



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 AM UTC

PDB ID : 3QEM / pdb_00003qem
Title : Crystal structure of amino terminal domains of the NMDA receptor subunit GluN1 and GluN2B in complex with Ro 25-6981
Authors : Karakas, E.; Simorowski, N.; Furukawa, H.
Deposited on : 2011-01-20
Resolution : 3.00 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

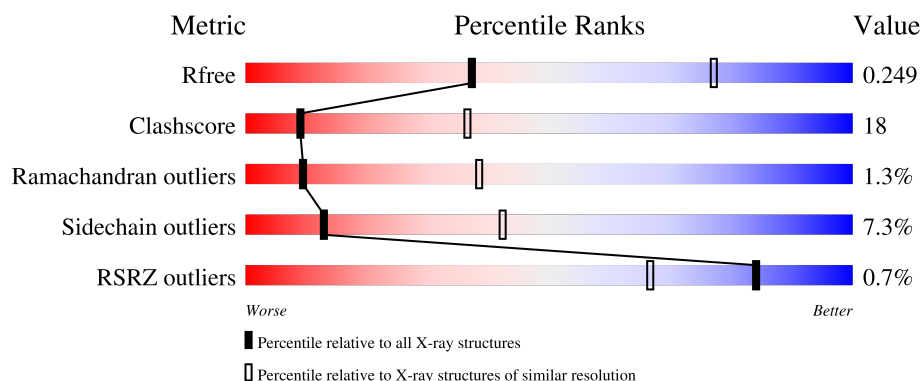
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	383	68% 22% • 7%
1	C	383	% 63% 27% • 8%
2	B	364	% 59% 33% 6% •
2	D	364	% 58% 32% • 5%
3	E	5	60% 40%

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
4	NAG	A	406	X	-	-	-
4	NAG	B	395	X	-	-	-
4	NAG	C	1	X	-	-	-
4	NAG	D	1	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10273 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 NMDA glutamate receptor subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2635	1684	456	485	10			
1	C	352	Total	C	N	O	S	0	0	0
			2483	1589	427	457	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	engineered mutation	UNP Q91977
A	371	GLN	ASN	engineered mutation	UNP Q91977
C	61	GLN	ASN	engineered mutation	UNP Q91977
C	371	GLN	ASN	engineered mutation	UNP Q91977

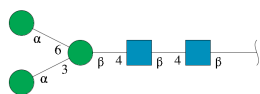
- Molecule 2 is a protein called Glutamate [NMDA] receptor subunit epsilon-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2548	1641	410	482	15			
2	D	345	Total	C	N	O	S	0	0	0
			2424	1560	393	456	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ASP	ASN	engineered mutation	UNP Q00960
D	348	ASP	ASN	engineered mutation	UNP Q00960

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

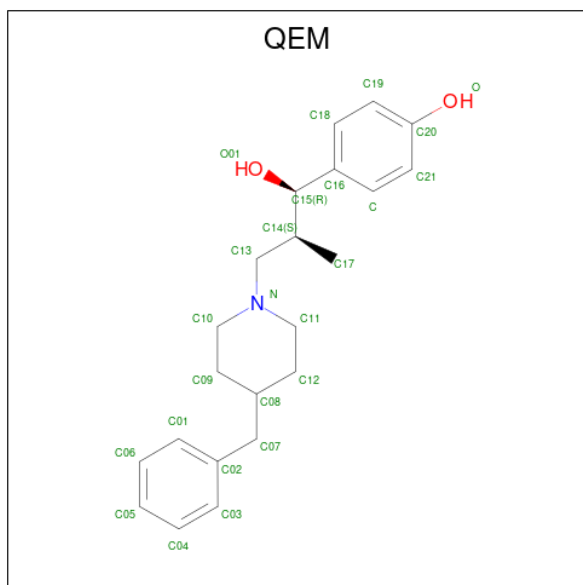
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is 4-[(1R,2S)-3-(4-benzylpiperidin-1-yl)-1-hydroxy-2-methylpropyl]phenol (CCD ID: QEM) (formula: C₂₂H₂₉NO₂).

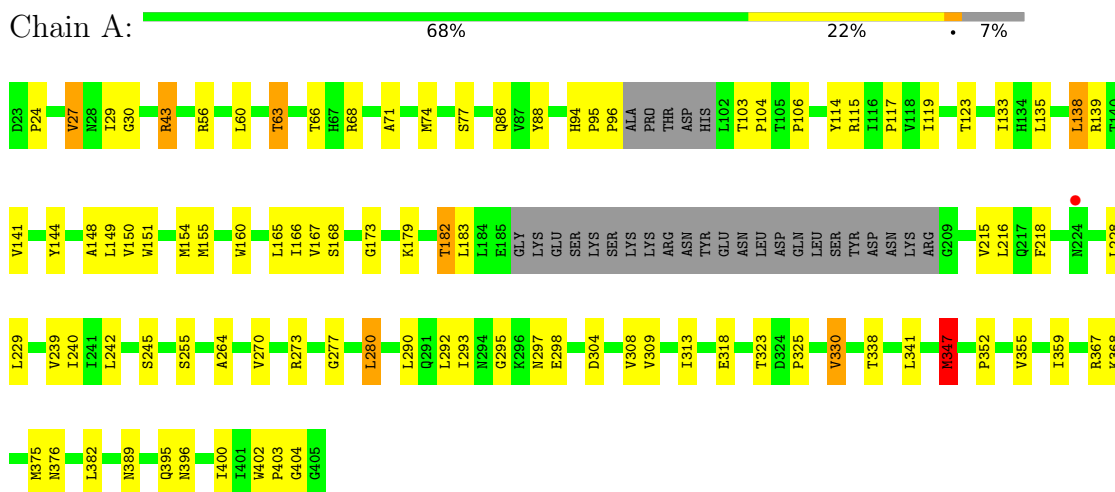


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			25	22	1	2		
6	D	1	Total	C	N	O	0	0
			25	22	1	2		

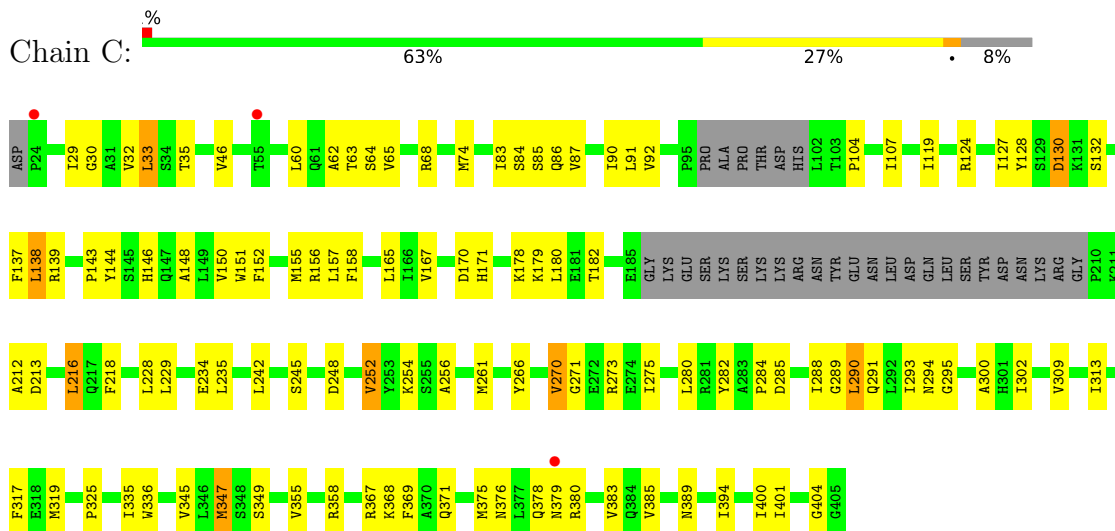
3 Residue-property plots

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: NMDA glutamate receptor subunit

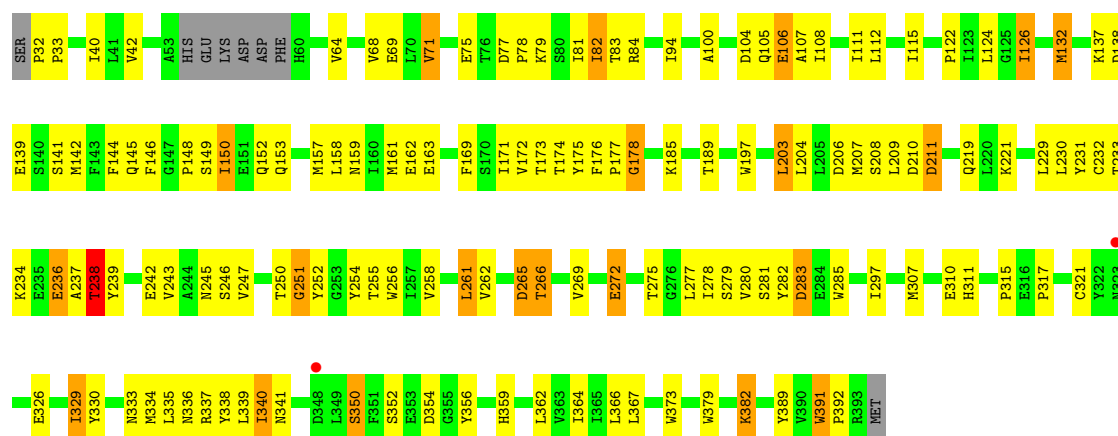


• Molecule 1: NMDA glutamate receptor subunit

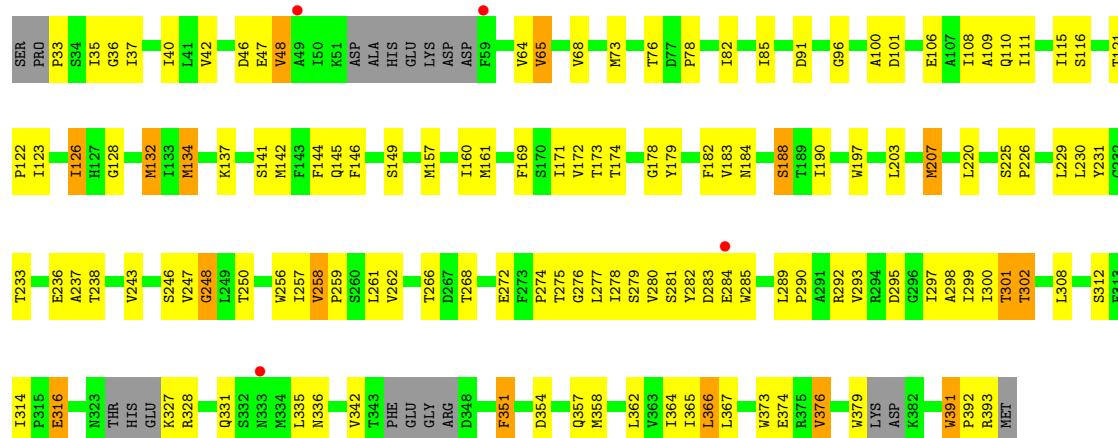


• Molecule 2: Glutamate [NMDA] receptor subunit epsilon-2





• Molecule 2: Glutamate [NMDA] receptor subunit epsilon-2



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.03Å 61.26Å 144.42Å 90.00° 116.32° 90.00°	Depositor
Resolution (Å)	29.94 – 3.00 29.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.94-3.00) 99.3 (29.94-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.192 , 0.250 0.193 , 0.249	Depositor DCC
R_{free} test set	2144 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10273	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NAG, QEM, MAN, BMA

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	0.70	0/2692	0.99	3/3677 (0.1%)
1	C	0.52	0/2536	0.91	6/3480 (0.2%)
2	B	0.59	0/2606	0.99	6/3577 (0.2%)
2	D	0.53	0/2475	0.95	9/3396 (0.3%)
All	All	0.59	0/10309	0.96	24/14130 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	LYS	N-CA-C	-7.48	101.25	112.54
2	B	238	THR	N-CA-C	-7.18	103.39	111.07
2	B	391	TRP	CA-C-N	6.83	127.22	119.92
2	B	391	TRP	C-N-CA	6.83	127.22	119.92
2	D	336	ASN	N-CA-C	6.68	118.56	111.28
2	D	132	MET	CB-CA-C	6.32	121.17	109.54
2	D	391	TRP	CA-C-N	6.18	126.53	119.92
2	D	391	TRP	C-N-CA	6.18	126.53	119.92
1	C	68	ARG	CA-C-N	6.01	127.35	119.84
1	C	68	ARG	C-N-CA	6.01	127.35	119.84
1	A	68	ARG	CA-C-N	5.98	125.19	118.97
1	A	68	ARG	C-N-CA	5.98	125.19	118.97
1	C	252	VAL	CB-CA-C	-5.92	104.41	111.81
1	C	404	GLY	N-CA-C	5.91	125.99	114.16
2	D	336	ASN	CB-CA-C	-5.80	101.15	110.79
1	C	394	ILE	N-CA-C	5.78	114.68	106.53
1	C	29	ILE	N-CA-C	-5.63	102.31	109.58
2	D	316	GLU	CA-C-N	5.62	125.89	119.83
2	D	316	GLU	C-N-CA	5.62	125.89	119.83
2	D	328	ARG	N-CA-C	5.54	117.78	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	351	PHE	N-CA-C	5.43	117.65	109.23
2	B	178	GLY	N-CA-C	-5.28	107.72	114.37
2	B	132	MET	CB-CA-C	5.22	119.14	109.54
1	A	318	GLU	N-CA-C	-5.04	106.64	112.89

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	2635	0	2507	67	0
1	C	2483	0	2251	85	0
2	B	2548	0	2261	111	0
2	D	2424	0	2100	102	0
3	E	61	0	52	1	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	25	0	29	1	0
6	D	25	0	29	0	0
All	All	10273	0	9294	359	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 18.

All (359) 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)
2:D:173:THR:HG22	2:D:231:TYR:HB3	1.36	1.06
2:D:157:MET:HE3	2:D:229:LEU:HD22	1.43	0.98
2:B:68:VAL:HG21	2:B:297:ILE:HD13	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:ILE:HA	2:D:146:PHE:HD1	1.31	0.94
2:D:160:ILE:HD11	2:D:364:ILE:HG12	1.55	0.88
2:B:354:ASP:HB2	2:B:356:TYR:CE2	2.09	0.87
2:D:33:PRO:HB2	2:D:64:VAL:HG23	1.55	0.86
2:D:258:VAL:HG12	2:D:279:SER:HB2	1.54	0.86
1:C:92:VAL:HG11	1:C:104:PRO:HB3	1.57	0.84
2:D:220:LEU:HD12	2:D:243:VAL:HG12	1.60	0.83
2:B:173:THR:HG22	2:B:231:TYR:HB3	1.59	0.82
2:B:234:LYS:HD2	2:B:262:VAL:O	1.80	0.81
2:B:354:ASP:HB2	2:B:356:TYR:HE2	1.43	0.81
2:D:146:PHE:HD2	2:D:357:GLN:NE2	1.78	0.81
2:B:307:MET:HE3	2:B:334:MET:HG2	1.62	0.80
1:A:151:TRP:O	1:A:155:MET:HG3	1.81	0.79
1:A:264:ALA:HB2	1:A:404:GLY:HA3	1.65	0.79
1:C:376:ASN:HD21	1:C:401:ILE:H	1.30	0.78
2:D:68:VAL:HG21	2:D:297:ILE:HD13	1.65	0.78
2:D:362:LEU:HB2	2:D:379:TRP:HB3	1.68	0.76
1:A:135:LEU:HD21	2:B:208:SER:HA	1.66	0.76
2:B:329:ILE:HD12	2:D:314:ILE:HD11	1.67	0.76
2:B:256:TRP:O	2:B:277:LEU:HD12	1.86	0.75
1:C:271:GLY:HA2	1:C:290:LEU:HD12	1.68	0.75
2:B:148:PRO:HG2	2:B:153:GLN:HE21	1.52	0.74
1:A:119:ILE:HG12	1:A:138:LEU:HD13	1.70	0.74
2:B:232:CYS:O	2:B:261:LEU:HD21	1.88	0.74
2:D:230:LEU:HB3	2:D:258:VAL:HG23	1.69	0.72
2:D:233:THR:OG1	2:D:236:GLU:HG3	1.89	0.72
1:A:43:ARG:HG3	1:A:43:ARG:HH11	1.53	0.71
1:A:29:ILE:HD11	1:A:60:LEU:HD13	1.72	0.71
2:D:276:GLY:HA2	2:D:366:LEU:HD11	1.71	0.71
2:B:149:SER:HB3	2:B:356:TYR:CG	2.26	0.71
2:B:149:SER:HB3	2:B:356:TYR:CD2	2.26	0.71
1:C:138:LEU:HD12	1:C:138:LEU:N	2.06	0.71
1:C:293:ILE:O	1:C:294:ASN:HB2	1.89	0.71
1:A:229:LEU:HD12	1:A:255:SER:HB2	1.72	0.71
2:B:362:LEU:HB2	2:B:379:TRP:HB3	1.73	0.71
1:C:30:GLY:O	1:C:90:ILE:HA	1.91	0.71
1:A:138:LEU:HD12	1:A:138:LEU:H	1.54	0.70
1:A:30:GLY:HA2	1:A:63:THR:O	1.91	0.70
1:A:179:LYS:HD2	1:A:179:LYS:O	1.91	0.70
1:C:139:ARG:NH2	1:C:143:PRO:HB3	2.06	0.69
2:D:161:MET:HE1	2:D:229:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:GLN:HE21	1:C:389:ASN:HA	1.57	0.69
2:B:100:ALA:HB2	2:B:126:ILE:HD11	1.75	0.69
2:D:157:MET:CE	2:D:229:LEU:HD22	2.21	0.69
2:B:161:MET:HE2	2:B:197:TRP:HZ3	1.57	0.68
2:B:157:MET:HE2	2:B:229:LEU:HD13	1.75	0.68
2:B:122:PRO:HB3	2:B:339:LEU:HD11	1.75	0.68
1:C:218:PHE:HB3	1:C:228:LEU:HD12	1.76	0.67
1:A:103:THR:HB	1:A:104:PRO:HD2	1.75	0.67
2:B:68:VAL:CG2	2:B:297:ILE:HD13	2.24	0.67
1:A:341:LEU:HA	2:B:210:ASP:OD1	1.96	0.66
2:D:33:PRO:CB	2:D:64:VAL:HG23	2.25	0.66
1:A:138:LEU:HD12	1:A:138:LEU:N	2.11	0.66
1:C:119:ILE:HA	1:C:138:LEU:O	1.96	0.66
2:D:106:GLU:N	2:D:106:GLU:OE1	2.29	0.66
2:D:100:ALA:HB2	2:D:126:ILE:HG12	1.78	0.66
2:B:106:GLU:N	2:B:106:GLU:OE1	2.30	0.65
2:D:283:ASP:C	2:D:285:TRP:H	2.05	0.65
2:D:96:GLY:HA3	2:D:300:ILE:HD13	1.79	0.64
1:C:144:TYR:CE2	1:C:273:ARG:HD2	2.32	0.64
1:C:138:LEU:HD12	1:C:138:LEU:H	1.61	0.64
2:D:172:VAL:HG22	2:D:203:LEU:HB2	1.79	0.64
1:C:128:TYR:HB2	1:C:139:ARG:NH1	2.12	0.64
1:C:228:LEU:C	1:C:228:LEU:HD23	2.24	0.63
1:A:71:ALA:HB1	1:A:106:PRO:HG3	1.82	0.62
2:D:82:ILE:HA	2:D:115:ILE:HD11	1.81	0.62
1:A:304:ASP:HB3	1:A:359:ILE:HD11	1.82	0.62
1:C:291:GLN:NE2	1:C:375:MET:HE2	2.15	0.61
2:B:175:TYR:CE1	2:B:204:LEU:HD21	2.35	0.61
2:B:78:PRO:HA	2:B:111:ILE:HD13	1.83	0.61
1:A:148:ALA:HB3	1:A:179:LYS:HG3	1.82	0.61
1:A:182:THR:HG22	1:A:183:LEU:HD23	1.80	0.61
1:C:216:LEU:HD23	1:C:216:LEU:N	2.14	0.61
2:D:174:THR:HG21	2:D:207:MET:HG3	1.83	0.61
1:A:218:PHE:HB3	1:A:228:LEU:HD22	1.83	0.61
2:B:330:TYR:HB3	2:D:316:GLU:HB2	1.82	0.61
2:D:36:GLY:O	2:D:37:ILE:HG13	2.01	0.61
2:D:68:VAL:CG2	2:D:297:ILE:HD13	2.31	0.61
2:D:282:TYR:CD2	2:D:292:ARG:NH2	2.69	0.60
2:D:366:LEU:HD12	2:D:367:LEU:N	2.17	0.60
2:D:190:ILE:HG23	2:D:197:TRP:HB2	1.84	0.60
2:D:78:PRO:O	2:D:82:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:THR:HG22	2:B:373:TRP:CD1	2.37	0.59
1:C:83:ILE:C	1:C:85:SER:H	2.10	0.59
1:C:254:LYS:HE2	1:C:282:TYR:CE2	2.37	0.59
2:B:148:PRO:HG2	2:B:153:GLN:NE2	2.18	0.59
1:C:130:ASP:OD1	1:C:132:SER:HB3	2.03	0.58
2:D:132:MET:O	2:D:145:GLN:NE2	2.36	0.58
1:A:160:TRP:HB3	1:A:239:VAL:HG21	1.86	0.58
2:B:307:MET:HE3	2:B:334:MET:CG	2.32	0.58
1:C:376:ASN:ND2	1:C:401:ILE:H	2.00	0.57
2:B:379:TRP:CZ2	2:B:382:LYS:HA	2.39	0.57
2:B:150:ILE:HD13	2:B:178:GLY:HA3	1.85	0.57
2:D:64:VAL:HG22	2:D:65:VAL:H	1.69	0.57
1:C:139:ARG:HH21	1:C:143:PRO:HB3	1.70	0.57
1:A:119:ILE:HA	1:A:138:LEU:O	2.04	0.57
2:B:138:ASP:OD1	2:B:139:GLU:N	2.38	0.57
2:D:157:MET:HE1	2:D:182:PHE:HZ	1.69	0.57
1:A:119:ILE:HG12	1:A:138:LEU:CD1	2.34	0.57
2:B:68:VAL:HG21	2:B:297:ILE:CD1	2.30	0.57
2:B:174:THR:HG21	2:B:236:GLU:HG2	1.86	0.57
1:C:33:LEU:HD22	1:C:302:ILE:HD11	1.86	0.57
2:D:293:VAL:O	2:D:297:ILE:HG13	2.05	0.57
1:C:124:ARG:O	1:C:143:PRO:HA	2.05	0.57
1:C:379:ASN:C	1:C:380:ARG:HG2	2.30	0.56
1:A:229:LEU:CD1	1:A:255:SER:HB2	2.34	0.56
1:C:165:LEU:HD22	1:C:180:LEU:HD23	1.87	0.56
2:D:144:PHE:HB3	2:D:351:PHE:CE2	2.41	0.56
1:A:242:LEU:HB3	1:A:270:VAL:HG12	1.87	0.56
2:D:100:ALA:HB2	2:D:126:ILE:CG1	2.36	0.56
2:B:82:ILE:HA	2:B:115:ILE:HD11	1.87	0.56
1:C:270:VAL:HG13	1:C:271:GLY:N	2.22	0.55
2:D:126:ILE:HA	2:D:146:PHE:CD1	2.24	0.55
2:B:352:SER:CB	2:B:356:TYR:CE1	2.89	0.55
2:B:389:TYR:C	2:B:389:TYR:CD2	2.85	0.54
1:A:330:VAL:HG22	2:B:79:LYS:HD3	1.88	0.54
2:D:246:SER:C	2:D:248:GLY:H	2.14	0.54
1:C:144:TYR:CZ	1:C:273:ARG:HD2	2.43	0.54
1:C:218:PHE:HB3	1:C:228:LEU:CD1	2.38	0.54
1:C:248:ASP:O	1:C:252:VAL:HG23	2.07	0.54
1:C:46:VAL:HG21	1:C:62:ALA:HB2	1.89	0.54
2:D:42:VAL:HG11	2:D:76:THR:CG2	2.38	0.54
2:D:374:GLU:O	2:D:376:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HB3	1:A:56:ARG:O	2.07	0.54
1:C:137:PHE:HE2	1:C:139:ARG:HD3	1.73	0.54
1:C:124:ARG:HB2	1:C:144:TYR:CZ	2.43	0.54
2:D:146:PHE:CD2	2:D:357:GLN:NE2	2.68	0.54
1:C:151:TRP:O	1:C:155:MET:HG3	2.07	0.53
2:B:94:ILE:O	2:B:317:PRO:HB3	2.08	0.53
1:C:91:LEU:N	1:C:91:LEU:HD12	2.24	0.53
2:D:258:VAL:HG22	2:D:259:PRO:HD2	1.91	0.53
1:A:396:ASN:C	1:A:396:ASN:OD1	2.51	0.53
2:D:126:ILE:CD1	2:D:293:VAL:HG22	2.39	0.53
2:D:299:ILE:HA	2:D:342:VAL:HG11	1.90	0.53
1:A:74:MET:HE3	1:A:77:SER:HB3	1.90	0.53
2:B:333:ASN:O	2:B:333:ASN:ND2	2.41	0.53
2:D:220:LEU:HD12	2:D:243:VAL:CG1	2.36	0.52
1:C:275:ILE:HB	1:C:280:LEU:HD13	1.92	0.52
2:D:258:VAL:HG22	2:D:262:VAL:HG21	1.91	0.52
2:B:161:MET:HE1	2:B:169:PHE:CD2	2.45	0.52
2:B:77:ASP:O	2:B:81:ILE:HG13	2.09	0.52
2:D:78:PRO:HA	2:D:111:ILE:HD13	1.91	0.52
1:A:27:VAL:HG22	1:A:60:LEU:HD23	1.91	0.52
1:C:325:PRO:HG3	1:C:336:TRP:CZ2	2.45	0.52
2:D:283:ASP:C	2:D:285:TRP:N	2.68	0.52
2:D:298:ALA:O	2:D:302:THR:HB	2.10	0.52
1:C:378:GLN:HG2	1:C:401:ILE:HD12	1.91	0.52
2:D:169:PHE:HZ	2:D:190:ILE:HD11	1.75	0.52
2:B:33:PRO:O	2:B:64:VAL:HG23	2.11	0.51
2:B:230:LEU:HB3	2:B:258:VAL:HG12	1.91	0.51
2:D:207:MET:HA	2:D:207:MET:HE2	1.92	0.51
2:D:257:ILE:HA	2:D:278:ILE:O	2.09	0.51
2:B:185:LYS:HD2	2:B:185:LYS:O	2.10	0.51
1:A:86:GLN:HB3	1:A:325:PRO:HG2	1.93	0.51
2:B:269:VAL:HG11	2:B:367:LEU:HD11	1.93	0.51
2:B:206:ASP:OD2	2:B:209:LEU:HD12	2.11	0.51
1:C:317:PHE:C	1:C:319:MET:H	2.19	0.51
2:D:366:LEU:HD22	2:D:391:TRP:CZ2	2.46	0.50
2:B:278:ILE:HG22	2:B:279:SER:N	2.26	0.50
2:D:174:THR:CG2	2:D:207:MET:HG3	2.41	0.50
2:B:366:LEU:HD12	2:B:391:TRP:CZ2	2.46	0.50
2:B:107:ALA:O	2:B:111:ILE:HG13	2.11	0.50
2:D:327:LYS:O	2:D:331:GLN:NE2	2.43	0.50
2:B:159:ASN:ND2	2:B:379:TRP:CZ3	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:MET:HE1	2:D:229:LEU:HB3	1.93	0.49
2:B:207:MET:HA	2:B:207:MET:HE2	1.94	0.49
2:D:256:TRP:O	2:D:277:LEU:HD12	2.13	0.49
1:C:138:LEU:N	1:C:138:LEU:CD1	2.75	0.49
1:A:71:ALA:HB1	1:A:106:PRO:CG	2.42	0.49
2:B:40:ILE:HA	2:B:71:VAL:O	2.13	0.49
2:B:307:MET:HG3	2:B:338:TYR:CE2	2.48	0.49
2:B:122:PRO:HB3	2:B:339:LEU:CD1	2.43	0.48
2:B:340:ILE:HG22	2:B:341:ASN:N	2.27	0.48
2:D:146:PHE:HD2	2:D:357:GLN:HE21	1.60	0.48
1:C:368:LYS:O	1:C:369:PHE:HB2	2.13	0.48
1:C:124:ARG:HB2	1:C:144:TYR:CE2	2.48	0.48
1:C:254:LYS:HE2	1:C:282:TYR:CD2	2.49	0.48
2:D:258:VAL:HG13	2:D:262:VAL:HB	1.95	0.48
1:C:83:ILE:C	1:C:85:SER:N	2.72	0.48
1:C:385:VAL:HG11	1:C:400:ILE:HG12	1.96	0.48
2:D:171:ILE:HG21	2:D:183:VAL:HG22	1.95	0.48
2:B:280:VAL:HG12	2:B:281:SER:H	1.79	0.47
2:D:137:LYS:HD2	2:D:354:ASP:O	2.15	0.47
1:C:63:THR:HG22	1:C:64:SER:H	1.80	0.47
1:A:168:SER:O	1:A:173:GLY:HA3	2.14	0.47
2:B:272:GLU:OE2	2:B:272:GLU:N	2.42	0.47
1:A:150:VAL:HG12	1:A:154:MET:HE2	1.95	0.47
2:B:68:VAL:CG1	2:B:69:GLU:N	2.77	0.47
2:B:233:THR:HG22	2:B:261:LEU:HD11	1.95	0.47
1:A:375:MET:HB3	1:A:382:LEU:HD22	1.96	0.47
2:B:272:GLU:H	2:B:272:GLU:CD	2.23	0.47
2:B:280:VAL:HG12	2:B:281:SER:N	2.30	0.47
1:C:371:GLN:HE21	1:C:389:ASN:CA	2.24	0.47
2:D:82:ILE:HG12	2:D:115:ILE:HD11	1.97	0.47
2:D:101:ASP:OD2	2:D:128:GLY:HA3	2.14	0.47
1:C:74:MET:HE3	1:C:74:MET:HA	1.95	0.47
2:D:266:THR:C	2:D:268:THR:H	2.23	0.47
1:A:29:ILE:CD1	1:A:60:LEU:HD13	2.42	0.46
1:A:135:LEU:HD12	6:B:396:QEM:C18	2.45	0.46
2:D:351:PHE:C	2:D:358:MET:HG2	2.40	0.46
2:D:40:ILE:CG2	2:D:73:MET:HE2	2.45	0.46
2:B:104:ASP:HA	2:B:132:MET:CE	2.45	0.46
2:D:42:VAL:HG21	2:D:101:ASP:HB3	1.96	0.46
1:C:152:PHE:CE2	1:C:156:ARG:HD2	2.50	0.46
2:D:40:ILE:HG21	2:D:73:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:ILE:O	2:D:301:THR:HB	2.16	0.46
1:A:149:LEU:HD23	1:A:183:LEU:HD11	1.96	0.46
2:D:42:VAL:HG11	2:D:76:THR:HG22	1.97	0.46
2:B:176:PHE:CD1	2:B:177:PRO:HD2	2.50	0.46
2:B:307:MET:SD	2:B:315:PRO:HD3	2.55	0.46
1:A:402:TRP:HB3	1:A:403:PRO:CD	2.46	0.46
2:B:278:ILE:HG22	2:B:279:SER:H	1.81	0.46
1:C:234:GLU:O	1:C:235:LEU:HD23	2.16	0.46
1:C:300:ALA:HB1	1:C:355:VAL:HG11	1.97	0.45
2:D:178:GLY:O	2:D:179:TYR:C	2.58	0.45
2:B:173:THR:CG2	2:B:231:TYR:HB3	2.39	0.45
1:C:289:GLY:C	1:C:290:LEU:HG	2.41	0.45
2:D:100:ALA:HB2	2:D:126:ILE:CD1	2.46	0.45
1:A:103:THR:HB	1:A:104:PRO:CD	2.45	0.45
1:A:179:LYS:HD2	1:A:179:LYS:C	2.41	0.45
2:B:336:ASN:O	2:B:337:ARG:C	2.60	0.45
2:D:280:VAL:HG12	2:D:281:SER:H	1.81	0.45
2:D:308:LEU:O	2:D:312:SER:HA	2.15	0.45
1:C:86:GLN:HG2	1:C:325:PRO:O	2.17	0.45
1:C:245:SER:HB3	1:C:273:ARG:NH2	2.31	0.45
1:C:345:VAL:O	1:C:349:SER:HB2	2.17	0.45
2:B:275:THR:HA	2:B:367:LEU:HD23	1.98	0.45
2:B:132:MET:O	2:B:145:GLN:NE2	2.49	0.45
2:B:171:ILE:HG22	2:B:172:VAL:N	2.32	0.45
1:C:150:VAL:HG11	1:C:290:LEU:CD2	2.47	0.45
2:B:100:ALA:HB2	2:B:126:ILE:CD1	2.43	0.44
1:C:229:LEU:HD13	1:C:256:ALA:HA	1.99	0.44
1:A:347:MET:HE3	1:A:347:MET:HB3	1.80	0.44
2:B:307:MET:HG3	2:B:338:TYR:HE2	1.81	0.44
1:A:308:VAL:HG21	1:A:359:ILE:HG21	1.99	0.44
2:B:237:ALA:O	2:B:238:THR:C	2.61	0.44
2:D:68:VAL:HG21	2:D:297:ILE:CD1	2.40	0.44
2:D:225:SER:HA	2:D:226:PRO:HD3	1.79	0.44
2:B:239:TYR:O	2:B:243:VAL:HG23	2.18	0.44
1:C:228:LEU:C	1:C:228:LEU:CD2	2.90	0.44
2:B:310:GLU:C	2:B:311:HIS:ND1	2.76	0.44
2:D:161:MET:HE1	2:D:229:LEU:CD1	2.46	0.44
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.65	0.44
1:C:358:ARG:O	1:C:367:ARG:NH1	2.51	0.44
2:B:252:TYR:C	2:B:254:TYR:H	2.25	0.44
1:C:92:VAL:CG2	1:C:107:ILE:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LYS:O	2:B:238:THR:HG23	2.18	0.44
1:C:46:VAL:HG11	1:C:62:ALA:HB2	2.00	0.44
1:C:288:ILE:HA	1:C:375:MET:O	2.18	0.44
2:B:157:MET:HE1	2:B:229:LEU:HB3	1.99	0.43
2:D:250:THR:HB	2:D:274:PRO:HB3	2.00	0.43
2:B:283:ASP:C	2:B:285:TRP:N	2.74	0.43
1:C:32:VAL:HG22	1:C:65:VAL:HG22	2.00	0.43
2:B:68:VAL:HG12	2:B:69:GLU:N	2.32	0.43
2:D:126:ILE:HG22	2:D:146:PHE:HE1	1.83	0.43
1:A:144:TYR:CE2	1:A:273:ARG:HD3	2.54	0.43
2:D:33:PRO:HB2	2:D:64:VAL:CG2	2.39	0.43
2:D:110:GLN:O	2:D:111:ILE:C	2.60	0.43
2:D:365:ILE:HG13	2:D:373:TRP:CE3	2.54	0.43
2:D:122:PRO:HA	2:D:142:MET:O	2.18	0.43
1:A:135:LEU:HD21	2:B:208:SER:CA	2.43	0.43
2:B:221:LYS:HA	2:B:247:VAL:HG11	1.99	0.43
2:B:245:ASN:C	2:B:247:VAL:H	2.27	0.43
1:C:157:LEU:HD12	1:C:157:LEU:O	2.17	0.43
2:B:146:PHE:HB3	2:B:282:TYR:HE2	1.84	0.43
1:C:170:ASP:O	1:C:171:HIS:C	2.60	0.43
2:D:391:TRP:HA	2:D:392:PRO:HD2	1.73	0.43
1:A:389:ASN:O	3:E:1:NAG:H82	2.18	0.43
2:D:246:SER:C	2:D:248:GLY:N	2.77	0.43
1:A:368:LYS:HB3	1:A:368:LYS:HE2	1.83	0.43
1:C:127:ILE:HA	1:C:171:HIS:CE1	2.54	0.43
1:A:297:ASN:O	1:A:298:GLU:C	2.61	0.43
1:A:304:ASP:HB3	1:A:359:ILE:CD1	2.48	0.43
1:A:396:ASN:OD1	1:A:396:ASN:O	2.37	0.43
2:B:173:THR:HA	2:B:231:TYR:O	2.18	0.43
2:B:336:ASN:C	2:B:338:TYR:N	2.76	0.43
1:A:367:ARG:HD2	1:A:368:LYS:O	2.19	0.42
2:B:157:MET:HE3	2:B:229:LEU:HD22	2.02	0.42
2:B:242:GLU:O	2:B:242:GLU:HG2	2.17	0.42
2:B:272:GLU:N	2:B:272:GLU:CD	2.77	0.42
2:B:83:THR:O	2:B:84:ARG:C	2.59	0.42
2:B:175:TYR:CZ	2:B:204:LEU:HD21	2.53	0.42
1:C:104:PRO:HD2	1:C:128:TYR:OH	2.19	0.42
1:C:146:HIS:C	1:C:148:ALA:H	2.28	0.42
1:A:88:TYR:O	1:A:117:PRO:HD2	2.18	0.42
2:D:100:ALA:HB2	2:D:126:ILE:HD11	2.00	0.42
2:D:116:SER:HB2	2:D:123:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:CB	1:A:228:LEU:HD11	2.49	0.42
1:A:376:ASN:ND2	1:A:400:ILE:HG23	2.35	0.42
1:C:284:PRO:O	1:C:285:ASP:C	2.62	0.42
1:C:371:GLN:NE2	1:C:389:ASN:HA	2.30	0.42
2:D:280:VAL:HG12	2:D:281:SER:N	2.34	0.42
2:D:289:LEU:HB3	2:D:290:PRO:CD	2.50	0.42
2:D:366:LEU:HD12	2:D:366:LEU:C	2.45	0.42
1:A:264:ALA:CB	1:A:404:GLY:HA3	2.43	0.42
2:B:32:PRO:HA	2:B:33:PRO:HD3	1.86	0.42
2:B:211:ASP:HB3	2:B:239:TYR:OH	2.20	0.42
2:B:282:TYR:HD1	2:B:282:TYR:HA	1.62	0.42
2:D:173:THR:HA	2:D:231:TYR:O	2.19	0.42
2:D:184:ASN:O	2:D:188:SER:HB3	2.18	0.42
2:B:203:LEU:HD13	2:B:219:GLN:HB3	2.01	0.42
1:A:166:ILE:HD12	1:A:240:ILE:CG2	2.50	0.42
2:D:35:ILE:HG23	2:D:64:VAL:HG21	2.02	0.42
1:A:43:ARG:HG3	1:A:43:ARG:NH1	2.28	0.42
1:A:86:GLN:HG2	1:A:325:PRO:O	2.20	0.42
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.73	0.42
2:B:149:SER:O	2:B:152:GLN:N	2.50	0.42
1:C:261:MET:HA	1:C:266:TYR:CE1	2.54	0.42
1:A:114:TYR:O	1:A:115:ARG:HB2	2.20	0.42
1:A:165:LEU:HB3	1:A:215:VAL:HG22	2.02	0.42
1:C:325:PRO:HG3	1:C:336:TRP:CE2	2.55	0.42
1:A:338:THR:O	1:A:338:THR:HG22	2.20	0.42
1:C:130:ASP:OD1	1:C:130:ASP:C	2.63	0.42
2:D:142:MET:HE2	2:D:142:MET:HB3	1.88	0.42
1:C:294:ASN:O	1:C:295:GLY:C	2.63	0.41
2:D:46:ASP:O	2:D:48:VAL:N	2.52	0.41
1:C:347:MET:HB3	1:C:347:MET:HE2	1.58	0.41
1:C:119:ILE:HD12	1:C:309:VAL:CG2	2.50	0.41
2:D:295:ASP:HA	2:D:298:ALA:HB3	2.02	0.41
2:B:266:THR:HG22	2:B:373:TRP:CG	2.55	0.41
1:C:157:LEU:HD23	1:C:158:PHE:CE2	2.56	0.41
1:A:293:ILE:C	1:A:295:GLY:H	2.28	0.41
2:B:105:GLN:HB2	2:B:108:ILE:HG13	2.03	0.41
2:B:250:THR:O	2:B:251:GLY:O	2.38	0.41
2:B:340:ILE:O	2:B:350:SER:HA	2.20	0.41
1:A:309:VAL:O	1:A:313:ILE:HG12	2.20	0.41
1:C:178:LYS:O	1:C:179:LYS:C	2.63	0.41
1:C:242:LEU:HB3	1:C:270:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:SER:HB3	2:B:356:TYR:CD1	2.56	0.41
2:D:40:ILE:HG21	2:D:73:MET:CE	2.51	0.41
2:B:75:GLU:HA	2:B:75:GLU:OE1	2.21	0.41
1:C:148:ALA:C	1:C:150:VAL:N	2.78	0.41
2:D:110:GLN:HA	2:D:134:MET:SD	2.61	0.41
2:B:104:ASP:OD1	2:B:265:ASP:HB3	2.20	0.41
2:B:112:LEU:HD23	2:B:112:LEU:HA	1.88	0.41
2:B:149:SER:HB3	2:B:356:TYR:CE2	2.56	0.41
2:B:231:TYR:CD2	2:B:231:TYR:C	2.99	0.41
2:B:122:PRO:HG3	2:B:142:MET:HE2	2.03	0.40
2:B:124:LEU:HD23	2:B:144:PHE:HB2	2.02	0.40
1:C:212:ALA:O	1:C:213:ASP:C	2.62	0.40
2:D:268:THR:O	2:D:268:THR:HG22	2.21	0.40
1:A:95:PRO:HB2	1:A:96:PRO:CD	2.51	0.40
1:A:139:ARG:HG3	1:A:141:VAL:O	2.21	0.40
1:C:33:LEU:HD22	1:C:302:ILE:CD1	2.49	0.40
1:C:228:LEU:HD23	1:C:228:LEU:O	2.20	0.40
2:B:158:LEU:HD13	2:B:189:THR:HG21	2.02	0.40
2:B:162:GLU:O	2:B:163:GLU:C	2.64	0.40
2:B:391:TRP:CD2	2:B:392:PRO:HD2	2.56	0.40
1:A:94:HIS:HD2	1:A:95:PRO:O	2.04	0.40
1:A:292:LEU:HD23	1:A:295:GLY:HA3	2.04	0.40
2:B:364:ILE:N	2:B:364:ILE:HD12	2.37	0.40
1:C:91:LEU:N	1:C:91:LEU:CD1	2.84	0.40
1:C:275:ILE:O	1:C:275:ILE:HG13	2.22	0.40
1:C:378:GLN:OE1	1:C:383:VAL:HG21	2.22	0.40
2:D:108:ILE:O	2:D:109:ALA:C	2.65	0.40
2:D:237:ALA:O	2:D:238:THR:C	2.64	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	349/383 (91%)	314 (90%)	32 (9%)	3 (1%)	14	48
1	C	346/383 (90%)	310 (90%)	34 (10%)	2 (1%)	21	56
2	B	352/364 (97%)	297 (84%)	49 (14%)	6 (2%)	7	32
2	D	335/364 (92%)	283 (84%)	45 (13%)	7 (2%)	5	27
All	All	1382/1494 (92%)	1204 (87%)	160 (12%)	18 (1%)	9	38

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	GLY
2	D	247	VAL
2	B	283	ASP
2	D	47	GLU
1	A	347	MET
2	B	246	SER
1	C	130	ASP
2	D	91	ASP
2	D	284	GLU
1	C	84	SER
2	D	149	SER
2	B	326	GLU
1	A	277	GLY
2	B	340	ILE
2	D	48	VAL
1	A	352	PRO
2	D	248	GLY
2	B	150	ILE

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	262/329 (80%)	245 (94%)	17 (6%)	15	47
1	C	226/329 (69%)	213 (94%)	13 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	238/327 (73%)	217 (91%)	21 (9%)	9	35
2	D	215/327 (66%)	197 (92%)	18 (8%)	10	37
All	All	941/1312 (72%)	872 (93%)	69 (7%)	13	42

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	43	ARG
1	A	63	THR
1	A	66	THR
1	A	123	THR
1	A	133	ILE
1	A	138	LEU
1	A	167	VAL
1	A	182	THR
1	A	245	SER
1	A	280	LEU
1	A	290	LEU
1	A	323	THR
1	A	330	VAL
1	A	347	MET
1	A	355	VAL
1	A	395	GLN
2	B	42	VAL
2	B	71	VAL
2	B	82	ILE
2	B	106	GLU
2	B	126	ILE
2	B	137	LYS
2	B	141	SER
2	B	203	LEU
2	B	211	ASP
2	B	236	GLU
2	B	238	THR
2	B	255	THR
2	B	261	LEU
2	B	265	ASP
2	B	266	THR
2	B	272	GLU
2	B	321	CYS

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Mol	Chain	Res	Type
2	B	329	ILE
2	B	335	LEU
2	B	350	SER
2	B	359	HIS
1	C	33	LEU
1	C	35	THR
1	C	60	LEU
1	C	87	VAL
1	C	138	LEU
1	C	167	VAL
1	C	182	THR
1	C	216	LEU
1	C	270	VAL
1	C	290	LEU
1	C	313	ILE
1	C	335	ILE
1	C	347	MET
2	D	65	VAL
2	D	85	ILE
2	D	121	THR
2	D	126	ILE
2	D	134	MET
2	D	141	SER
2	D	188	SER
2	D	207	MET
2	D	258	VAL
2	D	261	LEU
2	D	272	GLU
2	D	275	THR
2	D	301	THR
2	D	302	THR
2	D	335	LEU
2	D	366	LEU
2	D	376	VAL
2	D	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	146	HIS
1	A	371	GLN

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Mol	Chain	Res	Type
2	B	105	GLN
2	B	331	GLN
1	C	67	HIS
1	C	147	GLN
1	C	171	HIS
1	C	371	GLN
1	C	376	ASN
2	D	152	GLN
2	D	311	HIS
2	D	359	HIS

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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.60	0	17,19,21	0.93	0
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	0.70	0
3	BMA	E	3	3	11,11,12	1.07	1 (9%)	15,15,17	1.94	5 (33%)
3	MAN	E	4	3	11,11,12	0.61	0	15,15,17	0.61	0
3	MAN	E	5	3	11,11,12	0.70	0	15,15,17	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	C4-C5	2.28	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	O2-C2-C3	3.64	117.69	110.15
3	E	3	BMA	O5-C5-C6	3.13	113.76	107.66
3	E	3	BMA	O3-C3-C2	2.99	116.17	110.05
3	E	3	BMA	O3-C3-C4	2.45	116.16	110.38
3	E	3	BMA	O2-C2-C1	2.27	114.41	109.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

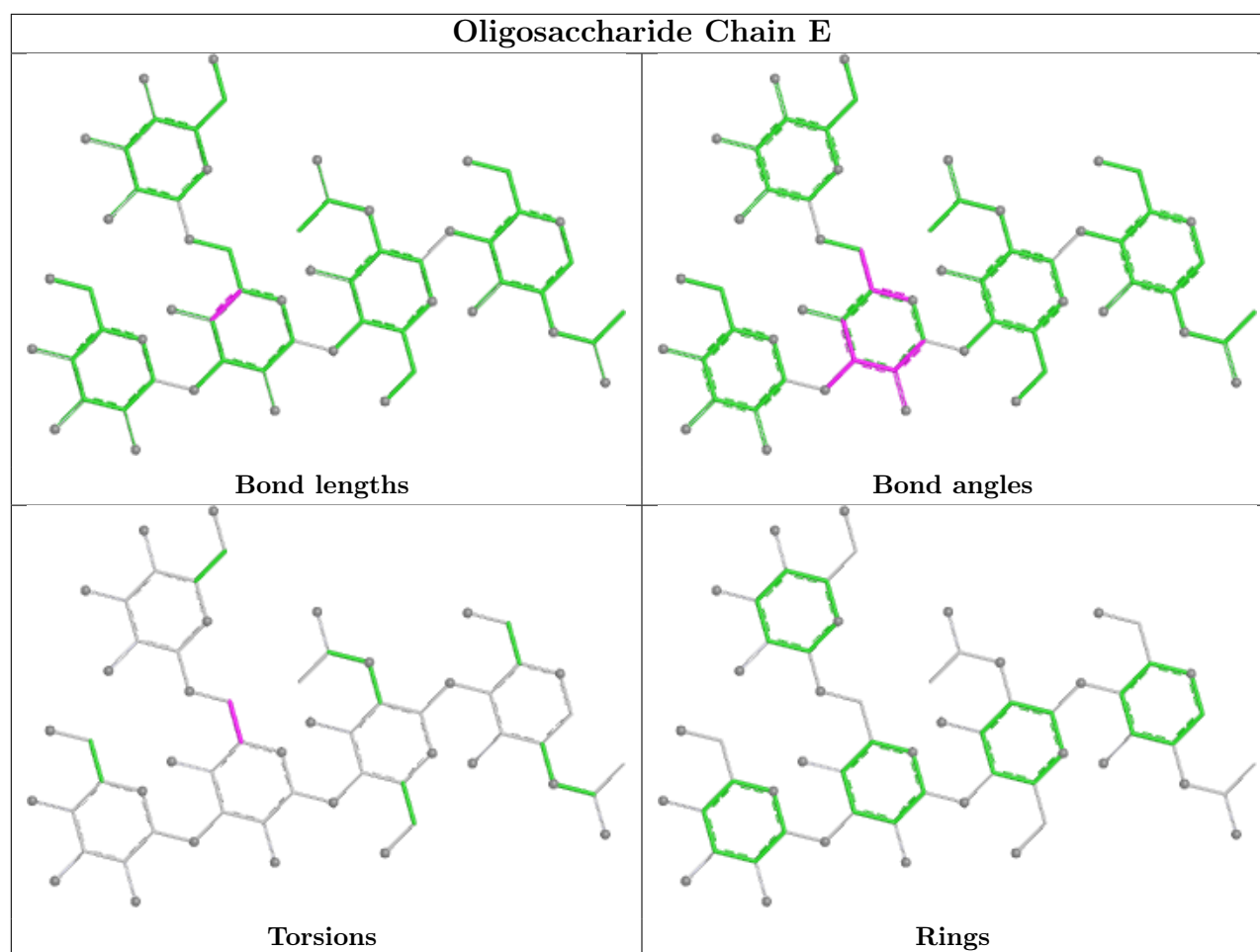
Mol	Chain	Res	Type	Atoms
3	E	3	BMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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



5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	395	2	14,14,15	0.63	0	17,19,21	1.21	1 (5%)
4	NAG	B	1	2	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
4	NAG	D	1	2	14,14,15	0.45	0	17,19,21	0.73	0
6	QEM	D	2	-	27,27,27	1.27	3 (11%)	35,36,36	2.14	4 (11%)
4	NAG	C	1	1	14,14,15	0.59	0	17,19,21	1.46	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	QEM	B	396	-	27,27,27	1.30	3 (11%)	35,36,36	2.05	4 (11%)
4	NAG	A	406	1	14,14,15	0.54	0	17,19,21	1.04	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
4	NAG	B	395	2	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	B	1	2	-	2/6/23/26	0/1/1/1
4	NAG	D	1	2	1/1/5/7	2/6/23/26	0/1/1/1
6	QEM	D	2	-	-	3/16/26/26	0/3/3/3
4	NAG	C	1	1	1/1/5/7	4/6/23/26	0/1/1/1
6	QEM	B	396	-	-	4/16/26/26	0/3/3/3
4	NAG	A	406	1	1/1/5/7	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	396	QEM	O-C20	3.05	1.43	1.37
6	D	2	QEM	C09-C08	-2.91	1.44	1.52
6	D	2	QEM	O-C20	2.81	1.43	1.37
6	B	396	QEM	C09-C08	-2.77	1.44	1.52
6	D	2	QEM	C14-C15	-2.16	1.49	1.53
6	B	396	QEM	C14-C15	-2.06	1.49	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	QEM	C10-N-C13	9.86	138.68	111.35
6	B	396	QEM	C10-N-C13	9.07	136.48	111.35
6	B	396	QEM	C11-N-C13	-4.93	97.68	111.35
4	C	1	NAG	C2-N2-C7	-4.24	117.22	122.90
6	D	2	QEM	C11-N-C13	-4.16	99.83	111.35
4	B	395	NAG	C4-C3-C2	3.88	116.71	111.02
6	D	2	QEM	C16-C15-C14	3.47	118.95	113.01
4	B	1	NAG	C1-O5-C5	2.89	116.06	112.19
4	A	406	NAG	C1-O5-C5	2.81	115.95	112.19
6	B	396	QEM	O01-C15-C16	-2.80	105.13	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	396	QEM	C09-C08-C07	-2.45	105.57	112.01
6	D	2	QEM	C09-C08-C07	-2.42	105.67	112.01
4	C	1	NAG	O5-C1-C2	-2.36	107.64	111.29

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	406	NAG	C1
4	B	395	NAG	C1
4	C	1	NAG	C1
4	D	1	NAG	C1

All (22) torsion outliers are listed below:

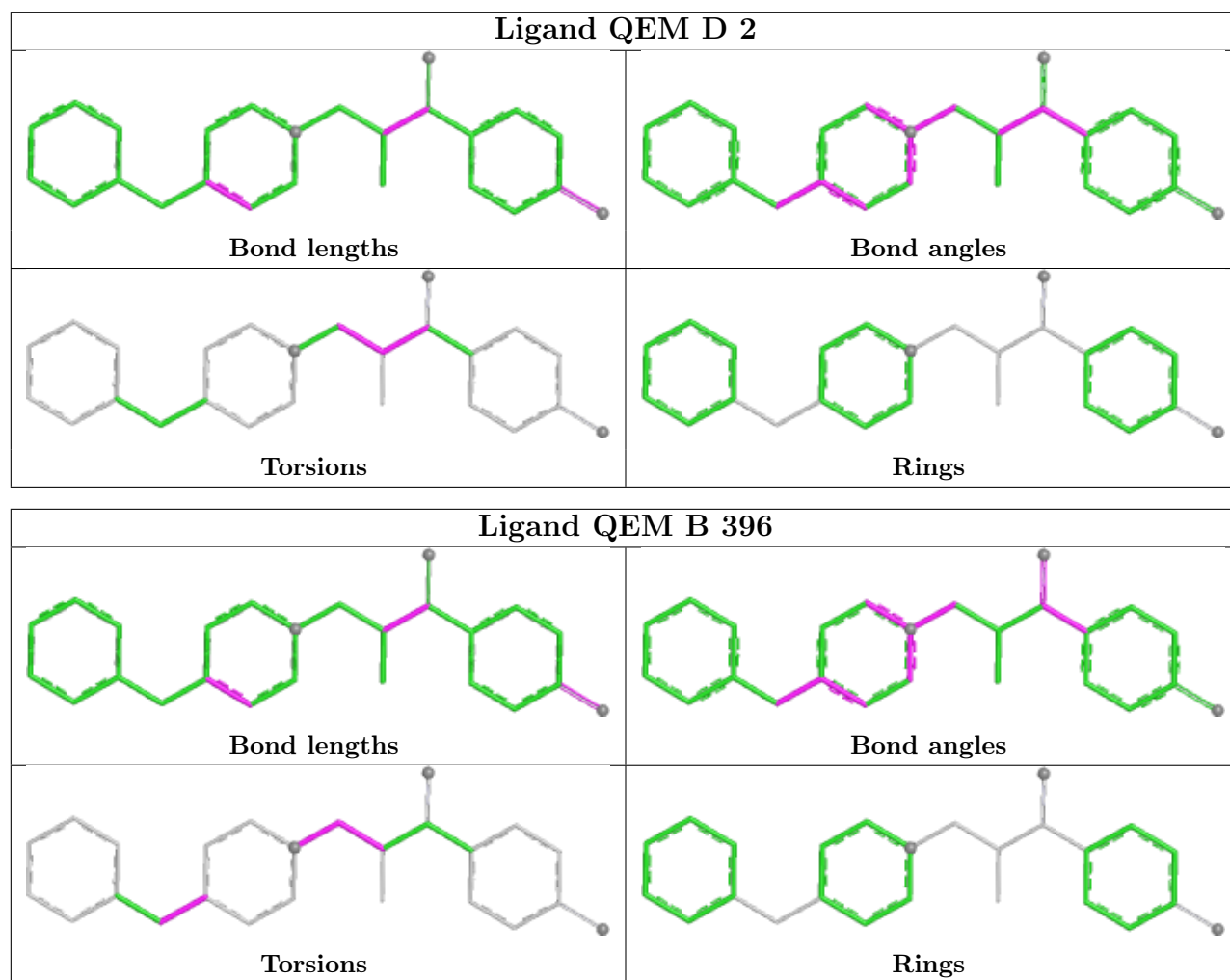
Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
6	B	396	QEM	N-C13-C14-C17
6	D	2	QEM	N-C13-C14-C17
4	A	406	NAG	O7-C7-N2-C2
4	A	406	NAG	O5-C5-C6-O6
4	A	406	NAG	C8-C7-N2-C2
4	B	395	NAG	C8-C7-N2-C2
4	B	395	NAG	O7-C7-N2-C2
4	C	1	NAG	O5-C5-C6-O6
4	A	406	NAG	C4-C5-C6-O6
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	C	1	NAG	C4-C5-C6-O6
6	D	2	QEM	N-C13-C14-C15
6	D	2	QEM	C13-C14-C15-O01
6	B	396	QEM	C02-C07-C08-C12
4	B	395	NAG	C4-C5-C6-O6
6	B	396	QEM	C14-C13-N-C10
6	B	396	QEM	C02-C07-C08-C09

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	396	QEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/383 (92%)	-0.56	1 (0%) 90 79	25, 53, 88, 116	0
1	C	352/383 (91%)	-0.23	3 (0%) 81 61	46, 77, 115, 146	0
2	B	356/364 (97%)	-0.21	2 (0%) 85 69	32, 69, 111, 144	0
2	D	345/364 (94%)	-0.14	4 (1%) 76 55	49, 76, 123, 153	0
All	All	1408/1494 (94%)	-0.29	10 (0%) 84 66	25, 70, 112, 153	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	333	ASN	3.8
1	C	24	PRO	2.8
2	D	49	ALA	2.8
1	C	379	ASN	2.7
2	B	323	ASN	2.6
2	B	348	ASP	2.5
2	D	284	GLU	2.4
2	D	59	PHE	2.3
1	A	224	ASN	2.2
1	C	55	THR	2.0

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

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

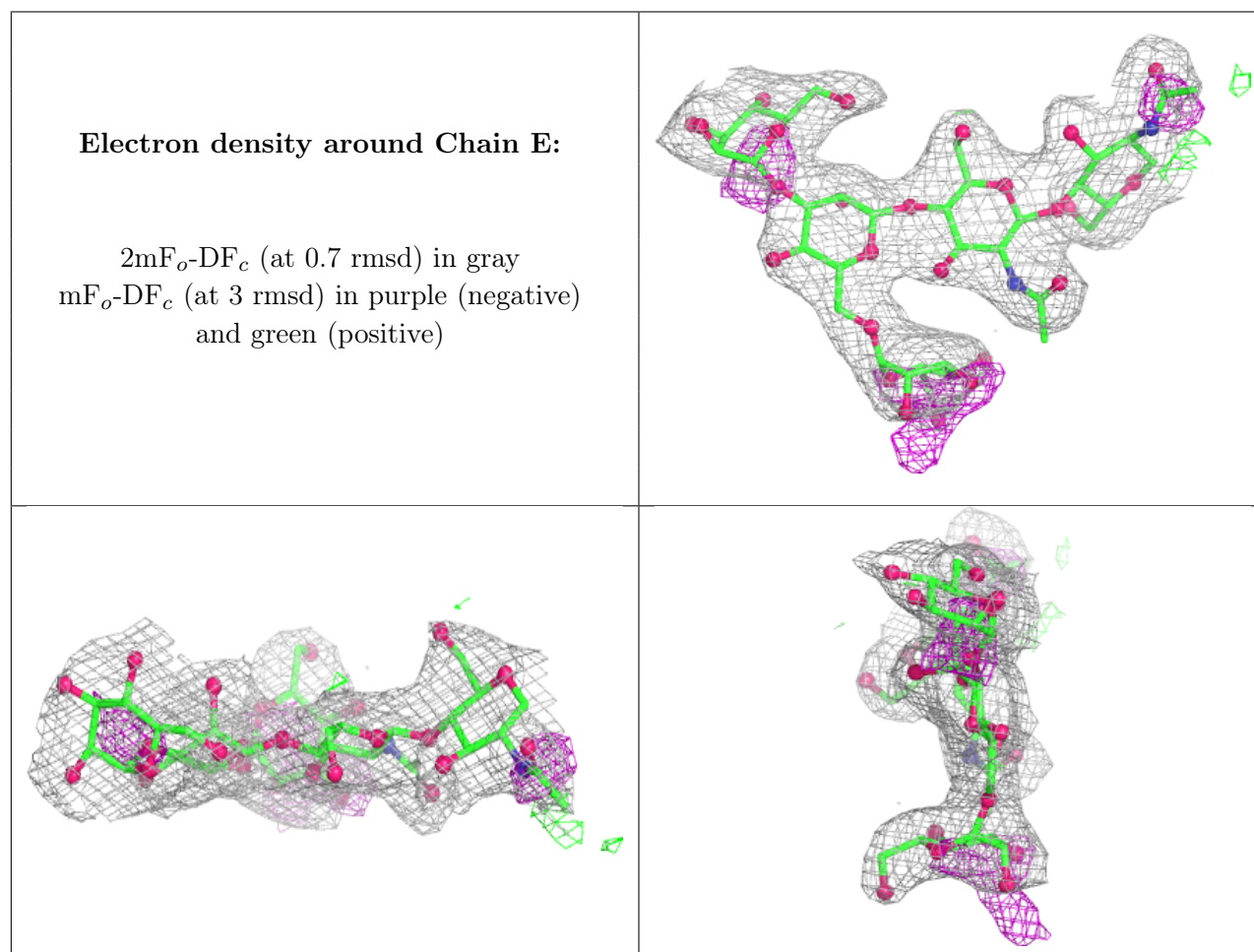
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	4	11/12	0.75	0.11	83,86,89,90	0
3	MAN	E	5	11/12	0.86	0.12	52,55,60,62	0
3	NAG	E	1	14/15	0.89	0.10	44,60,67,67	0
3	BMA	E	3	11/12	0.90	0.08	57,69,75,77	0
3	NAG	E	2	14/15	0.91	0.08	63,65,71,71	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.

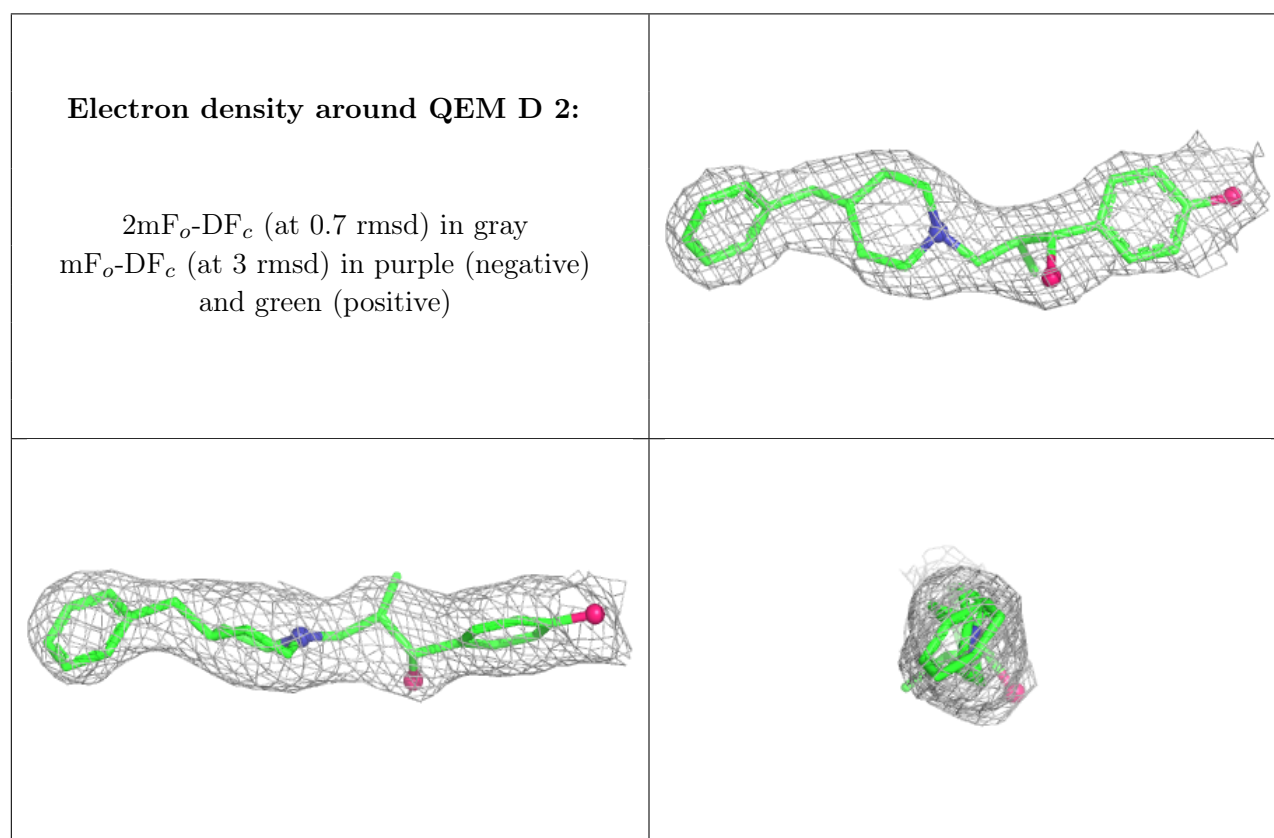


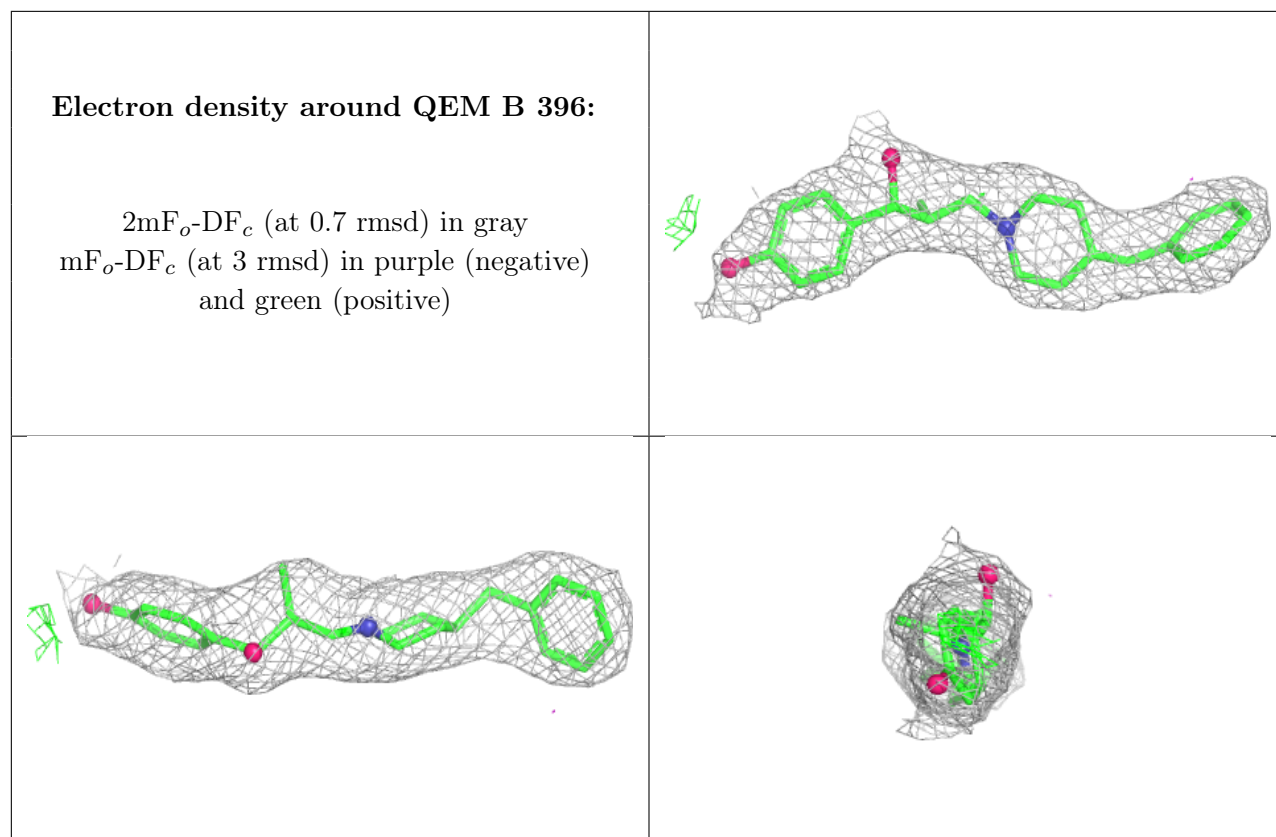
6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
4	NAG	D	1	14/15	0.46	0.12	100,121,125,125	0
4	NAG	B	395	14/15	0.58	0.12	92,104,108,109	0
4	NAG	B	1	14/15	0.62	0.12	100,110,114,117	0
5	NA	C	406	1/1	0.68	0.33	97,97,97,97	0
4	NAG	C	1	14/15	0.79	0.13	71,79,88,88	0
5	NA	A	407	1/1	0.81	0.17	67,67,67,67	0
4	NAG	A	406	14/15	0.91	0.12	45,49,58,58	0
6	QEM	D	2	25/25	0.95	0.11	52,58,63,64	0
6	QEM	B	396	25/25	0.96	0.08	36,42,49,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.