



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:39 AM UTC

PDB ID : 3H5V / pdb_00003h5v
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

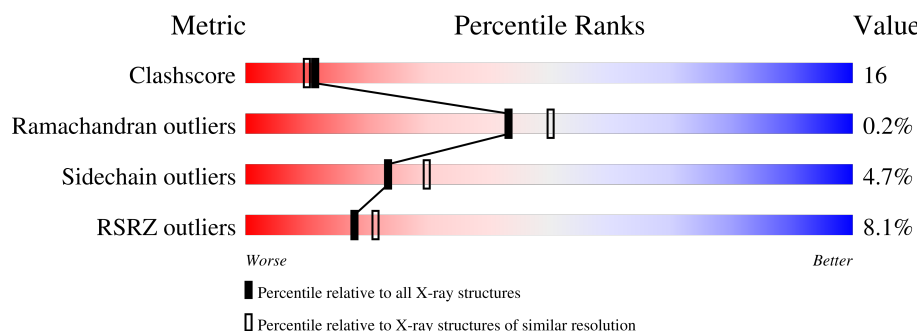
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	74% 21% • 5%
1	B	394	3% 67% 26% • 5%
1	C	394	19% 57% 35% • 5%
2	D	2	50% 50%
2	E	2	100%

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

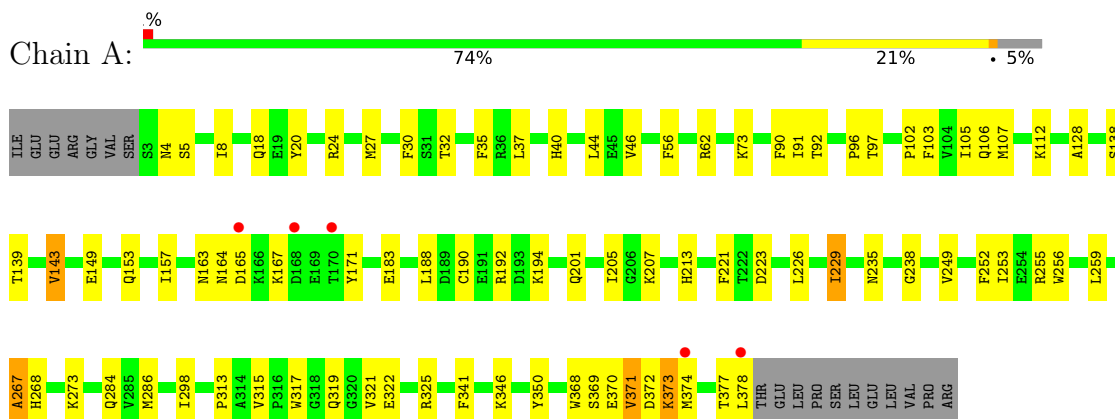
- Molecule 3 is water.

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

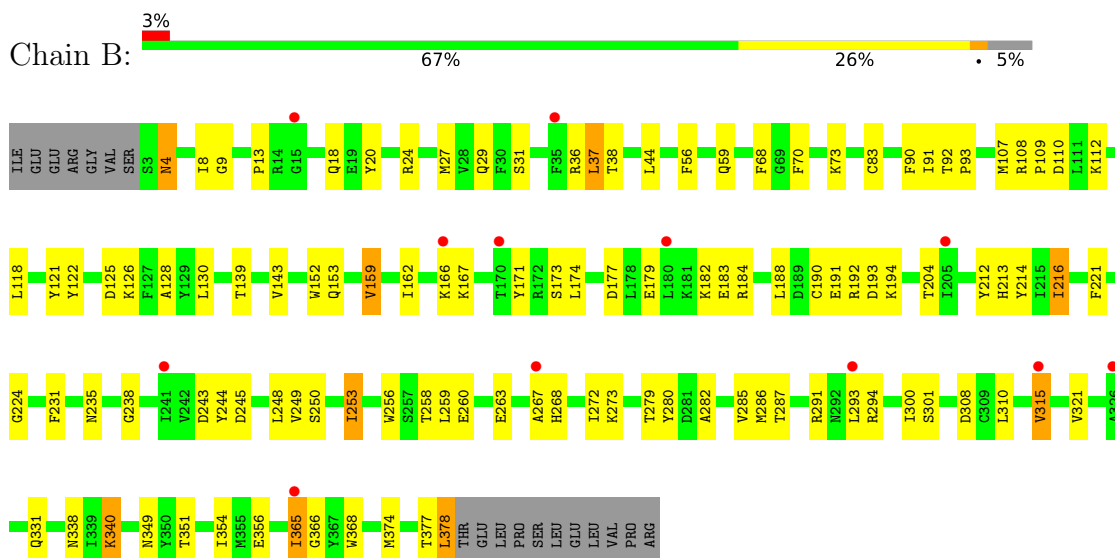
3 Residue-property plots

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

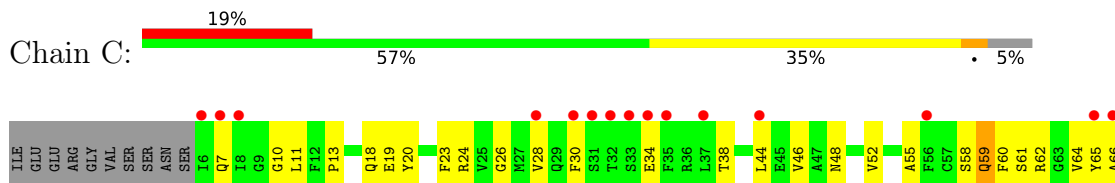
• Molecule 1: Glutamate receptor 2

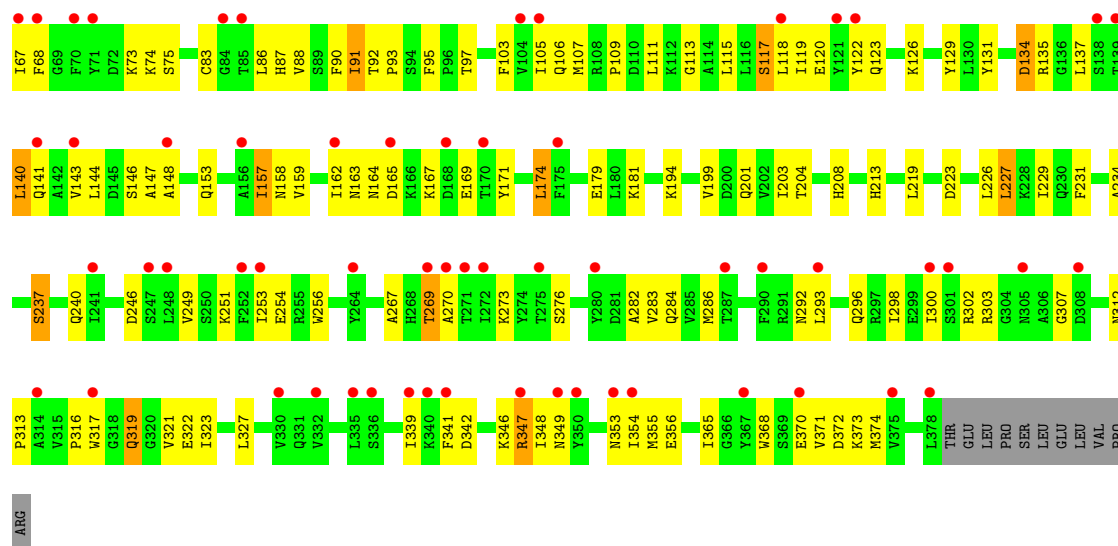


• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



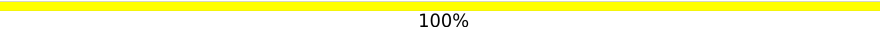


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50%



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

Chain E:  100%



4 Data and refinement statistics

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 19.91 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.91-2.33) 93.7 (19.91-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.186 , 0.235 (Not available) , (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)	0.29 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.67	0/3058	0.90	2/4136 (0.0%)
1	B	0.53	0/3058	0.83	1/4136 (0.0%)
1	C	0.37	0/3038	0.80	4/4109 (0.1%)
All	All	0.54	0/9154	0.84	7/12381 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ALA	N-CA-C	6.58	120.95	112.26
1	C	67	ILE	N-CA-C	6.16	117.16	108.17
1	C	147	ALA	N-CA-C	-5.78	105.94	112.87
1	B	44	LEU	N-CA-C	5.60	117.59	109.07
1	A	157	ILE	N-CA-C	5.22	115.64	108.12
1	C	157	ILE	CB-CA-C	-5.12	104.87	111.53
1	C	73	LYS	N-CA-C	-5.08	105.86	111.71

There are no chirality outliers.

There are no planarity outliers.

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	2996	0	2952	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2996	0	2952	93	0
1	C	2976	0	2937	128	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	284	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 16.

All (284) 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:B:107:MET:HE3	1:B:282:ALA:HA	1.46	0.98
1:A:373:LYS:HD3	1:A:373:LYS:N	1.81	0.96
1:C:91:ILE:HD13	1:C:286:MET:HE3	1.58	0.86
1:C:107:MET:HE3	1:C:282:ALA:HA	1.56	0.84
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:C:44:LEU:HD12	1:C:44:LEU:C	2.16	0.71
1:C:118:LEU:HD12	1:C:374:MET:HE1	1.73	0.70
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:HD3	1:A:373:LYS:H	1.55	0.69
1:B:8:ILE:CD1	1:B:286:MET:HE1	2.23	0.69
1:C:131:TYR:CZ	1:C:158:ASN:HB2	2.29	0.68
1:B:91:ILE:CG2	1:B:107:MET:HE2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:331:GLN:CD	1:B:340:LYS:HG3	2.23	0.63
1:B:8:ILE:HD12	1:B:286:MET:HE1	1.80	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:C:97:THR:HG23	1:C:106:GLN:NE2	2.13	0.62
1:B:107:MET:HE3	1:B:282:ALA:CA	2.24	0.62
1:A:105:ILE:HG22	1:A:107:MET:CE	2.29	0.62
1:B:378:LEU:CD1	1:B:378:LEU:C	2.73	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
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: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:A:107:MET:HE1	1:A:341:PHE:CZ	2.37	0.59
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:121:TYR:HB2	1:B:374:MET:HE3	1.85	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:C:44:LEU:HD12	1:C:44:LEU:O	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:N	1:C:91:ILE:HD12	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:A:106:GLN:HE22	1:A:346:LYS:HZ3	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:91:ILE:HG23	1:B:107:MET:HE2	1.87	0.57
1:C:97:THR:HG23	1:C:106:GLN:HE21	1.70	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:A:317:TRP:CE3	1:A:319:GLN:HG2	2.40	0.57
1:C:317:TRP:HB2	1:C:319:GLN:OE1	2.03	0.57
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:44:LEU:HD12	1:A:44:LEU:C	2.31	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
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:C:370:GLU:CD	1:C:370:GLU:H	2.14	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:B:107:MET:CE	1:B:282:ALA:HA	2.29	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:59:GLN:CD	3:B:471:HOH:O	2.50	0.54
1:B:36:ARG:HD2	1:B:38:THR:HG22	1.88	0.54
1:C:146:SER:C	1:C:148:ALA:N	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:ASN:C	1:C:165:ASP:H	2.17	0.53
1:B:27:MET:O	1:B:31:SER:HB3	2.08	0.53
1:C:26:GLY:C	1:C:283:VAL:HG11	2.33	0.53
1:A:91:ILE:HG23	1:A:107:MET:HE3	1.91	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: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:B:8:ILE:HD13	1:B:286:MET:HE1	1.91	0.51
1:C:10:GLY:HA2	1:C:68:PHE:O	2.11	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:B:121:TYR:CB	1:B:374:MET:HE3	2.41	0.51
1:C:174:LEU:HD12	1:C:174:LEU:O	2.11	0.51
1:C:317:TRP:H	1:C:317:TRP:CD1	2.29	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
1:C:162:ILE:HD11	1:C:194:LYS:HZ1	1.77	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: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:44:LEU:C	1:C:44:LEU:CD1	2.83	0.49
1:C:87:HIS:ND1	1:C:316:PRO:HB3	2.27	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:HD12	1:B:354:ILE:N	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:40:HIS:CE1	3:A:565:HOH:O	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:O	1:A:149:GLU:HG2	2.12	0.48
1:C:134:ASP:N	1:C:134:ASP:OD1	2.43	0.48
1:C:208:HIS:C	1:C:234:ALA:HB2	2.38	0.48
1:C:292:ASN:O	1:C:296:GLN:HG3	2.14	0.48
1:A:374:MET:HE3	1:A:374:MET:HB2	1.74	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:A:163:ASN:C	1:A:165:ASP:H	2.22	0.47
1:B:248:LEU:C	1:B:248:LEU:HD23	2.39	0.47
1:B:29:GLN:HG2	1:B:280:TYR:OH	2.14	0.47
1:B:177:ASP:C	1:B:179:GLU:N	2.72	0.47
1:C:157:ILE:HG12	3:C:393:HOH:O	2.14	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:356:GLU:CD	1:B:365:ILE:HD12	2.40	0.47
1:C:167:LYS:C	1:C:169:GLU:H	2.22	0.47
1:C:342:ASP:OD1	1:C:342:ASP:C	2.58	0.47
1:B:73:LYS:NZ	3:B:506:HOH:O	2.47	0.47
1:C:91:ILE:CD1	1:C:286:MET:HE3	2.38	0.47
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:B:378:LEU:C	1:B:378:LEU:HD13	2.40	0.46
1:A:171:TYR:CD2	1:A:201:GLN:HG2	2.51	0.46
1:C:113:GLY:HA3	1:C:368:TRP:CZ2	2.50	0.46
1:C:120:GLU:O	1:C:123:GLN:N	2.42	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
1:C:229:ILE:HG12	1:C:229:ILE:O	2.15	0.46
1:B:308:ASP:C	1:B:310:LEU:H	2.25	0.45
1:C:58:SER:O	1:C:62:ARG:HB2	2.17	0.45
1:C:293:LEU:HD21	1:C:300:ILE:HG21	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:27:MET:HE1	1:A:37:LEU:HB2	1.99	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:A:107:MET:HE1	1:A:341:PHE:HZ	1.80	0.44
1:C:7:GLN:HG2	1:C:38:THR:CG2	2.47	0.44
1:C:146:SER:C	1:C:148:ALA:H	2.24	0.44
1:C:46:VAL:O	1:C:75:SER:HB3	2.18	0.44
1:C:61:SER:HB3	1:C:307:GLY:O	2.18	0.44
1:A:4:ASN:HB2	1:A:35:PHE:HA	1.99	0.44
1:C:118:LEU:HD12	1:C:374:MET:CE	2.45	0.44
1:C:158:ASN:C	1:C:158:ASN:OD1	2.60	0.44
1:C:10:GLY:C	1:C:11:LEU:HD12	2.43	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:B:56:PHE:CD2	1:B:56:PHE:C	2.96	0.44
1:B:92:THR:HA	1:B:93:PRO:HD3	1.82	0.44
1:B:354:ILE:HG22	1:B:365:ILE:HG22	2.00	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:B:308:ASP:CG	1:B:310:LEU:H	2.25	0.43
1:A:139:THR:O	1:A:143:VAL:HG13	2.18	0.43
1:B:107:MET:HE1	1:B:285:VAL:HB	1.99	0.43
1:C:91:ILE:HG13	1:C:105:ILE:HG13	2.00	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: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
1:B:244:TYR:HA	1:B:249:VAL:CG1	2.49	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:C:144:LEU:C	1:C:146:SER:H	2.27	0.42
1:B:159:VAL:HG13	1:B:159:VAL:O	2.17	0.42
1:B:27:MET:HE1	1:B:37:LEU:O	2.19	0.42
1:B:91:ILE:HG21	1:B:107:MET:HE2	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:THR:HA	1:C:93:PRO:HD3	1.85	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:B:166:LYS:O	1:B:167:LYS:HB3	2.18	0.42
1:B:174:LEU:C	1:B:174:LEU:HD23	2.44	0.42
1:B:378:LEU:C	1:B:378:LEU:HD12	2.44	0.42
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.54	0.42
1:A:163:ASN:O	1:A:167:LYS:HB2	2.20	0.42
1:B:308:ASP:C	1:B:310:LEU:N	2.76	0.42
1:C:201:GLN:OE1	1:C:201:GLN:HA	2.19	0.42
1:B:125:ASP:OD1	1:B:126:LYS:N	2.53	0.42
1:B:27:MET:HE3	1:B:27:MET:HB3	1.84	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:C:240:GLN:HB3	1:C:355:MET:HE2	2.02	0.42
1:B:110:ASP:OD1	1:B:112:LYS:HG3	2.20	0.41
1:C:342:ASP:HB3	1:C:348:ILE:HG21	2.01	0.41
1:B:4:ASN:H	1:B:4:ASN:HD22	1.68	0.41
1:B:177:ASP:C	1:B:179:GLU:H	2.28	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:C:163:ASN:C	1:C:165:ASP:N	2.79	0.41
1:A:30:PHE:CZ	1:A:284:GLN:HB2	2.55	0.41
1:A:102:PRO:HB2	1:A:103:PHE:CD2	2.56	0.41
1:C:109:PRO:HG3	1:C:347:ARG:HE	1.85	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:A:164:ASN:N	1:A:164:ASN:HD22	2.18	0.41
1:B:118:LEU:HD13	1:B:374:MET:HE1	2.02	0.41
1:C:87:HIS:CD2	1:C:103:PHE:CZ	3.09	0.41
1:C:90:PHE:CE2	1:C:92:THR:HB	2.56	0.41
1:C:373:LYS:HB3	1:C:373:LYS:HE2	1.90	0.41
1:A:62:ARG:HG2	1:A:62:ARG:HH11	1.85	0.41
1:A:90:PHE:CE2	1:A:92:THR:HB	2.56	0.41
1:A:313:PRO:HD2	3:A:520:HOH:O	2.20	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:56:PHE:CD2	1:A:56:PHE:C	2.98	0.40
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: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:C:169:GLU:HG3	3:C:408:HOH:O	2.20	0.40
1:B:83:CYS:SG	1:B:90:PHE:HB2	2.61	0.40
1:B:130:LEU:N	1:B:130:LEU:HD23	2.36	0.40
1:B:253:ILE:HD13	1:B:253:ILE:HA	1.74	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	24	26
All	All	1119/1182 (95%)	1049 (94%)	68 (6%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	GLU
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%)	314 (97%)	11 (3%)	32	42
1	B	325/342 (95%)	307 (94%)	18 (6%)	19	23
1	C	322/342 (94%)	305 (95%)	17 (5%)	20	25
All	All	972/1026 (95%)	926 (95%)	46 (5%)	23	30

All (46) 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	143	VAL
1	A	188	LEU
1	A	229	ILE
1	A	321	VAL
1	A	371	VAL
1	A	373	LYS
1	A	377	THR
1	B	4	ASN
1	B	37	LEU
1	B	139	THR
1	B	143	VAL
1	B	159	VAL
1	B	162	ILE
1	B	173	SER
1	B	216	ILE
1	B	250	SER
1	B	253	ILE
1	B	258	THR
1	B	272	ILE
1	B	301	SER
1	B	315	VAL
1	B	340	LYS

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Mol	Chain	Res	Type
1	B	351	THR
1	B	365	ILE
1	B	378	LEU
1	C	59	GLN
1	C	91	ILE
1	C	117	SER
1	C	134	ASP
1	C	140	LEU
1	C	143	VAL
1	C	159	VAL
1	C	174	LEU
1	C	226	LEU
1	C	227	LEU
1	C	237	SER
1	C	253	ILE
1	C	269	THR
1	C	319	GLN
1	C	323	ILE
1	C	347	ARG
1	C	365	ILE

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	18	GLN
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	A	338	ASN
1	B	4	ASN
1	B	7	GLN
1	B	18	GLN
1	B	59	GLN
1	B	141	GLN
1	B	153	GLN
1	B	268	HIS
1	B	292	ASN
1	B	338	ASN
1	B	343	GLN

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Mol	Chain	Res	Type
1	B	349	ASN
1	C	18	GLN
1	C	87	HIS
1	C	106	GLN
1	C	163	ASN
1	C	235	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.53	0	17,19,21	0.81	0
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	2.41	4 (23%)
2	NAG	E	1	1,2	14,14,15	0.49	0	17,19,21	1.78	3 (17%)
2	NAG	E	2	2	14,14,15	0.43	0	17,19,21	1.30	1 (5%)

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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	7.62	122.41	112.19
2	E	1	NAG	C1-O5-C5	5.07	118.98	112.19
2	D	2	NAG	O5-C1-C2	4.49	118.24	111.29
2	E	2	NAG	C1-O5-C5	4.30	117.95	112.19
2	E	1	NAG	C4-C3-C2	-3.23	106.28	111.02
2	E	1	NAG	C2-N2-C7	-2.89	119.03	122.90
2	D	2	NAG	C4-C3-C2	-2.75	106.98	111.02
2	D	2	NAG	C2-N2-C7	-2.13	120.04	122.90

There are no chirality outliers.

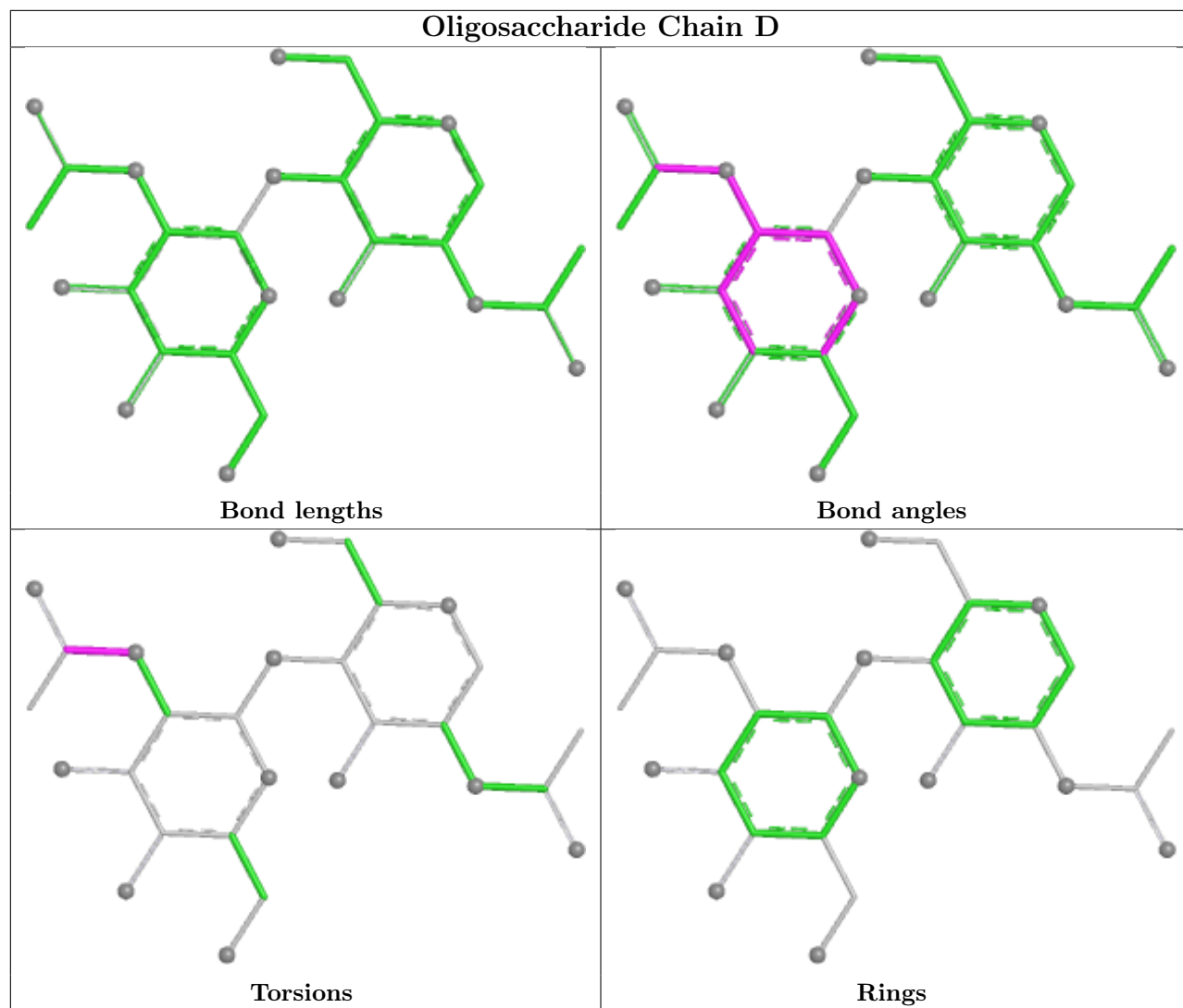
All (6) torsion outliers are listed below:

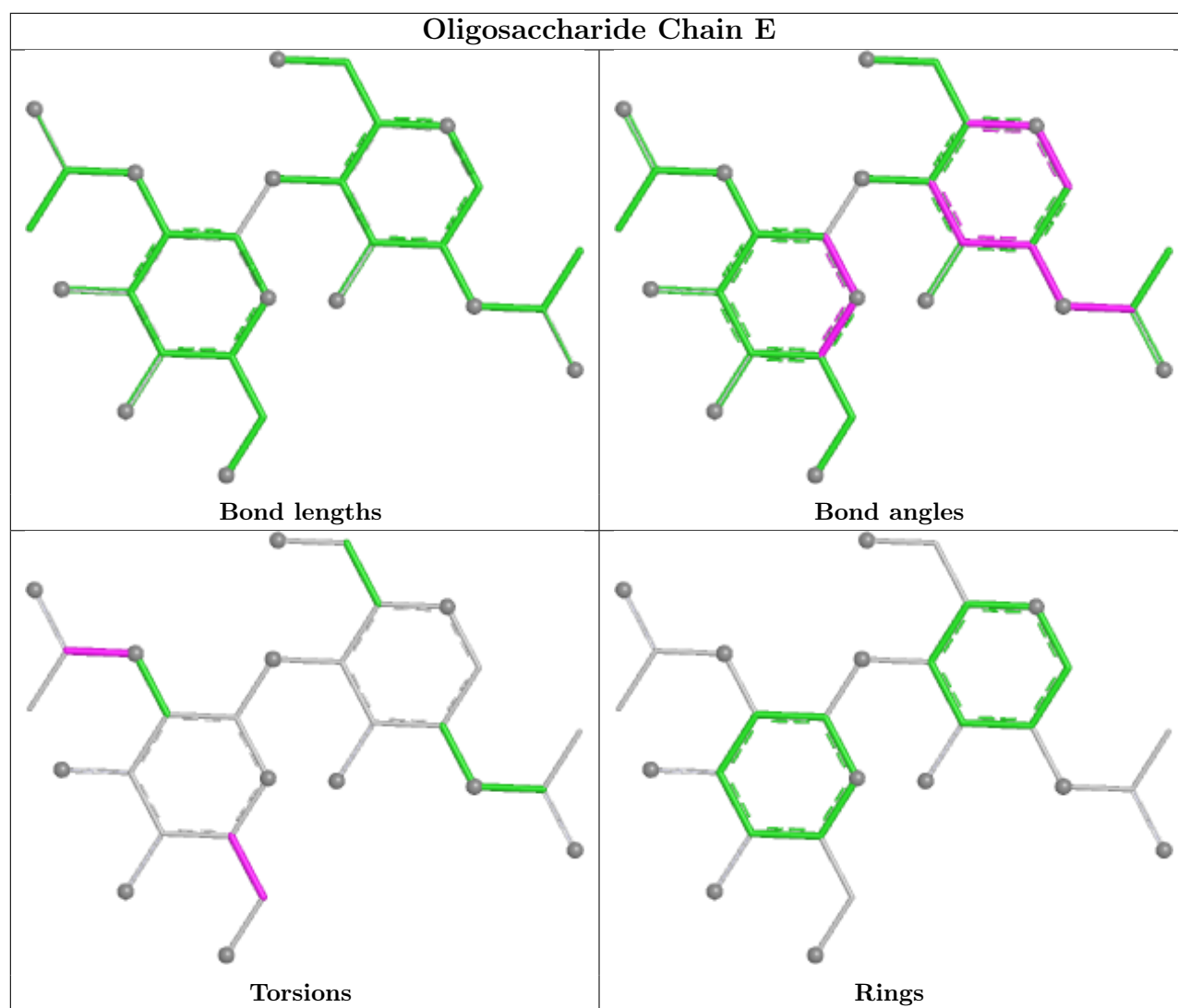
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

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.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/394 (95%)	0.07	5 (1%) 75 79	26, 50, 86, 134	11 (2%)
1	B	376/394 (95%)	0.58	12 (3%) 50 57	32, 67, 116, 178	10 (2%)
1	C	373/394 (94%)	1.30	74 (19%) 3 3	51, 120, 182, 220	10 (2%)
All	All	1125/1182 (95%)	0.65	91 (8%) 18 21	26, 73, 164, 220	31 (2%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	ASP	6.0
1	C	378	LEU	4.6
1	A	378	LEU	4.6
1	A	168	ASP	4.2
1	C	28	VAL	3.8
1	C	66	ALA	3.6
1	B	267	ALA	3.5
1	C	248	LEU	3.4
1	C	247	SER	3.3
1	C	264	TYR	3.3
1	C	31	SER	3.3
1	B	35	PHE	3.2
1	C	317	TRP	3.2
1	C	138	SER	3.2
1	A	165	ASP	3.1
1	C	170	THR	3.0
1	C	56	PHE	3.0
1	B	180	LEU	3.0
1	C	118	LEU	3.0
1	C	330	VAL	3.0
1	C	162	ILE	3.0
1	C	332	VAL	2.9
1	C	71	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	70	PHE	2.9
1	C	270	ALA	2.9
1	C	290	PHE	2.8
1	C	84	GLY	2.8
1	C	301	SER	2.8
1	C	375	VAL	2.8
1	C	272	ILE	2.8
1	B	170	THR	2.8
1	B	365	ILE	2.8
1	C	300	ILE	2.8
1	C	349	ASN	2.8
1	C	293	LEU	2.8
1	C	33	SER	2.7
1	C	6	ILE	2.7
1	C	35	PHE	2.6
1	C	104	VAL	2.6
1	C	350	TYR	2.6
1	C	241	ILE	2.6
1	C	37	LEU	2.6
1	C	335	LEU	2.6
1	C	175	PHE	2.6
1	C	143	VAL	2.6
1	C	105	ILE	2.6
1	C	65	TYR	2.5
1	C	271	THR	2.5
1	C	370	GLU	2.5
1	C	339	ILE	2.5
1	C	252	PHE	2.4
1	B	241	ILE	2.4
1	C	67	ILE	2.4
1	C	340	LYS	2.4
1	A	170	THR	2.4
1	C	8	ILE	2.4
1	C	148	ALA	2.3
1	C	341	PHE	2.3
1	C	287	THR	2.3
1	C	30	PHE	2.3
1	C	141	GLN	2.3
1	B	166	LYS	2.3
1	B	326	ALA	2.3
1	C	165	ASP	2.3
1	C	68	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	121	TYR	2.2
1	C	314	ALA	2.2
1	C	305	ASN	2.2
1	C	34	GLU	2.2
1	C	275	THR	2.2
1	C	122	TYR	2.2
1	C	7	GLN	2.2
1	C	139	THR	2.2
1	A	374	MET	2.1
1	B	293	LEU	2.1
1	C	44	LEU	2.1
1	C	308	ASP	2.1
1	B	315	VAL	2.1
1	C	269	THR	2.1
1	B	205	ILE	2.1
1	C	253	ILE	2.1
1	C	280	TYR	2.1
1	C	354	ILE	2.1
1	B	15	GLY	2.1
1	C	32	THR	2.1
1	C	85	THR	2.1
1	C	353	ASN	2.1
1	C	336	SER	2.0
1	C	367	TYR	2.0
1	C	347	ARG	2.0
1	C	156	ALA	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.

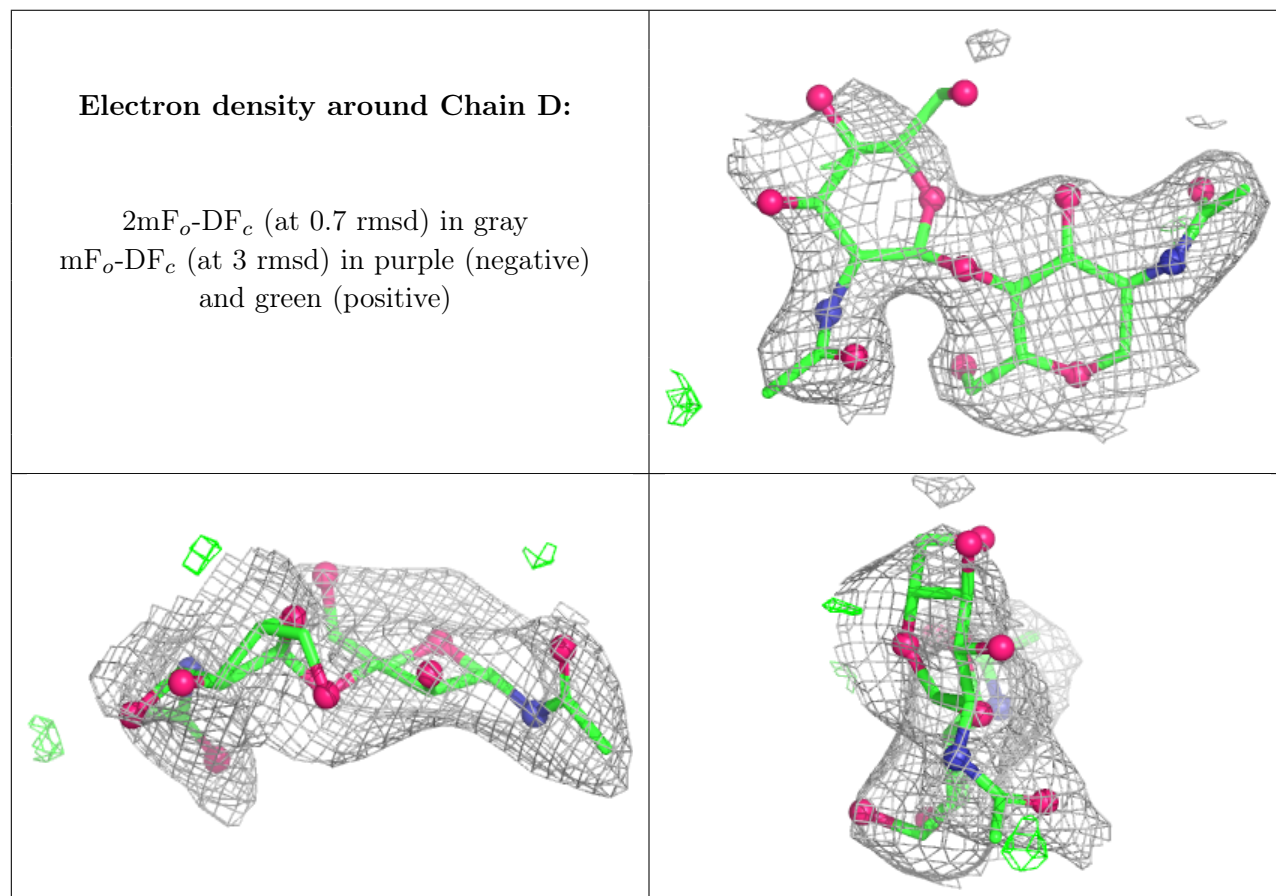
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.39	0.15	152,163,166,166	0
2	NAG	D	2	14/15	0.48	0.15	129,137,146,148	0

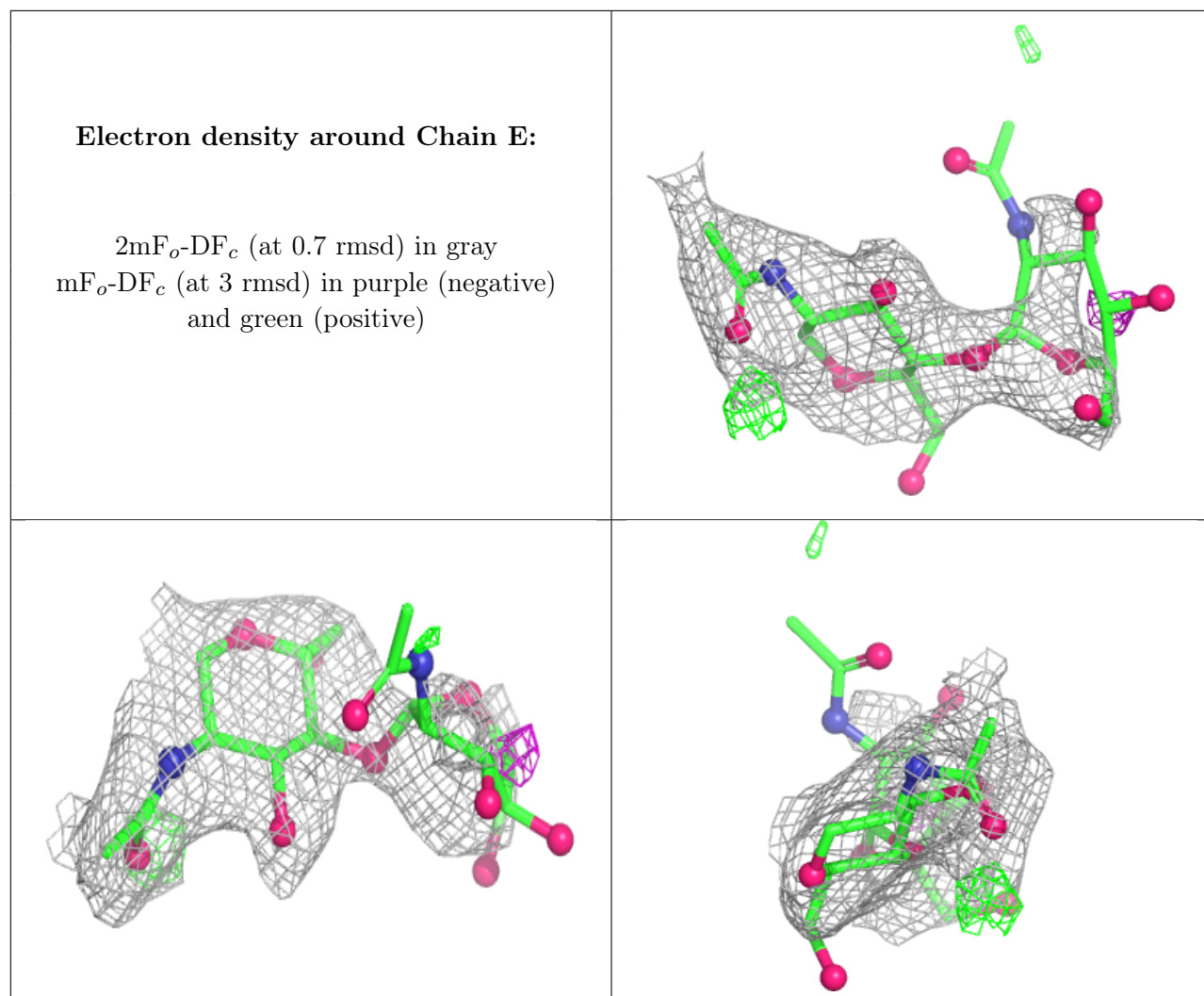
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	1	14/15	0.68	0.11	76,88,120,135	0
2	NAG	D	1	14/15	0.86	0.09	42,79,95,113	0

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.





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.