



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 AM UTC

PDB ID : 2CB3 / pdb_00002cb3
Title : Crystal structure of peptidoglycan recognition protein-LE in complex with tracheal cytotoxin (monomeric diaminopimelic acid-type peptidoglycan)
Authors : Lim, J.-H.; Kim, M.-S.; Oh, B.-H.
Deposited on : 2005-12-29
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

<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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

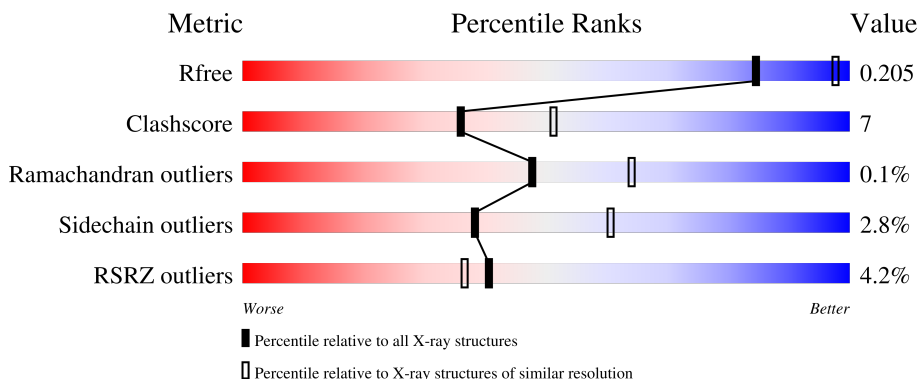
1 Overall quality at a glance i

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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	175	 3% 77% 21% ..
1	B	175	 3% 74% 21% . .
1	C	175	 6% 74% 23% ..
1	D	175	 5% 77% 19% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5942 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.

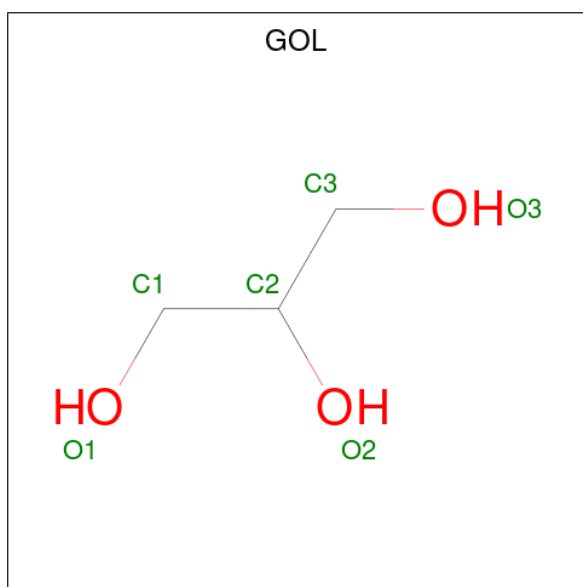
- Molecule 1 is a protein called PEPTIDOGLYCAN-RECOGNITION PROTEIN-LE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1365	862	242	251	10	0	0	1
1	B	170	1357	856	241	250	10	0	0	1
1	C	174	1388	875	247	256	10	0	0	1
1	D	171	1365	862	242	251	10	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

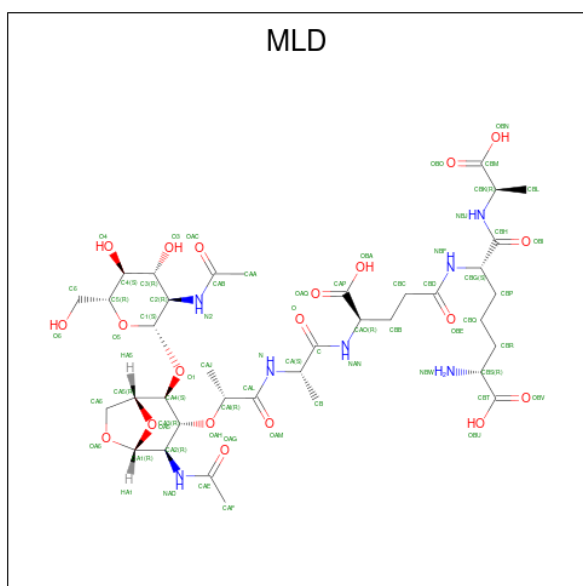
Chain	Residue	Modelled	Actual	Comment	Reference
A	227	SER	CYS	engineered mutation	UNP Q9VXN9
B	227	SER	CYS	engineered mutation	UNP Q9VXN9
C	227	SER	CYS	engineered mutation	UNP Q9VXN9
D	227	SER	CYS	engineered mutation	UNP Q9VXN9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is GLCNAC(BETA1-4)-MURNAC(1,6-ANHYDRO)-L-ALA-GAMMA-D-GLU-MESO-A2PM-D-ALA (CCD ID: MLD) (formula: $C_{37}H_{59}N_7O_{20}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			64	37	7	20		
3	B	1	Total	C	N	O	0	0
			64	37	7	20		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			64	37	7	20		
3	D	1	Total	C	N	O	0	0
			64	37	7	20		

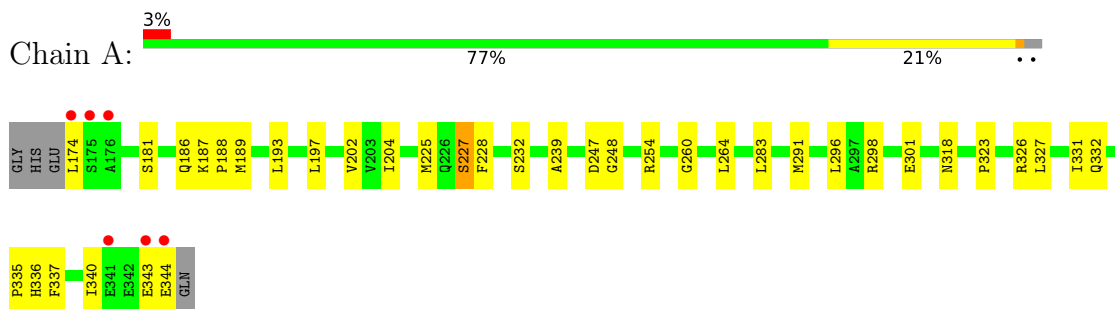
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	63	Total	O	0	0
			63	63		
4	C	50	Total	O	0	0
			50	50		
4	D	38	Total	O	0	0
			38	38		

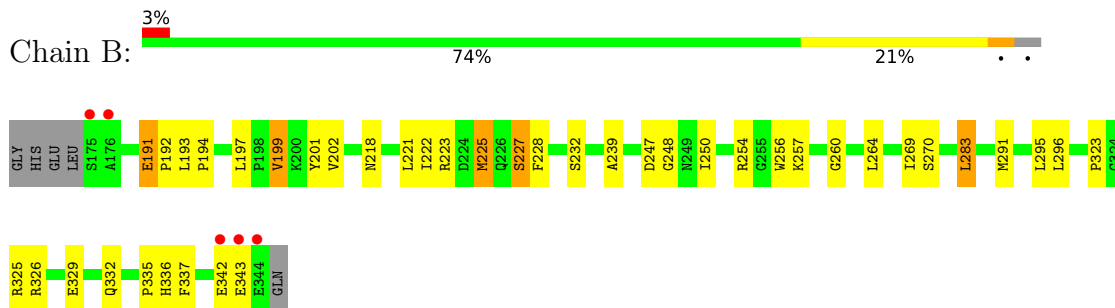
3 Residue-property plots [i](#)

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 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.

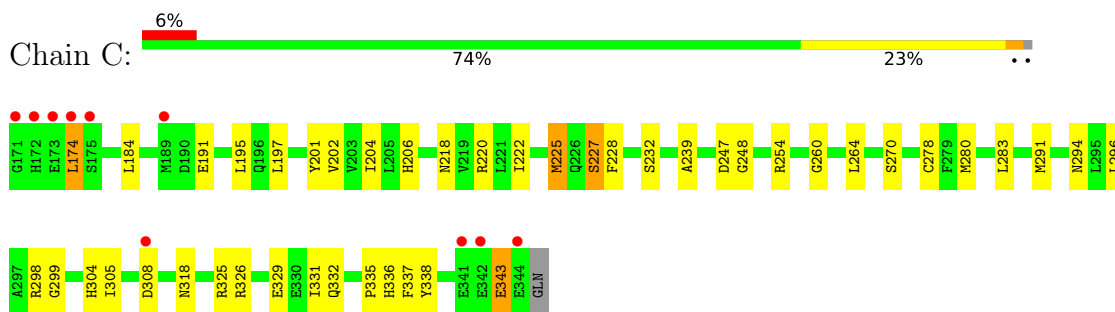
- Molecule 1: PEPTIDOGLYCAN-RECOGNITION PROTEIN-LE



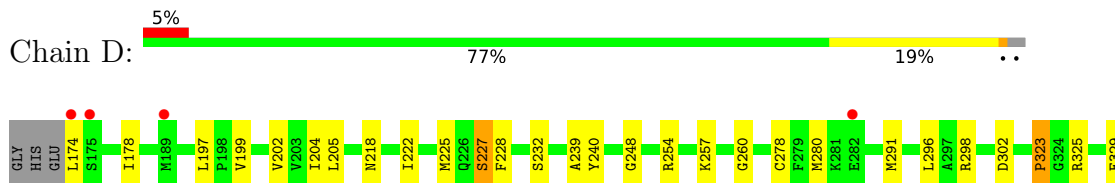
- Molecule 1: PEPTIDOGLYCAN-RECOGNITION PROTEIN-LE



- Molecule 1: PEPTIDOGLYCAN-RECOGNITION PROTEIN-LE



- Molecule 1: PEPTIDOGLYCAN-RECOGNITION PROTEIN-LE





4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	217.53Å 217.53Å 217.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.3 (30.00-2.40) 92.7 (30.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.39 (at 2.42Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.214 0.191 , 0.205	Depositor DCC
R_{free} test set	3107 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.030 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5942	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, MLD

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	0.65	4/1398 (0.3%)	0.92	2/1896 (0.1%)
1	B	0.64	4/1390 (0.3%)	0.91	4/1885 (0.2%)
1	C	0.67	3/1422 (0.2%)	0.91	3/1928 (0.2%)
1	D	0.66	3/1398 (0.2%)	0.92	5/1896 (0.3%)
All	All	0.65	14/5608 (0.2%)	0.91	14/7605 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	227	SER	CB-OG	18.00	1.78	1.42
1	C	227	SER	CB-OG	17.52	1.77	1.42
1	B	227	SER	CB-OG	17.19	1.76	1.42
1	A	227	SER	CB-OG	16.93	1.76	1.42
1	A	225	MET	SD-CE	6.10	1.94	1.79
1	D	225	MET	SD-CE	5.88	1.94	1.79
1	C	225	MET	SD-CE	5.82	1.94	1.79
1	B	225	MET	SD-CE	5.81	1.94	1.79
1	A	343	GLU	C-N	-5.74	1.25	1.33
1	B	343	GLU	C-N	-5.68	1.25	1.33
1	D	343	GLU	C-N	-5.54	1.25	1.33
1	C	343	GLU	C-N	-5.54	1.25	1.33
1	A	225	MET	CG-SD	5.25	1.93	1.80
1	B	225	MET	CG-SD	5.05	1.93	1.80

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	ALA	N-CA-C	8.36	120.39	111.28
1	B	239	ALA	N-CA-C	8.09	121.01	111.71
1	A	239	ALA	N-CA-C	7.35	120.35	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	ALA	N-CA-C	6.43	119.11	111.71
1	A	247	ASP	N-CA-C	-5.58	106.13	113.17
1	D	240	TYR	N-CA-C	5.39	118.50	110.52
1	B	247	ASP	N-CA-C	-5.27	106.62	113.16
1	C	247	ASP	N-CA-C	-5.27	106.82	113.20
1	B	257	LYS	N-CA-C	5.23	119.62	112.88
1	D	178	ILE	CA-C-N	5.18	125.16	120.03
1	D	178	ILE	C-N-CA	5.18	125.16	120.03
1	C	206	HIS	N-CA-C	-5.17	101.44	109.14
1	B	256	TRP	N-CA-C	5.06	117.53	111.71
1	D	257	LYS	N-CA-C	5.03	119.36	112.88

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	1365	0	1333	22	0
1	B	1357	0	1322	18	0
1	C	1388	0	1349	32	0
1	D	1365	0	1333	16	0
2	A	6	0	8	0	0
3	A	64	0	56	1	0
3	B	64	0	56	0	0
3	C	64	0	56	1	0
3	D	64	0	56	0	0
4	A	54	0	0	0	0
4	B	63	0	0	0	0
4	C	50	0	0	0	0
4	D	38	0	0	0	0
All	All	5942	0	5569	83	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 7.

All (83) 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:227:SER:CB	1:A:227:SER:OG	1.76	1.34
1:C:227:SER:OG	1:C:227:SER:CB	1.77	1.32
1:B:227:SER:CB	1:B:227:SER:OG	1.76	1.31
1:D:227:SER:OG	1:D:227:SER:CB	1.78	1.31
1:A:204:ILE:HG21	1:A:331:ILE:HD11	1.58	0.86
1:B:283:LEU:HD13	1:B:326:ARG:HG3	1.57	0.86
1:A:283:LEU:HD13	1:A:326:ARG:HG3	1.62	0.81
1:B:335:PRO:O	1:B:336:HIS:HB2	1.82	0.79
1:D:204:ILE:HG21	1:D:331:ILE:CD1	2.12	0.79
1:C:174:LEU:HG	1:C:298:ARG:HD3	1.65	0.76
1:C:335:PRO:O	1:C:336:HIS:HB2	1.87	0.74
1:D:204:ILE:HG21	1:D:331:ILE:HD11	1.71	0.73
1:D:278:CYS:SG	1:D:280:MET:HE2	2.30	0.72
1:C:204:ILE:HG21	1:C:331:ILE:CD1	2.20	0.71
1:D:339:ASN:HB3	1:D:342:GLU:HG2	1.72	0.71
1:D:248:GLY:O	1:D:291:MET:HG3	1.91	0.70
1:A:174:LEU:HG	1:A:298:ARG:HD2	1.73	0.70
1:A:204:ILE:HG21	1:A:331:ILE:CD1	2.21	0.70
1:C:204:ILE:HG21	1:C:331:ILE:HD11	1.74	0.70
1:C:248:GLY:O	1:C:291:MET:HG3	1.91	0.70
1:C:278:CYS:SG	1:C:280:MET:HE2	2.31	0.69
1:A:187:LYS:HG2	1:A:188:PRO:HD2	1.76	0.68
1:A:248:GLY:O	1:A:291:MET:HG3	1.95	0.67
1:C:283:LEU:HD13	1:C:326:ARG:HG3	1.76	0.67
1:D:335:PRO:O	1:D:336:HIS:HB2	1.93	0.66
1:B:248:GLY:O	1:B:291:MET:HG3	1.97	0.64
1:A:335:PRO:O	1:A:336:HIS:HB2	1.98	0.63
1:C:228:PHE:O	1:C:232:SER:HB2	1.98	0.62
1:B:191:GLU:OE1	1:B:192:PRO:HD2	2.01	0.60
1:D:254:ARG:HD2	1:D:260:GLY:HA2	1.83	0.60
1:B:254:ARG:HD2	1:B:260:GLY:HA2	1.83	0.59
1:A:186:GLN:NE2	1:C:280:MET:HE1	2.18	0.58
1:C:291:MET:HE2	1:C:294:ASN:HD22	1.72	0.54
1:A:228:PHE:O	1:A:232:SER:HB2	2.07	0.54
1:B:218:ASN:O	1:B:222:ILE:HG13	2.07	0.53
1:D:228:PHE:O	1:D:232:SER:HB2	2.08	0.53
1:C:202:VAL:HG11	1:C:296:LEU:HD21	1.90	0.53
1:C:338:TYR:CE1	1:C:343:GLU:HG3	2.44	0.52
1:C:254:ARG:HD2	1:C:260:GLY:HA2	1.92	0.52
1:A:202:VAL:HG11	1:A:296:LEU:HD21	1.92	0.52
1:A:323:PRO:HB2	1:A:327:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:VAL:HG11	1:D:296:LEU:HD21	1.92	0.50
1:B:325:ARG:O	1:B:329:GLU:HG3	2.11	0.50
1:C:195:LEU:O	1:C:197:LEU:HD22	2.11	0.50
1:C:298:ARG:HG3	1:C:298:ARG:HH11	1.76	0.49
1:A:254:ARG:HD2	1:A:260:GLY:HA2	1.95	0.49
1:B:228:PHE:O	1:B:232:SER:HB2	2.13	0.48
1:C:291:MET:CE	1:C:294:ASN:HD22	2.26	0.48
1:A:186:GLN:HG3	1:C:278:CYS:SG	2.54	0.47
1:A:340:ILE:O	1:A:344:GLU:N	2.47	0.47
1:C:325:ARG:O	1:C:329:GLU:HG3	2.14	0.47
1:A:186:GLN:HE22	1:C:280:MET:HE1	1.77	0.47
1:A:187:LYS:HG2	1:A:188:PRO:CD	2.44	0.47
1:D:174:LEU:HD11	1:D:302:ASP:OD2	2.16	0.46
1:D:332:GLN:HA	1:D:337:PHE:CG	2.51	0.46
1:C:218:ASN:O	1:C:222:ILE:HG13	2.15	0.46
1:C:332:GLN:HA	1:C:337:PHE:CG	2.51	0.46
1:B:250:ILE:HD13	1:B:295:LEU:HB2	1.97	0.46
1:B:202:VAL:HG11	1:B:296:LEU:HD21	1.98	0.45
1:B:193:LEU:HD23	1:B:194:PRO:HD2	1.97	0.45
1:B:335:PRO:O	1:B:336:HIS:CB	2.60	0.45
1:C:204:ILE:HG21	1:C:331:ILE:HD13	1.97	0.45
1:D:218:ASN:O	1:D:222:ILE:HG13	2.16	0.45
1:A:332:GLN:HA	1:A:337:PHE:CG	2.52	0.45
1:C:201:TYR:HB2	1:C:270:SER:HB3	1.99	0.44
1:B:221:LEU:HB3	1:B:225:MET:HE2	2.00	0.44
1:C:291:MET:HE2	1:C:294:ASN:ND2	2.32	0.43
1:A:318:ASN:ND2	3:A:1345:MLD:OBA	2.51	0.43
1:C:298:ARG:HG3	1:C:298:ARG:NH1	2.34	0.43
1:D:174:LEU:HG	1:D:298:ARG:HD2	2.01	0.43
1:A:189:MET:SD	1:C:280:MET:HE1	2.58	0.42
1:D:205:LEU:HA	1:D:323:PRO:HB3	2.00	0.42
1:B:201:TYR:HB2	1:B:270:SER:HB3	2.01	0.42
1:C:197:LEU:HD12	1:C:304:HIS:O	2.20	0.42
1:B:199:VAL:HG22	1:B:269:ILE:C	2.45	0.42
1:C:318:ASN:ND2	3:C:1344:MLD:OBA	2.53	0.42
1:C:299:GLY:HA3	1:C:305:ILE:HD12	2.02	0.41
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.87	0.41
1:C:222:ILE:HA	1:C:225:MET:HE3	2.02	0.41
1:D:325:ARG:O	1:D:329:GLU:HG3	2.21	0.41
1:A:181:SER:HB2	1:C:220:ARG:NH2	2.35	0.41
1:B:223:ARG:HA	1:B:223:ARG:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLN:HA	1:B:337:PHE:CG	2.57	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	169/175 (97%)	160 (95%)	9 (5%)	0	100	100
1	B	168/175 (96%)	160 (95%)	8 (5%)	0	100	100
1	C	172/175 (98%)	164 (95%)	7 (4%)	1 (1%)	21	32
1	D	169/175 (97%)	164 (97%)	5 (3%)	0	100	100
All	All	678/700 (97%)	648 (96%)	29 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	LEU

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	149/153 (97%)	146 (98%)	3 (2%)	48	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	148/153 (97%)	141 (95%)	7 (5%)	23	41
1	C	151/153 (99%)	147 (97%)	4 (3%)	40	63
1	D	149/153 (97%)	146 (98%)	3 (2%)	48	70
All	All	597/612 (98%)	580 (97%)	17 (3%)	38	60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
1	A	197	LEU
1	A	301	GLU
1	B	191	GLU
1	B	197	LEU
1	B	199	VAL
1	B	264	LEU
1	B	283	LEU
1	B	323	PRO
1	B	342	GLU
1	C	184	LEU
1	C	191	GLU
1	C	264	LEU
1	C	308	ASP
1	D	197	LEU
1	D	199	VAL
1	D	323	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	B	196	GLN
1	B	294	ASN
1	B	332	GLN
1	B	339	ASN
1	C	294	ASN
1	C	304	HIS
1	C	332	GLN
1	D	318	ASN
1	D	332	GLN

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](#)

5 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
3	MLD	A	1345	-	65,66,66	1.76	11 (16%)	88,93,93	1.87	18 (20%)
2	GOL	A	1344	-	5,5,5	0.26	0	5,5,5	0.53	0
3	MLD	D	1344	-	65,66,66	1.73	9 (13%)	88,93,93	1.90	18 (20%)
3	MLD	C	1344	-	65,66,66	1.73	11 (16%)	88,93,93	1.88	17 (19%)
3	MLD	B	1344	-	65,66,66	1.79	10 (15%)	88,93,93	1.88	17 (19%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLD	A	1345	-	-	9/69/114/114	0/4/3/3
2	GOL	A	1344	-	-	0/4/4/4	-
3	MLD	D	1344	-	-	7/69/114/114	0/4/3/3
3	MLD	C	1344	-	-	6/69/114/114	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLD	B	1344	-	-	6/69/114/114	0/4/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1344	MLD	C1-C2	8.30	1.66	1.53
3	A	1345	MLD	C1-C2	8.23	1.66	1.53
3	D	1344	MLD	C1-C2	8.12	1.65	1.53
3	C	1344	MLD	C1-C2	7.76	1.65	1.53
3	C	1344	MLD	OBV-CBT	4.31	1.34	1.22
3	D	1344	MLD	OBV-CBT	4.24	1.34	1.22
3	A	1345	MLD	OBV-CBT	4.16	1.34	1.22
3	B	1344	MLD	OBV-CBT	4.03	1.34	1.22
3	D	1344	MLD	CA1-CA2	4.00	1.59	1.53
3	C	1344	MLD	CA1-CA2	3.79	1.59	1.53
3	B	1344	MLD	CA1-CA2	3.66	1.58	1.53
3	A	1345	MLD	OA6-CA1	-3.56	1.34	1.41
3	A	1345	MLD	CA1-CA2	3.42	1.58	1.53
3	D	1344	MLD	OA6-CA1	-3.32	1.35	1.41
3	B	1344	MLD	OA6-CA1	-3.27	1.35	1.41
3	C	1344	MLD	OA6-CA1	-3.24	1.35	1.41
3	D	1344	MLD	CA4-CA5	3.20	1.61	1.52
3	B	1344	MLD	CA3-CA2	3.13	1.58	1.53
3	B	1344	MLD	C2-N2	3.08	1.50	1.45
3	C	1344	MLD	CA4-CA5	3.07	1.61	1.52
3	B	1344	MLD	CA4-CA5	3.06	1.61	1.52
3	C	1344	MLD	CA3-CA2	3.00	1.57	1.53
3	A	1345	MLD	CA3-CA2	3.00	1.57	1.53
3	B	1344	MLD	OBU-CBT	-2.93	1.21	1.30
3	D	1344	MLD	CA3-CA2	2.89	1.57	1.53
3	C	1344	MLD	OBU-CBT	-2.82	1.21	1.30
3	D	1344	MLD	OBU-CBT	-2.80	1.21	1.30
3	A	1345	MLD	OBU-CBT	-2.77	1.21	1.30
3	B	1344	MLD	CBK-CBM	2.77	1.56	1.52
3	A	1345	MLD	CA4-CA5	2.72	1.60	1.52
3	C	1344	MLD	CA3-CA4	2.45	1.57	1.52
3	A	1345	MLD	CA3-CA4	2.35	1.57	1.52
3	C	1344	MLD	C2-N2	2.35	1.49	1.45
3	B	1344	MLD	CA3-CA4	2.30	1.57	1.52
3	D	1344	MLD	CBK-CBM	2.24	1.55	1.52
3	D	1344	MLD	C2-N2	2.17	1.49	1.45
3	A	1345	MLD	C2-N2	2.16	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1344	MLD	CBK-CBM	2.11	1.55	1.52
3	A	1345	MLD	CBK-CBM	2.07	1.55	1.52
3	A	1345	MLD	CBG-NBF	2.07	1.50	1.45
3	C	1344	MLD	CBG-NBF	2.07	1.50	1.45

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1344	MLD	OA6-CA1-CA2	9.30	125.17	111.08
3	D	1344	MLD	OA6-CA1-CA2	9.13	124.92	111.08
3	C	1344	MLD	OA6-CA1-CA2	9.06	124.81	111.08
3	A	1345	MLD	OA6-CA1-CA2	8.72	124.29	111.08
3	C	1344	MLD	OA5-CA1-OA6	-5.47	101.68	105.97
3	D	1344	MLD	OA5-CA1-OA6	-5.46	101.69	105.97
3	D	1344	MLD	C1-O1-CA4	-5.30	105.41	117.98
3	C	1344	MLD	C1-O1-CA4	-5.14	105.80	117.98
3	A	1345	MLD	C1-O1-CA4	-5.08	105.95	117.98
3	B	1344	MLD	OA5-CA1-OA6	-5.06	102.00	105.97
3	A	1345	MLD	OA5-CA1-OA6	-5.01	102.04	105.97
3	B	1344	MLD	C1-O1-CA4	-4.91	106.33	117.98
3	A	1345	MLD	OA5-CA5-CA4	3.90	114.48	108.64
3	D	1344	MLD	OA5-CA5-CA4	3.87	114.44	108.64
3	C	1344	MLD	OA5-CA5-CA4	3.86	114.42	108.64
3	B	1344	MLD	OA5-CA5-CA4	3.75	114.26	108.64
3	B	1344	MLD	CA-N-CAL	3.70	129.11	121.32
3	D	1344	MLD	CA-N-CAL	3.61	128.91	121.32
3	A	1345	MLD	CA6-CA5-CA4	-3.44	105.44	112.59
3	C	1344	MLD	CA-N-CAL	3.44	128.55	121.32
3	D	1344	MLD	CA6-CA5-CA4	-3.13	106.08	112.59
3	A	1345	MLD	CA2-NAD-CAE	-3.12	115.81	123.11
3	B	1344	MLD	CA2-NAD-CAE	-3.09	115.86	123.11
3	A	1345	MLD	CA-N-CAL	3.07	127.78	121.32
3	C	1344	MLD	CA6-CA5-CA4	-3.06	106.23	112.59
3	B	1344	MLD	CA6-CA5-CA4	-3.03	106.29	112.59
3	C	1344	MLD	CA2-NAD-CAE	-2.92	116.27	123.11
3	D	1344	MLD	CA2-NAD-CAE	-2.90	116.31	123.11
3	B	1344	MLD	OBI-CBH-NBJ	2.81	127.98	122.96
3	A	1345	MLD	OBI-CBH-NBJ	2.77	127.91	122.96
3	C	1344	MLD	OBI-CBH-NBJ	2.76	127.90	122.96
3	D	1344	MLD	OBI-CBH-NBJ	2.70	127.80	122.96
3	B	1344	MLD	O1-C1-C2	-2.69	103.71	108.07
3	C	1344	MLD	O1-C1-C2	-2.61	103.84	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1344	MLD	OA5-CA5-CA6	-2.56	99.18	101.53
3	A	1345	MLD	CBK-NBJ-CBH	2.53	126.64	121.32
3	A	1345	MLD	O1-C1-C2	-2.47	104.06	108.07
3	D	1344	MLD	O1-C1-C2	-2.47	104.06	108.07
3	A	1345	MLD	OA5-CA5-CA6	-2.45	99.27	101.53
3	B	1344	MLD	OA5-CA5-CA6	-2.45	99.28	101.53
3	C	1344	MLD	CA6-OA6-CA1	2.41	109.99	106.82
3	B	1344	MLD	CBK-NBJ-CBH	2.40	126.37	121.32
3	B	1344	MLD	OBE-CBD-CBC	-2.40	117.67	122.02
3	D	1344	MLD	CBG-CBH-NBJ	-2.36	111.59	116.63
3	D	1344	MLD	CBK-NBJ-CBH	2.35	126.25	121.32
3	C	1344	MLD	OA6-CA6-CA5	-2.33	100.39	104.42
3	C	1344	MLD	OA5-CA5-CA6	-2.27	99.44	101.53
3	B	1344	MLD	CBG-CBH-NBJ	-2.27	111.79	116.63
3	B	1344	MLD	C6-C5-C4	-2.26	107.48	113.02
3	D	1344	MLD	OA6-CA6-CA5	-2.23	100.56	104.42
3	C	1344	MLD	OBE-CBD-CBC	-2.22	117.99	122.02
3	D	1344	MLD	C6-C5-C4	-2.22	107.56	113.02
3	D	1344	MLD	O5-C1-C2	-2.21	106.41	110.59
3	B	1344	MLD	O5-C1-C2	-2.21	106.42	110.59
3	D	1344	MLD	OBE-CBD-CBC	-2.21	118.02	122.02
3	C	1344	MLD	CBG-CBH-NBJ	-2.20	111.93	116.63
3	A	1345	MLD	CBG-CBH-NBJ	-2.19	111.96	116.63
3	A	1345	MLD	O5-C1-C2	-2.19	106.46	110.59
3	D	1344	MLD	CA6-OA6-CA1	2.17	109.67	106.82
3	B	1344	MLD	OA6-CA6-CA5	-2.14	100.71	104.42
3	A	1345	MLD	CBL-CBK-NBJ	2.14	114.31	110.38
3	A	1345	MLD	C6-C5-C4	-2.13	107.78	113.02
3	A	1345	MLD	CBM-CBK-NBJ	-2.12	105.70	110.40
3	A	1345	MLD	CA6-OA6-CA1	2.12	109.60	106.82
3	A	1345	MLD	OA6-CA6-CA5	-2.11	100.77	104.42
3	C	1344	MLD	O5-C1-C2	-2.11	106.61	110.59
3	C	1344	MLD	C6-C5-C4	-2.11	107.84	113.02
3	C	1344	MLD	O1-C1-O5	2.08	116.15	110.69
3	D	1344	MLD	CBM-CBK-NBJ	-2.06	105.83	110.40
3	B	1344	MLD	O1-C1-O5	2.05	116.08	110.69

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1344	MLD	C-CA-N-CAL

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Mol	Chain	Res	Type	Atoms
3	C	1344	MLD	C-CA-N-CAL
3	A	1345	MLD	C-CA-N-CAL
3	D	1344	MLD	C-CA-N-CAL
3	A	1345	MLD	NAN-CAO-CAP-OBA
3	A	1345	MLD	NAN-CAO-CAP-OAQ
3	C	1344	MLD	CBP-CBQ-CBR-CBS
3	B	1344	MLD	CB-CA-N-CAL
3	C	1344	MLD	CB-CA-N-CAL
3	D	1344	MLD	CBP-CBQ-CBR-CBS
3	B	1344	MLD	CBP-CBQ-CBR-CBS
3	A	1345	MLD	CB-CA-N-CAL
3	D	1344	MLD	CB-CA-N-CAL
3	A	1345	MLD	CBP-CBQ-CBR-CBS
3	B	1344	MLD	CA3-CA4-O1-C1
3	C	1344	MLD	CA3-CA4-O1-C1
3	D	1344	MLD	CA3-CA4-O1-C1
3	A	1345	MLD	CA3-CA4-O1-C1
3	A	1345	MLD	O5-C1-O1-CA4
3	D	1344	MLD	O5-C1-O1-CA4
3	C	1344	MLD	O5-C1-O1-CA4
3	B	1344	MLD	O5-C1-O1-CA4
3	A	1345	MLD	CBB-CAO-CAP-OBA
3	B	1344	MLD	CA5-CA4-O1-C1
3	A	1345	MLD	CBB-CAO-CAP-OAQ
3	C	1344	MLD	CA5-CA4-O1-C1
3	D	1344	MLD	CA5-CA4-O1-C1
3	D	1344	MLD	NAN-CAO-CAP-OAQ

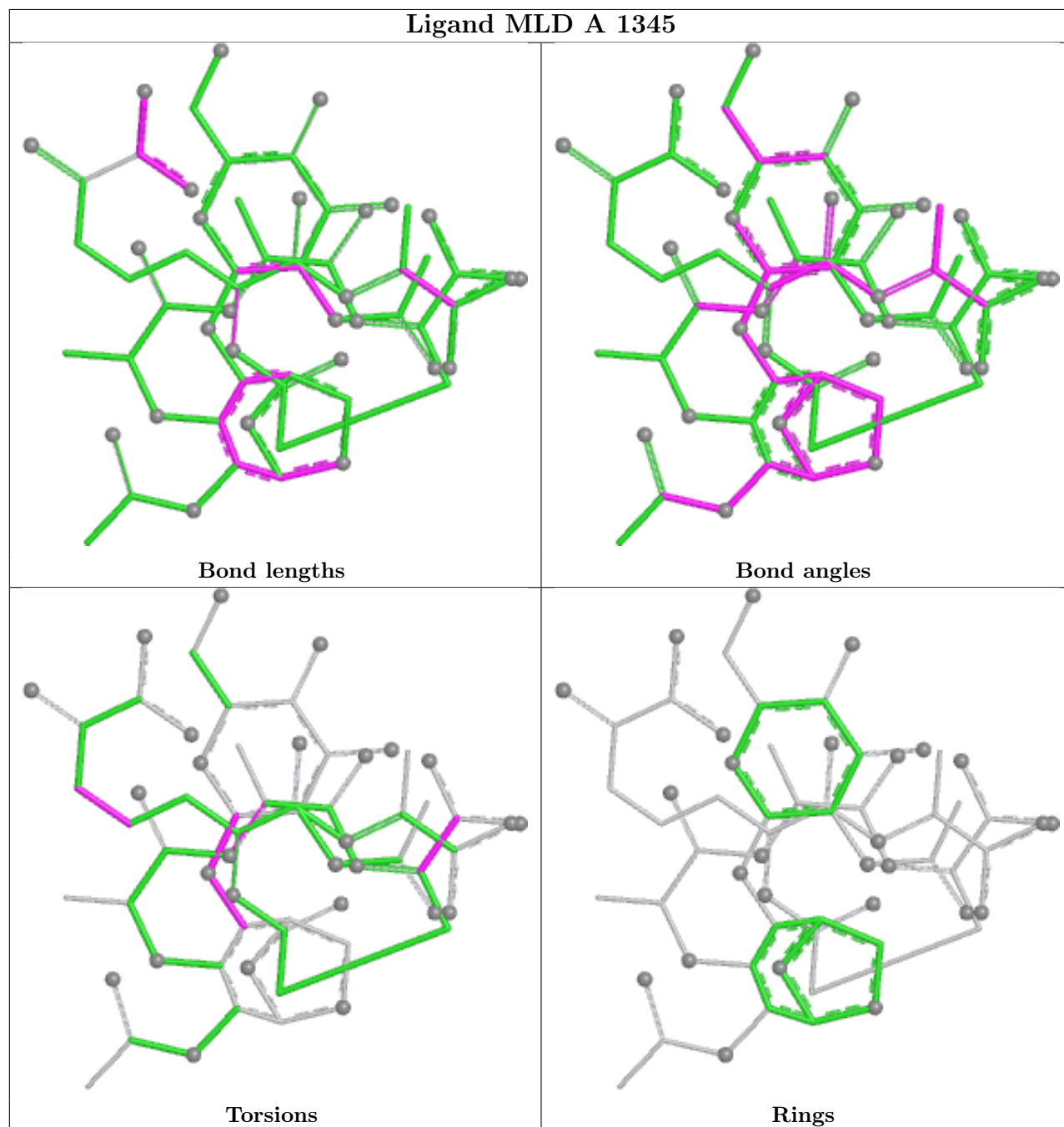
There are no ring outliers.

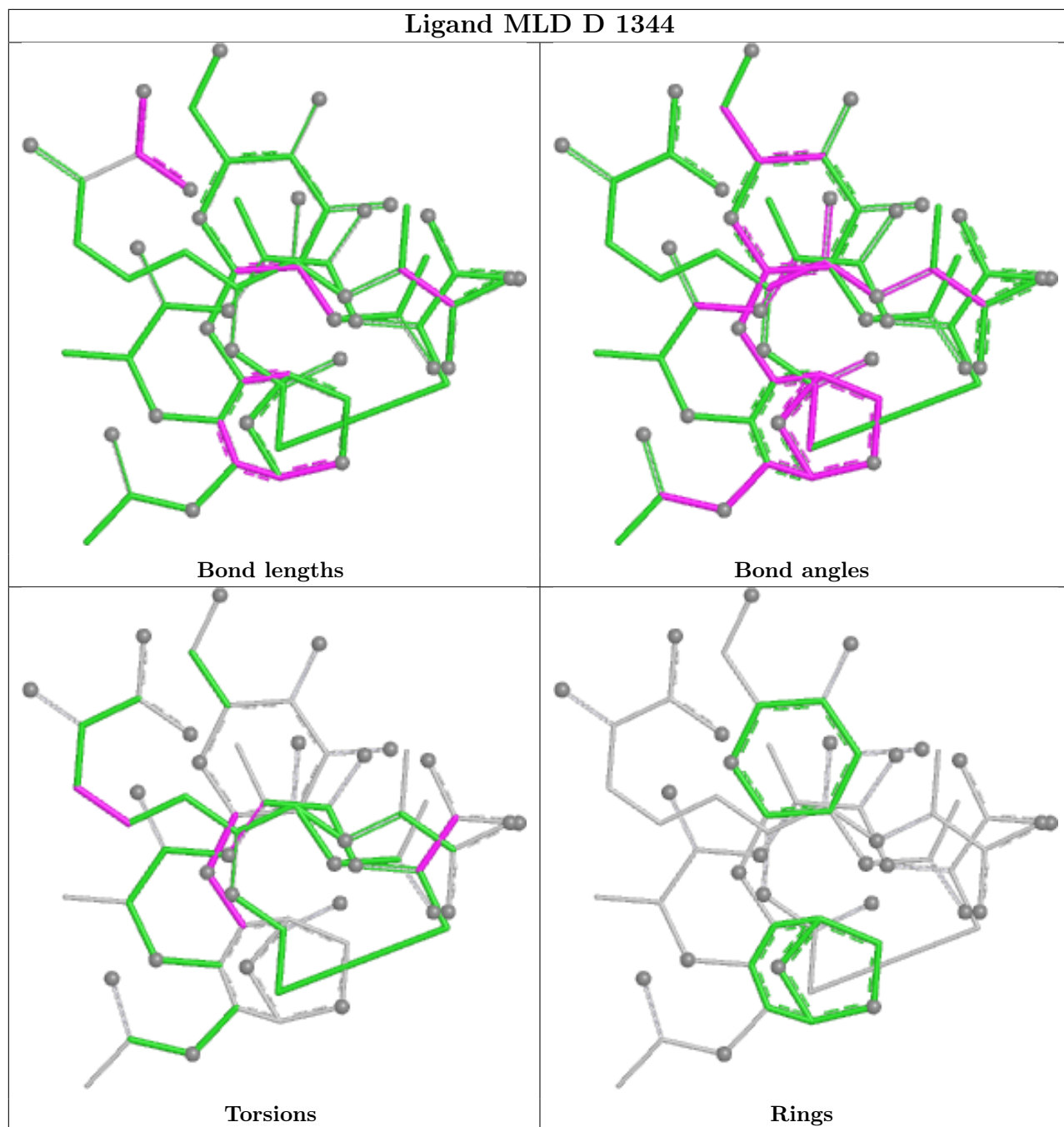
2 monomers are involved in 2 short contacts:

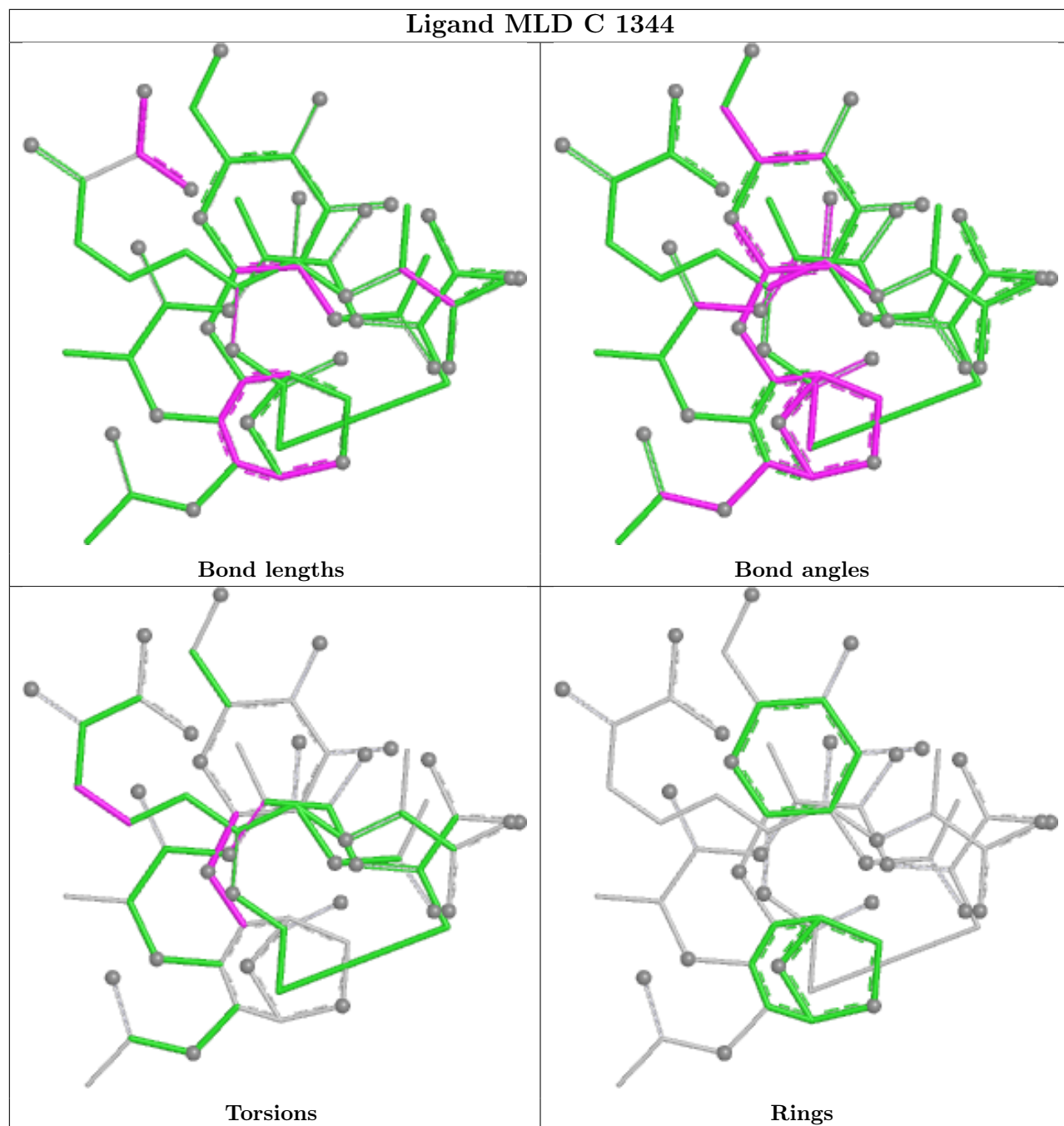
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1345	MLD	1	0
3	C	1344	MLD	1	0

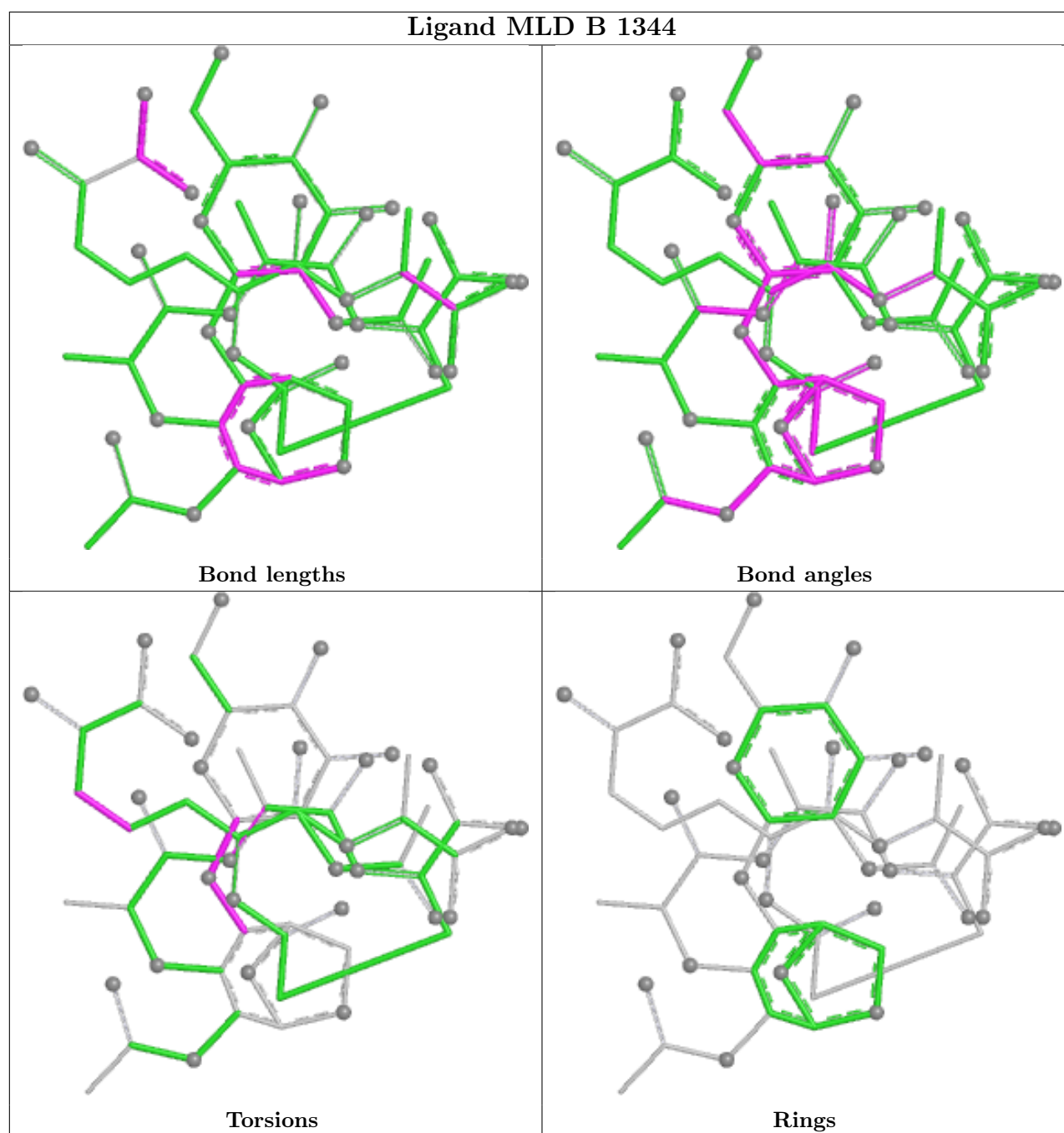
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/175 (97%)	-0.10	6 (3%) 47 43	12, 25, 44, 80	0
1	B	170/175 (97%)	-0.06	5 (2%) 53 50	14, 25, 44, 85	0
1	C	174/175 (99%)	0.09	10 (5%) 29 25	15, 27, 50, 64	0
1	D	171/175 (97%)	-0.01	8 (4%) 36 32	15, 27, 47, 86	0
All	All	686/700 (98%)	-0.02	29 (4%) 40 36	12, 26, 48, 86	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	344	GLU	7.6
1	B	175	SER	7.4
1	A	175	SER	6.6
1	B	344	GLU	6.6
1	C	171	GLY	6.0
1	C	344	GLU	5.8
1	D	342	GLU	4.9
1	A	174	LEU	4.8
1	B	176	ALA	3.8
1	D	343	GLU	3.6
1	A	176	ALA	3.5
1	D	341	GLU	3.4
1	C	175	SER	3.3
1	C	342	GLU	3.3
1	D	174	LEU	3.2
1	A	343	GLU	3.2
1	D	189	MET	3.2
1	A	344	GLU	3.0
1	C	174	LEU	2.6
1	B	342	GLU	2.6
1	B	343	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	172	HIS	2.5
1	D	175	SER	2.5
1	A	341	GLU	2.5
1	C	189	MET	2.4
1	C	173	GLU	2.4
1	D	282	GLU	2.3
1	C	341	GLU	2.3
1	C	308	ASP	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

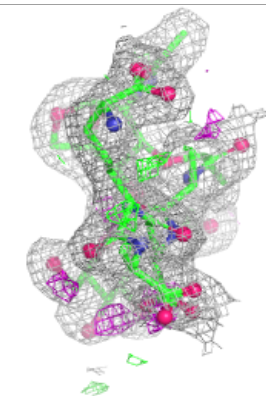
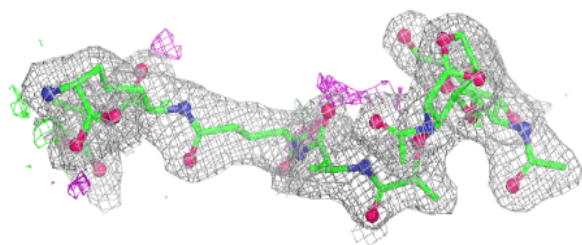
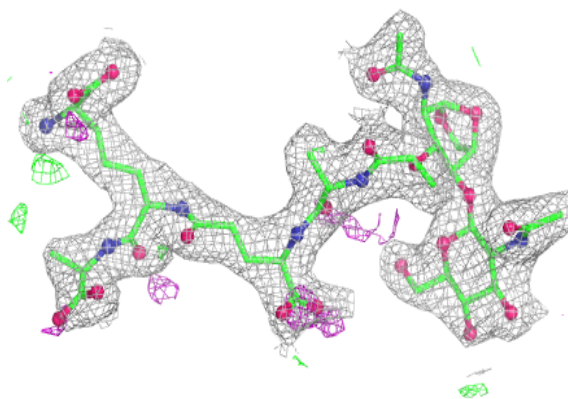
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	1344	6/6	0.84	0.27	49,55,57,60	0
3	MLD	A	1345	64/64	0.95	0.09	10,21,36,45	0
3	MLD	B	1344	64/64	0.95	0.09	16,23,37,43	0
3	MLD	C	1344	64/64	0.95	0.09	15,24,38,45	0
3	MLD	D	1344	64/64	0.95	0.09	14,23,37,40	0

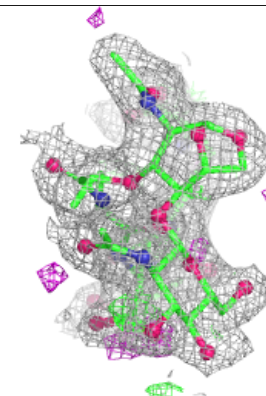
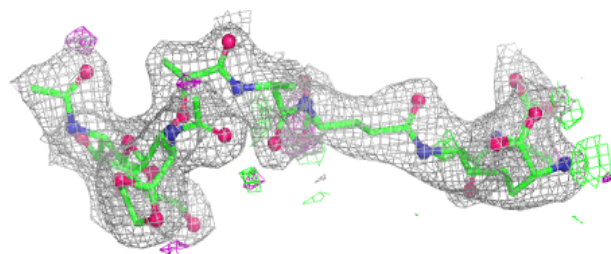
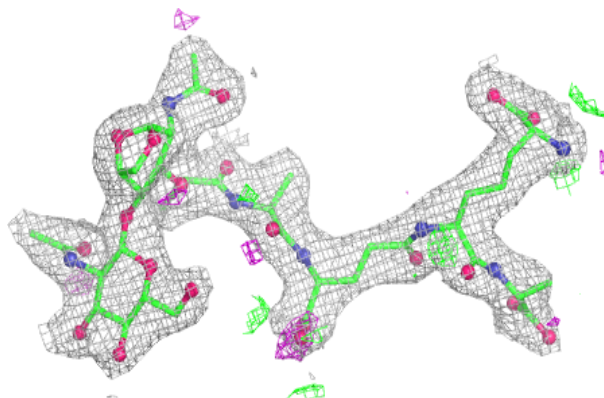
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MLD A 1345:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

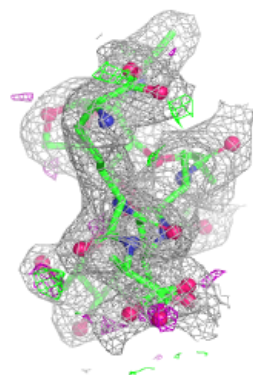
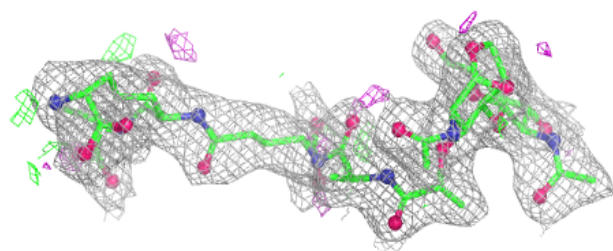
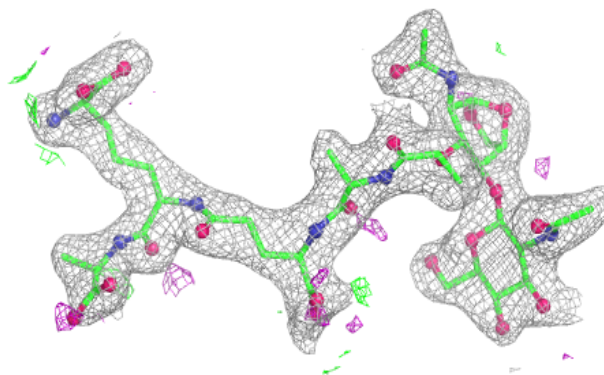
**Electron density around MLD B 1344:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

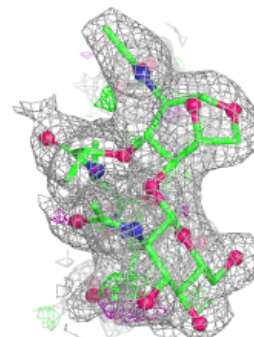
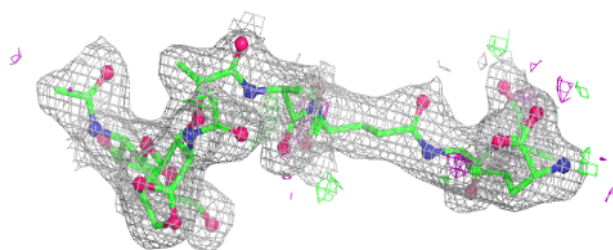
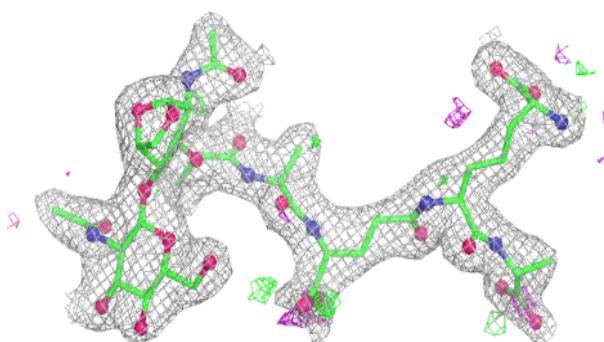


Electron density around MLD C 1344:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MLD D 1344:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.