



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:46 PM UTC

PDB ID : 3HRZ / pdb_00003hrz
Title : Cobra Venom Factor (CVF) in complex with human factor B
Authors : Janssen, B.J.C.; Gomes, L.; Koning, R.I.; Svergun, D.I.; Koster, A.J.;
Fritzinger, D.C.; Vogel, C.-W.; Gros, P.
Deposited on : 2009-06-10
Resolution : 2.20 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

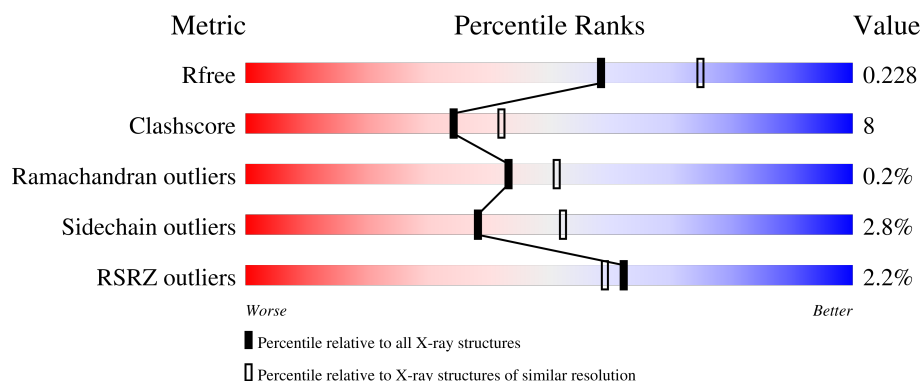
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

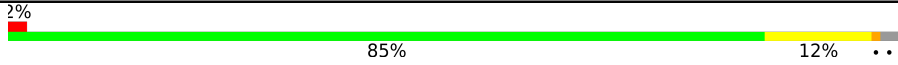
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	627	
2	B	252	
3	C	379	
4	D	741	
5	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	9324	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15938 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 Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	0
			4800	3071	804	910	15			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1856	1194	311	346	5			

- Molecule 3 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	362	Total	C	N	O	S	0	0	0
			2926	1847	490	570	19			

- Molecule 4 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	693	Total	C	N	O	S	0	0	0
			5469	3449	947	1040	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	254	GLY	ASP	engineered mutation	UNP P00751
D	260	ASP	ASN	engineered mutation	UNP P00751
D	740	ALA	-	insertion	UNP P00751
D	741	ALA	-	insertion	UNP P00751

- Molecule 5 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
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

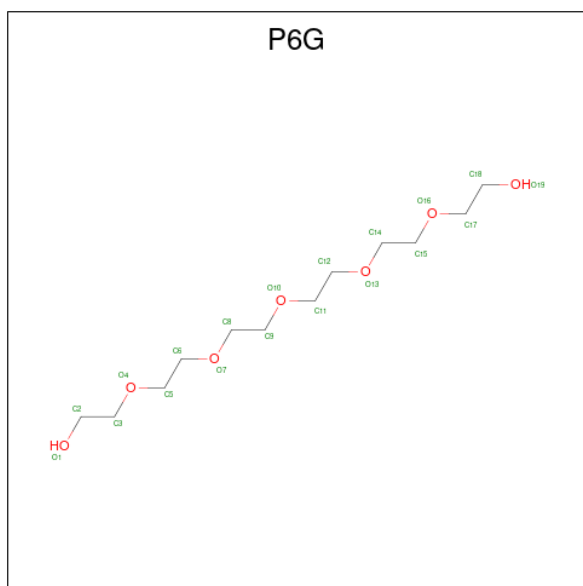
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

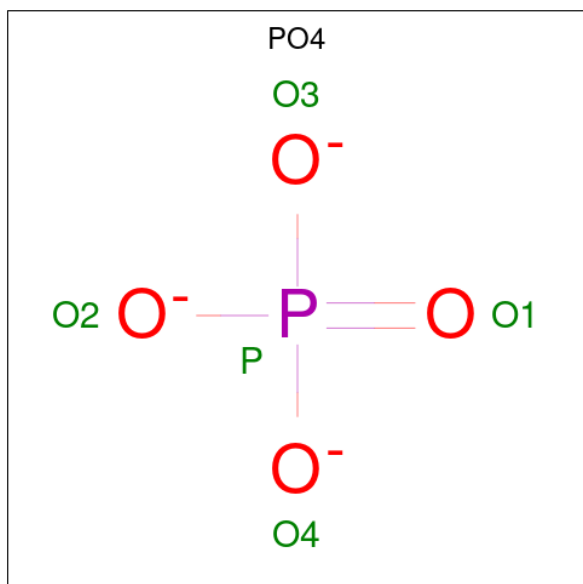
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0

- Molecule 9 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 19 12 7	0	0
9	C	1	Total C O 19 12 7	0	0

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	P	0	0
			5	4	1		
10	C	1	Total	O	P	0	0
			5	4	1		
10	D	1	Total	O	P	0	0
			5	4	1		
10	D	1	Total	O	P	0	0
			5	4	1		
10	D	1	Total	O	P	0	0
			5	4	1		

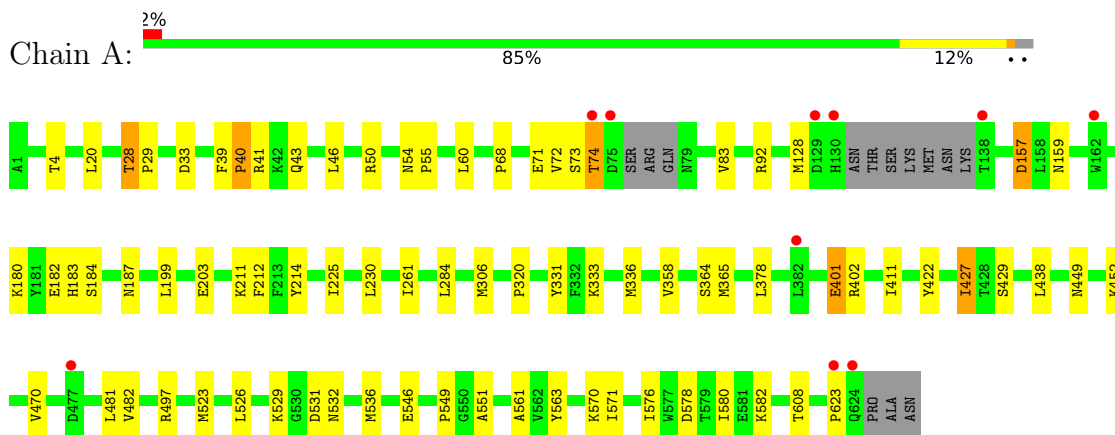
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	290	Total	O	0	0
			290	290		
11	B	100	Total	O	0	0
			100	100		
11	C	129	Total	O	0	0
			129	129		
11	D	232	Total	O	0	0
			232	232		

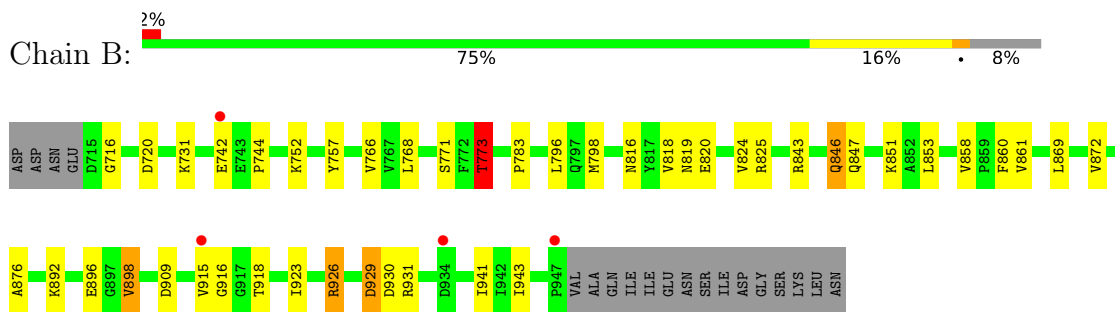
3 Residue-property plots

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

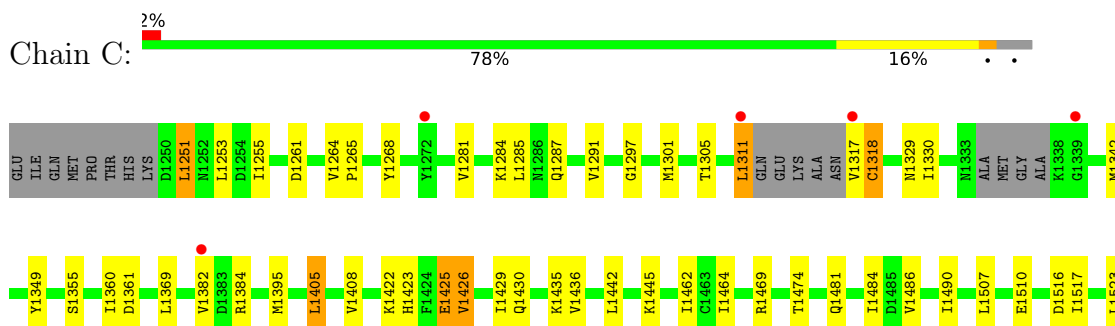
• Molecule 1: Cobra venom factor

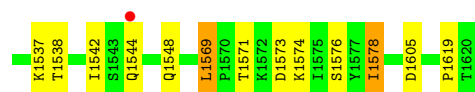


• Molecule 2: Cobra venom factor

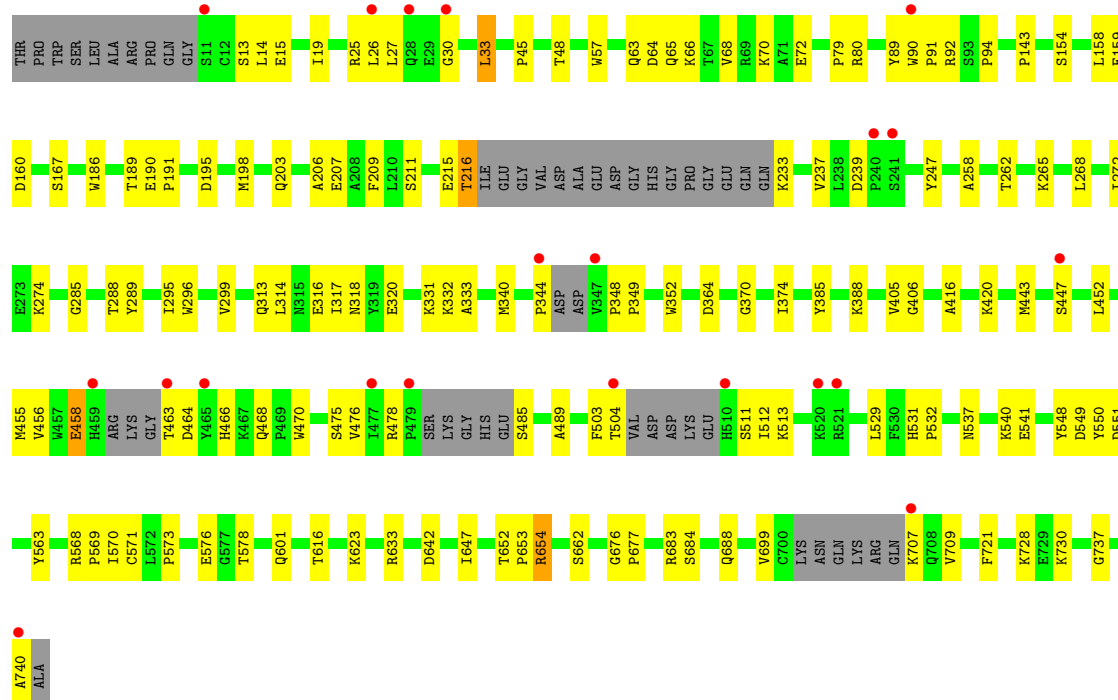
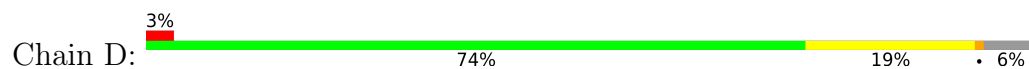


• Molecule 3: Cobra venom factor





• Molecule 4: Complement factor B



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.89Å 283.39Å 134.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.49 – 2.20 33.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.49-2.20) 99.5 (33.49-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.180 , 0.226 0.182 , 0.228	Depositor DCC
R_{free} test set	2486 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.9	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	0.96	EDS
Total number of atoms	15938	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: MG, P6G, K, NAG, PO4

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	0.49	0/4908	0.78	2/6678 (0.0%)
2	B	0.46	0/1894	0.86	8/2570 (0.3%)
3	C	0.46	0/2977	0.80	3/4026 (0.1%)
4	D	0.42	0/5591	0.77	3/7567 (0.0%)
All	All	0.46	0/15370	0.79	16/20841 (0.1%)

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
2	B	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	930	ASP	N-CA-C	-9.53	101.86	112.72
2	B	858	VAL	CA-C-N	6.60	126.36	119.76
2	B	858	VAL	C-N-CA	6.60	126.36	119.76
4	D	406	GLY	CA-C-N	6.44	126.01	119.19
4	D	406	GLY	C-N-CA	6.44	126.01	119.19
3	C	1578	ILE	CB-CA-C	-6.23	103.19	110.91
1	A	28	THR	CA-C-N	6.02	125.96	119.76
1	A	28	THR	C-N-CA	6.02	125.96	119.76
4	D	503	PHE	N-CA-C	5.21	117.73	109.50
2	B	716	GLY	N-CA-C	-5.19	108.46	115.21
2	B	773	THR	CA-C-N	5.18	126.32	119.84
2	B	773	THR	C-N-CA	5.18	126.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1569	LEU	CA-C-N	5.07	126.18	119.84
3	C	1569	LEU	C-N-CA	5.07	126.18	119.84
2	B	909	ASP	CA-C-N	5.05	124.66	119.05
2	B	909	ASP	C-N-CA	5.05	124.66	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	929	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	4800	0	4797	54	0
2	B	1856	0	1900	35	0
3	C	2926	0	2873	51	0
4	D	5469	0	5339	100	1
5	E	28	0	25	2	0
6	A	14	0	13	3	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
9	A	19	0	26	3	0
9	C	19	0	26	4	0
10	B	5	0	0	0	0
10	C	5	0	0	0	0
10	D	15	0	0	0	0
11	A	290	0	0	0	0
11	B	100	0	0	2	0
11	C	129	0	0	2	1
11	D	232	0	0	7	0
All	All	15938	0	15025	228	1

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 (228) 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)
3:C:1369:LEU:HB2	3:C:1395:MET:HE2	1.31	1.07
2:B:943:ILE:HD11	3:C:1301:MET:HE3	1.37	1.04
9:A:630:P6G:H91	9:A:630:P6G:C15	2.03	0.88
4:D:64:ASP:HB2	4:D:66:LYS:HG3	1.60	0.83
3:C:1445:LYS:HD3	9:C:100:P6G:H182	1.62	0.81
4:D:699:VAL:HG21	4:D:709:VAL:HG22	1.62	0.80
9:A:630:P6G:H91	9:A:630:P6G:H151	1.64	0.80
4:D:475:SER:HB3	4:D:513:LYS:HE3	1.62	0.79
1:A:333:LYS:CB	1:A:336:MET:HE3	2.16	0.76
2:B:943:ILE:HD11	3:C:1301:MET:CE	2.16	0.75
4:D:728:LYS:HE3	4:D:740:ALA:HB3	1.67	0.75
1:A:41:ARG:HH11	1:A:43:GLN:HG3	1.53	0.73
4:D:206:ALA:HA	4:D:443:MET:HE3	1.68	0.73
1:A:230:LEU:HD13	1:A:561:ALA:HB2	1.71	0.72
4:D:258:ALA:O	4:D:262:THR:HG23	1.89	0.71
4:D:209:PHE:CD2	4:D:443:MET:HE1	2.25	0.71
4:D:529:LEU:HD13	4:D:730:LYS:HD2	1.73	0.70
3:C:1251:LEU:HD13	3:C:1297:GLY:HA3	1.74	0.69
1:A:333:LYS:HB3	1:A:336:MET:HE3	1.73	0.69
2:B:861:VAL:H	3:C:1430:GLN:NE2	1.90	0.69
2:B:798:MET:HE1	2:B:872:VAL:HB	1.74	0.69
2:B:818:VAL:HG12	2:B:820:GLU:HG2	1.75	0.68
4:D:209:PHE:HD2	4:D:443:MET:HE1	1.56	0.68
4:D:489:ALA:HB2	4:D:677:PRO:HG3	1.76	0.68
4:D:299:VAL:HG13	4:D:340:MET:CE	2.24	0.68
3:C:1261:ASP:HB3	3:C:1285:LEU:HD12	1.75	0.68
1:A:429:SER:HB2	1:A:438:LEU:CD1	2.24	0.68
4:D:478:ARG:HH12	4:D:504:THR:HG22	1.60	0.67
9:A:630:P6G:H91	9:A:630:P6G:H152	1.74	0.67
4:D:299:VAL:H	4:D:340:MET:HE3	1.60	0.67
1:A:551:ALA:HA	2:B:773:THR:HG23	1.76	0.67
3:C:1619:PRO:HD2	11:C:484:HOH:O	1.96	0.65
4:D:26:LEU:HD22	4:D:30:GLY:HA2	1.79	0.65
4:D:550:TYR:CZ	4:D:654:ARG:HD3	2.32	0.65
4:D:299:VAL:HG13	4:D:340:MET:HE3	1.79	0.65
4:D:299:VAL:HG22	4:D:340:MET:HE3	1.77	0.65
4:D:475:SER:O	4:D:513:LYS:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASN:HD22	6:A:9187:NAG:H83	1.63	0.64
3:C:1571:THR:HG21	3:C:1576:SER:OG	1.98	0.64
4:D:195:ASP:HB2	4:D:198:MET:HE3	1.80	0.64
1:A:33:ASP:OD1	1:A:50:ARG:HD2	1.98	0.64
1:A:72:VAL:HG22	1:A:72:VAL:O	1.98	0.64
3:C:1422:LYS:HD3	3:C:1425:GLU:HG3	1.79	0.64
2:B:943:ILE:CD1	3:C:1301:MET:HE3	2.23	0.62
4:D:623:LYS:HE3	4:D:662:SER:O	1.99	0.62
4:D:233:LYS:NZ	4:D:233:LYS:HB3	2.14	0.61
4:D:374:ILE:HD11	4:D:416:ALA:HB1	1.82	0.61
2:B:898:VAL:HG21	3:C:1311:LEU:HD13	1.83	0.61
4:D:549:ASP:OD1	4:D:654:ARG:HD2	2.01	0.61
4:D:385:TYR:CD1	4:D:388:LYS:HD3	2.36	0.60
3:C:1573:ASP:O	3:C:1574:LYS:HG2	2.01	0.59
4:D:452:LEU:HD23	4:D:455:MET:HG3	1.84	0.59
3:C:1469:ARG:HG3	3:C:1578:ILE:HD11	1.83	0.59
3:C:1382:VAL:HG12	3:C:1382:VAL:O	2.00	0.59
4:D:285:GLY:HA3	4:D:340:MET:HE1	1.84	0.59
3:C:1330:ILE:HD13	3:C:1342:MET:HB2	1.85	0.59
4:D:203:GLN:HB3	4:D:458:GLU:HG3	1.85	0.59
4:D:265:LYS:HE3	4:D:314:LEU:O	2.03	0.58
4:D:296:TRP:CE2	4:D:317:ILE:HD12	2.38	0.58
4:D:563:TYR:CZ	4:D:569:PRO:HG3	2.38	0.58
1:A:20:LEU:HD13	1:A:470:VAL:HG11	1.85	0.57
4:D:247:TYR:CE1	4:D:340:MET:HE2	2.39	0.57
4:D:677:PRO:HD2	11:D:795:HOH:O	2.05	0.57
2:B:926:ARG:HD2	3:C:1305:THR:OG1	2.04	0.57
4:D:14:LEU:HD21	4:D:26:LEU:HD11	1.87	0.56
4:D:288:THR:HG21	4:D:317:ILE:HG21	1.85	0.56
1:A:41:ARG:NH1	1:A:43:GLN:HG3	2.21	0.56
1:A:449:ASN:HA	1:A:452:LYS:HE3	1.88	0.56
4:D:683:ARG:O	4:D:684:SER:HB2	2.05	0.56
3:C:1261:ASP:HB3	3:C:1285:LEU:CD1	2.36	0.56
3:C:1426:VAL:HG23	3:C:1429:ILE:HD13	1.88	0.56
4:D:570:ILE:HD13	4:D:688:GLN:HB2	1.88	0.55
1:A:128:MET:HE1	1:A:523:MET:HE2	1.89	0.55
1:A:549:PRO:HG3	2:B:744:PRO:HG3	1.88	0.55
4:D:247:TYR:HE1	4:D:340:MET:HE2	1.72	0.55
4:D:364:ASP:HB3	4:D:405:VAL:O	2.07	0.55
1:A:529:LYS:HE3	1:A:546:GLU:OE2	2.07	0.54
2:B:869:LEU:HD23	2:B:892:LYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:PRO:HG3	4:D:186:TRP:CZ2	2.42	0.54
2:B:898:VAL:CG2	3:C:1311:LEU:HD13	2.37	0.54
2:B:941:ILE:CG2	3:C:1301:MET:HE2	2.38	0.54
1:A:54:ASN:HB2	1:A:55:PRO:HD2	1.90	0.54
4:D:64:ASP:HB2	4:D:66:LYS:CG	2.37	0.53
4:D:216:THR:HG22	11:D:908:HOH:O	2.08	0.53
1:A:214:TYR:CE1	1:A:402:ARG:HD2	2.43	0.53
1:A:333:LYS:HB2	1:A:336:MET:HE3	1.89	0.53
4:D:699:VAL:HG22	4:D:699:VAL:O	2.09	0.53
1:A:358:VAL:HG12	1:A:365:MET:HG2	1.91	0.53
4:D:478:ARG:HH12	4:D:504:THR:CG2	2.22	0.52
4:D:313:GLN:O	4:D:316:GLU:HB2	2.09	0.52
4:D:80:ARG:HD3	4:D:94:PRO:O	2.10	0.52
3:C:1253:LEU:HD13	3:C:1255:ILE:HD11	1.91	0.52
3:C:1481:GLN:NE2	11:C:730:HOH:O	2.43	0.52
1:A:4:THR:HG22	1:A:608:THR:HG22	1.92	0.52
1:A:306:MET:HB3	9:C:100:P6G:H51	1.90	0.52
1:A:336:MET:HE1	1:A:422:TYR:HB3	1.92	0.52
3:C:1462:ILE:HD13	3:C:1542:ILE:HG22	1.92	0.52
4:D:344:PRO:HB2	11:D:972:HOH:O	2.09	0.52
2:B:818:VAL:CG1	2:B:820:GLU:HG2	2.38	0.51
4:D:207:GLU:O	4:D:211:SER:HB3	2.10	0.51
3:C:1251:LEU:CD1	3:C:1297:GLY:HA3	2.40	0.51
4:D:550:TYR:CE2	4:D:654:ARG:HD3	2.45	0.51
3:C:1395:MET:HE1	3:C:1423:HIS:HB2	1.93	0.51
5:E:1:NAG:O4	5:E:2:NAG:H61	2.11	0.51
4:D:571:CYS:HB3	4:D:578:THR:OG1	2.11	0.51
1:A:497:ARG:HG3	1:A:497:ARG:HH11	1.76	0.51
1:A:576:ILE:O	1:A:580:ILE:HG12	2.11	0.50
3:C:1464:ILE:HD11	3:C:1569:LEU:HD13	1.92	0.50
4:D:676:GLY:HA3	11:D:928:HOH:O	2.11	0.50
3:C:1486:VAL:O	3:C:1490:ILE:HG12	2.12	0.50
3:C:1382:VAL:O	3:C:1382:VAL:CG1	2.60	0.50
1:A:180:LYS:NZ	6:A:9187:NAG:H81	2.26	0.50
3:C:1442:LEU:O	9:C:100:P6G:H152	2.11	0.49
4:D:33:LEU:HD12	4:D:33:LEU:O	2.12	0.49
4:D:274:LYS:HE3	4:D:443:MET:O	2.12	0.49
4:D:388:LYS:HG2	11:D:807:HOH:O	2.11	0.49
2:B:720:ASP:CG	2:B:843:ARG:HH12	2.21	0.49
3:C:1291:VAL:HG21	3:C:1301:MET:HE1	1.93	0.49
4:D:45:PRO:HG3	4:D:68:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:929:ASP:C	2:B:931:ARG:H	2.21	0.48
3:C:1268:TYR:OH	3:C:1281:VAL:HG23	2.13	0.48
1:A:39:PHE:CD1	1:A:40:PRO:HA	2.49	0.48
1:A:73:SER:O	1:A:74:THR:OG1	2.27	0.48
1:A:578:ASP:O	1:A:582:LYS:HG2	2.13	0.47
3:C:1571:THR:HG23	3:C:1571:THR:O	2.13	0.47
4:D:314:LEU:O	4:D:317:ILE:HG12	2.14	0.47
3:C:1516:ASP:OD2	3:C:1548:GLN:HG2	2.15	0.47
1:A:427:ILE:CG2	1:A:438:LEU:HD11	2.45	0.47
2:B:796:LEU:HD21	2:B:798:MET:HE2	1.95	0.47
2:B:819:ASN:HA	2:B:853:LEU:HG	1.97	0.47
4:D:33:LEU:HD12	4:D:33:LEU:C	2.40	0.47
1:A:60:LEU:C	1:A:60:LEU:HD23	2.39	0.47
1:A:199:LEU:HD11	2:B:731:LYS:HG2	1.97	0.47
4:D:209:PHE:HD2	4:D:443:MET:CE	2.27	0.47
4:D:548:TYR:O	4:D:551:ASP:HB2	2.15	0.46
4:D:143:PRO:HG3	4:D:186:TRP:CE2	2.50	0.46
3:C:1285:LEU:HD13	3:C:1287:GLN:OE1	2.15	0.46
4:D:463:THR:HB	4:D:466:HIS:HB2	1.97	0.46
1:A:68:PRO:HB2	1:A:71:GLU:HG2	1.97	0.46
1:A:570:LYS:HG2	1:A:571:ILE:O	2.16	0.46
4:D:316:GLU:HA	4:D:316:GLU:OE1	2.16	0.46
1:A:83:VAL:HG13	1:A:83:VAL:O	2.16	0.46
1:A:563:TYR:OH	2:B:768:LEU:HD11	2.16	0.46
1:A:331:TYR:HA	1:A:411:ILE:O	2.16	0.46
3:C:1264:VAL:HA	3:C:1265:PRO:HD2	1.87	0.46
1:A:182:GLU:O	1:A:183:HIS:HB2	2.15	0.45
3:C:1464:ILE:HD13	3:C:1569:LEU:HD22	1.97	0.45
4:D:89:TYR:CE2	4:D:92:ARG:HG2	2.51	0.45
4:D:318:ASN:OD1	4:D:320:GLU:HG2	2.17	0.45
4:D:537:ASN:HB3	4:D:540:LYS:HD3	1.96	0.45
4:D:79:PRO:HG3	4:D:198:MET:HE1	1.98	0.45
4:D:348:PRO:HB2	4:D:352:TRP:CD1	2.52	0.45
1:A:212:PHE:CZ	1:A:320:PRO:HB3	2.52	0.45
4:D:25:ARG:NH2	4:D:27:LEU:HD21	2.31	0.45
1:A:481:LEU:HD23	1:A:482:VAL:N	2.32	0.45
4:D:730:LYS:HA	4:D:730:LYS:HD3	1.77	0.45
1:A:157:ASP:OD2	1:A:159:ASN:HB2	2.17	0.45
1:A:333:LYS:HD2	1:A:333:LYS:N	2.31	0.45
4:D:652:THR:HB	4:D:653:PRO:CD	2.47	0.45
2:B:851:LYS:HE3	2:B:851:LYS:HB3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:LEU:HD21	4:D:57:TRP:CZ2	2.52	0.44
2:B:766:VAL:CG1	2:B:783:PRO:HB3	2.47	0.44
3:C:1361:ASP:HB3	3:C:1435:LYS:HB2	1.99	0.44
2:B:860:PHE:HA	3:C:1430:GLN:HE22	1.82	0.44
4:D:158:LEU:O	4:D:159:GLU:HB2	2.18	0.44
3:C:1291:VAL:CG2	3:C:1301:MET:HE1	2.48	0.44
4:D:63:GLN:C	4:D:65:GLN:H	2.26	0.44
1:A:429:SER:HB2	1:A:438:LEU:HD12	1.97	0.44
3:C:1384:ARG:HG2	3:C:1405:LEU:HD12	1.98	0.44
1:A:225:ILE:HD12	1:A:261:ILE:HD11	2.00	0.43
1:A:73:SER:HB2	1:A:183:HIS:NE2	2.33	0.43
4:D:19:ILE:HG13	4:D:72:GLU:HA	2.00	0.43
4:D:207:GLU:HA	4:D:207:GLU:OE1	2.18	0.43
4:D:476:VAL:HG22	4:D:512:ILE:HG23	2.00	0.43
4:D:331:LYS:HD3	4:D:370:GLY:O	2.17	0.43
4:D:573:PRO:HB3	4:D:721:PHE:CZ	2.54	0.43
3:C:1537:LYS:HD2	3:C:1537:LYS:HA	1.82	0.43
5:E:2:NAG:O3	5:E:2:NAG:C7	2.66	0.43
1:A:39:PHE:CG	1:A:40:PRO:HA	2.54	0.43
1:A:333:LYS:HB3	1:A:336:MET:CE	2.45	0.43
3:C:1569:LEU:HD11	3:C:1578:ILE:HG12	2.00	0.43
4:D:215:GLU:CD	4:D:237:VAL:HG21	2.43	0.43
4:D:289:TYR:CG	4:D:333:ALA:HB2	2.54	0.43
3:C:1284:LYS:HE2	4:D:160:ASP:OD1	2.19	0.43
4:D:463:THR:HG22	4:D:464:ASP:N	2.34	0.43
1:A:28:THR:HA	1:A:29:PRO:HD3	1.89	0.43
2:B:926:ARG:NH1	3:C:1287:GLN:O	2.52	0.43
4:D:268:LEU:O	4:D:272:ILE:HG12	2.18	0.43
4:D:295:ILE:N	4:D:295:ILE:HD12	2.33	0.42
4:D:652:THR:HB	4:D:653:PRO:HD2	2.00	0.42
4:D:190:GLU:HA	4:D:191:PRO:HD3	1.81	0.42
2:B:825:ARG:O	2:B:876:ALA:HA	2.18	0.42
3:C:1510:GLU:HB2	3:C:1517:ILE:HB	2.02	0.42
4:D:470:TRP:HA	4:D:568:ARG:O	2.19	0.42
2:B:768:LEU:HB3	11:B:964:HOH:O	2.19	0.42
2:B:816:ASN:O	2:B:853:LEU:HA	2.20	0.42
3:C:1360:ILE:HD13	3:C:1436:VAL:HG22	2.02	0.42
2:B:846:GLN:HG3	11:B:272:HOH:O	2.20	0.42
2:B:824:VAL:O	2:B:847:GLN:HA	2.20	0.42
4:D:13:SER:OG	4:D:15:GLU:HG3	2.20	0.42
2:B:742:GLU:OE2	2:B:752:LYS:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:915:VAL:HB	2:B:916:GLY:H	1.72	0.41
4:D:70:LYS:HD2	4:D:70:LYS:HA	1.79	0.41
1:A:180:LYS:HZ1	6:A:9187:NAG:H81	1.85	0.41
2:B:923:ILE:N	2:B:923:ILE:HD12	2.35	0.41
3:C:1349:TYR:CG	3:C:1355:SER:HB3	2.55	0.41
4:D:730:LYS:HE3	11:D:938:HOH:O	2.20	0.41
3:C:1484:ILE:HB	3:C:1605:ASP:HB3	2.01	0.41
3:C:1405:LEU:HD23	3:C:1408:VAL:CG2	2.51	0.41
1:A:214:TYR:OH	1:A:320:PRO:HG3	2.21	0.41
1:A:401:GLU:H	1:A:401:GLU:HG2	1.62	0.41
1:A:549:PRO:CG	2:B:744:PRO:HG3	2.51	0.41
3:C:1517:ILE:HD13	3:C:1542:ILE:HG12	2.03	0.41
4:D:189:THR:HG22	4:D:420:LYS:HB3	2.03	0.41
4:D:576:GLU:HG3	4:D:737:GLY:O	2.20	0.41
1:A:180:LYS:HE3	1:A:184:SER:O	2.20	0.41
1:A:526:LEU:HD22	2:B:771:SER:HB3	2.02	0.41
1:A:531:ASP:O	1:A:532:ASN:HB2	2.21	0.41
4:D:274:LYS:HE2	4:D:447:SER:OG	2.21	0.41
4:D:468:GLN:HE21	4:D:468:GLN:HB2	1.76	0.41
4:D:531:HIS:CG	4:D:532:PRO:HD2	2.56	0.41
2:B:757:TYR:HB3	4:D:92:ARG:HD3	2.02	0.41
4:D:274:LYS:HD2	4:D:274:LYS:HA	1.84	0.41
4:D:90:TRP:HA	4:D:91:PRO:HA	1.93	0.40
9:C:100:P6G:H81	9:C:100:P6G:H52	1.37	0.40
4:D:348:PRO:HA	4:D:349:PRO:HD3	1.90	0.40
4:D:332:LYS:HE3	11:D:788:HOH:O	2.20	0.40
4:D:456:VAL:CG2	4:D:470:TRP:HZ3	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:633:ARG:NH1	11:C:574:HOH:O[3_455]	2.19	0.01

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	608/627 (97%)	597 (98%)	9 (2%)	2 (0%)	36	42
2	B	231/252 (92%)	223 (96%)	8 (4%)	0	100	100
3	C	356/379 (94%)	345 (97%)	10 (3%)	1 (0%)	36	42
4	D	679/741 (92%)	653 (96%)	26 (4%)	0	100	100
All	All	1874/1999 (94%)	1818 (97%)	53 (3%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1318	CYS
1	A	74	THR
1	A	623	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	536/548 (98%)	524 (98%)	12 (2%)	45	61
2	B	210/227 (92%)	204 (97%)	6 (3%)	37	51
3	C	332/345 (96%)	319 (96%)	13 (4%)	28	39
4	D	605/643 (94%)	589 (97%)	16 (3%)	40	55
All	All	1683/1763 (96%)	1636 (97%)	47 (3%)	38	52

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	46	LEU
1	A	92	ARG

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Mol	Chain	Res	Type
1	A	157	ASP
1	A	203	GLU
1	A	211	LYS
1	A	284	LEU
1	A	364	SER
1	A	378	LEU
1	A	401	GLU
1	A	427	ILE
1	A	536	MET
2	B	773	THR
2	B	846	GLN
2	B	896	GLU
2	B	898	VAL
2	B	918	THR
2	B	926	ARG
3	C	1251	LEU
3	C	1311	LEU
3	C	1317	VAL
3	C	1318	CYS
3	C	1329	ASN
3	C	1405	LEU
3	C	1425	GLU
3	C	1426	VAL
3	C	1474	THR
3	C	1507	LEU
3	C	1523	LEU
3	C	1538	THR
3	C	1544	GLN
4	D	33	LEU
4	D	48	THR
4	D	154	SER
4	D	167	SER
4	D	216	THR
4	D	239	ASP
4	D	458	GLU
4	D	485	SER
4	D	511	SER
4	D	541	GLU
4	D	601	GLN
4	D	616	THR
4	D	642	ASP
4	D	647	ILE

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Mol	Chain	Res	Type
4	D	654	ARG
4	D	707	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	54	ASN
1	A	80	GLN
1	A	346	ASN
1	A	414	GLN
1	A	506	ASN
2	B	846	GLN
3	C	1322	HIS
3	C	1331	HIS
3	C	1430	GLN
3	C	1441	ASN
3	C	1479	ASN
3	C	1481	GLN
3	C	1548	GLN
3	C	1552	ASN
4	D	82	HIS
4	D	165	HIS
4	D	448	GLN
4	D	533	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
5	NAG	E	1	5,4	14,14,15	0.46	0	17,19,21	1.57	1 (5%)
5	NAG	E	2	5	14,14,15	0.48	0	17,19,21	1.31	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
5	NAG	E	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	4.44	118.14	112.19
5	E	2	NAG	C1-O5-C5	3.27	116.57	112.19
5	E	2	NAG	O5-C5-C6	2.38	112.29	107.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

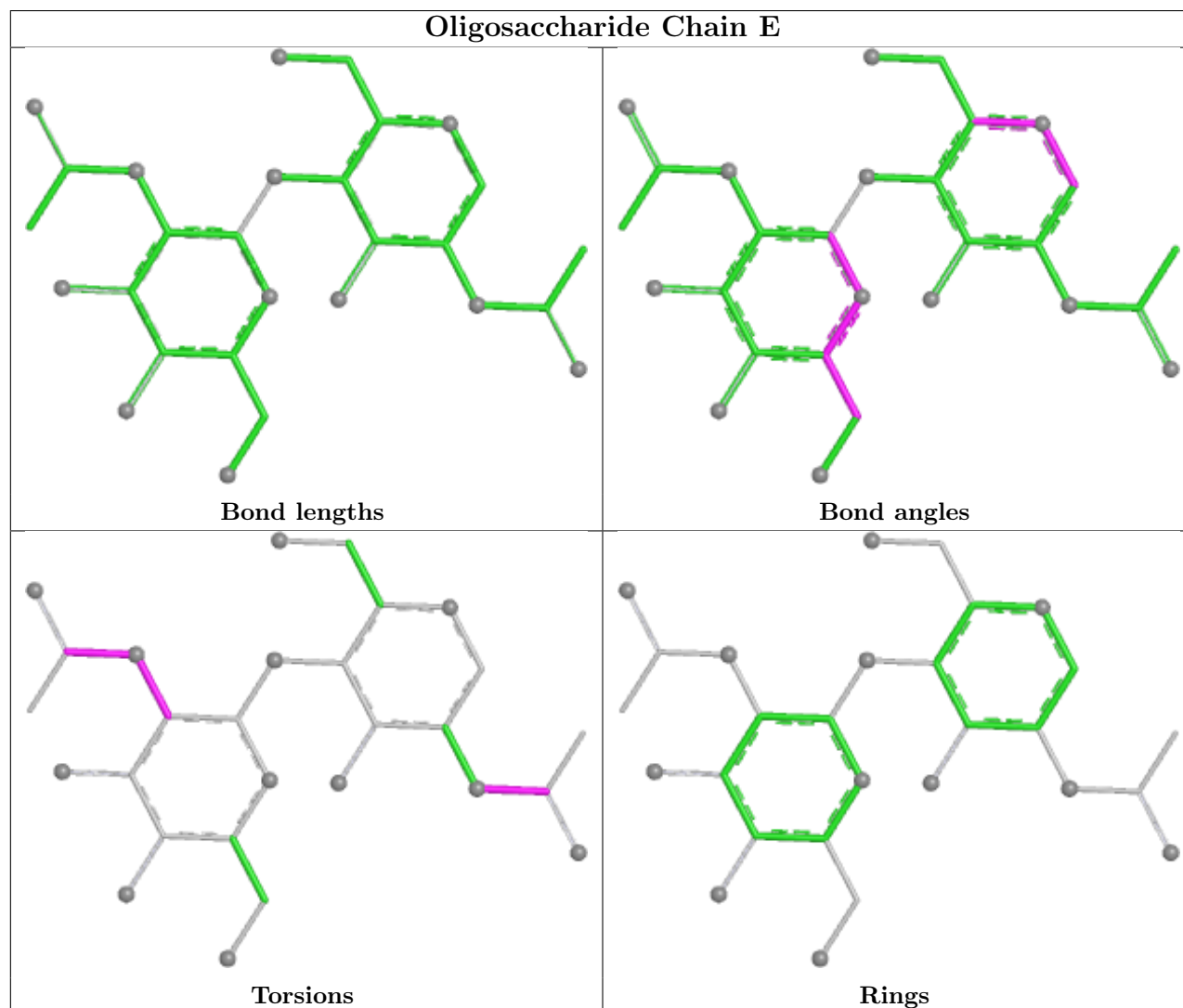
Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	2	0
5	E	1	NAG	1	0

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



5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	D	9117	4	14,14,15	0.45	0	17,19,21	1.39	2 (11%)
10	PO4	D	744	-	4,4,4	0.92	0	6,6,6	0.40	0
10	PO4	B	202	-	4,4,4	0.93	0	6,6,6	0.47	0
6	NAG	C	9324	3	14,14,15	0.64	0	17,19,21	1.19	1 (5%)
10	PO4	C	200	-	4,4,4	0.85	0	6,6,6	0.54	0
6	NAG	A	9187	1	14,14,15	0.40	0	17,19,21	1.03	1 (5%)
9	P6G	A	630	-	18,18,18	0.68	0	17,17,17	1.68	3 (17%)
10	PO4	D	743	-	4,4,4	0.91	0	6,6,6	0.63	0
9	P6G	C	100	-	18,18,18	0.46	0	17,17,17	1.76	4 (23%)
10	PO4	D	745	-	4,4,4	0.91	0	6,6,6	0.47	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
6	NAG	D	9117	4	-	2/6/23/26	0/1/1/1
6	NAG	C	9324	3	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	9187	1	-	3/6/23/26	0/1/1/1
9	P6G	A	630	-	-	4/16/16/16	-
9	P6G	C	100	-	-	5/16/16/16	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	630	P6G	O7-C6-C5	-4.58	89.47	110.35
6	C	9324	NAG	C1-O5-C5	3.93	117.45	112.19
9	C	100	P6G	C11-O10-C9	-3.84	96.46	113.26
9	C	100	P6G	O10-C11-C12	-3.72	93.40	110.35
6	D	9117	NAG	C1-O5-C5	3.23	116.52	112.19
6	D	9117	NAG	C2-N2-C7	-3.18	118.64	122.90
9	C	100	P6G	C8-O7-C6	-3.00	100.13	113.26
9	A	630	P6G	O4-C5-C6	2.98	123.95	110.35
6	A	9187	NAG	C1-O5-C5	2.94	116.12	112.19
9	C	100	P6G	O16-C15-C14	-2.57	98.64	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	630	P6G	O13-C14-C15	-2.13	100.65	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	9324	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	630	P6G	C12-C11-O10-C9
6	A	9187	NAG	C8-C7-N2-C2
6	C	9324	NAG	C8-C7-N2-C2
6	A	9187	NAG	O7-C7-N2-C2
6	C	9324	NAG	O7-C7-N2-C2
6	D	9117	NAG	C8-C7-N2-C2
6	D	9117	NAG	O7-C7-N2-C2
6	A	9187	NAG	O5-C5-C6-O6
9	C	100	P6G	C5-C6-O7-C8
9	C	100	P6G	O10-C11-C12-O13
9	C	100	P6G	C2-C3-O4-C5
9	A	630	P6G	O13-C14-C15-O16
9	C	100	P6G	C12-C11-O10-C9
9	C	100	P6G	O4-C5-C6-O7
9	A	630	P6G	C18-C17-O16-C15
9	A	630	P6G	O4-C5-C6-O7

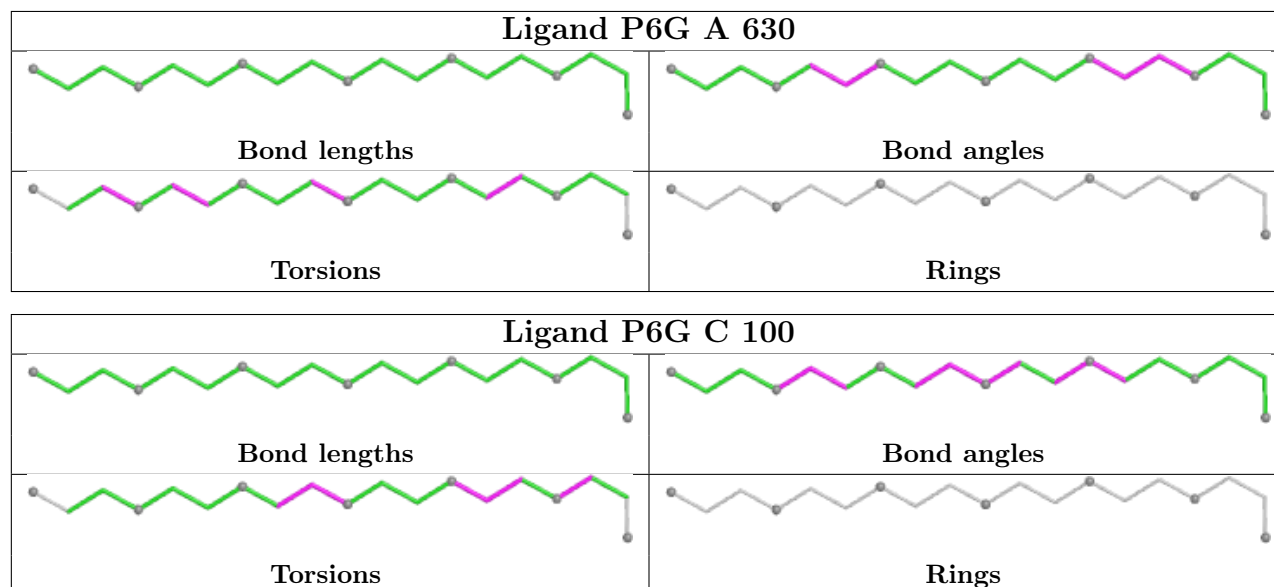
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	9187	NAG	3	0
9	A	630	P6G	3	0
9	C	100	P6G	4	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	614/627 (97%)	-0.43	10 (1%) 70 67	20, 35, 63, 113	0
2	B	233/252 (92%)	-0.36	4 (1%) 69 66	22, 37, 73, 106	0
3	C	362/379 (95%)	-0.16	6 (1%) 69 66	23, 42, 80, 108	0
4	D	693/741 (93%)	-0.06	21 (3%) 52 49	22, 45, 92, 121	0
All	All	1902/1999 (95%)	-0.24	41 (2%) 62 59	20, 40, 82, 121	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	344	PRO	4.9
4	D	504	THR	3.7
4	D	740	ALA	3.7
1	A	74	THR	3.5
4	D	463	THR	3.4
4	D	707	LYS	3.3
1	A	130	HIS	3.2
4	D	459	HIS	3.1
4	D	477	ILE	3.1
3	C	1339	GLY	3.0
4	D	479	PRO	3.0
4	D	241	SER	3.0
1	A	477	ASP	3.0
1	A	623	PRO	2.9
1	A	624	GLN	2.9
4	D	347	VAL	2.8
3	C	1382	VAL	2.8
1	A	75	ASP	2.8
1	A	138	THR	2.8
4	D	11	SER	2.8
4	D	447	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	90	TRP	2.7
3	C	1544	GLN	2.7
3	C	1311	LEU	2.7
4	D	30	GLY	2.7
2	B	934	ASP	2.6
4	D	521	ARG	2.6
4	D	240	PRO	2.6
2	B	915	VAL	2.5
3	C	1317	VAL	2.4
4	D	510	HIS	2.4
1	A	129	ASP	2.4
2	B	742	GLU	2.3
4	D	28	GLN	2.3
1	A	382	LEU	2.3
4	D	26	LEU	2.2
2	B	947	PRO	2.2
4	D	520	LYS	2.2
3	C	1272	TYR	2.2
4	D	465	TYR	2.1
1	A	162	TRP	2.1

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

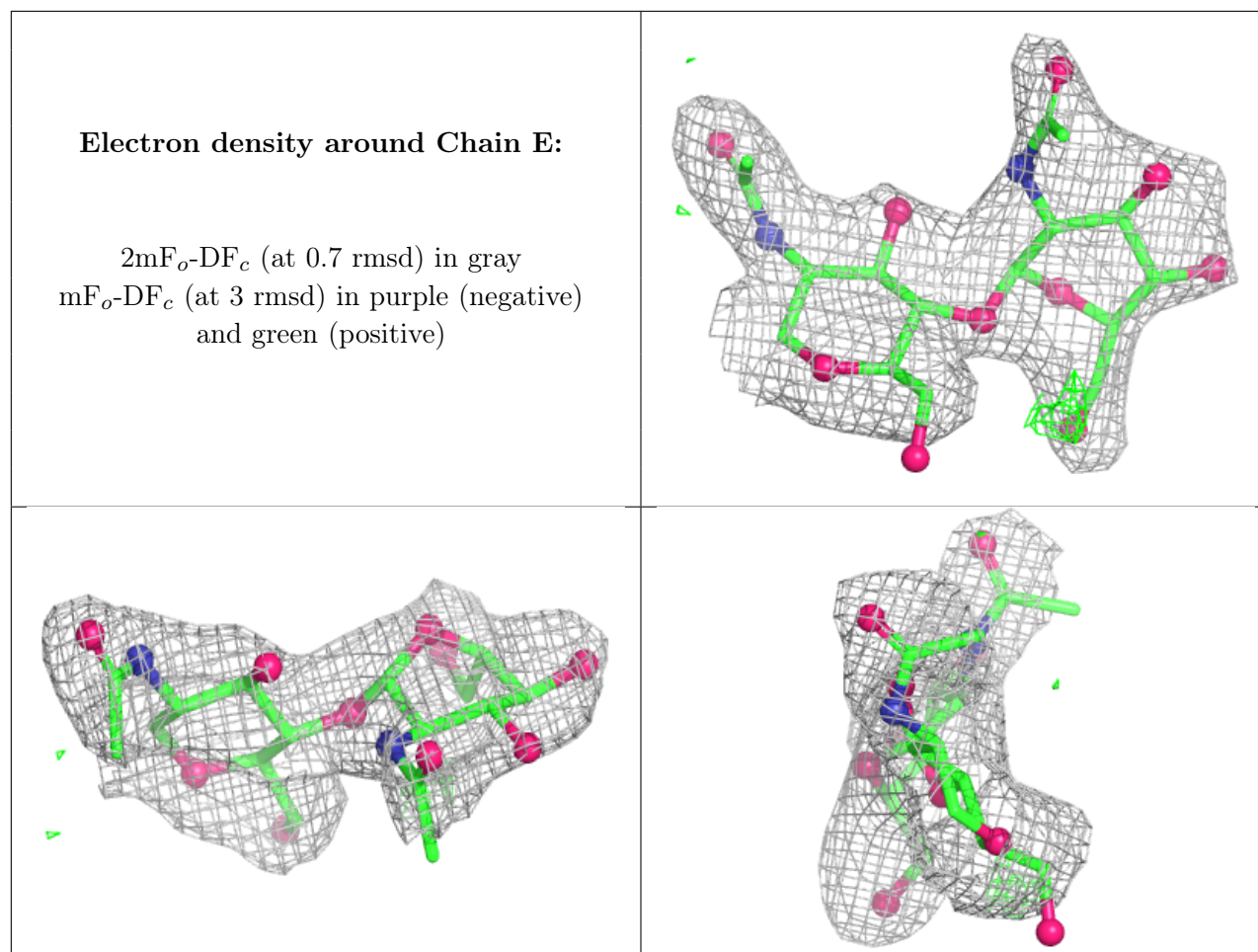
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	2	14/15	0.66	0.16	86,100,103,104	0
5	NAG	E	1	14/15	0.84	0.11	57,74,91,94	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
10	PO4	D	745	5/5	0.65	0.20	122,123,124,124	0
6	NAG	A	9187	14/15	0.72	0.14	61,81,87,91	0
9	P6G	A	630	19/19	0.77	0.21	53,85,98,98	0
6	NAG	C	9324	14/15	0.80	0.15	50,76,83,85	0
10	PO4	D	744	5/5	0.81	0.11	100,106,109,109	0
10	PO4	B	202	5/5	0.83	0.12	106,106,108,108	0
6	NAG	D	9117	14/15	0.85	0.13	56,68,82,84	0
10	PO4	C	200	5/5	0.89	0.12	45,64,68,72	0
9	P6G	C	100	19/19	0.90	0.14	29,49,65,68	0
10	PO4	D	743	5/5	0.91	0.12	75,79,80,80	0
8	K	A	629	1/1	0.95	0.19	49,49,49,49	0

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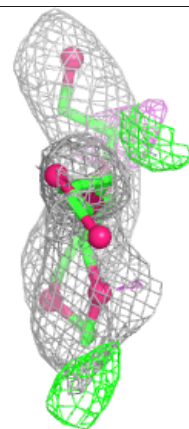
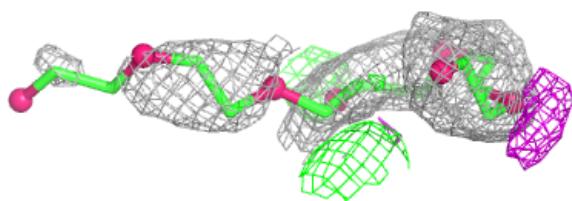
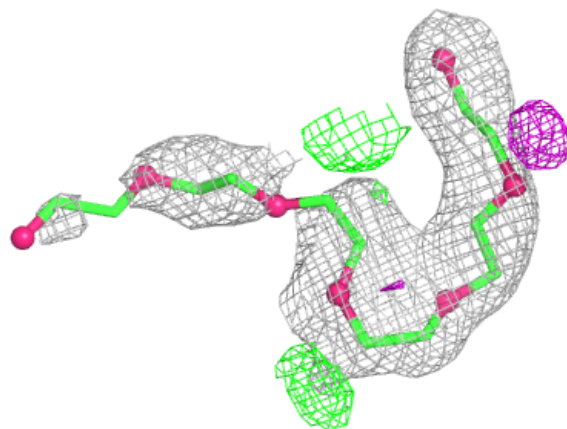
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	A	628	1/1	0.98	0.08	27,27,27,27	0
7	MG	D	742	1/1	0.99	0.02	29,29,29,29	0

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.

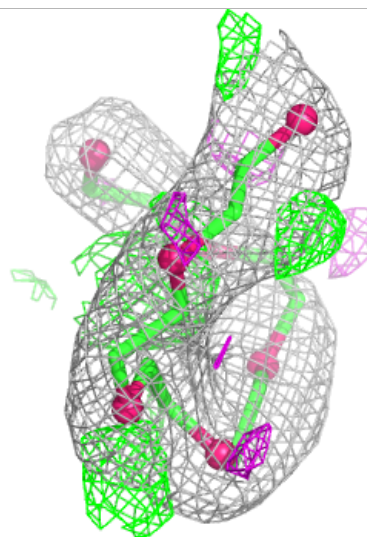
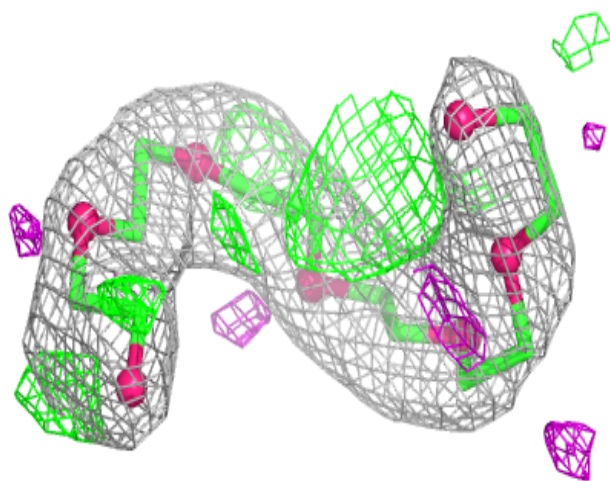
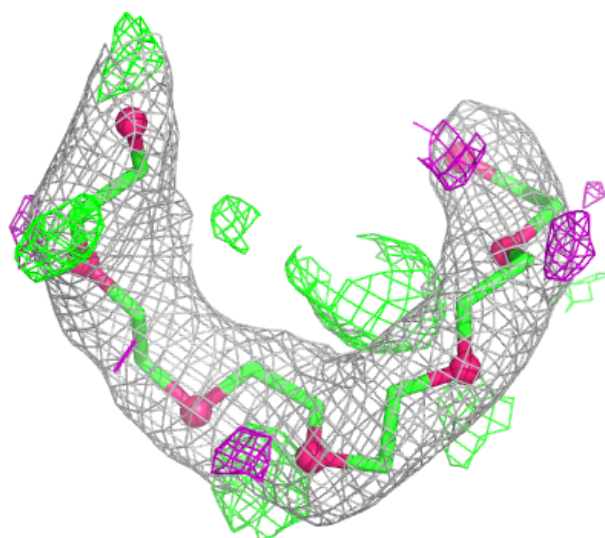
Electron density around P6G A 630:

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 P6G C 100:

$2mF_o-DF_c$ (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.