



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 AM UTC

PDB ID : 1UJW / pdb_00001ujw
Title : Structure of the complex between BtuB and Colicin E3 Receptor binding domain
Authors : Kurisu, G.; Zakharov, S.D.; Zhalnina, M.V.; Bano, S.; Eroukova, V.Y.; Rokitskaya, T.I.; Antonenko, Y.N.; Wiener, M.C.; Cramer, W.A.
Deposited on : 2003-08-12
Resolution : 2.75 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)	:	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

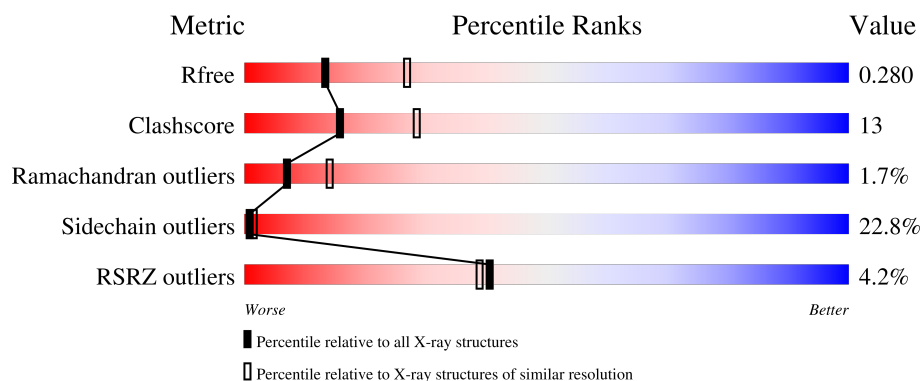
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	594	4% 60% 28% 8% • •
2	B	135	4% 55% 27% • • 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AAE	A	802	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5714 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.

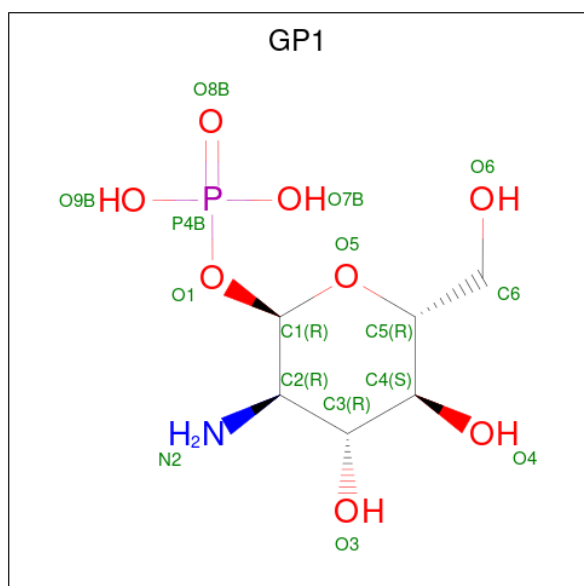
- Molecule 1 is a protein called Vitamin B12 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4567	2877	781	907	2			

- Molecule 2 is a protein called Colicin E3.

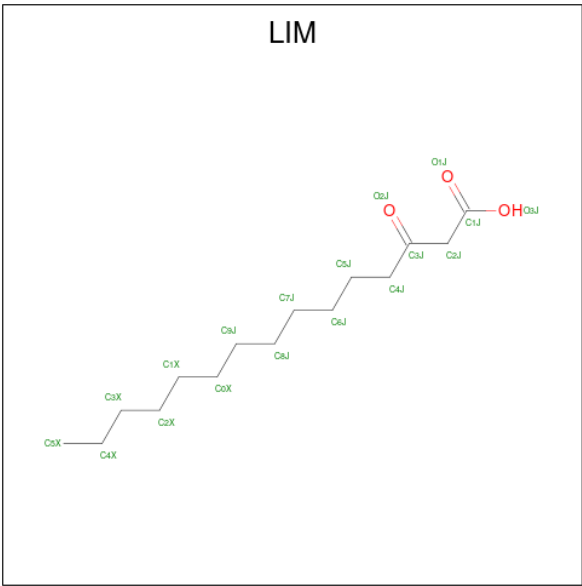
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			905	546	177	178	4			

- Molecule 3 is 2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose (CCD ID: GP1) (formula: $C_6H_{14}NO_8P$).



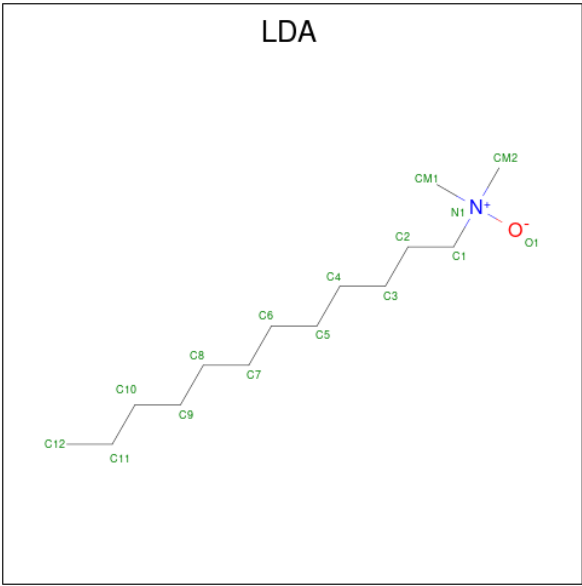
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 4 is 3-OXO-PENTADECANOIC ACID (CCD ID: LIM) (formula: C₁₅H₂₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	15	2		
4	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



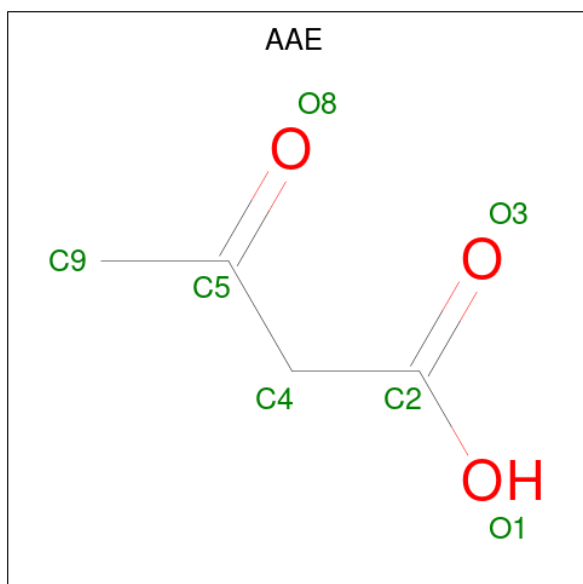
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			16	14	1	1		

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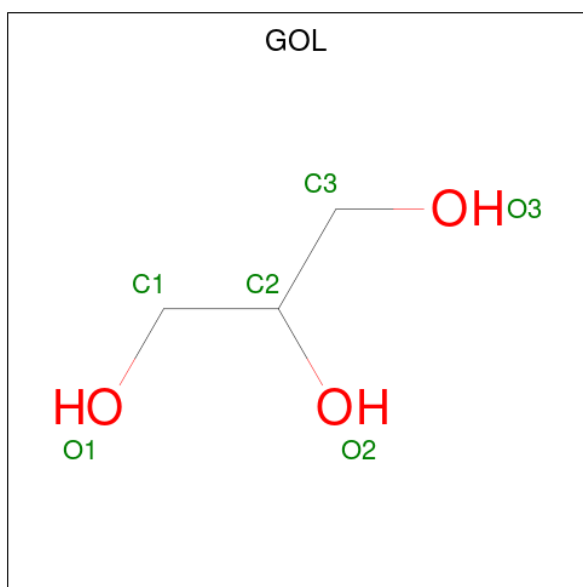
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is ACETOACETIC ACID (CCD ID: AAE) (formula: $C_4H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	9	Total O 9 9	0	0
8	B	1	Total O 1 1	0	0

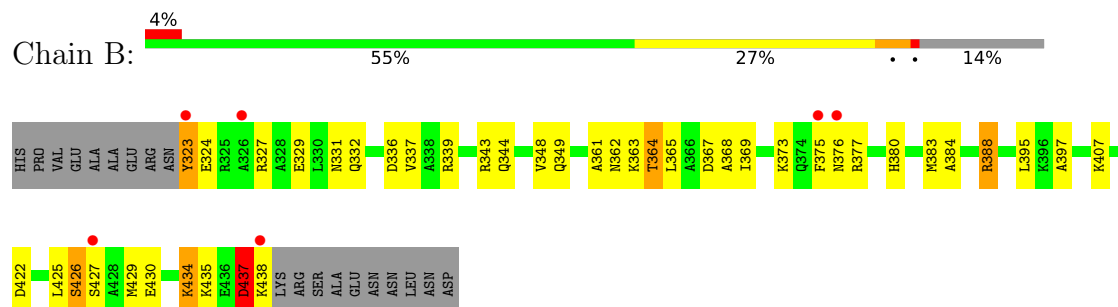
3 Residue-property plots

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 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: Vitamin B12 receptor



• Molecule 2: Colicin E3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.93Å 80.10Å 233.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.88 – 2.75 37.88 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.7 (37.88-2.75) 96.7 (37.88-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.244 , 0.293 0.233 , 0.280	Depositor DCC
R_{free} test set	1864 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5714	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GP1, AAE, LDA, LIM, GOL

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	1.04	7/4684 (0.1%)	1.11	10/6377 (0.2%)
2	B	0.82	0/914	1.11	3/1220 (0.2%)
All	All	1.00	7/5598 (0.1%)	1.11	13/7597 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	GLU	N-CA	6.38	1.53	1.45
1	A	531	TYR	CA-C	5.51	1.60	1.52
1	A	31	ARG	CA-C	-5.21	1.46	1.52
1	A	83	VAL	CA-CB	-5.10	1.47	1.54
1	A	129	ILE	CA-CB	-5.08	1.48	1.54
1	A	356	ALA	CA-CB	-5.05	1.45	1.53
1	A	302	ASN	CA-C	-5.01	1.46	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	VAL	CB-CA-C	-7.86	98.71	110.82
2	B	384	ALA	N-CA-C	6.24	118.16	111.36
1	A	261	ILE	CB-CA-C	-6.17	101.99	111.31
1	A	539	VAL	N-CA-C	5.93	121.68	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	ASP	N-CA-C	5.68	118.89	110.48
1	A	100	PRO	CB-CA-C	-5.38	106.50	111.40
1	A	495	LEU	N-CA-C	-5.36	101.92	109.96
1	A	219	ARG	N-CA-C	5.34	117.18	109.07
2	B	367	ASP	N-CA-C	-5.21	105.29	110.97
1	A	354	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	367	ARG	N-CA-C	5.15	118.46	110.17
2	B	395	LEU	N-CA-C	-5.07	105.83	111.36
1	A	459	ALA	N-CA-C	5.02	117.58	108.69

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	LEU	Peptide
1	A	229	TYR	Peptide
1	A	474	PRO	Peptide

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	4567	0	4287	140	0
2	B	905	0	885	10	0
3	A	32	0	0	0	0
4	A	34	0	54	2	0
5	A	112	0	217	6	0
6	A	6	0	5	0	0
7	A	48	0	63	6	0
8	A	9	0	0	2	0
8	B	1	0	0	0	0
All	All	5714	0	5511	149	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 13.

All (149) 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:13:ASN:H	1:A:13:ASN:HD22	1.10	1.00
1:A:506:GLN:HE21	1:A:506:GLN:HA	1.41	0.86
1:A:506:GLN:HE22	1:A:519:THR:HB	1.40	0.85
1:A:506:GLN:NE2	1:A:519:THR:HB	1.92	0.84
1:A:556:THR:HG21	7:A:708:GOL:O2	1.76	0.83
1:A:369:GLY:H	7:A:706:GOL:H32	1.45	0.81
1:A:556:THR:HG22	1:A:558:HIS:H	1.48	0.77
1:A:162:ASP:OD1	1:A:162:ASP:C	2.27	0.77
1:A:302:ASN:OD1	5:A:604:LDA:H121	1.84	0.77
1:A:299:GLN:HG2	1:A:316:ASP:HB3	1.69	0.75
1:A:546:LEU:HD11	1:A:573:TYR:OH	1.87	0.74
1:A:343:THR:HG23	8:A:910:HOH:O	1.87	0.74
1:A:426:THR:HG23	1:A:431:TRP:HE1	1.53	0.73
1:A:159:GLN:HE21	1:A:162:ASP:HA	1.53	0.73
1:A:267:THR:HG22	1:A:298:VAL:HG22	1.72	0.71
1:A:238:PRO:HG2	1:A:287:SER:HB3	1.73	0.69
1:A:411:ASP:H	1:A:455:ASN:HD21	1.40	0.69
1:A:203:TYR:CD1	1:A:203:TYR:C	2.73	0.67
1:A:13:ASN:H	1:A:13:ASN:ND2	1.88	0.67
1:A:105:GLN:HG3	1:A:133:ARG:HD2	1.78	0.65
1:A:383:TYR:OH	1:A:426:THR:HG22	1.97	0.65
1:A:397:ASN:H	1:A:400:GLN:HE21	1.44	0.65
1:A:246:TYR:OH	1:A:283:ARG:NH2	2.30	0.65
1:A:160:LEU:HD22	1:A:166:VAL:HB	1.78	0.64
1:A:354:GLU:HG3	1:A:355:GLY:N	2.12	0.64
1:A:283:ARG:HD2	1:A:284:TYR:CE1	2.33	0.63
1:A:68:ILE:HD13	1:A:76:VAL:CG2	2.28	0.63
1:A:528:ASP:O	1:A:538:THR:O	2.16	0.63
1:A:72:ASN:HD22	1:A:498:ARG:HH22	1.46	0.63
2:B:323:TYR:C	2:B:323:TYR:CD1	2.77	0.63
1:A:472:THR:O	1:A:475:LEU:CB	2.48	0.62
1:A:4:SER:O	1:A:7:THR:HG23	1.99	0.62
1:A:105:GLN:HG3	1:A:133:ARG:CD	2.30	0.61
1:A:159:GLN:HE21	1:A:162:ASP:CA	2.13	0.61
1:A:341:TYR:HB3	1:A:358:ARG:HG3	1.83	0.60
1:A:197:PHE:HD2	1:A:227:THR:HB	1.67	0.60
1:A:362:ASN:HD22	1:A:365:PHE:H	1.50	0.60
1:A:84:ARG:HH11	1:A:318:GLN:NE2	2.00	0.60
1:A:13:ASN:HD22	1:A:13:ASN:N	1.85	0.59
1:A:256:TYR:CZ	5:A:606:LDA:HM22	2.37	0.59
1:A:12:ALA:HB3	1:A:17:GLN:NE2	2.17	0.59
1:A:472:THR:O	1:A:475:LEU:HB3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HB	1:A:156:THR:OG1	2.03	0.58
1:A:479:VAL:HG23	1:A:505:TYR:CD2	2.38	0.58
1:A:343:THR:CG2	8:A:910:HOH:O	2.48	0.58
1:A:506:GLN:HE22	1:A:519:THR:CB	2.11	0.58
1:A:218:VAL:HG11	5:A:601:LDA:H61	1.87	0.57
1:A:383:TYR:CZ	1:A:426:THR:HG22	2.41	0.56
1:A:14:ARG:HD2	1:A:341:TYR:OH	2.06	0.55
1:A:12:ALA:HB3	1:A:17:GLN:HE22	1.71	0.55
1:A:84:ARG:HD2	1:A:318:GLN:HE22	1.71	0.55
2:B:368:ALA:HB1	2:B:397:ALA:HB2	1.90	0.54
1:A:203:TYR:CD1	1:A:204:GLY:N	2.75	0.54
1:A:169:LEU:HD12	1:A:169:LEU:C	2.33	0.54
1:A:477:HIS:HD2	1:A:505:TYR:OH	1.90	0.54
1:A:352:THR:O	1:A:375:ALA:HA	2.07	0.54
1:A:37:TRP:HB3	1:A:48:ARG:NH2	2.24	0.53
1:A:263:SER:OG	1:A:302:ASN:ND2	2.42	0.53
1:A:526:ARG:CD	1:A:541:MET:HE3	2.39	0.53
1:A:115:SER:O	1:A:358:ARG:HD3	2.08	0.53
1:A:477:HIS:N	1:A:477:HIS:ND1	2.57	0.53
1:A:411:ASP:H	1:A:455:ASN:ND2	2.06	0.53
1:A:260:LEU:HB2	7:A:704:GOL:H12	1.91	0.52
1:A:407:ASN:C	1:A:407:ASN:HD22	2.17	0.52
1:A:573:TYR:C	1:A:574:GLU:HG3	2.34	0.52
1:A:68:ILE:HD13	1:A:76:VAL:HG21	1.92	0.52
1:A:551:VAL:HG22	4:A:812:LIM:H5X3	1.92	0.51
1:A:13:ASN:O	1:A:14:ARG:HB2	2.09	0.51
1:A:196:GLY:HA3	1:A:228:ASN:HB2	1.92	0.50
1:A:582:ALA:HB1	1:A:585:GLU:OE1	2.12	0.50
1:A:72:ASN:HD22	1:A:498:ARG:NH2	2.10	0.50
1:A:475:LEU:HD22	1:A:509:TRP:HB3	1.92	0.50
1:A:285:ASP:OD1	1:A:285:ASP:C	2.53	0.50
1:A:229:TYR:OH	2:B:388:ARG:NH2	2.45	0.49
1:A:556:THR:HG21	7:A:708:GOL:HO2	1.76	0.49
1:A:29:VAL:HB	1:A:107:VAL:HB	1.95	0.49
1:A:510:GLN:CD	1:A:510:GLN:O	2.55	0.49
1:A:105:GLN:CG	1:A:133:ARG:HD3	2.43	0.48
1:A:112:GLY:O	1:A:125:GLY:HA2	2.13	0.48
1:A:240:LEU:HD12	1:A:240:LEU:N	2.28	0.48
1:A:361:ASP:OD2	5:A:604:LDA:HM12	2.13	0.48
1:A:17:GLN:HG3	1:A:21:THR:HG22	1.96	0.48
1:A:423:GLU:HB3	1:A:432:ARG:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASN:CG	1:A:365:PHE:CE2	2.92	0.48
1:A:544:VAL:HG21	1:A:573:TYR:CD1	2.48	0.48
1:A:397:ASN:H	1:A:400:GLN:NE2	2.10	0.47
1:A:174:HIS:ND1	1:A:175:THR:N	2.62	0.47
1:A:169:LEU:C	1:A:169:LEU:CD1	2.87	0.47
1:A:323:THR:HG22	1:A:326:THR:OG1	2.15	0.47
1:A:66:ILE:O	1:A:73:ALA:HA	2.14	0.47
1:A:149:TYR:OH	1:A:151:ASN:HB2	2.15	0.47
1:A:526:ARG:HD3	1:A:541:MET:HE3	1.97	0.47
1:A:25:PRO:HG2	1:A:111:ARG:HB2	1.97	0.47
1:A:455:ASN:O	1:A:456:GLU:C	2.57	0.46
2:B:373:LYS:HA	2:B:376:ASN:HB2	1.97	0.46
1:A:13:ASN:ND2	1:A:13:ASN:N	2.53	0.46
1:A:546:LEU:HD11	1:A:573:TYR:CZ	2.50	0.46
1:A:581:THR:O	1:A:582:ALA:C	2.58	0.46
1:A:193:ASP:OD2	1:A:193:ASP:N	2.48	0.46
2:B:425:LEU:HG	2:B:429:MET:HE2	1.96	0.46
1:A:68:ILE:CD1	1:A:76:VAL:HG21	2.45	0.46
1:A:315:VAL:HG21	5:A:604:LDA:H72	1.98	0.46
1:A:423:GLU:HB3	1:A:432:ARG:HG3	1.98	0.46
2:B:434:LYS:O	2:B:437:ASP:HB2	2.16	0.45
1:A:472:THR:O	1:A:475:LEU:HB2	2.16	0.45
1:A:520:TYR:HE1	1:A:545:SER:HG	1.64	0.45
2:B:365:LEU:HD11	2:B:369:ILE:HD11	1.99	0.45
1:A:256:TYR:OH	7:A:704:GOL:H31	2.17	0.45
1:A:196:GLY:HA2	1:A:228:ASN:HD22	1.82	0.45
1:A:383:TYR:OH	1:A:426:THR:CG2	2.65	0.45
1:A:506:GLN:HA	1:A:506:GLN:NE2	2.21	0.45
1:A:285:ASP:OD1	1:A:287:SER:OG	2.34	0.44
1:A:479:VAL:HG22	1:A:480:SER:N	2.31	0.44
1:A:527:TYR:CE2	1:A:540:LYS:HG3	2.51	0.44
1:A:567:ASN:O	1:A:568:LEU:C	2.58	0.44
1:A:558:HIS:ND1	7:A:708:GOL:H32	2.32	0.44
1:A:315:VAL:HG22	5:A:604:LDA:H91	2.00	0.44
1:A:470:PHE:CZ	1:A:477:HIS:CD2	3.05	0.44
1:A:216:GLY:HA2	1:A:253:GLY:O	2.17	0.44
1:A:509:TRP:CD1	1:A:511:LEU:HD12	2.53	0.44
1:A:300:TRP:CZ3	4:A:803:LIM:H2X1	2.53	0.43
1:A:380:ILE:HG22	1:A:381:GLU:N	2.32	0.43
1:A:510:GLN:HA	1:A:514:PHE:O	2.18	0.43
1:A:100:PRO:HG2	1:A:103:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:O	1:A:225:ASN:HA	2.19	0.43
1:A:11:THR:O	1:A:118:TYR:OH	2.36	0.42
1:A:519:THR:HG23	1:A:548:ASP:HB2	2.02	0.42
1:A:31:ARG:HG3	1:A:105:GLN:OE1	2.20	0.42
1:A:6:ASP:O	1:A:6:ASP:OD1	2.38	0.42
1:A:510:GLN:O	1:A:510:GLN:NE2	2.53	0.42
2:B:361:ALA:HA	2:B:364:THR:HG23	2.01	0.42
2:B:323:TYR:CD1	2:B:324:GLU:N	2.88	0.42
1:A:53:ASP:OD1	1:A:526:ARG:NH2	2.52	0.41
1:A:123:ILE:O	1:A:417:GLN:NE2	2.53	0.41
1:A:224:ASP:C	1:A:225:ASN:HD22	2.27	0.41
1:A:160:LEU:HD12	1:A:160:LEU:HA	1.92	0.41
1:A:348:VAL:O	1:A:348:VAL:HG22	2.19	0.41
1:A:360:ASP:O	1:A:367:ARG:HA	2.20	0.41
1:A:527:TYR:CE2	1:A:540:LYS:CG	3.03	0.41
1:A:194:ASN:O	1:A:196:GLY:N	2.53	0.41
1:A:13:ASN:ND2	1:A:17:GLN:NE2	2.68	0.41
1:A:407:ASN:C	1:A:407:ASN:ND2	2.79	0.41
1:A:468:ALA:O	1:A:469:ASN:HB3	2.21	0.41
2:B:422:ASP:O	2:B:426:SER:HB2	2.21	0.41
1:A:78:VAL:HG11	1:A:96:LEU:HD21	2.02	0.41
1:A:81:ASP:OD1	1:A:130:ILE:HA	2.21	0.40
1:A:199:SER:HA	1:A:225:ASN:ND2	2.36	0.40
1:A:161:GLY:C	1:A:163:LYS:H	2.29	0.40
1:A:573:TYR:CD2	1:A:573:TYR:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	572/594 (96%)	525 (92%)	36 (6%)	11 (2%)	6 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	114/135 (84%)	111 (97%)	2 (2%)	1 (1%)	14	28
All	All	686/729 (94%)	636 (93%)	38 (6%)	12 (2%)	7	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	539	VAL
1	A	197	PHE
1	A	283	ARG
1	A	363	SER
1	A	230	ASP
1	A	556	THR
2	B	437	ASP
1	A	146	SER
1	A	531	TYR
1	A	570	ASP
1	A	114	ARG

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	481/495 (97%)	379 (79%)	102 (21%)	1	2
2	B	88/104 (85%)	60 (68%)	28 (32%)	0	0
All	All	569/599 (95%)	439 (77%)	130 (23%)	1	1

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	7	THR
1	A	13	ASN
1	A	19	ARG

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Mol	Chain	Res	Type
1	A	21	THR
1	A	31	ARG
1	A	34	ILE
1	A	36	ARG
1	A	40	THR
1	A	47	ARG
1	A	54	ILE
1	A	63	LEU
1	A	68	ILE
1	A	85	LEU
1	A	93	SER
1	A	103	LEU
1	A	105	GLN
1	A	121	ASP
1	A	133	ARG
1	A	138	THR
1	A	141	SER
1	A	144	TRP
1	A	160	LEU
1	A	162	ASP
1	A	163	LYS
1	A	169	LEU
1	A	175	THR
1	A	193	ASP
1	A	198	LEU
1	A	199	SER
1	A	212	ASP
1	A	218	VAL
1	A	227	THR
1	A	239	LEU
1	A	245	LEU
1	A	251	ASP
1	A	257	ASN
1	A	260	LEU
1	A	261	ILE
1	A	265	LEU
1	A	268	SER
1	A	270	SER
1	A	283	ARG
1	A	285	ASP
1	A	287	SER
1	A	304	VAL

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Mol	Chain	Res	Type
1	A	315	VAL
1	A	323	THR
1	A	330	GLU
1	A	331	ASP
1	A	342	LEU
1	A	343	THR
1	A	345	LEU
1	A	348	VAL
1	A	350	ASP
1	A	354	GLU
1	A	363	SER
1	A	370	THR
1	A	374	SER
1	A	384	ARG
1	A	388	SER
1	A	398	LEU
1	A	407	ASN
1	A	416	LYS
1	A	418	TRP
1	A	425	LEU
1	A	426	THR
1	A	434	SER
1	A	440	VAL
1	A	441	SER
1	A	449	HIS
1	A	450	THR
1	A	451	LEU
1	A	452	LYS
1	A	456	GLU
1	A	475	LEU
1	A	477	HIS
1	A	485	ASP
1	A	493	THR
1	A	495	LEU
1	A	496	LEU
1	A	497	ARG
1	A	504	LYS
1	A	506	GLN
1	A	510	GLN
1	A	519	THR
1	A	526	ARG
1	A	529	LYS

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Mol	Chain	Res	Type
1	A	531	TYR
1	A	545	SER
1	A	551	VAL
1	A	556	THR
1	A	559	LEU
1	A	562	ARG
1	A	564	LYS
1	A	571	LYS
1	A	580	GLN
1	A	584	ARG
1	A	585	GLU
1	A	587	THR
1	A	588	LEU
1	A	589	SER
2	B	323	TYR
2	B	327	ARG
2	B	329	GLU
2	B	331	ASN
2	B	332	GLN
2	B	336	ASP
2	B	337	VAL
2	B	339	ARG
2	B	343	ARG
2	B	344	GLN
2	B	348	VAL
2	B	349	GLN
2	B	362	ASN
2	B	363	LYS
2	B	364	THR
2	B	375	PHE
2	B	377	ARG
2	B	380	HIS
2	B	383	MET
2	B	388	ARG
2	B	407	LYS
2	B	426	SER
2	B	427	SER
2	B	430	GLU
2	B	434	LYS
2	B	435	LYS
2	B	437	ASP
2	B	438	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	72	ASN
1	A	158	GLN
1	A	159	GLN
1	A	209	ASN
1	A	225	ASN
1	A	228	ASN
1	A	280	HIS
1	A	302	ASN
1	A	318	GLN
1	A	337	ASN
1	A	347	GLN
1	A	362	ASN
1	A	368	HIS
1	A	372	GLN
1	A	400	GLN
1	A	407	ASN
1	A	455	ASN
1	A	477	HIS
1	A	506	GLN
1	A	521	GLN
2	B	331	ASN
2	B	341	GLN
2	B	362	ASN
2	B	401	GLN
2	B	405	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

20 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	GP1	A	811	4	15,16,16	1.30	2 (13%)	24,24,24	2.87	9 (37%)
5	LDA	A	604	-	13,15,15	1.80	2 (15%)	14,17,17	0.76	0
5	LDA	A	605	-	13,15,15	1.78	1 (7%)	14,17,17	0.52	0
7	GOL	A	704	-	5,5,5	0.74	0	5,5,5	1.03	0
7	GOL	A	705	-	5,5,5	0.56	0	5,5,5	0.41	0
7	GOL	A	708	-	5,5,5	0.43	0	5,5,5	0.28	0
4	LIM	A	812	3	15,16,17	3.47	3 (20%)	15,16,18	2.95	3 (20%)
7	GOL	A	702	-	5,5,5	0.82	0	5,5,5	0.88	0
7	GOL	A	707	-	5,5,5	0.57	0	5,5,5	0.85	0
5	LDA	A	603	-	13,15,15	1.92	2 (15%)	14,17,17	0.75	0
4	LIM	A	803	3	15,16,17	3.45	2 (13%)	15,16,18	2.89	4 (26%)
5	LDA	A	607	-	13,15,15	1.92	2 (15%)	14,17,17	0.90	0
6	AAE	A	802	3	4,5,6	3.91	3 (75%)	5,5,7	3.57	3 (60%)
7	GOL	A	706	-	5,5,5	0.62	0	5,5,5	0.76	0
7	GOL	A	701	-	5,5,5	0.63	0	5,5,5	0.51	0
5	LDA	A	601	-	13,15,15	2.00	2 (15%)	14,17,17	0.81	0
7	GOL	A	703	-	5,5,5	0.52	0	5,5,5	0.54	0
3	GP1	A	801	6,4	15,16,16	1.38	1 (6%)	24,24,24	3.43	11 (45%)
5	LDA	A	606	-	13,15,15	1.82	2 (15%)	14,17,17	1.08	1 (7%)
5	LDA	A	602	-	13,15,15	2.16	2 (15%)	14,17,17	0.86	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
3	GP1	A	811	4	-	5/6/27/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LDA	A	604	-	-	9/13/13/13	-
5	LDA	A	605	-	-	8/13/13/13	-
7	GOL	A	704	-	-	4/4/4/4	-
7	GOL	A	705	-	-	2/4/4/4	-
7	GOL	A	708	-	-	0/4/4/4	-
4	LIM	A	812	3	-	6/15/15/16	-
7	GOL	A	702	-	-	2/4/4/4	-
7	GOL	A	707	-	-	2/4/4/4	-
5	LDA	A	603	-	-	7/13/13/13	-
4	LIM	A	803	3	-	6/15/15/16	-
5	LDA	A	607	-	-	6/13/13/13	-
6	AAE	A	802	3	-	2/3/3/4	-
7	GOL	A	706	-	-	1/4/4/4	-
7	GOL	A	701	-	-	0/4/4/4	-
5	LDA	A	601	-	-	2/13/13/13	-
7	GOL	A	703	-	-	3/4/4/4	-
3	GP1	A	801	6,4	-	3/6/27/27	0/1/1/1
5	LDA	A	606	-	-	4/13/13/13	-
5	LDA	A	602	-	-	8/13/13/13	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	LIM	O2J-C3J	12.53	1.43	1.21
4	A	812	LIM	O2J-C3J	11.73	1.42	1.21
5	A	602	LDA	O1-N1	-6.60	1.26	1.42
5	A	601	LDA	O1-N1	-6.46	1.26	1.42
5	A	605	LDA	O1-N1	-6.00	1.27	1.42
6	A	802	AAE	O8-C5	5.90	1.43	1.21
5	A	603	LDA	O1-N1	-5.83	1.27	1.42
5	A	604	LDA	O1-N1	-5.70	1.28	1.42
5	A	606	LDA	O1-N1	-5.55	1.28	1.42
5	A	607	LDA	O1-N1	-5.06	1.29	1.42
5	A	607	LDA	C1-N1	-4.68	1.46	1.51
4	A	812	LIM	C2J-C3J	4.64	1.56	1.52
4	A	812	LIM	O1J-C1J	4.36	1.44	1.20
3	A	801	GP1	P4B-O1	4.34	1.67	1.59
6	A	802	AAE	O3-C2	4.23	1.44	1.20
4	A	803	LIM	O1J-C1J	4.10	1.43	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	LDA	C1-N1	-4.05	1.47	1.51
5	A	603	LDA	C1-N1	-3.57	1.47	1.51
5	A	606	LDA	C1-N1	-3.40	1.48	1.51
5	A	601	LDA	C1-N1	-2.93	1.48	1.51
5	A	604	LDA	C1-N1	-2.86	1.48	1.51
6	A	802	AAE	C4-C5	2.67	1.54	1.52
3	A	811	GP1	P4B-O1	2.49	1.63	1.59
3	A	811	GP1	C4-C3	2.08	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	GP1	O5-C1-O1	-9.37	99.11	111.36
4	A	803	LIM	O1J-C1J-C2J	-7.55	102.96	126.34
3	A	801	GP1	C1-O5-C5	7.37	128.11	113.72
4	A	812	LIM	O2J-C3J-C2J	-7.14	110.48	121.17
4	A	812	LIM	O1J-C1J-C2J	-6.39	106.54	126.34
3	A	811	GP1	C1-O5-C5	6.28	125.98	113.72
3	A	801	GP1	C3-C4-C5	5.95	121.02	110.23
6	A	802	AAE	O3-C2-C4	5.75	144.16	126.34
4	A	803	LIM	O2J-C3J-C2J	-5.60	112.79	121.17
4	A	812	LIM	O2J-C3J-C4J	-5.46	107.07	121.40
3	A	811	GP1	C3-C4-C5	5.41	120.04	110.23
3	A	811	GP1	O5-C1-O1	-5.35	104.38	111.36
3	A	811	GP1	O5-C1-C2	5.22	121.62	110.08
3	A	811	GP1	C4-C3-C2	5.13	119.52	110.99
4	A	803	LIM	O2J-C3J-C4J	-4.88	108.60	121.40
3	A	801	GP1	O5-C1-C2	4.61	120.28	110.08
3	A	801	GP1	C4-C3-C2	4.30	118.12	110.99
6	A	802	AAE	O8-C5-C9	-4.17	111.05	121.48
3	A	811	GP1	O5-C5-C4	3.52	116.05	109.70
3	A	801	GP1	O3-C3-C2	3.25	116.05	110.22
3	A	811	GP1	O1-P4B-O8B	-3.22	97.87	109.33
3	A	801	GP1	P4B-O1-C1	3.16	132.01	123.54
3	A	801	GP1	C1-C2-N2	-3.12	104.59	110.20
4	A	803	LIM	C2J-C3J-C4J	-3.03	109.24	117.88
6	A	802	AAE	O8-C5-C4	-2.99	109.36	120.92
3	A	801	GP1	O5-C5-C4	2.61	114.41	109.70
3	A	801	GP1	C1-C2-C3	2.47	116.48	110.29
3	A	801	GP1	C6-C5-C4	2.39	118.89	113.02
3	A	811	GP1	O5-C5-C6	2.34	112.24	106.44
3	A	811	GP1	C1-C2-C3	2.12	115.61	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	606	LDA	CM1-N1-C1	-2.08	105.86	110.23

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	GP1	O5-C1-O1-P4B
3	A	811	GP1	O5-C1-O1-P4B
3	A	811	GP1	C1-O1-P4B-O8B
4	A	812	LIM	O1J-C1J-C2J-C3J
4	A	803	LIM	O1J-C1J-C2J-C3J
5	A	602	LDA	C2-C1-N1-CM2
5	A	602	LDA	N1-C1-C2-C3
5	A	603	LDA	C2-C1-N1-CM1
5	A	603	LDA	C2-C1-N1-CM2
5	A	604	LDA	C2-C1-N1-CM1
5	A	605	LDA	C2-C1-N1-CM2
5	A	607	LDA	C2-C1-N1-CM2
6	A	802	AAE	O3-C2-C4-C5
7	A	702	GOL	O1-C1-C2-O2
7	A	703	GOL	C1-C2-C3-O3
7	A	703	GOL	O2-C2-C3-O3
7	A	704	GOL	C1-C2-C3-O3
7	A	705	GOL	O1-C1-C2-C3
7	A	707	GOL	C1-C2-C3-O3
3	A	801	GP1	O5-C5-C6-O6
3	A	811	GP1	O5-C5-C6-O6
3	A	801	GP1	C4-C5-C6-O6
3	A	811	GP1	C4-C5-C6-O6
7	A	705	GOL	O1-C1-C2-O2
5	A	604	LDA	C6-C7-C8-C9
7	A	702	GOL	O1-C1-C2-C3
7	A	703	GOL	O1-C1-C2-C3
7	A	704	GOL	O1-C1-C2-C3
5	A	606	LDA	C2-C3-C4-C5
7	A	704	GOL	O2-C2-C3-O3
5	A	605	LDA	C4-C5-C6-C7
5	A	607	LDA	C2-C3-C4-C5
4	A	803	LIM	C5J-C6J-C7J-C8J
5	A	602	LDA	C11-C10-C9-C8
5	A	605	LDA	C6-C7-C8-C9
4	A	803	LIM	C9J-C0X-C1X-C2X

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Mol	Chain	Res	Type	Atoms
5	A	603	LDA	C4-C5-C6-C7
5	A	605	LDA	C1-C2-C3-C4
5	A	604	LDA	C4-C5-C6-C7
5	A	602	LDA	C4-C5-C6-C7
7	A	704	GOL	O1-C1-C2-O2
7	A	707	GOL	O2-C2-C3-O3
4	A	803	LIM	C1X-C0X-C9J-C8J
5	A	601	LDA	N1-C1-C2-C3
5	A	603	LDA	C9-C10-C11-C12
5	A	606	LDA	C3-C4-C5-C6
5	A	607	LDA	C3-C4-C5-C6
4	A	812	LIM	C9J-C0X-C1X-C2X
5	A	604	LDA	C9-C10-C11-C12
5	A	607	LDA	C4-C5-C6-C7
5	A	604	LDA	C1-C2-C3-C4
4	A	803	LIM	O2J-C3J-C4J-C5J
5	A	602	LDA	C2-C1-N1-CM1
5	A	604	LDA	C2-C1-N1-CM2
5	A	605	LDA	C2-C1-N1-CM1
5	A	607	LDA	C2-C1-N1-CM1
4	A	812	LIM	C2X-C3X-C4X-C5X
5	A	605	LDA	C2-C1-N1-O1
4	A	812	LIM	C1X-C2X-C3X-C4X
5	A	604	LDA	C5-C6-C7-C8
5	A	602	LDA	C6-C7-C8-C9
5	A	607	LDA	C5-C6-C7-C8
3	A	811	GP1	C1-O1-P4B-O7B
5	A	602	LDA	C1-C2-C3-C4
5	A	603	LDA	C3-C4-C5-C6
5	A	606	LDA	C7-C8-C9-C10
7	A	706	GOL	C1-C2-C3-O3
6	A	802	AAE	C2-C4-C5-C9
4	A	812	LIM	O2J-C3J-C4J-C5J
5	A	603	LDA	C7-C8-C9-C10
5	A	601	LDA	C6-C7-C8-C9
4	A	803	LIM	C2X-C3X-C4X-C5X
4	A	812	LIM	C4J-C5J-C6J-C7J
5	A	604	LDA	C3-C4-C5-C6
5	A	606	LDA	C6-C7-C8-C9
5	A	605	LDA	C2-C3-C4-C5
5	A	605	LDA	C11-C10-C9-C8
5	A	602	LDA	C2-C1-N1-O1

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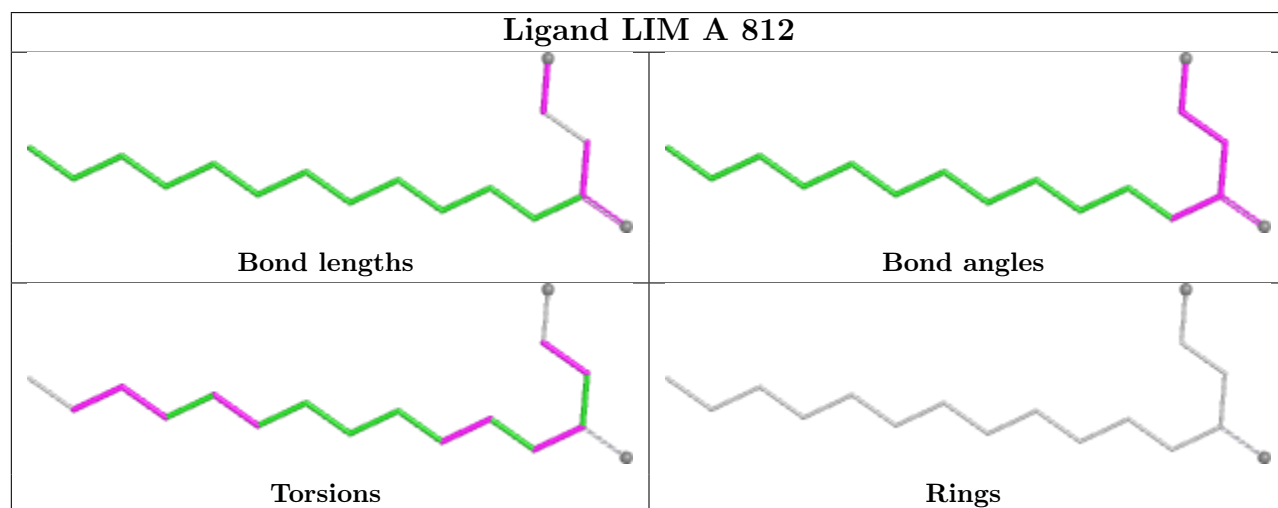
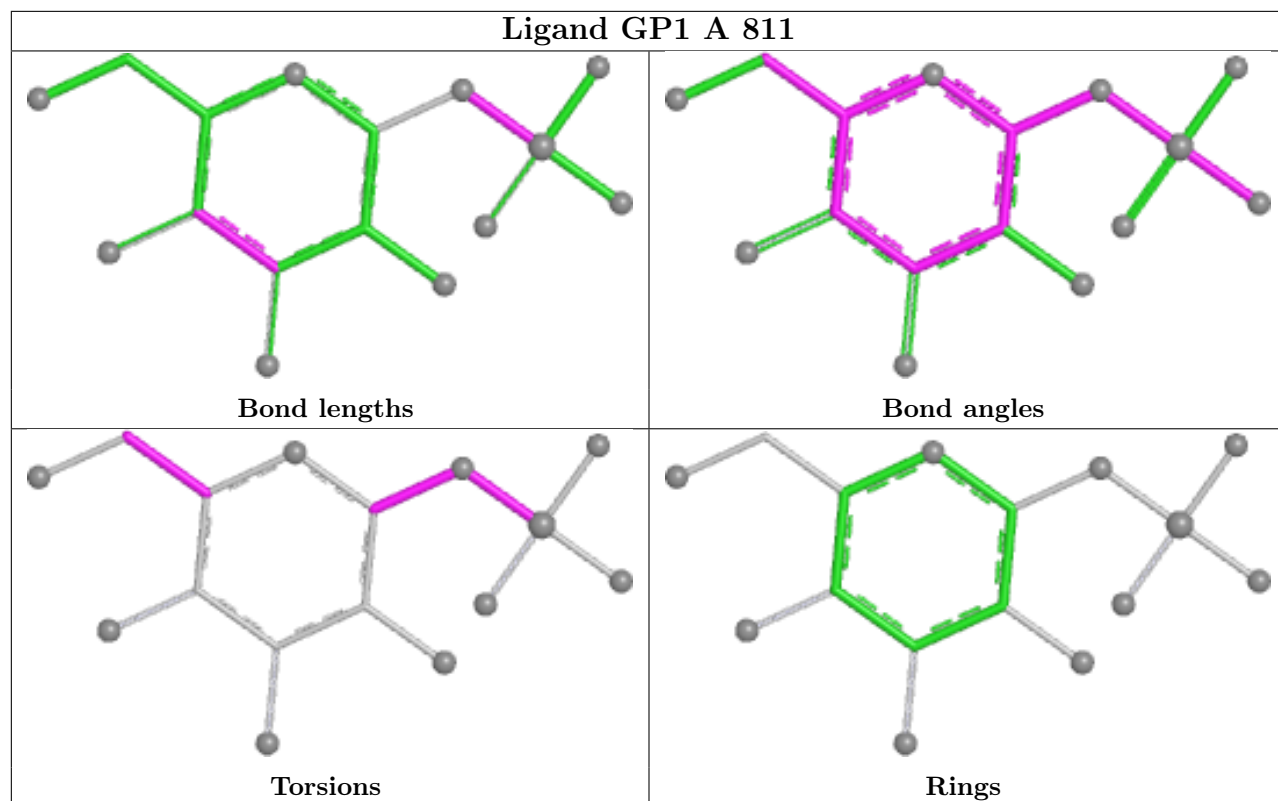
Mol	Chain	Res	Type	Atoms
5	A	603	LDA	C2-C1-N1-O1
5	A	604	LDA	C2-C1-N1-O1

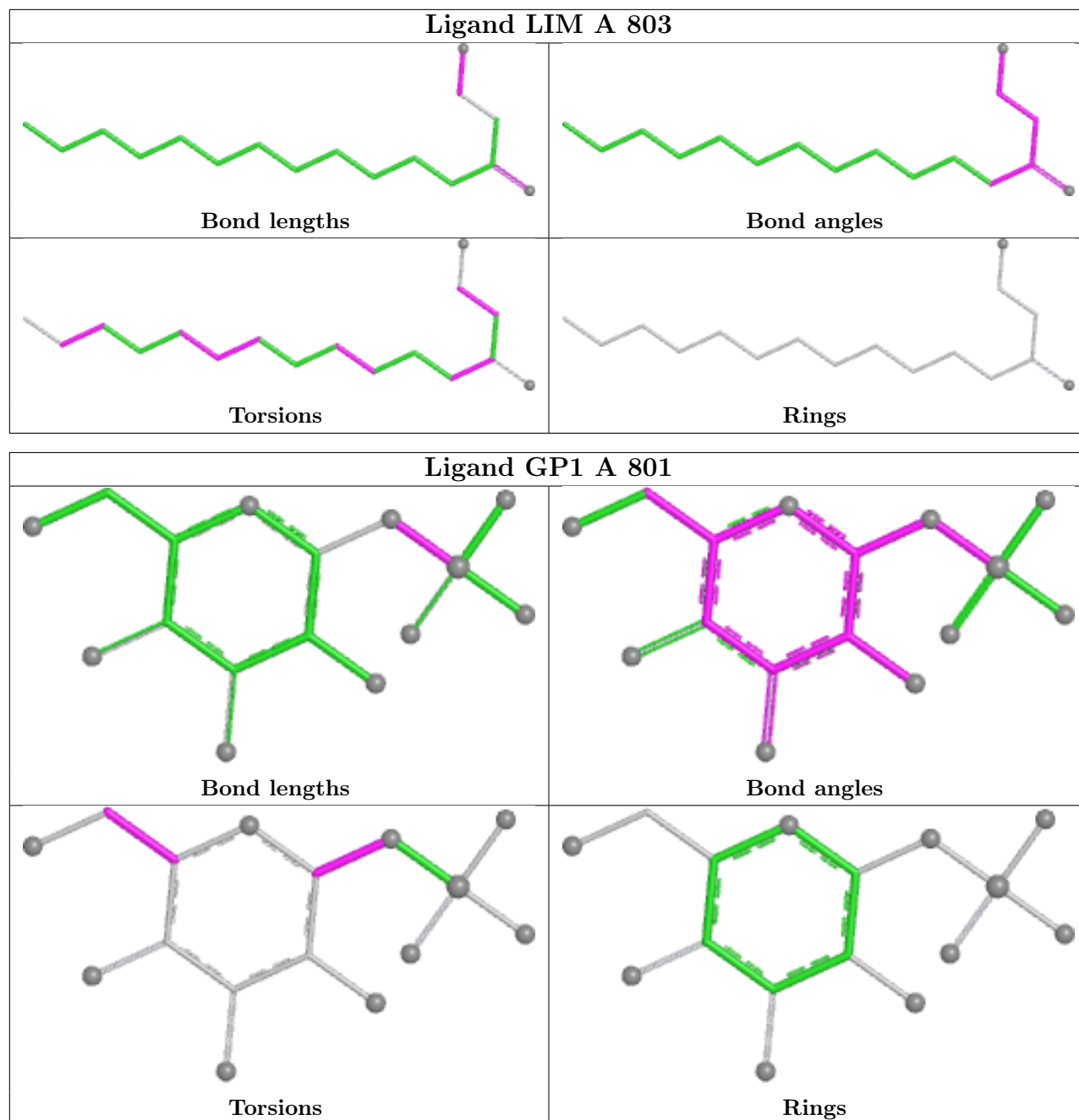
There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	LDA	4	0
7	A	704	GOL	2	0
7	A	708	GOL	3	0
4	A	812	LIM	1	0
4	A	803	LIM	1	0
7	A	706	GOL	1	0
5	A	601	LDA	1	0
5	A	606	LDA	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	576/594 (96%)	0.40	23 (3%) 42 40	22, 32, 40, 51	0
2	B	116/135 (85%)	0.66	6 (5%) 33 32	30, 35, 39, 41	0
All	All	692/729 (94%)	0.44	29 (4%) 40 39	22, 32, 40, 51	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	TYR	5.8
1	A	523	LEU	4.4
1	A	572	ASP	4.2
2	B	326	ALA	3.8
2	B	438	LYS	3.5
1	A	531	TYR	3.3
1	A	389	TYR	3.2
1	A	511	LEU	3.2
1	A	539	VAL	3.0
1	A	418	TRP	2.8
1	A	501	GLN	2.7
2	B	376	ASN	2.7
1	A	53	ASP	2.7
2	B	375	PHE	2.6
1	A	163	LYS	2.6
1	A	194	ASN	2.5
2	B	427	SER	2.5
1	A	454	TYR	2.4
1	A	177	GLY	2.4
1	A	510	GLN	2.4
1	A	215	SER	2.3
2	B	323	TYR	2.3
1	A	548	ASP	2.3
1	A	526	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	446	TYR	2.1
1	A	534	TYR	2.1
1	A	585	GLU	2.0
1	A	522	TYR	2.0
1	A	541	MET	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
3	GP1	A	811	16/16	0.29	0.20	84,87,95,95	0
3	GP1	A	801	16/16	0.52	0.19	77,83,91,91	0
6	AAE	A	802	6/7	0.61	0.23	80,81,84,86	0
7	GOL	A	703	6/6	0.67	0.14	64,67,69,72	0
7	GOL	A	707	6/6	0.68	0.17	76,77,78,78	0
7	GOL	A	706	6/6	0.70	0.18	61,65,68,69	0
7	GOL	A	705	6/6	0.75	0.16	73,75,75,76	0
5	LDA	A	605	16/16	0.77	0.20	67,70,76,78	0
4	LIM	A	812	17/18	0.80	0.19	66,71,84,86	0
4	LIM	A	803	17/18	0.82	0.18	63,69,76,77	0
5	LDA	A	607	16/16	0.86	0.17	53,65,75,75	0
7	GOL	A	701	6/6	0.86	0.20	62,64,64,65	0
5	LDA	A	606	16/16	0.88	0.16	53,56,62,63	0
5	LDA	A	601	16/16	0.89	0.17	59,65,68,69	0
7	GOL	A	702	6/6	0.89	0.18	56,58,59,60	0
5	LDA	A	604	16/16	0.89	0.14	60,64,69,70	0
5	LDA	A	603	16/16	0.90	0.13	53,55,65,65	0
5	LDA	A	602	16/16	0.90	0.15	52,57,64,66	0

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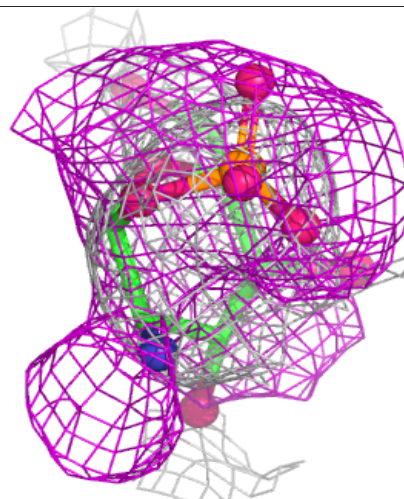
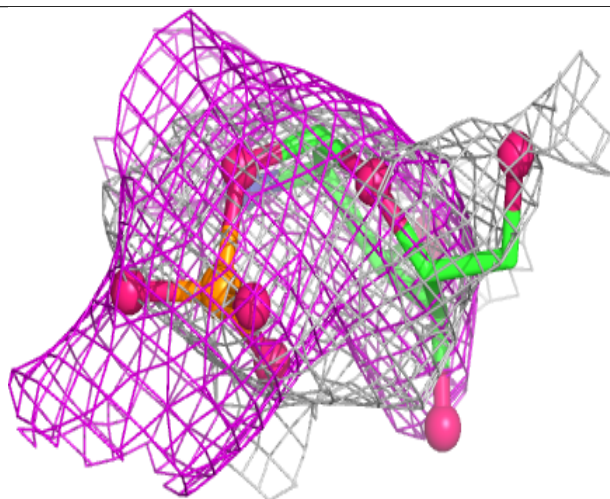
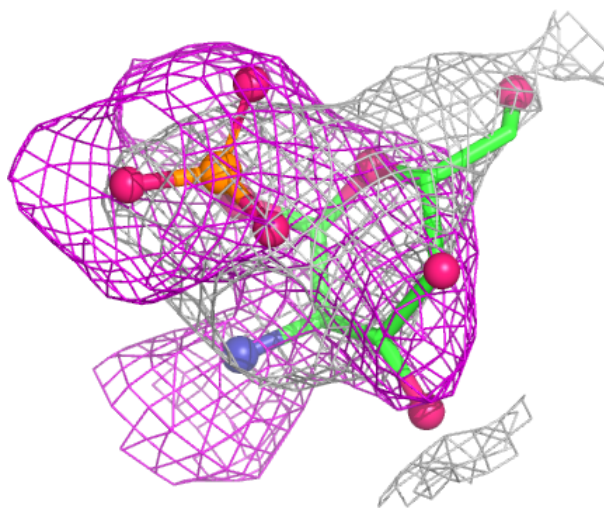
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	708	6/6	0.90	0.08	69,72,72,75	0
7	GOL	A	704	6/6	0.92	0.09	51,55,59,62	0

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.

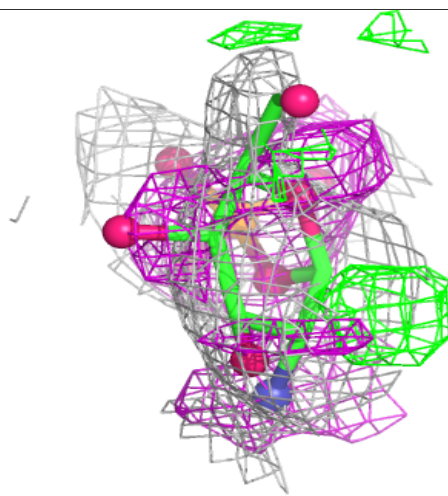
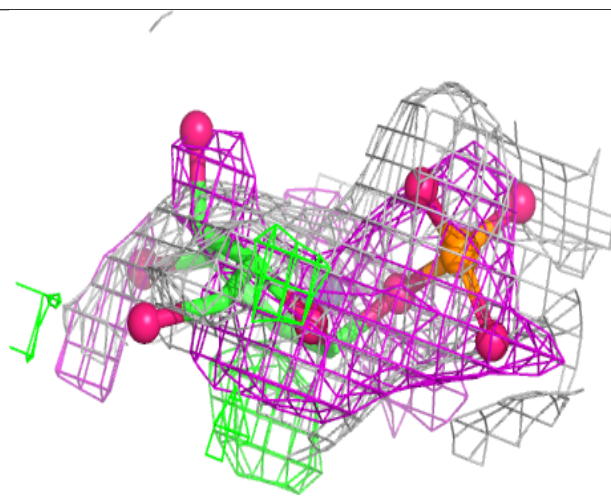
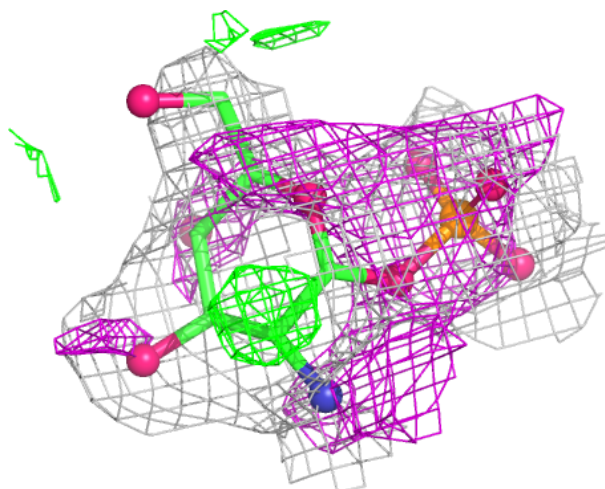
Electron density around GP1 A 811:

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



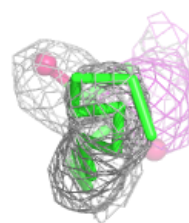
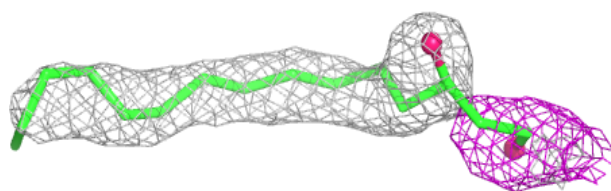
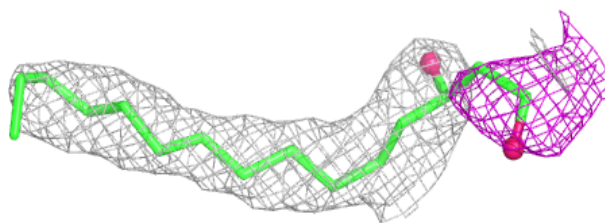
Electron density around GP1 A 801:

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

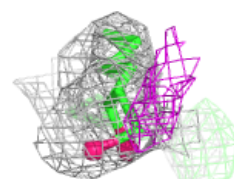
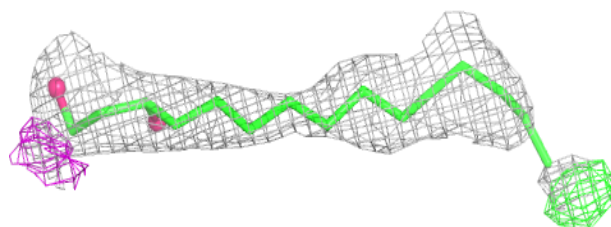
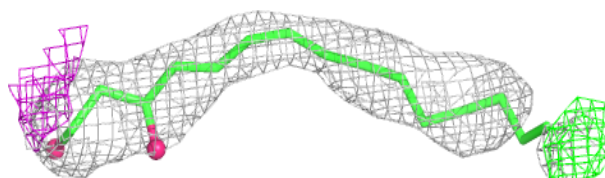


Electron density around LIM A 812:

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

**Electron density around LIM A 803:**

$2mF_o-DF_c$ (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.