



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:26 PM BST

PDB ID : 5ZID
Title : Crystal Structure of human DPP-IV in complex with HL2
Authors : Zhu, L.; Li, H.; Wu, F.
Deposited on : 2018-03-14
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

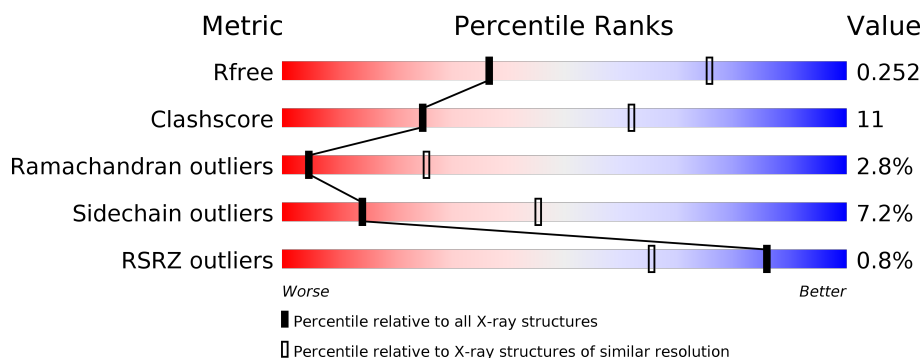
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	734	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	B	734	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>..</div> </div> </div>
2	C	4	<div> <div></div> <div>75%</div> <div>25%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12088 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
			5957	3824	981	1126	26			
1	B	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 14 discrepancies between the modelled and reference sequences:

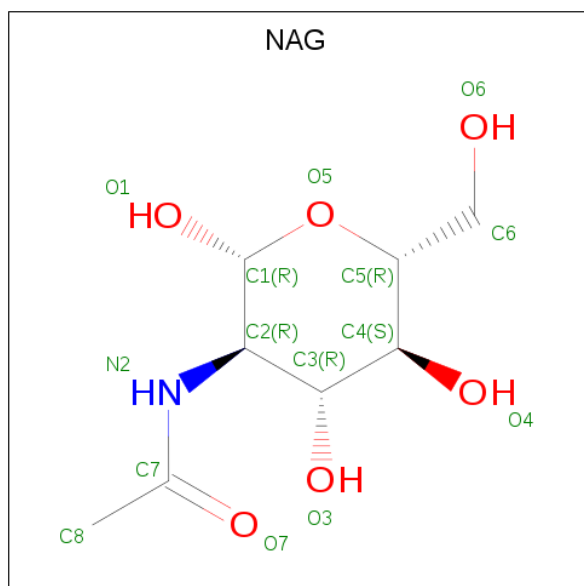
Chain	Residue	Modelled	Actual	Comment	Reference
A	767	GLY	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
B	767	GLY	-	expression tag	UNP P27487
B	768	HIS	-	expression tag	UNP P27487
B	769	HIS	-	expression tag	UNP P27487
B	770	HIS	-	expression tag	UNP P27487
B	771	HIS	-	expression tag	UNP P27487
B	772	HIS	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



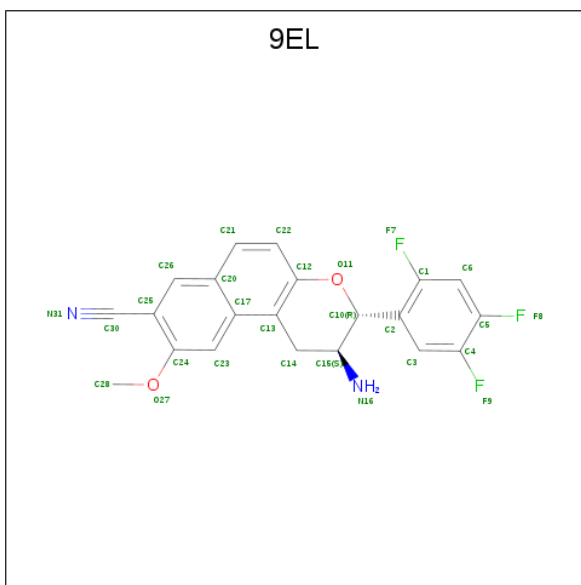
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is (2S,3R)-2-amino-9-methoxy-3-(2,4,5-trifluorophenyl)-2,3-dihydro-1H-naphtho[2,1-b]pyran-8-carbonitrile (three-letter code: 9EL) (formula: $C_{21}H_{15}F_3N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			28	21	3	2	2		
4	B	1	Total	C	F	N	O	0	0
			28	21	3	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	17	Total	O	0	0
			17	17		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:**

Amino Acid	Category	Percentage (%)
Lysine	Lysine	~12%
Isoleucine	Isoleucine	~8%
Methionine	Methionine	~5%
Aspartic Acid	Aspartic Acid	~10%
Glutamic Acid	Glutamic Acid	~10%
Alanine	Alanine	~16%
Valine	Valine	~5%
Proline	Proline	~2%
Glycine	Glycine	~1%
Serine	Serine	~1%
Threonine	Threonine	~1%
Cysteine	Cysteine	~1%
Histidine	Histidine	~1%
Tyrosine	Tyrosine	~1%
Phenylalanine	Phenylalanine	~1%
Tryptophan	Tryptophan	~1%
Selenocysteine	Selenocysteine	~1%

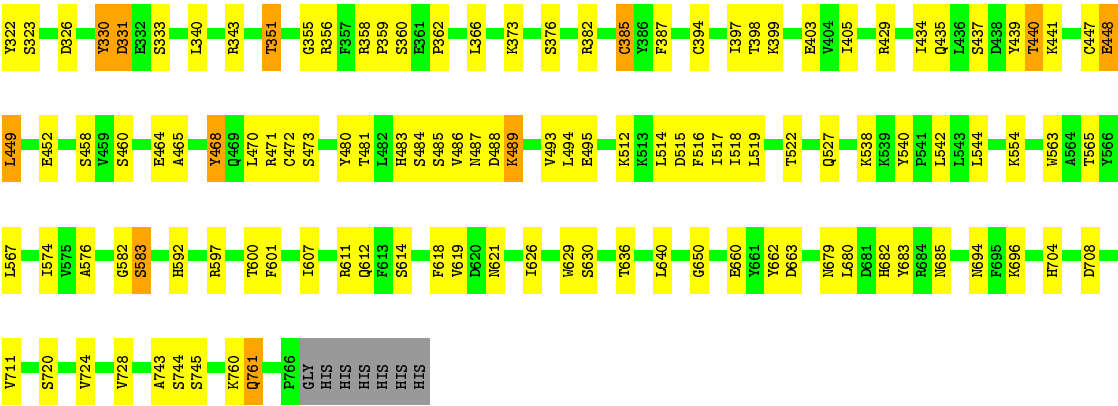
71% 26%

- Chain B:

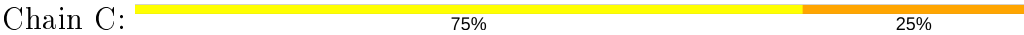
67% 28%

Chain B segments (from left to right):

 - R40
 - Y43
 - L49
 - L57
 - Y68
 - S59
 - L60
 - S64
 - E67
 - Y68
 - L69
 - Y70
 - K71
 - Q72
 - E73
 - N74
 - N75
 - L76
 - L77
 - W78
 - F79
 - N80
 - E81
 - E82
 - Y83
 - S84
 - N85
 - S86
 - S87
 - W88
 - F89
 - L90
 - E91
 - N92
 - S93
 - T94
 - F95
 - D96
 - E97
 - F98
 - G99
 - I102
 - N103
 - S106
 - I107
 - S108
 - P109
 - D110
 - G111
 - Q112
 - F113
 - L114
 - F115



• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.07Å 126.19Å 118.62Å 90.00° 99.30° 90.00°	Depositor
Resolution (Å)	85.82 – 3.00 55.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (85.82-3.00) 91.2 (55.16-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.191 , 0.253 0.201 , 0.252	Depositor DCC
R_{free} test set	1786 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12088	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: NAG, 9EL, MAN

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	0.73	0/6129	0.89	0/8336
1	B	0.72	0/6129	0.89	0/8336
All	All	0.72	0/12258	0.89	0/16672

There are no bond length outliers.

There are no bond angle outliers.

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	5957	0	5679	109	0
1	B	5957	0	5676	145	0
2	C	47	0	40	5	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
4	A	28	0	0	1	0
4	B	28	0	0	0	0
5	A	26	0	0	1	0
5	B	17	0	0	1	0
All	All	12088	0	11421	253	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 11.

All (253) 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:91:GLU:HG2	1:A:94:THR:OG1	1.46	1.15
1:B:77:LEU:HD22	1:B:86:SER:HB3	1.44	0.97
1:B:397:ILE:HD12	1:B:439:TYR:OH	1.74	0.88
1:B:397:ILE:HD12	1:B:439:TYR:CZ	2.11	0.85
1:A:91:GLU:CG	1:A:94:THR:OG1	2.24	0.85
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.59	0.83
1:A:231:THR:HG21	3:A:801:NAG:O6	1.80	0.81
1:B:515:ASP:OD1	1:B:516:PHE:N	2.14	0.81
1:B:272:ASN:C	1:B:272:ASN:OD1	2.18	0.80
1:B:267:LYS:HZ2	2:C:1:NAG:H81	1.47	0.78
1:B:307:THR:HG22	1:B:308:GLN:N	2.00	0.76
1:B:600:THR:OG1	1:B:601:PHE:N	2.20	0.74
1:B:544:LEU:HD12	1:B:576:ALA:O	1.88	0.73
1:B:351:THR:OG1	1:B:592:HIS:ND1	2.21	0.73
1:B:292:SER:O	1:B:317:ARG:NH2	2.22	0.72
1:A:487:ASN:HB3	1:A:489:LYS:HB2	1.72	0.71
1:B:267:LYS:NZ	2:C:1:NAG:H81	2.06	0.71
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.25	0.71
1:B:439:TYR:O	1:B:441:LYS:N	2.26	0.69
1:A:206:GLU:OE2	4:A:802:9EL:N16	2.26	0.69
1:A:630:SER:OG	1:A:740:HIS:NE2	2.25	0.69
1:A:84:GLY:O	1:A:86:SER:N	2.27	0.68
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.76	0.67
1:A:708:ASP:OD2	1:A:740:HIS:HA	1.94	0.67
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.77	0.66
1:B:582:GLY:O	1:B:583:SER:O	2.13	0.66
1:A:91:GLU:HG2	1:A:94:THR:HG1	1.57	0.66
1:B:267:LYS:NZ	2:C:1:NAG:C8	2.58	0.66
1:B:487:ASN:HB2	1:B:489:LYS:HB2	1.77	0.66
1:B:43:TYR:CD2	1:B:565:THR:HG22	2.31	0.65
1:B:481:THR:HG22	1:B:493:VAL:HG22	1.78	0.64
1:B:514:LEU:O	1:B:515:ASP:HB2	1.96	0.64
1:B:60:LEU:C	1:B:60:LEU:HD12	2.18	0.64
1:B:69:LEU:HD22	1:B:78:VAL:HG22	1.79	0.64
1:B:272:ASN:O	1:B:272:ASN:OD1	2.15	0.64
1:B:69:LEU:CD2	1:B:78:VAL:HG22	2.27	0.63
1:B:397:ILE:HG23	1:B:439:TYR:CE1	2.34	0.62
1:A:680:LEU:O	1:A:683:TYR:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:HG13	1:B:166:TYR:HB3	1.79	0.62
1:A:372:TYR:CE2	1:A:386:TYR:CD1	2.88	0.62
1:B:538:LYS:O	1:B:618:PHE:HA	1.99	0.62
1:A:196:ASN:OD1	1:A:227:GLN:HG3	1.99	0.61
1:A:231:THR:CG2	3:A:801:NAG:O6	2.48	0.61
1:A:422:TYR:CE1	1:A:447:CYS:HB3	2.35	0.60
1:A:484:SER:O	1:A:488:ASP:HA	2.01	0.60
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.37	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HB2	2.01	0.59
1:B:307:THR:HG22	1:B:308:GLN:H	1.67	0.59
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.84	0.59
1:B:155:VAL:HG22	1:B:166:TYR:HB2	1.85	0.58
1:B:582:GLY:O	1:B:583:SER:C	2.39	0.58
1:B:307:THR:CG2	1:B:308:GLN:N	2.67	0.58
1:B:468:TYR:CE1	1:B:483:HIS:HB2	2.39	0.57
1:A:702:LEU:HD11	1:A:716:SER:OG	2.04	0.57
1:A:680:LEU:HD21	1:A:684:ARG:NH1	2.20	0.56
1:A:500:LEU:HA	1:A:503:MET:CE	2.35	0.56
1:B:397:ILE:HG22	1:B:434:ILE:HD13	1.86	0.56
1:B:78:VAL:O	1:B:86:SER:O	2.23	0.56
1:A:328:CYS:HA	1:A:338:ASN:O	2.04	0.56
1:A:73:GLU:O	1:A:73:GLU:HG3	2.03	0.56
1:B:448:GLU:O	1:B:449:LEU:C	2.43	0.56
1:B:58:TYR:CZ	1:B:494:LEU:HD22	2.41	0.56
1:B:85:ASN:H	1:B:85:ASN:HD22	1.54	0.56
1:B:125:ARG:O	1:B:125:ARG:HG2	2.07	0.55
1:B:563:TRP:CE2	1:B:567:LEU:HD11	2.41	0.55
1:B:155:VAL:HG22	1:B:166:TYR:CB	2.37	0.55
1:A:94:THR:O	1:A:96:ASP:N	2.40	0.55
1:B:487:ASN:CB	1:B:489:LYS:HB2	2.37	0.54
1:A:310:ARG:NH1	1:A:368:GLY:O	2.40	0.54
1:A:461:PHE:CD1	1:A:468:TYR:HB3	2.42	0.54
1:B:597:ARG:O	1:B:600:THR:HG23	2.07	0.54
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.08	0.54
1:B:540:TYR:HB2	1:B:574:ILE:HD12	1.90	0.53
1:B:80:ASN:HB2	1:B:85:ASN:HB2	1.89	0.53
1:A:170:ASN:ND2	1:A:194:ILE:O	2.40	0.53
1:A:47:ASP:HA	1:A:52:THR:OG1	2.09	0.53
1:A:376:SER:HA	1:A:382:ARG:HA	1.90	0.53
1:B:267:LYS:HZ2	2:C:1:NAG:C8	2.19	0.52
1:B:267:LYS:HZ1	2:C:1:NAG:C8	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.75	0.51
1:A:518:ILE:HA	1:A:522:THR:O	2.11	0.51
1:A:582:GLY:HA2	1:A:594:ILE:HD13	1.92	0.51
1:A:318:ARG:NH2	1:A:668:GLU:OE2	2.42	0.51
1:A:289:ALA:HB1	1:A:290:PRO:HD2	1.93	0.51
1:A:653:VAL:O	1:A:654:ALA:C	2.49	0.51
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.93	0.51
1:A:82:GLU:OE1	1:A:467:TYR:OH	2.25	0.51
1:B:117:GLU:HG3	1:B:132:TYR:CE1	2.46	0.50
1:A:61:ARG:O	1:A:68:TYR:HB2	2.10	0.50
1:B:708:ASP:HB3	1:B:711:VAL:O	2.11	0.50
1:B:286:GLN:HG2	1:B:288:THR:HG22	1.92	0.50
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.47	0.50
1:A:334:SER:O	1:A:336:ARG:N	2.45	0.50
1:A:502:LYS:O	1:A:505:GLN:HG2	2.12	0.50
1:A:532:PRO:O	1:A:533:HIS:C	2.48	0.50
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.94	0.50
1:B:512:LYS:HE3	1:B:527:GLN:OE1	2.12	0.49
1:B:125:ARG:NH2	1:B:205:GLU:OE2	2.45	0.49
1:A:446:SER:HB2	1:A:457:TYR:CZ	2.47	0.49
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.12	0.49
1:A:131:SER:OG	1:A:150:ASN:ND2	2.46	0.49
1:A:91:GLU:O	1:A:92:ASN:C	2.51	0.49
1:B:106:SER:C	1:B:107:ILE:HD12	2.33	0.49
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.93	0.49
1:B:68:TYR:HD1	1:B:69:LEU:O	1.96	0.49
1:A:129:THR:HG23	1:A:151:ASN:HA	1.95	0.48
1:A:166:TYR:CE1	1:A:173:TYR:HB2	2.47	0.48
1:A:461:PHE:CE1	1:A:468:TYR:HB3	2.48	0.48
1:B:230:ASP:OD1	1:B:233:VAL:HG21	2.13	0.48
1:B:626:ILE:HG12	1:B:636:THR:HG23	1.94	0.48
1:A:269:PHE:HA	1:A:285:ILE:O	2.13	0.48
1:A:228:PHE:HA	1:A:265:THR:O	2.13	0.48
1:B:180:LEU:HD12	1:B:181:PRO:HD2	1.94	0.48
1:B:330:TYR:O	1:B:331:ASP:HB2	2.13	0.48
1:B:744:SER:O	1:B:745:SER:C	2.51	0.48
1:A:702:LEU:O	1:A:732:ALA:HA	2.13	0.48
1:B:222:PHE:HA	1:B:272:ASN:HA	1.96	0.48
1:A:187:TRP:CD1	1:A:187:TRP:N	2.82	0.47
1:B:399:LYS:HE3	5:B:909:HOH:O	2.13	0.47
1:A:745:SER:O	1:A:749:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.50	0.47
1:B:517:ILE:HD12	1:B:612:GLN:HG3	1.96	0.47
1:B:78:VAL:O	1:B:86:SER:HA	2.13	0.47
1:A:582:GLY:CA	1:A:594:ILE:HD13	2.43	0.47
1:A:500:LEU:HA	1:A:503:MET:HE3	1.96	0.47
1:B:285:ILE:HG22	1:B:286:GLN:O	2.15	0.47
1:A:291:ALA:O	1:A:295:ILE:HG23	2.15	0.46
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.97	0.46
1:B:439:TYR:O	1:B:440:THR:C	2.52	0.46
1:A:747:ALA:O	1:A:751:ILE:HG22	2.15	0.46
1:A:663:ASP:C	1:A:663:ASP:OD1	2.54	0.46
1:B:299:TYR:CE1	1:B:318:ARG:HA	2.51	0.46
1:B:682:HIS:O	1:B:683:TYR:C	2.54	0.46
1:B:73:GLU:O	1:B:75:ASN:N	2.48	0.46
1:A:449:LEU:O	1:A:450:ASN:HB2	2.15	0.46
1:B:85:ASN:N	1:B:85:ASN:HD22	2.14	0.45
1:A:237:GLU:HA	1:A:252:VAL:O	2.16	0.45
1:A:313:LEU:O	1:A:325:MET:HA	2.17	0.45
1:A:581:ARG:HE	1:A:601:PHE:HB3	1.80	0.45
1:A:752:TYR:O	1:A:756:SER:OG	2.25	0.45
1:A:73:GLU:O	1:A:92:ASN:ND2	2.49	0.45
1:A:745:SER:O	1:A:748:HIS:HB3	2.15	0.45
1:B:614:SER:HA	1:B:619:VAL:HB	1.98	0.45
1:B:82:GLU:HB2	1:B:83:TYR:CD1	2.51	0.45
1:A:140:ARG:HD3	1:A:140:ARG:HA	1.63	0.45
1:A:422:TYR:CE2	1:A:423:LYS:HD2	2.51	0.45
1:B:198:ILE:HA	1:B:211:TYR:O	2.17	0.45
1:B:471:ARG:HG2	1:B:480:TYR:CE2	2.52	0.45
1:B:72:GLN:HG3	1:B:75:ASN:HB3	1.98	0.45
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.98	0.45
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.52	0.45
1:B:468:TYR:CD1	1:B:468:TYR:N	2.85	0.45
1:B:84:GLY:O	1:B:85:ASN:C	2.54	0.45
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.89	0.45
1:A:192:ASP:O	1:A:193:ILE:HD13	2.17	0.45
1:B:203:TYR:CD1	1:B:228:PHE:CE1	3.05	0.45
1:B:694:ASN:C	1:B:696:LYS:N	2.70	0.45
1:A:75:ASN:OD1	1:A:92:ASN:ND2	2.50	0.44
1:B:107:ILE:HD12	1:B:107:ILE:N	2.32	0.44
1:B:172:ILE:HB	1:B:185:ILE:HB	1.99	0.44
1:B:219:ASN:HB3	1:B:308:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:THR:CG2	1:B:308:GLN:H	2.28	0.44
1:B:360:SER:O	1:B:373:LYS:HE2	2.17	0.44
1:A:512:LYS:NZ	1:A:558:VAL:O	2.51	0.44
1:A:714:GLN:HG3	1:B:249:PRO:HG3	1.99	0.44
1:B:257:PRO:O	1:B:663:ASP:HA	2.17	0.44
1:B:435:GLN:HG2	1:B:437:SER:OG	2.18	0.44
1:B:144:THR:O	1:B:147:ARG:HG2	2.17	0.44
1:B:113:PHE:CE2	1:B:178:PRO:CG	3.01	0.44
1:A:98:PHE:CD2	1:A:102:ILE:HD11	2.52	0.44
1:B:64:SER:OG	1:B:67:GLU:N	2.50	0.44
1:A:51:ASN:OD1	1:A:54:ARG:HG2	2.17	0.44
1:B:108:SER:O	1:B:111:GLY:N	2.46	0.44
1:A:186:THR:C	1:A:187:TRP:CD1	2.91	0.44
1:B:331:ASP:OD1	1:B:333:SER:OG	2.33	0.44
1:B:258:LYS:HA	1:B:662:TYR:O	2.18	0.44
1:B:468:TYR:CE1	1:B:483:HIS:CB	3.01	0.44
1:B:382:ARG:HG3	1:B:403:GLU:OE2	2.17	0.43
1:A:455:GLN:HG3	1:A:475:PRO:HD2	2.00	0.43
1:A:496:ASP:OD2	1:A:498:SER:HB3	2.18	0.43
1:B:397:ILE:CD1	1:B:439:TYR:OH	2.57	0.43
1:A:85:ASN:OD1	1:A:85:ASN:O	2.36	0.43
1:A:321:ASN:ND2	5:A:901:HOH:O	2.51	0.43
1:B:518:ILE:O	1:B:519:LEU:HD23	2.18	0.43
1:B:607:ILE:HG22	1:B:611:ARG:HD2	2.00	0.43
1:B:77:LEU:CD2	1:B:86:SER:HB3	2.29	0.43
1:B:93:SER:O	1:B:95:PHE:N	2.44	0.43
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.94	0.43
1:A:149:PRO:O	1:A:152:THR:OG1	2.36	0.43
1:A:230:ASP:O	1:A:231:THR:C	2.57	0.42
1:A:514:LEU:HD12	1:A:526:TYR:O	2.19	0.42
1:A:57:LEU:HA	1:A:480:TYR:CE1	2.54	0.42
1:B:405:ILE:HG13	1:B:429:ARG:HD2	2.00	0.42
1:B:607:ILE:O	1:B:611:ARG:HG3	2.19	0.42
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.01	0.42
1:B:102:ILE:CG2	1:B:103:ASN:N	2.82	0.42
1:B:154:TRP:C	1:B:155:VAL:CG2	2.87	0.42
1:A:430:ASN:OD1	1:A:446:SER:OG	2.28	0.42
1:B:330:TYR:O	1:B:331:ASP:CB	2.67	0.42
1:B:74:ASN:CB	1:B:92:ASN:HB2	2.50	0.42
1:A:66:HIS:C	1:A:67:GLU:HG3	2.39	0.42
1:B:154:TRP:C	1:B:155:VAL:HG23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.90	0.42
1:B:304:THR:HG21	1:B:362:PRO:HG2	2.01	0.42
1:A:94:THR:C	1:A:96:ASP:H	2.23	0.42
1:B:158:SER:HA	1:B:216:TRP:CD1	2.55	0.42
1:B:356:ARG:CZ	1:B:382:ARG:HD2	2.50	0.42
1:A:219:ASN:OD1	1:A:308:GLN:OE1	2.38	0.42
1:B:154:TRP:O	1:B:155:VAL:HG22	2.20	0.42
1:B:243:ASP:O	1:B:244:GLU:C	2.58	0.42
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.02	0.42
1:B:72:GLN:NE2	1:B:73:GLU:O	2.53	0.42
1:A:482:LEU:C	1:A:483:HIS:CD2	2.94	0.41
1:B:387:PHE:CZ	1:B:394:CYS:HB3	2.53	0.41
1:B:290:PRO:HD2	1:B:315:TRP:CD1	2.54	0.41
1:B:464:GLU:O	1:B:465:ALA:HB3	2.20	0.41
1:A:221:THR:O	1:A:273:THR:HB	2.20	0.41
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.85	0.41
1:B:136:ASP:OD2	1:B:139:LYS:HD3	2.21	0.41
1:A:546:VAL:HG12	1:A:547:TYR:N	2.35	0.41
1:B:518:ILE:C	1:B:519:LEU:HD23	2.41	0.41
1:B:69:LEU:O	1:B:70:TYR:HB2	2.20	0.41
1:A:316:LEU:HD12	1:A:317:ARG:N	2.35	0.41
1:B:106:SER:O	1:B:114:ILE:HA	2.21	0.41
1:B:116:LEU:O	1:B:132:TYR:HA	2.21	0.41
1:B:760:LYS:O	1:B:761:GLN:C	2.57	0.41
1:A:340:LEU:O	1:A:341:VAL:C	2.59	0.41
1:B:154:TRP:O	1:B:155:VAL:CG2	2.69	0.41
1:B:355:GLY:HA3	1:B:358:ARG:O	2.20	0.41
1:B:88:VAL:HG12	1:B:88:VAL:O	2.21	0.41
1:A:642:SER:OG	1:A:644:SER:HB3	2.21	0.41
1:A:638:MET:HE3	1:A:691:ARG:CZ	2.51	0.41
1:A:753:THR:O	1:A:756:SER:HB2	2.21	0.41
1:B:397:ILE:HD13	1:B:397:ILE:N	2.36	0.41
1:B:80:ASN:CB	1:B:85:ASN:HB2	2.50	0.41
1:A:524:PHE:CD1	1:A:580:GLY:HA2	2.56	0.40
1:A:600:THR:OG1	1:A:601:PHE:N	2.54	0.40
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.56	0.40
1:A:630:SER:OG	1:A:740:HIS:CE1	2.74	0.40
1:A:733:MET:HG3	1:A:734:TRP:O	2.21	0.40
1:B:720:SER:O	1:B:724:VAL:HG23	2.21	0.40
1:B:743:ALA:O	1:B:744:SER:C	2.58	0.40
1:B:484:SER:O	1:B:488:ASP:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.83	0.40
1:B:679:ASN:O	1:B:680:LEU:C	2.59	0.40
1:A:112:GLN:HB2	1:A:113:PHE:CD1	2.57	0.40
1:B:60:LEU:C	1:B:60:LEU:CD1	2.88	0.40
1:B:68:TYR:CE1	1:B:79:PHE:CD1	3.08	0.40
1:A:139:LYS:O	1:A:140:ARG:C	2.59	0.40
1:A:206:GLU:CD	1:A:666:TYR:HB2	2.41	0.40
1:A:88:VAL:HG12	1:A:88:VAL:O	2.20	0.40
1:B:124:TRP:CE3	1:B:124:TRP:HA	2.56	0.40
1:B:195:TYR:HB2	1:B:228:PHE:HB2	2.03	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	725/734 (99%)	646 (89%)	62 (9%)	17 (2%)	6	30
1	B	725/734 (99%)	621 (86%)	81 (11%)	23 (3%)	4	22
All	All	1450/1468 (99%)	1267 (87%)	143 (10%)	40 (3%)	5	25

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	93	SER
1	A	281	ASN
1	A	335	GLY
1	A	520	ASN
1	B	330	TYR
1	B	331	ASP
1	B	440	THR

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Mol	Chain	Res	Type
1	B	621	ASN
1	A	95	PHE
1	A	242	SER
1	A	450	ASN
1	A	714	GLN
1	B	74	ASN
1	B	87	SER
1	B	124	TRP
1	B	281	ASN
1	B	583	SER
1	A	146	GLU
1	B	70	TYR
1	B	85	ASN
1	B	94	THR
1	B	97	GLU
1	B	221	THR
1	B	366	LEU
1	A	191	GLU
1	A	63	ILE
1	A	140	ARG
1	A	231	THR
1	A	621	ASN
1	B	146	GLU
1	B	242	SER
1	B	322	TYR
1	B	447	CYS
1	B	449	LEU
1	B	452	GLU
1	A	690	SER
1	B	88	VAL
1	A	207	VAL
1	B	109	PRO

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	652/658 (99%)	614 (94%)	38 (6%)	20	55
1	B	652/658 (99%)	596 (91%)	56 (9%)	10	37
All	All	1304/1316 (99%)	1210 (93%)	94 (7%)	14	45

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	75	ASN
1	A	83	TYR
1	A	90	LEU
1	A	94	THR
1	A	97	GLU
1	A	106	SER
1	A	144	THR
1	A	160	VAL
1	A	182	SER
1	A	188	THR
1	A	212	SER
1	A	217	SER
1	A	273	THR
1	A	279	VAL
1	A	283	THR
1	A	309	GLU
1	A	312	SER
1	A	317	ARG
1	A	323	SER
1	A	326	ASP
1	A	336	ARG
1	A	366	LEU
1	A	385	CYS
1	A	442	VAL
1	A	448	GLU
1	A	458	SER
1	A	484	SER
1	A	486	VAL
1	A	489	LYS
1	A	505	GLN
1	A	511	SER
1	A	518	ILE
1	A	529	ILE
1	A	627	TRP

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Mol	Chain	Res	Type
1	A	649	CYS
1	A	662	TYR
1	A	745	SER
1	B	40	ARG
1	B	57	LEU
1	B	71	LYS
1	B	72	GLN
1	B	82	GLU
1	B	83	TYR
1	B	85	ASN
1	B	97	GLU
1	B	108	SER
1	B	109	PRO
1	B	129	THR
1	B	141	GLN
1	B	144	THR
1	B	145	GLU
1	B	147	ARG
1	B	160	VAL
1	B	179	ASN
1	B	182	SER
1	B	188	THR
1	B	202	VAL
1	B	211	TYR
1	B	212	SER
1	B	230	ASP
1	B	242	SER
1	B	250	LYS
1	B	256	TYR
1	B	272	ASN
1	B	279	VAL
1	B	302	ASP
1	B	312	SER
1	B	323	SER
1	B	326	ASP
1	B	351	THR
1	B	359	PRO
1	B	376	SER
1	B	385	CYS
1	B	398	THR
1	B	448	GLU
1	B	458	SER

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Mol	Chain	Res	Type
1	B	460	SER
1	B	468	TYR
1	B	472	CYS
1	B	473	SER
1	B	485	SER
1	B	486	VAL
1	B	489	LYS
1	B	495	GLU
1	B	522	THR
1	B	542	LEU
1	B	554	LYS
1	B	629	TRP
1	B	630	SER
1	B	660	GLU
1	B	685	ASN
1	B	704	HIS
1	B	761	GLN

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

Mol	Chain	Res	Type
1	A	85	ASN
1	A	92	ASN
1	A	150	ASN
1	A	595	ASN
1	A	748	HIS
1	B	85	ASN
1	B	487	ASN
1	B	621	ASN
1	B	697	GLN
1	B	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](#)

4 non-standard protein/DNA/RNA residues 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	MAN	C	3	2	11,11,12	0.52	0	15,15,17	1.19	3 (20%)
2	MAN	C	2	2	11,11,12	0.95	0	15,15,17	1.72	2 (13%)
3	NAG	B	801	1	14,14,15	0.58	0	17,19,21	1.83	4 (23%)
3	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	2	2	-	2/2/19/22	0/1/1/1
3	NAG	B	801	1	-	2/6/23/26	0/1/1/1
3	NAG	A	801	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MAN	C1-C2-C3	5.70	116.67	109.67
3	B	801	NAG	O5-C5-C6	4.56	114.35	107.20
3	B	801	NAG	C4-C3-C2	3.96	116.82	111.02
3	B	801	NAG	O5-C1-C2	-2.68	107.06	111.29
2	C	3	MAN	O5-C5-C6	2.58	111.24	107.20
2	C	3	MAN	C1-O5-C5	2.57	115.67	112.19
2	C	2	MAN	O5-C5-C4	-2.45	104.87	110.83
2	C	3	MAN	C1-C2-C3	2.25	112.43	109.67
3	B	801	NAG	O4-C4-C5	2.16	114.67	109.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	B	801	NAG	O5-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
2	C	2	MAN	C4-C5-C6-O6
2	C	2	MAN	O5-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6
3	B	801	NAG	C4-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	NAG	2	0

5.5 Carbohydrates

4 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	C	1	1,2	14,14,15	0.55	0	17,19,21	1.33	3 (17%)
2	MAN	C	2	2	11,11,12	0.95	0	15,15,17	1.72	2 (13%)
2	MAN	C	3	2	11,11,12	0.52	0	15,15,17	1.19	3 (20%)
2	MAN	C	4	2	11,11,12	0.62	0	15,15,17	1.19	3 (20%)

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	C	1	1,2	-	3/6/23/26	0/1/1/1
2	MAN	C	2	2	-	2/2/19/22	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MAN	C1-C2-C3	5.70	116.67	109.67
2	C	3	MAN	O5-C5-C6	2.58	111.24	107.20
2	C	3	MAN	C1-O5-C5	2.57	115.67	112.19
2	C	1	NAG	C8-C7-N2	2.56	120.44	116.10
2	C	4	MAN	C1-O5-C5	2.46	115.52	112.19
2	C	2	MAN	O5-C5-C4	-2.45	104.87	110.83
2	C	1	NAG	C1-O5-C5	2.33	115.35	112.19
2	C	4	MAN	C3-C4-C5	2.31	114.35	110.24
2	C	1	NAG	O5-C1-C2	-2.26	107.71	111.29
2	C	3	MAN	C1-C2-C3	2.25	112.43	109.67
2	C	4	MAN	O5-C1-C2	-2.16	107.44	110.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

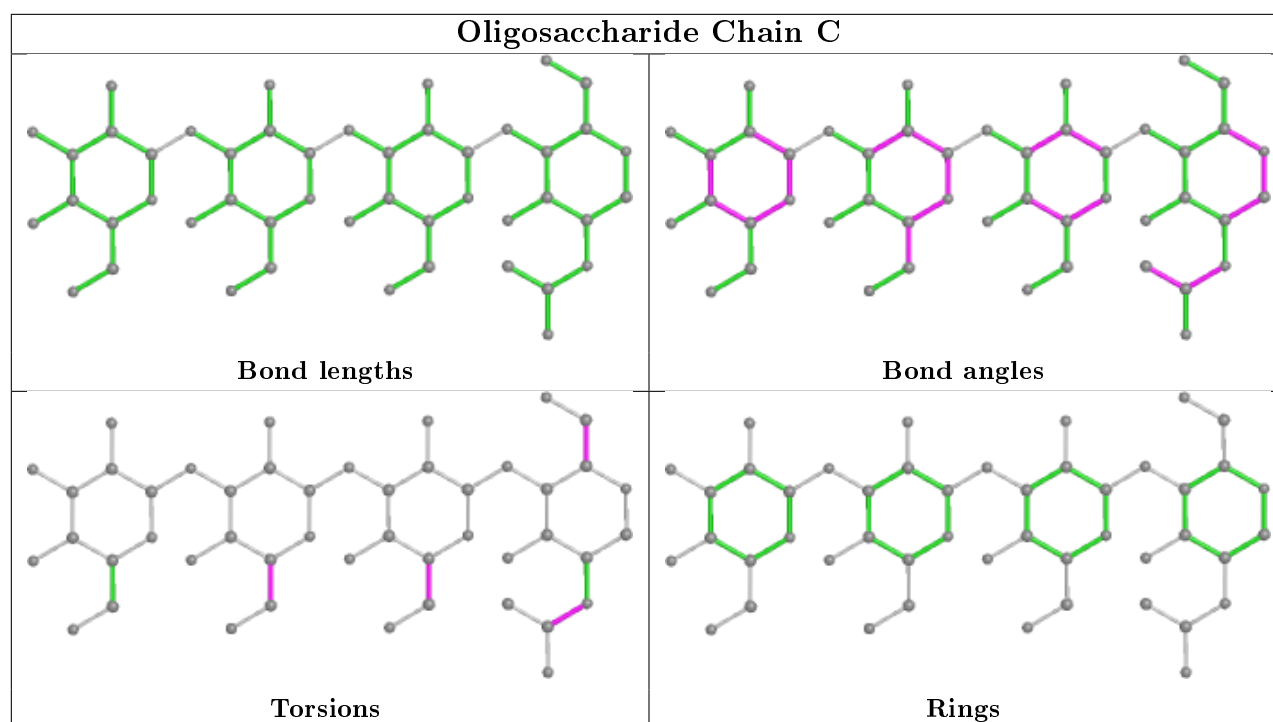
Mol	Chain	Res	Type	Atoms
2	C	2	MAN	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	MAN	O5-C5-C6-O6
2	C	3	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	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](#)

4 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	9EL	A	802	-	31,31,31	2.99	8 (25%)	43,46,46	1.76	10 (23%)
3	NAG	B	801	1	14,14,15	0.58	0	17,19,21	1.83	4 (23%)
3	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.61	0
4	9EL	B	806	-	31,31,31	3.05	9 (29%)	43,46,46	1.83	7 (16%)

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	9EL	A	802	-	-	1/8/20/20	0/4/4/4
3	NAG	B	801	1	-	2/6/23/26	0/1/1/1
3	NAG	A	801	1	-	4/6/23/26	0/1/1/1
4	9EL	B	806	-	-	1/8/20/20	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	9EL	C25-C30	-12.92	1.24	1.44
4	B	806	9EL	C25-C30	-12.35	1.25	1.44
4	A	802	9EL	C12-C13	6.73	1.49	1.38
4	B	806	9EL	C12-C13	5.61	1.47	1.38
4	B	806	9EL	C17-C20	4.22	1.50	1.43
4	B	806	9EL	C25-C24	3.98	1.48	1.40
4	B	806	9EL	O11-C10	-3.97	1.39	1.45
4	B	806	9EL	C13-C17	3.79	1.49	1.43
4	A	802	9EL	C17-C20	3.13	1.48	1.43
4	A	802	9EL	C25-C24	3.11	1.47	1.40
4	B	806	9EL	C2-C10	-2.97	1.45	1.51
4	A	802	9EL	C13-C17	2.95	1.48	1.43
4	A	802	9EL	O11-C10	-2.57	1.41	1.45
4	A	802	9EL	C2-C10	-2.56	1.46	1.51
4	B	806	9EL	C3-C4	2.31	1.41	1.37
4	B	806	9EL	C10-C15	-2.29	1.50	1.53
4	A	802	9EL	C23-C24	2.27	1.40	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	806	9EL	C3-C2-C1	5.69	121.21	116.48
4	B	806	9EL	C28-O27-C24	5.64	126.04	117.53
4	A	802	9EL	C13-C17-C20	-5.03	114.06	119.65
3	B	801	NAG	O5-C5-C6	4.56	114.35	107.20
4	B	806	9EL	C6-C1-C2	-4.23	118.77	123.83
3	B	801	NAG	C4-C3-C2	3.96	116.82	111.02
4	A	802	9EL	C3-C2-C1	3.58	119.46	116.48
4	A	802	9EL	C28-O27-C24	3.56	122.91	117.53
4	A	802	9EL	C21-C20-C26	-2.85	116.99	122.02
4	B	806	9EL	C13-C17-C20	-2.76	116.58	119.65
3	B	801	NAG	O5-C1-C2	-2.68	107.06	111.29
4	B	806	9EL	O11-C12-C22	2.54	120.81	116.29
4	A	802	9EL	C21-C20-C17	2.32	122.17	119.12
4	A	802	9EL	C25-C26-C20	-2.31	118.01	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	9EL	F7-C1-C6	2.27	123.14	118.61
4	B	806	9EL	O11-C12-C13	-2.24	118.39	122.39
3	B	801	NAG	O4-C4-C5	2.16	114.67	109.30
4	A	802	9EL	C6-C1-C2	-2.15	121.26	123.83
4	A	802	9EL	C26-C25-C30	-2.15	116.47	120.06
4	A	802	9EL	C26-C25-C24	2.11	122.86	119.43
4	B	806	9EL	C3-C4-C5	-2.05	118.69	121.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

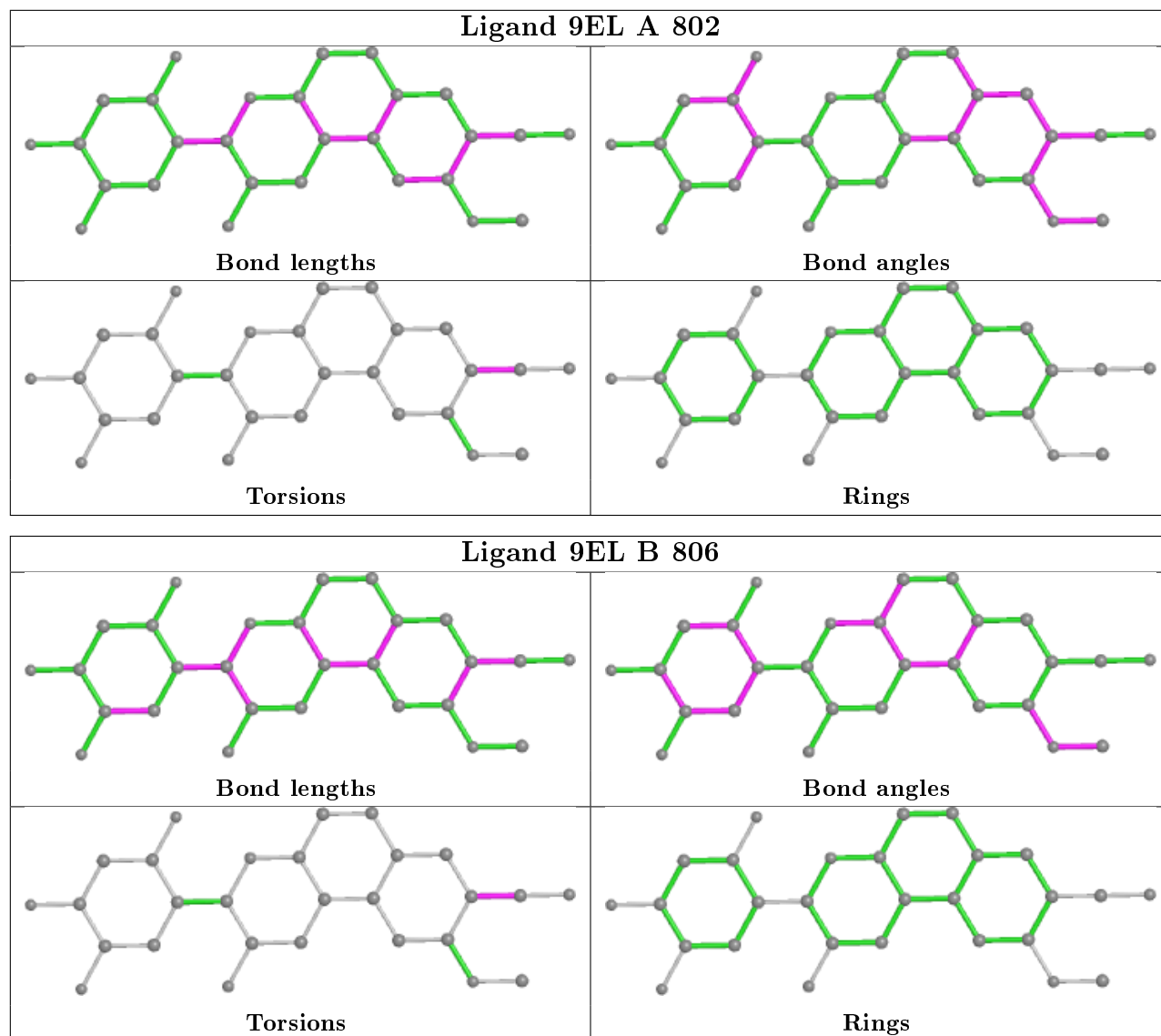
Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
4	B	806	9EL	C24-C25-C30-N31
3	B	801	NAG	O5-C5-C6-O6
3	A	801	NAG	O5-C5-C6-O6
3	A	801	NAG	C4-C5-C6-O6
3	B	801	NAG	C4-C5-C6-O6
4	A	802	9EL	C26-C25-C30-N31

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	9EL	1	0
3	A	801	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	727/734 (99%)	-0.37	4 (0%) 89 72	10, 27, 56, 92	2 (0%)
1	B	727/734 (99%)	-0.33	7 (0%) 82 59	11, 28, 62, 109	1 (0%)
All	All	1454/1468 (99%)	-0.35	11 (0%) 86 65	10, 27, 60, 109	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	SER	6.6
1	B	74	ASN	3.8
1	A	96	ASP	3.5
1	A	100	HIS	3.3
1	B	99	GLY	3.0
1	B	73	GLU	2.4
1	B	98	PHE	2.4
1	B	75	ASN	2.2
1	A	92	ASN	2.1
1	A	93	SER	2.1
1	B	96	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	MAN	C	3	11/12	0.70	0.35	54,56,57,59	0
3	NAG	A	801	14/15	0.80	0.30	32,33,35,41	0
3	NAG	B	801	14/15	0.82	0.31	40,54,64,64	0

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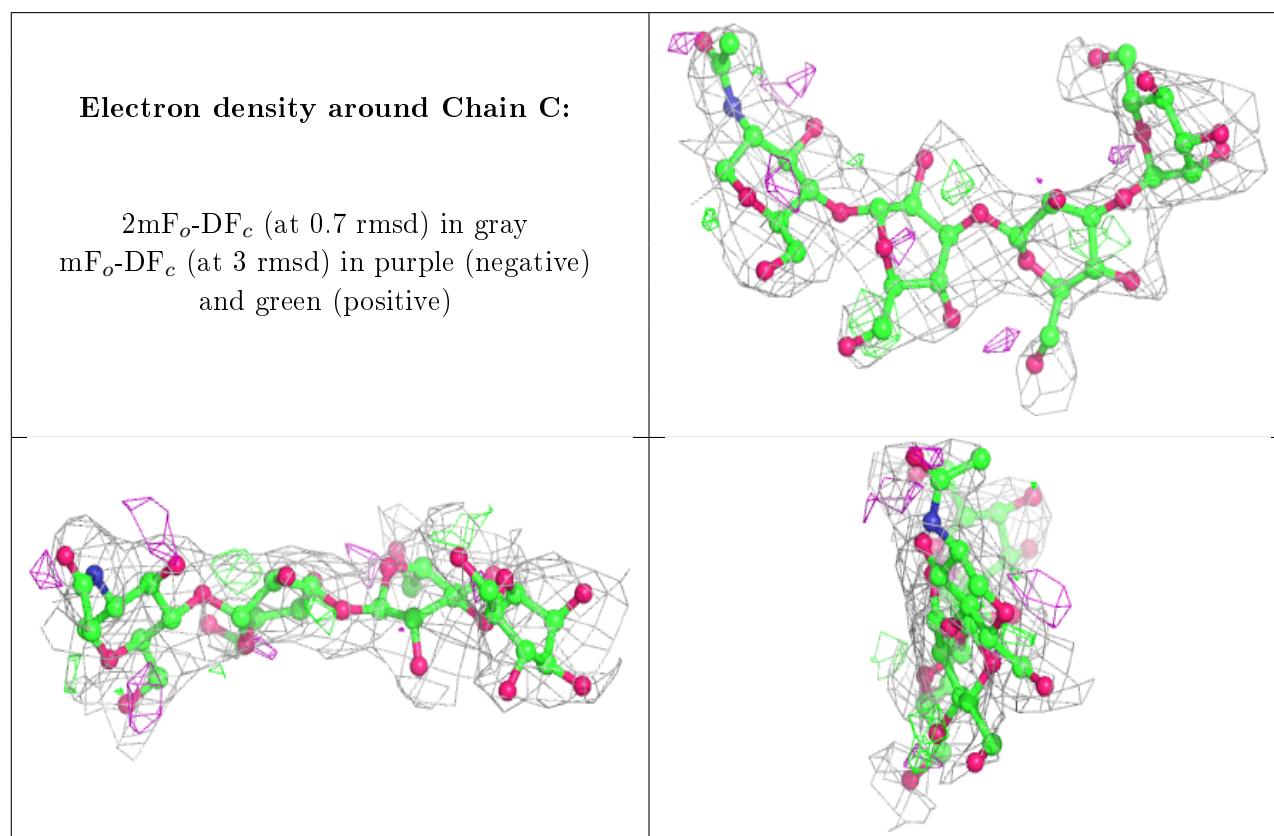
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	C	2	11/12	0.83	0.29	46,48,52,53	0

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(\AA^2)	Q<0.9
2	MAN	C	4	11/12	0.70	0.35	58,59,60,60	0
2	MAN	C	3	11/12	0.70	0.35	54,56,57,59	0
2	MAN	C	2	11/12	0.83	0.29	46,48,52,53	0
2	NAG	C	1	14/15	0.85	0.27	36,39,42,44	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.

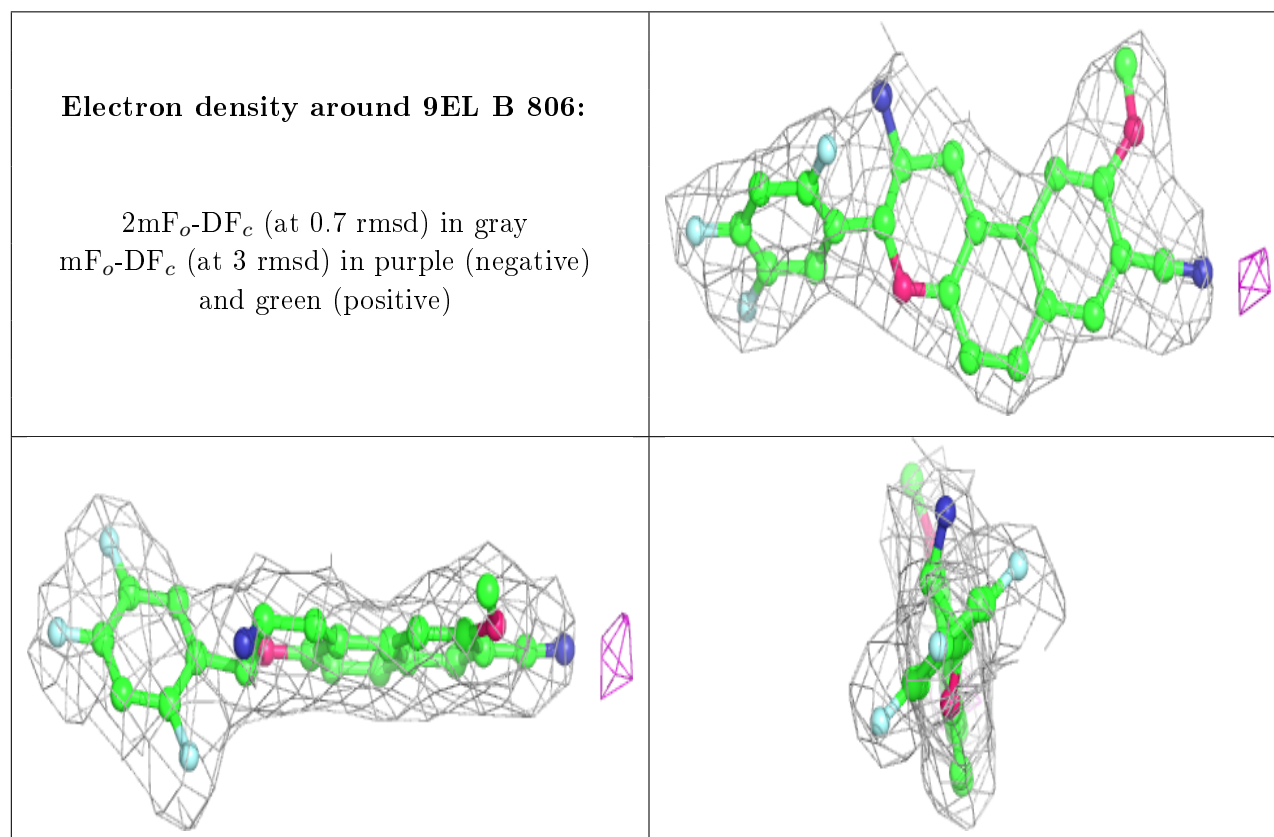


6.4 Ligands [i](#)

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.

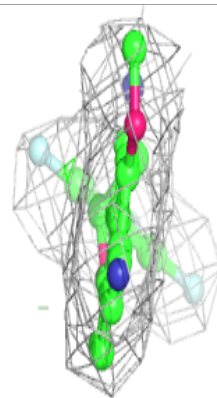
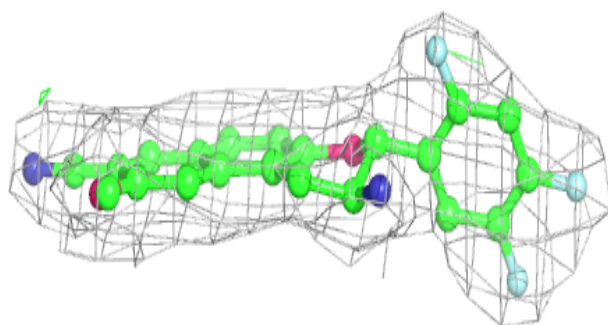
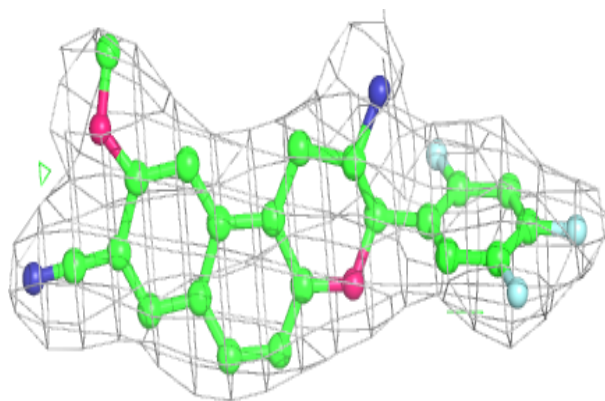
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	801	14/15	0.80	0.30	32,33,35,41	0
3	NAG	B	801	14/15	0.82	0.31	40,54,64,64	0
4	9EL	B	806	28/28	0.97	0.17	19,21,23,25	0
4	9EL	A	802	28/28	0.98	0.17	16,19,25,30	0

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 9EL A 802:

$2mF_o-DF_c$ (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.