



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 1QFF / pdb_00001qff
Title : E. COLI FERRIC HYDROXAMATE UPTAKE RECEPTOR (FHUA) IN
COMPLEX WITH BOUND FERRICHRONE-IRON
Authors : Ferguson, A.D.; Hofmann, E.; Coulton, J.W.; Diederichs, K.; Welte, W.
Deposited on : 1999-04-10
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

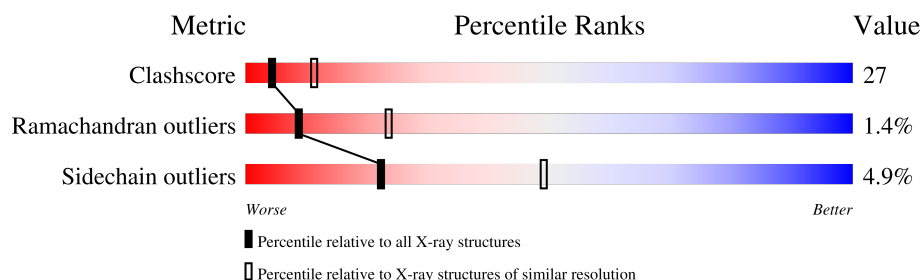
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	725	
2	B	9	

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
9	FCI	A	1050	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5972 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.

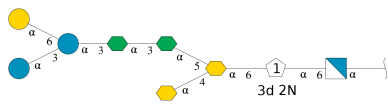
- Molecule 1 is a protein called FERRIC HYDROXAMATE UPTAKE RECEPTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	707	5524	3475	944	1091	4	10	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

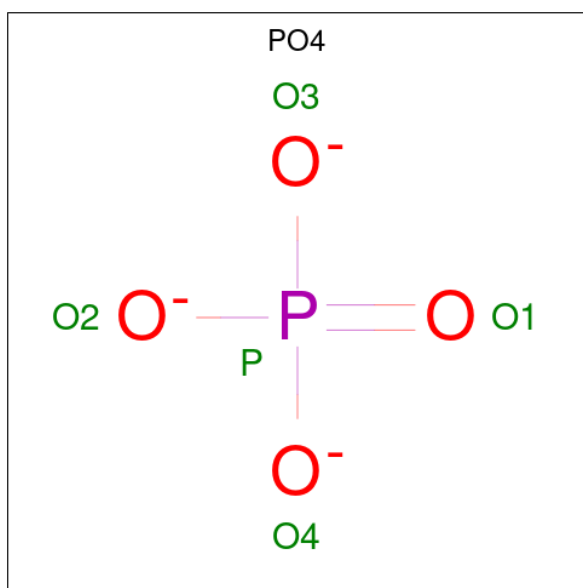
Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	expression tag	UNP P06971
A	407	SER	-	expression tag	UNP P06971
A	408	HIS	-	expression tag	UNP P06971
A	409	HIS	-	expression tag	UNP P06971
A	410	HIS	-	expression tag	UNP P06971
A	411	HIS	-	expression tag	UNP P06971
A	412	HIS	-	expression tag	UNP P06971
A	413	HIS	-	expression tag	UNP P06971
A	414	GLY	-	expression tag	UNP P06971
A	415	SER	-	expression tag	UNP P06971
A	416	SER	-	expression tag	UNP P06971

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-L-glycero-alpha-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-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



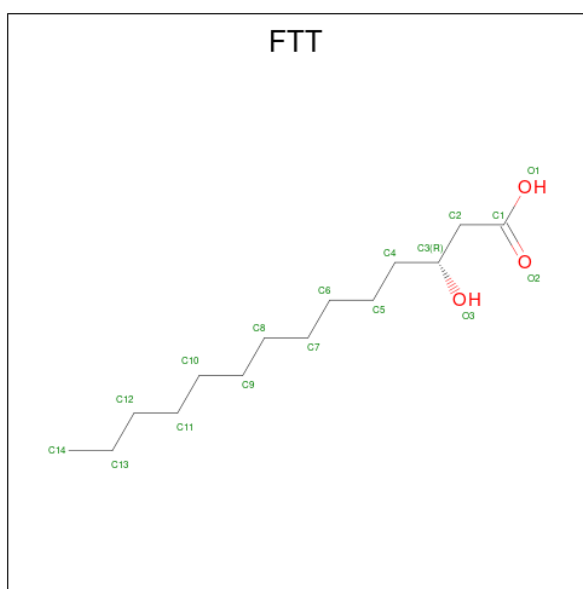
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	110	60	2	48	0	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



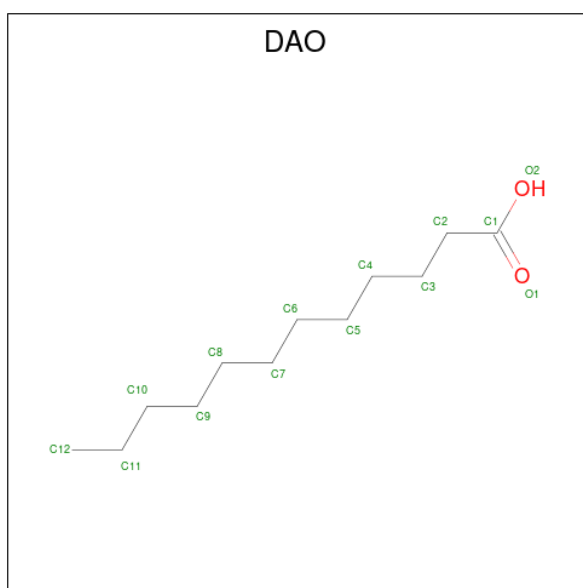
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			4	3	1		
3	A	1	Total	O	P	0	0
			4	3	1		

- Molecule 4 is 3-HYDROXY-TETRADECANOIC ACID (CCD ID: FTT) (formula: $C_{14}H_{28}O_3$).



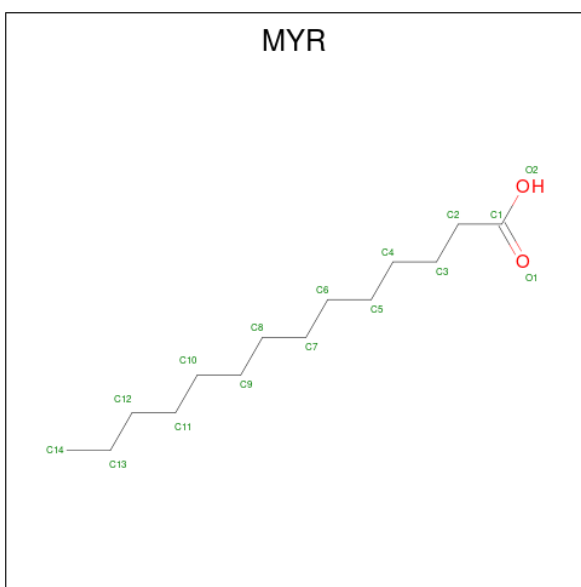
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 5 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



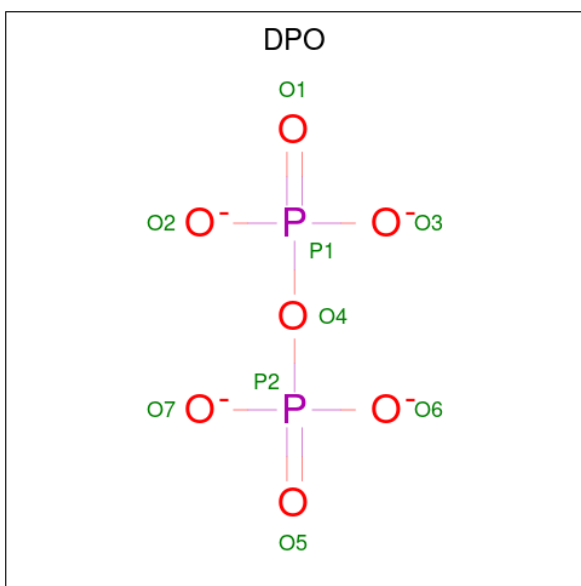
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



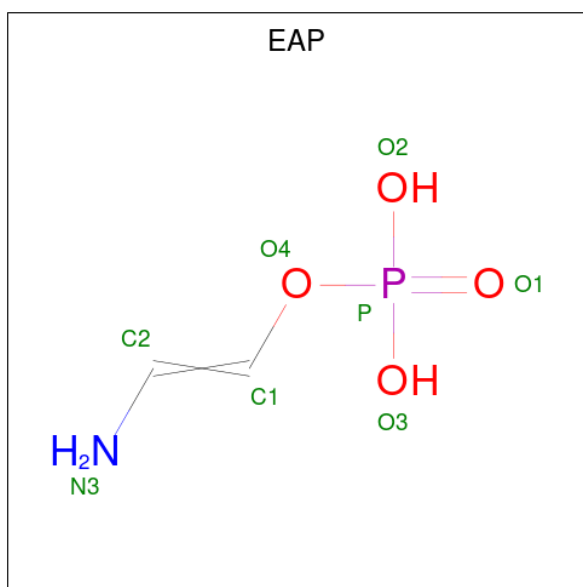
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is DIPHOSPHATE (CCD ID: DPO) (formula: O_7P_2).



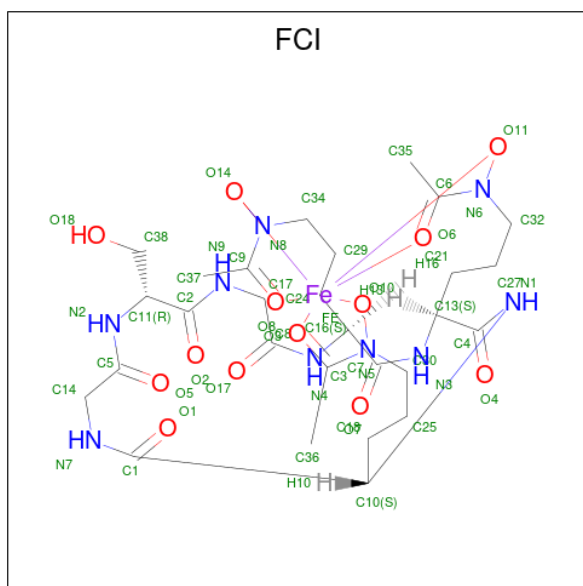
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 8 is 2-AMINO-VINYL-PHOSPHATE (CCD ID: EAP) (formula: $C_2H_6NO_4P$).



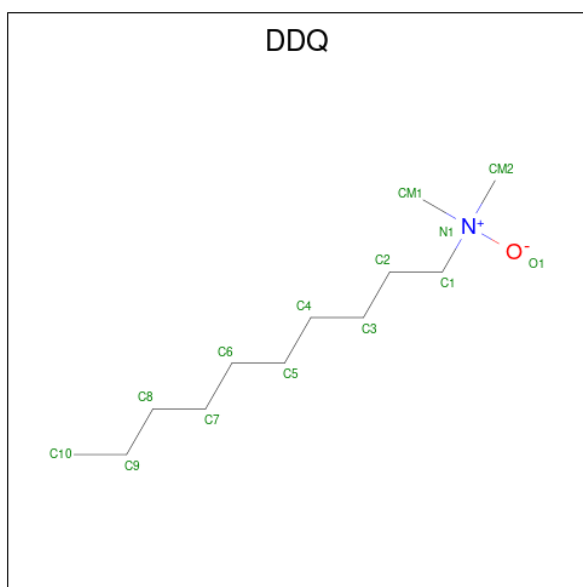
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			7	2	1	3	1		

- Molecule 9 is FERRICROCIN-IRON (CCD ID: FCI) (formula: $C_{28}H_{44}FeN_9O_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			51	28	1	9	13		

- Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	12	1	1		
10	A	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 11 is water.

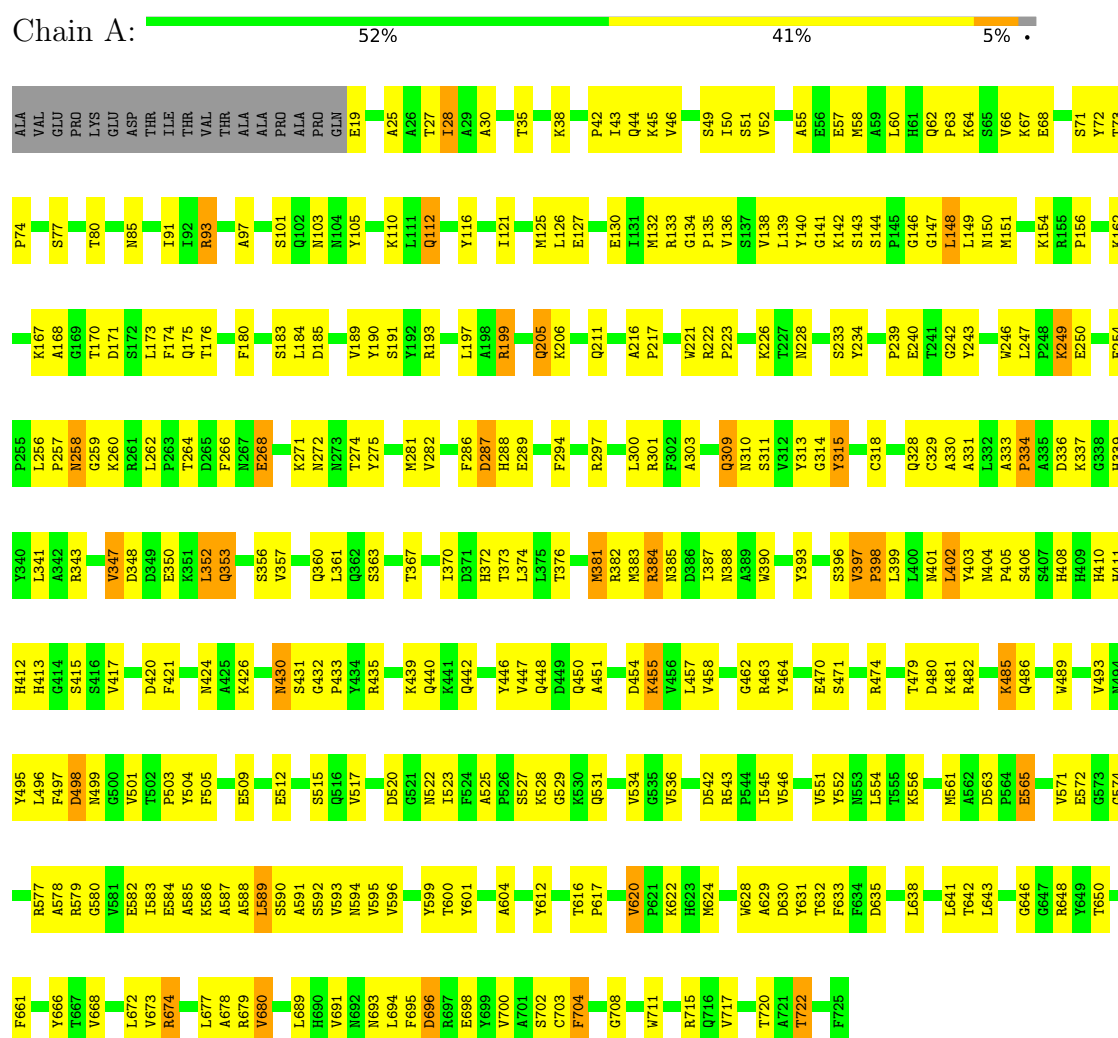
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	152	Total	O	0	0
			152	152		

3 Residue-property plots

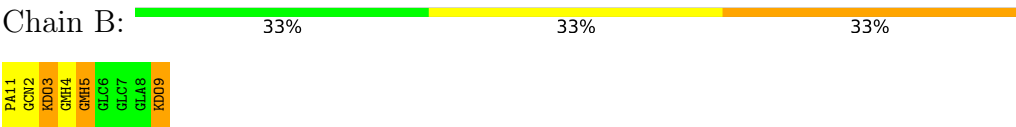
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: FERRIC HYDROXAMATE UPTAKE RECEPTOR



• Molecule 2: alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-L-glycero-alpha-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-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.40 Å 171.40 Å 85.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.3 (30.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5972	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GCN, MYR, DPO, PO4, GMH, DAO, DDQ, PA1, FTT, EAP, FCI, GLA, KDO

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	0.37	0/5654	0.90	19/7666 (0.2%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	HIS	N-CA-C	-7.98	103.53	113.18
1	A	127	GLU	N-CA-C	-7.63	104.50	113.88
1	A	249	LYS	N-CA-C	-6.30	104.85	112.54
1	A	485	LYS	N-CA-C	-6.20	99.09	109.07
1	A	46	VAL	CA-C-N	6.17	127.56	119.84
1	A	46	VAL	C-N-CA	6.17	127.56	119.84
1	A	25	ALA	N-CA-C	-6.12	98.43	108.41
1	A	591	ALA	N-CA-C	-6.12	105.80	113.20
1	A	311	SER	N-CA-C	5.97	118.85	108.76
1	A	515	SER	N-CA-C	-5.91	105.91	114.12
1	A	704	PHE	N-CA-C	-5.88	106.08	113.72
1	A	67	LYS	N-CA-C	-5.85	104.59	110.97
1	A	612	TYR	N-CA-C	5.79	119.91	112.26
1	A	309	GLN	N-CA-C	5.67	117.15	108.52
1	A	527	SER	N-CA-C	-5.36	102.58	110.52
1	A	595	VAL	N-CA-C	5.30	115.35	108.35
1	A	242	GLY	N-CA-C	5.13	119.55	112.52
1	A	700	VAL	N-CA-C	-5.08	101.03	108.54
1	A	347	VAL	N-CA-C	-5.04	101.11	108.17

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	5524	0	5223	296	0
2	B	110	0	84	5	0
3	A	8	0	0	1	0
4	A	56	0	83	4	0
5	A	13	0	23	0	0
6	A	15	0	27	0	0
7	A	8	0	0	0	0
8	A	7	0	4	2	0
9	A	51	0	44	2	0
10	A	28	0	54	1	0
11	A	152	0	0	11	0
All	All	5972	0	5542	305	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 27.

All (305) 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:121:ILE:HB	1:A:151:MSE:HE1	1.33	1.10
1:A:28:ILE:HD12	1:A:28:ILE:H	1.25	0.97
1:A:381:MSE:HE1	1:A:383:MSE:HB2	1.48	0.96
1:A:126:LEU:HD11	1:A:151:MSE:HE3	1.50	0.92
1:A:126:LEU:HD21	1:A:151:MSE:HE2	1.52	0.91
1:A:134:GLY:CA	1:A:146:GLY:HA2	2.01	0.91
4:A:1011:FTT:H72	4:A:1013:FTT:H62	1.56	0.86
1:A:121:ILE:HB	1:A:151:MSE:CE	2.04	0.86
1:A:274:THR:HG22	1:A:310:ASN:HB2	1.61	0.83
1:A:132:MSE:HE2	1:A:136:VAL:HG12	1.58	0.83
1:A:249:LYS:HG2	1:A:250:GLU:OE1	1.80	0.81
4:A:1011:FTT:H92	4:A:1013:FTT:H82	1.63	0.80
1:A:71:SER:HB3	1:A:648:ARG:HD2	1.64	0.79
1:A:384:ARG:HD2	11:A:2087:HOH:O	1.83	0.78
1:A:205:GLN:HG3	1:A:243:TYR:CG	2.20	0.77
1:A:397:VAL:HG23	1:A:398:PRO:HD2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:PHE:HB2	1:A:534:VAL:HG12	1.68	0.75
1:A:430:ASN:HD22	1:A:431:SER:N	1.85	0.75
1:A:503:PRO:HA	1:A:536:VAL:HG12	1.70	0.74
1:A:390:TRP:CD2	1:A:426:LYS:HD3	2.23	0.73
1:A:28:ILE:H	1:A:28:ILE:CD1	2.02	0.73
1:A:691:VAL:HG22	1:A:717:VAL:HG22	1.71	0.72
1:A:125:MSE:HG3	1:A:234:TYR:HE1	1.55	0.72
1:A:604:ALA:O	1:A:616:THR:HG22	1.90	0.71
1:A:228:ASN:HB3	1:A:287:ASP:OD1	1.89	0.71
1:A:35:THR:CG2	1:A:150:ASN:HD22	2.02	0.71
1:A:126:LEU:HD11	1:A:151:MSE:CE	2.19	0.71
1:A:199:ARG:HD2	11:A:2033:HOH:O	1.91	0.70
1:A:330:ALA:HA	1:A:337:LYS:NZ	2.06	0.70
1:A:715:ARG:HH11	1:A:715:ARG:HG2	1.54	0.70
1:A:66:VAL:HG21	1:A:151:MSE:HE3	1.73	0.70
1:A:309:GLN:HG2	1:A:348:ASP:HB3	1.74	0.70
1:A:134:GLY:C	1:A:146:GLY:HA2	2.17	0.70
1:A:404:ASN:HB3	1:A:405:PRO:HD3	1.75	0.69
1:A:373:THR:HB	1:A:450:GLN:HB2	1.74	0.69
1:A:545:ILE:HG22	1:A:587:ALA:HB1	1.76	0.68
1:A:300:LEU:HG	1:A:357:VAL:HG12	1.77	0.67
1:A:486:GLN:OE1	1:A:528:LYS:HE2	1.94	0.66
1:A:185:ASP:OD2	1:A:189:VAL:HG12	1.95	0.66
1:A:71:SER:HB3	1:A:648:ARG:CD	2.25	0.65
1:A:221:TRP:CE2	1:A:223:PRO:HG3	2.31	0.65
1:A:462:GLY:HA2	1:A:489:TRP:HA	1.79	0.64
1:A:167:LYS:HB2	1:A:175:GLN:HB3	1.78	0.64
1:A:134:GLY:N	1:A:146:GLY:HA2	2.11	0.64
1:A:352:LEU:C	1:A:352:LEU:HD12	2.22	0.64
1:A:390:TRP:CE2	1:A:426:LYS:HB3	2.33	0.64
1:A:470:GLU:HG3	1:A:481:LYS:HG2	1.78	0.64
1:A:590:SER:HB3	1:A:593:VAL:HB	1.80	0.64
8:A:2004:EAP:H11	2:B:4:GMH:H6	1.79	0.64
1:A:673:VAL:CG2	1:A:689:LEU:HB3	2.28	0.64
1:A:162:LYS:HA	1:A:180:PHE:CD1	2.33	0.63
1:A:74:PRO:HG3	1:A:584:GLU:HB2	1.81	0.63
1:A:430:ASN:HD22	1:A:430:ASN:C	2.06	0.63
1:A:52:VAL:HG22	1:A:130:GLU:HG2	1.81	0.63
1:A:185:ASP:CG	1:A:189:VAL:HG12	2.24	0.63
1:A:370:ILE:HG22	1:A:372:HIS:CD2	2.34	0.62
1:A:353:GLN:HG3	11:A:2087:HOH:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:HG21	4:A:1013:FTT:H81	1.80	0.62
1:A:300:LEU:CG	1:A:357:VAL:HG12	2.30	0.62
1:A:497:PHE:HB3	1:A:499:ASN:OD1	2.00	0.62
1:A:162:LYS:HA	1:A:180:PHE:HD1	1.65	0.61
1:A:148:LEU:C	1:A:148:LEU:HD23	2.24	0.61
1:A:49:SER:C	1:A:50:ILE:HD12	2.26	0.61
1:A:668:VAL:HG13	1:A:693:ASN:HA	1.81	0.61
1:A:446:TYR:HB3	1:A:463:ARG:HB2	1.83	0.61
1:A:64:LYS:HD2	1:A:85:ASN:HD22	1.66	0.61
1:A:226:LYS:HB3	1:A:289:GLU:HB3	1.82	0.61
1:A:35:THR:HG21	1:A:150:ASN:HD22	1.66	0.60
1:A:258:ASN:HD22	1:A:260:LYS:HD2	1.66	0.60
1:A:673:VAL:HG22	1:A:689:LEU:HB3	1.82	0.60
1:A:257:PRO:C	1:A:259:GLY:H	2.10	0.60
1:A:454:ASP:C	1:A:455:LYS:HE2	2.26	0.60
1:A:328:GLN:HB3	1:A:399:LEU:HD11	1.83	0.60
1:A:586:LYS:HG2	1:A:596:VAL:HG22	1.83	0.60
1:A:189:VAL:HG13	1:A:190:TYR:CD2	2.37	0.60
1:A:258:ASN:ND2	1:A:260:LYS:HD2	2.17	0.60
1:A:384:ARG:HD3	11:A:2078:HOH:O	2.00	0.60
1:A:217:PRO:HD2	1:A:233:SER:OG	2.02	0.59
1:A:168:ALA:HA	1:A:173:LEU:O	2.02	0.59
1:A:135:PRO:HB3	1:A:509:GLU:C	2.27	0.59
1:A:297:ARG:HD2	1:A:360:GLN:NE2	2.18	0.59
1:A:703:CYS:HA	1:A:708:GLY:O	2.02	0.58
1:A:64:LYS:HD2	1:A:85:ASN:ND2	2.18	0.58
1:A:300:LEU:C	1:A:300:LEU:HD23	2.28	0.58
1:A:628:TRP:CD1	1:A:646:GLY:HA3	2.38	0.58
1:A:55:ALA:HA	1:A:58:MSE:HE3	1.85	0.58
1:A:694:LEU:O	1:A:715:ARG:HD3	2.04	0.58
1:A:51:SER:OG	1:A:133:ARG:NH2	2.36	0.58
1:A:497:PHE:HB2	1:A:501:VAL:O	2.04	0.58
1:A:60:LEU:HD21	1:A:628:TRP:CZ3	2.40	0.57
8:A:2004:EAP:C1	2:B:4:GMH:H6	2.35	0.57
1:A:103:ASN:ND2	1:A:147:GLY:O	2.38	0.57
1:A:197:LEU:C	1:A:197:LEU:HD12	2.30	0.57
1:A:376:THR:HG22	1:A:447:VAL:HG13	1.87	0.57
1:A:673:VAL:HG23	1:A:673:VAL:O	2.05	0.57
1:A:105:TYR:CE2	1:A:110:LYS:HB2	2.41	0.56
1:A:383:MSE:HE1	1:A:440:GLN:NE2	2.21	0.56
1:A:154:LYS:HD3	1:A:193:ARG:NH2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD13	1:A:266:PHE:CD2	2.41	0.56
1:A:189:VAL:HG23	1:A:222:ARG:O	2.06	0.55
1:A:260:LYS:HB2	1:A:406:SER:OG	2.07	0.55
1:A:93:ARG:HG3	1:A:552:TYR:OH	2.06	0.55
1:A:497:PHE:HB2	1:A:501:VAL:HG23	1.89	0.55
1:A:134:GLY:HA2	1:A:146:GLY:HA2	1.86	0.55
1:A:272:ASN:HB3	1:A:420:ASP:OD1	2.07	0.55
1:A:531:GLN:HB2	1:A:554:LEU:CD1	2.37	0.54
1:A:45:LYS:HE2	1:A:496:LEU:HD21	1.88	0.54
1:A:125:MSE:HG3	1:A:234:TYR:CE1	2.38	0.54
1:A:517:VAL:HG23	1:A:522:ASN:N	2.21	0.54
1:A:72:TYR:HH	1:A:628:TRP:CD1	2.25	0.54
1:A:66:VAL:HG21	1:A:151:MSE:CE	2.37	0.54
1:A:628:TRP:CZ3	1:A:630:ASP:HB3	2.42	0.54
1:A:678:ALA:C	1:A:680:VAL:H	2.16	0.54
1:A:390:TRP:CZ2	1:A:426:LYS:HB3	2.43	0.53
1:A:561:MSE:HE2	1:A:574:GLY:N	2.23	0.53
1:A:633:PHE:HB2	1:A:638:LEU:O	2.08	0.53
1:A:580:GLY:HA3	1:A:601:TYR:O	2.09	0.53
1:A:592:SER:O	1:A:631:TYR:HA	2.09	0.53
1:A:455:LYS:HE2	1:A:455:LYS:N	2.23	0.53
1:A:408:HIS:O	1:A:412:HIS:HB2	2.09	0.53
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.73	0.52
1:A:424:ASN:O	1:A:426:LYS:HG3	2.08	0.52
1:A:693:ASN:HB3	1:A:715:ARG:HA	1.91	0.52
1:A:350:GLU:HG2	1:A:387:ILE:HG12	1.92	0.52
1:A:352:LEU:HB2	1:A:384:ARG:O	2.10	0.52
1:A:19:GLU:OE1	1:A:30:ALA:HB1	2.08	0.52
1:A:405:PRO:HA	1:A:410:HIS:CD2	2.45	0.52
1:A:58:MSE:C	1:A:60:LEU:H	2.18	0.52
1:A:643:LEU:HD22	1:A:673:VAL:HG12	1.92	0.51
1:A:125:MSE:HE3	1:A:216:ALA:HB2	1.90	0.51
1:A:583:ILE:HG12	1:A:599:TYR:HB3	1.92	0.51
1:A:341:LEU:HB2	1:A:402:LEU:HD11	1.91	0.51
1:A:480:ASP:HB3	1:A:523:ILE:HD11	1.91	0.51
1:A:313:TYR:HA	11:A:2129:HOH:O	2.10	0.51
1:A:356:SER:HB3	11:A:2030:HOH:O	2.11	0.51
1:A:374:LEU:HD12	1:A:448:GLN:O	2.10	0.51
1:A:93:ARG:HH11	1:A:582:GLU:CD	2.19	0.51
1:A:105:TYR:CZ	1:A:110:LYS:HB2	2.46	0.50
1:A:704:PHE:CE2	1:A:708:GLY:HA3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ASN:HB2	1:A:630:ASP:OD1	2.11	0.50
1:A:28:ILE:HD12	1:A:28:ILE:N	2.09	0.50
1:A:77:SER:OG	1:A:91:ILE:HB	2.12	0.50
1:A:256:LEU:HD11	1:A:402:LEU:HB3	1.93	0.50
1:A:631:TYR:HE2	1:A:633:PHE:CD1	2.30	0.50
1:A:390:TRP:CZ3	1:A:433:PRO:HG3	2.46	0.50
1:A:680:VAL:HG12	1:A:680:VAL:O	2.11	0.50
1:A:58:MSE:O	1:A:63:PRO:HD2	2.12	0.50
1:A:315:TYR:O	1:A:341:LEU:HD11	2.12	0.50
1:A:390:TRP:HE1	1:A:431:SER:CB	2.24	0.50
1:A:133:ARG:HD2	1:A:582:GLU:OE1	2.12	0.49
1:A:403:TYR:O	1:A:406:SER:HB3	2.11	0.49
1:A:38:LYS:HE3	1:A:139:LEU:O	2.13	0.49
1:A:628:TRP:CH2	1:A:630:ASP:HB3	2.47	0.49
1:A:49:SER:O	1:A:50:ILE:HD12	2.11	0.49
1:A:588:ALA:C	1:A:590:SER:H	2.20	0.49
1:A:205:GLN:HG3	1:A:243:TYR:CB	2.43	0.49
1:A:258:ASN:HB3	1:A:403:TYR:CZ	2.48	0.49
1:A:62:GLN:HB3	1:A:167:LYS:NZ	2.28	0.49
1:A:695:PHE:O	1:A:696:ASP:C	2.56	0.49
1:A:381:MSE:HE3	11:A:2007:HOH:O	2.13	0.49
1:A:44:GLN:HG2	1:A:45:LYS:N	2.27	0.49
1:A:505:PHE:HA	1:A:534:VAL:HA	1.94	0.49
1:A:650:THR:HB	1:A:666:TYR:CE1	2.48	0.48
1:A:97:ALA:HB3	1:A:101:SER:O	2.13	0.48
1:A:134:GLY:H	1:A:146:GLY:HA2	1.77	0.48
1:A:264:THR:HA	1:A:711:TRP:CD1	2.49	0.48
1:A:38:LYS:HG3	1:A:139:LEU:HD22	1.94	0.48
1:A:93:ARG:HG3	1:A:552:TYR:CZ	2.48	0.48
1:A:258:ASN:HB3	1:A:403:TYR:CE2	2.49	0.48
1:A:170:THR:HG22	1:A:171:ASP:N	2.28	0.48
1:A:206:LYS:HD3	1:A:415:SER:O	2.14	0.48
1:A:247:LEU:HD21	1:A:268:GLU:HG3	1.96	0.48
1:A:339:HIS:O	1:A:339:HIS:ND1	2.47	0.48
1:A:310:ASN:ND2	1:A:347:VAL:HG13	2.29	0.47
1:A:638:LEU:O	1:A:641:LEU:HB3	2.14	0.47
1:A:286:PHE:CZ	1:A:288:HIS:HB2	2.49	0.47
1:A:141:GLY:HA3	1:A:442:GLN:NE2	2.29	0.47
1:A:531:GLN:HB2	1:A:554:LEU:HD13	1.97	0.47
1:A:588:ALA:HA	1:A:594:ASN:HD22	1.80	0.47
1:A:617:PRO:HG2	1:A:620:VAL:HG11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD23	1:A:301:ARG:N	2.29	0.47
1:A:388:ASN:HD22	1:A:435:ARG:HG2	1.79	0.47
1:A:205:GLN:HG3	1:A:243:TYR:CD1	2.50	0.47
1:A:601:TYR:OH	1:A:622:LYS:NZ	2.48	0.47
1:A:715:ARG:HG2	1:A:715:ARG:NH1	2.28	0.47
1:A:211:GLN:OE1	1:A:239:PRO:HB2	2.15	0.46
1:A:579:ARG:HG3	1:A:579:ARG:HH11	1.79	0.46
2:B:4:GMH:H71	2:B:9:KDO:H32	1.96	0.46
1:A:455:LYS:HE2	1:A:455:LYS:CA	2.45	0.46
1:A:197:LEU:HD12	1:A:197:LEU:O	2.16	0.46
1:A:221:TRP:CZ2	1:A:223:PRO:HG3	2.50	0.46
1:A:72:TYR:CE2	1:A:628:TRP:HB2	2.50	0.46
1:A:93:ARG:NH1	1:A:582:GLU:OE1	2.49	0.46
1:A:130:GLU:O	1:A:149:LEU:HD12	2.16	0.46
1:A:138:VAL:HG13	1:A:139:LEU:HG	1.98	0.46
1:A:384:ARG:NH1	1:A:439:LYS:HE2	2.31	0.46
1:A:28:ILE:HD11	1:A:594:ASN:OD1	2.16	0.46
1:A:57:GLU:O	1:A:60:LEU:HB3	2.16	0.46
1:A:350:GLU:CD	1:A:387:ILE:HG12	2.41	0.46
1:A:702:SER:HB2	11:A:2016:HOH:O	2.16	0.46
1:A:482:ARG:CZ	1:A:525:ALA:HA	2.46	0.46
1:A:509:GLU:HA	1:A:529:GLY:O	2.16	0.46
1:A:631:TYR:HE2	1:A:633:PHE:CE1	2.33	0.46
1:A:257:PRO:C	1:A:259:GLY:N	2.75	0.46
1:A:352:LEU:HB3	1:A:385:ASN:OD1	2.16	0.45
1:A:458:VAL:HG23	1:A:493:VAL:HG22	1.98	0.45
1:A:505:PHE:CD1	1:A:505:PHE:C	2.94	0.45
1:A:66:VAL:CG2	1:A:151:MSE:HE3	2.43	0.45
1:A:249:LYS:HE2	1:A:254:GLU:OE1	2.17	0.45
1:A:430:ASN:ND2	11:A:2098:HOH:O	2.50	0.45
1:A:594:ASN:O	1:A:629:ALA:HA	2.16	0.45
1:A:333:ALA:O	1:A:336:ASP:N	2.48	0.45
1:A:352:LEU:C	1:A:352:LEU:CD1	2.87	0.45
1:A:27:THR:HG22	1:A:28:ILE:N	2.31	0.45
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.32	0.45
1:A:542:ASP:CG	1:A:543:ARG:H	2.24	0.45
1:A:563:ASP:OD2	1:A:565:GLU:HG2	2.17	0.45
3:A:2005:PO4:O3	2:B:5:GMH:C3	2.65	0.45
1:A:592:SER:HB2	1:A:632:THR:O	2.16	0.45
1:A:531:GLN:HB2	1:A:554:LEU:HD12	1.98	0.44
2:B:3:KDO:H7	2:B:4:GMH:C1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:CZ	1:A:133:ARG:HB3	2.48	0.44
1:A:585:ALA:O	1:A:596:VAL:HA	2.18	0.44
1:A:589:LEU:HB2	1:A:593:VAL:HG12	2.00	0.44
1:A:43:ILE:HD12	1:A:546:VAL:HG11	1.99	0.43
1:A:80:THR:O	1:A:80:THR:HG22	2.17	0.43
1:A:294:PHE:HE1	1:A:363:SER:HG	1.62	0.43
1:A:495:TYR:C	1:A:495:TYR:CD2	2.96	0.43
1:A:390:TRP:CG	1:A:426:LYS:HD3	2.52	0.43
1:A:720:THR:HG22	1:A:722:THR:HG22	2.00	0.43
1:A:264:THR:HG21	1:A:698:GLU:HG2	1.99	0.43
1:A:271:LYS:HB2	1:A:417:VAL:HG22	2.00	0.43
1:A:397:VAL:HG23	1:A:398:PRO:CD	2.43	0.43
1:A:520:ASP:OD2	1:A:522:ASN:HB2	2.19	0.43
1:A:571:VAL:HG12	1:A:572:GLU:N	2.33	0.43
1:A:309:GLN:O	1:A:347:VAL:HA	2.19	0.43
1:A:577:ARG:HG2	1:A:578:ALA:N	2.33	0.43
1:A:173:LEU:HD12	1:A:174:PHE:N	2.34	0.43
1:A:38:LYS:HE2	1:A:140:TYR:CE2	2.54	0.43
1:A:678:ALA:O	1:A:680:VAL:N	2.52	0.43
1:A:142:LYS:HG2	1:A:442:GLN:OE1	2.19	0.43
1:A:497:PHE:CB	1:A:501:VAL:HG23	2.48	0.43
1:A:126:LEU:HD22	1:A:151:MSE:HB3	2.01	0.42
1:A:367:THR:O	1:A:367:THR:HG22	2.18	0.42
1:A:464:TYR:OH	1:A:485:LYS:HB3	2.19	0.42
9:A:1050:FCI:HN9	9:A:1050:FCI:H382	1.61	0.42
1:A:495:TYR:C	1:A:495:TYR:HD2	2.27	0.42
1:A:353:GLN:HE21	1:A:353:GLN:HB3	1.66	0.42
1:A:116:TYR:CD1	9:A:1050:FCI:H353	2.54	0.42
1:A:281:MSE:HB3	1:A:303:ALA:HB2	2.01	0.42
1:A:383:MSE:HE3	1:A:440:GLN:CD	2.45	0.42
1:A:628:TRP:HH2	1:A:672:LEU:HD23	1.85	0.42
1:A:143:SER:HA	11:A:2127:HOH:O	2.20	0.42
1:A:393:TYR:OH	1:A:432:GLY:HA3	2.20	0.42
1:A:628:TRP:HD1	1:A:646:GLY:HA3	1.82	0.42
1:A:246:TRP:HB2	1:A:314:GLY:O	2.20	0.42
1:A:352:LEU:HD12	1:A:352:LEU:O	2.20	0.42
1:A:504:TYR:CD1	1:A:504:TYR:C	2.97	0.42
1:A:388:ASN:ND2	1:A:435:ARG:CD	2.83	0.42
1:A:183:SER:HA	1:A:191:SER:HA	2.02	0.42
1:A:329:CYS:C	1:A:331:ALA:H	2.28	0.42
1:A:471:SER:O	1:A:479:THR:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LYS:O	1:A:556:LYS:HA	2.19	0.42
1:A:112:GLN:HE21	1:A:112:GLN:CA	2.33	0.41
1:A:144:SER:HA	1:A:512:GLU:OE1	2.20	0.41
1:A:328:GLN:HB3	1:A:399:LEU:CD1	2.50	0.41
1:A:382:ARG:O	1:A:382:ARG:HG3	2.20	0.41
1:A:617:PRO:O	1:A:620:VAL:HG12	2.19	0.41
1:A:93:ARG:HD2	1:A:552:TYR:CE2	2.55	0.41
1:A:393:TYR:N	1:A:396:SER:HB3	2.35	0.41
1:A:176:THR:HG23	1:A:176:THR:O	2.21	0.41
1:A:396:SER:HA	1:A:430:ASN:HB2	2.02	0.41
1:A:93:ARG:CG	1:A:552:TYR:CZ	3.04	0.41
1:A:184:LEU:HD12	1:A:190:TYR:HB3	2.02	0.41
1:A:642:THR:HB	1:A:674:ARG:HB3	2.03	0.41
1:A:105:TYR:O	1:A:150:ASN:HA	2.21	0.41
1:A:382:ARG:HD2	4:A:1009:FTT:O3	2.20	0.41
1:A:205:GLN:NE2	11:A:2095:HOH:O	2.54	0.41
1:A:588:ALA:HA	1:A:594:ASN:ND2	2.35	0.41
1:A:50:ILE:HD11	1:A:132:MSE:HG3	2.03	0.41
1:A:294:PHE:HD1	1:A:361:LEU:HD11	1.86	0.41
1:A:339:HIS:HE1	1:A:401:ASN:HD21	1.69	0.41
1:A:350:GLU:HG2	1:A:387:ILE:HA	2.02	0.41
1:A:390:TRP:CH2	1:A:433:PRO:HG3	2.55	0.41
1:A:393:TYR:N	1:A:430:ASN:O	2.46	0.41
1:A:451:ALA:O	1:A:457:LEU:HD12	2.20	0.41
1:A:62:GLN:HB3	1:A:167:LYS:HZ1	1.86	0.41
1:A:148:LEU:HD23	1:A:149:LEU:N	2.35	0.41
1:A:205:GLN:HG3	1:A:243:TYR:HB2	2.03	0.41
1:A:297:ARG:HD2	1:A:360:GLN:HE21	1.84	0.41
1:A:297:ARG:HH11	1:A:360:GLN:HE21	1.68	0.41
1:A:240:GLU:HA	1:A:275:TYR:O	2.21	0.41
1:A:412:HIS:CD2	1:A:413:HIS:CE1	3.09	0.41
1:A:250:GLU:OE1	1:A:250:GLU:N	2.55	0.40
10:A:1101:DDQ:HM11	10:A:1101:DDQ:H22	1.88	0.40
1:A:397:VAL:HB	1:A:421:PHE:CE1	2.56	0.40
1:A:715:ARG:NH1	1:A:715:ARG:CG	2.84	0.40
1:A:138:VAL:HG23	1:A:489:TRP:HA	2.04	0.40
1:A:455:LYS:HE2	1:A:455:LYS:HA	2.02	0.40
1:A:661:PHE:H	1:A:661:PHE:HD1	1.66	0.40
1:A:42:PRO:CG	1:A:45:LYS:HD2	2.51	0.40
1:A:343:ARG:O	1:A:397:VAL:HG13	2.22	0.40
1:A:350:GLU:CG	1:A:387:ILE:HG12	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:TRP:NE1	1:A:431:SER:HB2	2.36	0.40
1:A:600:THR:HB	1:A:624:MSE:HB2	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	705/725 (97%)	637 (90%)	58 (8%)	10 (1%)	9 23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	PRO
1	A	679	ARG
1	A	334	PRO
1	A	498	ASP
1	A	589	LEU
1	A	696	ASP
1	A	258	ASN
1	A	318	CYS
1	A	474	ARG
1	A	680	VAL

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	587/591 (99%)	558 (95%)	29 (5%)	22	49

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

Mol	Chain	Res	Type
1	A	28	ILE
1	A	68	GLU
1	A	73	THR
1	A	93	ARG
1	A	112	GLN
1	A	148	LEU
1	A	156	PRO
1	A	199	ARG
1	A	205	GLN
1	A	268	GLU
1	A	287	ASP
1	A	315	TYR
1	A	334	PRO
1	A	352	LEU
1	A	353	GLN
1	A	381	MSE
1	A	384	ARG
1	A	397	VAL
1	A	402	LEU
1	A	430	ASN
1	A	455	LYS
1	A	498	ASP
1	A	551	VAL
1	A	565	GLU
1	A	620	VAL
1	A	635	ASP
1	A	674	ARG
1	A	677	LEU
1	A	722	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	165	GLN
1	A	202	ASN
1	A	205	GLN
1	A	310	ASN
1	A	328	GLN
1	A	354	ASN
1	A	360	GLN
1	A	388	ASN
1	A	404	ASN
1	A	409	HIS
1	A	412	HIS
1	A	430	ASN
1	A	438	ASN
1	A	448	GLN
1	A	522	ASN
1	A	594	ASN
1	A	686	ASN
1	A	716	GLN

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	PA1	B	1	2,7,4	11,11,12	0.64	0	15,15,17	0.78	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GCN	B	2	3,2,4	10,10,11	1.06	1 (10%)	13,13,15	2.64	2 (15%)
2	KDO	B	3	2	15,15,16	0.83	0	17,21,24	1.05	1 (5%)
2	GMH	B	4	2,8	13,13,14	0.79	0	16,18,20	0.65	0
2	GMH	B	5	3,2	13,13,14	1.03	1 (7%)	16,18,20	1.06	1 (6%)
2	GLC	B	6	2	11,11,12	0.57	0	15,15,17	0.71	0
2	GLC	B	7	2	11,11,12	0.55	0	15,15,17	0.52	0
2	GLA	B	8	2	11,11,12	0.45	0	15,15,17	0.53	0
2	KDO	B	9	2	15,15,16	0.70	0	17,21,24	1.01	1 (5%)

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	PA1	B	1	2,7,4	-	2/2/18/22	0/1/1/1
2	GCN	B	2	3,2,4	-	0/2/15/18	0/1/1/1
2	KDO	B	3	2	-	0/10/26/30	0/1/1/1
2	GMH	B	4	2,8	-	2/6/23/26	0/1/1/1
2	GMH	B	5	3,2	-	4/6/23/26	0/1/1/1
2	GLC	B	6	2	-	2/2/19/22	0/1/1/1
2	GLC	B	7	2	-	2/2/19/22	0/1/1/1
2	GLA	B	8	2	-	2/2/19/22	0/1/1/1
2	KDO	B	9	2	-	2/10/26/30	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GCN	C1-C2	2.82	1.55	1.52
2	B	5	GMH	O5-C5	2.31	1.46	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GCN	C3-C2-C1	8.71	116.91	109.87
2	B	5	GMH	C1-O5-C5	3.19	116.71	111.48
2	B	2	GCN	C1-O5-C5	2.58	115.64	112.19
2	B	1	PA1	O5-C1-C2	2.28	112.17	109.51
2	B	3	KDO	O1B-C1-C2	2.27	118.60	112.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	KDO	O1B-C1-C2	2.21	118.46	112.71

There are no chirality outliers.

All (16) torsion outliers are listed below:

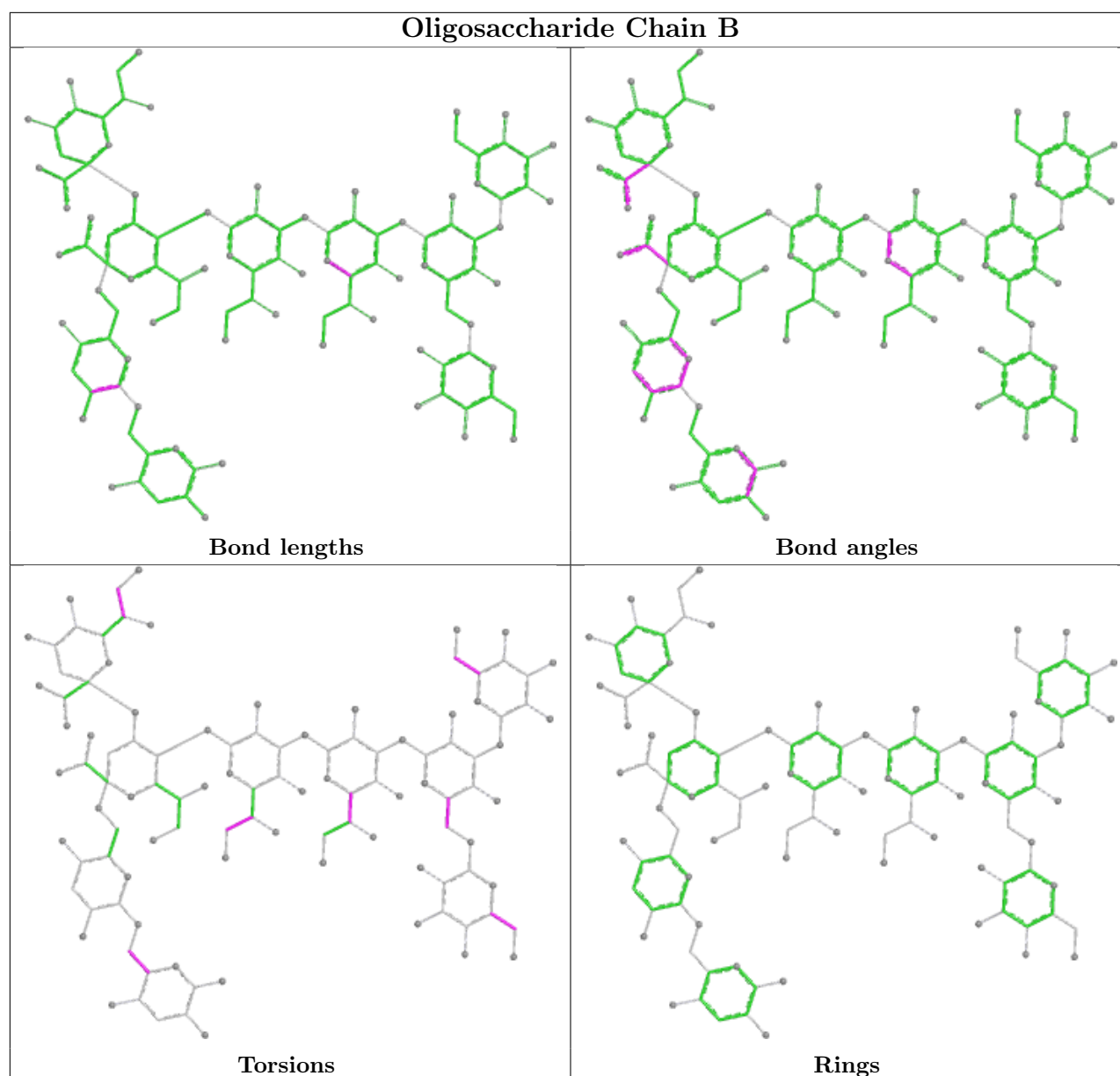
Mol	Chain	Res	Type	Atoms
2	B	4	GMH	O6-C6-C7-O7
2	B	5	GMH	C4-C5-C6-C7
2	B	5	GMH	C4-C5-C6-O6
2	B	5	GMH	O5-C5-C6-C7
2	B	5	GMH	O5-C5-C6-O6
2	B	1	PA1	C4-C5-C6-O6
2	B	1	PA1	O5-C5-C6-O6
2	B	7	GLC	O5-C5-C6-O6
2	B	8	GLA	O5-C5-C6-O6
2	B	4	GMH	C5-C6-C7-O7
2	B	7	GLC	C4-C5-C6-O6
2	B	8	GLA	C4-C5-C6-O6
2	B	9	KDO	O7-C7-C8-O8
2	B	9	KDO	C6-C7-C8-O8
2	B	6	GLC	C4-C5-C6-O6
2	B	6	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5	GMH	1	0
2	B	4	GMH	4	0
2	B	9	KDO	1	0
2	B	3	KDO	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 oligosaccharide.



5.6 Ligand geometry [i](#)

13 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
4	FTT	A	1009	2	14,15,16	0.41	0	15,15,17	0.69	1 (6%)
6	MYR	A	1014	4	14,14,15	1.01	1 (7%)	13,13,15	0.83	1 (7%)
3	PO4	A	2005	2	0,3,4	-	-	0,3,6	-	-
7	DPO	A	2000	2	4,7,8	2.50	1 (25%)	5,10,13	0.96	0
4	FTT	A	1011	5,2	14,15,16	0.32	0	15,15,17	0.81	0
4	FTT	A	1013	2,6	16,16,16	0.91	1 (6%)	16,17,17	0.56	0
3	PO4	A	2001	2	0,3,4	-	-	0,3,6	-	-
4	FTT	A	1010	2	6,6,16	1.32	1 (16%)	6,7,17	0.61	0
10	DDQ	A	1102	-	11,13,13	0.59	0	12,15,15	0.60	0
9	FCI	A	1050	-	56,56,56	1.40	4 (7%)	63,87,87	0.99	2 (3%)
10	DDQ	A	1101	-	11,13,13	0.65	0	12,15,15	0.60	0
5	DAO	A	1012	4	12,12,13	1.07	1 (8%)	11,11,13	0.83	1 (9%)
8	EAP	A	2004	2	3,6,7	3.08	2 (66%)	0,6,9	-	-

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	FTT	A	1009	2	-	0/14/14/15	-
6	MYR	A	1014	4	-	2/12/12/13	-
7	DPO	A	2000	2	-	0/2/5/6	-
4	FTT	A	1011	5,2	-	3/14/14/15	-
4	FTT	A	1013	2,6	-	1/15/15/15	-
4	FTT	A	1010	2	-	0/4/4/15	-
10	DDQ	A	1102	-	-	0/11/11/11	-
9	FCI	A	1050	-	3/3/17/23	11/62/116/116	0/4/6/6
10	DDQ	A	1101	-	-	0/11/11/11	-
5	DAO	A	1012	4	-	1/10/10/11	-
8	EAP	A	2004	2	-	0/0/4/5	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1050	FCI	O10-FE	5.97	2.12	1.99
9	A	1050	FCI	O3-FE	5.33	2.19	2.04
8	A	2004	EAP	P-O4	-4.70	1.49	1.63
7	A	2000	DPO	P1-O4	-4.47	1.50	1.63
6	A	1014	MYR	O2-C1	-3.74	1.23	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1012	DAO	O2-C1	-3.64	1.23	1.42
4	A	1013	FTT	O1-C1	3.33	1.41	1.30
4	A	1010	FTT	O1-C1	3.15	1.41	1.30
9	A	1050	FCI	O11-FE	3.06	2.05	1.99
9	A	1050	FCI	O14-FE	2.59	2.04	1.99
8	A	2004	EAP	O4-C1	2.51	1.44	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1050	FCI	C1-C10-N1	3.50	120.59	111.11
5	A	1012	DAO	O2-C1-C2	2.19	125.36	111.44
6	A	1014	MYR	O2-C1-C2	2.18	125.29	111.44
9	A	1050	FCI	O17-C8-N4	-2.15	119.31	122.95
4	A	1009	FTT	O2-C1-C2	-2.10	119.26	125.38

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1050	FCI	N6
9	A	1050	FCI	N8
9	A	1050	FCI	N5

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1050	FCI	C2-C11-C38-O18
9	A	1050	FCI	C24-C16-C7-N3
9	A	1050	FCI	C24-C16-C7-O7
9	A	1050	FCI	C38-C11-C2-O2
9	A	1050	FCI	C38-C11-C2-N9
4	A	1011	FTT	O3-C3-C4-C5
9	A	1050	FCI	N2-C11-C38-O18
4	A	1013	FTT	C11-C10-C9-C8
5	A	1012	DAO	O2-C1-C2-C3
9	A	1050	FCI	C25-C30-N5-O10
9	A	1050	FCI	N4-C16-C7-O7
4	A	1011	FTT	O2-C1-C2-C3
9	A	1050	FCI	N4-C16-C7-N3
6	A	1014	MYR	C2-C3-C4-C5
4	A	1011	FTT	C2-C3-C4-C5
9	A	1050	FCI	C25-C30-N5-C3

Continued on next page...

Continued from previous page...

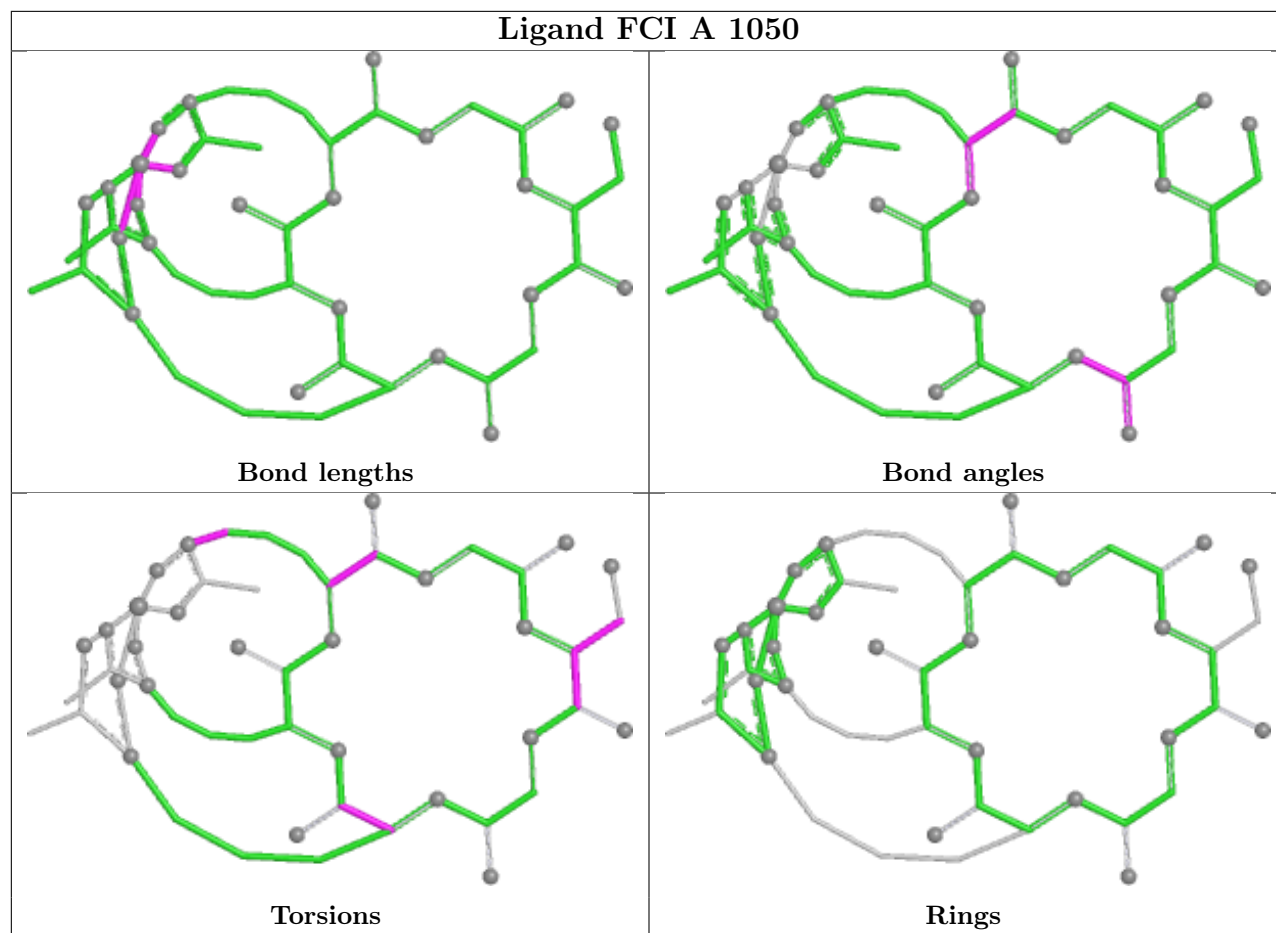
Mol	Chain	Res	Type	Atoms
9	A	1050	FCI	O1-C1-C10-C18
6	A	1014	MYR	O2-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1009	FTT	1	0
3	A	2005	PO4	1	0
4	A	1011	FTT	2	0
4	A	1013	FTT	3	0
9	A	1050	FCI	2	0
10	A	1101	DDQ	1	0
8	A	2004	EAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.