92	109.40
1	B	255	ILE	N-CA-C	5.16	115.37	110.42
1	A	156	GLN	N-CA-C	5.05	119.50	113.23
1	B	228	ASP	N-CA-C	5.04	120.15	112.54

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	5250	0	5194	137	0
1	B	5250	0	5194	116	0
2	A	20	0	28	1	0
2	B	20	0	28	4	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	511	0	0	17	0
5	B	502	0	0	17	0
All	All	11561	0	10444	250	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 (250) 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:606:VAL:HG12	1:B:607:ARG:HG3	1.46	0.97
1:A:691:ALA:O	1:A:692:GLU:HB2	1.75	0.85
1:A:299:ALA:HB2	1:A:418:ILE:HD13	1.64	0.80
1:A:502:LEU:HG	1:A:504:LEU:CD2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:ARG:HG3	1:B:653:ARG:HH11	1.47	0.78
1:B:161:ILE:HD12	1:B:172:MET:HE3	1.65	0.77
1:B:82:GLY:HA2	1:B:102:PRO:HB3	1.65	0.77
1:A:169:ARG:HD2	2:A:1015:BGL:H5	1.67	0.76
1:A:502:LEU:HG	1:A:504:LEU:HD21	1.67	0.76
1:A:600:VAL:HG23	1:A:686:LEU:HD21	1.69	0.75
1:A:570:ARG:HD3	1:A:588:ASP:OD1	1.85	0.74
1:A:303:ASP:HB3	1:A:305:ASN:ND2	2.02	0.74
1:A:657:ARG:HD3	5:A:1509:HOH:O	1.89	0.73
1:A:173:ILE:HD13	5:A:1344:HOH:O	1.88	0.72
1:B:570:ARG:HD3	1:B:588:ASP:OD1	1.88	0.72
1:A:449:ARG:HE	1:A:449:ARG:HA	1.52	0.72
1:A:82:GLY:HA2	1:A:102:PRO:HB3	1.70	0.72
1:A:325:SER:HB2	5:A:1455:HOH:O	1.89	0.71
1:B:526:ASN:H	1:B:526:ASN:HD22	1.38	0.71
1:A:167:THR:HG22	1:A:296:PHE:HB3	1.73	0.71
1:A:526:ASN:HD22	1:A:526:ASN:H	1.38	0.69
1:B:437:ASP:HB3	5:B:1124:HOH:O	1.92	0.69
1:B:492:LEU:HD12	2:B:1016:BGL:H4	1.74	0.69
1:A:122:ILE:HG13	1:B:619:PRO:HB3	1.75	0.68
1:B:509:ARG:HG2	5:B:1410:HOH:O	1.94	0.68
1:A:77:ASN:HA	1:A:86:VAL:HG13	1.75	0.67
1:B:235:ASN:ND2	1:B:237:SER:H	1.93	0.67
1:A:6:GLN:NE2	1:A:44:ASN:HA	2.11	0.66
1:B:449:ARG:O	1:B:453:GLN:HG2	1.96	0.65
1:A:139:ASN:HD22	1:A:140:VAL:H	1.44	0.65
1:B:235:ASN:C	1:B:235:ASN:HD22	2.05	0.65
1:B:418:ILE:HB	5:B:1128:HOH:O	1.97	0.65
1:B:576:LYS:HD3	1:B:582:GLU:HG3	1.80	0.64
1:A:606:VAL:HG22	1:A:607:ARG:HG3	1.80	0.64
1:A:382:ASN:HB3	1:A:383:PHE:CD1	2.33	0.63
1:A:635:GLY:HA3	5:A:1443:HOH:O	1.98	0.63
1:A:235:ASN:ND2	1:A:237:SER:H	1.97	0.63
1:A:337:PHE:CE1	1:A:350:GLN:HG3	2.34	0.63
1:A:526:ASN:HD22	1:A:526:ASN:N	1.93	0.63
1:B:102:PRO:HG2	1:B:105:ALA:HB2	1.79	0.63
1:A:9:ASN:HB3	1:A:40:LEU:HB2	1.80	0.62
1:A:235:ASN:C	1:A:235:ASN:HD22	2.07	0.62
1:B:526:ASN:HD22	1:B:526:ASN:N	1.96	0.62
1:B:111:THR:HG23	1:B:126:LYS:HE3	1.80	0.61
1:A:316:GLY:HA2	1:A:574:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:SER:HA	5:A:1170:HOH:O	2.00	0.61
1:A:668:LYS:HE2	5:A:1443:HOH:O	2.00	0.60
1:A:41:MET:HE1	1:A:55:PHE:CE2	2.36	0.60
1:B:77:ASN:OD1	1:B:86:VAL:HG13	2.02	0.60
1:B:337:PHE:CE1	1:B:350:GLN:HG3	2.36	0.60
1:B:488:VAL:HA	1:B:500:LEU:HD23	1.82	0.60
1:B:380:GLN:HG3	1:B:458:LYS:HD3	1.84	0.60
1:A:449:ARG:HA	1:A:449:ARG:NE	2.17	0.59
1:B:542:LEU:HD21	1:B:548:ALA:HB2	1.85	0.59
1:B:611:ASN:OD1	1:B:657:ARG:HD2	2.02	0.59
1:B:235:ASN:HD22	1:B:236:TRP:N	2.00	0.59
1:B:219:LEU:O	1:B:223:ILE:HG12	2.03	0.58
1:A:23:LYS:HE3	1:A:180:PHE:CE2	2.40	0.57
1:A:289:PRO:HB2	1:A:336:TRP:HB3	1.87	0.57
1:B:134:PHE:HB3	1:B:143:VAL:HG21	1.86	0.57
1:B:54:GLU:HB2	1:B:115:GLN:HB3	1.84	0.57
1:A:41:MET:HE3	1:A:97:ILE:HD12	1.86	0.56
1:B:169:ARG:O	1:B:169:ARG:HG3	2.03	0.56
1:A:396:ARG:HD3	1:A:417:THR:HG21	1.87	0.56
1:A:293:ILE:HG13	1:A:334:GLU:HG3	1.87	0.56
1:A:322:GLY:HA3	5:A:1456:HOH:O	2.03	0.56
1:B:653:ARG:HG3	1:B:653:ARG:NH1	2.19	0.56
1:B:259:TRP:CZ2	1:B:264:LEU:HD22	2.41	0.56
1:B:99:ILE:HD13	1:B:112:MET:HE1	1.88	0.56
1:A:446:ASP:O	1:A:450:GLN:HG3	2.07	0.55
1:A:382:ASN:HB3	1:A:383:PHE:CG	2.41	0.55
1:B:47:LEU:C	1:B:47:LEU:HD23	2.31	0.55
1:B:23:LYS:HE3	1:B:180:PHE:CE2	2.42	0.54
1:B:382:ASN:HB3	1:B:383:PHE:CG	2.42	0.54
1:A:137:TRP:CE2	1:A:151:ARG:HD3	2.42	0.54
1:A:627:CYS:HB3	1:A:674:PHE:CZ	2.43	0.54
1:A:602:ASN:N	1:A:602:ASN:HD22	2.04	0.54
1:A:138:LEU:HD22	1:A:140:VAL:HG22	1.89	0.54
1:A:102:PRO:HG2	1:A:105:ALA:HB2	1.90	0.53
1:A:117:PHE:CD1	1:B:651:LYS:HD2	2.44	0.53
1:A:167:THR:HG23	5:A:1077:HOH:O	2.07	0.53
1:B:623:PRO:HB3	1:B:649:GLY:HA2	1.90	0.53
1:B:648:LEU:HD22	1:B:654:SER:HB2	1.90	0.53
1:A:223:ILE:HB	1:A:354:ALA:HB1	1.90	0.53
1:B:36:ASN:C	1:B:36:ASN:HD22	2.16	0.53
1:A:235:ASN:HD22	1:A:236:TRP:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:VAL:HG23	1:A:660:ILE:CG1	2.39	0.52
1:A:502:LEU:CG	1:A:504:LEU:HD21	2.38	0.52
1:B:228:ASP:O	1:B:229:ASN:HB2	2.10	0.52
1:B:587:ARG:HD3	5:B:1126:HOH:O	2.10	0.52
1:B:289:PRO:HB2	1:B:336:TRP:HB3	1.91	0.51
1:A:139:ASN:HD22	1:A:140:VAL:N	2.07	0.51
1:B:196:LEU:HG	1:B:228:ASP:HB3	1.93	0.51
1:B:247:ARG:HG2	1:B:273:TRP:CZ2	2.46	0.51
1:A:219:LEU:O	1:A:223:ILE:HG12	2.11	0.51
1:A:623:PRO:HB3	1:A:649:GLY:HA2	1.93	0.51
1:A:447:GLN:O	1:A:451:VAL:HG23	2.10	0.51
1:B:526:ASN:H	1:B:526:ASN:ND2	2.08	0.51
1:B:8:ILE:HD12	1:B:41:MET:HE2	1.92	0.50
1:B:142:SER:HB2	1:B:338:VAL:HG22	1.92	0.50
1:B:380:GLN:CD	1:B:380:GLN:H	2.19	0.50
1:B:169:ARG:HD2	2:B:1016:BGL:H62	1.93	0.50
1:B:382:ASN:HB3	1:B:383:PHE:CD1	2.46	0.50
1:B:655:ARG:HB2	5:B:1448:HOH:O	2.10	0.50
1:A:691:ALA:O	1:A:692:GLU:CB	2.54	0.50
1:A:65:GLU:O	1:A:68:MET:HE2	2.12	0.49
1:B:167:THR:HG23	5:B:1285:HOH:O	2.12	0.49
1:A:235:ASN:HD22	1:A:237:SER:H	1.59	0.49
1:A:390:ALA:HB3	5:A:1101:HOH:O	2.12	0.49
1:A:316:GLY:HA2	1:A:574:VAL:CG2	2.43	0.49
1:A:41:MET:HE1	1:A:55:PHE:HE2	1.78	0.49
1:A:524:ILE:HB	1:A:526:ASN:HD21	1.78	0.49
1:A:512:LYS:HD2	1:A:577:VAL:HG11	1.95	0.48
1:A:679:PHE:HB3	1:A:682:ILE:HD11	1.95	0.48
1:A:611:ASN:OD1	1:A:657:ARG:HD2	2.13	0.48
1:B:524:ILE:HB	1:B:526:ASN:ND2	2.27	0.48
1:A:139:ASN:ND2	1:A:140:VAL:H	2.10	0.48
1:A:664:ARG:NH1	5:A:1073:HOH:O	2.45	0.48
1:B:137:TRP:CE2	1:B:151:ARG:HD3	2.48	0.48
1:A:167:THR:HG22	1:A:296:PHE:CB	2.43	0.48
1:B:161:ILE:HD12	1:B:172:MET:CE	2.41	0.48
1:A:201:ASP:HB3	5:A:1129:HOH:O	2.13	0.48
1:B:235:ASN:HD22	1:B:237:SER:H	1.58	0.48
1:A:139:ASN:HD22	1:A:139:ASN:N	2.12	0.48
1:A:351:VAL:O	1:A:368:PRO:HA	2.13	0.48
1:A:524:ILE:HB	1:A:526:ASN:ND2	2.29	0.48
1:A:173:ILE:HG21	5:A:1344:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:VAL:HB	1:B:369:ALA:HB3	1.96	0.47
1:A:44:ASN:OD1	1:A:45:LYS:HG2	2.15	0.47
1:A:375:ARG:HG3	1:A:440:LYS:HA	1.96	0.47
1:B:300:HIS:HB2	5:B:1068:HOH:O	2.14	0.47
1:B:640:ASN:ND2	5:B:1150:HOH:O	2.47	0.47
1:A:174:GLY:HA3	1:A:671:LEU:HD21	1.96	0.47
1:B:503:LEU:HD23	1:B:504:LEU:N	2.29	0.47
1:A:293:ILE:HD13	1:A:424:THR:HB	1.95	0.47
1:B:520:ALA:HB3	1:B:534:TRP:HB3	1.96	0.47
1:B:351:VAL:O	1:B:368:PRO:HA	2.14	0.47
1:B:316:GLY:HA2	1:B:574:VAL:HG23	1.97	0.47
1:B:491:MET:CG	1:B:496:LYS:HE2	2.45	0.47
1:A:134:PHE:HB3	1:A:143:VAL:HG21	1.97	0.47
1:B:655:ARG:HD3	5:B:1175:HOH:O	2.15	0.47
1:B:524:ILE:HB	1:B:526:ASN:HD21	1.80	0.47
1:B:401:TYR:HD2	1:B:408:GLN:HB2	1.80	0.46
1:B:293:ILE:CG1	1:B:334:GLU:HG3	2.45	0.46
1:A:502:LEU:HG	1:A:504:LEU:HD22	1.97	0.46
1:B:595:THR:HG22	1:B:596:LEU:N	2.31	0.46
1:B:680:PRO:HB3	5:B:1488:HOH:O	2.14	0.46
1:A:610:VAL:HG23	1:A:660:ILE:HG12	1.98	0.46
1:A:630:MET:O	1:A:672:ALA:HA	2.16	0.46
1:A:107:ILE:HD13	1:A:134:PHE:CE2	2.51	0.45
1:A:228:ASP:O	1:A:229:ASN:HB2	2.16	0.45
1:A:559:TYR:CD1	1:A:559:TYR:C	2.94	0.45
1:B:9:ASN:HB3	1:B:40:LEU:HB2	1.97	0.45
1:B:375:ARG:HD3	5:B:1482:HOH:O	2.15	0.45
1:B:578:PRO:O	1:B:579:ASP:HB2	2.15	0.45
1:A:58:SER:HB2	1:A:63:PRO:HB3	1.98	0.45
1:A:139:ASN:ND2	1:A:140:VAL:N	2.65	0.45
1:A:424:THR:O	1:A:433:MET:HB3	2.16	0.45
1:B:75:LEU:HD13	1:B:75:LEU:O	2.17	0.45
1:A:416:HIS:CD2	1:A:443:GLU:OE1	2.69	0.45
1:A:602:ASN:N	1:A:602:ASN:ND2	2.65	0.45
1:A:247:ARG:HD2	5:A:1033:HOH:O	2.16	0.45
1:A:415:SER:O	1:A:416:HIS:HD2	1.99	0.45
1:A:606:VAL:HG12	1:A:692:GLU:CB	2.46	0.45
1:B:293:ILE:HG13	1:B:334:GLU:HG3	1.97	0.45
1:B:382:ASN:HA	1:B:383:PHE:HA	1.74	0.45
1:B:480:PRO:HD3	5:B:1487:HOH:O	2.17	0.45
1:A:481:SER:OG	1:A:508:SER:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:HA	1:A:230:GLY:N	2.32	0.45
1:A:246:PRO:CB	1:A:271:GLN:HG3	2.47	0.45
1:A:41:MET:HE1	1:A:55:PHE:CZ	2.52	0.45
1:A:328:ASN:ND2	1:A:568:MET:HE2	2.32	0.45
1:A:196:LEU:HG	1:A:228:ASP:HB3	2.00	0.44
1:A:303:ASP:O	1:A:304:ARG:HB2	2.16	0.44
1:A:578:PRO:O	1:A:579:ASP:HB2	2.17	0.44
1:B:82:GLY:CA	1:B:102:PRO:HB3	2.43	0.44
1:B:41:MET:HE1	1:B:55:PHE:CE2	2.53	0.44
1:B:481:SER:HB3	1:B:508:SER:HB2	1.99	0.44
1:A:483:ILE:HD13	1:A:507:LEU:HD11	1.98	0.44
1:A:568:MET:SD	1:A:590:ILE:HB	2.57	0.44
1:A:328:ASN:ND2	1:A:525:TYR:HA	2.32	0.44
1:A:448:GLU:OE2	1:A:449:ARG:NE	2.51	0.44
1:A:606:VAL:HG13	1:A:607:ARG:NH1	2.33	0.44
1:B:173:ILE:HA	5:B:1342:HOH:O	2.18	0.44
1:B:347:GLY:HA3	5:B:1096:HOH:O	2.18	0.44
1:A:541:SER:HB3	5:A:1283:HOH:O	2.18	0.44
1:A:312:TYR:CD2	1:A:572:THR:HG21	2.53	0.43
1:A:614:MET:O	1:A:614:MET:HE2	2.18	0.43
1:A:500:LEU:HB2	1:A:552:ILE:HB	2.00	0.43
1:B:303:ASP:HB2	1:B:305:ASN:ND2	2.33	0.43
1:A:62:TYR:N	1:A:63:PRO:HD3	2.33	0.43
1:A:300:HIS:NE2	1:A:302:THR:HG22	2.33	0.43
1:A:611:ASN:HD22	1:A:612:VAL:H	1.66	0.43
1:B:268:ARG:HA	1:B:269:TYR:HA	1.67	0.43
1:B:503:LEU:HD23	1:B:503:LEU:C	2.44	0.43
1:A:526:ASN:N	1:A:526:ASN:ND2	2.65	0.43
1:A:313:ASP:OD2	1:A:317:ASN:HB2	2.18	0.43
1:A:526:ASN:H	1:A:526:ASN:ND2	2.10	0.43
1:A:679:PHE:CB	1:A:682:ILE:HD11	2.49	0.43
1:B:213:LYS:HB2	1:B:213:LYS:NZ	2.34	0.43
1:A:480:PRO:HG2	5:A:1457:HOH:O	2.17	0.43
1:B:601:LEU:O	1:B:602:ASN:HB2	2.19	0.43
1:A:73:PHE:HA	1:A:74:PRO:HD3	1.84	0.42
1:A:328:ASN:HD22	1:A:525:TYR:HA	1.83	0.42
1:B:136:PRO:HG3	1:B:287:GLY:O	2.19	0.42
1:B:381:LEU:O	1:B:385:MET:HG3	2.19	0.42
1:A:615:LEU:HD23	1:A:655:ARG:HG2	2.01	0.42
1:A:363:VAL:HG22	1:A:365:GLN:NE2	2.34	0.42
1:B:630:MET:O	1:B:672:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:PHE:HB3	1:B:651:LYS:HD2	2.00	0.42
1:B:83:TRP:HA	1:B:100:SER:O	2.18	0.42
1:B:454:LYS:O	1:B:458:LYS:HG3	2.19	0.42
1:B:41:MET:HE1	1:B:55:PHE:HE2	1.85	0.42
1:B:82:GLY:HA3	5:B:1269:HOH:O	2.20	0.42
1:B:380:GLN:CG	1:B:458:LYS:HD3	2.48	0.42
1:A:297:ASN:O	1:A:418:ILE:HG23	2.20	0.42
1:A:334:GLU:HA	1:A:350:GLN:O	2.20	0.42
1:B:79:SER:C	1:B:81:GLY:H	2.28	0.42
1:B:172:MET:HE2	1:B:685:MET:HE1	2.02	0.42
1:B:259:TRP:CE2	1:B:264:LEU:HD22	2.54	0.42
1:A:268:ARG:HA	1:A:269:TYR:HA	1.66	0.42
1:B:393:ASN:CG	5:B:1432:HOH:O	2.63	0.42
1:B:653:ARG:NH1	1:B:653:ARG:CG	2.79	0.42
1:B:139:ASN:HA	1:B:144:PHE:CD1	2.55	0.41
1:B:526:ASN:ND2	1:B:528:THR:H	2.18	0.41
1:B:518:MET:HE1	1:B:550:HIS:CE1	2.55	0.41
1:A:10:TRP:O	1:A:11:GLN:C	2.63	0.41
1:A:280:ASN:HD22	1:A:333:ASN:HD22	1.68	0.41
1:A:601:LEU:HD11	1:A:613:GLN:NE2	2.35	0.41
1:A:604:ALA:HA	1:A:610:VAL:HG11	2.03	0.41
1:A:627:CYS:HB2	1:A:645:VAL:HB	2.01	0.41
1:B:447:GLN:CD	1:B:447:GLN:H	2.27	0.41
1:B:487:LYS:HG2	2:B:1016:BGL:H8'1	2.02	0.41
1:B:76:SER:O	1:B:77:ASN:O	2.39	0.41
1:B:318:PRO:HG2	1:B:570:ARG:HG2	2.02	0.41
1:A:621:ASP:OD1	1:A:651:LYS:NZ	2.48	0.41
1:A:20:HIS:HD2	5:A:1092:HOH:O	2.02	0.41
1:A:34:GLY:HA2	1:A:101:SER:O	2.21	0.41
1:A:268:ARG:HB3	1:A:269:TYR:CD1	2.55	0.41
1:B:223:ILE:HB	1:B:354:ALA:HB1	2.03	0.41
1:A:606:VAL:CG1	1:A:692:GLU:HG2	2.51	0.40
1:B:299:ALA:O	1:B:391:GLU:HA	2.21	0.40
1:B:590:ILE:H	2:B:1016:BGL:C6	2.33	0.40
1:A:84:SER:OG	1:A:100:SER:HB3	2.20	0.40
1:A:229:ASN:HA	5:A:1097:HOH:O	2.20	0.40
1:B:50:ASN:HB3	5:B:1041:HOH:O	2.20	0.40
1:B:23:LYS:HE3	1:B:180:PHE:CZ	2.56	0.40
1:B:175:TRP:CE2	1:B:251:GLY:HA2	2.56	0.40
1:B:627:CYS:HB2	1:B:645:VAL:HB	2.04	0.40
1:B:504:LEU:HD12	1:B:540:MET:HE1	2.02	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	669/692 (97%)	643 (96%)	25 (4%)	1 (0%)	48	50
1	B	669/692 (97%)	638 (95%)	30 (4%)	1 (0%)	48	50
All	All	1338/1384 (97%)	1281 (96%)	55 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	ASN
1	A	77	ASN

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	565/595 (95%)	548 (97%)	17 (3%)	36	41
1	B	551/595 (93%)	540 (98%)	11 (2%)	48	56
All	All	1116/1190 (94%)	1088 (98%)	28 (2%)	42	48

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

Mol	Chain	Res	Type
1	A	8	ILE

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Mol	Chain	Res	Type
1	A	138	LEU
1	A	139	ASN
1	A	227	ASP
1	A	380	GLN
1	A	400	LEU
1	A	449	ARG
1	A	503	LEU
1	A	509	ARG
1	A	526	ASN
1	A	545	GLU
1	A	577	VAL
1	A	601	LEU
1	A	602	ASN
1	A	614	MET
1	A	629	LEU
1	A	655	ARG
1	B	36	ASN
1	B	75	LEU
1	B	138	LEU
1	B	380	GLN
1	B	400	LEU
1	B	448	GLU
1	B	526	ASN
1	B	601	LEU
1	B	629	LEU
1	B	653	ARG
1	B	655	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	11	GLN
1	A	20	HIS
1	A	38	GLN
1	A	93	ASN
1	A	115	GLN
1	A	139	ASN
1	A	168	ASN
1	A	235	ASN
1	A	280	ASN
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	382	ASN
1	A	408	GLN
1	A	411	ASN
1	A	416	HIS
1	A	450	GLN
1	A	506	ASN
1	A	517	ASN
1	A	526	ASN
1	A	550	HIS
1	A	602	ASN
1	A	613	GLN
1	A	640	ASN
1	B	6	GLN
1	B	36	ASN
1	B	115	GLN
1	B	148	HIS
1	B	168	ASN
1	B	176	ASN
1	B	226	ASN
1	B	229	ASN
1	B	235	ASN
1	B	280	ASN
1	B	297	ASN
1	B	328	ASN
1	B	357	GLN
1	B	382	ASN
1	B	408	GLN
1	B	526	ASN
1	B	640	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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
2	BGL	B	1016	-	20,20,20	1.50	2 (10%)	24,25,25	1.69	6 (25%)
2	BGL	A	1015	-	20,20,20	1.47	2 (10%)	24,25,25	1.59	6 (25%)

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	BGL	B	1016	-	-	9/11/31/31	0/1/1/1
2	BGL	A	1015	-	-	9/11/31/31	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1015	BGL	O2-C1'	4.06	1.54	1.43
2	B	1016	BGL	C1-C2	3.94	1.56	1.52
2	B	1016	BGL	O2-C1'	3.93	1.53	1.43
2	A	1015	BGL	C1-C2	3.58	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1016	BGL	C6-C5-C4	3.52	121.66	113.02
2	A	1015	BGL	C6-C5-C4	3.38	121.31	113.02
2	B	1016	BGL	C1'-O2-C2	3.30	121.34	114.02
2	A	1015	BGL	C1'-O2-C2	3.27	121.28	114.02
2	B	1016	BGL	O6-C6-C5	3.19	122.19	111.33
2	A	1015	BGL	O6-C6-C5	3.09	121.85	111.33
2	B	1016	BGL	O4-C4-C3	2.71	116.76	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1015	BGL	O4-C4-C3	2.59	116.49	110.38
2	B	1016	BGL	O2-C2-C3	2.48	114.83	109.83
2	B	1016	BGL	O3-C3-C2	2.29	115.80	109.94
2	A	1015	BGL	O2-C2-C3	2.25	114.35	109.83
2	A	1015	BGL	O3-C3-C2	2.03	115.15	109.94

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1015	BGL	C2'-C1'-O2-C2
2	A	1015	BGL	O5-C5-C6-O6
2	B	1016	BGL	O5-C5-C6-O6
2	A	1015	BGL	C4-C5-C6-O6
2	B	1016	BGL	C4-C5-C6-O6
2	A	1015	BGL	C3'-C4'-C5'-C6'
2	A	1015	BGL	O2-C1'-C2'-C3'
2	B	1016	BGL	C4'-C5'-C6'-C7'
2	B	1016	BGL	C3'-C4'-C5'-C6'
2	B	1016	BGL	C5'-C6'-C7'-C8'
2	A	1015	BGL	C4'-C5'-C6'-C7'
2	A	1015	BGL	C1'-C2'-C3'-C4'
2	A	1015	BGL	C5'-C6'-C7'-C8'
2	B	1016	BGL	O2-C1'-C2'-C3'
2	B	1016	BGL	C1'-C2'-C3'-C4'
2	A	1015	BGL	C1-C2-O2-C1'
2	B	1016	BGL	C1-C2-O2-C1'
2	B	1016	BGL	C3-C2-O2-C1'

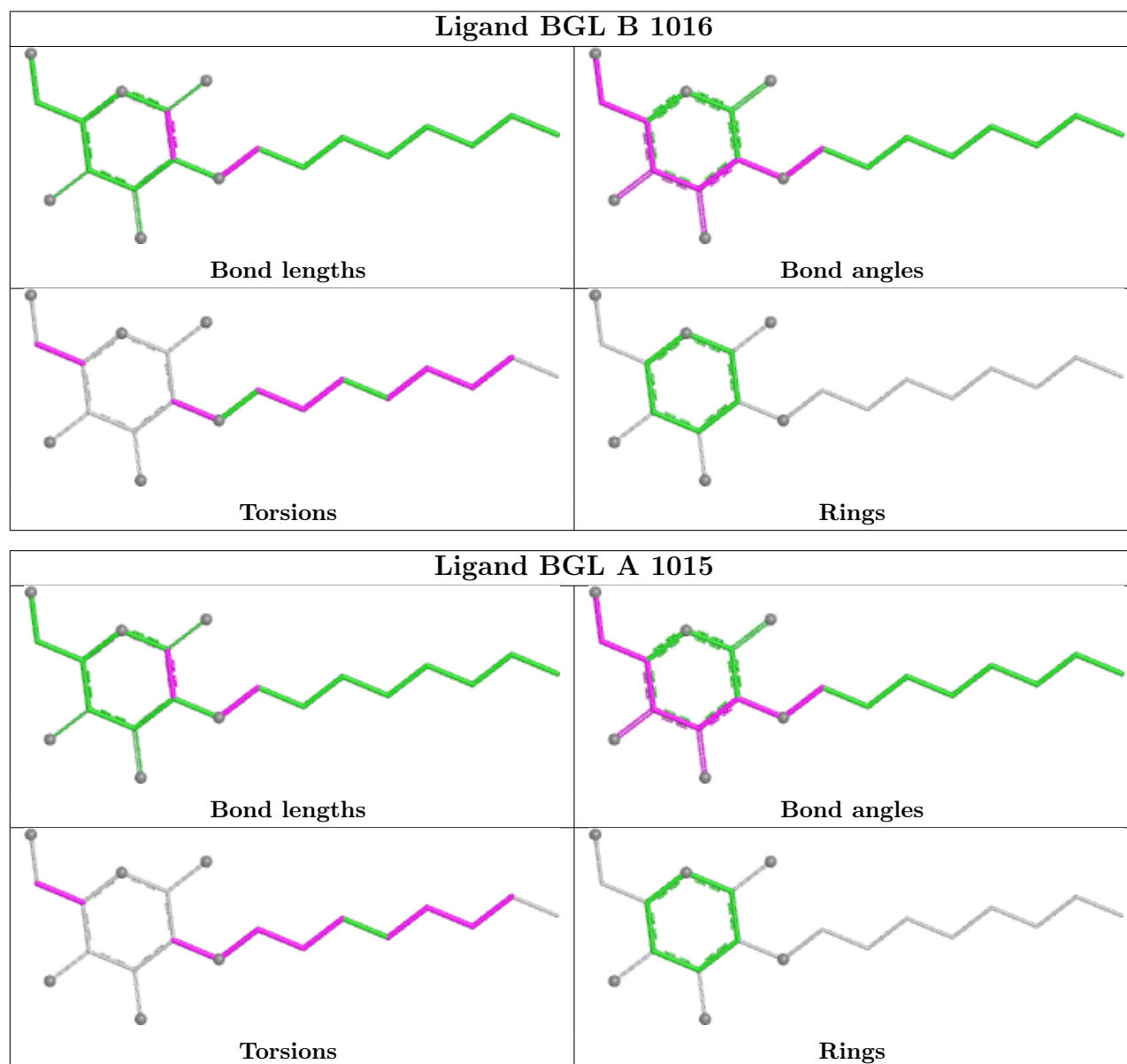
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1016	BGL	4	0
2	A	1015	BGL	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 ⓘ

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

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.