



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:26 PM UTC

PDB ID : 3OPM / pdb_00003opm
Title : Crystal Structure of Human DPP4 Bound to TAK-294
Authors : Yano, J.K.; Aertgeerts, K.
Deposited on : 2010-09-01
Resolution : 2.72 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

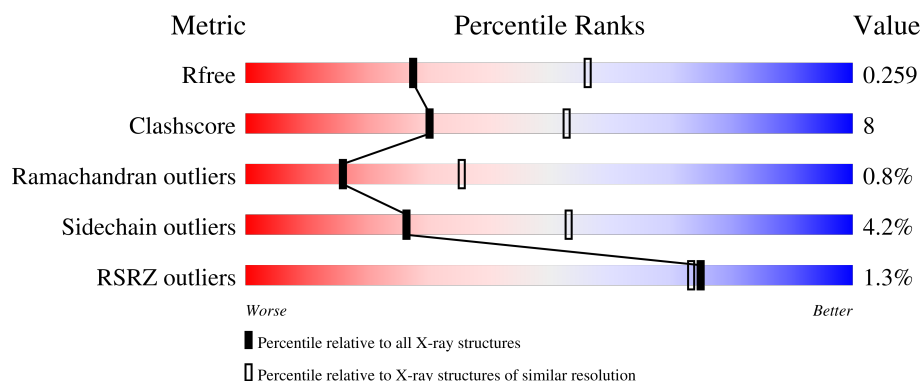
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	740	% 79% 17% ..
1	B	740	% 79% 19% ..
1	C	740	2% 75% 21% ..
1	D	740	% 81% 16% ..
2	E	2	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24713 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5950	3821	977	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	725	Total	C	N	O	S	0	0	0
			5937	3810	979	1122	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

Continued on next page...

Continued from previous page...

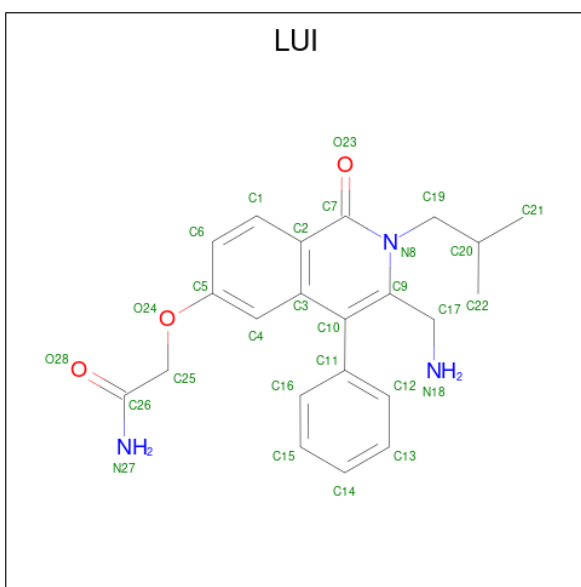
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



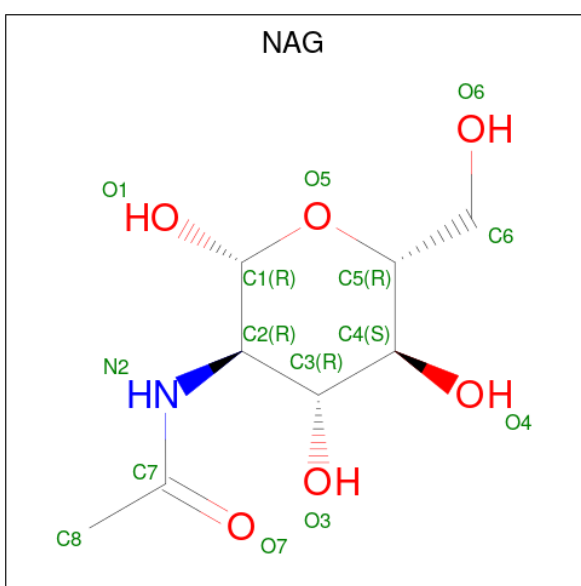
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-{[3-(aminomethyl)-2-(2-methylpropyl)-1-oxo-4-phenyl-1,2-dihydroisoquinolin-6-yl]oxy}acetamide (CCD ID: LUI) (formula: C₂₂H₂₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	3	3		
3	B	1	Total	C	N	O	0	0
			28	22	3	3		
3	C	1	Total	C	N	O	0	0
			28	22	3	3		
3	D	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

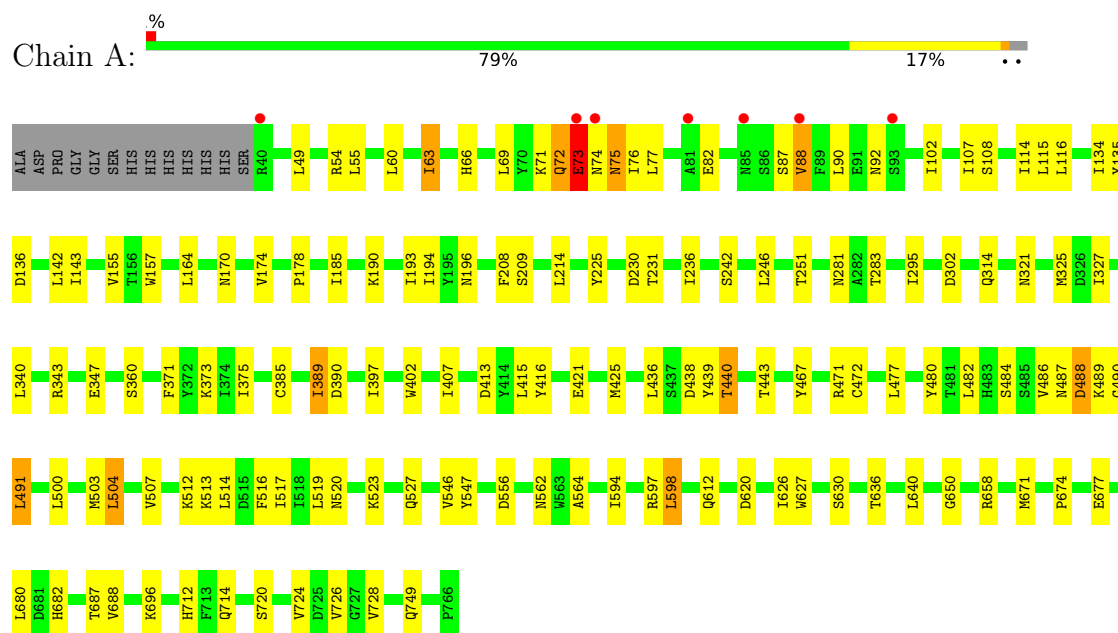
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	152	Total O 152 152	0	0
5	B	142	Total O 142 142	0	0
5	C	84	Total O 84 84	0	0
5	D	128	Total O 128 128	0	0

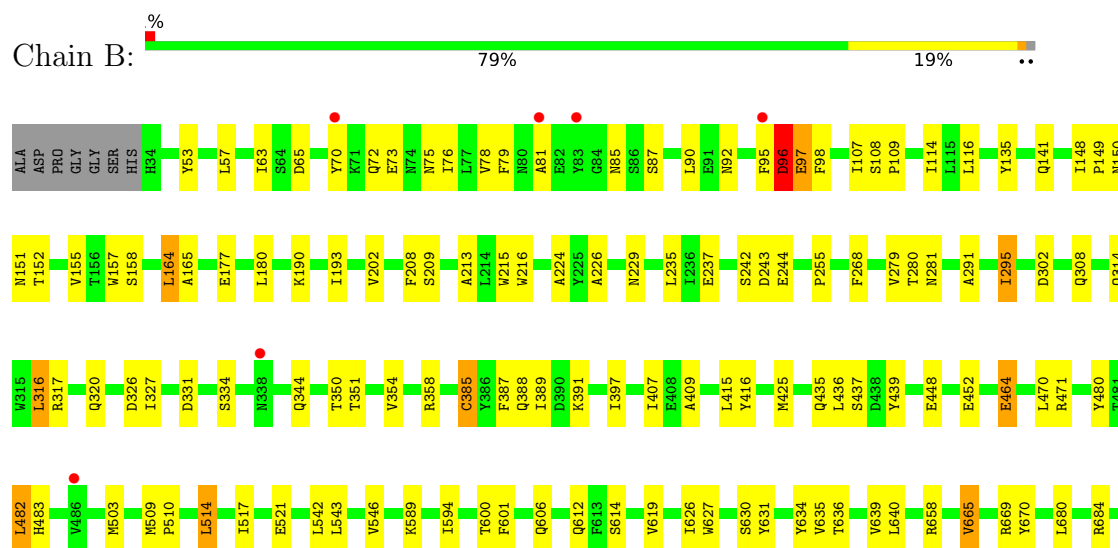
3 Residue-property plots [i](#)

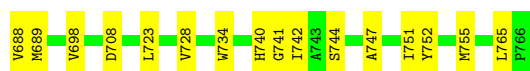
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Dipeptidyl peptidase 4

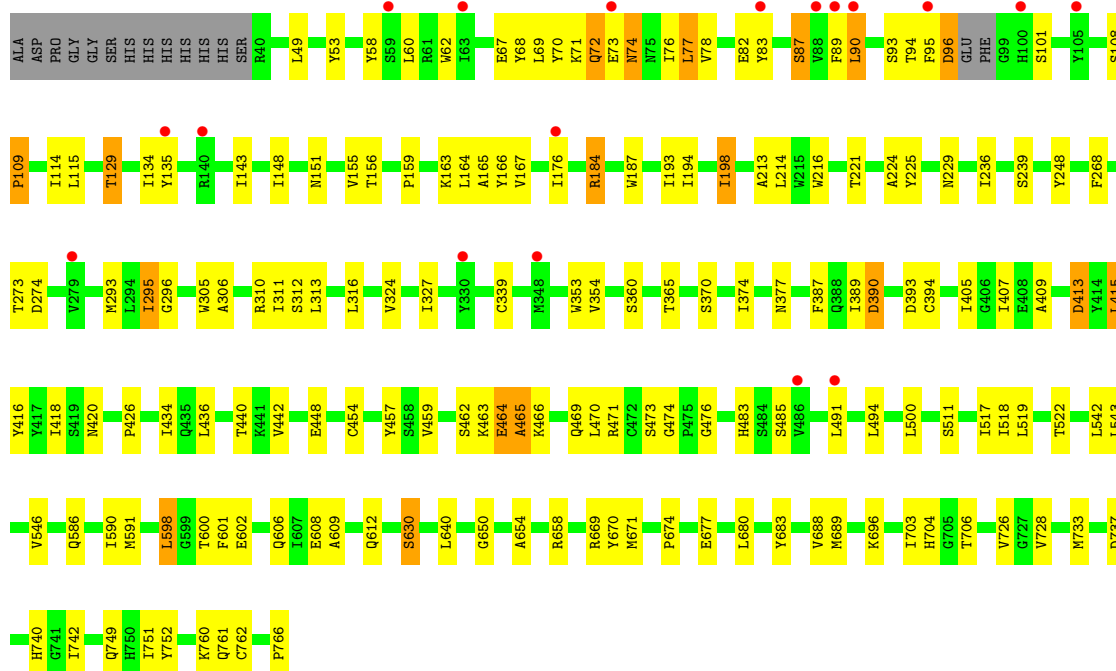
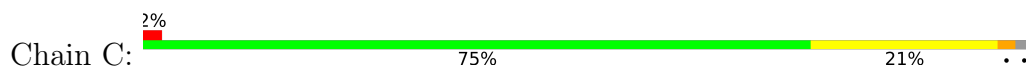


• Molecule 1: Dipeptidyl peptidase 4

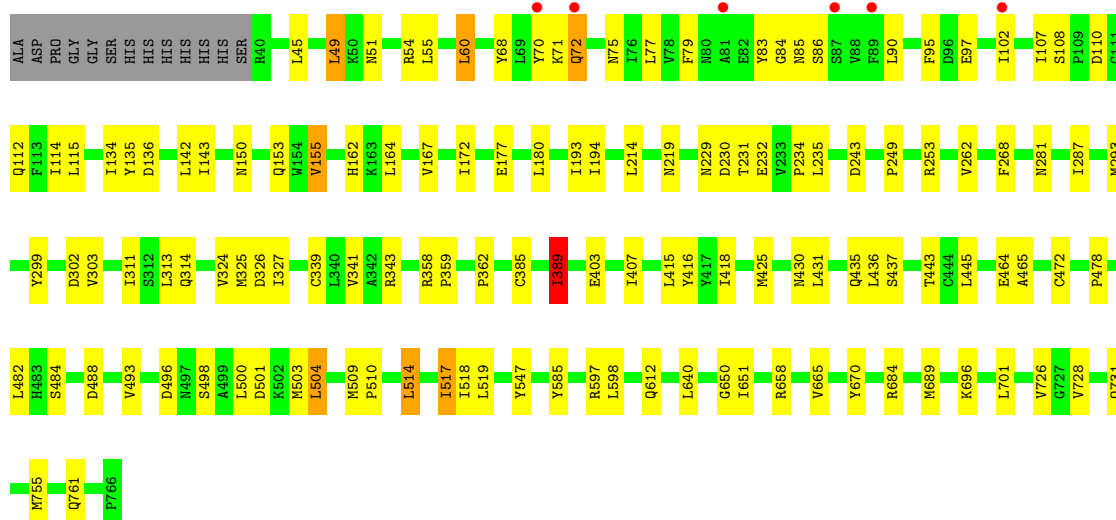
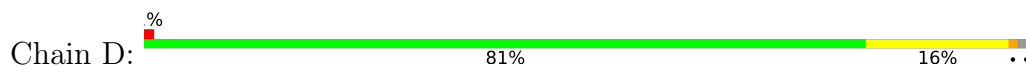




• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.77Å 122.56Å 144.74Å 90.00° 115.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.72 35.00 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.00-2.72) 97.4 (35.00-2.72)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.195 , 0.254 0.199 , 0.259	Depositor DCC
R_{free} test set	5038 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24713	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LUI, NAG

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	0.63	0/6122	0.79	1/8327 (0.0%)
1	B	0.62	0/6190	0.79	1/8419 (0.0%)
1	C	0.57	0/6107	0.75	2/8305 (0.0%)
1	D	0.61	0/6129	0.78	0/8336
All	All	0.61	0/24548	0.78	4/33387 (0.0%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	630	SER	CB-CA-C	-7.07	108.43	116.63
1	B	97	GLU	N-CA-C	-6.78	103.69	112.23
1	C	630	SER	CB-CA-C	-5.67	109.52	117.23
1	C	213	ALA	N-CA-C	-5.28	104.11	110.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	ASP	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	5950	0	5664	87	0
1	B	6013	0	5718	99	0
1	C	5937	0	5664	110	0
1	D	5957	0	5679	84	0
2	E	28	0	26	5	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	3	0
3	D	28	0	25	0	0
4	A	84	0	78	8	0
4	B	70	0	65	10	0
4	D	56	0	52	9	0
5	A	152	0	0	2	0
5	B	142	0	0	4	0
5	C	84	0	0	2	0
5	D	128	0	0	3	0
All	All	24713	0	23046	384	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 8.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HD21	4:B:1501:NAG:C1	1.09	1.57
1:C:229:ASN:HD21	2:E:1:NAG:C1	1.07	1.55
1:B:229:ASN:HD21	4:B:2291:NAG:C1	0.94	1.54
1:B:281:ASN:HD21	4:B:2811:NAG:C1	1.16	1.51
1:D:229:ASN:HD21	4:D:2291:NAG:C1	1.15	1.51
1:A:281:ASN:HD21	4:A:2811:NAG:C1	0.89	1.50
1:D:281:ASN:HD21	4:D:2811:NAG:C1	1.29	1.42
1:D:219:ASN:HD21	4:D:2191:NAG:C1	1.44	1.27
1:B:150:ASN:HD21	4:B:1501:NAG:C2	1.72	1.02
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.45	0.99
4:A:2291:NAG:O4	4:A:2292:NAG:C1	2.21	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:HG23	1:B:351:THR:HG23	1.54	0.88
1:A:82:GLU:OE2	1:A:467:TYR:OH	1.93	0.87
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.11	0.85
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.62	0.81
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.62	0.80
1:B:751:ILE:HG12	1:B:755:MET:HE2	1.63	0.80
1:C:470:LEU:HD12	1:C:483:HIS:NE2	1.98	0.79
1:B:327:ILE:HD13	1:B:389:ILE:CD1	2.12	0.79
1:A:63:ILE:HD11	1:A:69:LEU:HD12	1.63	0.79
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.64	0.78
1:A:321:ASN:CG	4:A:3211:NAG:C1	2.56	0.78
1:B:229:ASN:CG	4:B:2291:NAG:C1	2.58	0.77
1:C:72:GLN:HB2	1:C:77:LEU:HD11	1.66	0.77
1:C:630:SER:OG	1:C:740:HIS:NE2	2.19	0.75
1:A:347:GLU:OE1	1:A:373:LYS:NZ	2.18	0.74
1:B:327:ILE:HD13	1:B:389:ILE:HD11	1.70	0.74
1:B:327:ILE:HG21	1:B:389:ILE:HD11	1.69	0.73
1:D:425:MET:HE3	1:D:514:LEU:HD12	1.72	0.72
1:D:193:ILE:HG22	1:D:194:ILE:CD1	2.19	0.72
1:C:407:ILE:HG23	1:C:415:LEU:HD21	1.73	0.70
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.72	0.70
1:B:53:TYR:CE1	1:B:503:MET:HE2	2.26	0.70
1:C:71:LYS:HA	1:C:76:ILE:HD13	1.73	0.70
1:C:115:LEU:HD21	1:C:155:VAL:HG11	1.74	0.70
1:D:219:ASN:CG	4:D:2191:NAG:C1	2.64	0.69
1:A:500:LEU:HA	1:A:503:MET:HE3	1.74	0.69
1:D:45:LEU:HG	1:D:49:LEU:HD22	1.72	0.69
1:D:107:ILE:HG22	1:D:108:SER:O	1.92	0.69
1:C:156:THR:HG23	1:C:216:TRP:HE1	1.57	0.69
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.75	0.68
1:B:85:ASN:CG	4:B:901:NAG:C1	2.64	0.68
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.76	0.68
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.76	0.67
1:D:60:LEU:HD12	1:D:60:LEU:C	2.19	0.67
1:D:95:PHE:O	1:D:102:ILE:HD11	1.94	0.67
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.75	0.67
1:C:434:ILE:HG13	1:C:442:VAL:HG22	1.76	0.67
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.77	0.67
1:B:517:ILE:HD12	1:B:612:GLN:HG3	1.77	0.67
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.76	0.67
1:D:407:ILE:HG23	1:D:415:LEU:HD21	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:CG	4:B:1501:NAG:C1	2.68	0.66
1:C:511:SER:HB3	5:C:816:HOH:O	1.96	0.66
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.31	0.65
1:C:94:THR:HA	1:C:101:SER:HA	1.78	0.65
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.79	0.65
1:C:415:LEU:O	1:C:434:ILE:HG22	1.97	0.65
1:C:114:ILE:HG22	1:C:135:TYR:HB2	1.77	0.65
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.79	0.64
1:C:518:ILE:O	1:C:519:LEU:HD23	1.97	0.64
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.80	0.64
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.27	0.64
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.79	0.64
1:C:658:ARG:HG2	1:C:689:MET:HE1	1.80	0.64
1:B:208:PHE:O	1:B:209:SER:C	2.42	0.63
1:A:194:ILE:HD12	4:A:2291:NAG:H82	1.81	0.63
1:C:229:ASN:CG	2:E:1:NAG:C1	2.69	0.63
1:C:542:LEU:HD23	1:C:543:LEU:N	2.13	0.63
1:C:464:GLU:O	1:C:465:ALA:CB	2.47	0.63
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.34	0.62
1:A:546:VAL:HG12	1:A:627:TRP:O	1.99	0.62
1:B:327:ILE:HD13	1:B:389:ILE:HD12	1.81	0.62
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.82	0.62
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.81	0.62
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.82	0.62
3:C:800:LUI:C16	3:C:800:LUI:HN18	2.12	0.62
1:B:542:LEU:C	1:B:542:LEU:HD23	2.26	0.61
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.83	0.61
1:B:281:ASN:ND2	5:B:891:HOH:O	2.35	0.60
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.36	0.60
1:C:94:THR:HG22	5:C:809:HOH:O	2.00	0.60
1:C:167:VAL:HG11	1:C:198:ILE:HD13	1.83	0.60
1:A:281:ASN:CG	4:A:2811:NAG:C1	2.70	0.60
1:B:635:VAL:O	1:B:639:VAL:HG23	2.02	0.60
1:C:517:ILE:HD12	1:C:612:GLN:HG3	1.83	0.60
1:D:229:ASN:CG	4:D:2291:NAG:C1	2.70	0.60
1:B:152:THR:HG21	1:B:155:VAL:CG2	2.31	0.60
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.82	0.60
1:C:464:GLU:O	1:C:465:ALA:HB2	2.02	0.60
1:D:268:PHE:CD2	1:D:313:LEU:HD11	2.37	0.60
1:C:470:LEU:HD12	1:C:483:HIS:HE2	1.67	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:HE2	1:A:556:ASP:O	2.02	0.60
3:C:800:LUI:HN18	3:C:800:LUI:C11	2.15	0.59
1:D:84:GLY:O	1:D:86:SER:N	2.35	0.59
1:C:193:ILE:HG22	1:C:194:ILE:CD1	2.30	0.58
1:D:299:TYR:CE1	1:D:665:VAL:HG22	2.38	0.58
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.38	0.58
1:D:518:ILE:O	1:D:519:LEU:HD23	2.03	0.58
1:D:60:LEU:HB2	1:D:68:TYR:CD2	2.38	0.58
1:C:71:LYS:HZ2	1:C:74:ASN:HA	1.69	0.58
1:C:390:ASP:OD1	1:C:390:ASP:N	2.35	0.58
1:C:96:ASP:N	1:C:96:ASP:OD2	2.36	0.58
1:D:55:LEU:HD12	1:D:500:LEU:CD2	2.34	0.58
1:C:306:ALA:HB3	1:C:310:ARG:HB3	1.85	0.58
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.39	0.57
1:B:279:VAL:HG23	1:B:280:THR:HG23	1.86	0.57
1:B:471:ARG:HG2	1:B:480:TYR:CE1	2.39	0.57
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.87	0.57
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.86	0.57
2:E:1:NAG:C4	2:E:2:NAG:C1	2.83	0.57
1:A:517:ILE:HD12	1:A:612:GLN:HG3	1.88	0.56
1:A:174:VAL:HG23	1:A:185:ILE:HD11	1.86	0.56
1:B:190:LYS:HD3	1:B:193:ILE:HD12	1.88	0.56
1:C:608:GLU:O	1:C:612:GLN:HG2	2.06	0.56
1:A:486:VAL:HG13	1:A:487:ASN:H	1.71	0.56
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.88	0.56
4:A:2291:NAG:C4	4:A:2292:NAG:C1	2.84	0.56
1:C:459:VAL:HG23	1:C:469:GLN:O	2.05	0.56
1:B:202:VAL:HG22	1:B:665:VAL:HG13	1.89	0.55
1:B:752:TYR:HA	1:B:755:MET:HE3	1.87	0.55
1:C:60:LEU:C	1:C:60:LEU:HD12	2.32	0.55
1:D:136:ASP:HB2	1:D:143:ILE:HD11	1.88	0.55
1:C:312:SER:C	1:C:313:LEU:HD12	2.32	0.55
1:D:75:ASN:O	1:D:77:LEU:HD12	2.07	0.55
1:A:325:MET:CE	1:A:327:ILE:HD11	2.36	0.55
4:D:1501:NAG:H81	5:D:835:HOH:O	2.08	0.54
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.43	0.54
4:A:2811:NAG:H2	5:A:866:HOH:O	2.08	0.54
1:D:281:ASN:HD21	4:D:2811:NAG:C2	2.12	0.54
1:B:202:VAL:HG22	1:B:665:VAL:CG1	2.38	0.54
1:A:620:ASP:OD2	1:A:620:ASP:C	2.49	0.54
1:D:79:PHE:HA	1:D:86:SER:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:MET:CE	1:B:514:LEU:HD13	2.38	0.53
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.44	0.53
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.43	0.53
1:C:71:LYS:NZ	1:C:74:ASN:HA	2.24	0.53
1:A:55:LEU:HD23	1:A:500:LEU:HD23	1.88	0.53
1:B:242:SER:OG	1:B:243:ASP:N	2.40	0.53
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.90	0.53
1:A:415:LEU:HD23	1:A:416:TYR:N	2.24	0.53
1:A:69:LEU:HD22	1:A:76:ILE:HG22	1.90	0.52
1:A:325:MET:HE1	1:A:371:PHE:CE2	2.44	0.52
1:B:316:LEU:HD13	1:B:320:GLN:HG2	1.91	0.52
1:C:69:LEU:HD22	1:C:76:ILE:CG2	2.39	0.52
1:D:509:MET:HE3	1:D:510:PRO:HD2	1.90	0.52
1:C:70:TYR:O	1:C:77:LEU:HD12	2.10	0.52
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.44	0.52
1:D:500:LEU:HG	1:D:504:LEU:HD22	1.92	0.52
1:A:54:ARG:O	1:A:500:LEU:HD22	2.09	0.52
1:D:303:VAL:HG22	1:D:313:LEU:HD22	1.92	0.52
1:C:78:VAL:HG13	1:C:78:VAL:O	2.10	0.52
1:C:293:MET:CE	1:C:324:VAL:HG23	2.40	0.52
3:C:800:LUI:C11	3:C:800:LUI:N18	2.72	0.52
1:D:658:ARG:HB2	1:D:689:MET:HE1	1.92	0.52
1:D:232:GLU:CB	1:D:262:VAL:HG11	2.40	0.51
1:A:720:SER:O	1:A:724:VAL:HG23	2.11	0.51
1:C:184:ARG:HD2	1:C:187:TRP:CZ2	2.45	0.51
1:D:435:GLN:HE21	1:D:437:SER:HG	1.57	0.51
1:B:546:VAL:HG12	1:B:606:GLN:OE1	2.10	0.51
1:B:723:LEU:HD22	1:B:728:VAL:HG11	1.93	0.51
1:A:71:LYS:O	1:A:73:GLU:N	2.44	0.51
1:C:60:LEU:HD22	1:C:68:TYR:CG	2.45	0.51
1:B:81:ALA:HB1	1:B:482:LEU:HD11	1.93	0.51
1:C:360:SER:OG	1:C:374:ILE:O	2.27	0.51
1:C:229:ASN:ND2	2:E:1:NAG:O5	2.43	0.50
1:C:518:ILE:HA	1:C:522:THR:O	2.11	0.50
1:D:153:GLN:OE1	1:D:167:VAL:HG12	2.10	0.50
1:D:235:LEU:HD13	1:D:253:ARG:HB3	1.93	0.50
1:A:519:LEU:O	1:A:520:ASN:C	2.54	0.50
1:B:92:ASN:ND2	5:B:854:HOH:O	2.44	0.50
1:A:503:MET:HE2	5:A:902:HOH:O	2.12	0.50
1:D:232:GLU:HB2	1:D:262:VAL:HG11	1.93	0.49
1:A:107:ILE:HD11	1:A:114:ILE:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:OG1	1:B:237:GLU:OE2	2.25	0.49
1:D:325:MET:HE1	1:D:362:PRO:HB3	1.94	0.49
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.94	0.49
1:A:321:ASN:ND2	4:A:3211:NAG:C2	2.64	0.49
1:A:598:LEU:O	1:A:682:HIS:NE2	2.44	0.49
1:A:562:ASN:OD1	1:A:564:ALA:HB3	2.12	0.49
1:D:194:ILE:HG12	4:D:2291:NAG:H82	1.94	0.49
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.41	0.49
1:B:107:ILE:HD12	1:B:107:ILE:N	2.27	0.49
1:D:343:ARG:HD2	1:D:389:ILE:CG2	2.43	0.49
1:A:477:LEU:HD12	1:A:477:LEU:H	1.77	0.49
1:D:72:GLN:HG3	1:D:77:LEU:HD13	1.95	0.49
1:A:69:LEU:HD22	1:A:76:ILE:CG2	2.43	0.48
1:B:107:ILE:HG22	1:B:108:SER:O	2.13	0.48
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.28	0.48
1:C:671:MET:HE3	1:C:683:TYR:CD2	2.48	0.48
1:A:185:ILE:N	1:A:185:ILE:HD12	2.28	0.48
1:C:387:PHE:CD1	1:C:394:CYS:HB3	2.47	0.48
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.95	0.48
1:A:107:ILE:HG22	1:A:108:SER:O	2.13	0.48
1:C:353:TRP:CZ2	1:C:591:MET:HE3	2.48	0.48
1:C:248:TYR:OH	1:D:234:PRO:HG2	2.14	0.48
1:B:509:MET:HE3	1:B:510:PRO:HD2	1.96	0.48
1:C:163:LYS:HE2	1:C:176:ILE:HD12	1.96	0.48
1:C:465:ALA:O	1:C:485:SER:OG	2.20	0.48
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.79	0.48
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.96	0.48
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.49	0.48
1:D:281:ASN:CG	4:D:2811:NAG:C1	2.83	0.47
1:A:484:SER:O	1:A:488:ASP:HA	2.14	0.47
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.96	0.47
1:C:760:LYS:NZ	1:C:766:PRO:O	2.46	0.47
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.45	0.47
1:C:415:LEU:C	1:C:415:LEU:HD13	2.39	0.47
1:D:303:VAL:CG1	1:D:311:ILE:HD11	2.45	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.95	0.47
1:A:425:MET:CE	1:A:514:LEU:HD23	2.44	0.47
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.47
1:C:193:ILE:C	1:C:194:ILE:HD12	2.39	0.47
1:C:586:GLN:HB3	1:C:590:ILE:HD12	1.97	0.47
1:A:242:SER:HB3	1:A:246:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.49	0.47
1:B:640:LEU:HB3	1:B:698:VAL:HG21	1.96	0.47
1:C:78:VAL:HG12	1:C:87:SER:O	2.13	0.47
1:D:415:LEU:C	1:D:415:LEU:HD23	2.40	0.47
1:B:150:ASN:ND2	4:B:1501:NAG:C2	2.54	0.47
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.96	0.47
1:D:472:CYS:O	1:D:478:PRO:HA	2.15	0.47
2:E:1:NAG:O4	2:E:2:NAG:O5	2.32	0.47
1:B:165:ALA:HB2	1:B:216:TRP:CZ2	2.50	0.47
1:C:295:ILE:HG13	1:C:296:GLY:N	2.30	0.47
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.95	0.47
1:B:85:ASN:ND2	4:B:901:NAG:O5	2.41	0.47
1:B:409:ALA:HB3	1:B:416:TYR:HB2	1.97	0.47
1:C:327:ILE:HD13	1:C:389:ILE:CD1	2.45	0.46
1:C:474:GLY:HA2	1:C:476:GLY:O	2.15	0.46
1:C:248:TYR:CZ	1:D:234:PRO:HG2	2.50	0.46
1:B:73:GLU:C	1:B:75:ASN:H	2.22	0.46
1:B:81:ALA:CB	1:B:482:LEU:HD11	2.45	0.46
1:B:600:THR:OG1	1:B:601:PHE:N	2.47	0.46
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.96	0.46
1:D:484:SER:O	1:D:488:ASP:HA	2.15	0.46
1:D:701:LEU:HD13	1:D:731:GLN:HB2	1.97	0.46
1:A:75:ASN:ND2	1:A:88:VAL:HG13	2.30	0.46
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.96	0.46
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.97	0.46
1:D:162:HIS:NE2	1:D:177:GLU:OE1	2.43	0.46
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.97	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.51	0.46
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.98	0.46
1:C:115:LEU:HD21	1:C:155:VAL:CG1	2.42	0.46
1:C:268:PHE:CE2	1:C:313:LEU:HD21	2.50	0.46
1:D:110:ASP:OD2	1:D:112:GLN:NE2	2.49	0.46
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.42	0.46
1:A:415:LEU:HB2	1:A:436:LEU:HD21	1.98	0.46
1:B:235:LEU:HD23	1:B:255:PRO:HA	1.97	0.46
1:C:602:GLU:OE2	1:C:602:GLU:N	2.44	0.46
1:D:598:LEU:HD21	1:D:670:TYR:HB3	1.98	0.46
1:B:78:VAL:HG12	1:B:87:SER:O	2.16	0.46
1:C:89:PHE:O	1:C:90:LEU:CB	2.63	0.46
1:C:600:THR:OG1	1:C:601:PHE:N	2.48	0.46
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LEU:HD23	1:B:543:LEU:N	2.31	0.45
1:D:155:VAL:HG12	1:D:164:LEU:HD22	1.99	0.45
1:B:81:ALA:HB1	1:B:482:LEU:CD1	2.47	0.45
1:D:415:LEU:HD23	1:D:416:TYR:N	2.32	0.45
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.99	0.45
1:A:208:PHE:O	1:A:209:SER:C	2.59	0.45
1:A:327:ILE:HD12	1:A:343:ARG:O	2.17	0.45
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.51	0.45
1:A:63:ILE:CD1	1:A:69:LEU:HD12	2.42	0.45
1:B:53:TYR:CD1	1:B:503:MET:HE2	2.52	0.45
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.98	0.45
1:D:431:LEU:CD2	1:D:445:LEU:HD12	2.47	0.45
1:D:231:THR:HG23	5:D:861:HOH:O	2.17	0.45
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.16	0.45
1:A:60:LEU:HD12	1:A:60:LEU:C	2.42	0.45
1:A:486:VAL:HG13	1:A:487:ASN:N	2.31	0.45
1:A:490:GLY:O	1:A:491:LEU:C	2.60	0.45
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.47	0.45
1:B:281:ASN:HD21	4:B:2811:NAG:C2	2.10	0.45
1:B:614:SER:HA	1:B:619:VAL:HB	1.99	0.45
1:C:221:THR:HG23	1:C:274:ASP:OD1	2.17	0.45
1:A:598:LEU:HD22	1:A:671:MET:CG	2.45	0.45
1:D:293:MET:HE3	1:D:324:VAL:HG23	1.99	0.45
1:D:418:ILE:HA	1:D:430:ASN:O	2.17	0.45
1:C:457:TYR:HA	1:C:471:ARG:O	2.18	0.44
1:B:658:ARG:NH1	5:B:817:HOH:O	2.43	0.44
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.53	0.44
1:B:543:LEU:HD21	1:B:627:TRP:CD1	2.52	0.44
1:D:293:MET:CE	1:D:324:VAL:HG23	2.48	0.44
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.99	0.44
1:A:598:LEU:HB2	1:A:671:MET:SD	2.57	0.44
1:B:744:SER:HB2	1:B:747:ALA:HB3	1.98	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.44
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.48	0.44
1:B:631:TYR:O	1:B:634:TYR:HB3	2.17	0.44
1:C:313:LEU:HD12	1:C:313:LEU:N	2.33	0.44
1:C:409:ALA:HB3	1:C:416:TYR:HB2	2.00	0.44
1:D:115:LEU:HD12	1:D:134:ILE:HG12	1.98	0.44
1:B:734:TRP:CD1	1:B:734:TRP:C	2.96	0.44
1:A:69:LEU:HD23	1:A:77:LEU:O	2.18	0.44
1:B:388:GLN:HB2	1:B:391:LYS:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:ALA:HA	1:C:704:HIS:CE1	2.53	0.43
1:A:487:ASN:HD21	1:A:489:LYS:HD3	1.83	0.43
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.00	0.43
1:B:150:ASN:O	1:B:151:ASN:HB2	2.19	0.43
1:B:765:LEU:HD22	5:B:867:HOH:O	2.17	0.43
1:A:170:ASN:O	1:A:196:ASN:HB2	2.18	0.43
1:B:326:ASP:OD2	1:B:344:GLN:HG2	2.18	0.43
1:C:405:ILE:HG22	1:C:405:ILE:O	2.18	0.43
1:C:674:PRO:O	1:C:680:LEU:HD13	2.17	0.43
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.53	0.43
1:A:102:ILE:HG21	1:A:116:LEU:HD22	2.00	0.43
1:A:107:ILE:CD1	1:A:114:ILE:HD12	2.48	0.43
1:A:115:LEU:HD21	1:A:155:VAL:CG2	2.48	0.43
1:D:684:ARG:HG3	5:D:825:HOH:O	2.18	0.43
1:A:136:ASP:HB2	1:A:143:ILE:HD11	2.01	0.43
1:A:230:ASP:O	1:A:231:THR:C	2.62	0.43
1:A:674:PRO:O	1:A:680:LEU:HD13	2.19	0.43
1:B:658:ARG:HB2	1:B:689:MET:HE1	2.00	0.43
1:C:72:GLN:HE21	1:C:72:GLN:C	2.25	0.43
1:C:155:VAL:HG23	1:C:166:TYR:HB3	2.00	0.43
1:C:387:PHE:CZ	1:C:394:CYS:SG	3.12	0.43
1:B:291:ALA:O	1:B:295:ILE:HG23	2.18	0.43
1:C:415:LEU:HB2	1:C:436:LEU:HD11	2.01	0.43
1:C:58:TYR:CD1	1:C:494:LEU:HD13	2.54	0.43
1:A:90:LEU:HD21	1:A:114:ILE:HD13	2.01	0.42
1:B:723:LEU:CD2	1:B:728:VAL:HG11	2.48	0.42
1:A:190:LYS:HE2	1:A:193:ILE:HD12	2.00	0.42
1:C:761:GLN:NE2	1:D:761:GLN:HE22	2.17	0.42
1:D:54:ARG:HB2	1:D:54:ARG:NH1	2.35	0.42
1:D:60:LEU:HD13	1:D:68:TYR:HB2	2.02	0.42
1:C:129:THR:HG23	1:C:151:ASN:HA	2.02	0.42
1:C:413:ASP:OD1	1:C:413:ASP:N	2.52	0.42
1:D:493:VAL:HG11	1:D:496:ASP:HB3	2.01	0.42
1:B:148:ILE:HG23	1:B:149:PRO:HD2	2.02	0.42
1:C:72:GLN:CB	1:C:77:LEU:HD11	2.43	0.42
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.42
1:C:236:ILE:HD12	1:D:249:PRO:HD2	2.00	0.42
1:C:293:MET:HE2	1:C:324:VAL:HG23	2.01	0.42
1:C:706:THR:HG1	1:C:737:ASP:H	1.67	0.42
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.55	0.42
1:B:157:TRP:CZ3	1:B:164:LEU:HD13	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ILE:HD11	1:B:317:ARG:NH1	2.35	0.42
1:C:751:ILE:HG23	1:C:752:TYR:N	2.35	0.42
1:B:213:ALA:HB1	1:B:226:ALA:HB3	2.01	0.42
1:C:95:PHE:O	1:C:96:ASP:C	2.62	0.42
1:B:471:ARG:CG	1:B:480:TYR:CE1	3.02	0.41
1:C:703:ILE:HA	1:C:733:MET:O	2.20	0.41
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.84	0.41
1:D:134:ILE:HD11	1:D:164:LEU:CD1	2.50	0.41
1:A:236:ILE:HD13	1:A:712:HIS:ND1	2.35	0.41
1:A:438:ASP:OD2	1:A:440:THR:HB	2.20	0.41
1:B:76:ILE:HD12	1:B:90:LEU:CD2	2.50	0.41
1:C:165:ALA:HB2	1:C:216:TRP:CZ2	2.55	0.41
1:C:606:GLN:O	1:C:609:ALA:HB3	2.21	0.41
1:A:72:GLN:O	1:A:74:ASN:N	2.52	0.41
1:C:377:ASN:OD1	1:C:377:ASN:C	2.62	0.41
1:D:651:ILE:HD13	1:D:755:MET:HG2	2.00	0.41
1:A:658:ARG:CB	1:A:687:THR:HG22	2.47	0.41
1:B:109:PRO:HG3	1:B:158:SER:O	2.20	0.41
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.35	0.41
1:D:70:TYR:HB3	1:D:79:PHE:CE1	2.56	0.41
1:D:358:ARG:O	1:D:359:PRO:C	2.61	0.41
1:B:65:ASP:OD2	1:B:464:GLU:N	2.47	0.41
1:B:397:ILE:HG22	1:B:439:TYR:CZ	2.56	0.41
1:C:62:TRP:CD2	1:C:462:SER:HA	2.56	0.41
1:B:331:ASP:HB3	1:B:334:SER:HB3	2.03	0.41
1:C:108:SER:O	1:C:109:PRO:C	2.63	0.41
1:C:305:TRP:CZ2	1:C:311:ILE:HD12	2.55	0.41
1:D:79:PHE:HA	1:D:86:SER:CB	2.50	0.41
1:D:287:ILE:CG2	1:D:339:CYS:SG	3.09	0.41
1:B:215:TRP:HB2	1:B:224:ALA:HB3	2.03	0.41
1:B:308:GLN:HA	1:B:308:GLN:OE1	2.20	0.40
1:C:407:ILE:CG2	1:C:415:LEU:HD21	2.47	0.40
1:D:115:LEU:HD21	1:D:155:VAL:HG11	2.02	0.40
1:B:435:GLN:NE2	1:B:437:SER:OG	2.50	0.40
1:C:454:CYS:HB3	1:C:457:TYR:CZ	2.56	0.40
1:D:303:VAL:HG22	1:D:313:LEU:CD2	2.52	0.40
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.56	0.40
1:B:708:ASP:OD1	1:B:740:HIS:HA	2.21	0.40
1:D:230:ASP:O	1:D:231:THR:C	2.62	0.40
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.89	0.40
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.56	0.40
1:B:95:PHE:C	1:B:97:GLU:H	2.29	0.40
1:C:155:VAL:HG22	1:C:164:LEU:HD11	2.04	0.40
1:D:464:GLU:O	1:D:465:ALA:HB3	2.22	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	725/740 (98%)	677 (93%)	42 (6%)	6 (1%)	16	35
1	B	731/740 (99%)	691 (94%)	39 (5%)	1 (0%)	48	72
1	C	721/740 (97%)	673 (93%)	39 (5%)	9 (1%)	10	25
1	D	725/740 (98%)	674 (93%)	45 (6%)	6 (1%)	16	35
All	All	2902/2960 (98%)	2715 (94%)	165 (6%)	22 (1%)	16	35

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	GLU
1	C	90	LEU
1	C	93	SER
1	C	465	ALA
1	D	85	ASN
1	A	92	ASN
1	D	503	MET
1	A	491	LEU
1	C	393	ASP
1	D	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	72	GLN
1	A	714	GLN
1	B	96	ASP
1	C	73	GLU
1	C	463	LYS
1	D	389	ILE
1	C	82	GLU
1	D	150	ASN
1	C	109	PRO
1	A	88	VAL
1	C	742	ILE

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	651/662 (98%)	624 (96%)	27 (4%)	27	54
1	B	658/662 (99%)	633 (96%)	25 (4%)	29	56
1	C	650/662 (98%)	617 (95%)	33 (5%)	21	46
1	D	652/662 (98%)	628 (96%)	24 (4%)	30	57
All	All	2611/2648 (99%)	2502 (96%)	109 (4%)	26	53

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	66	HIS
1	A	73	GLU
1	A	75	ASN
1	A	87	SER
1	A	142	LEU
1	A	283	THR
1	A	295	ILE
1	A	340	LEU
1	A	360	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	375	ILE
1	A	385	CYS
1	A	389	ILE
1	A	390	ASP
1	A	413	ASP
1	A	440	THR
1	A	443	THR
1	A	472	CYS
1	A	482	LEU
1	A	488	ASP
1	A	504	LEU
1	A	547	TYR
1	A	594	ILE
1	A	597	ARG
1	A	598	LEU
1	A	677	GLU
1	A	688	VAL
1	B	57	LEU
1	B	63	ILE
1	B	72	GLN
1	B	96	ASP
1	B	98	PHE
1	B	141	GLN
1	B	164	LEU
1	B	244	GLU
1	B	295	ILE
1	B	316	LEU
1	B	354	VAL
1	B	358	ARG
1	B	385	CYS
1	B	436	LEU
1	B	448	GLU
1	B	452	GLU
1	B	464	GLU
1	B	482	LEU
1	B	514	LEU
1	B	521	GLU
1	B	589	LYS
1	B	594	ILE
1	B	630	SER
1	B	665	VAL
1	B	688	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	67	GLU
1	C	72	GLN
1	C	74	ASN
1	C	77	LEU
1	C	83	TYR
1	C	87	SER
1	C	96	ASP
1	C	129	THR
1	C	143	ILE
1	C	184	ARG
1	C	198	ILE
1	C	239	SER
1	C	295	ILE
1	C	316	LEU
1	C	339	CYS
1	C	354	VAL
1	C	365	THR
1	C	370	SER
1	C	390	ASP
1	C	413	ASP
1	C	415	LEU
1	C	418	ILE
1	C	440	THR
1	C	448	GLU
1	C	464	GLU
1	C	466	LYS
1	C	473	SER
1	C	491	LEU
1	C	546	VAL
1	C	598	LEU
1	C	677	GLU
1	C	688	VAL
1	C	762	CYS
1	D	49	LEU
1	D	60	LEU
1	D	71	LYS
1	D	83	TYR
1	D	97	GLU
1	D	142	LEU
1	D	155	VAL
1	D	180	LEU
1	D	243	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	326	ASP
1	D	327	ILE
1	D	341	VAL
1	D	385	CYS
1	D	389	ILE
1	D	436	LEU
1	D	443	THR
1	D	482	LEU
1	D	498	SER
1	D	501	ASP
1	D	504	LEU
1	D	514	LEU
1	D	517	ILE
1	D	547	TYR
1	D	597	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	119	ASN
1	A	123	GLN
1	A	196	ASN
1	A	281	ASN
1	A	344	GLN
1	A	388	GLN
1	A	505	GLN
1	A	586	GLN
1	A	749	GLN
1	B	51	ASN
1	B	150	ASN
1	B	169	ASN
1	B	229	ASN
1	B	281	ASN
1	B	314	GLN
1	B	508	GLN
1	B	731	GLN
1	B	748	HIS
1	C	72	GLN
1	C	74	ASN
1	C	100	HIS
1	C	229	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	314	GLN
1	C	435	GLN
1	C	450	ASN
1	C	592	HIS
1	D	92	ASN
1	D	112	GLN
1	D	141	GLN
1	D	196	ASN
1	D	227	GLN
1	D	229	ASN
1	D	281	ASN
1	D	430	ASN
1	D	435	GLN
1	D	748	HIS
1	D	761	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

2 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	NAG	E	1	1,2	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.43	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	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	O5-C1-C2	-3.29	106.21	111.29
2	E	1	NAG	C1-C2-N2	3.07	115.27	110.43
2	E	2	NAG	O7-C7-N2	2.35	126.13	121.98
2	E	1	NAG	O4-C4-C3	-2.18	105.25	110.38

There are no chirality outliers.

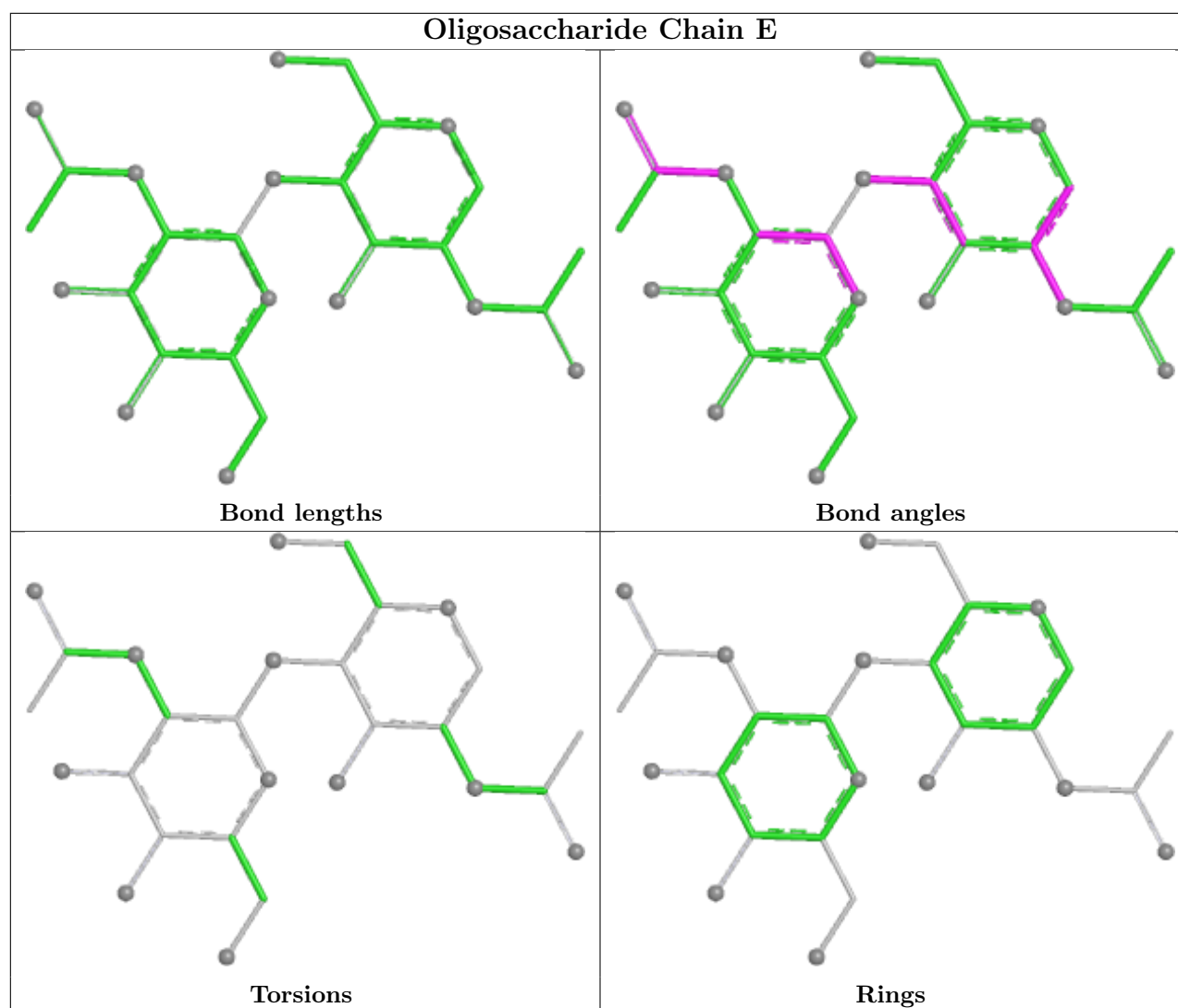
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	2	0
2	E	1	NAG	5	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](#)

19 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	NAG	A	2291	1	14,14,15	0.66	0	17,19,21	1.32	2 (11%)
4	NAG	B	2811	1	14,14,15	0.51	0	17,19,21	0.88	0
4	NAG	B	901	1	14,14,15	0.79	0	17,19,21	2.14	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LUI	A	800	-	29,30,30	0.86	2 (6%)	38,42,42	1.36	4 (10%)
4	NAG	D	1501	1	14,14,15	0.88	0	17,19,21	1.65	3 (17%)
4	NAG	D	2811	1	14,14,15	0.87	0	17,19,21	1.98	4 (23%)
3	LUI	D	800	-	29,30,30	0.84	1 (3%)	38,42,42	1.47	4 (10%)
4	NAG	A	2811	1	14,14,15	0.89	0	17,19,21	1.39	5 (29%)
4	NAG	A	2292	-	14,14,15	0.66	0	17,19,21	1.22	2 (11%)
4	NAG	D	2291	1	14,14,15	0.51	0	17,19,21	2.53	6 (35%)
4	NAG	D	2191	1	14,14,15	0.61	0	17,19,21	1.06	1 (5%)
3	LUI	C	800	-	29,30,30	0.85	1 (3%)	38,42,42	1.33	3 (7%)
4	NAG	B	3211	1	14,14,15	0.72	0	17,19,21	1.32	1 (5%)
4	NAG	A	1501	1	14,14,15	0.68	0	17,19,21	2.04	5 (29%)
3	LUI	B	800	-	29,30,30	0.84	1 (3%)	38,42,42	1.41	3 (7%)
4	NAG	A	3211	1	14,14,15	0.59	0	17,19,21	0.85	0
4	NAG	A	2191	1	14,14,15	0.67	0	17,19,21	0.94	1 (5%)
4	NAG	B	1501	1	14,14,15	0.59	0	17,19,21	1.25	1 (5%)
4	NAG	B	2291	1	14,14,15	0.51	0	17,19,21	1.09	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
4	NAG	A	2291	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	B	901	1	-	1/6/23/26	0/1/1/1
3	LUI	A	800	-	-	4/13/15/15	0/3/3/3
4	NAG	D	1501	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2811	1	-	0/6/23/26	0/1/1/1
3	LUI	D	800	-	-	3/13/15/15	0/3/3/3
4	NAG	A	2811	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2292	-	-	2/6/23/26	0/1/1/1
4	NAG	D	2291	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2191	1	-	0/6/23/26	0/1/1/1
3	LUI	C	800	-	-	2/13/15/15	0/3/3/3
4	NAG	B	3211	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LUI	B	800	-	-	1/13/15/15	0/3/3/3
4	NAG	A	3211	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2291	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	LUI	C7-N8	-2.54	1.34	1.40
3	B	800	LUI	C7-N8	-2.28	1.35	1.40
3	A	800	LUI	C9-N8	-2.23	1.35	1.39
3	C	800	LUI	C7-N8	-2.21	1.35	1.40
3	D	800	LUI	C7-N8	-2.15	1.35	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2291	NAG	C1-O5-C5	7.19	121.82	112.19
3	B	800	LUI	C2-C7-N8	5.02	122.62	115.26
3	D	800	LUI	C2-C7-N8	5.01	122.60	115.26
3	A	800	LUI	C2-C7-N8	4.86	122.38	115.26
3	C	800	LUI	C2-C7-N8	4.74	122.20	115.26
4	B	901	NAG	C4-C3-C2	4.71	117.92	111.02
4	D	2291	NAG	O5-C1-C2	4.63	118.45	111.29
4	D	2811	NAG	O5-C1-C2	4.51	118.27	111.29
3	C	800	LUI	C25-O24-C5	4.46	125.62	117.63
4	B	901	NAG	C1-O5-C5	4.43	118.13	112.19
4	A	1501	NAG	C1-C2-N2	4.35	117.29	110.43
4	D	2811	NAG	C1-C2-N2	-4.16	103.89	110.43
4	B	3211	NAG	C4-C3-C2	4.14	117.08	111.02
4	A	1501	NAG	O5-C1-C2	-3.78	105.44	111.29
4	A	2291	NAG	C3-C4-C5	3.60	116.75	110.23
4	A	1501	NAG	C2-N2-C7	3.41	127.47	122.90
4	B	1501	NAG	C1-O5-C5	3.39	116.73	112.19
4	D	2291	NAG	C1-C2-N2	-3.38	105.11	110.43
4	D	1501	NAG	C2-N2-C7	3.37	127.41	122.90
3	D	800	LUI	C12-C11-C10	-3.33	115.18	120.91
4	D	2811	NAG	C4-C3-C2	3.23	115.75	111.02
4	B	901	NAG	O5-C1-C2	3.19	116.23	111.29
3	B	800	LUI	C12-C11-C10	-3.16	115.47	120.91
4	D	1501	NAG	C1-C2-N2	3.07	115.27	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	800	LUI	C7-N8-C9	-3.03	120.43	123.68
3	A	800	LUI	C12-C11-C10	-3.01	115.72	120.91
4	A	2292	NAG	O5-C1-C2	-2.77	107.00	111.29
4	B	2291	NAG	C1-C2-N2	2.72	114.71	110.43
4	A	1501	NAG	C4-C3-C2	-2.69	107.07	111.02
4	B	901	NAG	O7-C7-C8	-2.69	117.27	122.05
4	A	2811	NAG	C3-C4-C5	2.66	115.05	110.23
3	B	800	LUI	C7-N8-C9	-2.60	120.89	123.68
4	A	1501	NAG	C1-O5-C5	2.53	115.58	112.19
3	A	800	LUI	C7-N8-C9	-2.46	121.05	123.68
4	A	2811	NAG	C1-C2-N2	-2.43	106.61	110.43
4	A	2811	NAG	C4-C3-C2	2.41	114.56	111.02
4	D	2291	NAG	C3-C4-C5	2.40	114.59	110.23
4	D	2811	NAG	C2-N2-C7	2.32	126.01	122.90
3	D	800	LUI	C16-C11-C10	2.30	124.86	120.91
4	A	2811	NAG	C1-O5-C5	2.25	115.21	112.19
4	A	2811	NAG	O5-C1-C2	2.24	114.75	111.29
4	D	2191	NAG	C2-N2-C7	2.22	125.88	122.90
4	D	1501	NAG	O4-C4-C5	2.21	114.77	109.32
4	A	2292	NAG	O7-C7-N2	2.17	125.81	121.98
4	A	2191	NAG	O5-C1-C2	-2.10	108.05	111.29
4	D	2291	NAG	O7-C7-N2	2.07	125.64	121.98
4	D	2291	NAG	O5-C5-C4	2.06	115.83	110.83
4	A	2291	NAG	C1-C2-N2	-2.05	107.20	110.43
3	C	800	LUI	C20-C19-N8	-2.05	109.40	112.38
3	A	800	LUI	C9-C17-N18	-2.03	108.62	113.12

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	800	LUI	O24-C25-C26-N27
4	A	1501	NAG	C3-C2-N2-C7
4	D	1501	NAG	C1-C2-N2-C7
4	B	2811	NAG	O5-C5-C6-O6
4	B	1501	NAG	O5-C5-C6-O6
4	D	1501	NAG	O5-C5-C6-O6
4	B	2811	NAG	C4-C5-C6-O6
4	B	1501	NAG	C4-C5-C6-O6
4	D	1501	NAG	C4-C5-C6-O6
4	A	2292	NAG	C4-C5-C6-O6
4	A	2292	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	2291	NAG	C4-C5-C6-O6
4	A	1501	NAG	C4-C5-C6-O6
4	A	2811	NAG	C4-C5-C6-O6
4	A	1501	NAG	O5-C5-C6-O6
3	A	800	LUI	N8-C19-C20-C21
4	A	2811	NAG	O5-C5-C6-O6
4	B	901	NAG	O5-C5-C6-O6
3	D	800	LUI	N8-C19-C20-C21
4	B	3211	NAG	O5-C5-C6-O6
3	A	800	LUI	N8-C19-C20-C22
4	D	2291	NAG	O5-C5-C6-O6
3	B	800	LUI	O24-C25-C26-O28
4	A	2291	NAG	C4-C5-C6-O6
3	D	800	LUI	N8-C19-C20-C22
3	C	800	LUI	O24-C25-C26-O28
4	B	3211	NAG	C4-C5-C6-O6
3	D	800	LUI	O24-C25-C26-O28
3	A	800	LUI	O24-C25-C26-O28
3	A	800	LUI	C4-C5-O24-C25

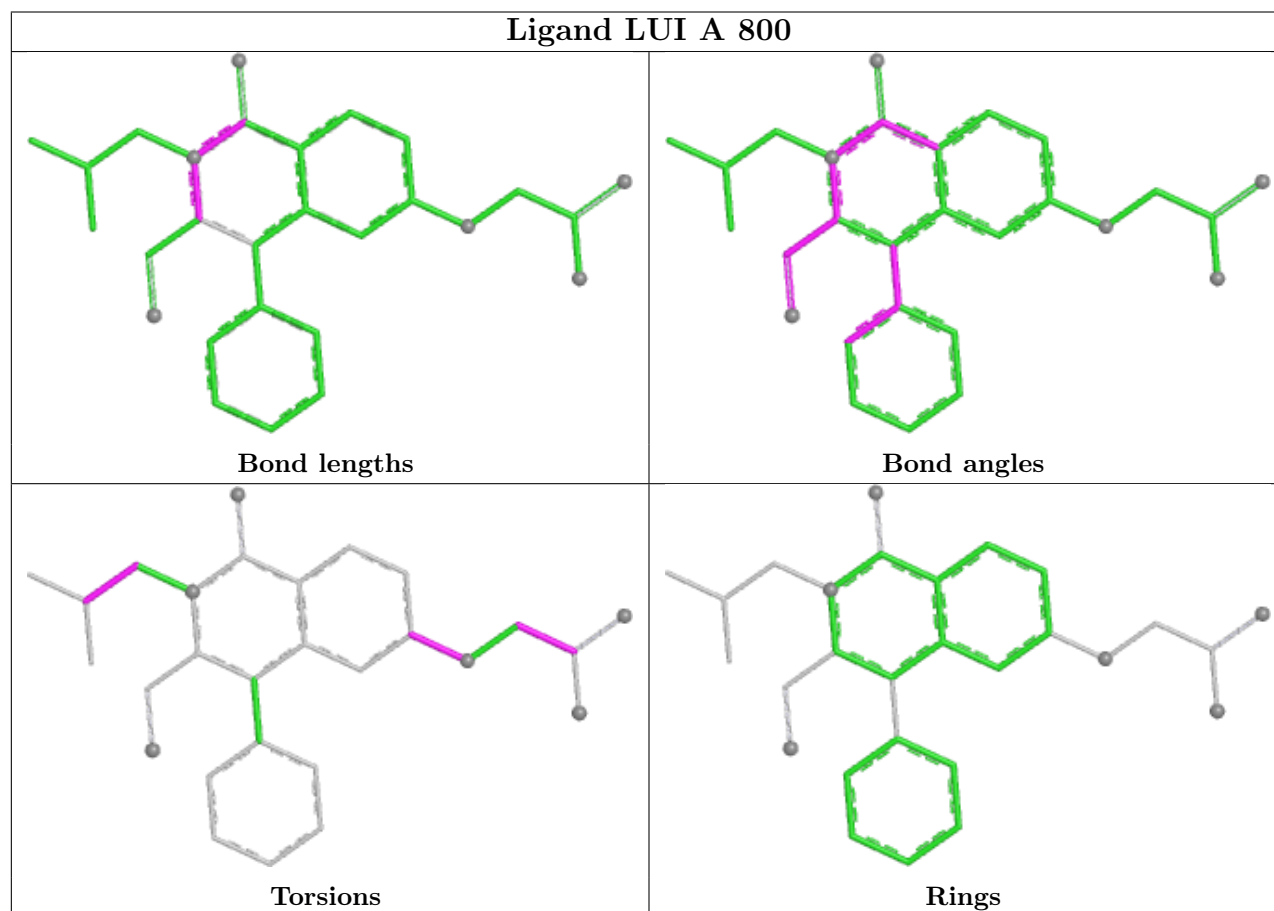
There are no ring outliers.

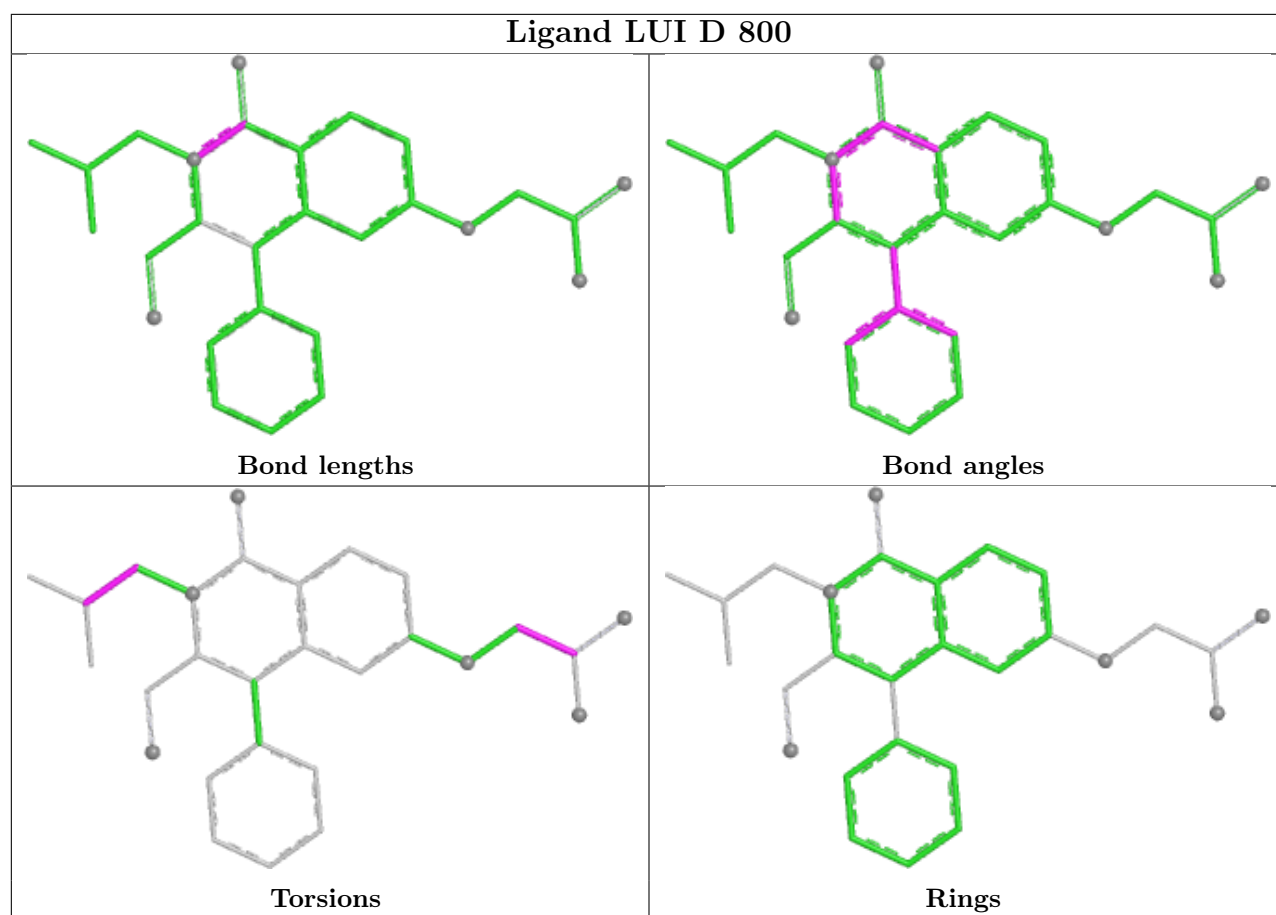
13 monomers are involved in 30 short contacts:

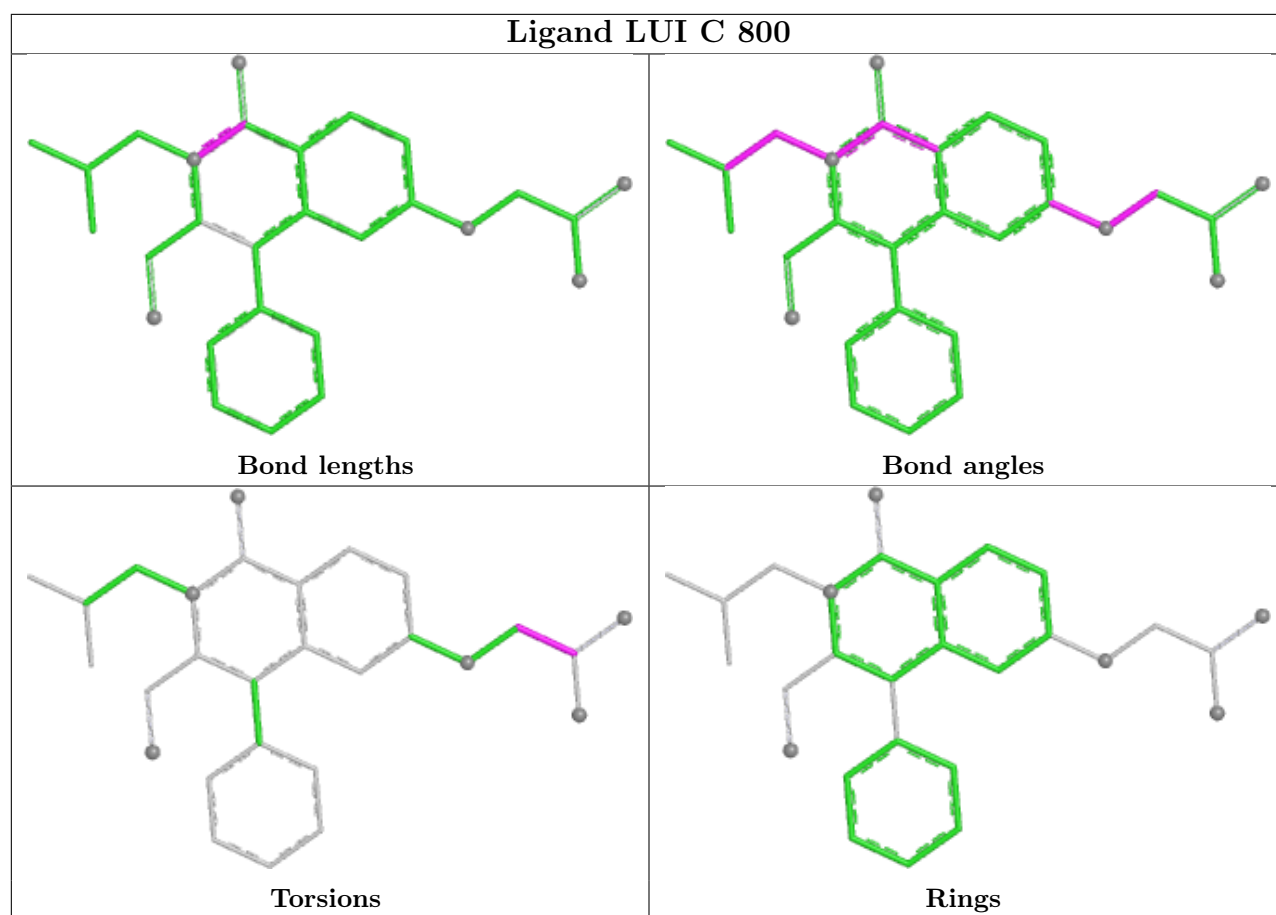
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2291	NAG	3	0
4	B	2811	NAG	2	0
4	B	901	NAG	2	0
4	D	1501	NAG	1	0
4	D	2811	NAG	3	0
4	A	2811	NAG	3	0
4	A	2292	NAG	2	0
4	D	2291	NAG	3	0
4	D	2191	NAG	2	0
3	C	800	LUI	3	0
4	A	3211	NAG	2	0
4	B	1501	NAG	4	0
4	B	2291	NAG	2	0

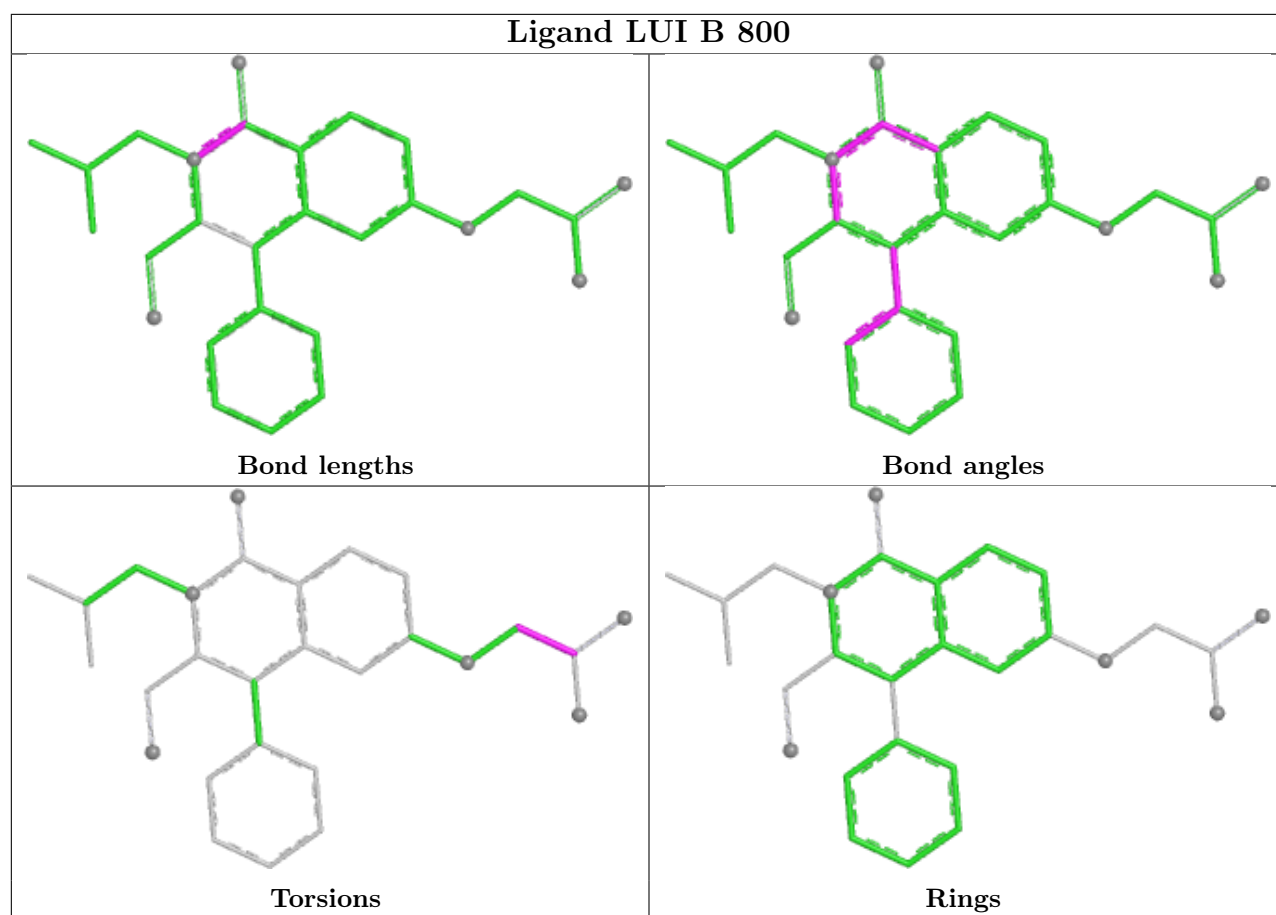
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	727/740 (98%)	-0.23	7 (0%) 79 78	21, 42, 79, 100	0
1	B	733/740 (99%)	-0.22	6 (0%) 82 81	24, 46, 69, 85	0
1	C	725/740 (97%)	0.15	18 (2%) 58 55	25, 61, 101, 122	0
1	D	727/740 (98%)	-0.12	6 (0%) 82 81	24, 47, 91, 117	0
All	All	2912/2960 (98%)	-0.11	37 (1%) 75 73	21, 48, 91, 122	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	3.9
1	C	83	TYR	3.4
1	C	486	VAL	3.3
1	C	348	MET	3.3
1	B	70	TYR	3.1
1	A	81	ALA	3.0
1	C	88	VAL	2.9
1	D	81	ALA	2.9
1	D	102	ILE	2.8
1	A	40	ARG	2.8
1	C	89	PHE	2.8
1	B	338	ASN	2.5
1	C	59	SER	2.5
1	C	105	TYR	2.5
1	A	74	ASN	2.5
1	A	85	ASN	2.4
1	C	279	VAL	2.4
1	B	83	TYR	2.3
1	C	135	TYR	2.3
1	B	486	VAL	2.3
1	D	89	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	2.3
1	B	81	ALA	2.3
1	C	176	ILE	2.2
1	B	95	PHE	2.2
1	C	73	GLU	2.2
1	C	330	TYR	2.2
1	A	73	GLU	2.2
1	D	72	GLN	2.2
1	A	93	SER	2.2
1	C	63	ILE	2.1
1	C	140	ARG	2.1
1	C	100	HIS	2.1
1	C	491	LEU	2.1
1	D	70	TYR	2.1
1	D	87	SER	2.0
1	A	88	VAL	2.0

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

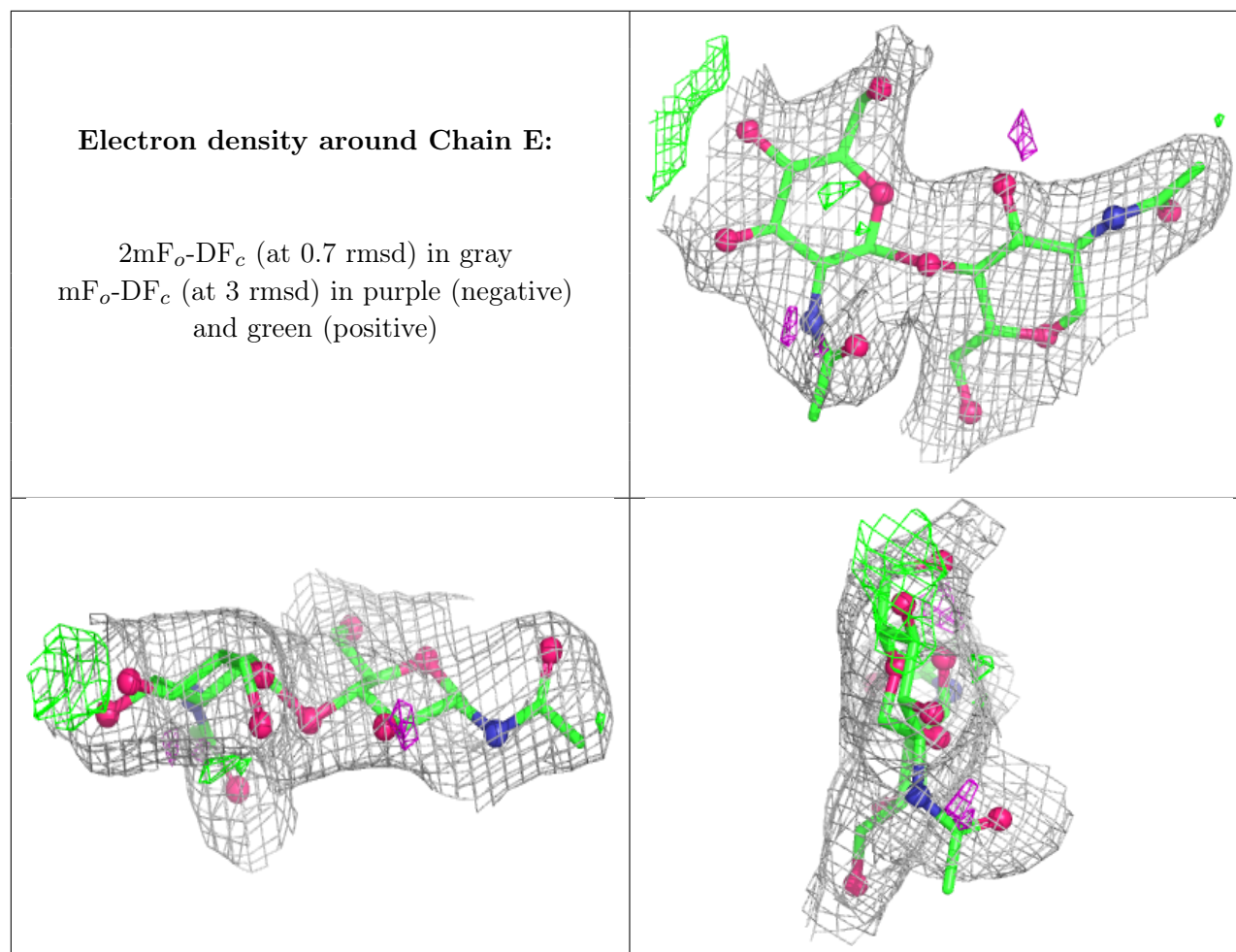
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	E	2	14/15	0.79	0.12	55,55,56,56	0
2	NAG	E	1	14/15	0.90	0.08	42,44,46,46	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 [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($\text{\AA}^2$)	Q<0.9
4	NAG	A	2811	14/15	0.68	0.15	48,51,54,54	0
4	NAG	D	1501	14/15	0.68	0.13	51,53,54,54	0
4	NAG	A	1501	14/15	0.70	0.13	53,55,57,59	0
4	NAG	B	901	14/15	0.73	0.12	53,54,55,55	0
4	NAG	B	3211	14/15	0.75	0.13	55,57,57,58	0
4	NAG	A	2191	14/15	0.77	0.12	53,56,59,60	0
4	NAG	D	2191	14/15	0.78	0.11	51,53,57,58	0
4	NAG	D	2811	14/15	0.78	0.12	52,53,54,54	0
4	NAG	B	1501	14/15	0.82	0.10	50,51,52,52	0
4	NAG	B	2811	14/15	0.82	0.11	51,52,55,55	0
4	NAG	A	2292	14/15	0.84	0.09	50,51,52,52	0

Continued on next page...

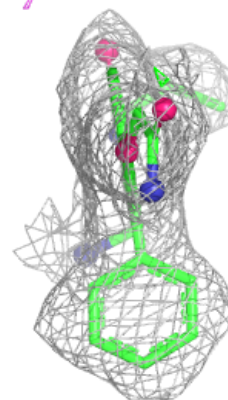
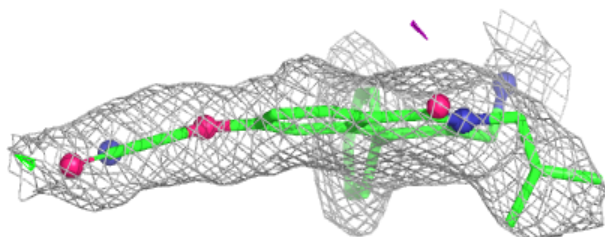
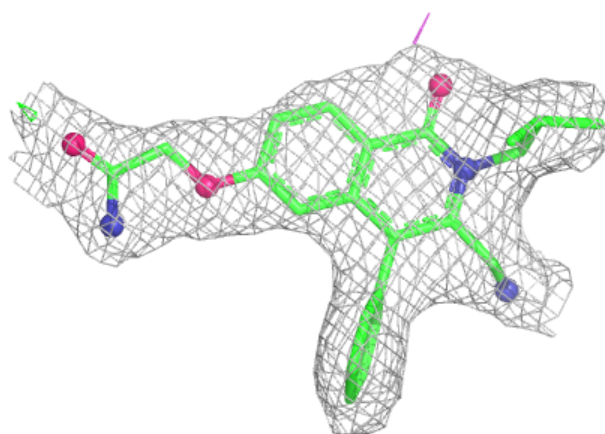
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	D	2291	14/15	0.86	0.10	50,51,53,54	0
4	NAG	B	2291	14/15	0.86	0.10	45,48,49,49	0
4	NAG	A	3211	14/15	0.87	0.11	49,52,54,55	0
4	NAG	A	2291	14/15	0.89	0.11	45,48,50,51	0
3	LUI	D	800	28/28	0.94	0.09	35,38,42,43	0
3	LUI	C	800	28/28	0.94	0.08	39,41,46,47	0
3	LUI	B	800	28/28	0.95	0.08	37,39,40,40	0
3	LUI	A	800	28/28	0.95	0.09	36,40,47,50	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.

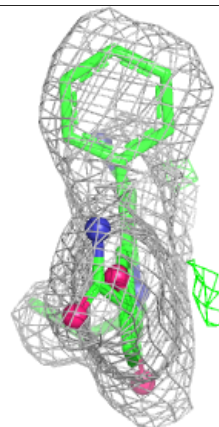
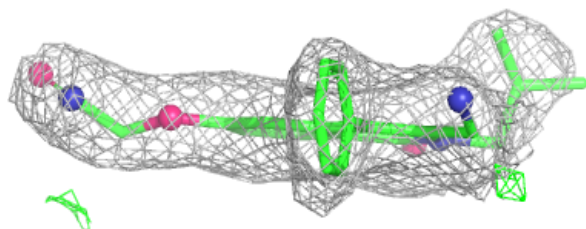
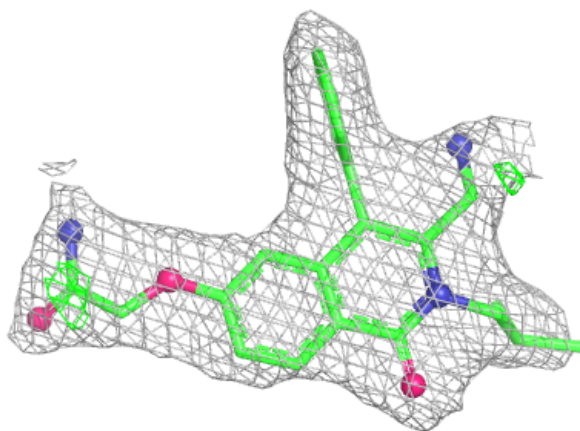
Electron density around LUI D 800:

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

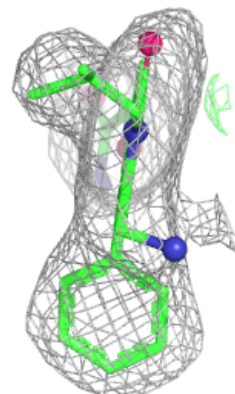
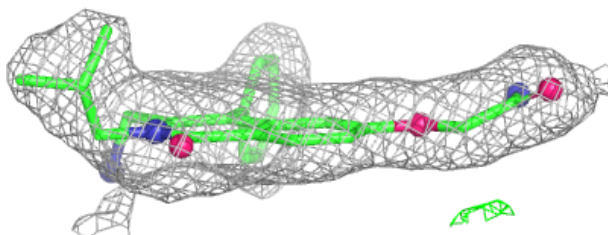
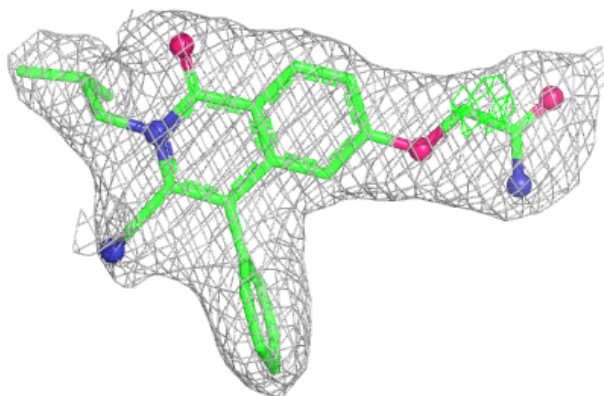


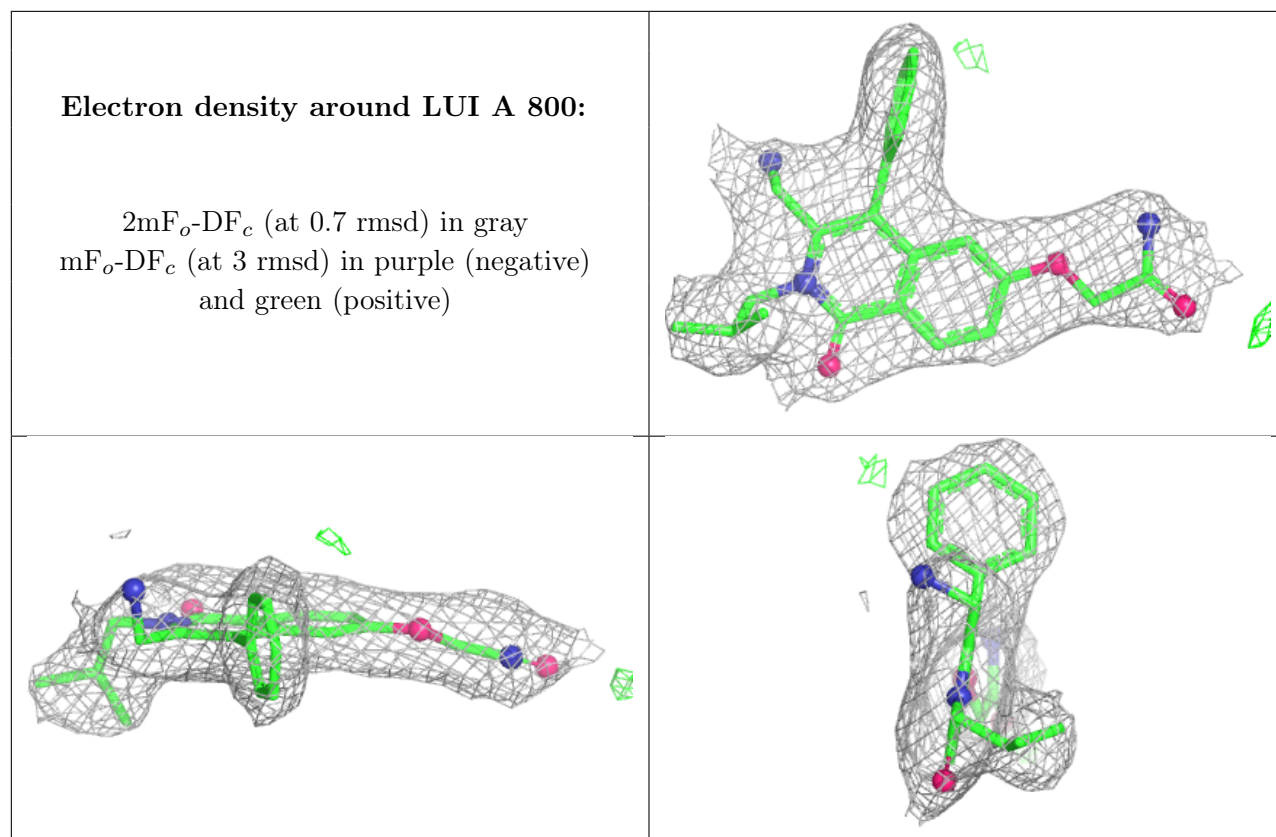
Electron density around LUI C 800:

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

**Electron density around LUI B 800:**

$2mF_o-DF_c$ (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.