Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:55 PM BST

PDB ID	:	3H5V
Title	:	Crystal structure of the GluR2-ATD
Authors	:	Jin, R.; Singh, S.K.; Gu, S.; Furukawa, H.; Sobolevsky, A.; Zhou, J.; Jin, Y.; Gouaux, E.
Deposited on	:	2009-04-22
Resolution	:	2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

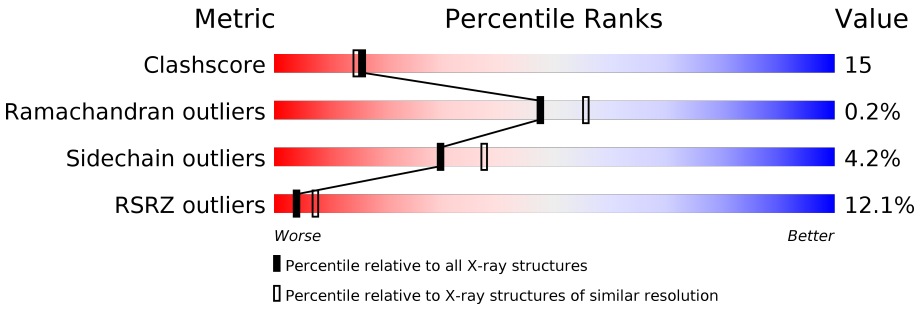
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.33 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))
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	394	3% 75% 19% • 5%
1	B	394	7% 69% 26% • 5%
1	C	394	25% 57% 35% • 5%
2	D	2	50% 50%
2	E	2	100%

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
2	NAG	E	2	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9392 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	43	0	0
			2996	1907	512	568	9			
1	B	376	Total	C	N	O	S	34	0	0
			2996	1907	512	568	9			
1	C	373	Total	C	N	O	S	35	0	0
			2976	1897	508	562	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ILE	-	expression tag	UNP P19491
A	-3	GLU	-	expression tag	UNP P19491
A	-2	GLU	-	expression tag	UNP P19491
A	-1	ARG	-	expression tag	UNP P19491
A	384	LEU	-	expression tag	UNP P19491
A	385	GLU	-	expression tag	UNP P19491
A	386	LEU	-	expression tag	UNP P19491
A	387	VAL	-	expression tag	UNP P19491
A	388	PRO	-	expression tag	UNP P19491
A	389	ARG	-	expression tag	UNP P19491
B	-4	ILE	-	expression tag	UNP P19491
B	-3	GLU	-	expression tag	UNP P19491
B	-2	GLU	-	expression tag	UNP P19491
B	-1	ARG	-	expression tag	UNP P19491
B	384	LEU	-	expression tag	UNP P19491
B	385	GLU	-	expression tag	UNP P19491
B	386	LEU	-	expression tag	UNP P19491
B	387	VAL	-	expression tag	UNP P19491
B	388	PRO	-	expression tag	UNP P19491
B	389	ARG	-	expression tag	UNP P19491
C	-4	ILE	-	expression tag	UNP P19491
C	-3	GLU	-	expression tag	UNP P19491
C	-2	GLU	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ARG	-	expression tag	UNP P19491
C	384	LEU	-	expression tag	UNP P19491
C	385	GLU	-	expression tag	UNP P19491
C	386	LEU	-	expression tag	UNP P19491
C	387	VAL	-	expression tag	UNP P19491
C	388	PRO	-	expression tag	UNP P19491
C	389	ARG	-	expression tag	UNP P19491

- 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
2	D	2	Total C N O 28 16 2 10	0	0	0
2	E	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is water.

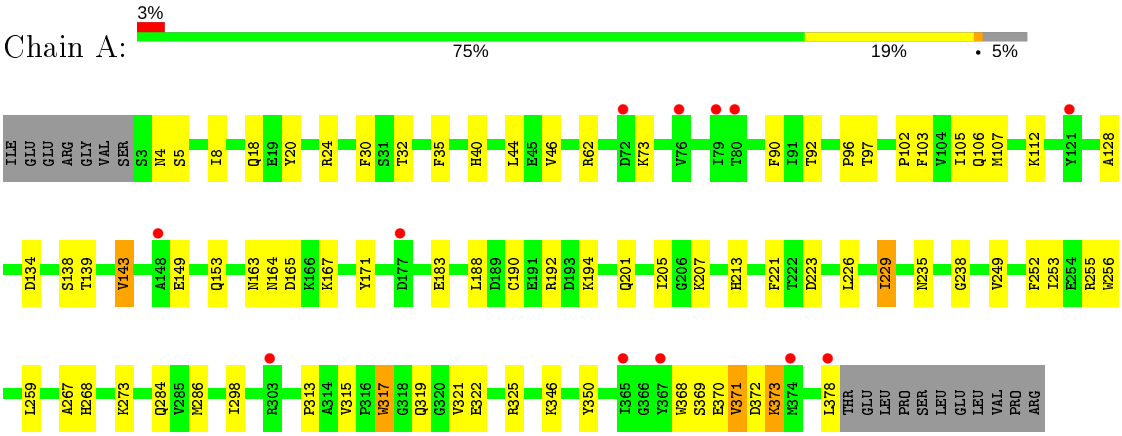
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	229	Total O 229 229	0	0
3	B	118	Total O 118 118	0	0
3	C	21	Total O 21 21	0	0

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.

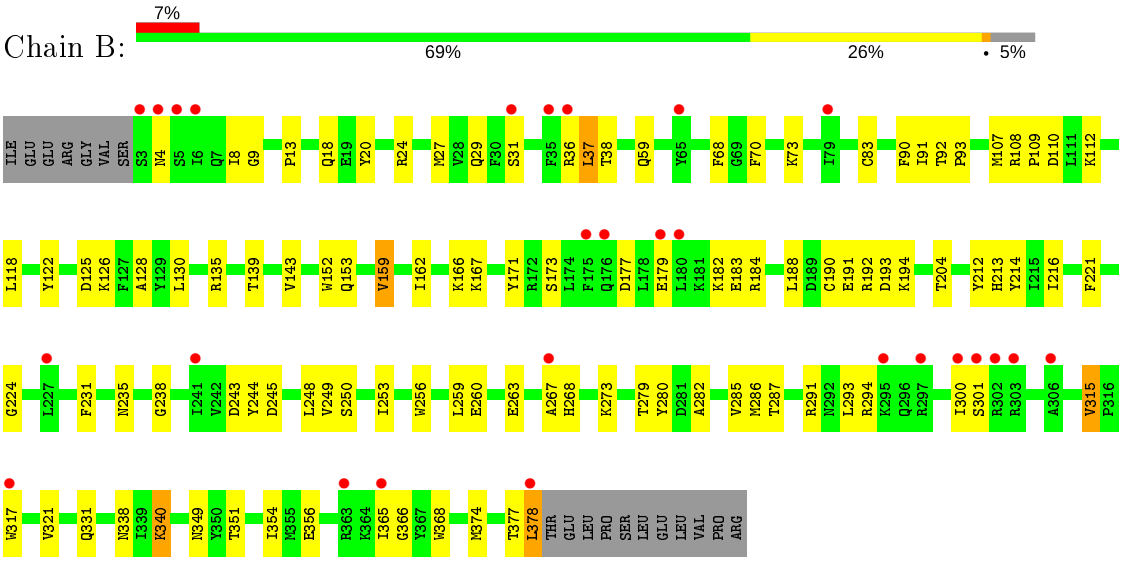
- Molecule 1: Glutamate receptor 2

Chain A:



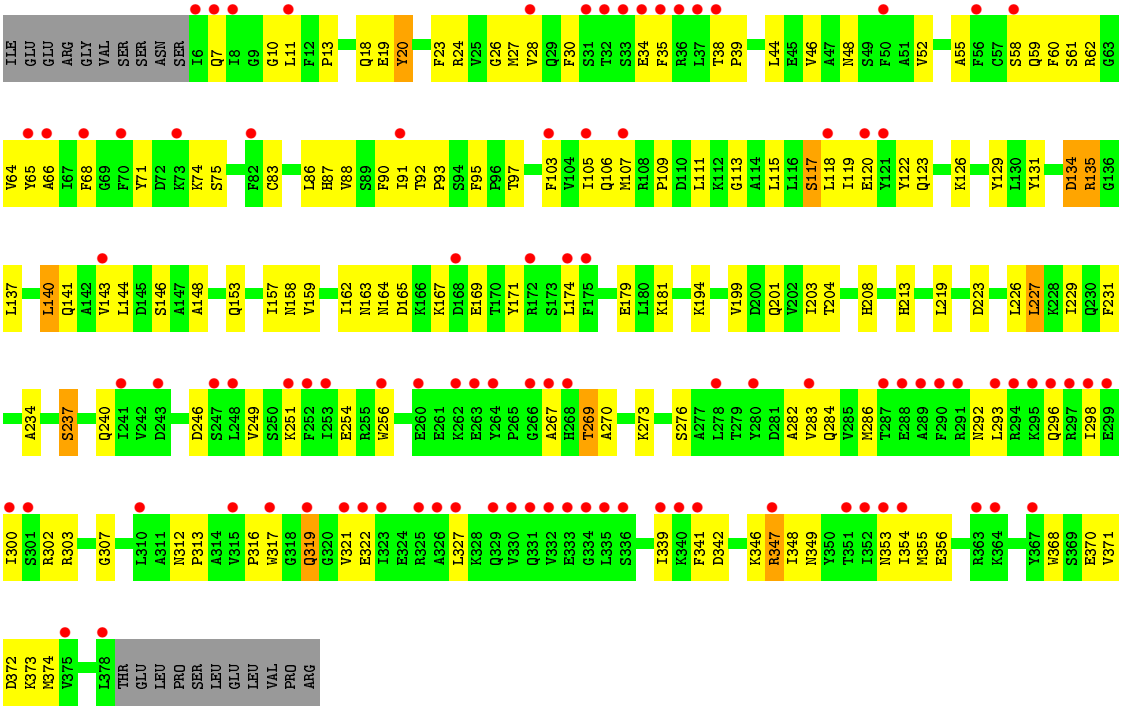
- Molecule 1: Glutamate receptor 2

Chain B:



- Molecule 1: Glutamate receptor 2

Chain C:

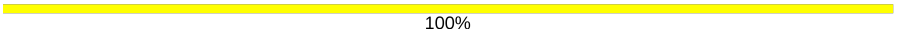


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	64.00Å 362.99Å 61.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.33 46.90 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.91-2.33) 92.4 (46.90-2.28)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.186 , 0.235 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9392	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

5.1 Standard geometry

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	0.52	0/3058	0.61	0/4136
1	B	0.43	0/3058	0.56	0/4136
1	C	0.30	0/3038	0.47	0/4109
All	All	0.43	0/9154	0.55	0/12381

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	2952	62	0
1	B	2996	0	2952	78	0
1	C	2976	0	2937	123	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	229	0	0	5	0
3	B	118	0	0	8	0
3	C	21	0	0	4	0
All	All	9392	0	8891	259	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 15.

All (259) 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:373:LYS:HD3	1:A:373:LYS:N	1.81	0.96
1:C:246:ASP:HB2	1:C:249:VAL:HG22	1.57	0.84
1:A:97:THR:H	1:A:106:GLN:NE2	1.77	0.82
1:B:4:ASN:HB3	1:B:294:ARG:HH22	1.46	0.81
1:A:259:LEU:O	1:A:268:HIS:HD2	1.68	0.77
1:A:378:LEU:HD23	1:A:378:LEU:H	1.50	0.77
1:B:366:GLY:HA2	1:B:377:THR:OG1	1.84	0.76
1:B:128:ALA:HB2	1:B:183:GLU:HG2	1.69	0.74
1:B:315:VAL:HG22	1:B:315:VAL:O	1.88	0.73
1:C:7:GLN:HA	1:C:38:THR:O	1.90	0.71
1:C:368:TRP:HA	1:C:373:LYS:O	1.90	0.71
1:B:18:GLN:HE22	1:B:273:LYS:H	1.39	0.70
1:C:339:ILE:HG12	1:C:347:ARG:HH12	1.56	0.70
1:A:97:THR:H	1:A:106:GLN:HE21	1.39	0.70
1:B:293:LEU:HD13	1:B:300:ILE:HG21	1.73	0.69
1:A:373:LYS:H	1:A:373:LYS:HD3	1.55	0.69
1:C:131:TYR:CZ	1:C:158:ASN:HB2	2.29	0.68
1:B:213:HIS:CG	1:B:235:ASN:HB2	2.30	0.67
1:C:237:SER:HB3	1:C:356:GLU:HG2	1.77	0.66
1:C:44:LEU:C	1:C:44:LEU:HD12	2.16	0.66
1:A:252:PHE:HD2	1:A:253:ILE:HD12	1.61	0.66
1:C:97:THR:H	1:C:106:GLN:HE21	1.43	0.66
1:C:269:THR:HG22	1:C:270:ALA:H	1.60	0.66
1:C:126:LYS:NZ	1:C:181:LYS:HB3	2.11	0.65
1:C:66:ALA:HB1	1:C:88:VAL:HG13	1.78	0.65
1:A:106:GLN:HE22	1:A:346:LYS:NZ	1.95	0.64
1:C:129:TYR:CE1	1:C:131:TYR:HB3	2.32	0.64
1:A:18:GLN:HE22	1:A:273:LYS:H	1.44	0.63
1:C:87:HIS:HD2	1:C:321:VAL:HG22	1.62	0.63
1:B:188:LEU:HD12	1:B:216:ILE:HD13	1.80	0.63
1:C:83:CYS:SG	1:C:90:PHE:HB2	2.38	0.63
1:A:112:LYS:HE2	1:A:138:SER:OG	1.98	0.62
1:B:107:MET:CE	1:B:282:ALA:HA	2.29	0.62
1:C:97:THR:HG23	1:C:106:GLN:NE2	2.13	0.62
1:A:105:ILE:HG22	1:A:107:MET:CE	2.29	0.62
1:B:159:VAL:HG13	1:B:194:LYS:HE3	1.80	0.62
1:A:213:HIS:CG	1:A:235:ASN:HB2	2.34	0.62
1:C:13:PRO:HA	1:C:44:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HG21	1:A:322:GLU:HG2	1.81	0.61
1:B:191:GLU:HG2	1:B:193:ASP:H	1.64	0.61
1:B:107:MET:HE3	1:B:282:ALA:HA	1.81	0.61
1:C:105:ILE:HG22	1:C:341:PHE:CE2	2.37	0.60
1:B:260:GLU:OE2	1:B:263:GLU:HB2	2.01	0.60
1:C:90:PHE:O	1:C:105:ILE:HG12	2.00	0.60
1:B:9:GLY:HA3	3:B:471:HOH:O	2.01	0.60
1:C:317:TRP:CE3	1:C:319:GLN:HG2	2.36	0.60
1:C:157:ILE:HA	3:C:393:HOH:O	2.03	0.59
1:C:339:ILE:CG1	1:C:347:ARG:HH12	2.16	0.59
1:B:130:LEU:O	1:B:188:LEU:O	2.20	0.59
1:C:20:TYR:O	1:C:23:PHE:HB3	2.02	0.59
1:B:331:GLN:CD	1:B:340:LYS:HG3	2.23	0.59
1:C:44:LEU:O	1:C:44:LEU:HD12	2.03	0.59
1:B:20:TYR:CE2	1:B:24:ARG:HD2	2.38	0.58
1:B:321:VAL:HG23	3:B:396:HOH:O	2.03	0.58
1:C:91:ILE:HD12	1:C:91:ILE:N	2.18	0.58
1:A:171:TYR:CG	1:A:201:GLN:HG2	2.38	0.58
1:B:68:PHE:CZ	1:B:279:THR:HG23	2.38	0.58
1:C:317:TRP:HE3	1:C:319:GLN:OE1	1.86	0.58
1:C:162:ILE:O	1:C:162:ILE:HG13	2.03	0.58
1:A:226:LEU:O	1:A:229:ILE:HD12	2.04	0.58
1:B:378:LEU:C	1:B:378:LEU:CD1	2.73	0.57
1:C:55:ALA:O	1:C:59:GLN:HG2	2.04	0.57
1:C:97:THR:H	1:C:106:GLN:NE2	2.02	0.57
1:C:59:GLN:HB3	1:C:64:VAL:HG11	1.87	0.57
1:A:97:THR:N	1:A:106:GLN:NE2	2.51	0.57
1:C:97:THR:HG23	1:C:106:GLN:HE21	1.70	0.57
1:A:317:TRP:CE3	1:A:319:GLN:HG2	2.40	0.57
1:A:106:GLN:HE22	1:A:346:LYS:HZ3	1.53	0.57
1:A:97:THR:N	1:A:106:GLN:HE21	2.02	0.57
1:A:153:GLN:HE21	1:B:153:GLN:NE2	2.03	0.57
1:C:317:TRP:HB2	1:C:319:GLN:OE1	2.03	0.57
1:B:27:MET:HE1	1:B:37:LEU:O	2.05	0.56
1:A:153:GLN:HE21	1:B:153:GLN:HE21	1.53	0.56
1:B:204:THR:HG22	1:C:231:PHE:HB2	1.87	0.56
1:C:223:ASP:OD2	1:C:273:LYS:HA	2.05	0.56
1:C:179:GLU:HA	3:C:401:HOH:O	2.05	0.56
1:A:249:VAL:O	1:A:253:ILE:HD13	2.06	0.56
1:C:109:PRO:HG3	1:C:347:ARG:HD2	1.87	0.56
1:B:244:TYR:HA	1:B:249:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LEU:HD12	1:C:374:MET:HE1	1.88	0.55
1:B:179:GLU:HA	3:B:504:HOH:O	2.06	0.55
1:C:11:LEU:HD23	1:C:44:LEU:HD21	1.88	0.55
1:A:205:ILE:HD11	1:A:207:LYS:HD2	1.89	0.55
1:B:287:THR:HG22	1:B:291:ARG:HH12	1.71	0.55
1:C:129:TYR:HE1	1:C:131:TYR:HB3	1.72	0.55
1:C:65:TYR:N	1:C:66:ALA:HA	2.21	0.54
1:C:13:PRO:HB3	1:C:46:VAL:HG13	1.89	0.54
1:A:350:TYR:CE2	1:A:370:GLU:HG3	2.42	0.54
1:B:190:CYS:HB3	1:B:194:LYS:HB3	1.89	0.54
1:C:339:ILE:HA	1:C:347:ARG:NH1	2.23	0.54
1:A:138:SER:HB2	3:A:528:HOH:O	2.08	0.54
1:B:36:ARG:HD2	1:B:38:THR:HG22	1.88	0.54
1:C:87:HIS:CD2	1:C:321:VAL:HG22	2.42	0.54
1:A:255:ARG:HD2	1:A:255:ARG:O	2.08	0.53
1:C:106:GLN:OE1	1:C:346:LYS:HD3	2.08	0.53
1:C:348:ILE:HD12	1:C:349:ASN:HB2	1.88	0.53
1:A:221:PHE:CD1	1:A:238:GLY:HA3	2.43	0.53
1:A:190:CYS:HB3	1:A:194:LYS:HB3	1.91	0.53
1:C:146:SER:C	1:C:148:ALA:N	2.62	0.53
1:B:27:MET:O	1:B:31:SER:HB3	2.08	0.53
1:C:240:GLN:O	1:C:353:ASN:HB2	2.09	0.53
1:C:115:LEU:O	1:C:119:ILE:HG13	2.09	0.52
1:C:162:ILE:HD11	1:C:194:LYS:HZ1	1.75	0.52
1:B:259:LEU:O	1:B:268:HIS:HD2	1.92	0.52
1:C:122:TYR:CE2	1:C:213:HIS:HE1	2.27	0.52
1:A:40:HIS:HE1	3:A:565:HOH:O	1.92	0.52
1:C:18:GLN:HE22	1:C:273:LYS:H	1.59	0.51
1:A:317:TRP:CE3	1:A:319:GLN:CG	2.93	0.51
1:C:10:GLY:HA2	1:C:68:PHE:O	2.11	0.51
1:C:134:ASP:OD1	1:C:134:ASP:N	2.43	0.51
1:A:371:VAL:O	1:A:371:VAL:HG23	2.11	0.51
1:C:109:PRO:HG3	1:C:347:ARG:CD	2.40	0.51
1:A:112:LYS:CE	1:A:138:SER:OG	2.59	0.51
1:B:159:VAL:O	1:B:194:LYS:HE3	2.11	0.51
1:C:131:TYR:CE1	1:C:140:LEU:HD13	2.46	0.51
1:B:184:ARG:HD3	1:B:212:TYR:CE2	2.46	0.51
1:C:174:LEU:HD12	1:C:174:LEU:O	2.11	0.51
1:B:221:PHE:CD1	1:B:238:GLY:HA3	2.46	0.50
1:C:48:ASN:O	1:C:52:VAL:HG23	2.11	0.50
1:C:44:LEU:HD23	1:C:55:ALA:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:GLU:CD	1:C:370:GLU:H	2.14	0.50
1:A:44:LEU:HD12	1:A:44:LEU:C	2.31	0.50
1:A:96:PRO:HA	1:A:106:GLN:HE21	1.76	0.50
1:A:298:ILE:HG21	1:A:322:GLU:CG	2.41	0.49
1:C:91:ILE:HD13	1:C:286:MET:CE	2.42	0.49
1:A:205:ILE:HG13	1:A:207:LYS:HG3	1.94	0.49
1:C:30:PHE:CE1	1:C:284:GLN:HG3	2.47	0.49
1:C:87:HIS:ND1	1:C:316:PRO:HB3	2.27	0.49
1:B:59:GLN:CD	3:B:471:HOH:O	2.50	0.49
1:C:109:PRO:HG3	1:C:347:ARG:NE	2.27	0.49
1:C:111:LEU:HD13	1:C:219:LEU:CD2	2.43	0.49
1:B:354:ILE:N	1:B:354:ILE:HD12	2.28	0.49
1:C:106:GLN:HE22	1:C:346:LYS:NZ	2.11	0.49
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.77	0.49
1:C:140:LEU:O	1:C:140:LEU:HG	2.13	0.49
1:A:149:GLU:O	1:A:149:GLU:HG2	2.12	0.48
1:A:40:HIS:CE1	3:A:565:HOH:O	2.66	0.48
1:C:292:ASN:O	1:C:296:GLN:HG3	2.14	0.48
1:C:26:GLY:C	1:C:283:VAL:HG11	2.33	0.48
1:B:191:GLU:HG2	1:B:192:ARG:N	2.27	0.48
1:B:8:ILE:HD13	1:B:286:MET:CE	2.43	0.48
1:C:317:TRP:CZ3	1:C:319:GLN:HG2	2.49	0.48
1:C:137:LEU:O	1:C:141:GLN:HG3	2.13	0.48
1:C:163:ASN:C	1:C:165:ASP:H	2.17	0.48
1:B:29:GLN:HG2	1:B:280:TYR:OH	2.14	0.47
1:C:157:ILE:HG12	3:C:393:HOH:O	2.14	0.47
1:B:8:ILE:HD13	1:B:286:MET:HE2	1.96	0.47
1:C:95:PHE:CD2	1:C:135:ARG:HA	2.50	0.47
1:A:62:ARG:NH1	1:A:62:ARG:HG2	2.29	0.47
1:C:251:LYS:HD2	1:C:254:GLU:OE1	2.14	0.47
1:B:91:ILE:CG2	1:B:107:MET:HE2	2.45	0.46
1:B:182:LYS:HA	3:B:504:HOH:O	2.15	0.46
1:C:131:TYR:OH	1:C:158:ASN:HB2	2.15	0.46
1:B:354:ILE:HD11	1:B:368:TRP:HB2	1.97	0.46
1:C:118:LEU:HD12	1:C:374:MET:CE	2.45	0.46
1:A:171:TYR:CD2	1:A:201:GLN:HG2	2.51	0.46
1:C:120:GLU:O	1:C:123:GLN:N	2.42	0.46
1:C:113:GLY:HA3	1:C:368:TRP:CZ2	2.50	0.46
1:B:248:LEU:HD23	1:B:248:LEU:O	2.16	0.46
1:B:260:GLU:HG3	1:B:263:GLU:HB3	1.96	0.46
1:B:338:ASN:ND2	1:B:349:ASN:HD22	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ILE:O	1:C:229:ILE:HG12	2.15	0.46
1:B:73:LYS:NZ	3:B:506:HOH:O	2.47	0.45
1:C:293:LEU:HD21	1:C:300:ILE:HG21	1.98	0.45
1:C:58:SER:O	1:C:62:ARG:HB2	2.17	0.45
1:A:315:VAL:HG12	3:A:500:HOH:O	2.15	0.45
1:B:20:TYR:CZ	1:B:24:ARG:HD2	2.51	0.45
1:C:162:ILE:HD13	1:C:171:TYR:OH	2.17	0.45
1:B:224:GLY:HA3	3:B:466:HOH:O	2.17	0.45
1:A:8:ILE:HG21	1:A:286:MET:CE	2.47	0.45
1:B:256:TRP:CH2	1:B:267:ALA:HB2	2.52	0.45
1:B:159:VAL:HG22	1:B:171:TYR:HE2	1.82	0.45
1:C:90:PHE:HE2	1:C:92:THR:HB	1.82	0.45
1:B:13:PRO:HD3	1:B:70:PHE:CD1	2.52	0.44
1:C:60:PHE:CE1	1:C:86:LEU:HD13	2.52	0.44
1:C:74:LYS:HE3	1:C:74:LYS:HB2	1.64	0.44
1:C:7:GLN:HG2	1:C:38:THR:CG2	2.47	0.44
1:C:61:SER:HB3	1:C:307:GLY:O	2.18	0.44
1:C:46:VAL:O	1:C:75:SER:HB3	2.18	0.44
1:A:4:ASN:HB2	1:A:35:PHE:HA	1.99	0.44
1:A:128:ALA:HB2	1:A:183:GLU:HG2	1.99	0.44
1:A:259:LEU:O	1:A:268:HIS:CD2	2.59	0.44
1:C:44:LEU:CD1	1:C:44:LEU:C	2.83	0.44
1:B:166:LYS:O	1:B:167:LYS:HB3	2.18	0.44
1:B:354:ILE:HG22	1:B:365:ILE:HG22	2.00	0.44
1:B:92:THR:HA	1:B:93:PRO:HD3	1.82	0.44
1:C:113:GLY:O	1:C:117:SER:HB2	2.17	0.44
1:C:339:ILE:HG12	1:C:347:ARG:NH1	2.30	0.44
1:B:231:PHE:HB2	1:C:204:THR:HG22	2.00	0.43
1:C:208:HIS:C	1:C:234:ALA:HB2	2.38	0.43
1:A:139:THR:O	1:A:143:VAL:HG13	2.18	0.43
1:B:248:LEU:HD23	1:B:248:LEU:C	2.39	0.43
1:B:177:ASP:C	1:B:179:GLU:N	2.72	0.43
1:C:91:ILE:HG13	1:C:105:ILE:HG13	2.00	0.43
1:A:8:ILE:HG21	1:A:286:MET:HE2	1.99	0.43
1:C:65:TYR:CZ	1:C:302:ARG:NH1	2.87	0.43
1:C:126:LYS:HG3	1:C:153:GLN:HB3	2.01	0.43
1:C:163:ASN:O	1:C:164:ASN:HB3	2.18	0.43
1:C:371:VAL:HG23	1:C:372:ASP:H	1.84	0.43
1:A:163:ASN:C	1:A:165:ASP:H	2.22	0.43
1:B:36:ARG:HD2	1:B:38:THR:CG2	2.49	0.43
1:A:256:TRP:O	1:A:267:ALA:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:TYR:HA	1:B:249:VAL:CG1	2.49	0.43
1:B:378:LEU:HD13	1:B:378:LEU:C	2.40	0.43
1:C:24:ARG:O	1:C:28:VAL:HG23	2.19	0.43
1:C:65:TYR:CE2	1:C:302:ARG:NH1	2.86	0.43
1:B:159:VAL:HG13	1:B:159:VAL:O	2.17	0.42
1:B:213:HIS:HD2	1:B:214:TYR:N	2.17	0.42
1:C:105:ILE:HG13	1:C:327:LEU:HD13	2.00	0.42
1:C:27:MET:HE1	1:C:39:PRO:HD3	2.01	0.42
1:C:92:THR:HA	1:C:93:PRO:HD3	1.85	0.42
1:C:167:LYS:C	1:C:169:GLU:H	2.22	0.42
1:C:339:ILE:HG23	1:C:347:ARG:NH1	2.34	0.42
1:A:255:ARG:HD3	1:A:255:ARG:HA	1.76	0.42
1:C:353:ASN:HB3	1:C:355:MET:HE2	2.01	0.42
1:A:163:ASN:O	1:A:167:LYS:HB2	2.20	0.42
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.54	0.42
1:B:356:GLU:CD	1:B:365:ILE:HD12	2.40	0.42
1:C:201:GLN:OE1	1:C:201:GLN:HA	2.19	0.42
1:C:342:ASP:OD1	1:C:342:ASP:C	2.58	0.42
1:B:125:ASP:OD1	1:B:126:LYS:N	2.53	0.42
1:B:118:LEU:HD11	1:B:122:TYR:CE1	2.55	0.42
1:A:368:TRP:CZ2	1:A:373:LYS:HD2	2.54	0.42
1:B:110:ASP:OD1	1:B:112:LYS:HG3	2.20	0.41
1:C:107:MET:CE	1:C:282:ALA:HA	2.49	0.41
1:C:342:ASP:HB3	1:C:348:ILE:HG21	2.01	0.41
1:B:4:ASN:HD22	1:B:4:ASN:H	1.68	0.41
1:B:108:ARG:HA	1:B:109:PRO:HD2	1.96	0.41
1:B:243:ASP:OD1	1:B:245:ASP:HB2	2.20	0.41
1:B:349:ASN:ND2	3:B:487:HOH:O	2.49	0.41
1:A:102:PRO:HB2	1:A:103:PHE:CD2	2.56	0.41
1:A:30:PHE:CZ	1:A:284:GLN:HB2	2.55	0.41
1:C:256:TRP:CZ2	1:C:267:ALA:HA	2.56	0.41
1:C:312:ASN:HA	1:C:313:PRO:HA	1.92	0.41
1:C:109:PRO:HG3	1:C:347:ARG:HE	1.85	0.41
1:A:164:ASN:N	1:A:164:ASN:HD22	2.18	0.41
1:C:87:HIS:CD2	1:C:103:PHE:CZ	3.09	0.41
1:C:373:LYS:HE2	1:C:373:LYS:HB3	1.90	0.41
1:C:90:PHE:CE2	1:C:92:THR:HB	2.56	0.41
1:A:313:PRO:HD2	3:A:520:HOH:O	2.20	0.41
1:A:62:ARG:HH11	1:A:62:ARG:HG2	1.85	0.41
1:B:107:MET:HE3	1:B:285:VAL:HB	2.02	0.41
1:A:90:PHE:CE2	1:A:92:THR:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ILE:N	1:C:354:ILE:HD12	2.36	0.41
1:A:192:ARG:HH22	1:A:223:ASP:HB3	1.86	0.41
1:A:369:SER:HB3	1:A:372:ASP:HB2	2.03	0.41
1:C:199:VAL:O	1:C:203:ILE:HG13	2.20	0.41
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.84	0.41
1:B:118:LEU:HA	1:B:374:MET:CE	2.51	0.40
1:C:19:GLU:HG3	1:C:276:SER:HA	2.03	0.40
1:C:146:SER:C	1:C:148:ALA:H	2.24	0.40
1:C:298:ILE:HG21	1:C:322:GLU:HG2	2.04	0.40
1:B:125:ASP:O	1:B:152:TRP:HA	2.22	0.40
1:B:8:ILE:CD1	1:B:286:MET:HE1	2.51	0.40
1:C:169:GLU:HG3	3:C:408:HOH:O	2.20	0.40
1:B:130:LEU:N	1:B:130:LEU:HD23	2.36	0.40
1:B:253:ILE:HA	1:B:253:ILE:HD13	1.74	0.40
1:B:83:CYS:SG	1:B:90:PHE:HB2	2.61	0.40
1:C:140:LEU:O	1:C:144:LEU:HG	2.22	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	374/394 (95%)	362 (97%)	12 (3%)	0	100	100
1	B	374/394 (95%)	355 (95%)	19 (5%)	0	100	100
1	C	371/394 (94%)	332 (90%)	37 (10%)	2 (0%)	29	31
All	All	1119/1182 (95%)	1049 (94%)	68 (6%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	GLU

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Mol	Chain	Res	Type
1	C	303	ARG

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	325/342 (95%)	313 (96%)	12 (4%)	34	43
1	B	325/342 (95%)	311 (96%)	14 (4%)	29	36
1	C	322/342 (94%)	307 (95%)	15 (5%)	26	33
All	All	972/1026 (95%)	931 (96%)	41 (4%)	30	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	32	THR
1	A	46	VAL
1	A	73	LYS
1	A	134	ASP
1	A	143	VAL
1	A	188	LEU
1	A	229	ILE
1	A	317	TRP
1	A	321	VAL
1	A	371	VAL
1	A	373	LYS
1	B	37	LEU
1	B	135	ARG
1	B	139	THR
1	B	143	VAL
1	B	159	VAL
1	B	162	ILE
1	B	173	SER
1	B	250	SER
1	B	301	SER

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Mol	Chain	Res	Type
1	B	315	VAL
1	B	317	TRP
1	B	340	LYS
1	B	351	THR
1	B	378	LEU
1	C	20	TYR
1	C	35	PHE
1	C	71	TYR
1	C	117	SER
1	C	134	ASP
1	C	135	ARG
1	C	140	LEU
1	C	143	VAL
1	C	159	VAL
1	C	226	LEU
1	C	227	LEU
1	C	237	SER
1	C	269	THR
1	C	319	GLN
1	C	347	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	106	GLN
1	A	164	ASN
1	A	268	HIS
1	A	284	GLN
1	A	292	ASN
1	A	296	GLN
1	B	4	ASN
1	B	7	GLN
1	B	18	GLN
1	B	59	GLN
1	B	153	GLN
1	B	268	HIS
1	B	292	ASN
1	B	338	ASN
1	B	343	GLN
1	C	18	GLN

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Mol	Chain	Res	Type
1	C	87	HIS
1	C	106	GLN
1	C	163	ASN
1	C	268	HIS
1	C	292	ASN
1	C	296	GLN
1	C	331	GLN
1	C	349	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)

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	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.54	0	17,19,21	0.87	0
2	NAG	D	2	2	14,14,15	0.50	0	17,19,21	2.39	4 (23%)
2	NAG	E	1	1,2	14,14,15	0.48	0	17,19,21	1.75	3 (17%)
2	NAG	E	2	2	14,14,15	0.42	0	17,19,21	1.37	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	C1-O5-C5	7.54	122.41	112.19
2	E	1	NAG	C1-O5-C5	5.01	118.98	112.19
2	D	2	NAG	O5-C1-C2	4.40	118.24	111.29
2	E	2	NAG	C1-O5-C5	4.25	117.95	112.19
2	E	1	NAG	C4-C3-C2	-3.23	106.28	111.02
2	D	2	NAG	C4-C3-C2	-2.75	106.98	111.02
2	E	2	NAG	O5-C5-C6	2.73	111.49	107.20
2	E	1	NAG	C2-N2-C7	-2.72	119.03	122.90
2	D	2	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

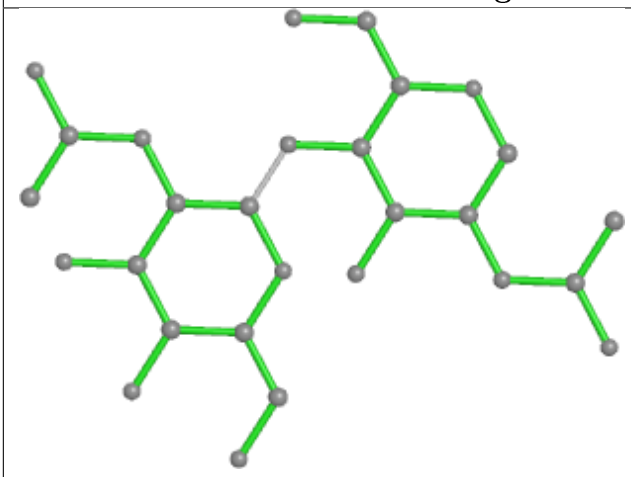
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

There are no ring outliers.

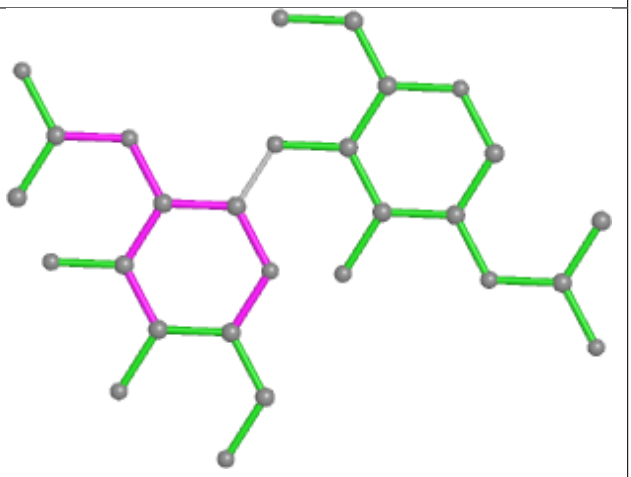
No monomer is involved in short contacts.

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

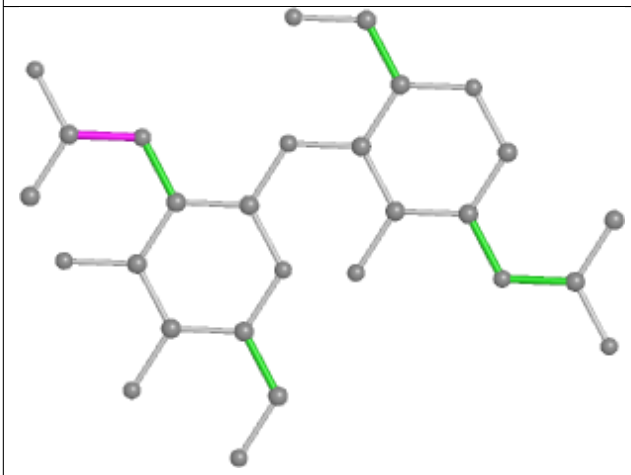
Oligosaccharide Chain D



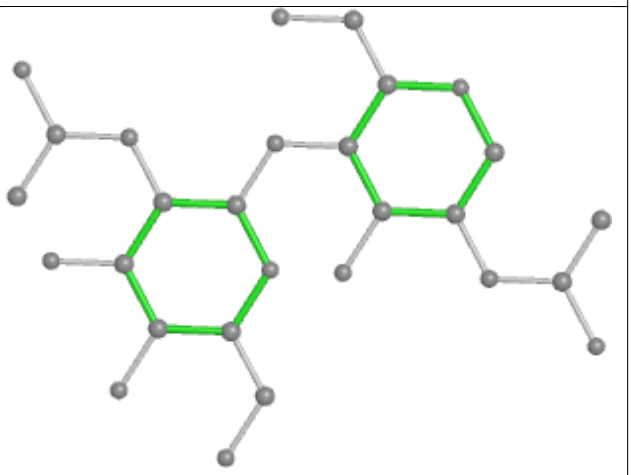
Bond lengths



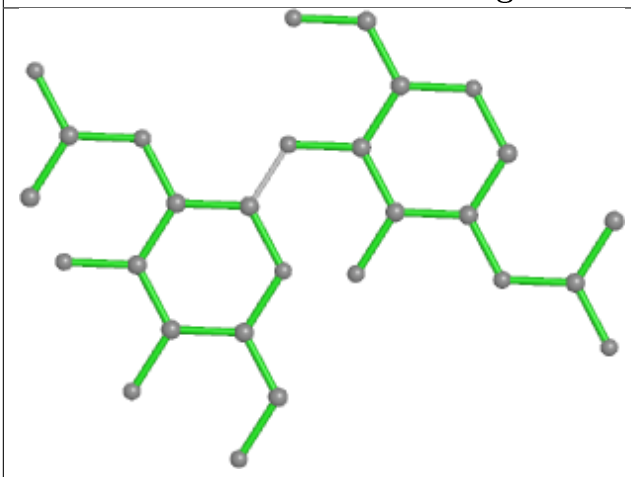
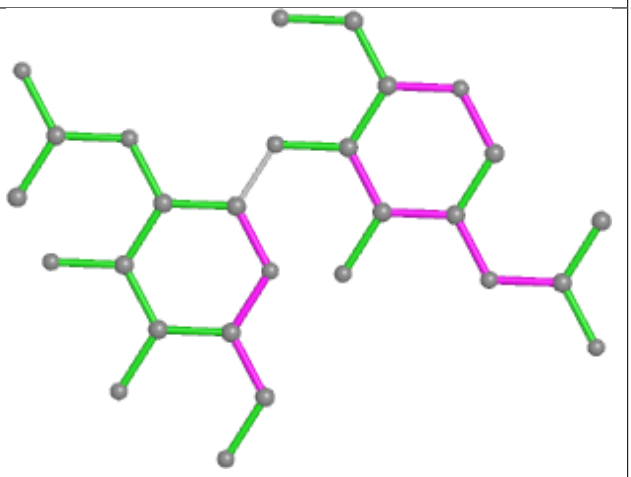
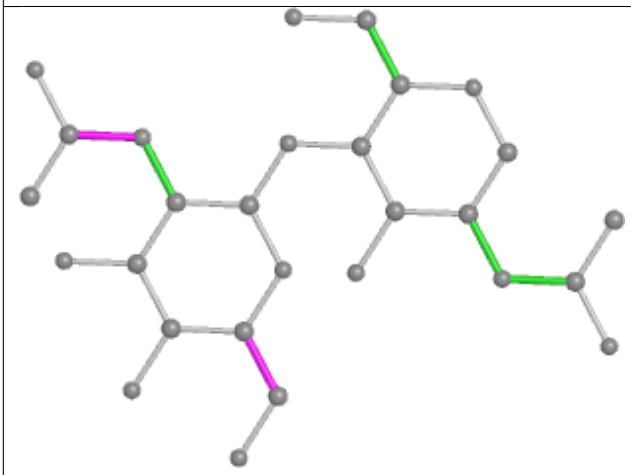
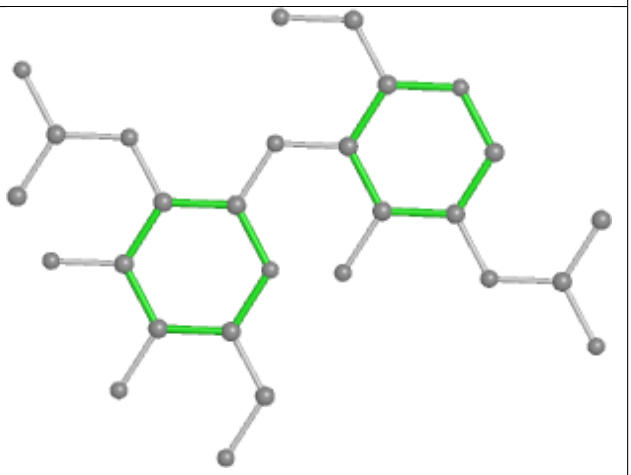
Bond angles



Torsions



Rings

Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	376/394 (95%)	0.27	12 (3%) 47 58	29, 50, 91, 155	11 (2%)
1	B	376/394 (95%)	0.61	27 (7%) 15 22	32, 67, 117, 178	10 (2%)
1	C	373/394 (94%)	1.53	97 (26%) 0 1	69, 121, 182, 220	10 (2%)
All	All	1125/1182 (95%)	0.80	136 (12%) 4 7	29, 74, 164, 220	31 (2%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	332	VAL	10.9
1	C	31	SER	10.3
1	C	335	LEU	8.3
1	C	66	ALA	7.5
1	C	293	LEU	7.5
1	B	3	SER	7.0
1	B	303	ARG	6.8
1	C	248	LEU	6.7
1	C	290	PHE	6.6
1	C	36	ARG	6.5
1	C	32	THR	6.4
1	C	247	SER	6.2
1	C	326	ALA	5.9
1	C	65	TYR	5.9
1	C	294	ARG	5.7
1	C	28	VAL	5.6
1	C	35	PHE	5.4
1	B	5	SER	5.4
1	C	327	LEU	5.3
1	C	325	ARG	5.1
1	C	375	VAL	5.1
1	B	36	ARG	4.9
1	C	34	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	180	LEU	4.9
1	C	6	ILE	4.8
1	C	91	ILE	4.7
1	C	253	ILE	4.7
1	B	300	ILE	4.6
1	C	105	ILE	4.5
1	C	339	ILE	4.3
1	C	319	GLN	4.3
1	C	289	ALA	4.2
1	C	264	TYR	4.1
1	C	287	THR	3.9
1	C	268	HIS	3.9
1	C	323	ILE	3.9
1	A	148	ALA	3.8
1	C	8	ILE	3.7
1	C	341	PHE	3.7
1	A	374	MET	3.6
1	C	322	GLU	3.6
1	C	378	LEU	3.6
1	B	267	ALA	3.5
1	B	35	PHE	3.4
1	C	262	LYS	3.3
1	C	297	ARG	3.3
1	C	172	ARG	3.2
1	C	103	PHE	3.2
1	C	329	GLN	3.2
1	B	179	GLU	3.2
1	B	378	LEU	3.2
1	C	321	VAL	3.2
1	C	291	ARG	3.2
1	C	267	ALA	3.1
1	B	6	ILE	3.1
1	B	65	TYR	3.1
1	C	296	GLN	3.1
1	C	33	SER	3.0
1	A	378	LEU	3.0
1	C	288	GLU	3.0
1	C	331	GLN	3.0
1	C	107	MET	3.0
1	C	56	PHE	3.0
1	C	330	VAL	3.0
1	A	367	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	260	GLU	2.9
1	C	280	TYR	2.9
1	B	297	ARG	2.9
1	C	121	TYR	2.9
1	C	7	GLN	2.9
1	C	38	THR	2.9
1	C	354	ILE	2.8
1	B	302	ARG	2.8
1	B	317	TRP	2.8
1	C	73	LYS	2.8
1	B	365	ILE	2.8
1	C	68	PHE	2.8
1	A	121	TYR	2.8
1	C	82	PHE	2.8
1	C	352	ILE	2.8
1	B	4	ASN	2.7
1	B	31	SER	2.7
1	B	175	PHE	2.7
1	C	174	LEU	2.7
1	B	176	GLN	2.7
1	A	76	VAL	2.7
1	C	315	VAL	2.6
1	C	317	TRP	2.6
1	C	299	GLU	2.6
1	C	301	SER	2.6
1	C	353	ASN	2.6
1	C	251	LYS	2.6
1	C	11	LEU	2.6
1	C	263	GLU	2.6
1	C	37	LEU	2.6
1	C	118	LEU	2.5
1	B	306	ALA	2.5
1	B	241	ILE	2.5
1	C	243	ASP	2.5
1	A	365	ILE	2.5
1	A	303	ARG	2.5
1	C	241	ILE	2.5
1	C	168	ASP	2.5
1	C	278	LEU	2.5
1	C	70	PHE	2.4
1	C	252	PHE	2.4
1	C	363	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	300	ILE	2.4
1	C	347	ARG	2.3
1	C	58	SER	2.3
1	A	80	THR	2.3
1	C	295	LYS	2.3
1	C	334	GLY	2.3
1	A	79	ILE	2.3
1	C	340	LYS	2.2
1	A	177	ASP	2.2
1	C	367	TYR	2.2
1	C	143	VAL	2.2
1	C	364	LYS	2.2
1	C	50	PHE	2.2
1	B	79	ILE	2.2
1	C	266	GLY	2.2
1	C	283	VAL	2.1
1	C	256	TRP	2.1
1	B	363	ARG	2.1
1	C	333	GLU	2.1
1	A	72	ASP	2.1
1	C	120	GLU	2.1
1	C	298	ILE	2.1
1	B	295	LYS	2.1
1	C	336	SER	2.1
1	B	227	LEU	2.0
1	C	351	THR	2.0
1	B	301	SER	2.0
1	C	175	PHE	2.0
1	C	310	LEU	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)

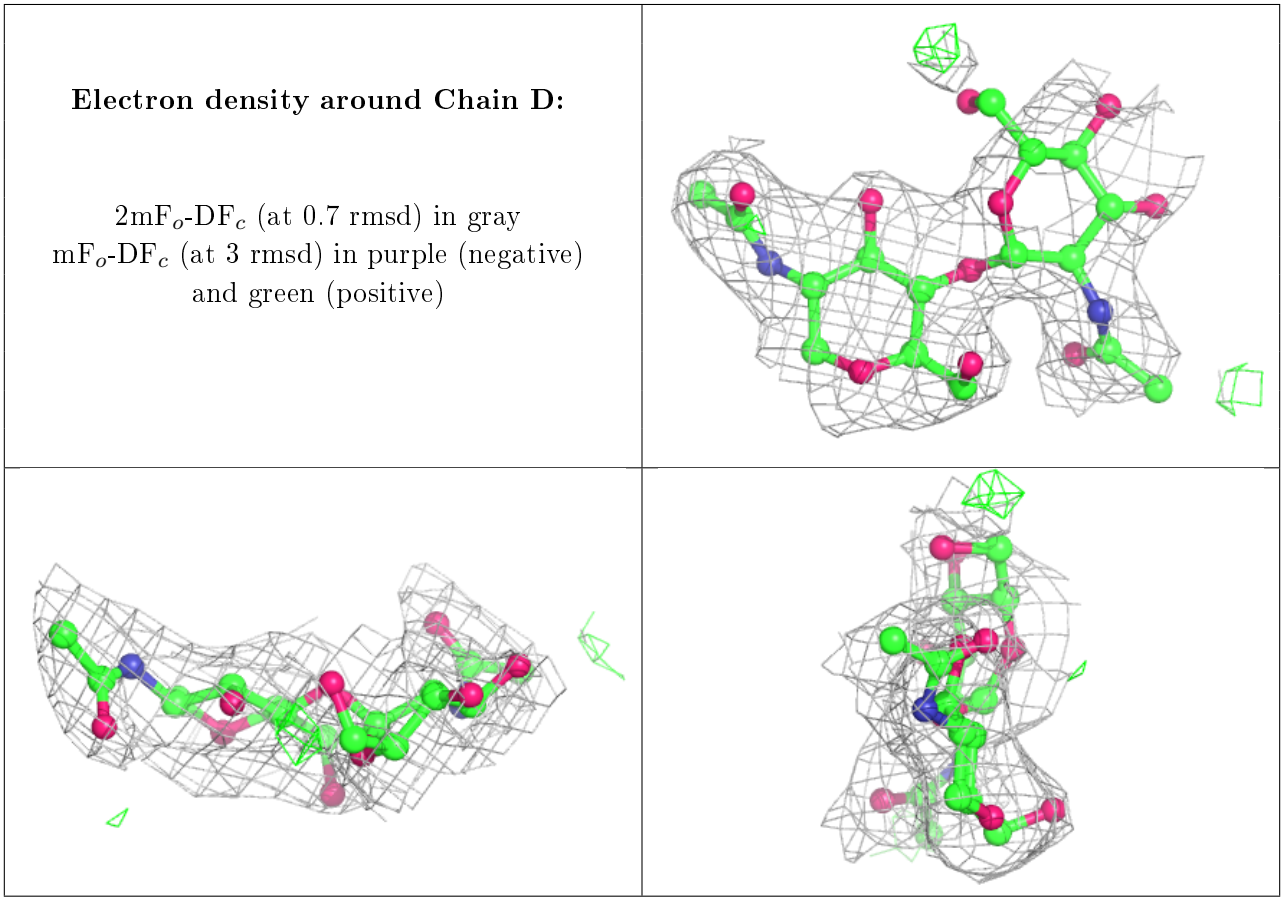
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	E	2	14/15	0.60	0.50	152,163,166,166	0
2	NAG	D	2	14/15	0.77	0.21	129,137,146,148	0
2	NAG	E	1	14/15	0.87	0.23	76,88,120,135	0
2	NAG	D	1	14/15	0.91	0.14	42,79,95,113	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.

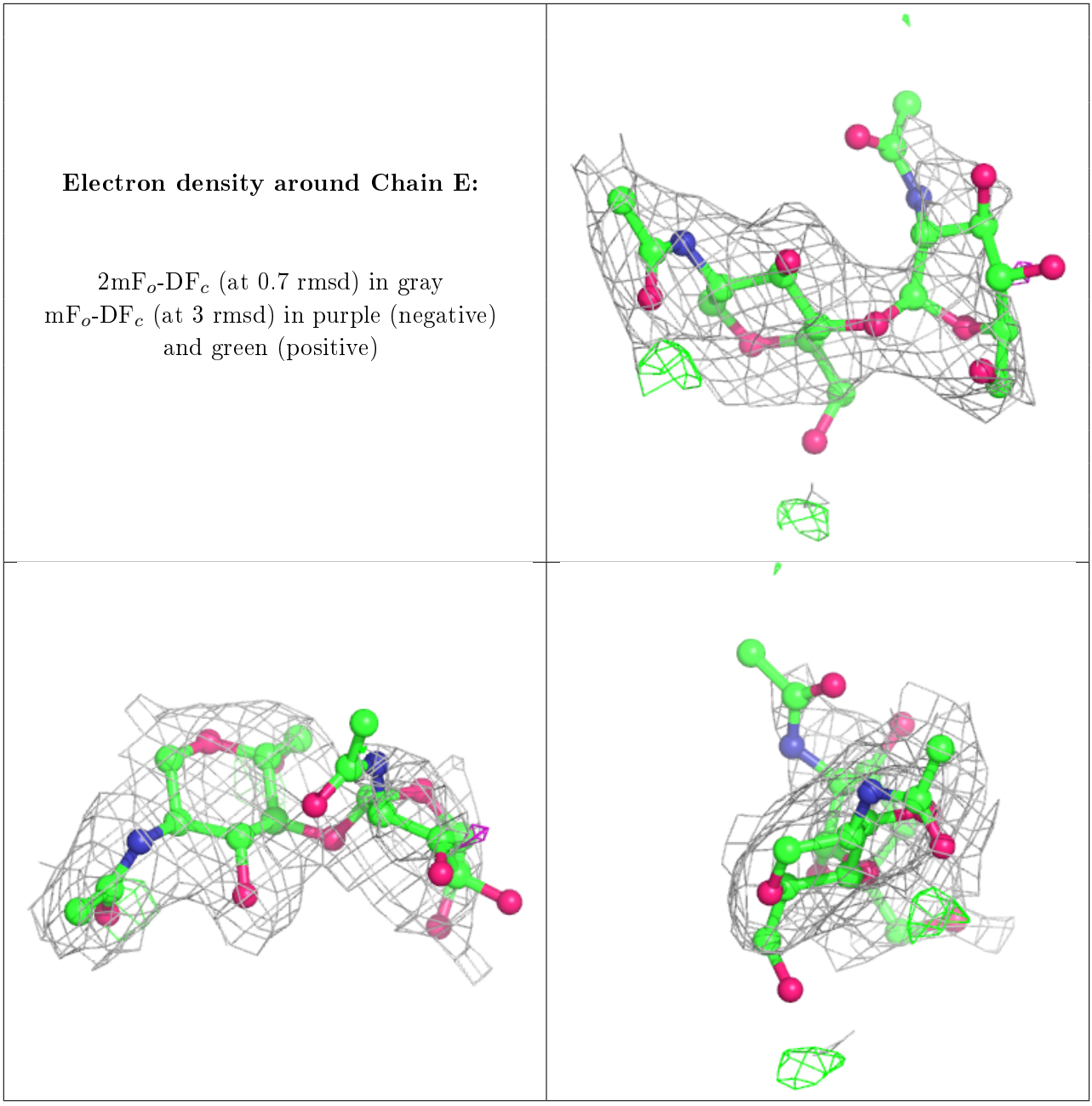
Electron density around Chain D:

$2mF_o$-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 E:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.