



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:59 PM UTC

PDB ID : 5ZID / pdb_00005zid
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 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

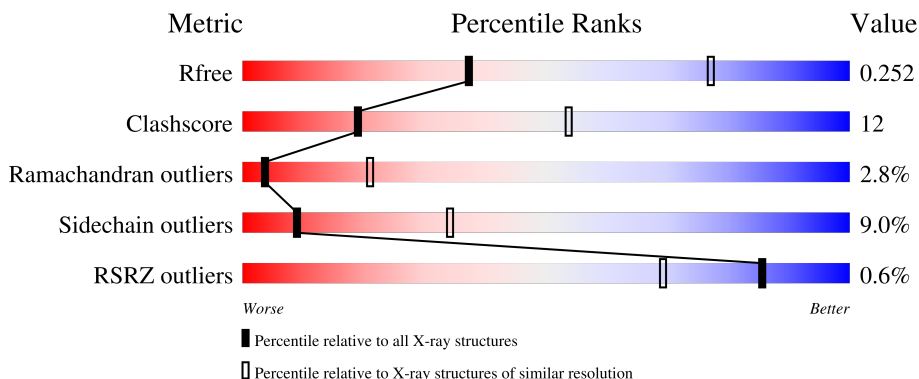
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	734	 66% 29% . .
1	B	734	 63% 30% 6% .
2	C	4	 75% 25%

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.

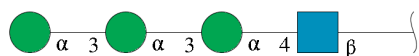
- Molecule 1 is a protein called Dipeptidyl peptidase 4.

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.



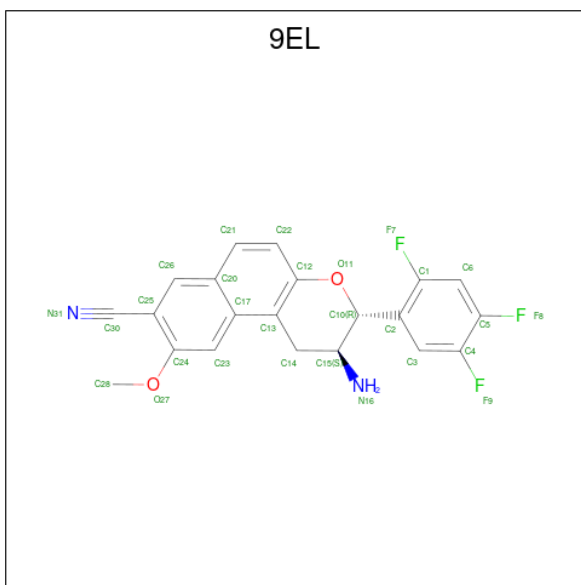
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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 (CCD ID: 9EL) (formula: $C_{21}H_{15}F_3N_2O_2$).



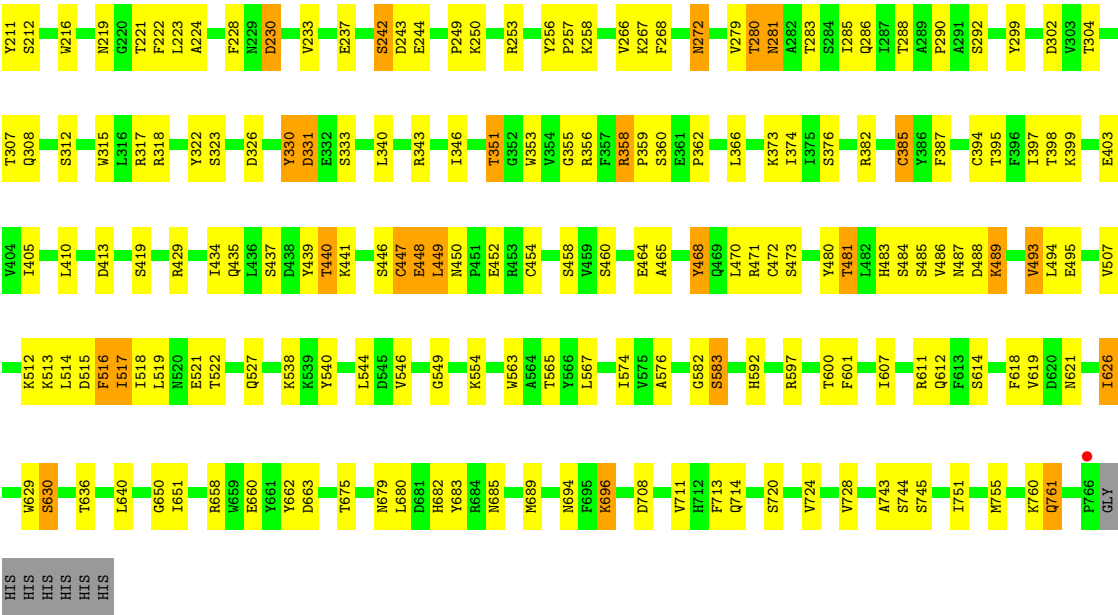
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			28	21	3	2	2		
4	B	1	Total	C	F	N	O	0	0
			28	21	3	2	2		

- Molecule 5 is water.

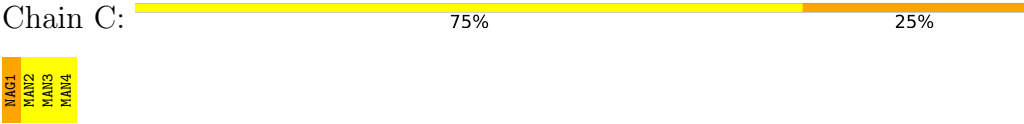
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	17	Total	O	0	0
			17	17		

- Molecule 1: Dipeptidyl peptidase 4





● 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 85.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.2 (85.82-3.00) 91.2 (85.82-3.00)	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 (4.64%)	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)	0.37 , 53.8	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, 9EL

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	0.99	5/6129 (0.1%)	1.15	23/8336 (0.3%)
1	B	0.96	1/6129 (0.0%)	1.15	19/8336 (0.2%)
All	All	0.97	6/12258 (0.0%)	1.15	42/16672 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	TRP	CA-C	6.36	1.60	1.52
1	A	630	SER	CA-C	-6.23	1.47	1.52
1	A	520	ASN	CA-C	6.16	1.61	1.52
1	A	123	GLN	CA-C	5.80	1.55	1.52
1	A	210	ALA	N-CA	-5.66	1.38	1.46
1	A	521	GLU	CA-C	5.58	1.59	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	VAL	N-CA-C	9.48	119.52	110.42
1	B	413	ASP	N-CA-C	7.07	120.02	111.40
1	A	254	VAL	CA-C-N	-6.87	111.78	120.23
1	A	254	VAL	C-N-CA	-6.87	111.78	120.23
1	B	156	THR	N-CA-C	6.82	120.41	108.75
1	A	400	GLY	N-CA-C	6.79	119.04	110.96
1	A	67	GLU	N-CA-C	6.61	119.11	109.07
1	B	87	SER	N-CA-C	6.39	124.42	110.80
1	B	202	VAL	CB-CA-C	-6.25	103.97	111.97
1	A	177	GLU	CA-C-N	6.19	126.65	119.47
1	A	177	GLU	C-N-CA	6.19	126.65	119.47
1	B	419	SER	N-CA-C	5.91	117.76	108.96
1	B	283	THR	N-CA-C	5.87	118.77	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	SER	N-CA-C	5.85	117.92	108.32
1	B	516	PHE	N-CA-C	5.82	117.81	109.14
1	B	358	ARG	N-CA-C	5.80	113.23	108.07
1	A	498	SER	N-CA-C	5.79	117.67	111.36
1	B	546	VAL	N-CA-C	5.78	116.44	108.12
1	B	374	ILE	CB-CA-C	-5.74	103.79	110.91
1	A	630	SER	CB-CA-C	-5.66	109.53	117.23
1	A	587	GLY	CA-C-O	-5.66	118.38	122.45
1	A	521	GLU	N-CA-C	5.63	121.68	113.40
1	A	94	THR	N-CA-C	-5.58	98.92	110.80
1	A	130	ALA	N-CA-C	5.46	117.09	108.96
1	A	549	GLY	CA-C-N	5.44	126.64	119.84
1	A	549	GLY	C-N-CA	5.44	126.64	119.84
1	B	454	CYS	N-CA-C	5.42	117.66	108.02
1	A	664	SER	N-CA-C	5.38	117.57	111.11
1	B	132	TYR	N-CA-C	5.37	116.96	107.61
1	A	297	ASP	N-CA-C	-5.32	102.17	110.10
1	B	205	GLU	N-CA-C	5.28	116.72	111.07
1	A	454	CYS	N-CA-C	5.27	117.24	108.02
1	A	425	MET	N-CA-C	5.26	117.03	109.04
1	A	744	SER	N-CA-C	-5.18	102.71	110.23
1	B	266	VAL	N-CA-C	5.18	115.36	108.27
1	B	481	THR	N-CA-C	5.17	117.53	109.52
1	B	549	GLY	CA-C-N	5.12	126.23	119.84
1	B	549	GLY	C-N-CA	5.12	126.23	119.84
1	B	198	ILE	CB-CA-C	-5.09	106.95	111.74
1	A	583	SER	N-CA-C	5.07	117.08	110.43
1	A	409	ALA	N-CA-C	5.03	116.16	108.42
1	A	205	GLU	N-CA-C	5.02	116.60	111.03

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	116	0
1	B	5957	0	5676	161	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	276	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 12.

All (276) 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:272:ASN:OD1	1:B:272:ASN:C	2.18	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: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: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:600:THR:OG1	1:B:601:PHE:N	2.20	0.69
1:B:60:LEU:C	1:B:60:LEU:HD12	2.18	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:69:LEU:HD22	1:B:78:VAL:HG22	1.79	0.64
1:B:272:ASN:OD1	1:B:272:ASN:O	2.15	0.64
1:A:500:LEU:HA	1:A:503:MET:HE3	1.81	0.63
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
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:B:582:GLY:O	1:B:583:SER:C	2.39	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:B:448:GLU:O	1:B:449:LEU:C	2.43	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: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:73:GLU:O	1:A:73:GLU:HG3	2.03	0.56
1:A:328:CYS:HA	1:A:338:ASN:O	2.04	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:751:ILE:HG12	1:B:755:MET:HE2	1.87	0.56
1:A:653:VAL:O	1:A:654:ALA:C	2.49	0.55
1:B:125:ARG:O	1:B:125:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:532:PRO:O	1:A:533:HIS:C	2.48	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:91:GLU:O	1:A:92:ASN:C	2.51	0.54
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.08	0.54
1:B:106:SER:C	1:B:107:ILE:HD12	2.33	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:744:SER:O	1:B:745:SER:C	2.51	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
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:B:439:TYR:O	1:B:440:THR:C	2.52	0.51
1:A:663:ASP:OD1	1:A:663:ASP:C	2.54	0.51
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.93	0.51
1:B:682:HIS:O	1:B:683:TYR:C	2.54	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:694:ASN:C	1:B:696:LYS:N	2.70	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: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:84:GLY:O	1:B:85:ASN:C	2.54	0.49
1:B:125:ARG:NH2	1:B:205:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:SER:HB2	1:A:457:TYR:CZ	2.47	0.49
1:A:752:TYR:O	1:A:756:SER:OG	2.25	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: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:186:THR:C	1:A:187:TRP:CD1	2.91	0.48
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: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:A:638:MET:HE3	1:A:691:ARG:CZ	2.44	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
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.50	0.47
1:A:230:ASP:O	1:A:231:THR:C	2.57	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:B:154:TRP:C	1:B:155:VAL:HG23	2.40	0.47
1:A:66:HIS:C	1:A:67:GLU:HG3	2.39	0.47
1:B:154:TRP:C	1:B:155:VAL:CG2	2.87	0.47
1:B:285:ILE:HG22	1:B:286:GLN:O	2.15	0.47
1:A:94:THR:C	1:A:96:ASP:H	2.23	0.46
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.97	0.46
1:A:291:ALA:O	1:A:295:ILE:HG23	2.15	0.46
1:B:243:ASP:O	1:B:244:GLU:C	2.58	0.46
1:A:747:ALA:O	1:A:751:ILE:HG22	2.15	0.46
1:B:73:GLU:O	1:B:75:ASN:N	2.48	0.46
1:B:299:TYR:CE1	1:B:318:ARG:HA	2.51	0.46
1:B:518:ILE:C	1:B:519:LEU:HD23	2.41	0.46
1:B:760:LYS:O	1:B:761:GLN:C	2.57	0.46
1:A:340:LEU:O	1:A:341:VAL:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:C	1:A:483:HIS:CD2	2.94	0.46
1:A:449:LEU:O	1:A:450:ASN:HB2	2.15	0.46
1:B:85:ASN:HD22	1:B:85:ASN:N	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: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:82:GLU:HB2	1:B:83:TYR:CD1	2.51	0.45
1:B:614:SER:HA	1:B:619:VAL:HB	1.98	0.45
1:A:140:ARG:HD3	1:A:140:ARG:HA	1.63	0.45
1:B:743:ALA:O	1:B:744:SER:C	2.58	0.45
1:A:206:GLU:CD	1:A:666:TYR:HB2	2.41	0.45
1:A:353:TRP:CZ2	1:A:591:MET:HE3	2.52	0.45
1:A:422:TYR:CE2	1:A:423:LYS:HD2	2.51	0.45
1:B:72:GLN:HG3	1:B:75:ASN:HB3	1.98	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:A:139:LYS:O	1:A:140:ARG:C	2.59	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:N	1:B:468:TYR:CD1	2.85	0.45
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.89	0.45
1:B:60:LEU:C	1:B:60:LEU:CD1	2.88	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: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
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:113:PHE:CE2	1:B:178:PRO:CG	3.01	0.44
1:B:144:THR:O	1:B:145:GLU:C	2.58	0.44
1:B:144:THR:O	1:B:147:ARG:HG2	2.17	0.44
1:B:679:ASN:O	1:B:680:LEU:C	2.59	0.44
1:A:98:PHE:CD2	1:A:102:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:SER:OG	1:B:67:GLU:N	2.50	0.44
1:B:713:PHE:O	1:B:714:GLN:C	2.57	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:B:439:TYR:C	1:B:441:LYS:N	2.75	0.44
1:A:519:LEU:C	1:A:521:GLU:N	2.74	0.44
1:B:258:LYS:HA	1:B:662:TYR:O	2.18	0.44
1:B:331:ASP:OD1	1:B:333:SER:OG	2.33	0.44
1:A:477:LEU:O	1:A:478:PRO:C	2.61	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:B:629:TRP:O	1:B:630:SER:C	2.61	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:77:LEU:CD2	1:B:86:SER:HB3	2.29	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: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:B:450:ASN:OD1	1:B:450:ASN:C	2.60	0.43
1:A:149:PRO:O	1:A:152:THR:OG1	2.36	0.43
1:A:568:ALA:O	1:A:569:SER:C	2.61	0.43
1:B:658:ARG:HB2	1:B:689:MET:HE1	2.01	0.43
1:B:600:THR:HG1	1:B:601:PHE:H	1.64	0.42
1:A:57:LEU:HA	1:A:480:TYR:CE1	2.54	0.42
1:A:514:LEU:HD12	1:A:526:TYR:O	2.19	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:A:430:ASN:OD1	1:A:446:SER:OG	2.28	0.42
1:B:74:ASN:CB	1:B:92:ASN:HB2	2.50	0.42
1:B:330:TYR:O	1:B:331:ASP:CB	2.67	0.42
1:A:334:SER:O	1:A:335:GLY:C	2.61	0.42
1:B:470:LEU:HD23	1:B:470:LEU:HA	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:N	2.77	0.42
1:B:93:SER:C	1:B:95:PHE:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:SER:O	1:B:447:CYS:C	2.63	0.42
1:B:158:SER:HA	1:B:216:TRP:CD1	2.55	0.42
1:B:280:THR:O	1:B:281:ASN:C	2.63	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:A:360:SER:OG	1:A:374:ILE:O	2.37	0.42
1:B:72:GLN:NE2	1:B:73:GLU:O	2.53	0.42
1:B:154:TRP:O	1:B:155:VAL:HG22	2.20	0.42
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.02	0.42
1:B:582:GLY:C	1:B:583:SER:O	2.62	0.42
1:B:675:THR:C	1:B:680:LEU:HB2	2.44	0.42
1:B:387:PHE:CZ	1:B:394:CYS:HB3	2.53	0.41
1:B:694:ASN:C	1:B:696:LYS:H	2.28	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:B:208:PHE:O	1:B:209:SER:C	2.63	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:A:546:VAL:HG12	1:A:547:TYR: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:88:VAL:O	1:B:88:VAL:HG12	2.21	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:A:464:GLU:O	1:A:465:ALA:C	2.62	0.41
1:A:642:SER:OG	1:A:644:SER:HB3	2.21	0.41
1:A:753:THR:O	1:A:756:SER:HB2	2.21	0.41
1:B:80:ASN:CB	1:B:85:ASN:HB2	2.50	0.41
1:B:397:ILE:N	1:B:397:ILE:HD13	2.36	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:44:THR:O	1:B:45:LEU:C	2.59	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:49:LEU:HD23	1:B:49:LEU:HA	1.83	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:A:112:GLN:HB2	1:A:113:PHE:CD1	2.57	0.40
1:B:68:TYR:CE1	1:B:79:PHE:CD1	3.08	0.40
1:A:88:VAL:O	1:A:88:VAL:HG12	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/734 (99%)	646 (89%)	62 (9%)	17 (2%)	5	25
1	B	725/734 (99%)	621 (86%)	81 (11%)	23 (3%)	3	18
All	All	1450/1468 (99%)	1267 (87%)	143 (10%)	40 (3%)	4	21

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
1	B	621	ASN
1	A	95	PHE
1	A	242	SER
1	A	450	ASN
1	A	714	GLN

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Mol	Chain	Res	Type
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 ⓘ

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%)	602 (92%)	50 (8%)	12	40
1	B	652/658 (99%)	585 (90%)	67 (10%)	7	28
All	All	1304/1316 (99%)	1187 (91%)	117 (9%)	9	34

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	73	GLU
1	A	75	ASN
1	A	83	TYR
1	A	88	VAL
1	A	90	LEU
1	A	91	GLU
1	A	94	THR
1	A	97	GLU
1	A	106	SER
1	A	107	ILE
1	A	129	THR
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	316	LEU
1	A	317	ARG
1	A	323	SER
1	A	326	ASP
1	A	336	ARG
1	A	339	CYS
1	A	366	LEU
1	A	385	CYS
1	A	392	LYS
1	A	418	ILE
1	A	442	VAL
1	A	448	GLU
1	A	452	GLU
1	A	458	SER
1	A	484	SER
1	A	486	VAL
1	A	511	SER
1	A	518	ILE
1	A	529	ILE

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Mol	Chain	Res	Type
1	A	530	LEU
1	A	536	LYS
1	A	594	ILE
1	A	636	THR
1	A	649	CYS
1	A	662	TYR
1	A	745	SER
1	A	751	ILE
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	174	VAL
1	B	179	ASN
1	B	181	PRO
1	B	182	SER
1	B	188	THR
1	B	202	VAL
1	B	207	VAL
1	B	212	SER
1	B	223	LEU
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	280	THR
1	B	302	ASP
1	B	312	SER
1	B	323	SER

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Mol	Chain	Res	Type
1	B	326	ASP
1	B	346	ILE
1	B	351	THR
1	B	359	PRO
1	B	376	SER
1	B	385	CYS
1	B	395	THR
1	B	398	THR
1	B	410	LEU
1	B	448	GLU
1	B	458	SER
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	493	VAL
1	B	495	GLU
1	B	507	VAL
1	B	513	LYS
1	B	517	ILE
1	B	521	GLU
1	B	522	THR
1	B	554	LYS
1	B	626	ILE
1	B	630	SER
1	B	651	ILE
1	B	660	GLU
1	B	685	ASN
1	B	696	LYS
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	92	ASN
1	A	103	ASN
1	A	150	ASN
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	455	GLN
1	A	572	ASN
1	A	697	GLN
1	A	748	HIS
1	A	749	GLN
1	B	51	ASN
1	B	85	ASN
1	B	112	GLN
1	B	138	ASN
1	B	435	GLN
1	B	487	ASN
1	B	697	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	2	2	11,11,12	0.92	0	15,15,17	1.50	2 (13%)
3	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	B	801	1	14,14,15	0.58	0	17,19,21	1.69	4 (23%)
2	MAN	C	3	2	11,11,12	0.51	0	15,15,17	1.03	1 (6%)

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	2	2	-	2/2/19/22	0/1/1/1
3	NAG	A	801	1	-	4/6/23/26	0/1/1/1
3	NAG	B	801	1	-	2/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MAN	C1-C2-C3	4.83	116.67	109.64
3	B	801	NAG	C4-C3-C2	3.96	116.82	111.02
3	B	801	NAG	O5-C5-C6	3.44	114.35	107.66
3	B	801	NAG	O5-C1-C2	-2.73	107.06	111.29
2	C	3	MAN	C1-O5-C5	2.60	115.67	112.19
2	C	2	MAN	O5-C5-C4	-2.45	104.87	110.83
3	B	801	NAG	O4-C4-C5	2.17	114.67	109.32

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	0.54	0	17,19,21	1.36	3 (17%)
2	MAN	C	2	2	11,11,12	0.92	0	15,15,17	1.50	2 (13%)
2	MAN	C	3	2	11,11,12	0.51	0	15,15,17	1.03	1 (6%)
2	MAN	C	4	2	11,11,12	0.60	0	15,15,17	1.11	2 (13%)

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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	MAN	C1-C2-C3	4.83	116.67	109.64
2	C	1	NAG	C8-C7-N2	2.61	120.44	116.12
2	C	3	MAN	C1-O5-C5	2.60	115.67	112.19
2	C	4	MAN	C1-O5-C5	2.49	115.52	112.19
2	C	2	MAN	O5-C5-C4	-2.45	104.87	110.83
2	C	1	NAG	C1-O5-C5	2.36	115.35	112.19
2	C	1	NAG	O5-C1-C2	-2.31	107.71	111.29
2	C	4	MAN	C3-C4-C5	2.27	114.35	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

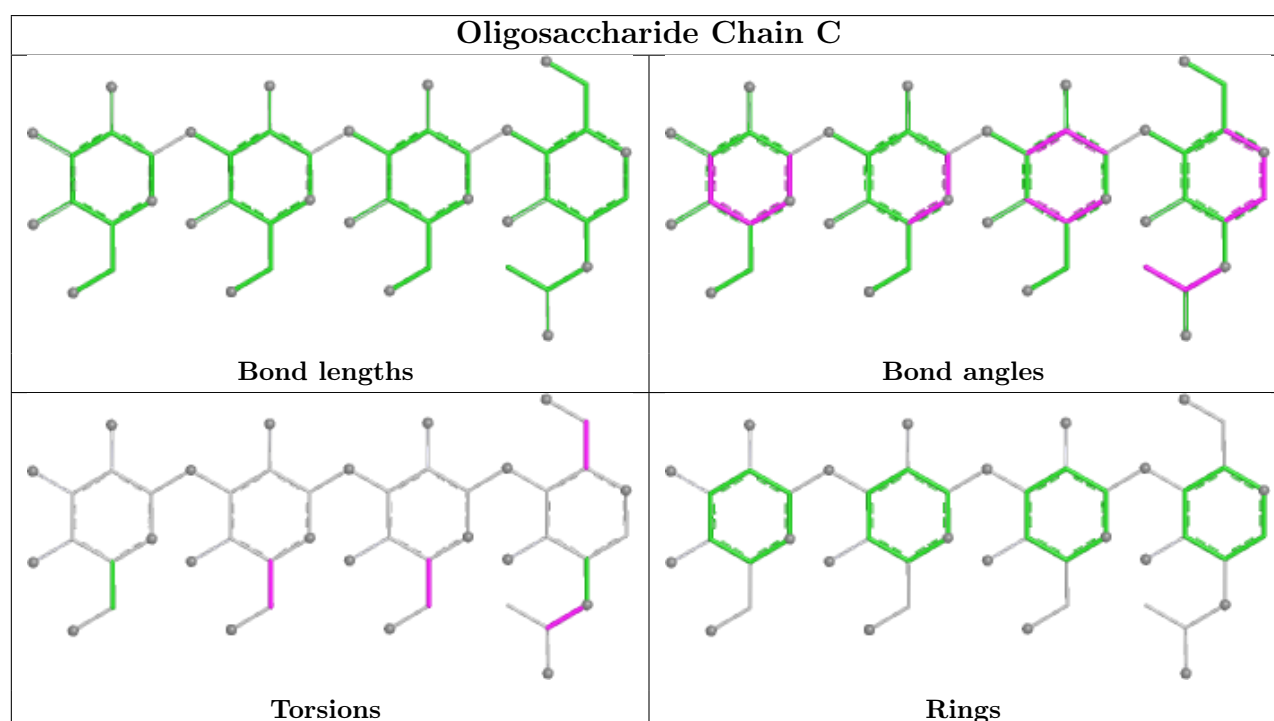
Mol	Chain	Res	Type	Atoms
2	C	2	MAN	C4-C5-C6-O6
2	C	2	MAN	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	MAN	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	MAN	O5-C5-C6-O6

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	3.08	10 (32%)	42,46,46	1.79	10 (23%)
4	9EL	B	806	-	31,31,31	3.13	9 (29%)	42,46,46	1.88	7 (16%)
3	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	B	801	1	14,14,15	0.58	0	17,19,21	1.69	4 (23%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	9EL	C25-C30	-13.59	1.24	1.44
4	B	806	9EL	C25-C30	-12.99	1.25	1.44
4	A	802	9EL	C12-C13	6.59	1.49	1.38
4	B	806	9EL	C12-C13	5.50	1.47	1.38
4	B	806	9EL	C25-C24	4.18	1.48	1.40
4	B	806	9EL	C17-C20	4.13	1.50	1.43
4	B	806	9EL	O11-C10	-4.04	1.39	1.45
4	B	806	9EL	C13-C17	3.27	1.49	1.43
4	A	802	9EL	C25-C24	3.26	1.47	1.40
4	B	806	9EL	C2-C10	-3.23	1.45	1.51
4	A	802	9EL	C17-C20	3.06	1.48	1.43
4	A	802	9EL	C2-C10	-2.78	1.46	1.51
4	A	802	9EL	O11-C10	-2.60	1.41	1.45
4	A	802	9EL	C13-C17	2.54	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	806	9EL	C3-C4	2.28	1.41	1.37
4	A	802	9EL	C23-C24	2.21	1.40	1.36
4	A	802	9EL	C2-C1	-2.21	1.34	1.38
4	B	806	9EL	C10-C15	-2.12	1.50	1.53
4	A	802	9EL	C21-C20	-2.05	1.37	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	806	9EL	C28-O27-C24	5.81	126.04	117.51
4	B	806	9EL	C3-C2-C1	5.73	121.21	116.42
4	B	806	9EL	C6-C1-C2	-4.65	118.77	123.93
4	A	802	9EL	C13-C17-C20	-4.51	114.06	119.66
3	B	801	NAG	C4-C3-C2	3.96	116.82	111.02
4	A	802	9EL	C28-O27-C24	3.68	122.91	117.51
4	A	802	9EL	C3-C2-C1	3.64	119.46	116.42
3	B	801	NAG	O5-C5-C6	3.44	114.35	107.66
4	A	802	9EL	C21-C20-C26	-2.91	116.99	122.00
3	B	801	NAG	O5-C1-C2	-2.73	107.06	111.29
4	B	806	9EL	O11-C12-C22	2.53	120.81	116.20
4	B	806	9EL	C13-C17-C20	-2.48	116.58	119.66
4	A	802	9EL	C25-C26-C20	-2.42	118.01	121.14
4	A	802	9EL	C6-C1-C2	-2.41	121.26	123.93
4	A	802	9EL	C26-C25-C30	-2.41	116.47	120.16
4	A	802	9EL	C21-C20-C17	2.36	122.17	119.12
4	B	806	9EL	O11-C12-C13	-2.34	118.39	122.28
4	A	802	9EL	F7-C1-C6	2.25	123.14	118.64
3	B	801	NAG	O4-C4-C5	2.17	114.67	109.32
4	A	802	9EL	C26-C25-C24	2.15	122.86	119.49
4	B	806	9EL	C23-C17-C20	2.08	120.94	118.64

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

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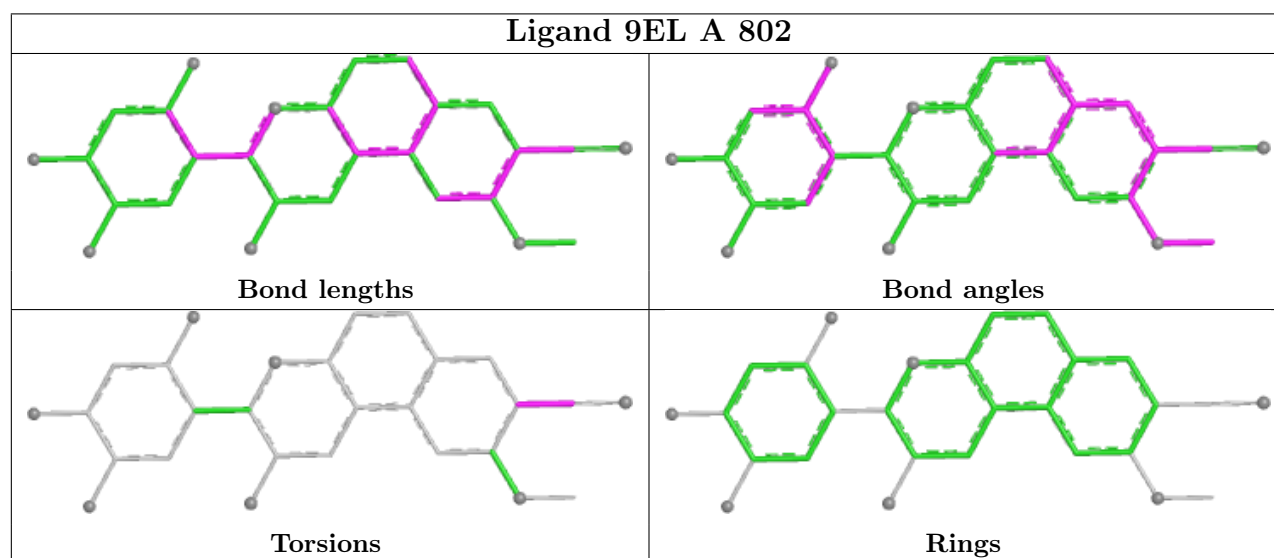
Mol	Chain	Res	Type	Atoms
4	A	802	9EL	C26-C25-C30-N31

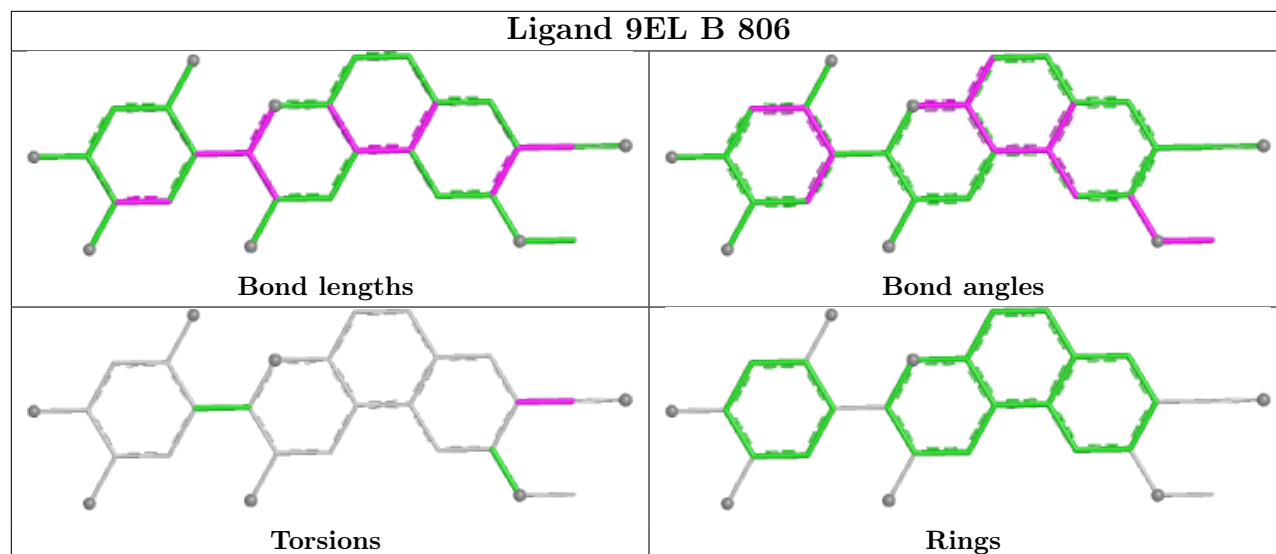
There are no ring outliers.

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%)	-0.23	2 (0%)	90 79	10, 27, 56, 92	2 (0%)
1	B	727/734 (99%)	-0.18	6 (0%)	82 64	11, 28, 62, 109	1 (0%)
All	All	1454/1468 (99%)	-0.21	8 (0%)	85 69	10, 27, 60, 109	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	SER	6.3
1	B	88	VAL	3.1
1	B	85	ASN	2.7
1	B	86	SER	2.5
1	A	473	SER	2.1
1	B	766	PRO	2.1
1	B	155	VAL	2.1
1	A	100	HIS	2.1

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.

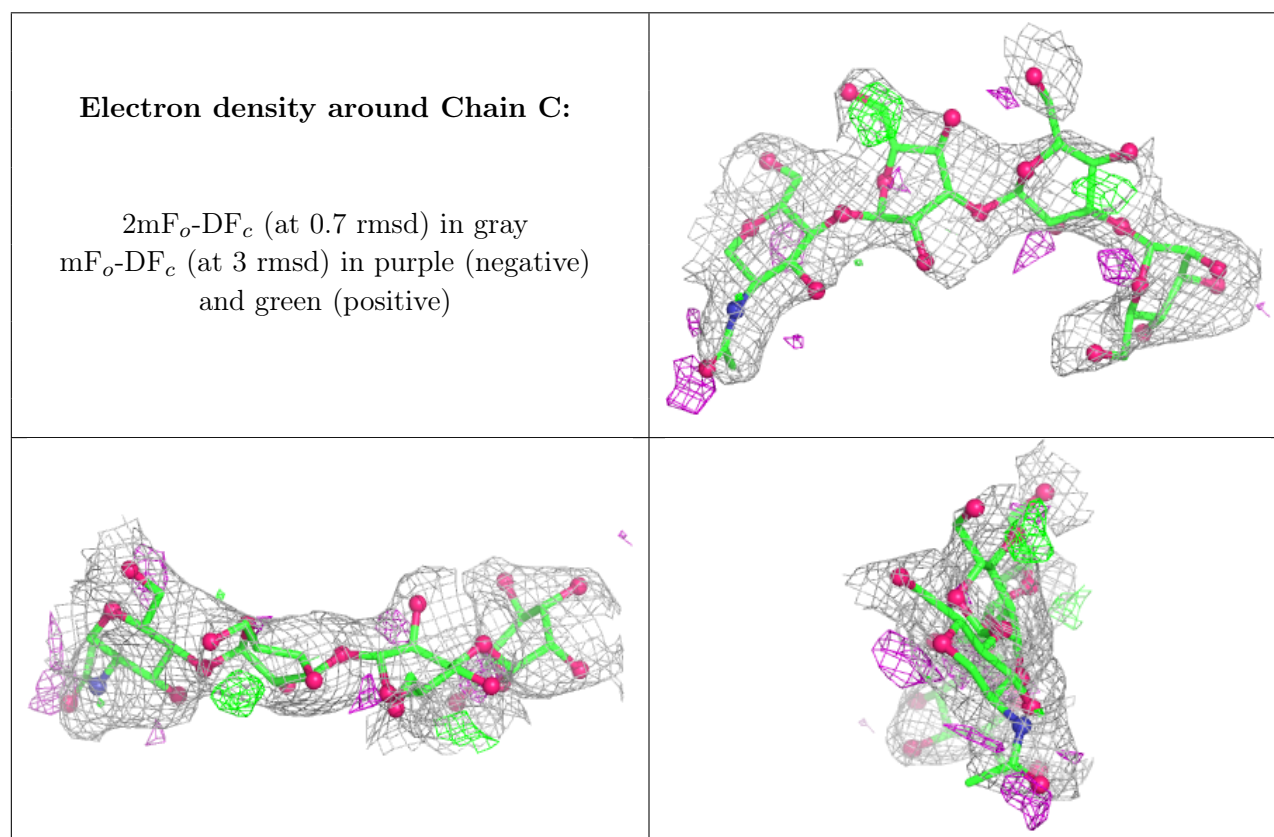
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	C	3	11/12	0.59	0.18	54,56,57,59	0
3	NAG	A	801	14/15	0.67	0.20	32,33,35,41	0
2	MAN	C	2	11/12	0.76	0.17	46,48,52,53	0
3	NAG	B	801	14/15	0.78	0.15	40,54,64,64	0

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(Å ²)	Q<0.9
2	MAN	C	3	11/12	0.59	0.18	54,56,57,59	0
2	MAN	C	4	11/12	0.75	0.15	58,59,60,60	0
2	MAN	C	2	11/12	0.76	0.17	46,48,52,53	0
2	NAG	C	1	14/15	0.77	0.17	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](#)

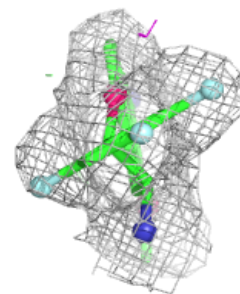
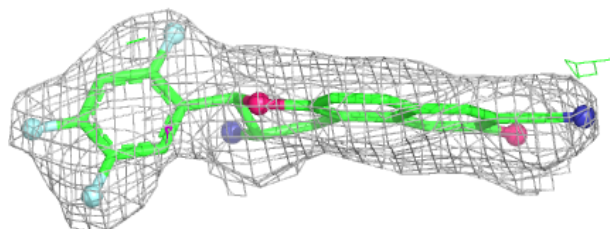
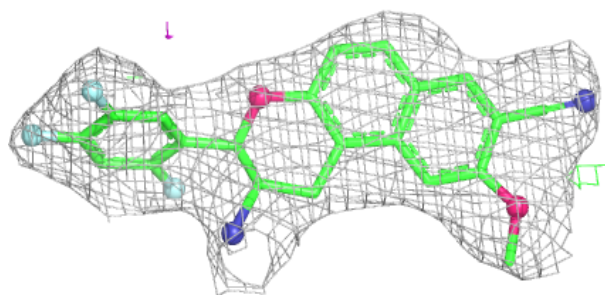
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	801	14/15	0.67	0.20	32,33,35,41	0
3	NAG	B	801	14/15	0.78	0.15	40,54,64,64	0
4	9EL	A	802	28/28	0.94	0.09	16,19,25,30	0
4	9EL	B	806	28/28	0.95	0.08	19,21,23,25	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.

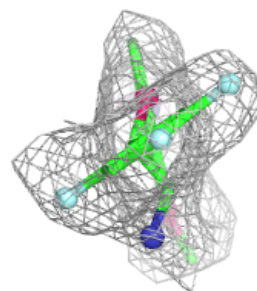
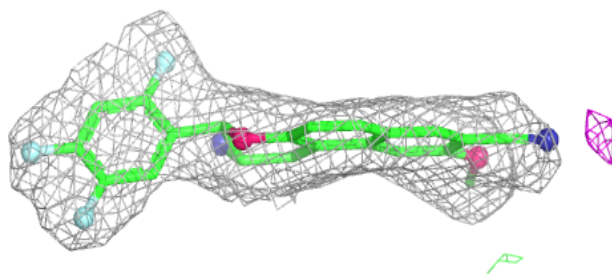
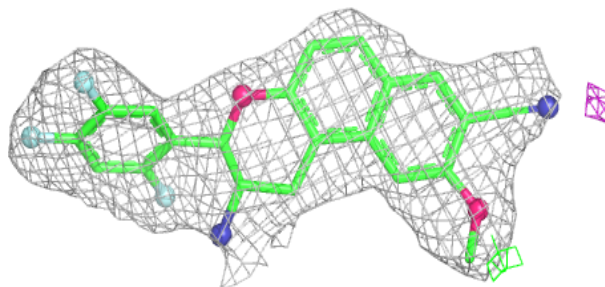
Electron density around 9EL A 802:

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



Electron density around 9EL B 806:

$2mF_o - DF_c$ (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.