



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:24 AM UTC

PDB ID : 4U4F / pdb_00004u4f
Title : Structure of GluA2* in complex with partial agonist (S)-5-Nitrowillardiine
Authors : Yelshanskaya, M.V.; Li, M.; Sobolevsky, A.I.
Deposited on : 2014-07-23
Resolution : 4.79 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

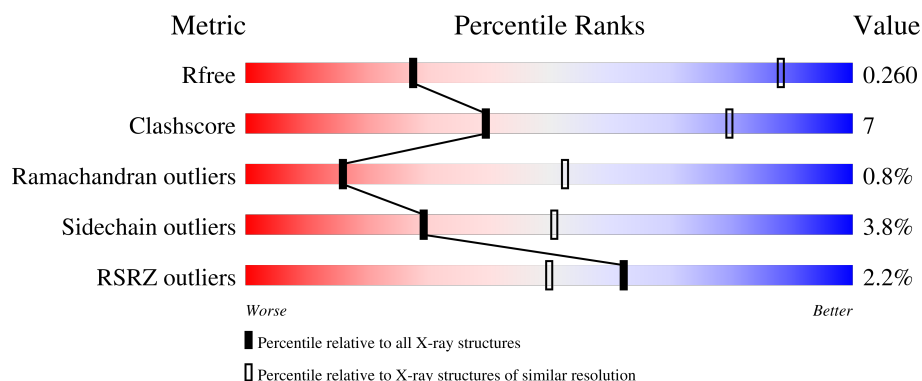
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	822	 2% 76% 17% • 7%
1	B	822	 3% 73% 19% • 7%
1	C	822	 2% 73% 19% • 7%
1	D	822	 2% 76% 16% • 7%
2	E	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	G	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24067 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	768	Total	C	N	O	S	0	0	0
			5979	3836	990	1125	28			
1	B	768	Total	C	N	O	S	0	0	0
			5974	3831	990	1125	28			
1	C	768	Total	C	N	O	S	0	0	0
			5974	3831	990	1125	28			
1	D	768	Total	C	N	O	S	0	0	0
			5974	3831	990	1125	28			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491

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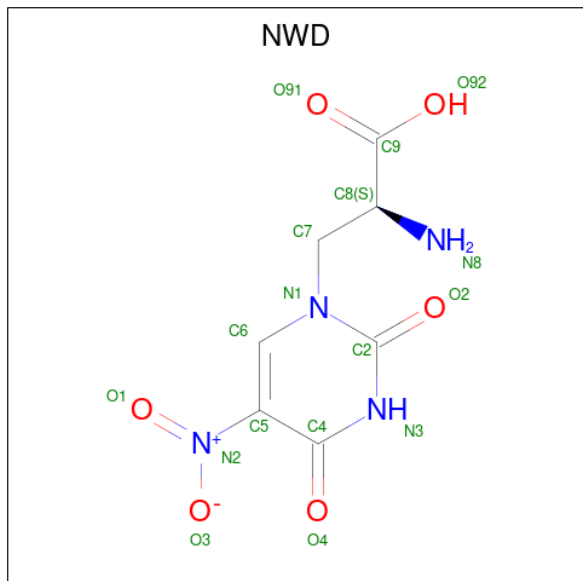
Chain	Residue	Modelled	Actual	Comment	Reference
D	831	ARG	-	expression tag	UNP P19491

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

- Molecule 3 is 3-(5-nitro-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-L-alanine (CCD ID: NWD) (formula: C₇H₈N₄O₆).



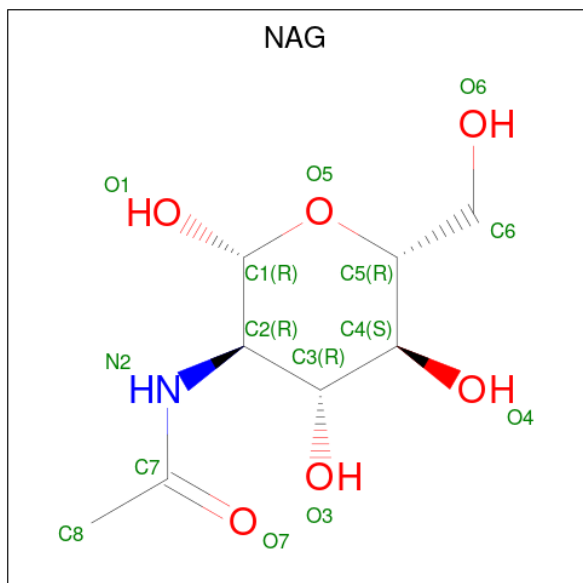
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	7	4	6		
3	B	1	Total	C	N	O	0	0
			17	7	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			17	7	4	6		
3	D	1	Total	C	N	O	0	0
			17	7	4	6		

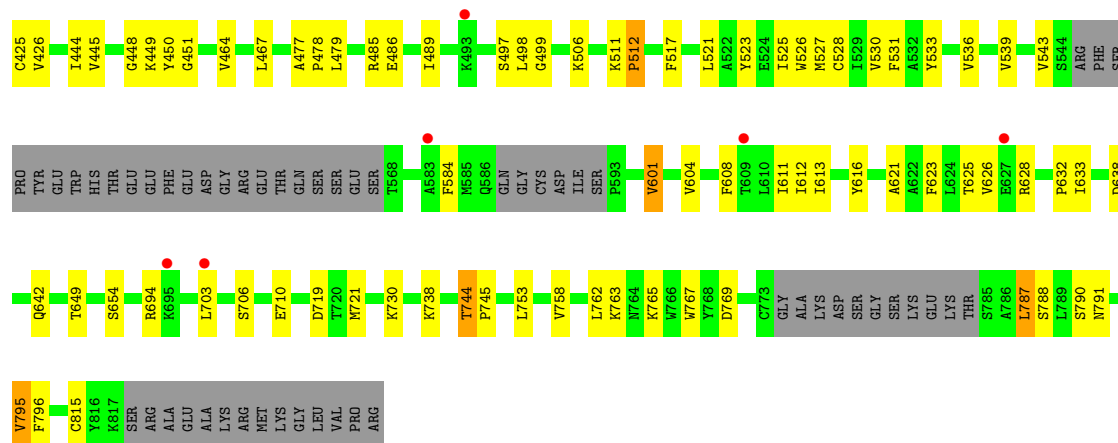
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



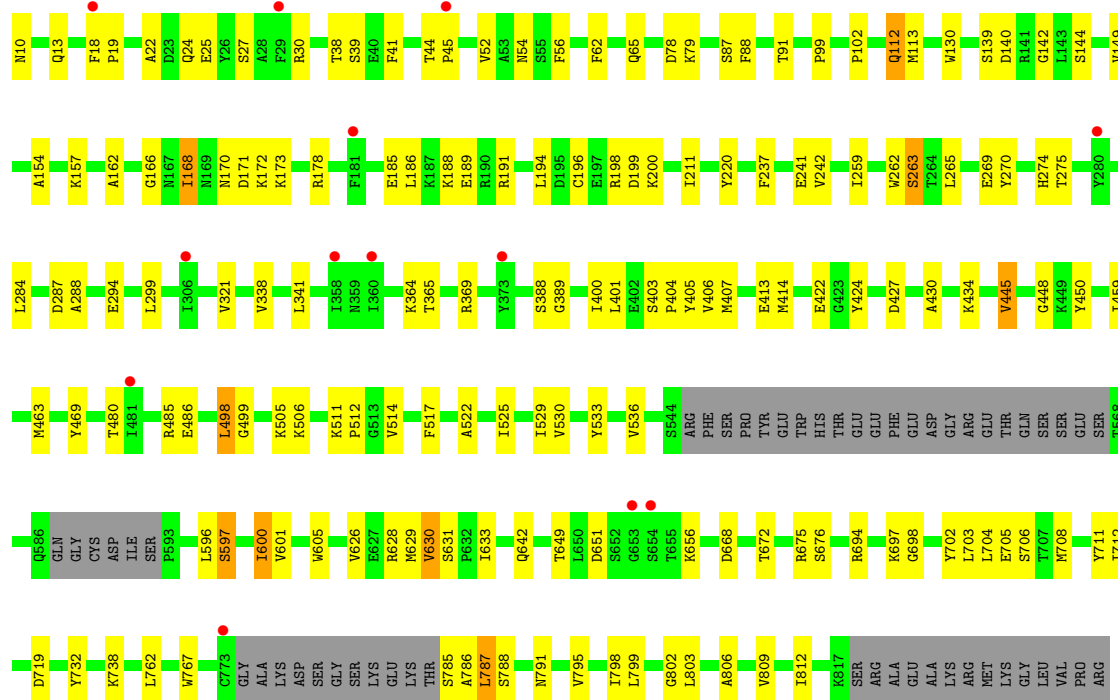
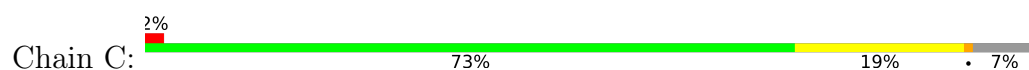
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: Glutamate receptor 2

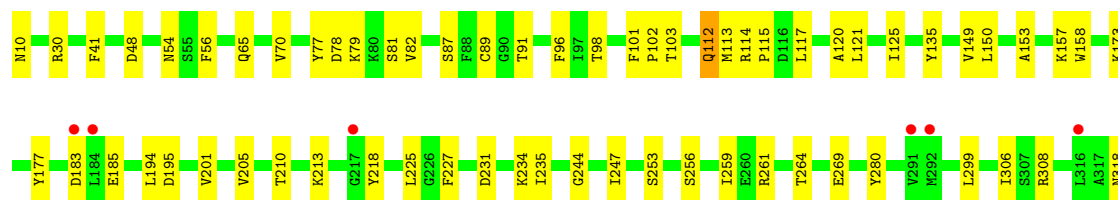
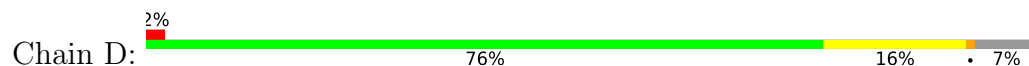


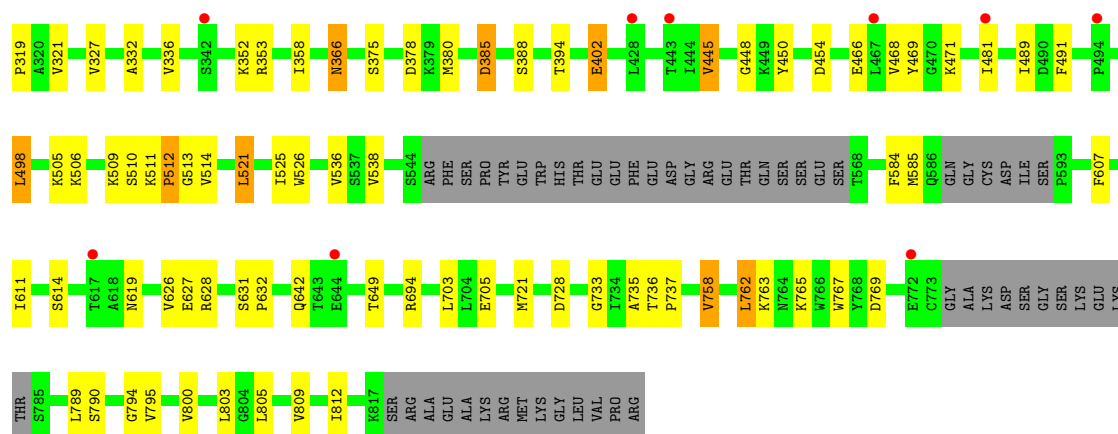


• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2





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

Chain E: 50% 50%



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

Chain F: 50% 50%



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

Chain G: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.37Å 166.57Å 566.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.95 – 4.79 39.95 – 4.79	Depositor EDS
% Data completeness (in resolution range)	89.8 (39.95-4.79) 89.7 (39.95-4.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.228 , 0.262 0.231 , 0.260	Depositor DCC
R_{free} test set	1515 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 182.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	24067	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NWD, 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	0.28	0/6100	0.75	2/8249 (0.0%)
1	B	0.28	0/6094	0.74	2/8241 (0.0%)
1	C	0.28	0/6094	0.73	1/8241 (0.0%)
1	D	0.28	0/6094	0.73	2/8241 (0.0%)
All	All	0.28	0/24382	0.74	7/32972 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	N-CA-C	-6.05	106.88	114.56
1	C	185	GLU	N-CA-C	-5.45	106.51	112.72
1	A	185	GLU	N-CA-C	-5.36	106.93	112.93
1	B	312	ALA	N-CA-C	-5.35	106.75	113.28
1	D	585	MET	N-CA-C	5.30	117.14	110.24
1	B	182	GLN	N-CA-C	-5.21	106.60	113.12
1	D	795	VAL	N-CA-C	-5.11	108.53	113.53

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	5979	0	5913	78	0
1	B	5974	0	5909	101	0
1	C	5974	0	5908	96	0
1	D	5974	0	5908	81	0
2	E	28	0	25	2	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	A	17	0	7	0	0
3	B	17	0	7	0	0
3	C	17	0	7	0	0
3	D	17	0	7	0	0
4	D	14	0	13	0	0
All	All	24067	0	23754	321	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 7.

All (321) 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:506:LYS:HB3	1:C:719:ASP:HB2	1.50	0.92
1:C:505:LYS:HD2	1:C:506:LYS:HG2	1.55	0.87
1:B:512:PRO:HA	1:B:790:SER:HB2	1.58	0.84
1:A:101:PHE:HA	1:A:114:ARG:HD3	1.66	0.78
1:C:166:GLY:HA2	1:C:200:LYS:HE2	1.72	0.71
1:B:744:THR:HG23	1:B:745:PRO:HD3	1.70	0.71
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.71	0.71
1:A:789:LEU:HD13	1:D:525:ILE:HG12	1.74	0.69
1:C:241:GLU:OE2	1:C:364:LYS:NZ	2.26	0.68
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.76	0.68
1:C:186:LEU:HD21	1:D:157:LYS:HE2	1.76	0.67
1:D:48:ASP:OD2	1:D:65:GLN:NE2	2.28	0.67
1:A:166:GLY:HA2	1:A:200:LYS:HE2	1.77	0.67
1:D:102:PRO:HD3	1:D:114:ARG:HD2	1.77	0.66
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.78	0.65
1:A:610:LEU:HD12	1:A:613:ILE:HD11	1.78	0.65
1:C:601:VAL:HG22	1:D:803:LEU:HD23	1.78	0.65
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.78	0.65
1:C:369:ARG:NH1	1:C:388:SER:OG	2.30	0.65
1:B:165:VAL:O	1:B:200:LYS:NZ	2.30	0.64
1:D:366:ASN:OD1	1:D:366:ASN:N	2.31	0.63
1:B:304:ILE:HG21	1:B:328:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TYR:OH	1:D:195:ASP:OD2	2.16	0.63
1:C:87:SER:OG	1:D:54:ASN:OD1	2.17	0.62
1:C:505:LYS:HZ2	1:C:697:LYS:HA	1.64	0.62
1:A:170:ASN:HA	1:A:173:LYS:HB2	1.80	0.62
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.81	0.61
1:A:196:CYS:HB3	1:A:200:LYS:HB3	1.81	0.61
1:B:506:LYS:HG3	1:B:721:MET:HE3	1.82	0.61
1:C:113:MET:HE3	1:C:288:ALA:HA	1.82	0.61
1:D:114:ARG:NH1	1:D:280:TYR:OH	2.34	0.60
1:D:70:VAL:O	1:D:308:ARG:NH1	2.35	0.60
1:C:102:PRO:HA	1:C:112:GLN:HG2	1.84	0.60
1:C:38:THR:OG1	1:C:39:SER:N	2.33	0.60
1:D:213:LYS:NZ	1:D:218:TYR:OH	2.30	0.60
1:C:530:VAL:HA	1:C:533:TYR:HB3	1.84	0.59
1:A:330:GLU:HG2	1:A:334:LYS:HE2	1.85	0.59
1:A:758:VAL:HA	1:A:761:LYS:HB3	1.84	0.59
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.84	0.59
1:C:54:ASN:OD1	1:D:87:SER:OG	2.21	0.59
1:B:134:ALA:HB2	1:B:189:GLU:HG2	1.85	0.59
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.84	0.58
1:B:486:GLU:O	1:B:738:LYS:NZ	2.33	0.58
1:C:78:ASP:OD1	1:C:79:LYS:N	2.35	0.58
1:A:135:TYR:OH	1:A:195:ASP:OD2	2.18	0.57
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.87	0.57
1:C:787:LEU:HD13	1:C:788:SER:H	1.70	0.57
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.87	0.57
1:A:803:LEU:HD21	1:D:536:VAL:HG22	1.87	0.56
1:A:205:VAL:HG13	1:A:235:ILE:HD12	1.88	0.56
1:B:517:PHE:HB2	1:B:791:ASN:OD1	2.05	0.56
1:B:528:CYS:HA	1:B:531:PHE:HB2	1.88	0.56
1:A:236:GLN:NE2	1:A:365:THR:O	2.37	0.55
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.88	0.55
1:C:27:SER:HB3	1:C:270:TYR:HB3	1.87	0.55
1:D:521:LEU:HD23	1:D:525:ILE:HB	1.89	0.55
1:A:113:MET:HG3	1:A:288:ALA:HB2	1.88	0.55
1:A:337:GLN:HE22	2:E:1:NAG:H2	1.72	0.54
1:A:407:MET:N	1:A:422:GLU:O	2.33	0.54
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.89	0.54
1:B:633:ILE:HG23	1:B:638:ASP:HB2	1.89	0.54
1:B:198:ARG:HH22	1:B:229:ASP:HB3	1.73	0.54
1:B:79:LYS:HZ1	1:B:80:LYS:HE3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HD2	1:A:354:ILE:HD11	1.90	0.53
1:A:602:GLY:HA2	1:A:605:TRP:HB3	1.89	0.53
1:A:198:ARG:HD3	1:A:279:LYS:HE3	1.88	0.53
1:B:17:LEU:HG	1:B:50:LEU:HD21	1.89	0.53
1:C:168:ILE:HD13	1:C:173:LYS:HG3	1.90	0.53
1:B:399:THR:HG23	1:B:444:ILE:HD13	1.91	0.53
1:A:754:SER:HB2	1:A:759:LEU:HD12	1.89	0.53
1:A:228:THR:OG1	1:A:246:GLN:NE2	2.41	0.53
1:D:402:GLU:OE1	1:D:450:TYR:OH	2.26	0.53
1:B:258:PHE:HD1	1:B:259:ILE:HD12	1.74	0.53
1:B:79:LYS:HE3	1:B:139:SER:HB2	1.90	0.52
1:A:225:LEU:HD13	1:A:247:ILE:HD11	1.90	0.52
1:B:530:VAL:HA	1:B:533:TYR:HB3	1.92	0.52
1:A:142:GLY:O	1:A:144:SER:N	2.41	0.52
1:D:185:GLU:OE1	1:D:213:LYS:NZ	2.43	0.52
1:D:225:LEU:HB3	1:D:247:ILE:HB	1.92	0.52
1:D:626:VAL:O	1:D:627:GLU:HG2	2.10	0.52
1:A:683:VAL:HG11	1:A:689:GLY:HA2	1.91	0.51
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.45	0.51
1:D:332:ALA:O	1:D:336:VAL:HG23	2.11	0.51
1:C:162:ALA:HB3	1:D:150:LEU:HD13	1.91	0.51
1:C:651:ASP:OD1	1:C:656:LYS:NZ	2.43	0.51
1:A:366:ASN:OD1	1:A:366:ASN:N	2.31	0.51
1:B:344:ASN:O	1:B:353:ARG:NH2	2.43	0.51
1:B:654:SER:OG	1:B:730:LYS:NZ	2.40	0.51
1:D:113:MET:O	1:D:353:ARG:NH1	2.44	0.51
1:C:505:LYS:HG2	1:C:698:GLY:N	2.26	0.51
1:B:521:LEU:HD22	1:B:526:TRP:CD2	2.46	0.51
1:A:511:LYS:HG2	1:A:512:PRO:HD2	1.92	0.51
1:B:383:THR:O	1:B:385:ASP:N	2.44	0.51
1:D:102:PRO:HA	1:D:112:GLN:HG2	1.93	0.51
1:B:173:LYS:HZ1	1:B:200:LYS:HE3	1.76	0.51
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.76	0.50
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.93	0.50
1:A:375:SER:HB3	1:A:378:ASP:HB2	1.94	0.50
1:A:114:ARG:NH2	1:A:280:TYR:OH	2.44	0.50
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.93	0.50
1:B:788:SER:C	1:B:790:SER:H	2.20	0.50
1:C:171:ASP:OD1	1:C:172:LYS:N	2.45	0.50
1:D:78:ASP:N	1:D:81:SER:OG	2.44	0.50
1:B:450:TYR:HE2	1:B:478:PRO:HG2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TYR:HB2	1:C:242:VAL:HG22	1.95	0.49
1:D:10:ASN:HB2	1:D:41:PHE:HA	1.93	0.49
1:C:694:ARG:NE	1:C:719:ASP:OD1	2.43	0.49
1:D:489:ILE:HD12	1:D:735:ALA:HB1	1.94	0.49
1:A:528:CYS:HB3	1:B:796:PHE:CZ	2.48	0.49
1:B:79:LYS:HZ2	1:B:140:ASP:HA	1.77	0.49
1:C:188:LYS:HD3	1:C:469:TYR:CZ	2.48	0.49
1:C:196:CYS:HB3	1:C:200:LYS:HB3	1.95	0.49
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.48	0.49
1:B:621:ALA:O	1:B:625:THR:OG1	2.28	0.48
1:A:405:TYR:HA	1:A:424:TYR:HB3	1.94	0.48
1:D:509:LYS:O	1:D:511:LYS:N	2.46	0.48
1:A:537:SER:HB3	1:A:583:ALA:HB2	1.94	0.48
1:B:405:TYR:HA	1:B:424:TYR:HB3	1.95	0.48
1:B:477:ALA:O	1:B:479:LEU:N	2.45	0.48
1:D:809:VAL:HG13	1:D:812:ILE:HD11	1.95	0.48
1:B:275:THR:OG1	1:B:277:THR:O	2.28	0.48
1:C:22:ALA:HB1	1:C:25:GLU:HB2	1.95	0.48
1:C:154:ALA:HB1	1:D:183:ASP:HB3	1.94	0.48
1:B:601:VAL:HG22	1:C:803:LEU:HD23	1.95	0.48
1:B:628:ARG:HG2	1:C:628:ARG:HH12	1.77	0.48
1:A:445:VAL:HG13	1:A:448:GLY:HA2	1.94	0.48
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.95	0.48
1:C:445:VAL:HG13	1:C:448:GLY:HA2	1.96	0.48
1:D:173:LYS:NZ	1:D:177:TYR:OH	2.46	0.48
1:A:207:GLN:O	1:A:211:ILE:HG13	2.14	0.47
1:D:231:ASP:HB3	1:D:234:LYS:HE2	1.96	0.47
1:B:103:THR:N	1:B:112:GLN:OE1	2.38	0.47
1:B:449:LYS:HG2	1:B:450:TYR:H	1.78	0.47
1:B:694:ARG:NE	1:B:719:ASP:OD1	2.48	0.47
1:C:294:GLU:HG3	1:C:338:VAL:HG11	1.96	0.47
1:C:596:LEU:HB3	1:D:809:VAL:HG11	1.96	0.47
1:D:498:LEU:HD23	1:D:705:GLU:HB3	1.95	0.47
1:D:173:LYS:HG2	1:D:177:TYR:HE2	1.79	0.47
1:B:29:PHE:O	1:B:33:MET:HG2	2.13	0.47
1:C:112:GLN:H	1:C:112:GLN:HE21	1.63	0.47
1:B:325:GLN:CD	1:B:325:GLN:H	2.23	0.47
1:B:338:VAL:HG23	1:B:345:ILE:HD12	1.97	0.47
1:B:626:VAL:HB	1:C:628:ARG:HE	1.79	0.47
1:D:521:LEU:HD22	1:D:526:TRP:CD2	2.49	0.47
1:A:29:PHE:O	1:A:33:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:HG2	1:A:766:TRP:HH2	1.80	0.47
1:A:667:PHE:CE1	1:A:727:LEU:HB3	2.50	0.47
1:D:103:THR:O	1:D:352:LYS:NZ	2.48	0.46
1:A:527:MET:HE3	1:A:531:PHE:HE2	1.80	0.46
1:B:521:LEU:HD23	1:B:525:ILE:HB	1.97	0.46
1:C:498:LEU:HD23	1:C:705:GLU:HB3	1.97	0.46
1:B:753:LEU:HD22	1:B:758:VAL:HG21	1.97	0.46
1:C:705:GLU:OE1	1:C:732:TYR:OH	2.27	0.46
1:C:711:TYR:HB2	1:C:767:TRP:NE1	2.31	0.46
1:D:445:VAL:HG13	1:D:448:GLY:HA2	1.97	0.46
1:A:337:GLN:NE2	2:E:1:NAG:H2	2.31	0.46
1:B:114:ARG:NH1	1:B:280:TYR:OH	2.48	0.46
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.96	0.46
1:C:629:MET:O	1:C:631:SER:N	2.48	0.46
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.70	0.46
1:D:800:VAL:HA	1:D:803:LEU:HB2	1.97	0.46
1:C:427:ASP:HB2	1:C:762:LEU:HD21	1.96	0.46
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.51	0.46
1:B:608:PHE:CD1	1:C:799:LEU:HD22	2.50	0.46
1:A:171:ASP:OD1	1:A:172:LYS:N	2.49	0.46
1:C:597:SER:O	1:C:600:ILE:HG12	2.15	0.46
1:D:512:PRO:HB2	1:D:513:GLY:H	1.54	0.46
1:B:138:ASP:HB3	1:B:166:GLY:HA3	1.98	0.46
1:C:517:PHE:HB2	1:C:791:ASN:OD1	2.16	0.46
1:A:79:LYS:HD3	1:A:139:SER:O	2.16	0.45
1:A:683:VAL:HB	1:A:688:GLU:HB3	1.98	0.45
1:B:763:LYS:O	1:B:767:TRP:HB2	2.16	0.45
1:B:451:GLY:O	1:B:485:ARG:NH2	2.50	0.45
1:C:198:ARG:NH2	1:C:199:ASP:OD1	2.49	0.45
1:C:480:THR:O	1:C:485:ARG:NH1	2.44	0.45
1:D:89:CYS:SG	1:D:96:PHE:HB2	2.57	0.45
1:A:705:GLU:OE1	1:A:732:TYR:OH	2.21	0.45
1:C:263:SER:OG	1:C:275:THR:O	2.32	0.45
1:C:52:VAL:HG22	1:C:78:ASP:HB2	1.98	0.45
1:C:178:ARG:HA	1:C:211:ILE:HD11	1.98	0.45
1:D:607:PHE:O	1:D:611:ILE:HG12	2.16	0.45
1:D:763:LYS:O	1:D:767:TRP:HB2	2.16	0.45
1:C:30:ARG:NH2	1:C:269:GLU:OE2	2.49	0.45
1:B:406:VAL:HG23	1:B:425:CYS:HB2	1.98	0.45
1:B:499:GLY:O	1:B:706:SER:N	2.50	0.45
1:B:521:LEU:HB2	1:B:616:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:OG1	1:A:39:SER:N	2.50	0.45
1:C:708:MET:O	1:C:712:ILE:HG12	2.17	0.45
1:C:130:TRP:CE2	1:C:191:ARG:HD3	2.52	0.44
1:D:481:ILE:HD11	1:D:733:GLY:HA3	1.98	0.44
1:B:539:VAL:HG21	1:C:803:LEU:HB3	1.99	0.44
1:A:711:TYR:HB2	1:A:767:TRP:NE1	2.32	0.44
1:B:205:VAL:O	1:B:209:ILE:HG13	2.17	0.44
1:C:407:MET:N	1:C:422:GLU:O	2.43	0.44
1:A:332:ALA:O	1:A:336:VAL:HG23	2.17	0.44
1:C:188:LYS:HD2	1:C:459:ILE:HG23	1.99	0.44
1:C:626:VAL:O	1:C:630:VAL:HG23	2.18	0.44
1:A:382:LEU:HD22	1:A:382:LEU:O	2.18	0.44
1:B:366:ASN:OD1	1:B:366:ASN:N	2.46	0.44
1:A:529:ILE:HD12	1:A:612:ILE:HG21	1.99	0.44
1:B:372:GLY:HA3	1:B:382:LEU:HA	2.00	0.44
1:C:450:TYR:O	1:C:463:MET:N	2.49	0.44
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.99	0.44
1:D:758:VAL:O	1:D:762:LEU:HB2	2.17	0.44
1:A:195:ASP:HA	1:A:223:ALA:HB3	2.00	0.44
1:B:539:VAL:O	1:B:543:VAL:HG23	2.18	0.44
1:B:604:VAL:HG11	1:C:802:GLY:HA3	2.00	0.44
1:C:18:PHE:HA	1:C:19:PRO:HD3	1.90	0.44
1:C:486:GLU:O	1:C:738:LYS:NZ	2.51	0.44
1:A:422:GLU:HG2	1:A:766:TRP:CH2	2.53	0.44
1:A:628:ARG:C	1:D:626:VAL:HG21	2.43	0.44
1:B:232:LEU:HD22	1:B:363:LEU:HD22	2.00	0.44
1:C:91:THR:HG21	1:D:56:PHE:CZ	2.53	0.44
1:A:142:GLY:C	1:A:144:SER:H	2.23	0.43
1:B:18:PHE:HA	1:B:19:PRO:HD3	1.86	0.43
1:D:728:ASP:N	1:D:728:ASP:OD1	2.50	0.43
1:B:48:ASP:OD2	1:B:65:GLN:NE2	2.41	0.43
1:B:102:PRO:HD3	1:B:114:ARG:HD2	1.98	0.43
1:C:511:LYS:HG2	1:C:512:PRO:HD2	2.01	0.43
1:C:795:VAL:O	1:C:798:ILE:HG22	2.18	0.43
1:D:466:GLU:HG2	1:D:471:LYS:HD2	2.00	0.43
1:B:638:ASP:OD1	1:B:638:ASP:N	2.52	0.43
1:A:118:LYS:HB2	1:A:118:LYS:HE3	1.80	0.43
1:B:523:TYR:O	1:B:527:MET:HG2	2.19	0.43
1:C:62:PHE:CE2	1:C:88:PHE:HB3	2.53	0.43
1:D:299:LEU:HD13	1:D:306:ILE:HG21	2.01	0.43
1:C:44:THR:HA	1:C:45:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.99	0.43
1:D:765:LYS:HA	1:D:769:ASP:HB2	2.01	0.43
1:D:121:LEU:O	1:D:125:ILE:HG13	2.18	0.43
1:D:491:PHE:CE1	1:D:735:ALA:HB2	2.54	0.43
1:C:405:TYR:HA	1:C:424:TYR:HB3	2.00	0.43
1:C:499:GLY:O	1:C:706:SER:N	2.47	0.43
1:D:96:PHE:HE1	1:D:98:THR:HB	1.84	0.43
1:A:62:PHE:HE2	1:A:92:LEU:HD12	1.84	0.43
1:A:101:PHE:HA	1:A:102:PRO:HD3	1.87	0.43
1:A:102:PRO:HA	1:A:112:GLN:HG2	1.99	0.43
1:C:142:GLY:C	1:C:144:SER:H	2.27	0.43
1:A:610:LEU:HD21	1:B:613:ILE:HG21	2.01	0.42
1:D:201:VAL:O	1:D:205:VAL:HG23	2.19	0.42
1:D:253:SER:HA	1:D:256:SER:HB3	2.00	0.42
1:A:686:THR:HG21	1:A:708:MET:SD	2.59	0.42
1:B:445:VAL:HG13	1:B:448:GLY:HA2	2.02	0.42
1:B:601:VAL:HG23	1:C:806:ALA:HB3	2.00	0.42
1:D:505:LYS:NZ	1:D:694:ARG:O	2.48	0.42
1:A:405:TYR:CD2	1:A:478:PRO:HG3	2.55	0.42
1:B:38:THR:OG1	1:B:39:SER:N	2.52	0.42
1:D:512:PRO:HA	1:D:790:SER:HB2	2.01	0.42
1:A:36:PHE:CZ	1:A:290:GLN:HB2	2.54	0.42
1:A:99:PRO:O	1:A:114:ARG:HD2	2.20	0.42
1:A:400:ILE:HG22	1:A:477:ALA:HB1	2.01	0.42
1:C:400:ILE:HA	1:C:445:VAL:HG12	2.02	0.42
1:B:219:HIS:ND1	1:B:241:GLU:O	2.46	0.42
1:B:464:VAL:HG13	1:B:489:ILE:HD13	2.02	0.42
1:D:385:ASP:OD1	1:D:385:ASP:N	2.52	0.42
1:B:628:ARG:HG2	1:C:628:ARG:NH1	2.35	0.42
1:C:13:GLN:HG3	1:C:44:THR:O	2.20	0.42
1:C:672:THR:HG23	1:C:675:ARG:NH2	2.35	0.42
1:D:506:LYS:HE2	1:D:721:MET:HE3	2.00	0.42
1:A:162:ALA:HB3	1:B:150:LEU:HD13	2.01	0.42
1:C:56:PHE:CE1	1:D:91:THR:HG21	2.55	0.42
1:D:114:ARG:HA	1:D:115:PRO:HD3	1.90	0.42
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.55	0.41
1:B:79:LYS:NZ	1:B:80:LYS:HE3	2.34	0.41
1:B:96:PHE:HE1	1:B:98:THR:HB	1.85	0.41
1:B:706:SER:O	1:B:710:GLU:HG2	2.20	0.41
1:A:323:TRP:H	1:A:323:TRP:CD1	2.38	0.41
1:B:115:PRO:HA	1:B:353:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:OD2	1:C:341:LEU:N	2.52	0.41
1:D:261:ARG:NH2	1:D:264:THR:OG1	2.53	0.41
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.82	0.41
1:A:500:ILE:O	1:A:727:LEU:HG	2.20	0.41
1:D:30:ARG:HH22	1:D:269:GLU:HG3	1.84	0.41
1:A:656:LYS:HE3	1:A:682:PHE:CZ	2.56	0.41
1:A:115:PRO:HA	1:A:353:ARG:HB2	2.01	0.41
1:B:213:LYS:O	1:B:220:TYR:OH	2.34	0.41
1:B:787:LEU:HD22	1:B:787:LEU:HA	1.92	0.41
1:C:401:LEU:HD23	1:C:406:VAL:HG12	2.03	0.41
1:C:702:TYR:CE2	1:C:704:LEU:HB3	2.56	0.41
1:A:154:ALA:HB1	1:B:183:ASP:HB3	2.03	0.41
1:A:181:PHE:C	1:A:183:ASP:H	2.29	0.41
1:B:521:LEU:HB2	1:B:616:TYR:HD1	1.84	0.41
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.88	0.41
1:B:181:PHE:HA	1:B:184:LEU:HB2	2.02	0.41
1:B:200:LYS:HD2	1:B:200:LYS:HA	1.88	0.41
1:B:364:LYS:HB3	1:B:365:THR:H	1.73	0.41
1:B:467:LEU:HD23	1:B:467:LEU:HA	1.90	0.41
1:C:24:GLN:HG3	1:C:262:TRP:HZ2	1.85	0.41
1:C:403:SER:HA	1:C:404:PRO:HA	1.72	0.41
1:A:626:VAL:O	1:A:630:VAL:HG23	2.21	0.41
1:A:787:LEU:HB2	1:D:619:ASN:ND2	2.35	0.41
1:B:406:VAL:HG22	1:B:426:VAL:HG23	2.03	0.41
1:C:30:ARG:HH22	1:C:269:GLU:HG3	1.86	0.41
1:D:101:PHE:HA	1:D:114:ARG:HD2	2.03	0.41
1:D:805:LEU:O	1:D:809:VAL:HG23	2.21	0.41
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.56	0.40
1:A:659:PHE:CE2	1:A:703:LEU:HD13	2.56	0.40
1:B:25:GLU:OE1	1:B:25:GLU:N	2.53	0.40
1:B:173:LYS:HG2	1:B:177:TYR:HE2	1.86	0.40
1:C:10:ASN:HB2	1:C:41:PHE:HA	2.03	0.40
1:C:91:THR:HG21	1:D:56:PHE:CE2	2.56	0.40
1:B:511:LYS:HA	1:B:512:PRO:HD3	1.90	0.40
1:C:265:LEU:O	1:C:274:HIS:ND1	2.45	0.40
1:C:430:ALA:O	1:C:434:LYS:N	2.53	0.40
1:C:522:ALA:HB3	1:C:525:ILE:HG13	2.02	0.40
1:D:468:VAL:HG23	1:D:469:TYR:CD1	2.57	0.40
1:D:489:ILE:HG22	1:D:737:PRO:HA	2.02	0.40
1:A:803:LEU:HD23	1:A:803:LEU:HA	1.96	0.40
1:D:153:ALA:HA	1:D:158:TRP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ILE:HD13	1:D:358:ILE:HG12	2.03	0.40
1:D:318:ASN:HA	1:D:319:PRO:HA	1.84	0.40
1:D:375:SER:HB3	1:D:378:ASP:HB2	2.02	0.40
1:D:514:VAL:HG13	1:D:794:GLY:HA3	2.03	0.40
1:B:623:PHE:CZ	1:C:786:ALA:HA	2.56	0.40
1:C:237:PHE:CD1	1:C:365:THR:HG23	2.56	0.40
1:A:528:CYS:HB3	1:B:796:PHE:HZ	1.86	0.40
1:A:628:ARG:NH2	1:D:628:ARG:HG2	2.37	0.40
1:B:136:LEU:HD22	1:B:163:ILE:HB	2.04	0.40
1:B:237:PHE:HB2	1:D:210:THR:HG22	2.04	0.40
1:B:360:ILE:HG22	1:B:371:ILE:HG12	2.03	0.40
1:C:536:VAL:HG21	1:C:605:TRP:CE3	2.57	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	760/822 (92%)	693 (91%)	61 (8%)	6 (1%)	16	52
1	B	760/822 (92%)	703 (92%)	50 (7%)	7 (1%)	14	49
1	C	760/822 (92%)	698 (92%)	57 (8%)	5 (1%)	18	55
1	D	760/822 (92%)	702 (92%)	52 (7%)	6 (1%)	16	52
All	All	3040/3288 (92%)	2796 (92%)	220 (7%)	24 (1%)	16	52

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	512	PRO
1	C	597	SER
1	D	512	PRO

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Mol	Chain	Res	Type
1	A	143	LEU
1	B	390	LEU
1	B	393	LYS
1	C	140	ASP
1	C	630	VAL
1	D	510	SER
1	A	597	SER
1	B	384	GLU
1	D	385	ASP
1	A	584	PHE
1	B	394	THR
1	B	584	PHE
1	B	632	PRO
1	C	633	ILE
1	A	142	GLY
1	A	198	ARG
1	A	387	THR
1	D	82	VAL
1	D	584	PHE
1	D	632	PRO
1	C	389	GLY

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	636/702 (91%)	611 (96%)	25 (4%)	28	50
1	B	635/702 (90%)	610 (96%)	25 (4%)	28	50
1	C	635/702 (90%)	612 (96%)	23 (4%)	31	52
1	D	635/702 (90%)	611 (96%)	24 (4%)	29	51
All	All	2541/2808 (90%)	2444 (96%)	97 (4%)	29	51

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	60	ASN
1	A	65	GLN
1	A	82	VAL
1	A	112	GLN
1	A	165	VAL
1	A	183	ASP
1	A	194	LEU
1	A	219	HIS
1	A	248	VAL
1	A	275	THR
1	A	289	VAL
1	A	308	ARG
1	A	366	ASN
1	A	380	MET
1	A	382	LEU
1	A	396	VAL
1	A	401	LEU
1	A	413	GLU
1	A	484	VAL
1	A	498	LEU
1	A	514	VAL
1	A	642	GLN
1	A	643	THR
1	A	678	GLU
1	B	79	LYS
1	B	84	THR
1	B	87	SER
1	B	139	SER
1	B	140	ASP
1	B	210	THR
1	B	248	VAL
1	B	252	ASP
1	B	308	ARG
1	B	328	GLU
1	B	380	MET
1	B	387	THR
1	B	390	LEU
1	B	394	THR
1	B	413	GLU
1	B	497	SER
1	B	498	LEU
1	B	601	VAL

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Mol	Chain	Res	Type
1	B	612	ILE
1	B	642	GLN
1	B	744	THR
1	B	762	LEU
1	B	787	LEU
1	B	795	VAL
1	B	815	CYS
1	C	65	GLN
1	C	112	GLN
1	C	139	SER
1	C	149	VAL
1	C	157	LYS
1	C	168	ILE
1	C	189	GLU
1	C	194	LEU
1	C	259	ILE
1	C	263	SER
1	C	321	VAL
1	C	413	GLU
1	C	414	MET
1	C	445	VAL
1	C	498	LEU
1	C	514	VAL
1	C	529	ILE
1	C	600	ILE
1	C	642	GLN
1	C	668	ASP
1	C	676	SER
1	C	785	SER
1	C	787	LEU
1	D	79	LYS
1	D	112	GLN
1	D	149	VAL
1	D	194	LEU
1	D	235	ILE
1	D	259	ILE
1	D	321	VAL
1	D	327	VAL
1	D	366	ASN
1	D	380	MET
1	D	388	SER
1	D	394	THR

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Mol	Chain	Res	Type
1	D	402	GLU
1	D	445	VAL
1	D	454	ASP
1	D	498	LEU
1	D	521	LEU
1	D	538	VAL
1	D	614	SER
1	D	631	SER
1	D	642	GLN
1	D	736	THR
1	D	758	VAL
1	D	762	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	337	GLN
1	B	290	GLN
1	C	350	ASN
1	C	392	GLN
1	C	411	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](#)

6 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	E	1	2,1	14,14,15	0.53	0	17,19,21	0.70	0
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	0.71	0
2	NAG	F	1	2,1	14,14,15	0.66	0	17,19,21	0.94	1 (5%)
2	NAG	F	2	2	14,14,15	0.53	0	17,19,21	0.65	0
2	NAG	G	1	2,1	14,14,15	0.52	0	17,19,21	0.84	0
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	0.59	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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C4-C3-C2	2.03	113.99	111.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2

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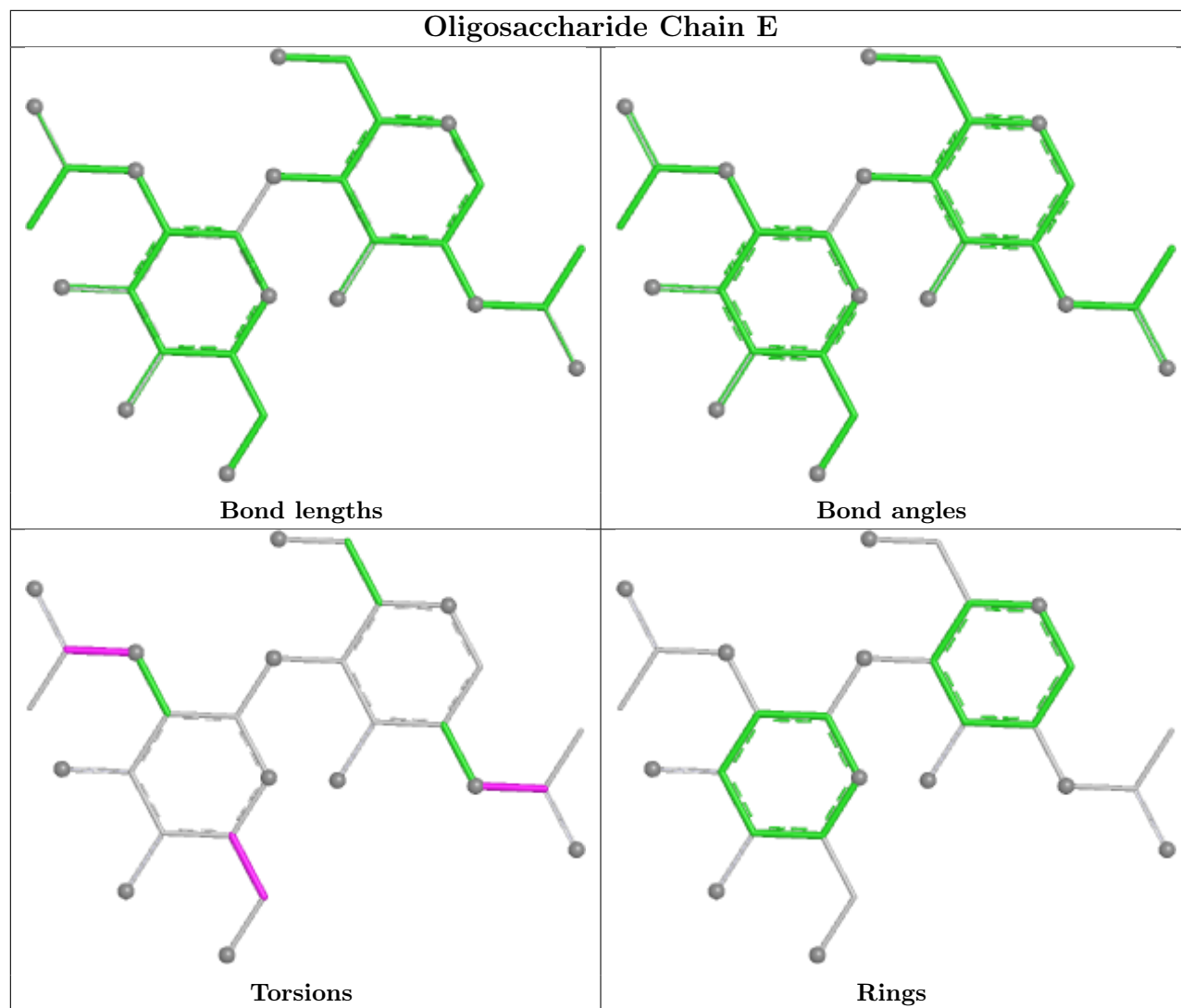
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

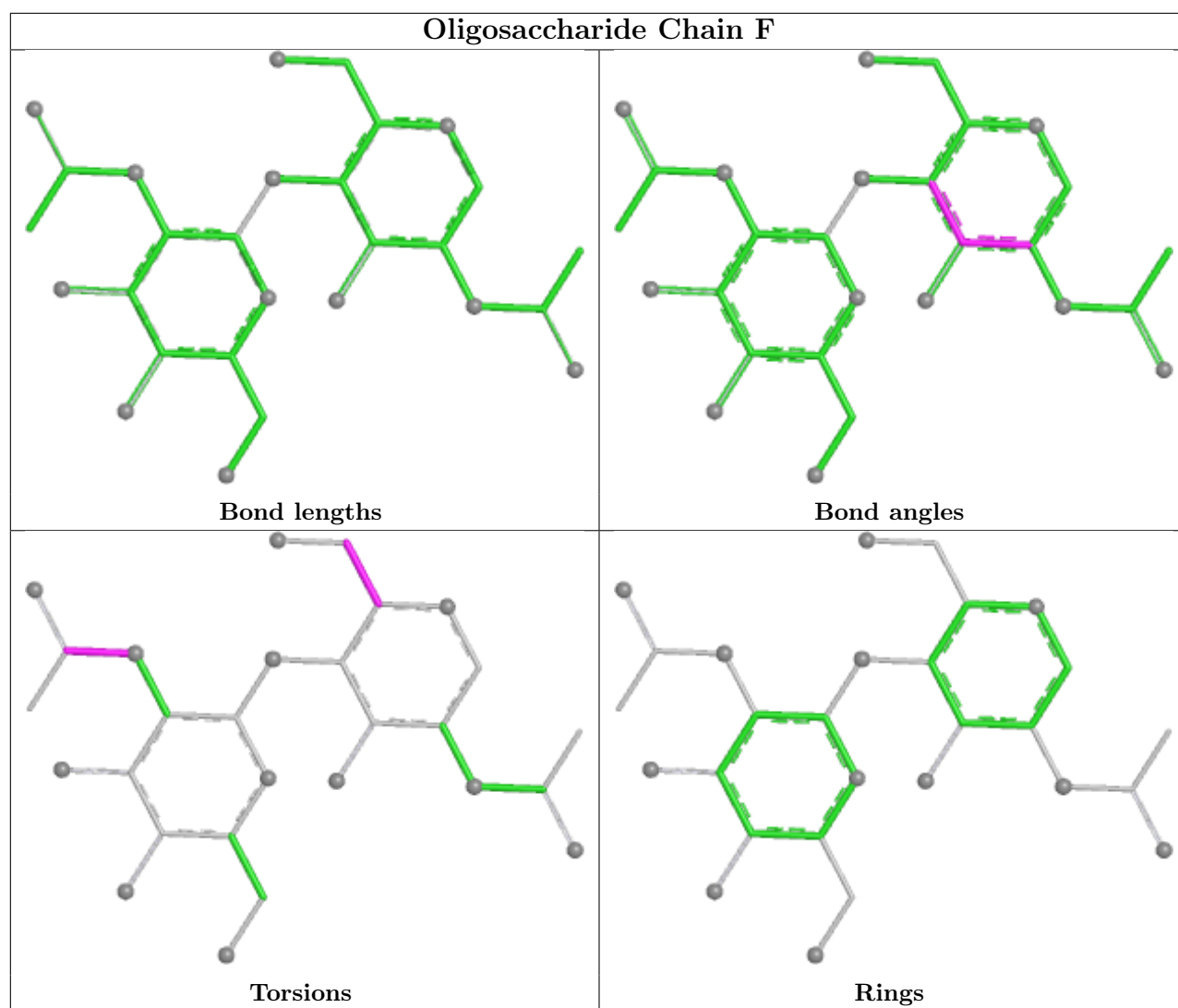
There are no ring outliers.

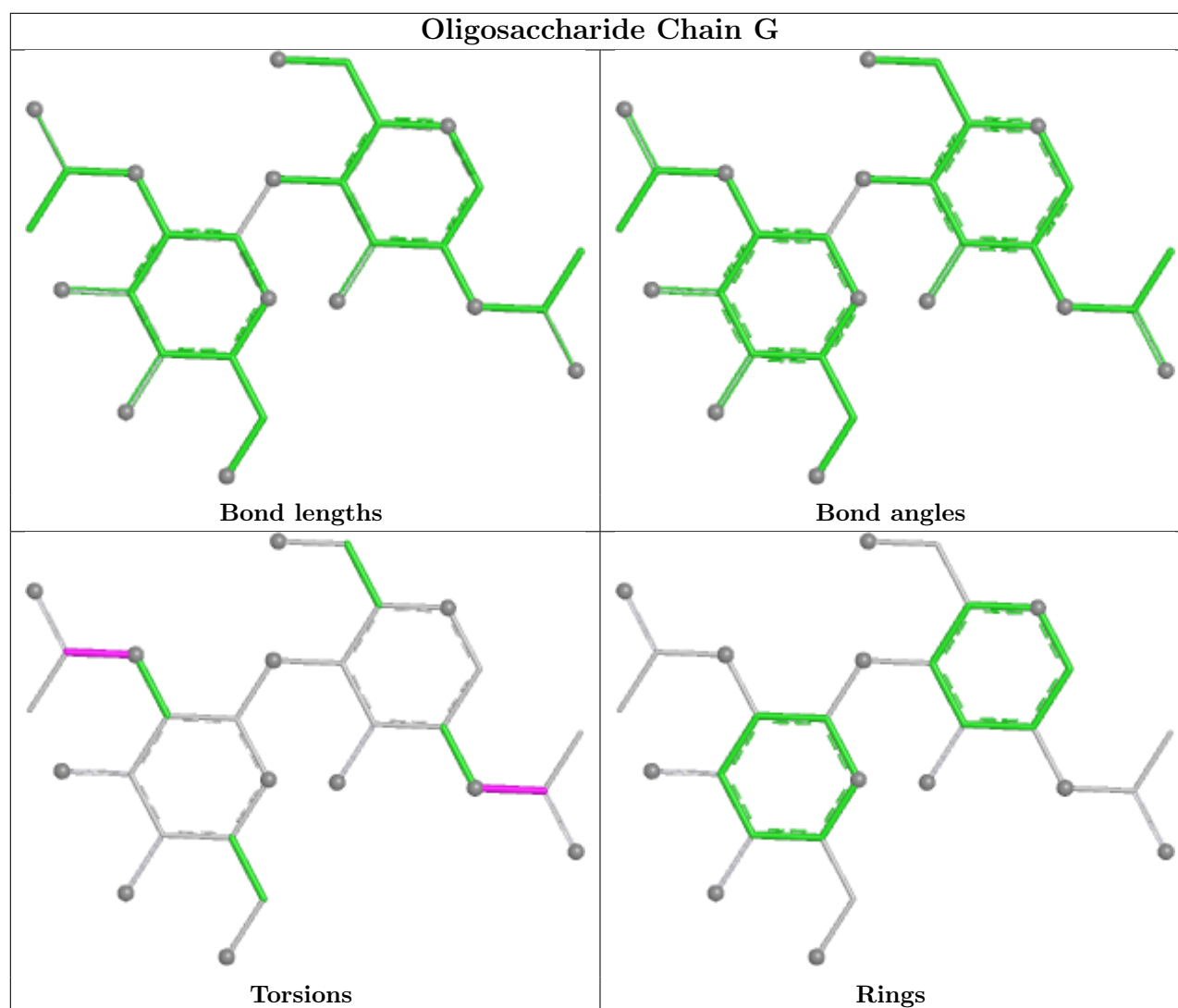
1 monomer is involved in 2 short contacts:

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

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







5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	NWD	D	902	-	15,17,17	2.19	5 (33%)	12,24,24	3.82	4 (33%)
3	NWD	B	903	-	15,17,17	2.21	5 (33%)	12,24,24	4.01	5 (41%)
3	NWD	A	903	-	15,17,17	2.17	5 (33%)	12,24,24	4.00	5 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	901	1	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
3	NWD	C	903	-	15,17,17	2.15	4 (26%)	12,24,24	3.82	5 (41%)

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	NWD	D	902	-	-	2/10/12/12	0/1/1/1
3	NWD	B	903	-	-	3/10/12/12	0/1/1/1
3	NWD	A	903	-	-	2/10/12/12	0/1/1/1
4	NAG	D	901	1	-	4/6/23/26	0/1/1/1
3	NWD	C	903	-	-	4/10/12/12	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	NWD	C6-N1	4.18	1.45	1.37
3	A	903	NWD	C2-N1	4.09	1.43	1.37
3	D	902	NWD	C2-N1	4.09	1.43	1.37
3	B	903	NWD	C6-N1	4.03	1.44	1.37
3	C	903	NWD	C2-N1	4.00	1.43	1.37
3	A	903	NWD	C6-N1	3.98	1.44	1.37
3	B	903	NWD	C7-N1	-3.97	1.42	1.47
3	D	902	NWD	C6-N1	3.88	1.44	1.37
3	B	903	NWD	C2-N1	3.71	1.42	1.37
3	D	902	NWD	C7-N1	-3.62	1.43	1.47
3	A	903	NWD	C7-N1	-3.53	1.43	1.47
3	B	903	NWD	C7-C8	-3.41	1.49	1.53
3	C	903	NWD	C7-N1	-3.13	1.43	1.47
3	C	903	NWD	C7-C8	-3.07	1.49	1.53
3	D	902	NWD	C7-C8	-3.01	1.49	1.53
3	A	903	NWD	C7-C8	-3.00	1.49	1.53
3	D	902	NWD	C5-C4	2.11	1.50	1.47
3	A	903	NWD	C5-C4	2.06	1.49	1.47
3	B	903	NWD	C5-C4	2.06	1.49	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	NWD	C5-C4-N3	12.51	118.44	112.19
3	B	903	NWD	C5-C4-N3	12.35	118.35	112.19
3	C	903	NWD	C5-C4-N3	12.00	118.18	112.19
3	D	902	NWD	C5-C4-N3	11.86	118.11	112.19
3	B	903	NWD	C6-N1-C2	3.36	124.61	121.29
3	A	903	NWD	C4-N3-C2	-3.35	122.95	127.34
3	D	902	NWD	C4-N3-C2	-3.32	122.99	127.34
3	B	903	NWD	C7-N1-C2	-3.24	115.26	118.43
3	A	903	NWD	C6-N1-C2	3.13	124.38	121.29
3	B	903	NWD	C4-N3-C2	-3.10	123.28	127.34
3	C	903	NWD	C4-N3-C2	-3.09	123.29	127.34
3	D	902	NWD	C6-N1-C2	2.71	123.97	121.29
3	D	902	NWD	O4-C4-C5	2.47	122.33	118.90
3	B	903	NWD	O4-C4-C5	2.31	122.11	118.90
4	D	901	NAG	O5-C1-C2	2.29	114.83	111.29
3	C	903	NWD	O4-C4-C5	2.29	122.07	118.90
3	A	903	NWD	O4-C4-C5	2.24	122.01	118.90
3	A	903	NWD	C7-N1-C2	-2.21	116.26	118.43
3	C	903	NWD	C7-N1-C2	-2.14	116.34	118.43
3	C	903	NWD	C6-N1-C2	2.05	123.31	121.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	NWD	C4-C5-N2-O1
3	A	903	NWD	C6-C5-N2-O1
3	B	903	NWD	C6-C5-N2-O1
3	C	903	NWD	C8-C7-N1-C2
3	C	903	NWD	C8-C7-N1-C6
4	D	901	NAG	C8-C7-N2-C2
4	D	901	NAG	O7-C7-N2-C2
4	D	901	NAG	O5-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
3	B	903	NWD	C4-C5-N2-O1
3	D	902	NWD	C4-C5-N2-O1
3	D	902	NWD	C6-C5-N2-O1
3	C	903	NWD	C6-C5-N2-O1
3	C	903	NWD	C4-C5-N2-O1
3	B	903	NWD	N8-C8-C9-O92

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 ⓘ

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	768/822 (93%)	-0.25	17 (2%)	62 50	5, 118, 276, 550	0
1	B	768/822 (93%)	-0.09	23 (2%)	52 42	3, 118, 270, 550	0
1	C	768/822 (93%)	-0.23	13 (1%)	69 55	24, 155, 280, 493	0
1	D	768/822 (93%)	-0.19	15 (1%)	65 52	6, 147, 286, 550	0
All	All	3072/3288 (93%)	-0.19	68 (2%)	62 50	3, 137, 280, 550	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	358	ILE	5.4
1	B	124	LEU	4.4
1	A	103	THR	4.3
1	A	102	PRO	4.2
1	B	338	VAL	4.2
1	A	220	TYR	4.2
1	A	181	PHE	4.2
1	A	174	ASP	4.1
1	D	183	ASP	3.9
1	B	113	MET	3.9
1	B	341	LEU	3.8
1	D	481	ILE	3.8
1	C	373	TYR	3.8
1	C	360	ILE	3.8
1	B	703	LEU	3.7
1	A	609	THR	3.4
1	B	306	ILE	3.2
1	B	609	THR	3.1
1	B	380	MET	3.1
1	C	773	CYS	3.0
1	A	178	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	204	ILE	2.9
1	A	43	LEU	2.9
1	C	654	SER	2.8
1	D	494	PRO	2.8
1	D	644	GLU	2.8
1	B	299	LEU	2.7
1	B	104	ASP	2.7
1	B	127	TYR	2.7
1	B	151	ASP	2.7
1	B	284	LEU	2.6
1	D	291	VAL	2.6
1	B	122	LEU	2.4
1	C	181	PHE	2.4
1	D	428	LEU	2.4
1	A	248	VAL	2.4
1	B	291	VAL	2.3
1	C	653	GLY	2.3
1	B	493	LYS	2.3
1	B	695	LYS	2.3
1	B	43	LEU	2.3
1	D	292	MET	2.3
1	D	342	SER	2.2
1	A	104	ASP	2.2
1	D	772	GLU	2.2
1	C	18	PHE	2.2
1	A	708	MET	2.2
1	C	45	PRO	2.2
1	D	443	THR	2.2
1	A	197	GLU	2.2
1	B	287	ASP	2.1
1	D	217	GLY	2.1
1	C	29	PHE	2.1
1	B	627	GLU	2.1
1	C	280	TYR	2.1
1	A	651	ASP	2.1
1	A	678	GLU	2.1
1	B	360	ILE	2.1
1	B	583	ALA	2.1
1	D	184	LEU	2.1
1	C	306	ILE	2.0
1	D	617	THR	2.0
1	D	467	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	101	PHE	2.0
1	C	481	ILE	2.0
1	A	654	SER	2.0
1	A	117	LEU	2.0
1	D	316	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](#)

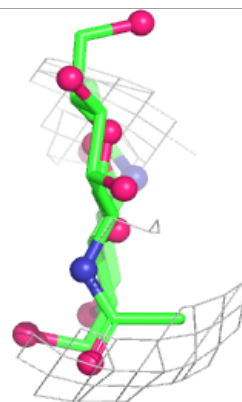
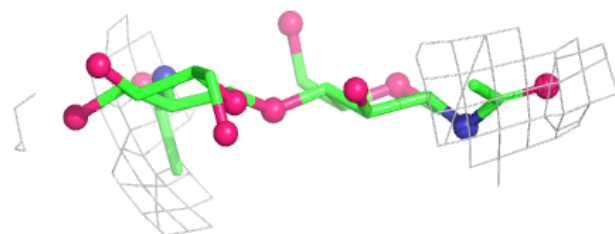
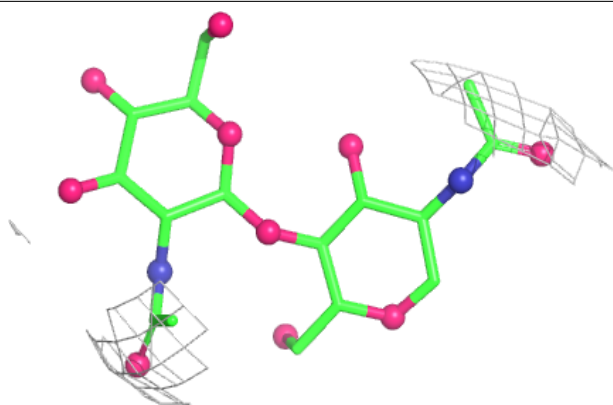
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F	2	14/15	0.56	0.11	170,170,170,170	0
2	NAG	G	2	14/15	0.75	0.09	249,249,249,249	0
2	NAG	E	2	14/15	0.76	0.06	165,165,165,165	0
2	NAG	F	1	14/15	0.78	0.07	174,174,174,174	0
2	NAG	E	1	14/15	0.86	0.06	176,176,176,176	0
2	NAG	G	1	14/15	0.90	0.08	239,239,239,239	0

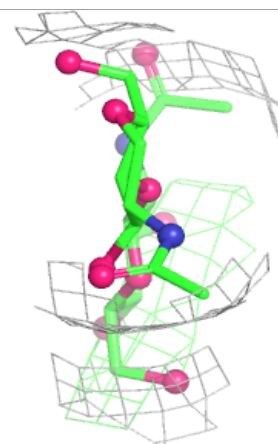
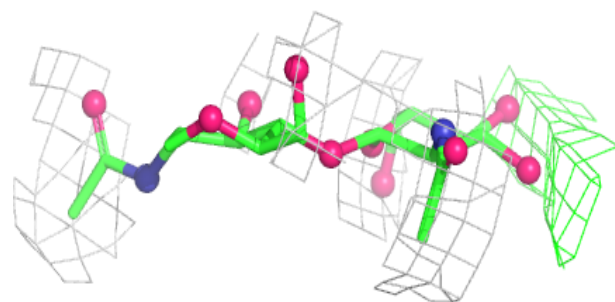
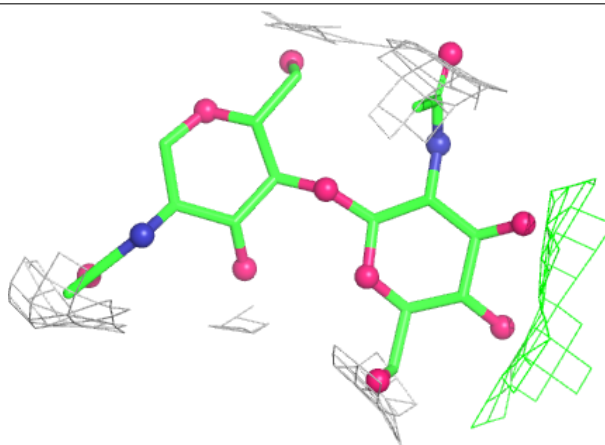
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

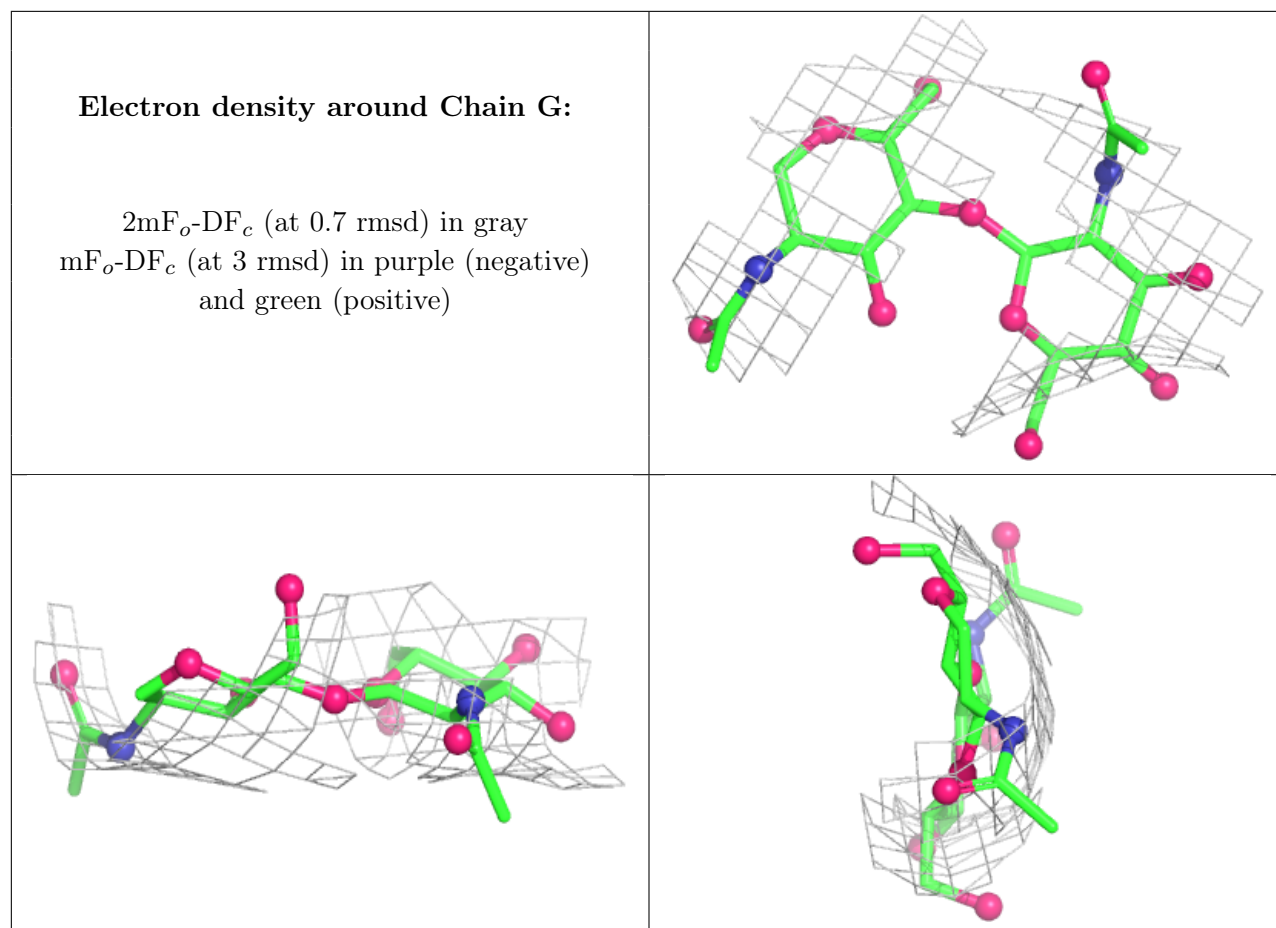
Electron density around Chain E:

$2mF_o-DF_c$ (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
3	NWD	C	903	17/17	0.59	0.23	124,124,124,124	0
3	NWD	D	902	17/17	0.62	0.10	199,199,199,199	0
4	NAG	D	901	14/15	0.76	0.07	176,176,176,176	0
3	NWD	A	903	17/17	0.82	0.17	136,136,136,136	0
3	NWD	B	903	17/17	0.91	0.08	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.