Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:34 PM EDT

PDB ID	:	3R4D
Title	:	Crystal structure of mouse coronavirus receptor-binding domain complexed with its murine receptor
Authors	:	Peng, G.Q.; Sun, D.W.; Rajashankar, K.R.; Qian, Z.H.; Holmes, K.V.; Li, F.
Deposited on	:	2011-03-17
Resolution	:	3.10 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:

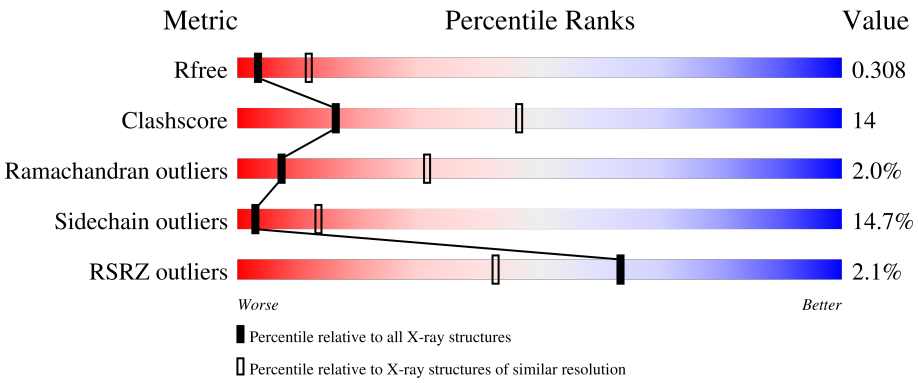
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	208	5% 61% 27% 5% • •
1	C	208	3% 49% 37% 9% • •
2	B	288	58% 19% • 20%
2	D	288	52% 24% • 20%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	50% 50%

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
3	NAG	E	2	-	-	-	X
3	NAG	F	2	-	-	-	X
4	NAG	C	300	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6982 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 CEA-related cell adhesion molecule 1, isoform 1/2S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1577	990	272	307	8	0	0	0
1	C	199	1577	990	272	307	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	HIS	-	expression tag	UNP Q3LFS8
A	204	HIS	-	expression tag	UNP Q3LFS8
A	205	HIS	-	expression tag	UNP Q3LFS8
A	206	HIS	-	expression tag	UNP Q3LFS8
A	207	HIS	-	expression tag	UNP Q3LFS8
A	208	HIS	-	expression tag	UNP Q3LFS8
C	203	HIS	-	expression tag	UNP Q3LFS8
C	204	HIS	-	expression tag	UNP Q3LFS8
C	205	HIS	-	expression tag	UNP Q3LFS8
C	206	HIS	-	expression tag	UNP Q3LFS8
C	207	HIS	-	expression tag	UNP Q3LFS8
C	208	HIS	-	expression tag	UNP Q3LFS8

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	229	1810	1189	286	328	7	0	0	0
2	D	229	1810	1189	286	328	7	0	0	0

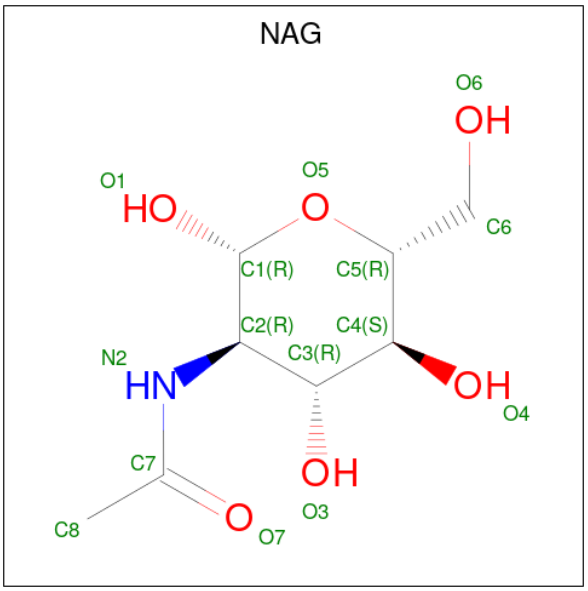
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	HIS	-	expression tag	UNP S5ZBM1
B	298	HIS	-	expression tag	UNP S5ZBM1
B	299	HIS	-	expression tag	UNP S5ZBM1
B	300	HIS	-	expression tag	UNP S5ZBM1
B	301	HIS	-	expression tag	UNP S5ZBM1
B	302	HIS	-	expression tag	UNP S5ZBM1
D	297	HIS	-	expression tag	UNP S5ZBM1
D	298	HIS	-	expression tag	UNP S5ZBM1
D	299	HIS	-	expression tag	UNP S5ZBM1
D	300	HIS	-	expression tag	UNP S5ZBM1
D	301	HIS	-	expression tag	UNP S5ZBM1
D	302	HIS	-	expression tag	UNP S5ZBM1

- Molecule 3 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			
3	E	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0

- Molecule 4 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		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
			Total	C	N	O		
4	D	1	14	8	1	5	0	0

- Molecule 5 is water.

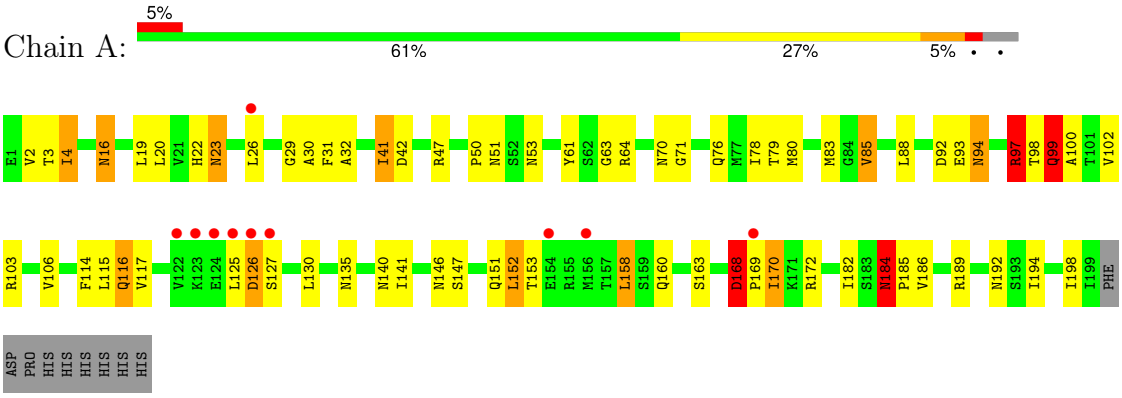
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	11	11	11	0	0
			Total	O		
5	B	17	17	17	0	0
			Total	O		
5	C	14	14	14	0	0
			Total	O		
5	D	26	26	26	0	0

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.

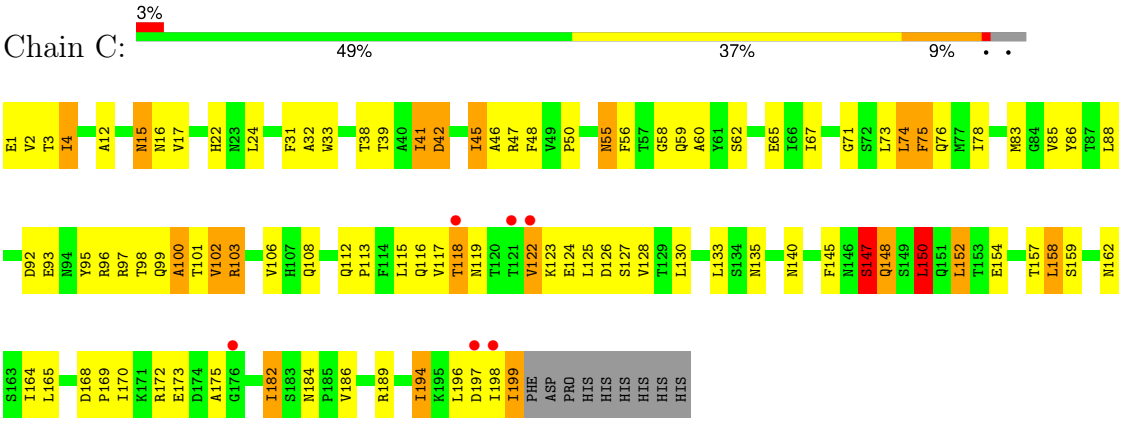
• Molecule 1: CEA-related cell adhesion molecule 1, isoform 1/2S

Chain A:



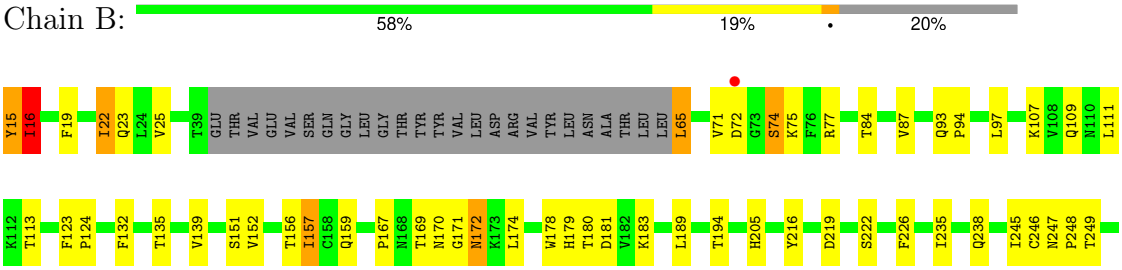
• Molecule 1: CEA-related cell adhesion molecule 1, isoform 1/2S

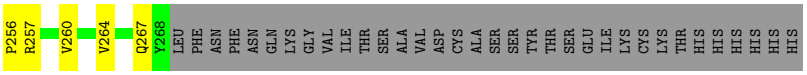
Chain C:



• Molecule 2: Spike glycoprotein

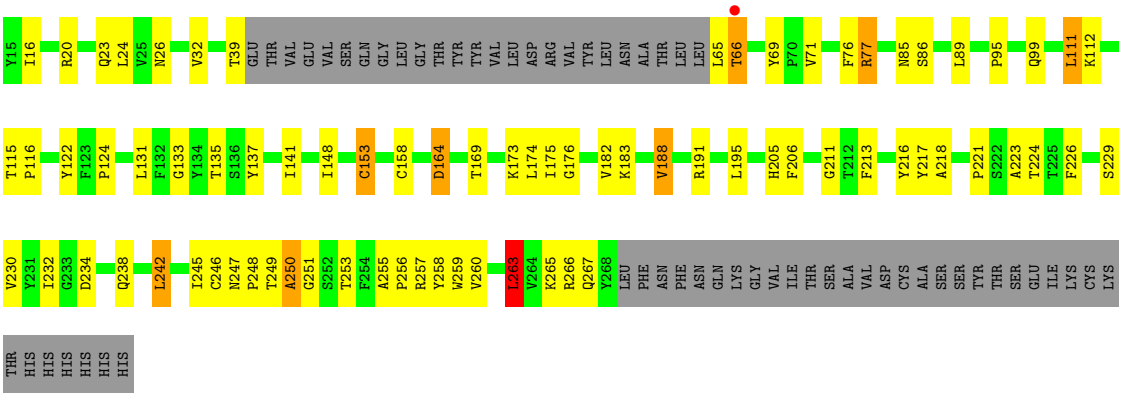
Chain B:





• Molecule 2: Spike glycoprotein

Chain D:



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

Chain E:

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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	76.38Å 76.38Å 942.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.10 39.25 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-3.10) 92.8 (39.25-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	19.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.308 0.247 , 0.308	Depositor DCC
R_{free} test set	1689 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6982	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.58	0/1604	0.74	0/2182
1	C	0.69	0/1604	0.84	4/2182 (0.2%)
2	B	0.66	0/1870	0.73	0/2560
2	D	0.71	1/1870 (0.1%)	0.79	2/2560 (0.1%)
All	All	0.66	1/6948 (0.0%)	0.77	6/9484 (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
1	A	0	2
2	B	0	1
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	153	CYS	CB-SG	-5.62	1.72	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	55	ASN	CB-CA-C	-8.61	93.17	110.40
2	D	263	LEU	CA-CB-CG	8.28	134.33	115.30
1	C	150	LEU	CA-CB-CG	7.25	131.98	115.30
2	D	164	ASP	CB-CG-OD1	-6.49	112.45	118.30
1	C	24	LEU	CA-CB-CG	6.32	129.84	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	158	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	97	ARG	Peptide
1	A	99	GLN	Peptide
2	B	15	TYR	Peptide
2	D	251	GLY	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	1577	0	1564	62	0
1	C	1577	0	1564	81	0
2	B	1810	0	1745	27	0
2	D	1810	0	1745	33	0
3	E	28	0	26	5	0
3	F	28	0	25	0	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
4	C	28	0	26	0	0
4	D	14	0	13	0	0
5	A	11	0	0	1	0
5	B	17	0	0	2	0
5	C	14	0	0	0	0
5	D	26	0	0	0	0
All	All	6982	0	6747	196	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 14.

All (196) 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:C:99:GLN:HA	1:C:100:ALA:HB2	1.31	1.11
1:C:99:GLN:HA	1:C:100:ALA:CB	1.80	1.09
2:B:132:PHE:HB3	2:B:157:ILE:HG21	1.36	1.01
1:C:98:THR:O	1:C:100:ALA:HB2	1.58	1.00
1:A:2:VAL:HG12	1:A:97:ARG:HH21	1.28	0.98
1:C:45:ILE:HG12	1:C:46:ALA:N	1.77	0.96
2:B:132:PHE:HB3	2:B:157:ILE:CG2	1.98	0.92
1:A:168:ASP:HB3	1:A:169:PRO:HD3	1.52	0.91
1:C:45:ILE:HG12	1:C:46:ALA:H	1.39	0.87
1:A:98:THR:O	1:A:99:GLN:HB2	1.74	0.87
3:E:1:NAG:C4	3:E:2:NAG:C1	2.53	0.85
1:C:103:ARG:CG	1:C:103:ARG:HH11	1.93	0.81
1:C:99:GLN:CA	1:C:100:ALA:HB2	2.10	0.81
1:A:83:MET:HB3	1:A:106:VAL:HG12	1.63	0.80
1:A:2:VAL:HG12	1:A:97:ARG:NH2	1.98	0.79
2:B:132:PHE:O	2:B:157:ILE:HG22	1.83	0.79
1:C:39:THR:O	2:D:20:ARG:NH2	2.16	0.78
1:C:4:ILE:HG13	1:C:102:VAL:HG13	1.65	0.78
1:C:123:LYS:HD2	1:C:199:ILE:HB	1.65	0.76
1:C:41:ILE:HD12	1:C:41:ILE:N	2.00	0.76
2:D:246:CYS:O	2:D:248:PRO:HD3	1.86	0.75
1:C:4:ILE:HG13	1:C:102:VAL:CG1	2.17	0.74
2:B:65:LEU:O	2:B:267:GLN:HA	1.88	0.72
1:A:168:ASP:CB	1:A:169:PRO:HD3	2.21	0.71
1:C:128:VAL:HG12	1:C:170:ILE:HD11	1.72	0.71
2:D:99:GLN:HE22	2:D:238:GLN:HE21	1.43	0.67
1:A:30:ALA:HB2	2:B:22:ILE:HD12	1.76	0.67
1:A:88:LEU:HB3	1:A:100:ALA:HB3	1.77	0.66
1:C:103:ARG:HH11	1:C:103:ARG:HG3	1.61	0.66
1:A:16:ASN:ND2	1:A:76:GLN:O	2.28	0.65
1:C:99:GLN:HA	1:C:100:ALA:HB3	1.74	0.65
1:C:41:ILE:HD13	1:C:42:ASP:OD1	1.97	0.65
1:C:98:THR:O	1:C:100:ALA:CB	2.43	0.63
1:C:127:SER:HB2	1:C:168:ASP:HB2	1.79	0.63
1:A:115:LEU:H	1:A:192:ASN:HD21	1.46	0.63
1:A:168:ASP:HB3	1:A:169:PRO:CD	2.24	0.63
1:A:127:SER:HB3	1:A:168:ASP:OD1	1.99	0.63
1:C:41:ILE:HD12	1:C:41:ILE:H	1.64	0.63
2:B:16:ILE:HD12	2:B:238:GLN:HE22	1.62	0.62
1:A:98:THR:O	1:A:99:GLN:CB	2.48	0.62
1:C:74:LEU:CD1	1:C:76:GLN:HG3	2.30	0.62
1:C:113:PRO:HG3	1:C:182:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HD13	1:C:76:GLN:HG3	1.83	0.61
1:A:16:ASN:HD22	1:A:16:ASN:N	1.98	0.61
1:C:32:ALA:HB2	1:C:47:ARG:HG3	1.82	0.60
2:D:164:ASP:HB2	2:D:245:ILE:O	2.00	0.60
1:C:3:THR:HB	1:C:22:HIS:HB2	1.81	0.60
1:C:47:ARG:NH2	2:D:23:GLN:O	2.33	0.60
1:A:78:ILE:HG22	1:A:106:VAL:HG21	1.83	0.60
1:C:115:LEU:HD11	1:C:130:LEU:HB3	1.84	0.60
2:B:156:THR:HB	2:B:180:THR:O	2.02	0.59
1:A:41:ILE:O	1:A:41:ILE:HG13	2.02	0.59
3:E:1:NAG:H4	3:E:2:NAG:C1	2.33	0.58
3:E:1:NAG:HO4	3:E:2:NAG:C1	2.10	0.58
2:B:139:VAL:HG22	2:B:152:VAL:HG22	1.85	0.58
1:A:184:ASN:O	1:A:186:VAL:N	2.36	0.58
1:A:19:LEU:HG	1:A:102:VAL:HG11	1.85	0.58
1:C:103:ARG:HH11	1:C:103:ARG:HG2	1.68	0.58
1:C:103:ARG:CG	1:C:103:ARG:NH1	2.62	0.57
1:C:41:ILE:HD13	1:C:42:ASP:H	1.70	0.56
1:A:151:GLN:O	1:A:153:THR:HG23	2.05	0.56
1:A:23:ASN:N	1:A:23:ASN:OD1	2.39	0.55
1:A:114:PHE:HE2	1:A:116:GLN:HG3	1.72	0.55
1:A:29:GLY:O	1:A:50:PRO:HD2	2.06	0.55
1:A:3:THR:O	1:A:22:HIS:O	2.25	0.55
1:C:175:ALA:HB2	1:C:198:ILE:HG12	1.88	0.55
2:B:205:HIS:CD2	5:B:315:HOH:O	2.59	0.54
1:A:85:VAL:HG12	1:A:103:ARG:HH12	1.72	0.54
1:C:31:PHE:CE2	1:C:71:GLY:HA2	2.43	0.54
1:C:83:MET:HE3	1:C:106:VAL:H	1.72	0.54
1:A:158:LEU:HD22	1:A:158:LEU:H	1.73	0.54
2:B:25:VAL:HG21	2:B:87:VAL:HG13	1.89	0.53
1:C:41:ILE:N	1:C:41:ILE:CD1	2.67	0.53
1:C:98:THR:C	1:C:100:ALA:HB2	2.25	0.53
1:A:140:ASN:O	1:A:182:ILE:HA	2.09	0.52
1:C:45:ILE:HD11	1:C:73:LEU:HD21	1.91	0.52
2:D:188:VAL:HG13	2:D:230:VAL:HG21	1.90	0.52
1:C:145:PHE:HB3	1:C:150:LEU:HB3	1.92	0.52
1:C:17:VAL:HG13	1:C:75:PHE:HB2	1.91	0.51
1:C:1:GLU:HA	1:C:97:ARG:HH12	1.75	0.50
1:A:4:ILE:HD12	1:A:20:LEU:O	2.11	0.50
2:D:124:PRO:HG2	2:D:258:TYR:HD1	1.77	0.50
1:A:31:PHE:CE2	1:A:71:GLY:HA2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASP:C	1:C:93:GLU:OE1	2.50	0.50
1:A:3:THR:N	1:A:22:HIS:O	2.44	0.50
1:C:55:ASN:O	1:C:56:PHE:CG	2.65	0.49
1:A:61:TYR:CE1	1:A:63:GLY:HA2	2.47	0.49
1:C:4:ILE:HG13	1:C:102:VAL:HG11	1.95	0.49
2:D:66:THR:HB	2:D:267:GLN:NE2	2.28	0.49
2:D:255:ALA:HB1	2:D:257:ARG:NH2	2.27	0.49
1:A:97:ARG:O	1:A:97:ARG:CG	2.60	0.49
1:A:160:GLN:HB2	1:A:163:SER:HB3	1.94	0.49
1:A:80:MET:HA	1:A:106:VAL:HG13	1.94	0.48
1:C:45:ILE:O	1:C:58:GLY:N	2.41	0.48
1:C:15:ASN:HD22	1:C:16:ASN:H	1.60	0.48
1:C:55:ASN:O	1:C:56:PHE:CD1	2.67	0.48
1:C:45:ILE:HG22	1:C:60:ALA:HB3	1.95	0.48
1:A:85:VAL:HG12	1:A:103:ARG:NH1	2.28	0.48
1:C:78:ILE:CG2	1:C:106:VAL:HG21	2.42	0.48
2:D:206:PHE:HB3	2:D:213:PHE:CZ	2.48	0.48
2:B:71:VAL:O	2:B:74:SER:HB2	2.12	0.48
1:A:117:VAL:HG12	1:A:130:LEU:HD23	1.94	0.48
2:D:26:ASN:HB2	2:D:86:SER:OG	2.13	0.48
2:D:115:THR:HB	2:D:116:PRO:HD2	1.96	0.48
1:C:103:ARG:HG2	1:C:103:ARG:NH1	2.28	0.48
2:D:205:HIS:HB2	2:D:216:TYR:HB2	1.94	0.48
2:B:216:TYR:CD1	2:B:226:PHE:HA	2.49	0.47
1:A:116:GLN:NE2	1:C:133:LEU:HB3	2.29	0.47
2:B:15:TYR:HB3	2:B:159:GLN:O	2.14	0.47
2:B:246:CYS:O	2:B:248:PRO:HD3	2.15	0.47
1:A:117:VAL:HG12	1:A:130:LEU:CD2	2.45	0.47
1:C:112:GLN:HA	1:C:189:ARG:HG2	1.96	0.47
1:A:114:PHE:CE2	1:A:116:GLN:HG3	2.50	0.47
2:B:151:SER:HA	2:B:189:LEU:O	2.15	0.47
2:B:19:PHE:HB2	2:B:156:THR:HG22	1.98	0.46
1:C:92:ASP:OD1	1:C:93:GLU:N	2.48	0.46
2:D:218:ALA:HB2	2:D:224:THR:HA	1.98	0.46
1:A:168:ASP:CB	1:A:169:PRO:CD	2.88	0.46
1:C:119:ASN:HB3	1:C:122:VAL:HG22	1.97	0.46
2:B:111:LEU:HD11	2:B:256:PRO:HA	1.98	0.46
2:D:111:LEU:HD21	2:D:256:PRO:HA	1.97	0.46
1:A:78:ILE:CG2	1:A:106:VAL:HG21	2.47	0.45
1:A:135:ASN:HD21	1:C:116:GLN:HA	1.80	0.45
2:B:169:THR:O	2:B:171:GLY:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:O	1:C:119:ASN:HB2	2.17	0.45
2:D:211:GLY:O	2:D:232:ILE:O	2.34	0.45
2:D:242:LEU:CD1	2:D:242:LEU:N	2.80	0.45
1:A:116:GLN:HA	1:C:135:ASN:HD21	1.81	0.45
1:C:41:ILE:CD1	1:C:42:ASP:H	2.29	0.45
1:A:116:GLN:HG2	1:C:135:ASN:ND2	2.32	0.45
1:C:12:ALA:O	1:C:15:ASN:HB2	2.16	0.45
2:D:77:ARG:NH2	2:D:95:PRO:O	2.50	0.45
2:D:137:TYR:CD2	2:D:232:ILE:HG23	2.51	0.45
2:B:178:TRP:CZ3	2:B:179:HIS:CD2	3.05	0.45
1:C:147:SER:O	1:C:148:GLN:HB2	2.17	0.45
1:A:80:MET:HA	1:A:106:VAL:CG1	2.47	0.44
2:D:248:PRO:C	2:D:250:ALA:H	2.20	0.44
2:D:16:ILE:O	2:D:158:CYS:O	2.35	0.44
1:A:2:VAL:HG13	1:A:2:VAL:O	2.16	0.44
2:B:219:ASP:OD2	2:B:219:ASP:N	2.51	0.44
1:C:56:PHE:CZ	2:D:24:LEU:HA	2.52	0.44
1:C:152:LEU:H	1:C:152:LEU:HG	1.48	0.44
1:C:158:LEU:HA	1:C:164:ILE:O	2.17	0.44
2:D:131:LEU:C	2:D:133:GLY:H	2.21	0.44
1:A:92:ASP:CG	1:A:93:GLU:H	2.21	0.44
1:C:4:ILE:CG1	1:C:102:VAL:CG1	2.92	0.44
1:C:168:ASP:HA	1:C:169:PRO:HA	1.62	0.44
1:A:184:ASN:OD1	1:A:186:VAL:HG12	2.18	0.44
1:C:150:LEU:HD21	1:C:165:LEU:HD21	1.99	0.44
1:A:126:ASP:O	1:A:170:ILE:HG12	2.17	0.43
1:C:42:ASP:O	1:C:59:GLN:HB3	2.18	0.43
1:A:146:ASN:O	1:A:147:SER:HB2	2.18	0.43
2:D:112:LYS:HG3	2:D:122:TYR:CZ	2.53	0.43
1:C:124:GLU:O	1:C:125:LEU:HB2	2.18	0.43
1:C:140:ASN:O	1:C:182:ILE:HA	2.19	0.43
1:A:26:LEU:HD12	1:A:26:LEU:N	2.34	0.43
3:E:2:NAG:C8	3:E:2:NAG:O3	2.66	0.43
1:C:4:ILE:CG1	1:C:102:VAL:HG13	2.43	0.43
1:A:16:ASN:ND2	1:A:16:ASN:N	2.66	0.42
2:D:76:PHE:HB3	2:D:259:TRP:HB3	2.01	0.42
1:C:158:LEU:HD13	1:C:162:ASN:OD1	2.19	0.42
2:D:175:ILE:HG22	2:D:176:GLY:N	2.34	0.42
1:A:83:MET:CB	1:A:106:VAL:HG12	2.41	0.42
2:D:148:ILE:HG13	2:D:195:LEU:HG	2.01	0.42
1:C:65:GLU:HB3	1:C:73:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:HA	1:A:94:ASN:HA	1.84	0.42
2:D:217:TYR:CG	2:D:218:ALA:N	2.87	0.42
2:D:263:LEU:O	2:D:263:LEU:HD23	2.18	0.42
1:C:117:VAL:HG11	1:C:194:ILE:HG12	2.00	0.42
1:C:45:ILE:HD11	1:C:73:LEU:CD2	2.50	0.42
1:C:86:TYR:O	1:C:101:THR:HA	2.19	0.42
1:C:93:GLU:OE1	1:C:93:GLU:N	2.53	0.41
1:A:41:ILE:HG22	5:A:210:HOH:O	2.19	0.41
1:C:78:ILE:HG21	1:C:106:VAL:HG21	2.01	0.41
1:A:184:ASN:OD1	1:A:184:ASN:C	2.59	0.41
2:B:123:PHE:HB2	2:B:124:PRO:HD2	2.01	0.41
1:C:48:PHE:CE1	1:C:50:PRO:HA	2.56	0.41
1:C:67:ILE:HG23	1:C:67:ILE:O	2.21	0.41
1:A:47:ARG:HH12	2:B:23:GLN:H	1.68	0.41
1:A:184:ASN:C	1:A:186:VAL:H	2.22	0.41
2:D:111:LEU:HB2	2:D:122:TYR:O	2.20	0.41
1:A:32:ALA:HB2	1:A:47:ARG:HG3	2.03	0.41
1:C:74:LEU:HD22	1:C:75:PHE:N	2.36	0.41
1:C:96:ARG:CZ	2:D:20:ARG:HE	2.33	0.41
2:B:15:TYR:O	2:B:16:ILE:O	2.40	0.40
2:B:205:HIS:HD2	5:B:315:HOH:O	1.98	0.40
1:C:33:TRP:CE2	1:C:88:LEU:HD13	2.56	0.40
2:D:217:TYR:CD2	2:D:218:ALA:N	2.89	0.40
1:A:92:ASP:CG	1:A:93:GLU:N	2.75	0.40
1:A:135:ASN:ND2	1:C:117:VAL:H	2.19	0.40
1:A:92:ASP:OD1	1:A:93:GLU:N	2.54	0.40
2:B:93:GLN:HB2	2:B:94:PRO:HD2	2.02	0.40
2:B:181:ASP:HB3	2:B:183:LYS:O	2.22	0.40
1:A:20:LEU:HD12	3:E:1:NAG:H83	2.02	0.40
2:B:169:THR:CG2	2:B:172:ASN:HB3	2.51	0.40
2:D:226:PHE:HZ	2:D:229:SER:HB3	1.87	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	197/208 (95%)	175 (89%)	16 (8%)	6 (3%)	4	23
1	C	197/208 (95%)	174 (88%)	20 (10%)	3 (2%)	10	39
2	B	225/288 (78%)	200 (89%)	21 (9%)	4 (2%)	8	34
2	D	225/288 (78%)	204 (91%)	17 (8%)	4 (2%)	8	34
All	All	844/992 (85%)	753 (89%)	74 (9%)	17 (2%)	7	31

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
2	B	16	ILE
2	B	72	ASP
1	C	100	ALA
1	C	147	SER
1	C	148	GLN
2	D	223	ALA
2	D	234	ASP
1	A	168	ASP
1	A	185	PRO
2	B	170	ASN
1	A	152	LEU
1	A	184	ASN
2	D	250	ALA
2	D	221	PRO
2	B	247	ASN
1	A	198	ILE

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	180/189 (95%)	154 (86%)	26 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	180/189 (95%)	147 (82%)	33 (18%)	1 7
2	B	198/252 (79%)	174 (88%)	24 (12%)	5 20
2	D	198/252 (79%)	170 (86%)	28 (14%)	3 15
All	All	756/882 (86%)	645 (85%)	111 (15%)	3 13

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	16	ASN
1	A	23	ASN
1	A	41	ILE
1	A	42	ASP
1	A	51	ASN
1	A	53	ASN
1	A	64	ARG
1	A	70	ASN
1	A	79	THR
1	A	85	VAL
1	A	94	ASN
1	A	97	ARG
1	A	99	GLN
1	A	116	GLN
1	A	125	LEU
1	A	126	ASP
1	A	141	ILE
1	A	152	LEU
1	A	158	LEU
1	A	168	ASP
1	A	170	ILE
1	A	172	ARG
1	A	184	ASN
1	A	189	ARG
1	A	194	ILE
2	B	16	ILE
2	B	22	ILE
2	B	65	LEU
2	B	74	SER
2	B	75	LYS
2	B	77	ARG
2	B	84	THR

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Mol	Chain	Res	Type
2	B	97	LEU
2	B	107	LYS
2	B	109	GLN
2	B	113	THR
2	B	135	THR
2	B	157	ILE
2	B	167	PRO
2	B	172	ASN
2	B	174	LEU
2	B	194	THR
2	B	222	SER
2	B	235	ILE
2	B	245	ILE
2	B	249	THR
2	B	257	ARG
2	B	260	VAL
2	B	264	VAL
1	C	2	VAL
1	C	4	ILE
1	C	15	ASN
1	C	38	THR
1	C	41	ILE
1	C	42	ASP
1	C	45	ILE
1	C	62	SER
1	C	74	LEU
1	C	75	PHE
1	C	85	VAL
1	C	95	TYR
1	C	102	VAL
1	C	103	ARG
1	C	108	GLN
1	C	118	THR
1	C	122	VAL
1	C	126	ASP
1	C	147	SER
1	C	150	LEU
1	C	152	LEU
1	C	154	GLU
1	C	157	THR
1	C	159	SER
1	C	172	ARG

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Mol	Chain	Res	Type
1	C	173	GLU
1	C	182	ILE
1	C	184	ASN
1	C	186	VAL
1	C	194	ILE
1	C	196	LEU
1	C	197	ASP
1	C	199	ILE
2	D	32	VAL
2	D	39	THR
2	D	65	LEU
2	D	66	THR
2	D	69	TYR
2	D	71	VAL
2	D	77	ARG
2	D	85	ASN
2	D	89	LEU
2	D	111	LEU
2	D	135	THR
2	D	141	ILE
2	D	153	CYS
2	D	169	THR
2	D	173	LYS
2	D	174	LEU
2	D	182	VAL
2	D	183	LYS
2	D	188	VAL
2	D	191	ARG
2	D	242	LEU
2	D	247	ASN
2	D	249	THR
2	D	253	THR
2	D	260	VAL
2	D	263	LEU
2	D	265	LYS
2	D	266	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	16	ASN

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Mol	Chain	Res	Type
1	A	135	ASN
1	A	140	ASN
1	A	162	ASN
1	A	179	GLN
1	A	192	ASN
2	B	99	GLN
2	B	172	ASN
2	B	179	HIS
2	B	196	ASN
2	B	238	GLN
1	C	15	ASN
1	C	22	HIS
1	C	59	GLN
1	C	108	GLN
1	C	135	ASN
1	C	161	ASN
1	C	184	ASN
2	D	85	ASN
2	D	99	GLN
2	D	179	HIS
2	D	247	ASN
2	D	267	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
3	NAG	E	1	3,1	14,14,15	0.60	0	17,19,21	2.95	7 (41%)
3	NAG	E	2	3	14,14,15	1.06	1 (7%)	17,19,21	2.48	4 (23%)
3	NAG	F	1	3,1	14,14,15	0.67	0	17,19,21	1.28	2 (11%)
3	NAG	F	2	3	14,14,15	0.45	0	17,19,21	0.86	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
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	-2.36	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	-6.64	103.28	112.19
3	E	1	NAG	C1-C2-N2	6.25	120.28	110.43
3	E	1	NAG	C2-N2-C7	6.19	131.19	122.90
3	E	2	NAG	C2-N2-C7	5.02	129.63	122.90
3	E	1	NAG	C4-C3-C2	-4.67	104.18	111.02
3	E	2	NAG	C1-C2-N2	-4.07	104.01	110.43
3	E	1	NAG	O5-C1-C2	-3.84	105.35	111.29
3	F	1	NAG	O3-C3-C2	-3.77	101.56	109.40
3	E	1	NAG	C8-C7-N2	3.55	122.01	116.12
3	E	1	NAG	C1-O5-C5	3.00	116.21	112.19
3	E	2	NAG	C8-C7-N2	2.21	119.78	116.12
3	F	1	NAG	O4-C4-C3	2.09	115.31	110.38
3	E	1	NAG	O3-C3-C2	2.09	113.74	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
3	F	2	NAG	O5-C5-C6-O6

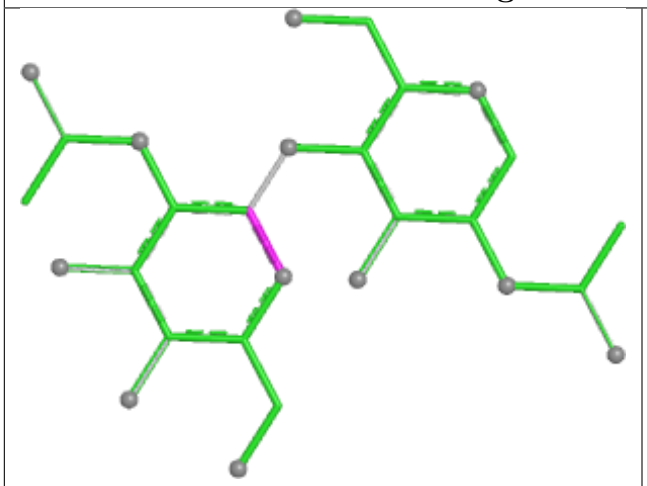
There are no ring outliers.

2 monomers are involved in 5 short contacts:

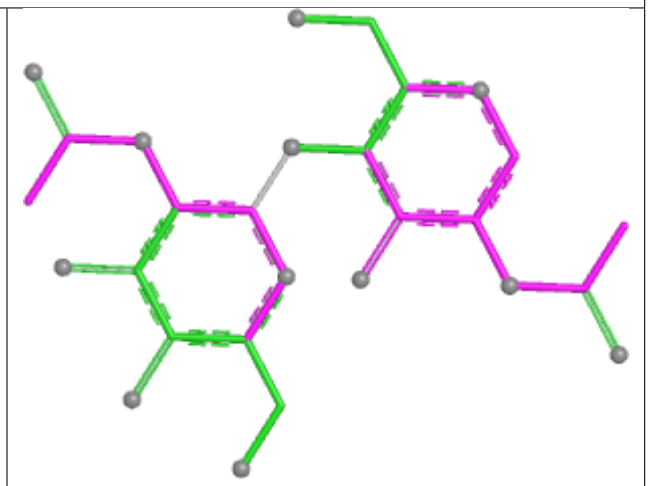
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	4	0
3	E	1	NAG	4	0

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

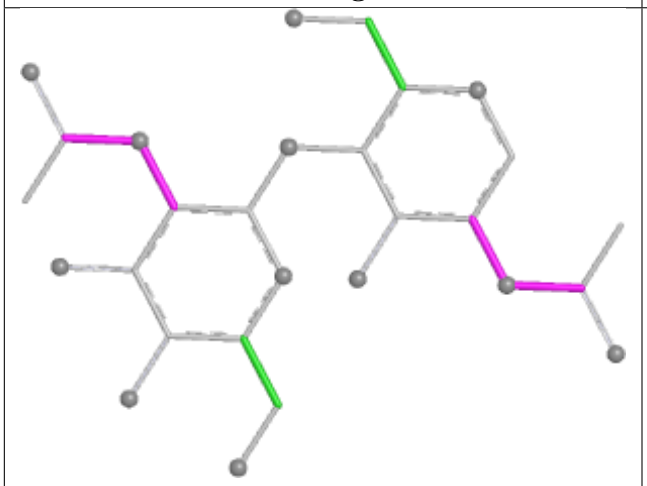
Oligosaccharide Chain E



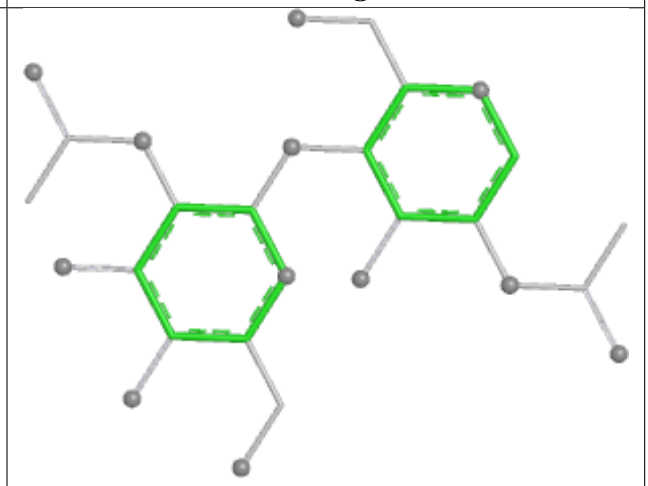
Bond lengths



Bond angles

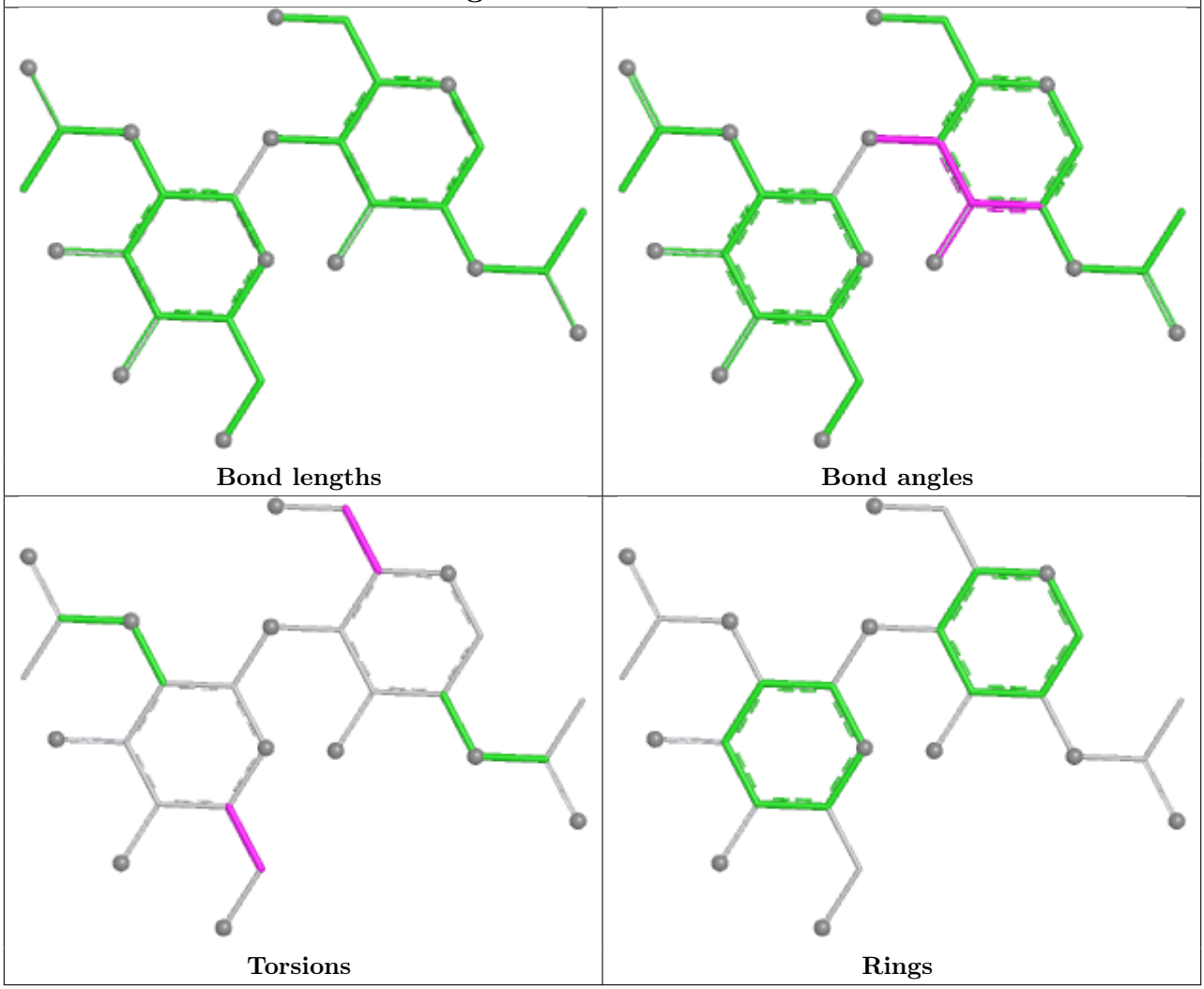


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	304	1	14,14,15	0.74	1 (7%)	17,19,21	1.02	1 (5%)
4	NAG	A	300	1	14,14,15	0.52	0	17,19,21	1.71	3 (17%)
4	NAG	C	300	1	14,14,15	0.63	0	17,19,21	2.08	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	303	2	14,14,15	0.53	0	17,19,21	1.61	1 (5%)
4	NAG	D	303	2	14,14,15	0.58	0	17,19,21	1.33	3 (17%)
4	NAG	C	304	1	14,14,15	0.59	0	17,19,21	1.33	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
4	NAG	A	304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	300	1	-	3/6/23/26	0/1/1/1
4	NAG	C	300	1	-	5/6/23/26	0/1/1/1
4	NAG	B	303	2	-	1/6/23/26	0/1/1/1
4	NAG	D	303	2	-	0/6/23/26	0/1/1/1
4	NAG	C	304	1	-	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)
4	A	304	NAG	C1-C2	2.11	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	300	NAG	C2-N2-C7	6.65	131.81	122.90
4	B	303	NAG	C1-O5-C5	5.53	119.60	112.19
4	A	300	NAG	C1-O5-C5	5.02	118.91	112.19
4	C	300	NAG	C8-C7-N2	3.16	121.35	116.12
4	A	304	NAG	C1-O5-C5	3.09	116.33	112.19
4	D	303	NAG	C1-O5-C5	2.99	116.19	112.19
4	A	300	NAG	O5-C1-C2	-2.83	106.92	111.29
4	C	304	NAG	O5-C1-C2	2.64	115.38	111.29
4	C	300	NAG	O5-C5-C6	2.55	112.62	107.66
4	D	303	NAG	O3-C3-C2	-2.25	104.73	109.40
4	A	300	NAG	C8-C7-N2	2.12	119.64	116.12
4	D	303	NAG	O7-C7-N2	2.10	125.70	121.98
4	C	304	NAG	O7-C7-C8	-2.10	118.32	122.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	300	NAG	C3-C2-N2-C7
4	C	300	NAG	O5-C5-C6-O6
4	C	300	NAG	C4-C5-C6-O6
4	A	300	NAG	C8-C7-N2-C2
4	A	300	NAG	O7-C7-N2-C2
4	C	300	NAG	C8-C7-N2-C2
4	C	300	NAG	O7-C7-N2-C2
4	B	303	NAG	O5-C5-C6-O6
4	A	300	NAG	O5-C5-C6-O6

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	199/208 (95%)	0.25	10 (5%)	28	13	50, 72, 125, 156	0
1	C	199/208 (95%)	-0.11	6 (3%)	50	27	48, 71, 113, 149	0
2	B	229/288 (79%)	-0.31	1 (0%)	92	84	45, 61, 92, 133	0
2	D	229/288 (79%)	-0.45	1 (0%)	92	84	34, 51, 81, 107	0
All	All	856/992 (86%)	-0.17	18 (2%)	63	43	34, 63, 107, 156	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	122	VAL	4.3
1	A	124	GLU	3.7
1	A	125	LEU	3.6
1	A	123	LYS	3.4
1	A	169	PRO	3.4
1	C	197	ASP	3.2
1	A	122	VAL	3.2
1	A	156	MET	3.1
1	A	26	LEU	2.9
1	C	176	GLY	2.8
1	C	198	ILE	2.7
1	C	118	THR	2.7
1	C	121	THR	2.6
1	A	126	ASP	2.6
2	B	72	ASP	2.4
1	A	127	SER	2.3
1	A	154	GLU	2.2
2	D	66	THR	2.0

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

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

6.3 Carbohydrates (i)

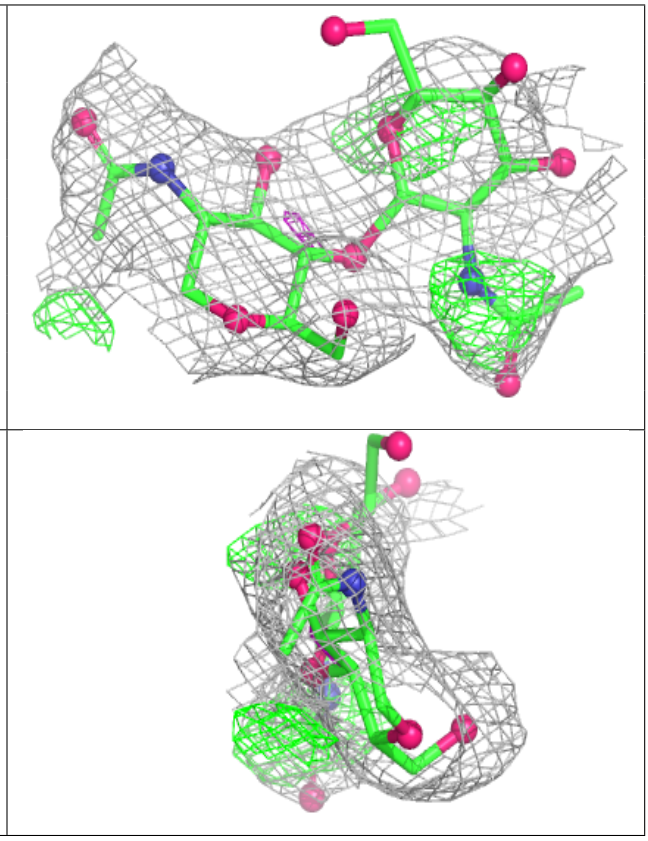
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.56	0.47	258,258,258,258	0
3	NAG	F	2	14/15	0.71	0.42	253,254,254,254	0
3	NAG	F	1	14/15	0.89	0.25	35,48,52,54	0
3	NAG	E	1	14/15	0.89	0.23	33,49,53,54	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.

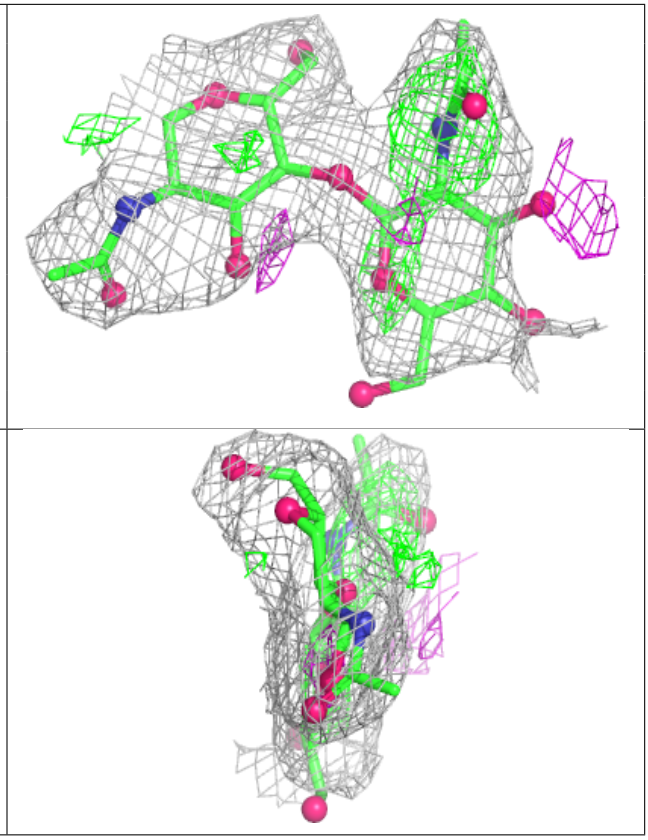
Electron density around Chain E:

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 F:

$2mF_o$-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
4	NAG	C	300	14/15	0.73	0.43	53,71,75,75	0
4	NAG	A	300	14/15	0.82	0.31	48,65,72,72	0
4	NAG	A	304	14/15	0.86	0.34	45,61,65,67	0
4	NAG	B	303	14/15	0.90	0.23	33,49,53,59	0
4	NAG	C	304	14/15	0.92	0.16	33,49,53,53	0
4	NAG	D	303	14/15	0.92	0.20	29,43,59,62	0

6.5 Other polymers (i)

There are no such residues in this entry.