



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:46 PM UTC

PDB ID : 1FCP / pdb_00001fcp
Title : FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) FROM E.COLI
IN COMPLEX WITH BOUND FERRICHROME-IRON
Authors : Hofmann, E.; Ferguson, A.D.; Diederichs, K.; Welte, W.
Deposited on : 1998-10-14
Resolution : 2.70 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

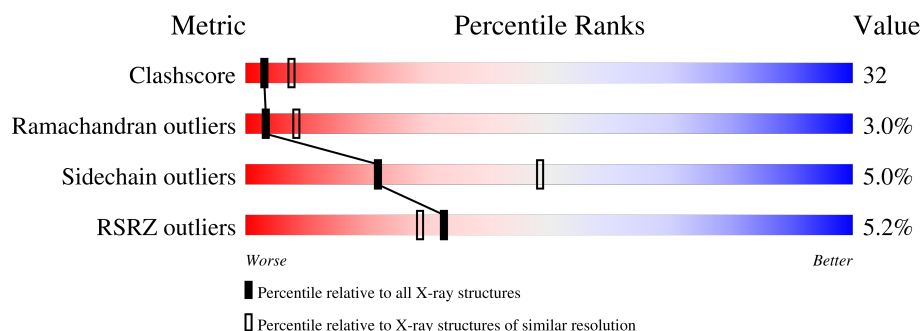
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	705	5% 50% 43% 7%
2	B	9	67% 33%

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
4	LIL	A	904	X	-	-	-
8	FCI	A	750	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5832 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.

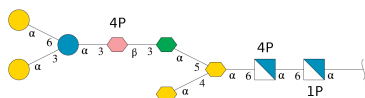
- Molecule 1 is a protein called PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	Se	0	0	0
			5512	3469	942	1087	4	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	insertion	UNP P06971
A	407	HIS	-	insertion	UNP P06971
A	408	HIS	-	insertion	UNP P06971
A	409	HIS	-	insertion	UNP P06971
A	410	HIS	-	insertion	UNP P06971
A	411	HIS	-	insertion	UNP P06971
A	412	HIS	-	insertion	UNP P06971
A	413	GLY	-	insertion	UNP P06971
A	414	SER	-	insertion	UNP P06971

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-4-O-phosphono-D-glycero-beta-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.

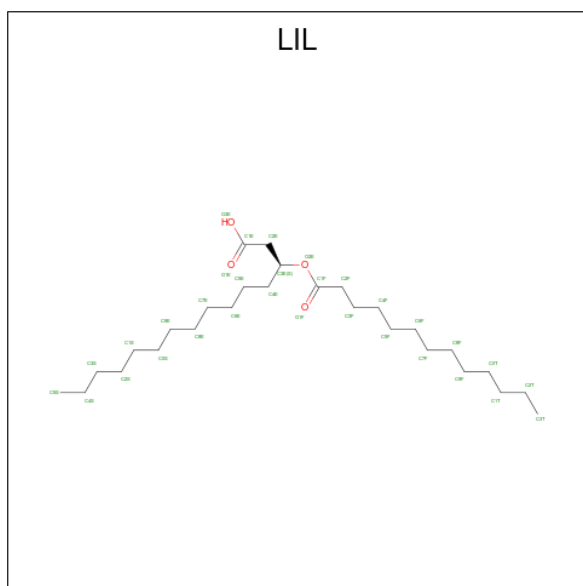


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			124	60	2	59	3			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

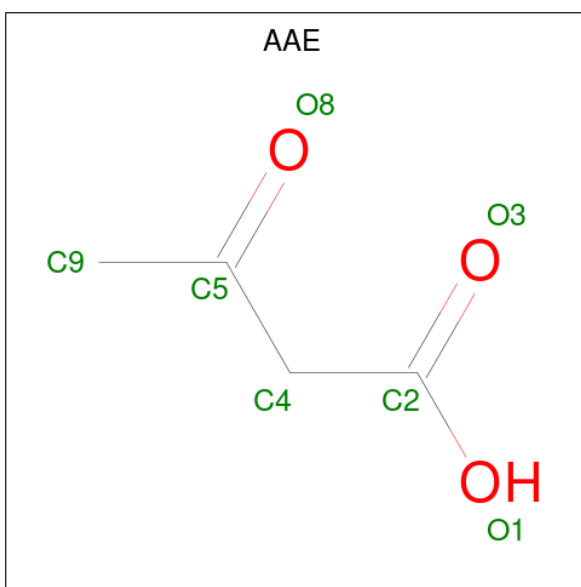
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ni 2 2	0	0

- Molecule 4 is 2-TRIDECANOYLOXY-PENTADECANOIC ACID (CCD ID: LIL) (formula: C₂₈H₅₄O₄).



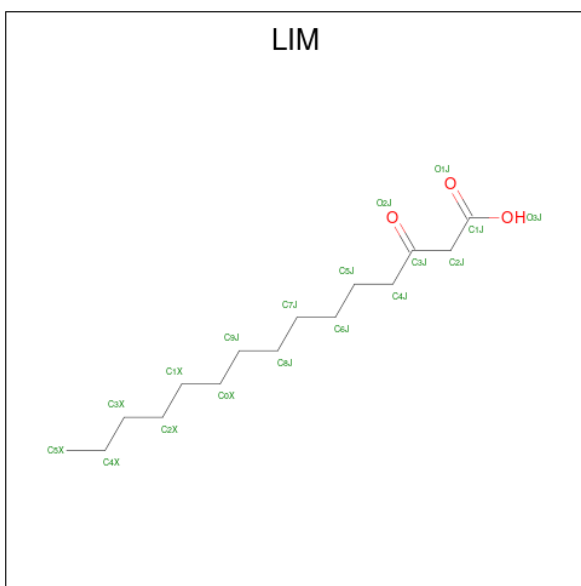
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 31 28 3	0	0
4	A	1	Total C O 31 28 3	0	0

- Molecule 5 is ACETOACETIC ACID (CCD ID: AAE) (formula: C₄H₆O₃).



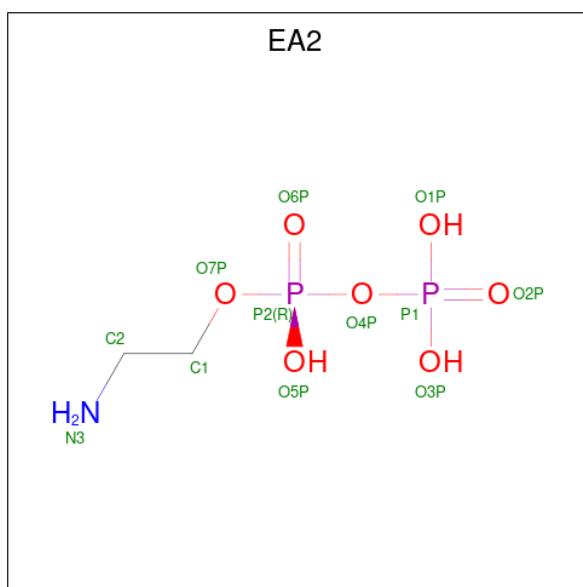
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is 3-OXO-PENTADECANOIC ACID (CCD ID: LIM) (formula: $C_{15}H_{28}O_3$).



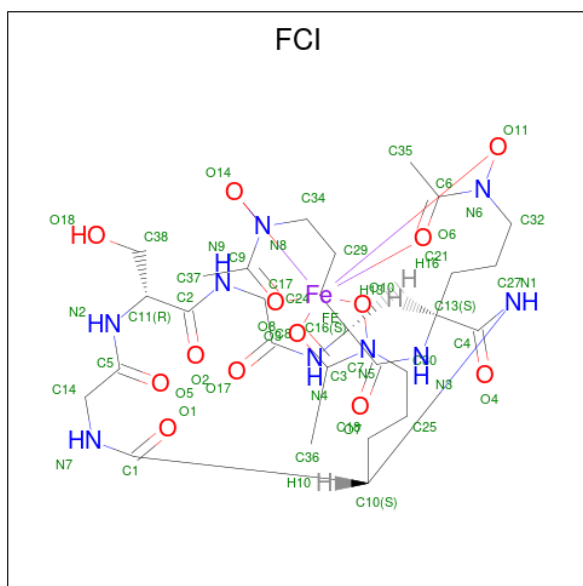
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 7 is AMINOETHANOLPYROPHOSPHATE (CCD ID: EA2) (formula: $C_2H_9NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			11	2	1	6	2		

- Molecule 8 is FERRICROCIN-IRON (CCD ID: FCI) (formula: $C_{28}H_{44}FeN_9O_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			46	24	1	9	12		

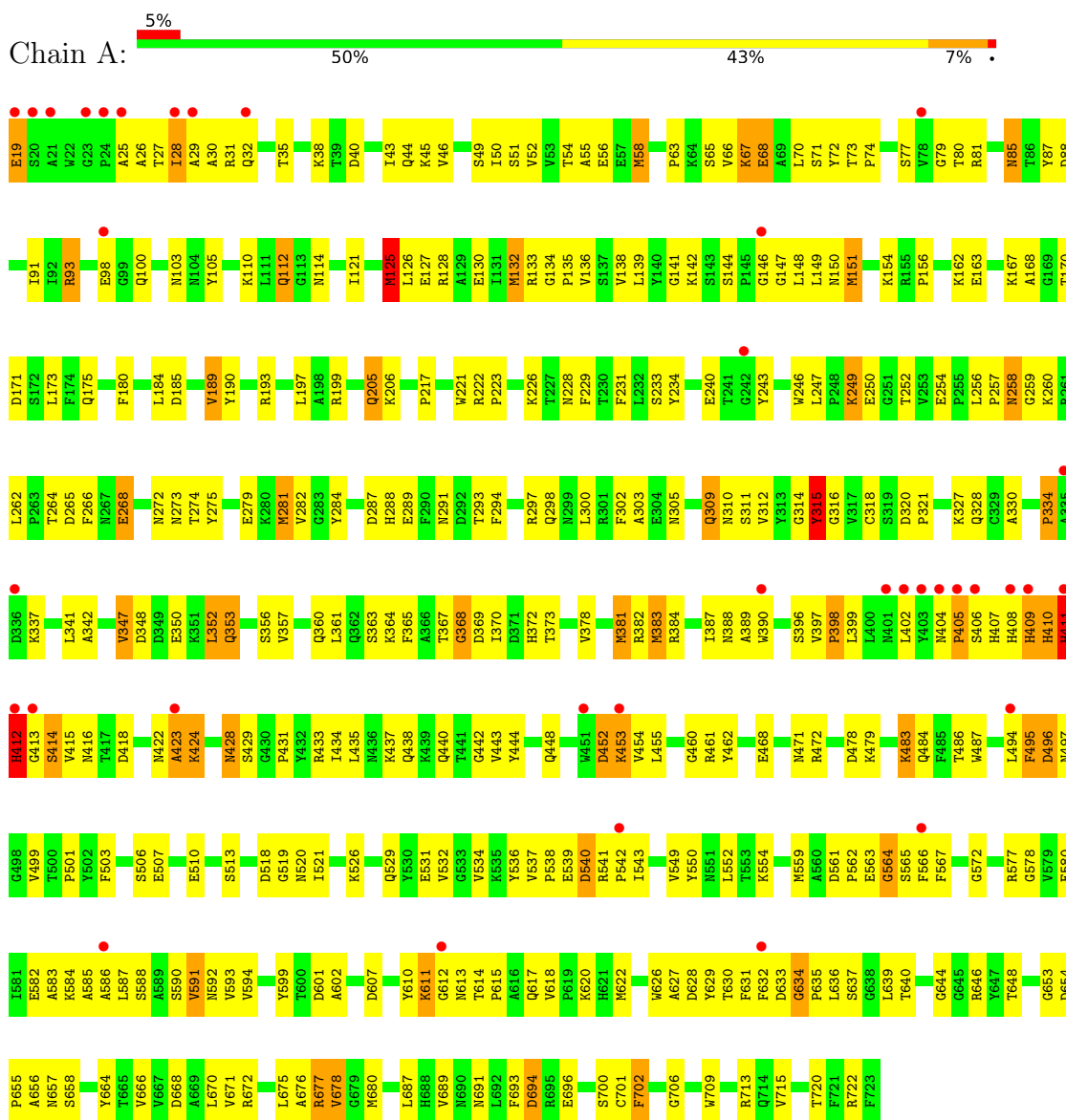
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	52	Total	O	0	0
			52	52		

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: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)



• Molecule 2: alpha-D-galactopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-4-O-phosphono-D-glycero-beta-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-

manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



GP11
GP42
KDD3
GME4
GPH5
GLC6
GLA7
GLA8
KDD9

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.40Å 171.40Å 85.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-2.70) 98.3 (40.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.69Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.232 , 0.281 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5832	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: LIL, GP4, LIM, KDO, EA2, GLC, FCI, GMH, GP1, AAE, GLA, GPH, NI

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	0.57	11/5642 (0.2%)	1.03	30/7650 (0.4%)

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	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	MSE	SE-CE	-7.76	1.72	1.95
1	A	125	MSE	SE-CE	-7.08	1.74	1.95
1	A	132	MSE	SE-CE	-6.84	1.75	1.95
1	A	125	MSE	CG-SE	-6.49	1.75	1.95
1	A	151	MSE	SE-CE	-6.42	1.76	1.95
1	A	381	MSE	SE-CE	-6.10	1.77	1.95
1	A	58	MSE	SE-CE	-6.10	1.77	1.95
1	A	680	MSE	CG-SE	-5.87	1.77	1.95
1	A	383	MSE	SE-CE	-5.48	1.79	1.95
1	A	622	MSE	SE-CE	-5.37	1.79	1.95
1	A	132	MSE	CG-SE	-5.25	1.79	1.95

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	HIS	N-CA-C	19.41	152.14	110.80
1	A	409	HIS	N-CA-C	-14.29	92.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	TYR	N-CA-C	-13.78	97.48	108.78
1	A	411	HIS	N-CA-C	-12.54	92.82	113.50
1	A	315	TYR	CA-C-N	-9.22	111.69	122.85
1	A	315	TYR	C-N-CA	-9.22	111.69	122.85
1	A	127	GLU	N-CA-C	-8.31	103.66	113.88
1	A	612	GLY	N-CA-C	-7.04	106.47	115.42
1	A	632	PHE	N-CA-C	-6.93	104.10	114.64
1	A	411	HIS	CA-C-N	6.89	134.71	121.54
1	A	411	HIS	C-N-CA	6.89	134.71	121.54
1	A	249	LYS	N-CA-C	-6.54	104.40	112.38
1	A	497	ASN	N-CA-C	-6.46	105.37	113.18
1	A	412	HIS	CA-C-O	6.37	129.62	120.51
1	A	311	SER	N-CA-C	6.16	119.17	108.76
1	A	412	HIS	CB-CA-C	-6.04	98.41	110.42
1	A	314	GLY	CA-C-N	-5.96	116.61	123.04
1	A	314	GLY	C-N-CA	-5.96	116.61	123.04
1	A	483	LYS	N-CA-C	-5.79	99.47	108.90
1	A	410	HIS	CA-C-N	5.61	128.81	120.17
1	A	410	HIS	C-N-CA	5.61	128.81	120.17
1	A	411	HIS	CA-C-O	5.50	124.54	118.65
1	A	513	SER	N-CA-C	-5.23	106.29	113.30
1	A	46	VAL	CA-C-N	5.23	126.38	119.84
1	A	46	VAL	C-N-CA	5.23	126.38	119.84
1	A	347	VAL	N-CA-C	-5.22	100.86	108.17
1	A	309	GLN	N-CA-C	5.08	116.79	108.76
1	A	702	PHE	N-CA-C	-5.08	106.77	113.17
1	A	189	VAL	N-CA-C	-5.03	105.50	112.50
1	A	591	VAL	N-CA-C	5.01	115.19	108.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	TYR	Sidechain
1	A	412	HIS	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5512	0	5213	340	0
2	B	124	0	70	4	0
3	A	2	0	0	0	0
4	A	62	0	106	16	0
5	A	6	0	5	0	0
6	A	17	0	27	6	0
7	A	11	0	6	0	0
8	A	46	0	31	2	0
9	A	52	0	0	6	0
All	All	5832	0	5458	354	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 32.

All (354) 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:410:HIS:HA	1:A:412:HIS:ND1	1.69	1.06
1:A:121:ILE:HB	1:A:151:MSE:HE1	1.40	1.01
1:A:28:ILE:HD12	1:A:28:ILE:H	1.24	1.00
1:A:410:HIS:H	1:A:412:HIS:HB3	1.27	0.97
1:A:410:HIS:CA	1:A:412:HIS:ND1	2.29	0.95
1:A:132:MSE:HE2	1:A:136:VAL:HG12	1.49	0.95
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.00	0.91
1:A:66:VAL:HG21	1:A:151:MSE:HE3	1.51	0.90
1:A:199:ARG:HD2	9:A:1054:HOH:O	1.75	0.86
1:A:341:LEU:HB2	1:A:402:LEU:HD11	1.58	0.84
1:A:453:LYS:N	1:A:453:LYS:HE2	1.93	0.83
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.61	0.83
1:A:121:ILE:HB	1:A:151:MSE:CE	2.10	0.81
1:A:206:LYS:HD3	1:A:414:SER:H	1.45	0.81
1:A:468:GLU:HG3	1:A:479:LYS:HG2	1.62	0.81
1:A:125:MSE:HG3	1:A:234:TYR:HE1	1.46	0.80
1:A:206:LYS:CD	1:A:413:GLY:HA3	2.11	0.80
1:A:373:THR:HB	1:A:448:GLN:HB2	1.65	0.79
1:A:453:LYS:HE2	1:A:453:LYS:H	1.48	0.78
1:A:228:ASN:HB3	1:A:287:ASP:OD1	1.83	0.78
1:A:309:GLN:HG2	1:A:348:ASP:HB3	1.66	0.77
1:A:206:LYS:HG3	1:A:413:GLY:HA3	1.67	0.75
1:A:410:HIS:HA	1:A:412:HIS:CE1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ASN:HB2	1:A:628:ASP:OD1	1.85	0.75
1:A:542:PRO:HG2	1:A:586:ALA:HB3	1.68	0.75
1:A:35:THR:HG21	1:A:150:ASN:HD22	1.50	0.74
1:A:71:SER:HB3	1:A:646:ARG:HD2	1.69	0.74
1:A:494:LEU:HD11	9:A:1047:HOH:O	1.87	0.74
1:A:410:HIS:N	1:A:412:HIS:HB3	2.02	0.74
1:A:31:ARG:HH12	1:A:539:GLU:HA	1.52	0.74
1:A:249:LYS:HG2	1:A:250:GLU:OE1	1.88	0.73
1:A:126:LEU:HD11	1:A:151:MSE:CE	2.18	0.73
2:B:6:GLC:H61	2:B:8:GLA:H5	1.69	0.73
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.02	0.73
1:A:503:PHE:HB2	1:A:532:VAL:HG12	1.71	0.73
1:A:126:LEU:HD11	1:A:151:MSE:HE3	1.70	0.72
1:A:602:ALA:O	1:A:614:THR:HG22	1.91	0.71
1:A:67:LYS:HZ2	1:A:67:LYS:HB2	1.54	0.71
1:A:330:ALA:HA	1:A:337:LYS:NZ	2.06	0.70
1:A:93:ARG:HD3	1:A:133:ARG:HG2	1.73	0.70
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.26	0.70
1:A:409:HIS:O	1:A:410:HIS:HB2	1.90	0.70
1:A:134:GLY:C	1:A:146:GLY:HA2	2.18	0.69
1:A:444:TYR:HB3	1:A:461:ARG:HB2	1.74	0.69
1:A:206:LYS:CG	1:A:413:GLY:HA3	2.22	0.69
4:A:903:LIL:H8E1	4:A:904:LIL:H8E1	1.74	0.68
1:A:384:ARG:NH1	1:A:437:LYS:HE2	2.08	0.68
1:A:415:VAL:HG22	1:A:416:ASN:N	2.08	0.68
1:A:28:ILE:H	1:A:28:ILE:CD1	2.02	0.67
1:A:390:TRP:CZ3	1:A:431:PRO:HB3	2.28	0.67
1:A:407:HIS:O	1:A:409:HIS:O	2.13	0.67
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.11	0.66
1:A:134:GLY:HA2	1:A:146:GLY:HA2	1.78	0.66
1:A:217:PRO:HD2	1:A:233:SER:OG	1.95	0.66
1:A:98:GLU:OE2	1:A:554:LYS:NZ	2.27	0.66
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.78	0.65
1:A:415:VAL:HG22	1:A:416:ASN:H	1.62	0.65
1:A:410:HIS:H	1:A:412:HIS:CB	2.05	0.65
1:A:713:ARG:HH11	1:A:713:ARG:HG2	1.63	0.64
1:A:565:SER:C	1:A:567:PHE:H	2.05	0.64
1:A:297:ARG:HG3	1:A:360:GLN:HG3	1.80	0.63
1:A:125:MSE:HG3	1:A:234:TYR:CE1	2.32	0.63
1:A:19:GLU:O	1:A:32:GLN:HG3	1.97	0.63
1:A:126:LEU:HD21	1:A:151:MSE:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:GLC:H61	2:B:8:GLA:C5	2.29	0.63
1:A:282:VAL:HG21	4:A:903:LIL:H9E1	1.81	0.63
1:A:352:LEU:HB2	1:A:384:ARG:O	1.99	0.63
1:A:197:LEU:C	1:A:197:LEU:HD12	2.24	0.62
1:A:590:SER:HB2	1:A:630:THR:O	2.00	0.62
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.35	0.62
1:A:381:MSE:HE1	1:A:383:MSE:HB2	1.82	0.62
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.82	0.62
4:A:903:LIL:H2E2	4:A:904:LIL:H4E2	1.82	0.62
1:A:79:GLY:C	1:A:81:ARG:H	2.08	0.62
1:A:49:SER:C	1:A:50:ILE:HD12	2.25	0.61
1:A:626:TRP:CH2	1:A:628:ASP:HB3	2.34	0.61
1:A:58:MSE:O	1:A:63:PRO:HD2	2.00	0.61
1:A:666:VAL:HG13	1:A:691:ASN:HA	1.81	0.61
1:A:543:ILE:HG22	1:A:585:ALA:HB1	1.82	0.61
1:A:611:LYS:C	1:A:613:ASN:H	2.08	0.61
1:A:105:TYR:O	1:A:150:ASN:HA	2.01	0.60
1:A:671:VAL:CG2	1:A:687:LEU:HB3	2.31	0.60
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.37	0.60
1:A:148:LEU:C	1:A:148:LEU:HD23	2.27	0.59
1:A:297:ARG:HD2	1:A:360:GLN:NE2	2.17	0.59
1:A:559:MSE:HE2	1:A:572:GLY:N	2.17	0.59
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.66	0.59
1:A:28:ILE:HG13	1:A:56:GLU:OE1	2.02	0.59
1:A:66:VAL:HG21	1:A:151:MSE:CE	2.29	0.59
1:A:93:ARG:HG3	1:A:550:TYR:OH	2.02	0.59
1:A:231:PHE:CZ	4:A:903:LIL:H4S2	2.36	0.59
1:A:460:GLY:HA2	1:A:487:TRP:HA	1.84	0.59
1:A:565:SER:O	1:A:567:PHE:N	2.32	0.59
1:A:93:ARG:HH11	1:A:580:GLU:CD	2.10	0.59
1:A:71:SER:HB3	1:A:646:ARG:CD	2.31	0.59
1:A:353:GLN:OE1	1:A:384:ARG:HD3	2.03	0.58
1:A:138:VAL:HG13	1:A:139:LEU:HG	1.86	0.58
1:A:282:VAL:HG11	4:A:903:LIL:H7F2	1.85	0.58
1:A:390:TRP:HE1	1:A:429:SER:CB	2.15	0.58
1:A:133:ARG:HD2	1:A:580:GLU:OE1	2.03	0.58
1:A:501:PRO:HA	1:A:534:VAL:HG12	1.84	0.58
1:A:134:GLY:N	1:A:146:GLY:HA2	2.17	0.58
4:A:903:LIL:H9E2	4:A:904:LIL:H0S1	1.85	0.58
1:A:135:PRO:HB2	1:A:506:SER:OG	2.04	0.58
1:A:300:LEU:C	1:A:300:LEU:HD23	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:ARG:HG3	1:A:577:ARG:HH11	1.68	0.57
1:A:74:PRO:HG3	1:A:582:GLU:HB2	1.87	0.57
1:A:384:ARG:HH12	1:A:437:LYS:HE2	1.68	0.57
1:A:352:LEU:C	1:A:352:LEU:HD12	2.28	0.57
1:A:434:ILE:HD13	1:A:471:ASN:HA	1.87	0.57
1:A:689:VAL:HG22	1:A:715:VAL:HG22	1.86	0.57
1:A:316:GLY:O	1:A:341:LEU:HD12	2.05	0.57
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.40	0.56
1:A:206:LYS:HG3	1:A:413:GLY:CA	2.35	0.56
1:A:294:PHE:HE1	1:A:363:SER:HG	1.53	0.56
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.39	0.56
1:A:388:ASN:HD22	1:A:433:ARG:HG2	1.70	0.56
1:A:350:GLU:HG2	1:A:387:ILE:HG12	1.87	0.56
1:A:25:ALA:O	1:A:26:ALA:HB3	2.05	0.56
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.40	0.56
1:A:529:GLN:HB2	1:A:552:LEU:HD13	1.88	0.56
4:A:904:LIL:H9F1	6:A:906:LIM:H5X2	1.87	0.56
1:A:330:ALA:HA	1:A:337:LYS:HZ1	1.71	0.55
1:A:615:PRO:O	1:A:618:VAL:HG12	2.06	0.55
1:A:67:LYS:HE3	1:A:87:TYR:O	2.07	0.55
1:A:185:ASP:OD2	1:A:189:VAL:HG12	2.07	0.55
1:A:607:ASP:HB3	1:A:610:TYR:O	2.06	0.55
1:A:135:PRO:HB3	1:A:507:GLU:C	2.32	0.55
1:A:407:HIS:C	1:A:409:HIS:O	2.49	0.55
1:A:247:LEU:HD21	1:A:268:GLU:HG3	1.88	0.55
1:A:249:LYS:HE2	1:A:254:GLU:OE1	2.07	0.55
1:A:258:ASN:HD22	1:A:260:LYS:HD2	1.72	0.55
1:A:93:ARG:NH1	1:A:580:GLU:OE1	2.41	0.55
1:A:654:ASP:OD2	1:A:658:SER:HB3	2.07	0.55
1:A:79:GLY:C	1:A:81:ARG:N	2.65	0.54
1:A:52:VAL:HG22	1:A:130:GLU:HG2	1.88	0.54
1:A:676:ALA:C	1:A:678:VAL:H	2.15	0.54
1:A:19:GLU:OE2	1:A:30:ALA:HA	2.06	0.54
1:A:390:TRP:CD2	1:A:424:LYS:HG3	2.42	0.54
1:A:672:ARG:HD2	9:A:1028:HOH:O	2.06	0.54
1:A:300:LEU:CG	1:A:357:VAL:HG12	2.38	0.54
1:A:590:SER:O	1:A:629:TYR:HA	2.08	0.54
1:A:531:GLU:HG3	1:A:550:TYR:HB3	1.90	0.54
1:A:257:PRO:C	1:A:259:GLY:H	2.16	0.53
1:A:265:ASP:CG	1:A:412:HIS:HD2	2.16	0.53
1:A:341:LEU:CB	1:A:402:LEU:HD11	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:CG	1:A:360:GLN:HG3	2.38	0.53
1:A:310:ASN:ND2	1:A:347:VAL:HG13	2.24	0.53
1:A:408:HIS:O	1:A:411:HIS:HB2	2.08	0.53
1:A:51:SER:OG	1:A:133:ARG:NH2	2.39	0.53
1:A:66:VAL:CG2	1:A:151:MSE:HE3	2.31	0.53
1:A:189:VAL:HG23	1:A:222:ARG:O	2.07	0.53
1:A:49:SER:O	1:A:50:ILE:HD12	2.08	0.53
1:A:368:GLY:O	1:A:369:ASP:HB2	2.08	0.52
1:A:288:HIS:ND1	1:A:289:GLU:N	2.57	0.52
1:A:646:ARG:NH1	1:A:668:ASP:OD2	2.42	0.52
1:A:484:GLN:OE1	1:A:526:LYS:HE2	2.08	0.52
1:A:264:THR:HA	1:A:709:TRP:CD1	2.45	0.52
1:A:409:HIS:O	1:A:410:HIS:CB	2.54	0.52
1:A:637:SER:HB3	1:A:677:ARG:HH21	1.75	0.52
4:A:904:LIL:H7F1	6:A:906:LIM:C0X	2.40	0.52
1:A:264:THR:HG21	1:A:696:GLU:HG2	1.92	0.51
1:A:294:PHE:CD1	1:A:361:LEU:HD11	2.45	0.51
1:A:279:GLU:HA	1:A:305:ASN:OD1	2.11	0.51
1:A:631:PHE:HB2	1:A:636:LEU:O	2.10	0.51
1:A:298:GLN:HE22	6:A:906:LIM:H3X1	1.73	0.51
1:A:205:GLN:HG3	1:A:243:TYR:HB2	1.92	0.51
1:A:565:SER:C	1:A:567:PHE:N	2.68	0.51
1:A:103:ASN:ND2	1:A:147:GLY:O	2.44	0.51
1:A:170:THR:HG22	1:A:171:ASP:N	2.27	0.50
1:A:540:ASP:OD2	1:A:541:ARG:HG3	2.11	0.50
1:A:462:TYR:OH	1:A:483:LYS:HB3	2.12	0.50
1:A:542:PRO:CG	1:A:586:ALA:HB3	2.40	0.50
1:A:67:LYS:HD3	9:A:1043:HOH:O	2.11	0.50
1:A:229:PHE:HZ	4:A:904:LIL:H5S2	1.77	0.50
1:A:701:CYS:HA	1:A:706:GLY:O	2.11	0.50
1:A:281:MSE:HB3	1:A:303:ALA:HB2	1.94	0.50
1:A:410:HIS:N	1:A:412:HIS:ND1	2.60	0.50
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.41	0.50
1:A:670:LEU:HD12	1:A:671:VAL:N	2.26	0.50
1:A:142:LYS:NZ	1:A:438:GLN:OE1	2.45	0.50
1:A:413:GLY:O	1:A:414:SER:HB2	2.11	0.50
1:A:402:LEU:C	1:A:405:PRO:HD2	2.36	0.50
1:A:168:ALA:HA	1:A:173:LEU:O	2.12	0.49
1:A:671:VAL:HG22	1:A:687:LEU:HB3	1.93	0.49
1:A:80:THR:HG22	1:A:80:THR:O	2.12	0.49
1:A:588:SER:HB3	1:A:591:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:CG	1:A:412:HIS:CD2	2.91	0.49
1:A:302:PHE:HZ	4:A:903:LIL:H2E1	1.77	0.49
1:A:67:LYS:HG3	1:A:88:ASP:HA	1.93	0.49
1:A:529:GLN:HB2	1:A:552:LEU:CD1	2.42	0.49
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.38	0.49
1:A:32:GLN:O	1:A:128:ARG:NH2	2.44	0.49
1:A:383:MSE:HE1	1:A:438:GLN:NE2	2.27	0.49
1:A:671:VAL:HG23	1:A:671:VAL:O	2.12	0.49
1:A:65:SER:OG	1:A:67:LYS:HB2	2.13	0.49
1:A:130:GLU:O	1:A:149:LEU:HD12	2.12	0.49
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.95	0.48
1:A:294:PHE:HD1	1:A:361:LEU:HD11	1.78	0.48
1:A:302:PHE:CZ	4:A:903:LIL:H2E1	2.47	0.48
1:A:390:TRP:CE2	1:A:424:LYS:HB2	2.48	0.48
1:A:610:TYR:O	1:A:611:LYS:HB2	2.13	0.48
1:A:72:TYR:CE2	1:A:626:TRP:HB2	2.48	0.48
1:A:626:TRP:CD1	1:A:644:GLY:HA3	2.48	0.48
1:A:45:LYS:HB3	1:A:455:LEU:CD2	2.44	0.48
1:A:258:ASN:ND2	1:A:260:LYS:HD2	2.28	0.48
1:A:265:ASP:OD1	1:A:412:HIS:CD2	2.67	0.48
1:A:93:ARG:HG3	1:A:550:TYR:CZ	2.48	0.48
1:A:282:VAL:HG21	4:A:903:LIL:C9E	2.43	0.48
1:A:415:VAL:CG2	1:A:416:ASN:H	2.26	0.48
1:A:67:LYS:HB2	1:A:67:LYS:NZ	2.27	0.48
1:A:252:THR:HG22	1:A:709:TRP:CE2	2.48	0.48
1:A:256:LEU:HD11	1:A:402:LEU:HB3	1.96	0.48
1:A:594:VAL:O	1:A:626:TRP:N	2.44	0.48
1:A:610:TYR:CZ	1:A:655:PRO:HB2	2.49	0.48
1:A:184:LEU:HD12	1:A:190:TYR:HB3	1.95	0.48
1:A:406:SER:O	1:A:410:HIS:HD2	1.97	0.48
1:A:284:TYR:OH	6:A:906:LIM:H5X3	2.14	0.48
1:A:415:VAL:CG2	1:A:416:ASN:N	2.75	0.48
1:A:578:GLY:HA3	1:A:599:TYR:O	2.13	0.48
1:A:297:ARG:HG3	1:A:360:GLN:CG	2.44	0.48
1:A:478:ASP:HB3	1:A:521:ILE:HD11	1.96	0.48
1:A:134:GLY:H	1:A:146:GLY:HA2	1.78	0.47
1:A:38:LYS:HE3	1:A:139:LEU:O	2.14	0.47
1:A:611:LYS:C	1:A:613:ASN:N	2.72	0.47
1:A:114:ASN:HB2	9:A:1023:HOH:O	2.14	0.47
1:A:27:THR:HG22	1:A:28:ILE:N	2.30	0.47
1:A:262:LEU:HD13	1:A:266:PHE:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASP:C	1:A:454:VAL:H	2.22	0.47
1:A:68:GLU:C	1:A:70:LEU:H	2.23	0.47
1:A:246:TRP:HB3	1:A:706:GLY:HA2	1.94	0.47
1:A:342:ALA:HA	1:A:399:LEU:HD22	1.96	0.47
1:A:367:THR:HG22	1:A:367:THR:O	2.15	0.47
1:A:593:VAL:HG12	1:A:627:ALA:HB2	1.96	0.47
4:A:904:LIL:H2F2	6:A:906:LIM:O1J	2.14	0.47
1:A:31:ARG:NH2	1:A:541:ARG:O	2.48	0.47
1:A:615:PRO:HG2	1:A:618:VAL:HG11	1.97	0.47
1:A:678:VAL:HG12	1:A:678:VAL:O	2.14	0.47
1:A:320:ASP:OD1	1:A:321:PRO:HD2	2.14	0.47
1:A:636:LEU:HD22	1:A:639:LEU:HD22	1.97	0.47
1:A:27:THR:C	1:A:29:ALA:H	2.21	0.46
1:A:356:SER:HB3	9:A:1051:HOH:O	2.14	0.46
1:A:390:TRP:HE1	1:A:429:SER:HB2	1.80	0.46
1:A:68:GLU:C	1:A:70:LEU:N	2.72	0.46
1:A:112:GLN:HE21	1:A:112:GLN:CA	2.28	0.46
1:A:206:LYS:HD3	1:A:413:GLY:HA3	1.93	0.46
1:A:495:PHE:HB2	1:A:499:VAL:O	2.16	0.46
1:A:347:VAL:O	1:A:389:ALA:HB1	2.16	0.46
1:A:693:PHE:O	1:A:694:ASP:C	2.59	0.46
1:A:77:SER:OG	1:A:91:ILE:HB	2.15	0.46
1:A:518:ASP:OD2	1:A:520:ASN:HB2	2.16	0.46
1:A:577:ARG:O	1:A:601:ASP:HB3	2.16	0.46
1:A:154:LYS:HD3	1:A:193:ARG:CZ	2.46	0.46
1:A:297:ARG:HD2	1:A:360:GLN:HE21	1.81	0.46
1:A:126:LEU:HD11	1:A:151:MSE:HE2	1.97	0.46
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.80	0.46
1:A:300:LEU:CB	1:A:357:VAL:HG12	2.46	0.46
4:A:903:LIL:H3E1	4:A:903:LIL:H2F2	1.72	0.46
1:A:114:ASN:OD1	1:A:387:ILE:HD11	2.16	0.45
1:A:27:THR:C	1:A:29:ALA:N	2.74	0.45
1:A:536:TYR:CD2	1:A:538:PRO:HD3	2.51	0.45
1:A:390:TRP:CE2	1:A:424:LYS:HG3	2.51	0.45
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.52	0.45
1:A:402:LEU:O	1:A:405:PRO:HD2	2.17	0.45
1:A:265:ASP:OD2	1:A:413:GLY:HA2	2.17	0.45
1:A:288:HIS:ND1	1:A:288:HIS:C	2.75	0.45
1:A:599:TYR:OH	1:A:620:LYS:NZ	2.50	0.45
1:A:617:GLN:HG2	1:A:700:SER:HB2	1.99	0.45
1:A:240:GLU:HA	1:A:275:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD12	1:A:197:LEU:O	2.18	0.44
2:B:6:GLC:C6	2:B:8:GLA:C5	2.95	0.44
1:A:722:ARG:HG3	1:A:722:ARG:HH11	1.82	0.44
1:A:65:SER:HB3	1:A:85:ASN:OD1	2.16	0.44
1:A:100:GLN:HG3	8:A:750:FCI:C9	2.48	0.44
1:A:258:ASN:HD22	1:A:260:LYS:CD	2.31	0.44
1:A:422:ASN:O	1:A:423:ALA:C	2.58	0.44
1:A:44:GLN:HG2	1:A:45:LYS:N	2.32	0.44
1:A:519:GLY:O	1:A:520:ASN:ND2	2.51	0.44
1:A:565:SER:O	1:A:566:PHE:HB2	2.18	0.44
1:A:653:GLY:O	1:A:654:ASP:HB3	2.17	0.44
1:A:691:ASN:HB3	1:A:713:ARG:HA	2.00	0.44
1:A:320:ASP:O	1:A:321:PRO:C	2.61	0.44
1:A:406:SER:O	1:A:410:HIS:CD2	2.70	0.44
1:A:592:ASN:O	1:A:627:ALA:HA	2.18	0.44
1:A:713:ARG:HG2	1:A:713:ARG:NH1	2.32	0.44
1:A:300:LEU:HG	1:A:357:VAL:HG12	1.99	0.44
1:A:634:GLY:HA3	1:A:635:PRO:HD2	1.90	0.44
1:A:378:VAL:HA	1:A:442:GLY:O	2.19	0.43
1:A:562:PRO:HB2	1:A:563:GLU:OE1	2.18	0.43
1:A:309:GLN:O	1:A:347:VAL:HA	2.17	0.43
1:A:141:GLY:HA3	1:A:440:GLN:NE2	2.33	0.43
1:A:273:ASN:HD21	1:A:312:VAL:H	1.65	0.43
4:A:904:LIL:H1T1	6:A:906:LIM:H5X1	1.99	0.43
1:A:352:LEU:HD12	1:A:352:LEU:O	2.19	0.43
4:A:903:LIL:H4F1	4:A:903:LIL:H5E2	1.99	0.43
1:A:93:ARG:HD2	1:A:580:GLU:OE2	2.19	0.43
1:A:559:MSE:SE	1:A:607:ASP:HA	2.68	0.43
1:A:676:ALA:O	1:A:678:VAL:N	2.47	0.43
1:A:144:SER:HA	1:A:510:GLU:OE1	2.18	0.43
1:A:206:LYS:HD2	1:A:413:GLY:HA3	1.99	0.43
1:A:226:LYS:HB3	1:A:289:GLU:HB3	1.99	0.43
1:A:388:ASN:ND2	1:A:433:ARG:CD	2.82	0.43
1:A:702:PHE:CE2	1:A:706:GLY:HA3	2.54	0.43
1:A:364:LYS:CD	1:A:373:THR:HG23	2.48	0.43
2:B:5:GPH:O2	2:B:6:GLC:H5	2.19	0.43
1:A:443:VAL:HG23	1:A:443:VAL:O	2.18	0.43
1:A:303:ALA:O	1:A:353:GLN:HA	2.19	0.42
1:A:410:HIS:H	1:A:412:HIS:CG	2.37	0.42
1:A:291:ASN:OD1	1:A:293:THR:HG22	2.19	0.42
1:A:563:GLU:O	1:A:564:GLY:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:SER:HB3	1:A:677:ARG:HE	1.84	0.42
1:A:300:LEU:HB2	1:A:357:VAL:HG12	2.01	0.42
1:A:388:ASN:ND2	1:A:433:ARG:HD3	2.34	0.42
1:A:536:TYR:CZ	1:A:538:PRO:HB3	2.54	0.42
1:A:640:THR:HB	1:A:672:ARG:HB3	2.02	0.42
1:A:112:GLN:HE21	1:A:112:GLN:C	2.27	0.42
1:A:648:THR:HB	1:A:664:TYR:CE1	2.54	0.42
1:A:396:SER:HA	1:A:428:ASN:HB2	2.02	0.42
1:A:656:ALA:O	1:A:657:ASN:HB2	2.19	0.42
1:A:197:LEU:C	1:A:197:LEU:CD1	2.93	0.42
1:A:424:LYS:HD3	1:A:424:LYS:N	2.35	0.42
8:A:750:FCI:H212	8:A:750:FCI:O11	2.19	0.42
1:A:365:PHE:HE1	1:A:372:HIS:ND1	2.18	0.41
1:A:382:ARG:O	1:A:382:ARG:HG3	2.20	0.41
1:A:428:ASN:C	1:A:428:ASN:HD22	2.27	0.41
1:A:31:ARG:NH1	1:A:539:GLU:HA	2.27	0.41
1:A:453:LYS:HE2	1:A:453:LYS:CA	2.50	0.41
1:A:43:ILE:HG13	1:A:537:VAL:HG21	2.02	0.41
1:A:163:GLU:HB2	1:A:722:ARG:HD3	2.02	0.41
1:A:350:GLU:CG	1:A:387:ILE:HG12	2.50	0.41
1:A:586:ALA:HA	1:A:592:ASN:HD22	1.85	0.41
1:A:350:GLU:CD	1:A:387:ILE:HG12	2.45	0.41
1:A:561:ASP:OD1	1:A:562:PRO:HD2	2.21	0.41
1:A:618:VAL:HG13	1:A:618:VAL:O	2.20	0.41
1:A:79:GLY:O	1:A:81:ARG:N	2.54	0.41
1:A:148:LEU:HD23	1:A:149:LEU:N	2.36	0.41
1:A:327:LYS:O	1:A:328:GLN:C	2.62	0.41
1:A:272:ASN:HB3	1:A:418:ASP:OD1	2.20	0.41
1:A:365:PHE:CD1	1:A:365:PHE:C	2.99	0.41
1:A:434:ILE:HG22	1:A:435:LEU:N	2.35	0.41
1:A:577:ARG:HG3	1:A:577:ARG:NH1	2.34	0.41
1:A:583:ALA:O	1:A:594:VAL:HA	2.21	0.41
1:A:126:LEU:HD13	1:A:151:MSE:HB3	2.03	0.41
1:A:352:LEU:C	1:A:352:LEU:CD1	2.92	0.41
1:A:543:ILE:CG2	1:A:585:ALA:HB1	2.48	0.41
1:A:390:TRP:NE1	1:A:424:LYS:HB2	2.37	0.40
1:A:494:LEU:O	1:A:495:PHE:O	2.40	0.40
1:A:378:VAL:HG12	1:A:443:VAL:HG12	2.03	0.40
1:A:55:ALA:HA	1:A:58:MSE:HE3	2.02	0.40
1:A:526:LYS:O	1:A:554:LYS:HA	2.21	0.40
1:A:300:LEU:HG	1:A:357:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ALA:C	1:A:588:SER:H	2.30	0.40
1:A:390:TRP:NE1	1:A:429:SER:HB2	2.36	0.40
1:A:584:LYS:HG2	1:A:594:VAL:HG22	2.03	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	703/705 (100%)	624 (89%)	58 (8%)	21 (3%)	3 8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	PHE
1	A	633	ASP
1	A	634	GLY
1	A	368	GLY
1	A	414	SER
1	A	452	ASP
1	A	564	GLY
1	A	611	LYS
1	A	677	ARG
1	A	694	ASP
1	A	258	ASN
1	A	334	PRO
1	A	412	HIS
1	A	587	LEU
1	A	678	VAL
1	A	40	ASP
1	A	423	ALA
1	A	472	ARG

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Mol	Chain	Res	Type
1	A	496	ASP
1	A	318	CYS
1	A	398	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	585/575 (102%)	556 (95%)	29 (5%)	22	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	28	ILE
1	A	54	THR
1	A	67	LYS
1	A	68	GLU
1	A	73	THR
1	A	85	ASN
1	A	93	ARG
1	A	112	GLN
1	A	125	MSE
1	A	156	PRO
1	A	205	GLN
1	A	268	GLU
1	A	315	TYR
1	A	334	PRO
1	A	352	LEU
1	A	353	GLN
1	A	404	ASN
1	A	405	PRO
1	A	411	HIS
1	A	424	LYS
1	A	428	ASN
1	A	453	LYS

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Mol	Chain	Res	Type
1	A	486	THR
1	A	496	ASP
1	A	540	ASP
1	A	549	VAL
1	A	675	LEU
1	A	720	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	85	ASN
1	A	112	GLN
1	A	150	ASN
1	A	202	ASN
1	A	205	GLN
1	A	258	ASN
1	A	310	ASN
1	A	328	GLN
1	A	354	ASN
1	A	388	ASN
1	A	410	HIS
1	A	428	ASN
1	A	520	ASN
1	A	592	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 ⓘ

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GP1	B	1	3,2	15,16,16	1.60	1 (6%)	24,24,24	1.21	1 (4%)
2	GP4	B	2	2	15,15,16	1.75	2 (13%)	20,22,24	1.42	2 (10%)
2	KDO	B	3	2	15,15,16	0.85	0	17,21,24	1.21	3 (17%)
2	GMH	B	4	2	13,13,14	0.85	0	16,18,20	0.94	1 (6%)
2	GPH	B	5	3,2	17,17,18	1.47	3 (17%)	24,25,27	1.41	4 (16%)
2	GLC	B	6	2	11,11,12	0.70	0	15,15,17	1.16	1 (6%)
2	GLA	B	7	2	11,11,12	0.66	0	15,15,17	1.04	1 (6%)
2	GLA	B	8	2	11,11,12	0.65	0	15,15,17	0.80	1 (6%)
2	KDO	B	9	2	15,15,16	0.67	0	17,21,24	1.09	2 (11%)

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	GP1	B	1	3,2	-	3/6/27/27	0/1/1/1
2	GP4	B	2	2	-	0/7/24/27	0/1/1/1
2	KDO	B	3	2	-	0/10/26/30	0/1/1/1
2	GMH	B	4	2	-	0/6/23/26	0/1/1/1
2	GPH	B	5	3,2	-	0/11/28/31	0/1/1/1
2	GLC	B	6	2	-	0/2/19/22	0/1/1/1
2	GLA	B	7	2	-	2/2/19/22	0/1/1/1
2	GLA	B	8	2	-	1/2/19/22	0/1/1/1
2	KDO	B	9	2	-	2/10/26/30	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GP4	P4A-O4	-5.41	1.50	1.59
2	B	1	GP1	P4B-O1	-5.07	1.50	1.59
2	B	5	GPH	P1-O4	-3.78	1.52	1.59
2	B	2	GP4	C1-C2	2.97	1.55	1.52
2	B	5	GPH	O5-C5	2.59	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GPH	C5-C4	2.14	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GP1	P4B-O1-C1	-4.57	111.28	123.54
2	B	2	GP4	P4A-O4-C4	-4.11	112.45	123.43
2	B	5	GPH	P1-O4-C4	-4.01	112.72	123.43
2	B	2	GP4	C1-O5-C5	3.49	116.87	112.19
2	B	7	GLA	C1-O5-C5	3.47	116.83	112.19
2	B	5	GPH	C6-C5-C4	-3.07	109.27	114.41
2	B	4	GMH	O3-C3-C2	2.59	115.34	110.05
2	B	6	GLC	C1-O5-C5	2.48	115.51	112.19
2	B	3	KDO	C4-C5-C6	-2.45	105.56	110.51
2	B	5	GPH	C1-C2-C3	2.34	113.05	109.64
2	B	3	KDO	O6-C6-C7	2.29	111.06	106.60
2	B	3	KDO	O1B-C1-C2	2.26	118.58	112.71
2	B	9	KDO	O1B-C1-C2	2.18	118.39	112.71
2	B	8	GLA	C1-O5-C5	2.18	115.11	112.19
2	B	9	KDO	O1A-C1-C2	-2.14	118.23	122.85
2	B	5	GPH	C1-O5-C5	2.08	114.89	111.48

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	GP1	C4-C5-C6-O6
2	B	1	GP1	O5-C5-C6-O6
2	B	9	KDO	C6-C7-C8-O8
2	B	9	KDO	O7-C7-C8-O8
2	B	7	GLA	C4-C5-C6-O6
2	B	8	GLA	C4-C5-C6-O6
2	B	1	GP1	C1-O1-P4B-O7B
2	B	7	GLA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

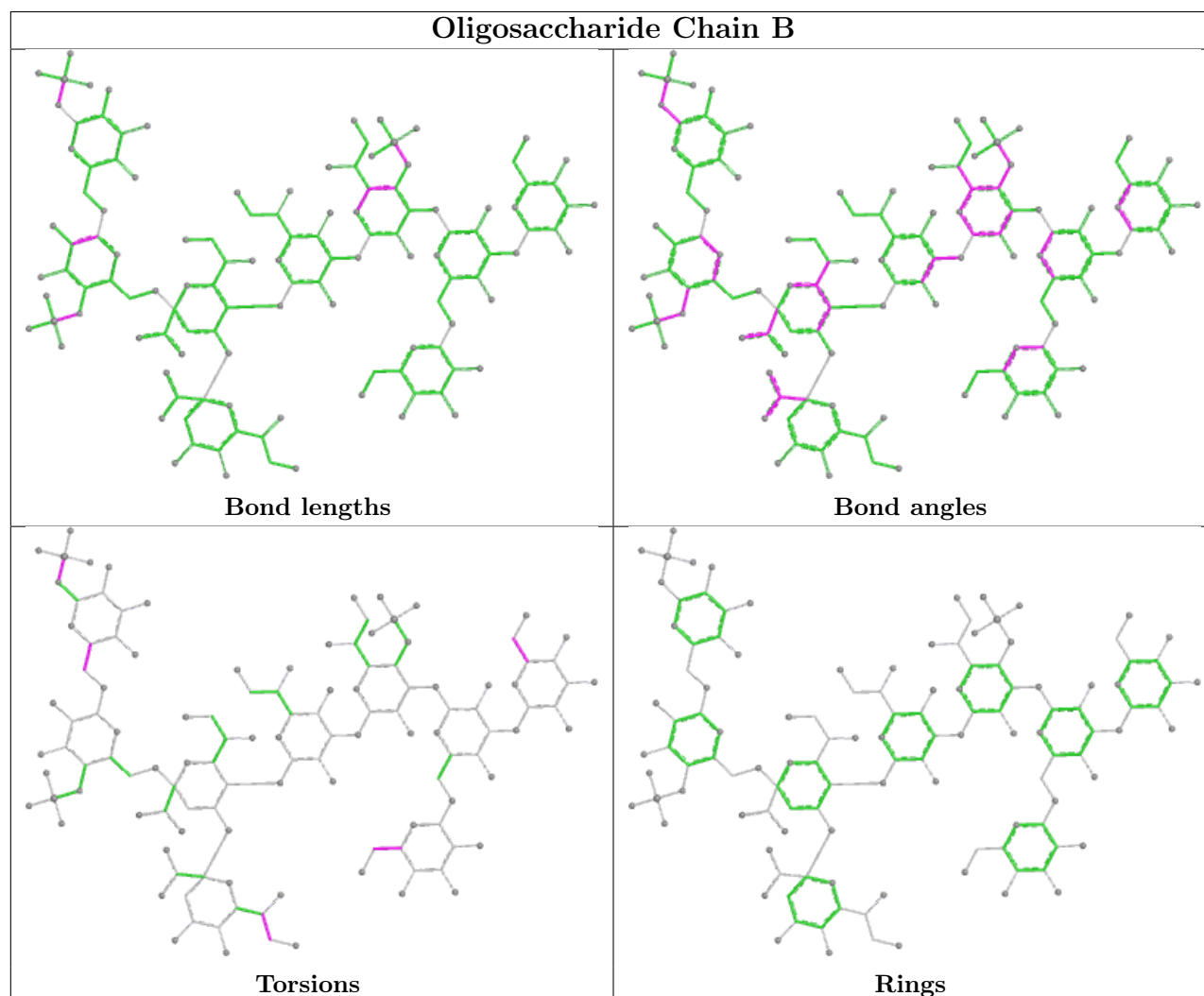
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	GLC	4	0
2	B	5	GPH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	GLA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	LIL	A	903	-	30,30,31	0.79	1 (3%)	31,31,33	1.09	1 (3%)
8	FCI	A	750	-	45,51,56	0.43	0	51,78,87	0.69	2 (3%)
7	EA2	A	1008	-	6,10,11	1.38	1 (16%)	8,13,16	0.88	1 (12%)
5	AAE	A	905	-	4,5,6	3.14	1 (25%)	5,5,7	2.81	3 (60%)
6	LIM	A	906	-	15,16,17	3.29	1 (6%)	15,16,18	2.49	4 (26%)
4	LIL	A	904	-	30,30,31	0.71	1 (3%)	31,31,33	1.20	3 (9%)

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
4	LIL	A	903	-	-	6/31/31/32	-
8	FCI	A	750	-	3/3/13/23	6/57/102/116	0/4/6/6
5	AAE	A	905	-	-	1/3/3/4	-
6	LIM	A	906	-	-	2/15/15/16	-
7	EA2	A	1008	-	-	1/8/10/11	-
4	LIL	A	904	-	1/1/2/3	4/31/31/32	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	906	LIM	O2J-C3J	12.59	1.43	1.21
5	A	905	AAE	O8-C5	5.96	1.43	1.21
4	A	903	LIL	O2E-C1F	3.88	1.45	1.34
4	A	904	LIL	O2E-C1F	3.50	1.44	1.34
7	A	1008	EA2	P2-O7P	-2.48	1.49	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	906	LIM	O2J-C3J-C2J	-7.67	109.68	121.17
5	A	905	AAE	O8-C5-C9	-4.80	109.47	121.48
4	A	903	LIL	O2E-C1F-O1F	-4.38	113.46	123.70
6	A	906	LIM	O2J-C3J-C4J	-4.37	109.93	121.40
4	A	904	LIL	O2E-C1F-O1F	-4.10	114.13	123.70
4	A	904	LIL	C4E-C3E-C2E	-3.22	110.00	114.08
5	A	905	AAE	O8-C5-C4	-2.92	109.64	120.92
8	A	750	FCI	C34-N8-C9	2.76	131.04	125.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	906	LIM	C2J-C3J-C4J	-2.53	110.66	117.88
8	A	750	FCI	C32-N6-C6	2.34	130.21	125.58
7	A	1008	EA2	P2-O7P-C1	-2.24	110.58	121.26
4	A	904	LIL	O1E-C1E-C2E	-2.18	119.02	125.38
6	A	906	LIM	O1J-C1J-C2J	-2.09	119.86	126.34
5	A	905	AAE	C9-C5-C4	-2.02	110.83	117.78

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	904	LIL	C3E
8	A	750	FCI	N5
8	A	750	FCI	N8
8	A	750	FCI	N6

All (20) torsion outliers are listed below:

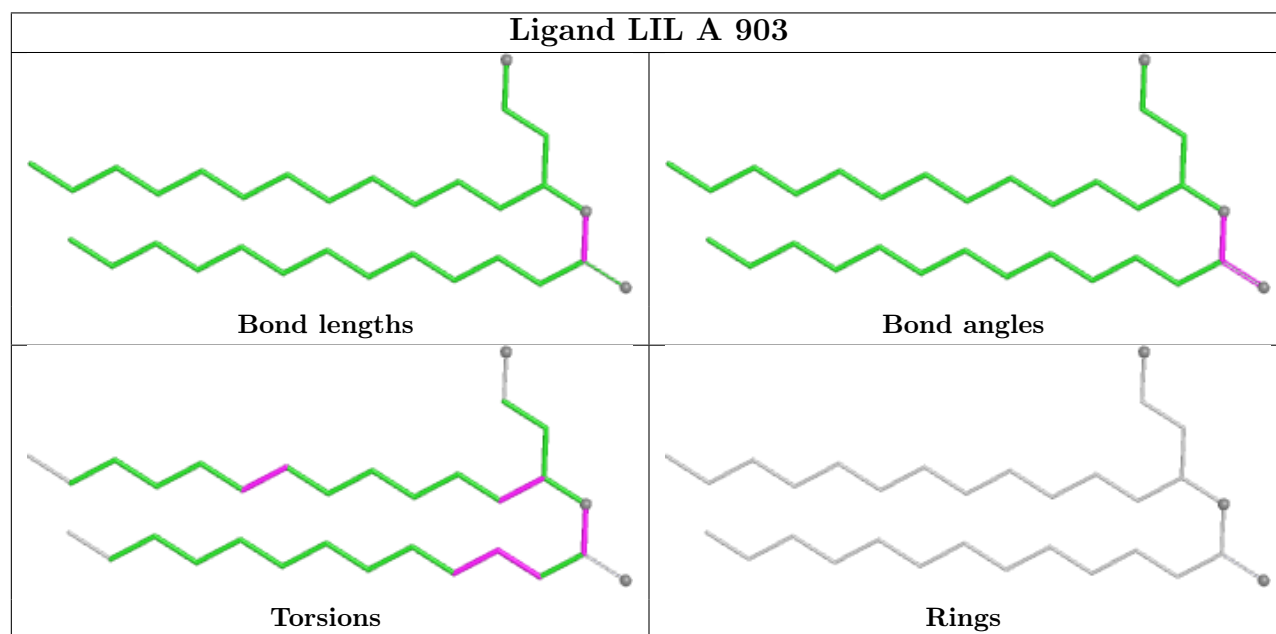
Mol	Chain	Res	Type	Atoms
4	A	903	LIL	O1F-C1F-O2E-C3E
4	A	903	LIL	C2F-C1F-O2E-C3E
8	A	750	FCI	C24-C16-C7-O7
8	A	750	FCI	C25-C30-N5-C3
8	A	750	FCI	C24-C16-C7-N3
4	A	904	LIL	C1F-C2F-C3F-C4F
8	A	750	FCI	N2-C11-C2-O2
4	A	904	LIL	C2F-C1F-O2E-C3E
8	A	750	FCI	N2-C11-C2-N9
4	A	903	LIL	C1S-C0S-C9E-C8E
4	A	903	LIL	C2F-C3F-C4F-C5F
4	A	904	LIL	O1E-C1E-C2E-C3E
4	A	903	LIL	C1F-C2F-C3F-C4F
7	A	1008	EA2	O7P-C1-C2-N3
4	A	904	LIL	O2E-C3E-C4E-C5E
6	A	906	LIM	O2J-C3J-C4J-C5J
6	A	906	LIM	C1X-C2X-C3X-C4X
8	A	750	FCI	C13-C21-C27-C32
4	A	903	LIL	C2E-C3E-C4E-C5E
5	A	905	AAE	C2-C4-C5-C9

There are no ring outliers.

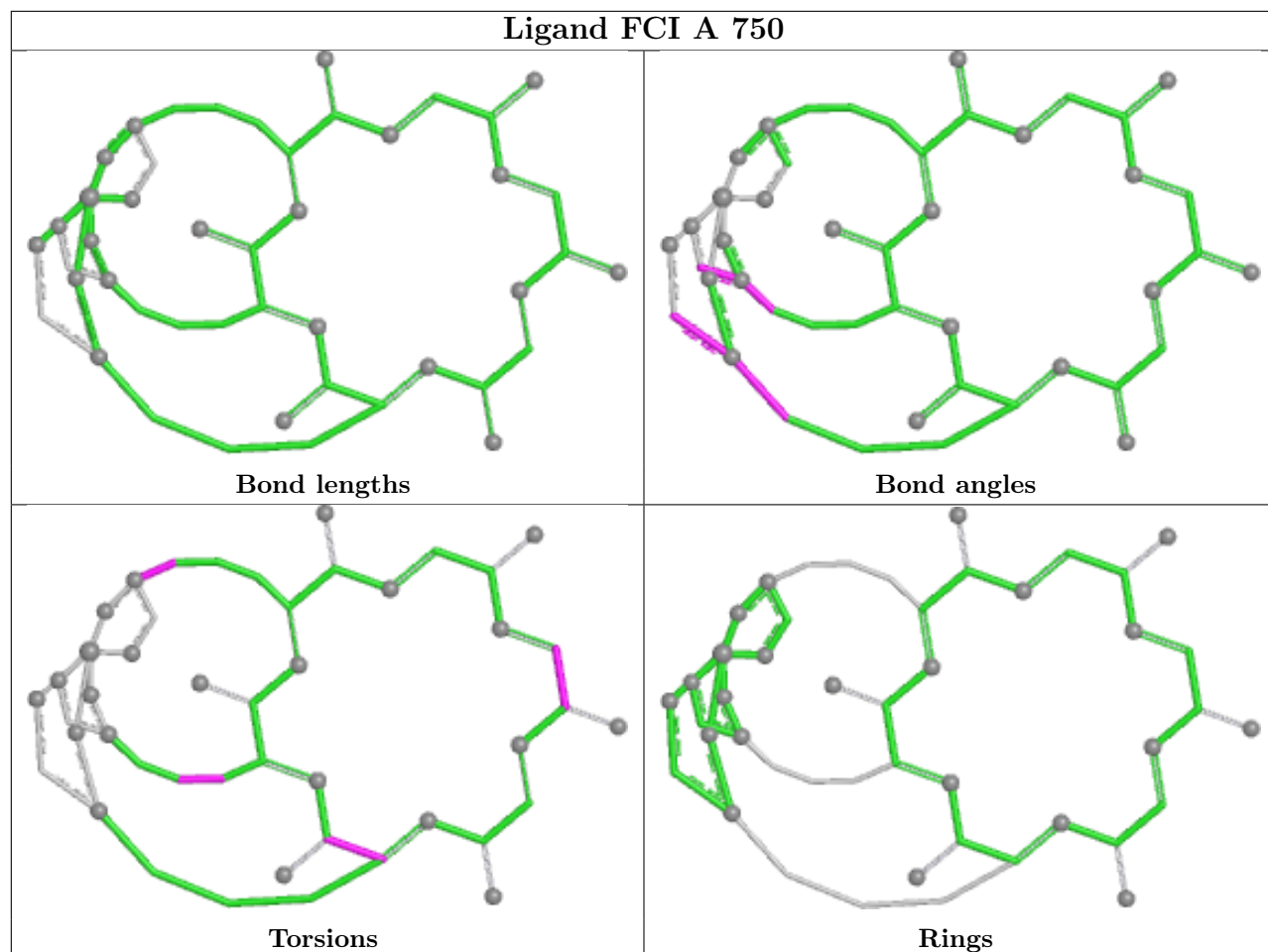
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	LIL	11	0
8	A	750	FCI	2	0
6	A	906	LIM	6	0
4	A	904	LIL	8	0

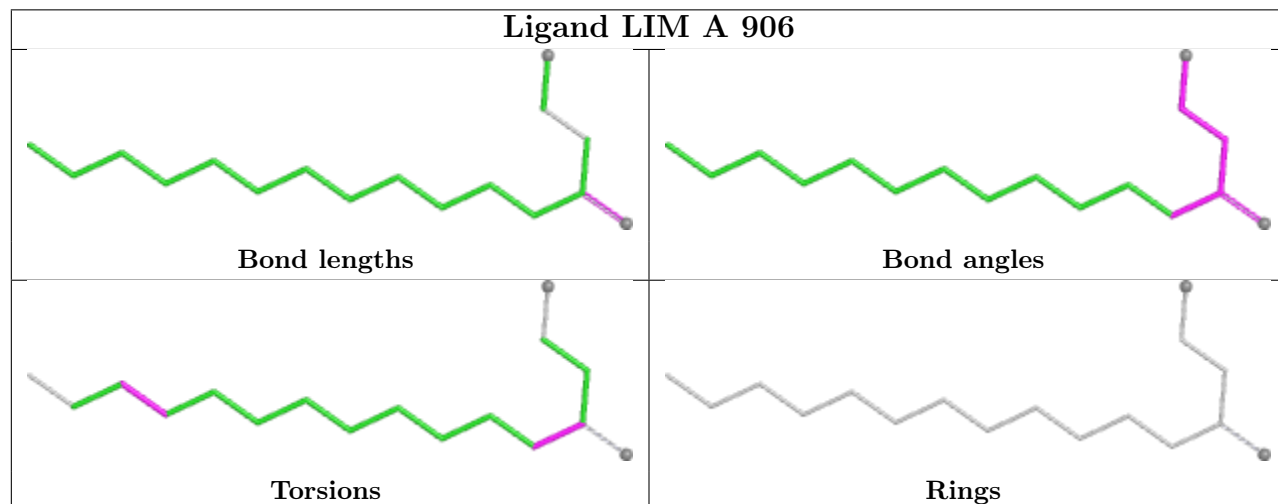
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

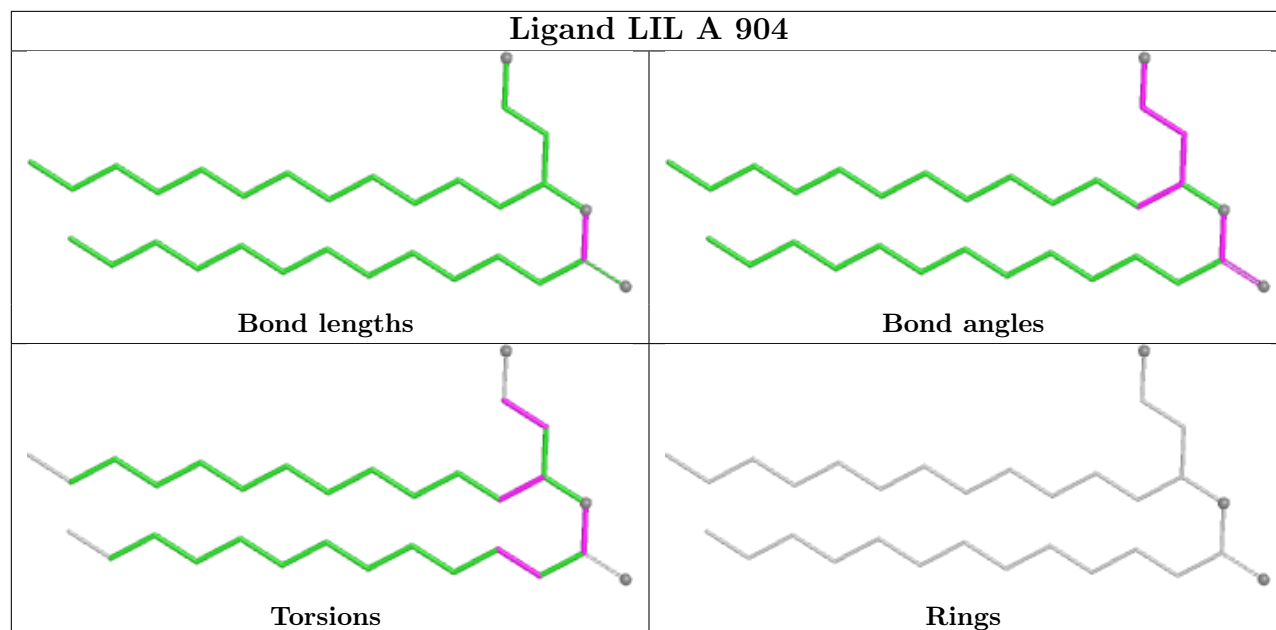


Ligand FCI A 750



Ligand LIM A 906





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	695/705 (98%)	0.44	36 (5%) 33 29	31, 62, 94, 113	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	HIS	8.4
1	A	23	GLY	5.0
1	A	403	TYR	4.9
1	A	566	PHE	4.8
1	A	404	ASN	4.2
1	A	405	PRO	3.9
1	A	19	GLU	3.9
1	A	24	PRO	3.8
1	A	29	ALA	3.4
1	A	28	ILE	3.4
1	A	406	SER	3.3
1	A	20	SER	3.3
1	A	413	GLY	3.2
1	A	411	HIS	2.9
1	A	78	VAL	2.9
1	A	542	PRO	2.9
1	A	390	TRP	2.7
1	A	242	GLY	2.7
1	A	632	PHE	2.7
1	A	409	HIS	2.6
1	A	612	GLY	2.6
1	A	451	TRP	2.5
1	A	21	ALA	2.5
1	A	423	ALA	2.5
1	A	586	ALA	2.5
1	A	453	LYS	2.3
1	A	146	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	402	LEU	2.2
1	A	494	LEU	2.2
1	A	336	ASP	2.2
1	A	408	HIS	2.2
1	A	25	ALA	2.1
1	A	335	ALA	2.1
1	A	401	ASN	2.1
1	A	98	GLU	2.0
1	A	32	GLN	2.0

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

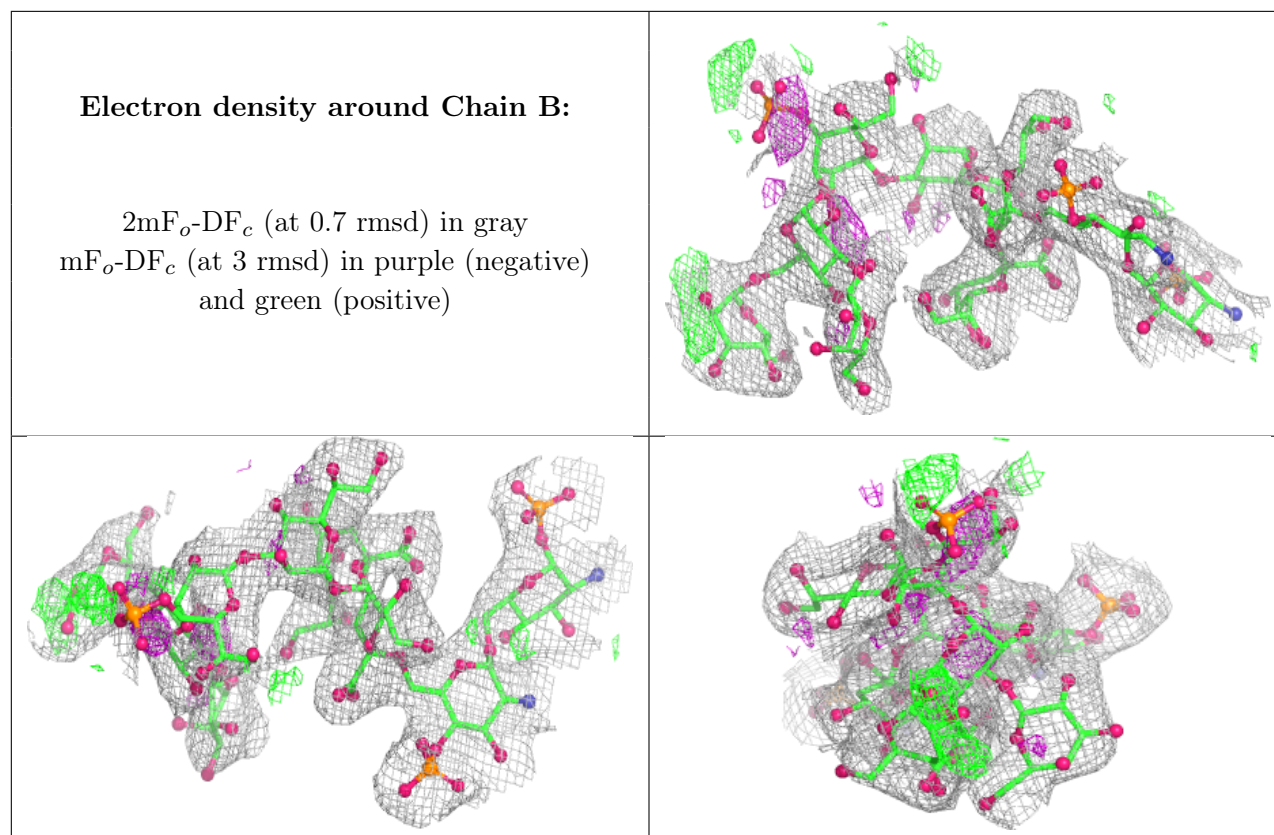
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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	GLA	B	8	11/12	0.63	0.17	81,91,107,107	0
2	GLA	B	7	11/12	0.75	0.15	74,96,110,120	0
2	GPH	B	5	17/18	0.77	0.17	55,82,120,120	0
2	GLC	B	6	11/12	0.81	0.15	74,83,102,110	0
2	KDO	B	9	15/16	0.90	0.09	49,64,80,85	0
2	GP1	B	1	16/16	0.93	0.08	50,63,90,103	0
2	GMH	B	4	13/14	0.94	0.09	43,59,80,83	0
2	KDO	B	3	15/16	0.95	0.07	45,59,70,92	0
2	GP4	B	2	15/16	0.96	0.07	32,46,71,73	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

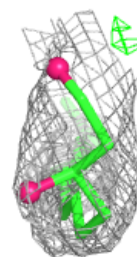
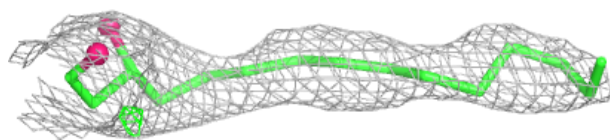
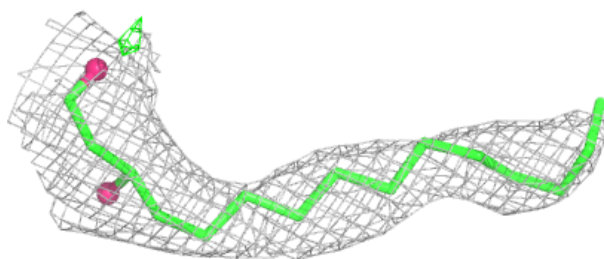
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	AAE	A	905	6/7	0.73	0.23	75,80,86,107	0
7	EA2	A	1008	11/12	0.88	0.15	52,109,120,120	0
6	LIM	A	906	17/18	0.90	0.18	54,65,82,97	0
4	LIL	A	903	31/32	0.90	0.19	48,78,93,96	0
4	LIL	A	904	31/32	0.94	0.14	48,59,76,83	0
3	NI	A	1012	1/1	0.96	0.09	113,113,113,113	0
3	NI	A	1011	1/1	0.96	0.07	98,98,98,98	0
8	FCI	A	750	46/51	0.97	0.08	21,47,64,69	0

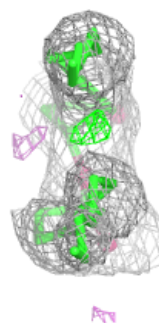
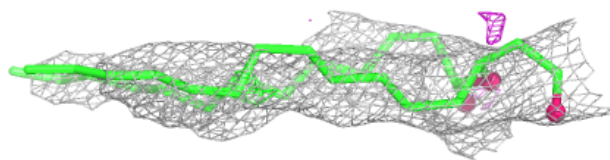
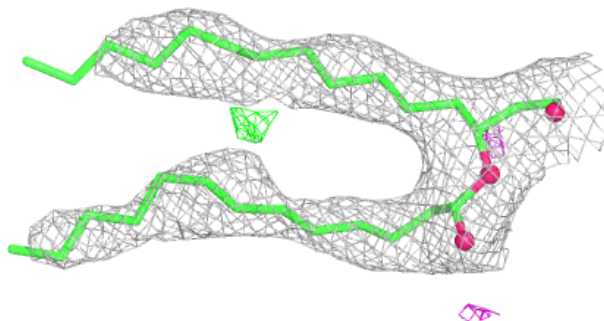
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LIM A 906:

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

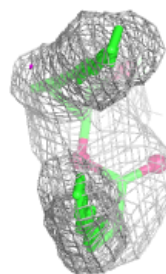
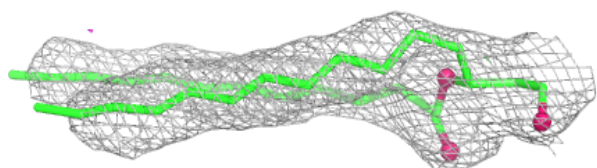
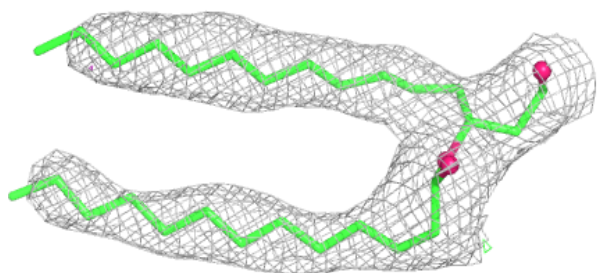
**Electron density around LIL A 903:**

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

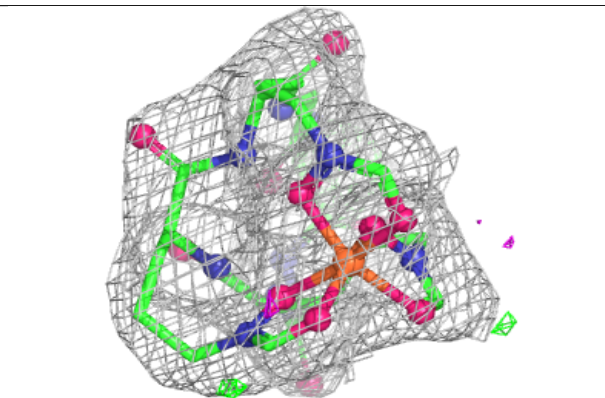
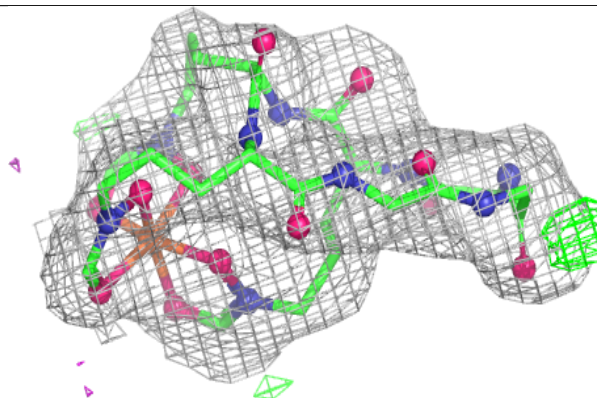
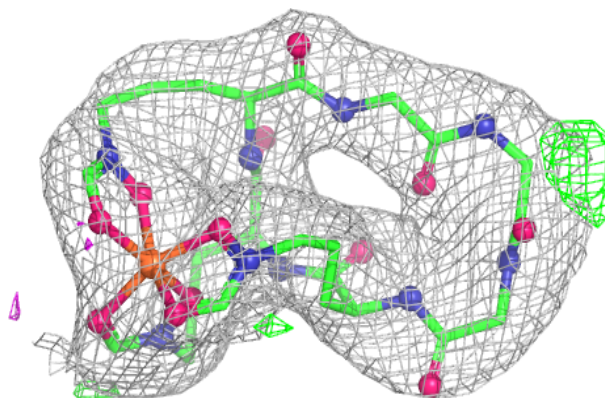


Electron density around LIL A 904:

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

**Electron density around FCI A 750:**

$2mF_o-DF_c$ (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.