Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 02:59 pm GMT

PDB ID	:	1US1
Title	:	Crystal structure of human vascular adhesion protein-1
Authors	:	Airenne, T.T.; Nymalm, Y.; Kidron, H.; Soderholm, A.; Johnson, M.S.; Salminen, T.A.
Deposited on	:	2003-11-17
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

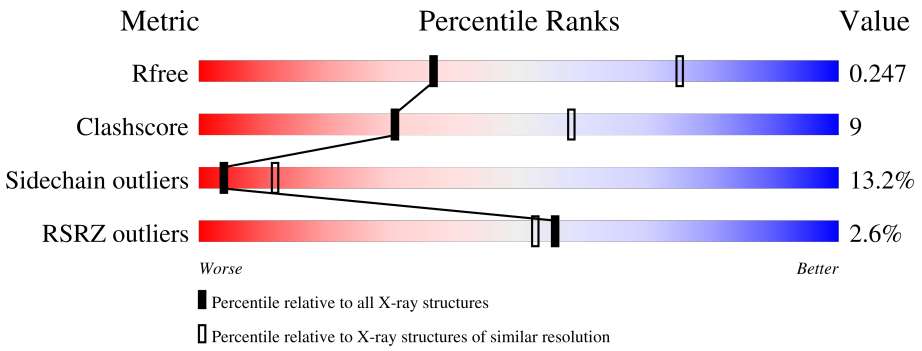
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	763	2%, 67%, 22%, •, 8%
1	B	763	3%, 67%, 21%, •, 8%
2	C	2	50%, 50%
2	D	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11153 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 MEMBRANE COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	704	5545	3560	953	1012	20	0	0	0
1	B	699	5518	3543	950	1005	20	0	0	0

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

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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	2	2	2	0	0

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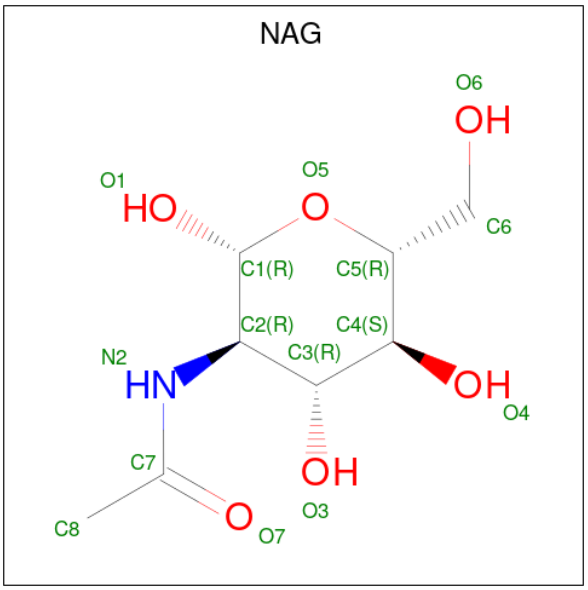
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	B	2	2	2	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



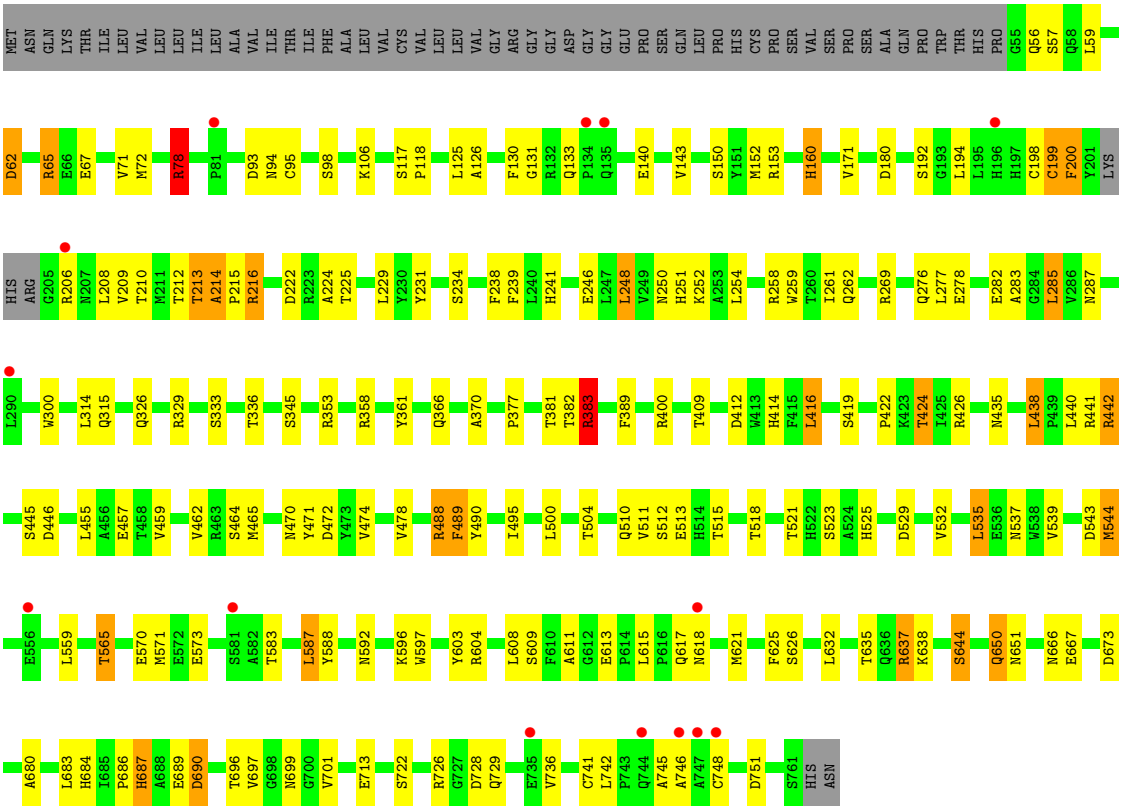
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

3 Residue-property plots (i)

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

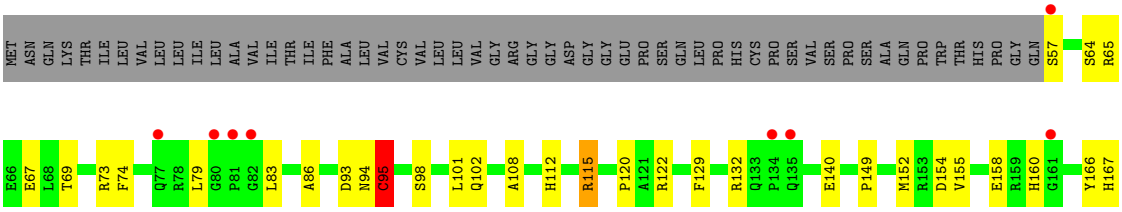
• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

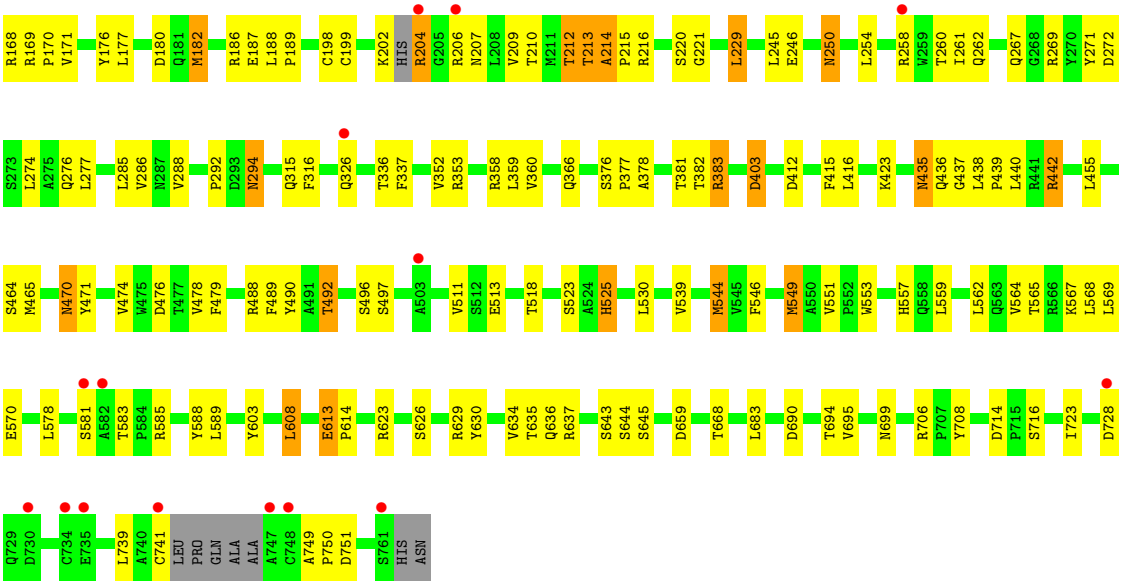
Chain A: 2% 67% 22% • 8%



• Molecule 1: MEMBRANE COPPER AMINE OXIDASE

Chain B: 3% 67% 21% • 8%



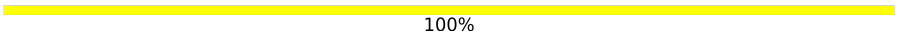


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	226.10Å 226.10Å 223.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.90 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.96-2.90) 93.6 (19.98-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.60 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.241 , 0.267 0.224 , 0.247	Depositor DCC
R_{free} test set	3477 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.789	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 27.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TPQ, CU, NAG, CA

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	0.94	4/5705 (0.1%)	1.00	19/7779 (0.2%)
1	B	0.91	2/5676 (0.0%)	0.99	16/7735 (0.2%)
All	All	0.93	6/11381 (0.1%)	1.00	35/15514 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	592	ASN	CB-CG	6.80	1.66	1.51
1	B	95	CYS	CB-SG	-5.81	1.72	1.81
1	A	214	ALA	CA-CB	-5.70	1.40	1.52
1	A	689	GLU	CD-OE1	5.25	1.31	1.25
1	A	457	GLU	CD-OE1	5.08	1.31	1.25
1	B	549	MET	SD-CE	5.01	2.06	1.77

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	383	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	A	383	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	B	154	ASP	CB-CG-OD2	8.23	125.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	637	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	62	ASP	CB-CG-OD2	7.85	125.36	118.30
1	B	690	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	543	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	751	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	728	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	403	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	529	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	93	ASP	CB-CG-OD2	6.14	123.82	118.30
1	B	412	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	637	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	751	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	180	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	168	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	728	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	216	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	353	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	690	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	65	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	544	MET	CG-SD-CE	-5.45	91.47	100.20
1	A	93	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	78	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	222	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	294	ASN	CB-CA-C	5.31	121.01	110.40
1	B	608	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	115	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	62	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	A	446	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	180	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	59	LEU	CB-CA-C	-5.07	100.56	110.20
1	B	476	ASP	CB-CG-OD2	5.06	122.86	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	THR	Peptide
1	A	438	LEU	Peptide
1	B	213	THR	Peptide
1	B	214	ALA	Peptide
1	B	292	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	57	SER	Peptide
1	B	94	ASN	Peptide

5.2 Too-close contacts (i)

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	5545	0	5293	119	0
1	B	5518	0	5270	105	0
2	C	28	0	25	1	0
2	D	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
All	All	11153	0	10639	200	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 9.

All (200) 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:621:MET:CE	1:A:621:MET:SD	2.01	1.48
1:A:571:MET:CE	1:A:571:MET:SD	2.05	1.44
1:B:549:MET:SD	1:B:549:MET:CE	2.05	1.44
1:A:441:ARG:HA	1:B:492:THR:HG21	1.56	0.86
1:A:500:LEU:HD22	1:A:510:GLN:HG3	1.61	0.82
1:A:336:THR:HG22	1:A:353:ARG:HB2	1.63	0.79
1:A:495:ILE:H	1:A:495:ILE:HD12	1.47	0.79
1:B:360:VAL:HG12	1:B:530:LEU:HD23	1.65	0.78
1:A:699:ASN:HD21	1:B:706:ARG:HH22	1.33	0.76
1:B:749:ALA:HB3	1:B:750:PRO:HD3	1.70	0.74
1:B:492:THR:HG22	1:B:694:THR:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:TYR:CD2	1:B:277:LEU:HD13	2.25	0.72
1:A:680:ALA:HB1	1:A:701:VAL:CG1	2.20	0.72
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.72	0.72
1:A:216:ARG:HD2	1:A:651:ASN:OD1	1.91	0.70
1:A:680:ALA:HB1	1:A:701:VAL:HG13	1.74	0.69
1:B:202:LYS:O	1:B:204:ARG:HA	1.94	0.68
1:A:573:GLU:OE2	1:A:666:ASN:N	2.26	0.68
1:A:495:ILE:HD12	1:A:495:ILE:N	2.09	0.68
1:A:214:ALA:CB	1:A:215:PRO:CD	2.72	0.67
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.78	0.66
1:A:212:THR:HG21	1:A:216:ARG:NH2	2.10	0.66
1:B:435:ASN:C	1:B:435:ASN:HD22	1.98	0.66
1:B:214:ALA:CB	1:B:215:PRO:CD	2.74	0.65
1:A:160:HIS:CD2	1:A:160:HIS:N	2.63	0.65
1:B:492:THR:CG2	1:B:694:THR:O	2.44	0.65
1:A:117:SER:HB3	1:A:118:PRO:HD2	1.79	0.64
1:A:214:ALA:HB3	1:A:215:PRO:CD	2.28	0.64
1:B:749:ALA:CB	1:B:750:PRO:HD3	2.28	0.64
1:A:212:THR:HG22	1:A:213:THR:N	2.14	0.63
1:A:611:ALA:O	1:B:585:ARG:NH1	2.30	0.63
1:A:212:THR:CG2	1:A:216:ARG:NH2	2.62	0.62
1:A:65:ARG:HD2	1:A:414:HIS:HD1	1.66	0.61
1:A:214:ALA:CB	1:A:215:PRO:HD3	2.30	0.61
1:A:194:LEU:HD23	1:A:277:LEU:HD21	1.83	0.61
1:B:214:ALA:CB	1:B:382:THR:HA	2.31	0.61
1:A:687:HIS:HD2	1:B:708:TYR:HD1	1.47	0.60
1:A:214:ALA:HB1	1:A:215:PRO:HD3	1.83	0.60
1:B:271:TYR:CE2	1:B:277:LEU:HD13	2.36	0.60
1:A:377:PRO:HB3	1:B:553:TRP:CZ3	2.37	0.60
1:A:687:HIS:CD2	1:B:708:TYR:HD1	2.19	0.60
1:B:250:ASN:ND2	1:B:250:ASN:C	2.55	0.60
1:A:67:GLU:O	1:A:71:VAL:HG23	2.02	0.60
1:A:366:GLN:HE21	1:A:644:SER:H	1.48	0.60
1:B:132:ARG:O	1:B:132:ARG:HG2	2.03	0.59
1:B:212:THR:HG21	1:B:216:ARG:NH2	2.18	0.59
1:B:435:ASN:ND2	1:B:437:GLY:H	2.01	0.59
1:B:636:GLN:NE2	1:B:668:THR:O	2.36	0.58
1:B:229:LEU:HD13	1:B:245:LEU:HD23	1.84	0.58
1:B:470:ASN:ND2	1:B:470:ASN:H	2.01	0.58
1:A:438:LEU:HD11	1:B:490:TYR:CZ	2.39	0.58
1:B:366:GLN:NE2	1:B:643:SER:OG	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:MET:HG2	1:B:683:LEU:HD22	1.86	0.57
1:B:272:ASP:HB2	1:B:276:GLN:HE22	1.68	0.57
1:B:214:ALA:HB3	1:B:215:PRO:CD	2.35	0.57
1:A:251:HIS:HA	1:A:259:TRP:CD1	2.40	0.57
1:A:500:LEU:CD2	1:A:510:GLN:HG3	2.33	0.57
1:B:95:CYS:HB3	1:B:129:PHE:HB2	1.88	0.56
1:B:166:TYR:O	1:B:169:ARG:HB3	2.05	0.56
1:B:250:ASN:HB2	1:B:262:GLN:NE2	2.21	0.56
1:B:214:ALA:HB1	1:B:383:ARG:H	1.70	0.56
1:A:465:MET:SD	1:B:442:ARG:HD2	2.46	0.55
1:B:182:MET:HB2	1:B:186:ARG:NH2	2.20	0.55
1:A:687:HIS:HD2	1:B:708:TYR:CD1	2.25	0.54
1:A:212:THR:HG21	1:A:216:ARG:HH22	1.71	0.54
1:A:687:HIS:CD2	1:B:708:TYR:CD1	2.96	0.54
1:B:212:THR:CG2	1:B:216:ARG:NH2	2.71	0.54
1:A:745:ALA:O	1:A:746:ALA:HB2	2.07	0.54
1:A:544:MET:HE2	1:B:683:LEU:HD13	1.89	0.54
1:B:438:LEU:HD22	1:B:439:PRO:HD2	1.90	0.53
1:A:160:HIS:N	1:A:160:HIS:HD2	2.06	0.53
1:A:224:ALA:HB1	1:A:248:LEU:HD11	1.90	0.53
1:B:108:ALA:HB1	1:B:120:PRO:HG3	1.90	0.53
1:A:495:ILE:HD11	1:A:690:ASP:O	2.08	0.53
1:B:623:ARG:HD2	1:B:659:ASP:OD2	2.09	0.53
1:A:239:PHE:CD1	1:A:470:ASN:HB3	2.45	0.52
1:B:250:ASN:C	1:B:250:ASN:HD22	2.13	0.52
1:A:314:LEU:HD23	1:B:316:PHE:CE2	2.44	0.52
1:B:415:PHE:CZ	1:B:423:LYS:HB2	2.44	0.52
1:A:117:SER:HB3	1:A:118:PRO:CD	2.39	0.52
1:B:435:ASN:C	1:B:435:ASN:ND2	2.63	0.52
1:B:64:SER:OG	1:B:67:GLU:HG3	2.10	0.52
1:B:132:ARG:O	1:B:132:ARG:CG	2.58	0.52
1:B:539:VAL:HG22	1:B:569:LEU:HB2	1.91	0.52
1:A:261:ILE:HG22	1:A:261:ILE:O	2.10	0.51
1:B:723:ILE:CD1	1:B:739:LEU:HG	2.40	0.51
1:A:565:THR:HG22	1:A:565:THR:O	2.10	0.50
1:A:696:THR:HG21	1:B:439:PRO:O	2.12	0.50
1:A:495:ILE:H	1:A:495:ILE:CD1	2.20	0.50
1:B:366:GLN:HG3	1:B:644:SER:HB2	1.92	0.50
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.93	0.50
1:B:214:ALA:HB1	1:B:215:PRO:HD3	1.93	0.50
1:A:194:LEU:CD2	1:A:277:LEU:HD21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:CB	1:A:382:THR:HA	2.42	0.50
1:A:699:ASN:ND2	1:B:706:ARG:HH22	2.05	0.50
1:A:248:LEU:HG	1:A:262:GLN:HB2	1.92	0.50
1:A:490:TYR:CZ	1:B:438:LEU:HD11	2.47	0.50
1:B:167:HIS:CE1	1:B:221:GLY:HA2	2.47	0.50
1:A:638:LYS:HZ1	1:A:667:GLU:CD	2.16	0.49
1:A:438:LEU:HD11	1:B:490:TYR:CE2	2.48	0.49
1:A:596:LYS:HD2	1:A:597:TRP:CH2	2.48	0.49
1:A:441:ARG:HA	1:B:492:THR:CG2	2.36	0.49
1:A:214:ALA:HB1	1:A:383:ARG:H	1.77	0.48
1:B:86:ALA:HA	1:B:95:CYS:SG	2.53	0.48
1:B:723:ILE:HD11	1:B:739:LEU:HG	1.96	0.48
1:B:381:THR:O	1:B:381:THR:HG22	2.15	0.47
1:A:442:ARG:HH11	1:B:403:ASP:CG	2.17	0.47
1:A:532:VAL:H	1:A:537:ASN:HD21	1.62	0.47
1:B:74:PHE:CD1	1:B:149:PRO:HB2	2.50	0.47
1:B:546:PHE:CZ	1:B:562:LEU:HD13	2.50	0.47
1:A:588:TYR:HB2	1:A:603:TYR:O	2.14	0.46
1:A:366:GLN:NE2	1:A:644:SER:H	2.14	0.46
1:A:745:ALA:O	1:A:746:ALA:CB	2.63	0.46
1:B:212:THR:HG21	1:B:216:ARG:HH22	1.80	0.46
1:A:241:HIS:CE1	1:A:300:TRP:CZ3	3.04	0.46
1:A:336:THR:CG2	1:A:353:ARG:HB2	2.42	0.46
1:A:621:MET:CE	1:A:621:MET:HB2	2.46	0.45
1:B:246:GLU:OE1	1:B:377:PRO:HD2	2.16	0.45
1:B:213:THR:HG21	1:B:378:ALA:HB1	1.98	0.45
1:B:171:VAL:HG11	1:B:176:TYR:CE1	2.52	0.45
1:A:94:ASN:ND2	1:A:130:PHE:HA	2.32	0.45
1:A:171:VAL:HG21	1:A:216:ARG:CZ	2.47	0.45
1:A:198:CYS:SG	1:A:199:CYS:N	2.89	0.45
1:B:359:LEU:HD13	1:B:603:TYR:CZ	2.52	0.45
1:A:94:ASN:HD22	1:A:131:GLY:H	1.64	0.45
1:A:440:LEU:HD23	1:A:455:LEU:HD23	1.99	0.45
1:A:442:ARG:HD2	1:B:465:MET:SD	2.57	0.45
1:A:133:GLN:OE1	2:C:1:NAG:O6	2.35	0.44
1:B:435:ASN:HD22	1:B:436:GLN:N	2.15	0.44
1:B:589:LEU:HD23	1:B:589:LEU:N	2.31	0.44
1:B:749:ALA:CB	1:B:750:PRO:CD	2.95	0.44
1:A:525:HIS:CE1	1:A:644:SER:HG	2.35	0.44
1:B:551:VAL:HG23	1:B:557:HIS:O	2.17	0.44
1:A:535:LEU:HD13	1:A:673:ASP:OD2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLU:O	1:B:274:LEU:HD12	2.18	0.44
1:B:699:ASN:HD22	1:B:699:ASN:N	2.15	0.44
1:A:246:GLU:OE1	1:A:377:PRO:HD2	2.17	0.44
1:A:389:PHE:HE1	1:A:650:GLN:OE1	2.00	0.44
1:A:315:GLN:NE2	1:B:315:GLN:HE21	2.16	0.44
1:A:251:HIS:HB2	1:A:259:TRP:CE2	2.53	0.44
1:A:488:ARG:HD3	1:A:488:ARG:HA	1.58	0.44
1:B:588:TYR:HB2	1:B:603:TYR:O	2.18	0.44
1:A:212:THR:HG22	1:A:213:THR:O	2.18	0.43
1:A:283:ALA:CB	1:A:285:LEU:HD12	2.47	0.43
1:A:98:SER:O	1:A:126:ALA:HA	2.18	0.43
1:A:224:ALA:HB1	1:A:248:LEU:CD1	2.48	0.43
1:A:250:ASN:HB2	1:A:262:GLN:NE2	2.33	0.43
1:A:214:ALA:HB2	1:A:382:THR:HG23	2.00	0.43
1:A:106:LYS:HG3	1:A:361:TYR:CE1	2.53	0.43
1:B:101:LEU:HD12	1:B:102:GLN:N	2.34	0.43
1:A:587:LEU:HD22	1:A:632:LEU:HD21	2.01	0.43
1:B:474:VAL:HB	1:B:490:TYR:HB2	2.01	0.43
1:A:212:THR:CG2	1:A:213:THR:N	2.82	0.42
1:A:414:HIS:ND1	1:A:424:THR:OG1	2.52	0.42
1:A:381:THR:O	1:A:383:ARG:HD2	2.19	0.42
1:A:465:MET:HG2	1:A:474:VAL:HG22	2.01	0.42
1:A:683:LEU:HB2	1:B:544:MET:CE	2.50	0.42
1:A:729:GLN:NE2	1:A:736:VAL:HG13	2.35	0.42
1:B:337:PHE:CZ	1:B:479:PHE:CE1	3.07	0.42
1:B:564:VAL:HG12	1:B:565:THR:N	2.33	0.42
1:A:65:ARG:HD2	1:A:414:HIS:ND1	2.33	0.42
1:B:169:ARG:HA	1:B:170:PRO:HD3	1.94	0.42
1:A:241:HIS:CE1	1:A:300:TRP:CE3	3.08	0.42
1:B:564:VAL:CG1	1:B:565:THR:N	2.81	0.42
1:B:578:LEU:HD23	1:B:630:TYR:CD2	2.55	0.42
1:B:714:ASP:OD1	1:B:716:SER:OG	2.36	0.42
1:B:352:VAL:HB	1:B:360:VAL:HG22	2.01	0.42
1:A:225:THR:OG1	1:A:251:HIS:HE1	2.03	0.42
1:A:474:VAL:HB	1:A:490:TYR:HB2	2.01	0.42
1:B:381:THR:O	1:B:381:THR:CG2	2.67	0.42
1:A:78:ARG:HH11	1:A:78:ARG:HB2	1.85	0.41
1:B:182:MET:HE2	1:B:187:GLU:OE2	2.19	0.41
1:B:286:VAL:O	1:B:286:VAL:HG12	2.20	0.41
1:A:238:PHE:C	1:A:238:PHE:CD1	2.93	0.41
1:B:271:TYR:CE2	1:B:277:LEU:CD1	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ASN:ND2	1:B:470:ASN:N	2.68	0.41
1:A:94:ASN:ND2	1:A:131:GLY:H	2.19	0.41
1:A:615:LEU:HD12	1:B:546:PHE:CE2	2.55	0.41
1:A:200:PHE:N	1:A:200:PHE:CD2	2.89	0.41
1:A:684:HIS:O	1:A:686:PRO:HD3	2.21	0.41
1:B:188:LEU:N	1:B:189:PRO:CD	2.83	0.41
1:B:440:LEU:HD23	1:B:455:LEU:HD23	2.03	0.41
1:B:525:HIS:CE1	1:B:644:SER:HG	2.36	0.41
1:B:613:GLU:HA	1:B:614:PRO:HD3	1.92	0.41
1:A:214:ALA:CB	1:A:383:ARG:H	2.33	0.41
1:A:315:GLN:HE21	1:B:315:GLN:HE21	1.69	0.41
1:A:416:LEU:HD12	1:A:422:PRO:HA	2.02	0.41
1:A:742:LEU:HA	1:A:746:ALA:HB3	2.03	0.41
1:B:539:VAL:HG11	1:B:634:VAL:HG11	2.03	0.41
1:A:94:ASN:ND2	1:A:131:GLY:N	2.69	0.41
1:A:512:SER:OG	1:A:515:THR:HB	2.21	0.41
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.90	0.40
1:A:199:CYS:HA	1:A:231:TYR:OH	2.21	0.40
1:A:416:LEU:HD12	1:A:422:PRO:CA	2.52	0.40
1:A:470:ASN:ND2	1:A:470:ASN:H	2.20	0.40
1:B:699:ASN:N	1:B:699:ASN:ND2	2.69	0.40
1:A:208:LEU:HD13	1:A:229:LEU:HD23	2.03	0.40
1:A:370:ALA:HA	1:A:521:THR:O	2.22	0.40
1:A:489:PHE:CD1	1:A:489:PHE:C	2.94	0.40
1:A:697:VAL:H	1:A:697:VAL:HG23	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

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	583/634 (92%)	500 (86%)	83 (14%)	3 10
1	B	581/634 (92%)	510 (88%)	71 (12%)	5 15
All	All	1164/1268 (92%)	1010 (87%)	154 (13%)	4 12

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	57	SER
1	A	62	ASP
1	A	65	ARG
1	A	72	MET
1	A	78	ARG
1	A	95	CYS
1	A	125	LEU
1	A	140	GLU
1	A	150	SER
1	A	152	MET
1	A	153	ARG
1	A	160	HIS
1	A	192	SER
1	A	199	CYS
1	A	200	PHE
1	A	206	ARG
1	A	209	VAL
1	A	210	THR
1	A	234	SER
1	A	248	LEU
1	A	252	LYS
1	A	254	LEU
1	A	258	ARG
1	A	269	ARG
1	A	276	GLN
1	A	278	GLU
1	A	282	GLU
1	A	285	LEU
1	A	287	ASN
1	A	326	GLN
1	A	329	ARG
1	A	333	SER

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Mol	Chain	Res	Type
1	A	345	SER
1	A	358	ARG
1	A	383	ARG
1	A	400	ARG
1	A	409	THR
1	A	416	LEU
1	A	419	SER
1	A	424	THR
1	A	426	ARG
1	A	435	ASN
1	A	442	ARG
1	A	445	SER
1	A	459	VAL
1	A	462	VAL
1	A	464	SER
1	A	472	ASP
1	A	478	VAL
1	A	488	ARG
1	A	489	PHE
1	A	504	THR
1	A	511	VAL
1	A	513	GLU
1	A	518	THR
1	A	523	SER
1	A	535	LEU
1	A	539	VAL
1	A	544	MET
1	A	559	LEU
1	A	565	THR
1	A	570	GLU
1	A	583	THR
1	A	587	LEU
1	A	604	ARG
1	A	608	LEU
1	A	609	SER
1	A	613	GLU
1	A	617	GLN
1	A	618	ASN
1	A	625	PHE
1	A	626	SER
1	A	635	THR
1	A	637	ARG

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Mol	Chain	Res	Type
1	A	644	SER
1	A	650	GLN
1	A	687	HIS
1	A	713	GLU
1	A	722	SER
1	A	726	ARG
1	A	741	CYS
1	A	748	CYS
1	B	69	THR
1	B	73	ARG
1	B	83	LEU
1	B	95	CYS
1	B	98	SER
1	B	112	HIS
1	B	115	ARG
1	B	122	ARG
1	B	140	GLU
1	B	152	MET
1	B	155	VAL
1	B	158	GLU
1	B	160	HIS
1	B	177	LEU
1	B	182	MET
1	B	198	CYS
1	B	199	CYS
1	B	204	ARG
1	B	206	ARG
1	B	207	ASN
1	B	209	VAL
1	B	210	THR
1	B	212	THR
1	B	220	SER
1	B	229	LEU
1	B	250	ASN
1	B	254	LEU
1	B	258	ARG
1	B	260	THR
1	B	261	ILE
1	B	267	GLN
1	B	269	ARG
1	B	285	LEU
1	B	288	VAL

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Mol	Chain	Res	Type
1	B	294	ASN
1	B	326	GLN
1	B	336	THR
1	B	358	ARG
1	B	376	SER
1	B	383	ARG
1	B	416	LEU
1	B	435	ASN
1	B	442	ARG
1	B	464	SER
1	B	470	ASN
1	B	478	VAL
1	B	488	ARG
1	B	489	PHE
1	B	492	THR
1	B	496	SER
1	B	497	SER
1	B	511	VAL
1	B	513	GLU
1	B	518	THR
1	B	523	SER
1	B	525	HIS
1	B	559	LEU
1	B	567	LYS
1	B	568	LEU
1	B	570	GLU
1	B	581	SER
1	B	583	THR
1	B	608	LEU
1	B	613	GLU
1	B	626	SER
1	B	629	ARG
1	B	635	THR
1	B	637	ARG
1	B	645	SER
1	B	695	VAL
1	B	741	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN

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Mol	Chain	Res	Type
1	A	160	HIS
1	A	185	ASN
1	A	207	ASN
1	A	242	HIS
1	A	251	HIS
1	A	262	GLN
1	A	287	ASN
1	A	315	GLN
1	A	319	GLN
1	A	366	GLN
1	A	435	ASN
1	A	470	ASN
1	A	537	ASN
1	A	617	GLN
1	A	687	HIS
1	A	699	ASN
1	B	94	ASN
1	B	167	HIS
1	B	207	ASN
1	B	250	ASN
1	B	251	HIS
1	B	262	GLN
1	B	276	GLN
1	B	366	GLN
1	B	435	ASN
1	B	436	GLN
1	B	470	ASN
1	B	699	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
1	TPQ	A	471	1,3	13,14,15	2.77	5 (38%)	15,19,21	2.25	4 (26%)
1	TPQ	B	471	1,3	13,14,15	3.17	5 (38%)	15,19,21	2.47	7 (46%)

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
1	TPQ	A	471	1,3	-	4/5/22/24	0/1/1/1
1	TPQ	B	471	1,3	-	4/5/22/24	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	TPQ	C3-C4	8.13	1.48	1.35
1	A	471	TPQ	C3-C4	7.37	1.46	1.35
1	B	471	TPQ	C6-C1	4.28	1.45	1.34
1	B	471	TPQ	O5-C5	4.21	1.35	1.24
1	B	471	TPQ	O2-C2	3.86	1.34	1.24
1	A	471	TPQ	O5-C5	3.73	1.34	1.24
1	A	471	TPQ	O2-C2	3.53	1.34	1.24
1	A	471	TPQ	C6-C1	3.46	1.43	1.34
1	A	471	TPQ	O4-C4	2.02	1.39	1.34
1	B	471	TPQ	C1-C2	2.01	1.52	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	TPQ	C3-C4-C5	-5.04	116.05	121.26
1	B	471	TPQ	C4-C3-C2	4.54	125.33	120.30
1	B	471	TPQ	C3-C4-C5	-4.33	116.78	121.26
1	A	471	TPQ	CA-CB-C1	-4.23	105.42	113.51
1	B	471	TPQ	CB-C1-C2	4.03	125.79	118.57
1	A	471	TPQ	C4-C3-C2	3.29	123.95	120.30
1	B	471	TPQ	C6-C1-C2	-2.76	116.52	118.64
1	B	471	TPQ	C1-C6-C5	2.63	127.45	122.52
1	B	471	TPQ	O5-C5-C4	2.60	123.64	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	471	TPQ	CB-CA-C	2.50	116.16	111.47
1	A	471	TPQ	O4-C4-C3	2.40	128.34	121.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C-CA-CB-C1
1	B	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C6-C1-CB-CA
1	A	471	TPQ	C6-C1-CB-CA
1	A	471	TPQ	N-CA-CB-C1
1	B	471	TPQ	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

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	2,1	14,14,15	0.62	0	17,19,21	2.38	6 (35%)
2	NAG	C	2	2	14,14,15	1.06	0	17,19,21	2.43	8 (47%)
2	NAG	D	1	2,1	14,14,15	0.55	0	17,19,21	1.89	7 (41%)
2	NAG	D	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.89	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
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C3-C2	2.24	1.57	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C1-O5-C5	6.98	121.66	112.19
2	C	2	NAG	O7-C7-C8	-4.92	112.93	122.06
2	D	2	NAG	O5-C1-C2	-4.20	104.66	111.29
2	D	2	NAG	O3-C3-C2	3.95	117.64	109.47
2	C	2	NAG	C3-C4-C5	-3.70	103.63	110.24
2	C	2	NAG	O7-C7-N2	3.47	128.34	121.95
2	D	1	NAG	O3-C3-C2	-3.23	102.79	109.47
2	C	2	NAG	C1-O5-C5	3.22	116.56	112.19
2	C	2	NAG	O4-C4-C3	3.22	117.80	110.35
2	D	1	NAG	C1-O5-C5	3.19	116.52	112.19
2	D	1	NAG	C4-C3-C2	3.00	115.42	111.02
2	C	2	NAG	O3-C3-C2	2.91	115.48	109.47
2	D	2	NAG	O4-C4-C5	2.89	116.47	109.30
2	D	1	NAG	O5-C1-C2	-2.85	106.79	111.29
2	C	1	NAG	C6-C5-C4	-2.80	106.45	113.00
2	C	1	NAG	C1-C2-N2	-2.68	105.91	110.49
2	C	1	NAG	O5-C5-C6	2.62	111.32	107.20
2	C	2	NAG	O4-C4-C5	2.42	115.31	109.30
2	C	1	NAG	O5-C5-C4	2.37	116.60	110.83
2	D	1	NAG	C8-C7-N2	2.33	120.04	116.10
2	C	1	NAG	O7-C7-N2	-2.32	117.69	121.95
2	C	2	NAG	C2-N2-C7	2.27	126.14	122.90
2	D	1	NAG	O7-C7-C8	-2.12	118.12	122.06
2	D	1	NAG	O5-C5-C6	2.12	110.52	107.20
2	D	2	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

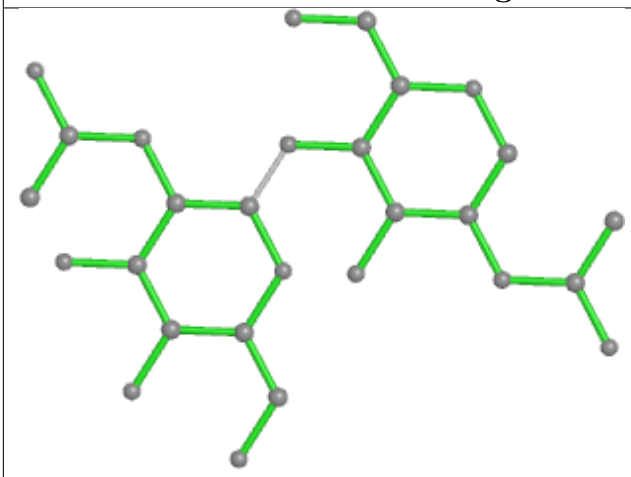
There are no ring outliers.

1 monomer is involved in 1 short contact:

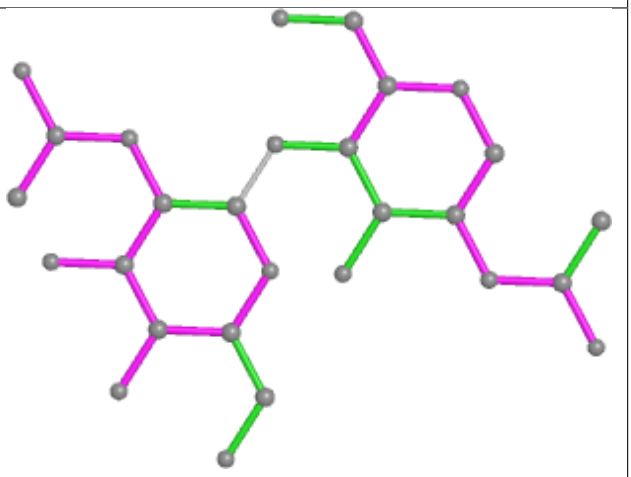
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

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

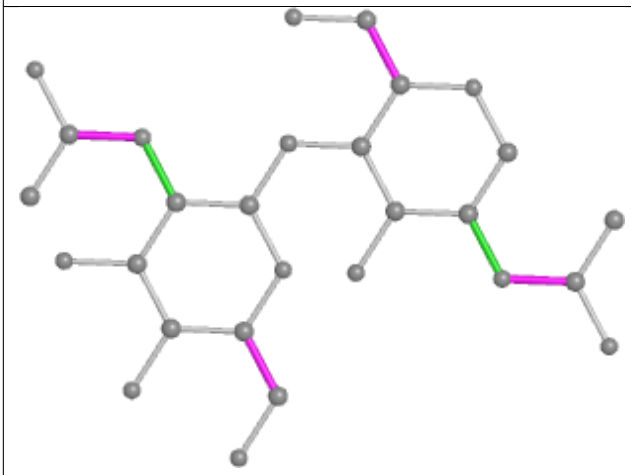
Oligosaccharide Chain C



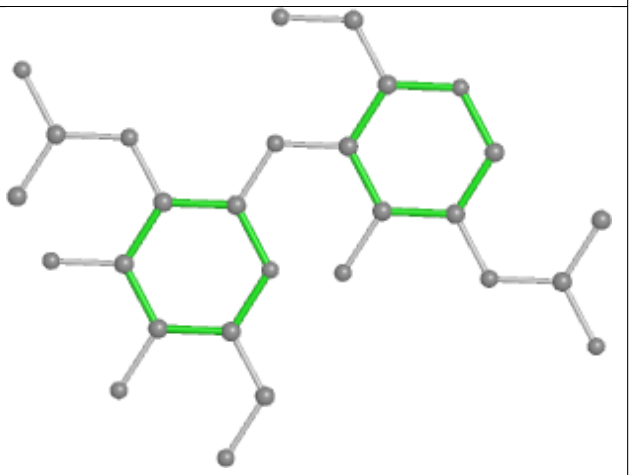
Bond lengths



Bond angles

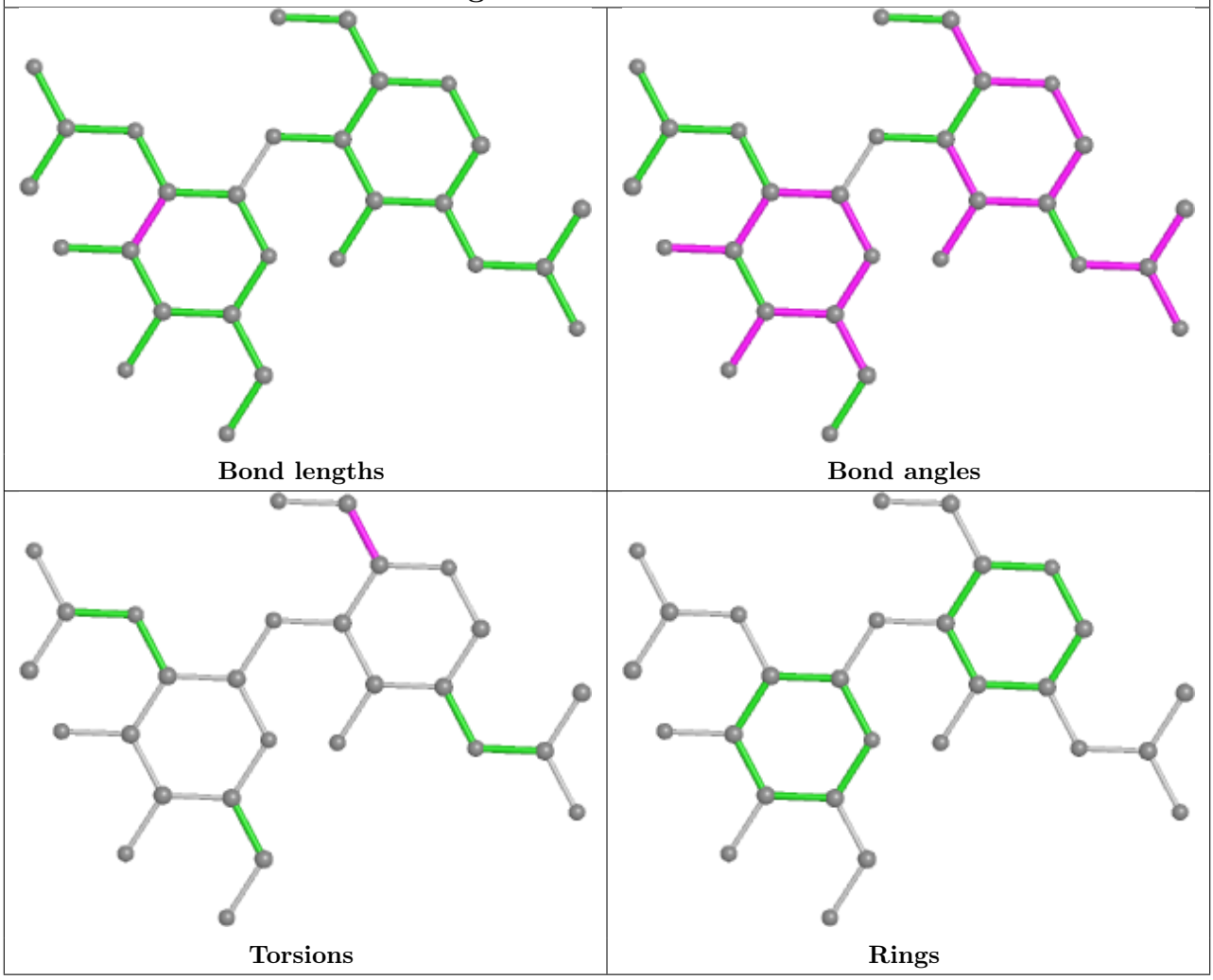


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	NAG	B	1767	1	14,14,15	1.14	0	17,19,21	1.87	5 (29%)
5	NAG	A	1767	1	14,14,15	0.84	0	17,19,21	2.24	5 (29%)

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	B	1767	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1767	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1767	NAG	O5-C5-C6	5.17	115.31	107.20
5	A	1767	NAG	C1-C2-N2	4.32	117.86	110.49
5	A	1767	NAG	C2-N2-C7	3.95	128.53	122.90
5	A	1767	NAG	O7-C7-C8	-3.58	115.41	122.06
5	A	1767	NAG	C4-C3-C2	-3.57	105.78	111.02
5	B	1767	NAG	C1-O5-C5	2.36	115.39	112.19
5	B	1767	NAG	O3-C3-C2	2.34	114.30	109.47
5	B	1767	NAG	O4-C4-C3	2.20	115.42	110.35
5	A	1767	NAG	O5-C5-C4	2.10	115.94	110.83
5	B	1767	NAG	C2-N2-C7	2.07	125.85	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1767	NAG	O5-C5-C6-O6
5	A	1767	NAG	C4-C5-C6-O6
5	B	1767	NAG	C8-C7-N2-C2
5	A	1767	NAG	O5-C5-C6-O6
5	B	1767	NAG	O7-C7-N2-C2
5	B	1767	NAG	C4-C5-C6-O6
5	A	1767	NAG	C1-C2-N2-C7
5	B	1767	NAG	C1-C2-N2-C7
5	B	1767	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	703/763 (92%)	-0.26	14 (1%)	65	63	27, 41, 58, 82	0
1	B	698/763 (91%)	-0.26	23 (3%)	46	41	26, 41, 58, 79	0
All	All	1401/1526 (91%)	-0.26	37 (2%)	56	52	26, 41, 58, 82	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	747	ALA	5.2
1	B	735	GLU	4.1
1	B	81	PRO	3.7
1	B	748	CYS	3.7
1	A	746	ALA	3.5
1	A	81	PRO	3.4
1	A	206	ARG	3.3
1	A	744	GLN	3.2
1	B	503	ALA	3.2
1	A	135	GLN	3.1
1	B	134	PRO	3.0
1	B	581	SER	2.9
1	B	326	GLN	2.8
1	B	741	CYS	2.8
1	A	134	PRO	2.7
1	B	57	SER	2.7
1	B	77	GLN	2.6
1	B	761	SER	2.6
1	B	582	ALA	2.6
1	A	556	GLU	2.5
1	B	135	GLN	2.5
1	B	82	GLY	2.5
1	B	728	ASP	2.4
1	A	747	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	80	GLY	2.3
1	B	258	ARG	2.3
1	A	735	GLU	2.3
1	B	730	ASP	2.2
1	B	734	CYS	2.2
1	B	206	ARG	2.1
1	A	290	LEU	2.1
1	A	618	ASN	2.1
1	A	581	SER	2.1
1	A	748	CYS	2.0
1	A	196	HIS	2.0
1	B	161	GLY	2.0
1	B	204	ARG	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
1	TPQ	B	471	14/15	0.90	0.17	29,35,42,42	0
1	TPQ	A	471	14/15	0.95	0.14	29,37,43,43	0

6.3 Carbohydrates (i)

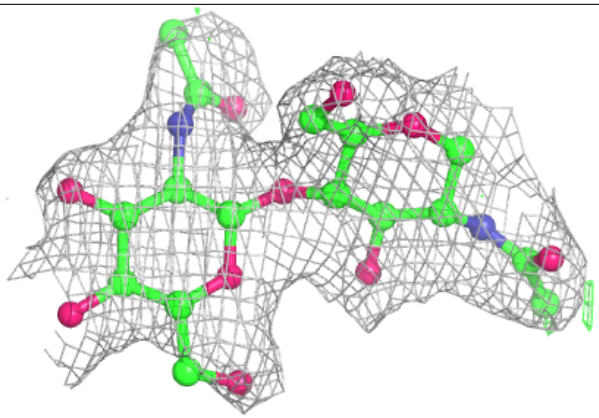
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

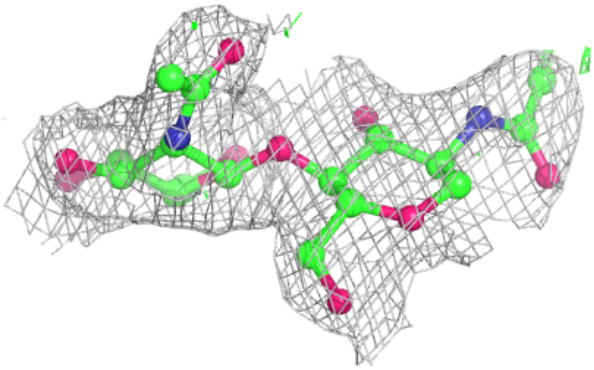
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.79	0.29	57,59,64,65	0
2	NAG	D	2	14/15	0.83	0.31	58,61,64,66	0
2	NAG	C	1	14/15	0.93	0.17	46,49,51,55	0
2	NAG	D	1	14/15	0.95	0.11	45,48,51,55	0

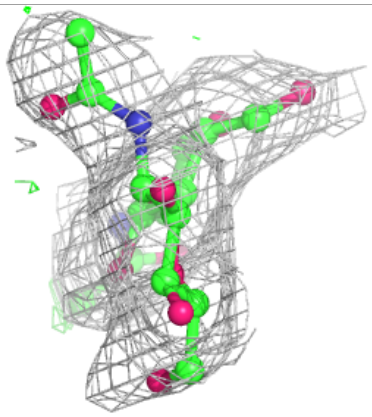
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

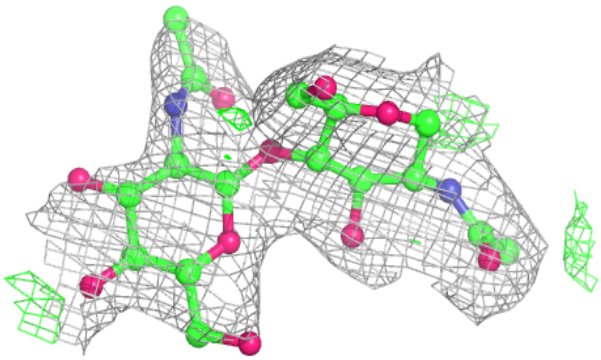


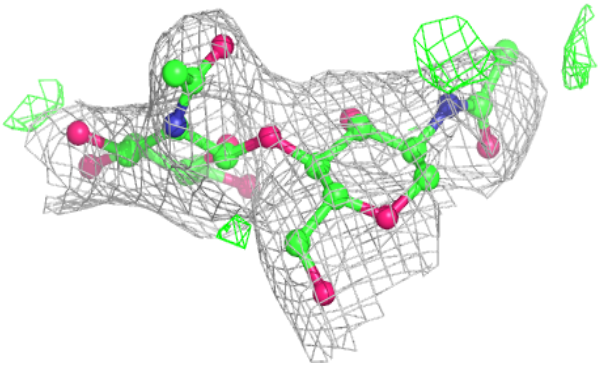


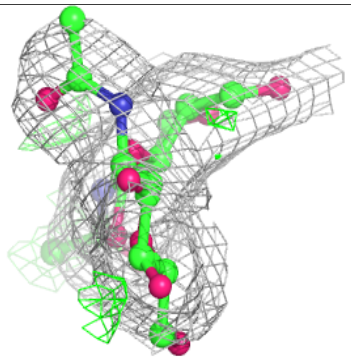


Electron density around Chain D:

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







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(Å^2)	Q<0.9
5	NAG	B	1767	14/15	0.84	0.28	61,64,66,66	0
5	NAG	A	1767	14/15	0.88	0.28	61,64,65,65	0
4	CA	A	1763	1/1	0.94	0.10	33,33,33,33	0
4	CA	B	1764	1/1	0.95	0.05	48,48,48,48	0
4	CA	B	1763	1/1	0.96	0.12	35,35,35,35	0
4	CA	A	1764	1/1	0.96	0.12	52,52,52,52	0
3	CU	A	1762	1/1	0.98	0.07	35,35,35,35	0
3	CU	B	1762	1/1	0.99	0.05	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.