



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:20 PM BST

PDB ID : 3NWD
Title : Glycoprotein B from Herpes simplex virus type 1, Y179S mutant, low-pH
Authors : Stampfer, S.D.; Lou, H.; Cohen, G.H.; Eisenberg, R.J.; Heldwein, E.E.
Deposited on : 2010-07-09
Resolution : 2.88 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

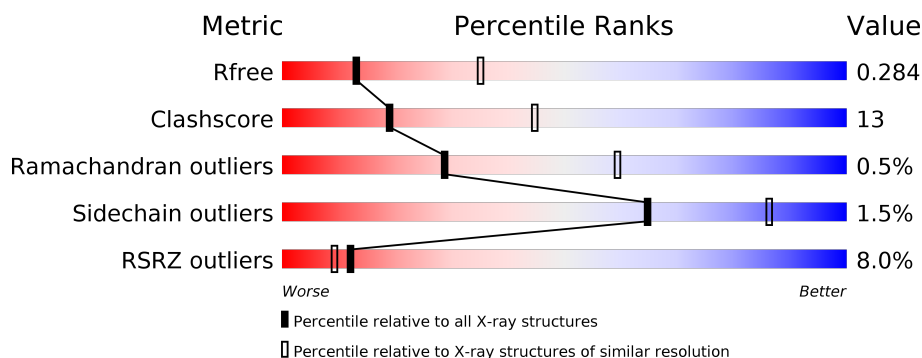
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	703	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>25%</div> <div>14%</div> </div> </div>
1	B	703	<div> <div>7%</div> <div> <div></div> <div>60%</div> <div>24%</div> <div>15%</div> </div> </div>
1	C	703	<div> <div>8%</div> <div> <div></div> <div>55%</div> <div>30%</div> <div>15%</div> </div> </div>
1	D	703	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>14%</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	1	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19481 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	597	Total	C	N	O	S	0	1	0
			4767	3000	835	910	22			
1	A	606	Total	C	N	O	S	0	1	0
			4843	3056	843	922	22			
1	C	601	Total	C	N	O	S	0	0	0
			4766	3003	831	910	22			
1	D	606	Total	C	N	O	S	0	1	0
			4829	3044	846	918	21			

There are 24 discrepancies between the modelled and reference sequences:

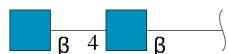
Chain	Residue	Modelled	Actual	Comment	Reference
B	28	ASP	-	expression tag	UNP P06437
B	29	PRO	-	expression tag	UNP P06437
B	58	ALA	PRO	SEE REMARK 999	UNP P06437
B	179	SER	TYR	engineered mutation	UNP P06437
B	313	SER	THR	SEE REMARK 999	UNP P06437
B	443	LEU	GLN	SEE REMARK 999	UNP P06437
A	28	ASP	-	expression tag	UNP P06437
A	29	PRO	-	expression tag	UNP P06437
A	58	ALA	PRO	SEE REMARK 999	UNP P06437
A	179	SER	TYR	engineered mutation	UNP P06437
A	313	SER	THR	SEE REMARK 999	UNP P06437
A	443	LEU	GLN	SEE REMARK 999	UNP P06437
C	28	ASP	-	expression tag	UNP P06437
C	29	PRO	-	expression tag	UNP P06437
C	58	ALA	PRO	SEE REMARK 999	UNP P06437
C	179	SER	TYR	engineered mutation	UNP P06437
C	313	SER	THR	SEE REMARK 999	UNP P06437
C	443	LEU	GLN	SEE REMARK 999	UNP P06437
D	28	ASP	-	expression tag	UNP P06437
D	29	PRO	-	expression tag	UNP P06437
D	58	ALA	PRO	SEE REMARK 999	UNP P06437

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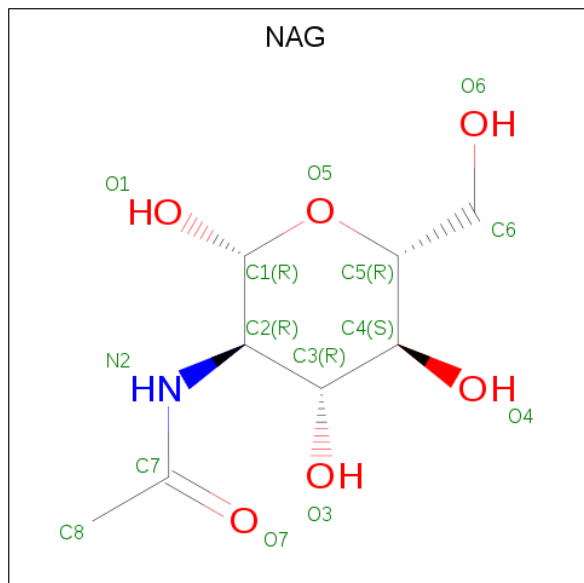
Chain	Residue	Modelled	Actual	Comment	Reference
D	179	SER	TYR	engineered mutation	UNP P06437
D	313	SER	THR	SEE REMARK 999	UNP P06437
D	443	LEU	GLN	SEE REMARK 999	UNP P06437

- 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			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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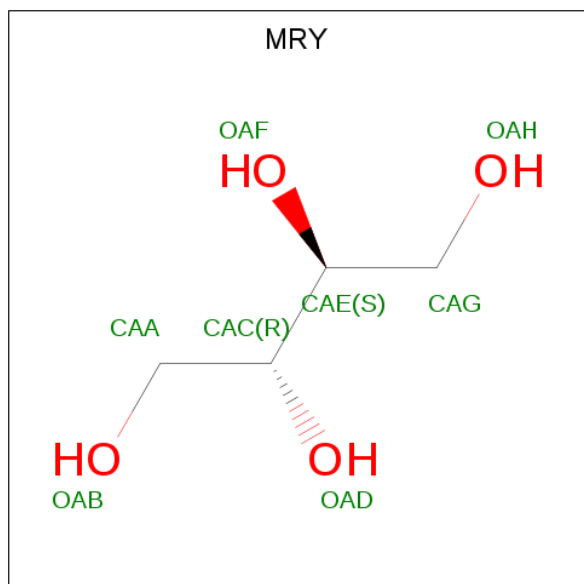
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
	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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: C₄H₁₀O₄).



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

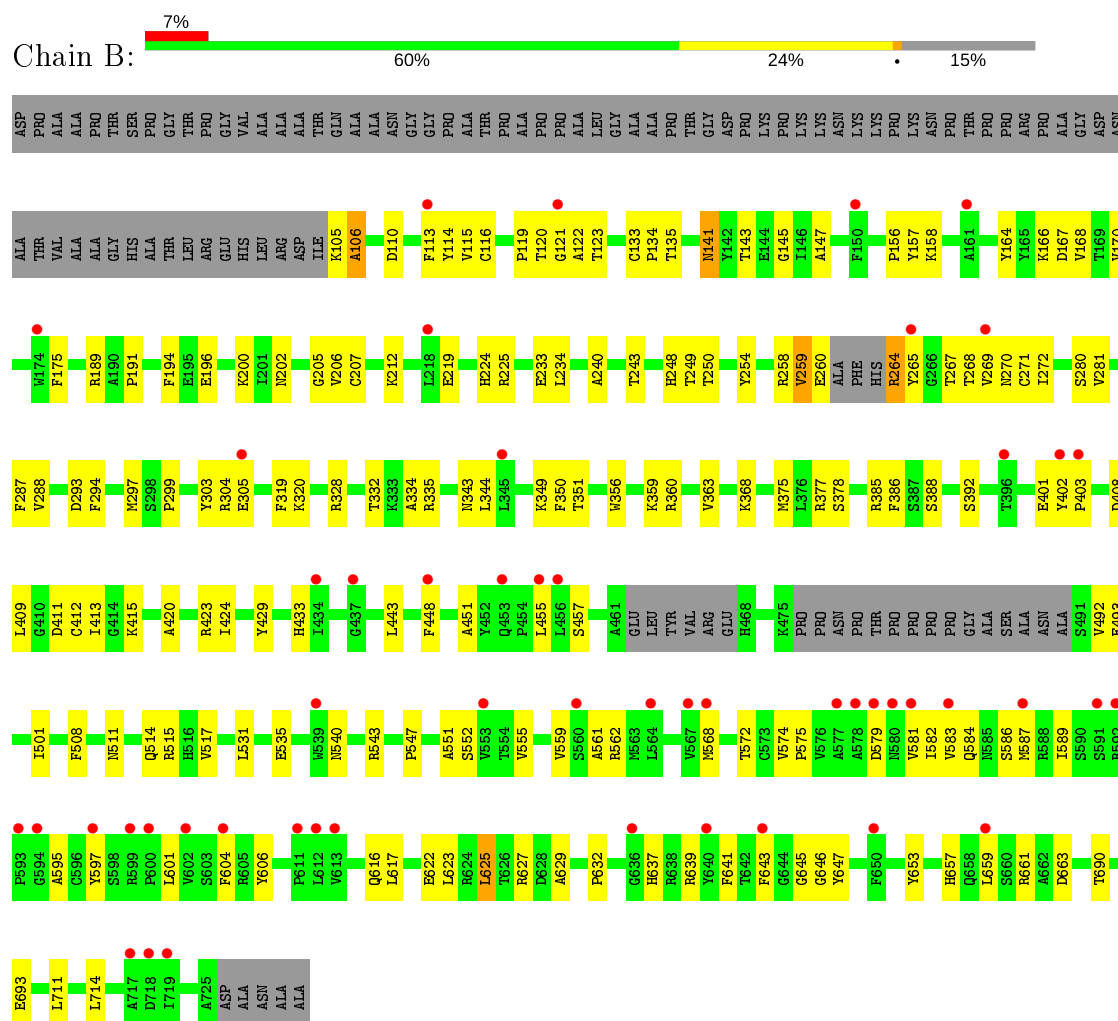
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	16	Total	O	0	0
			16	16		
6	A	25	Total	O	0	0
			25	25		
6	C	18	Total	O	0	0
			18	18		
6	D	25	Total	O	0	0
			25	25		

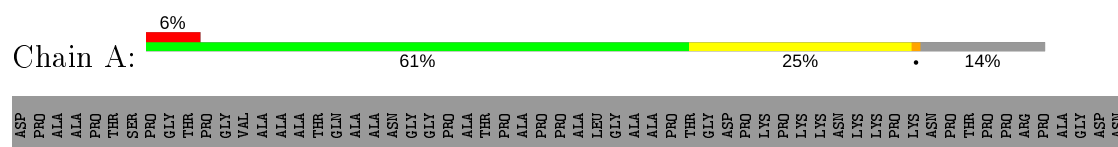
3 Residue-property plots

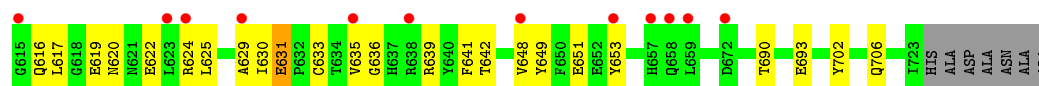
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Envelope glycoprotein B

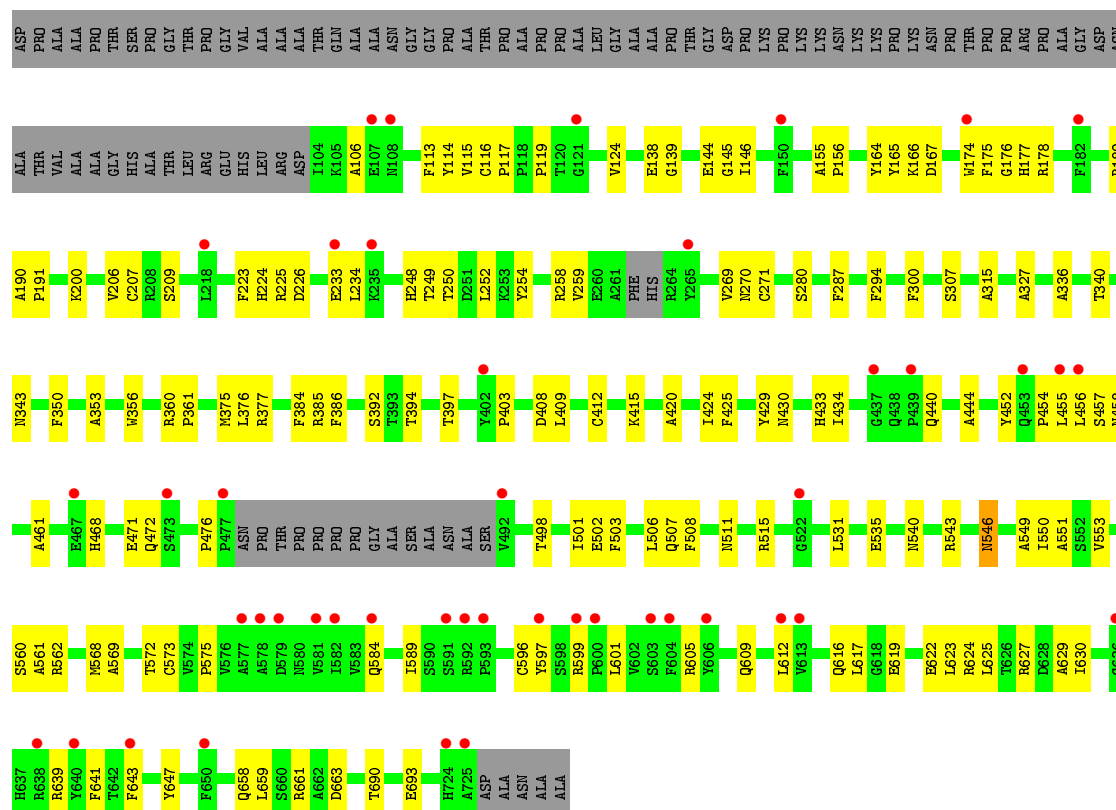


• Molecule 1: Envelope glycoprotein B





• Molecule 1: Envelope glycoprotein B



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



• Molecule 2: 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	P 3	Depositor
Cell constants a, b, c, α , β , γ	117.76Å 117.76Å 318.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.56 – 2.88 48.56 – 2.88	Depositor EDS
% Data completeness (in resolution range)	88.0 (48.56-2.88) 88.0 (48.56-2.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.238 , 0.283 0.235 , 0.284	Depositor DCC
R_{free} test set	5310 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l 0.468 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19481	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8395e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, MRY, 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	0.21	0/4966	0.39	0/6757
1	B	0.22	0/4879	0.38	0/6631
1	C	0.22	0/4880	0.38	0/6639
1	D	0.22	0/4948	0.38	0/6731
All	All	0.22	0/19673	0.38	0/26758

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	4843	0	4604	113	0
1	B	4767	0	4540	123	0
1	C	4766	0	4514	144	0
1	D	4829	0	4602	111	0
2	E	28	0	25	2	0
2	F	28	0	25	3	0
3	A	42	0	39	0	0
3	B	28	0	26	0	0
3	C	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	C	8	0	10	1	0
6	A	25	0	0	0	0
6	B	16	0	0	0	0
6	C	18	0	0	1	0
6	D	25	0	0	0	0
All	All	19481	0	18437	491	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 13.

All (491) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:H	1:A:184:GLY:HA3	1.20	1.05
1:A:183:MET:N	1:A:184:GLY:HA3	1.88	0.88
1:B:259:VAL:HG22	1:B:260:GLU:H	1.45	0.82
1:C:256:PRO:HD3	1:C:266:GLY:HA2	1.64	0.79
1:D:403:PRO:HG3	1:D:476:PRO:HB3	1.65	0.79
1:C:393:THR:HG22	1:C:505:ARG:HG2	1.66	0.77
1:A:150:PHE:HB2	1:A:449:LEU:HB3	1.68	0.75
1:C:599:ARG:HH12	1:C:617:LEU:HG	1.53	0.73
1:A:436:VAL:HB	1:A:454:PRO:HB2	1.70	0.71
1:B:166:LYS:HG2	1:B:271:CYS:HA	1.72	0.71
1:C:174:TRP:HB2	1:C:183:MET:SD	2.30	0.70
1:C:397:THR:HG22	1:C:444:ALA:HA	1.73	0.69
1:C:116:CYS:HB3	1:C:560:SER:HB2	1.74	0.69
1:D:375:MET:SD	1:D:386:PHE:HB3	2.33	0.68
1:A:298:SER:HB3	1:A:310:GLU:HB3	1.76	0.67
1:B:385:ARG:HH22	1:B:515:ARG:NH2	1.93	0.67
1:C:156:PRO:HG2	1:C:279:ARG:NH2	2.10	0.67
1:D:456:LEU:HD21	1:D:461:ALA:HA	1.75	0.67
1:D:224:HIS:HB2	1:D:269:VAL:HB	1.77	0.66
1:A:156:PRO:HG2	1:A:279:ARG:NH2	2.11	0.66
1:A:174:TRP:HB2	1:A:183:MET:SD	2.36	0.66
1:D:546:ASN:HB3	1:D:549:ALA:HB3	1.78	0.66
1:C:202:ASN:O	1:C:328:ARG:HB3	1.95	0.65
1:D:584:GLN:HG3	1:D:601:LEU:HB2	1.79	0.65
1:C:158:LYS:HD3	1:C:279:ARG:NH1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:LYS:HG2	1:D:271:CYS:HA	1.77	0.65
1:C:606:TYR:CD2	1:C:613:VAL:HG21	2.31	0.64
1:C:436:VAL:HB	1:C:454:PRO:HB2	1.79	0.64
1:D:166:LYS:HE3	1:D:207:CYS:SG	2.37	0.64
1:C:156:PRO:HG2	1:C:279:ARG:HH21	1.62	0.64
1:D:119:PRO:HG2	1:D:562:ARG:HG2	1.80	0.64
1:D:206:VAL:HG12	1:D:233:GLU:HG2	1.79	0.64
1:D:280:SER:HB2	1:D:287:PHE:HB3	1.80	0.63
1:A:105:LYS:HG2	1:A:582:ILE:HG22	1.81	0.63
1:C:166:LYS:HG2	1:C:271:CYS:HA	1.80	0.63
1:A:202:ASN:O	1:A:328:ARG:HB3	1.98	0.63
1:B:156:PRO:HB3	1:B:281:VAL:HG12	1.81	0.62
1:D:550:ILE:O	1:D:553:VAL:HG12	1.99	0.62
1:C:145:GLY:HA2	1:C:455:LEU:HG	1.81	0.62
1:C:583:VAL:HA	1:C:602:VAL:HG12	1.80	0.62
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.82	0.61
1:B:224:HIS:HB2	1:B:269:VAL:HB	1.81	0.61
1:A:235:LYS:HG2	1:A:248:HIS:O	2.00	0.61
1:A:464:TYR:O	1:A:468:HIS:HB2	2.00	0.61
1:D:223:PHE:HB2	1:D:226:ASP:HA	1.83	0.60
1:A:325:PHE:HE2	1:A:327:ALA:HB2	1.66	0.60
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.83	0.60
1:D:119:PRO:HG3	1:D:561:ALA:HA	1.82	0.60
1:C:386:PHE:HB2	1:C:395:PHE:HB2	1.83	0.60
1:C:601:LEU:HD23	1:C:616:GLN:HB3	1.83	0.60
1:B:105:LYS:N	1:B:582:ILE:HG13	2.16	0.60
1:A:237:ALA:HA	1:A:248:HIS:CD2	2.37	0.60
1:D:377:ARG:HD3	1:D:386:PHE:CZ	2.38	0.59
1:D:616:GLN:HG3	1:D:624:ARG:HB2	1.83	0.59
1:A:235:LYS:HE3	1:A:248:HIS:CE1	2.37	0.59
1:C:649:TYR:CE2	1:C:651:GLU:HB2	2.37	0.59
1:D:360:ARG:HG2	1:D:409:LEU:HD23	1.84	0.58
1:B:343:ASN:HD21	1:B:356:TRP:HD1	1.51	0.58
1:C:235:LYS:HE3	1:C:248:HIS:CE1	2.38	0.58
1:D:252:LEU:H	1:D:252:LEU:HD23	1.68	0.58
1:A:324:GLY:HA2	1:A:339:PRO:HB2	1.85	0.58
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.84	0.58
1:D:115:VAL:O	1:D:117:PRO:HD3	2.02	0.58
1:A:589:ILE:HG22	1:A:592:ARG:H	1.69	0.58
1:B:175:PHE:CD2	1:B:259:VAL:HG12	2.38	0.58
1:C:166:LYS:HD2	1:C:211:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LEU:O	1:B:535:GLU:HG2	2.04	0.58
1:A:253:LYS:HA	1:A:268:THR:HG21	1.86	0.58
1:D:377:ARG:HB2	1:D:386:PHE:CE2	2.39	0.58
1:A:314:TYR:HB3	1:A:318:ARG:HD2	1.84	0.57
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.04	0.57
1:C:511:ASN:O	1:C:515:ARG:HG2	2.04	0.57
1:A:600:PRO:O	1:A:616:GLN:HG3	2.04	0.57
1:B:170:VAL:HG22	1:B:267:THR:HG22	1.86	0.57
1:B:119:PRO:HG2	1:B:562:ARG:HG2	1.87	0.57
1:A:603:SER:HB3	1:A:612:LEU:HG	1.87	0.57
1:D:429:TYR:CE2	1:D:455:LEU:HD13	2.39	0.57
1:B:240:ALA:HB1	1:B:243:THR:OG1	2.05	0.57
1:B:375:MET:HE1	1:B:388:SER:HB2	1.86	0.56
1:D:248:HIS:HA	1:D:271:CYS:O	2.05	0.56
1:A:582:ILE:HD11	1:A:603:SER:HB2	1.87	0.56
1:A:401:GLU:HG2	1:A:441:TYR:O	2.06	0.56
1:A:588:ARG:HG2	1:A:596:CYS:SG	2.46	0.56
1:C:118:PRO:HD3	1:C:625:LEU:CD2	2.35	0.56
1:A:331:THR:HG22	1:A:332:THR:HG23	1.87	0.56
1:B:141:ASN:HD22	1:B:141:ASN:N	2.02	0.56
1:C:113:PHE:O	1:C:575:PRO:HA	2.04	0.56
1:D:343:ASN:HD21	1:D:356:TRP:HD1	1.54	0.56
1:A:325:PHE:CE2	1:A:327:ALA:HB2	2.41	0.56
1:A:147:ALA:HA	1:A:451:ALA:O	2.06	0.56
1:C:250:THR:HG22	1:C:252:LEU:H	1.72	0.55
1:A:539:TRP:O	1:A:543:ARG:HG3	2.06	0.55
1:B:205:GLY:O	1:B:233:GLU:HG3	2.06	0.55
1:B:540:ASN:O	1:B:543:ARG:HG2	2.07	0.55
1:B:625:LEU:H	1:B:625:LEU:HD22	1.72	0.55
1:B:595:ALA:HA	1:B:632:PRO:HA	1.89	0.55
1:C:241:THR:O	1:C:243:THR:HG23	2.07	0.55
1:A:597:TYR:HA	1:A:630:ILE:HA	1.89	0.55
1:A:649:TYR:CE2	1:A:651:GLU:HB2	2.41	0.55
1:C:516:HIS:O	1:C:520:MET:HG2	2.07	0.54
1:B:167:ASP:OD2	1:B:189:ARG:HG2	2.07	0.54
1:A:223:PHE:HB2	1:A:226:ASP:HA	1.89	0.54
1:B:234:LEU:HD23	1:B:249:THR:HG23	1.89	0.54
1:D:498:THR:HG21	1:D:503:PHE:HE2	1.73	0.54
1:C:200:LYS:HE3	1:C:208:ARG:CZ	2.37	0.54
1:A:360:ARG:HB2	1:A:361:PRO:HD3	1.89	0.54
1:C:633:CYS:HA	1:C:653:TYR:OH	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PRO:HA	1:B:350:PHE:HA	1.88	0.54
1:B:196:GLU:O	1:B:200:LYS:HB2	2.07	0.54
1:C:150:PHE:HB2	1:C:449:LEU:HB3	1.90	0.54
1:C:372:VAL:HG11	1:C:375:MET:HE2	1.90	0.54
1:B:711:LEU:HD12	1:B:714:LEU:HD12	1.89	0.53
1:C:597:TYR:CE1	1:C:601:LEU:HD11	2.43	0.53
1:A:285:ASP:HA	1:A:298:SER:HB2	1.89	0.53
1:C:105:LYS:HE2	1:C:579:ASP:O	2.08	0.53
1:B:551:ALA:O	1:B:555:VAL:HG23	2.09	0.53
1:D:225:ARG:HD2	1:D:254:TYR:CD1	2.43	0.53
1:B:559:VAL:HG12	1:B:572:THR:HA	1.91	0.53
1:B:647:TYR:HE2	1:B:661:ARG:HE	1.55	0.53
1:D:502:GLU:O	1:D:506:LEU:HB2	2.08	0.53
1:D:531:LEU:O	1:D:535:GLU:HG2	2.08	0.53
1:B:551:ALA:HB2	1:B:568:MET:SD	2.49	0.53
1:D:209:SER:HB2	1:D:224:HIS:HB3	1.91	0.53
1:B:250:THR:HB	1:B:270:ASN:HB2	1.90	0.52
1:B:639:ARG:HB3	1:B:641:PHE:CE1	2.44	0.52
1:D:124:VAL:HG12	1:D:569:ALA:HA	1.90	0.52
1:D:206:VAL:HA	1:D:233:GLU:HA	1.90	0.52
1:A:515:ARG:N	1:A:515:ARG:HD2	2.23	0.52
1:A:212:LYS:HE2	1:A:219:GLU:OE2	2.10	0.52
1:A:280:SER:HB2	1:A:287:PHE:HB3	1.91	0.52
1:A:145:GLY:HA2	1:A:455:LEU:HG	1.92	0.52
1:B:375:MET:SD	1:B:386:PHE:HB3	2.49	0.52
1:C:317:ASP:O	1:C:320:LYS:HE2	2.09	0.52
1:A:225:ARG:HD2	1:A:254:TYR:CD1	2.44	0.52
1:A:516:HIS:O	1:A:520:MET:HG2	2.10	0.52
1:B:206:VAL:HA	1:B:233:GLU:HA	1.91	0.52
1:C:225:ARG:HD2	1:C:254:TYR:CD1	2.45	0.52
1:A:343:ASN:O	1:A:353:ALA:HA	2.09	0.52
1:C:360:ARG:HB2	1:C:361:PRO:HD3	1.92	0.52
1:C:620:ASN:HA	1:C:642:THR:HG21	1.92	0.52
1:D:601:LEU:HB3	1:D:627:ARG:CZ	2.40	0.52
1:D:601:LEU:HD13	1:D:627:ARG:NH1	2.25	0.52
1:D:639:ARG:HB3	1:D:641:PHE:CE1	2.44	0.52
1:B:429:TYR:CD2	1:B:455:LEU:HD13	2.45	0.51
1:D:178:ARG:HG2	1:D:178:ARG:O	2.11	0.51
1:D:605:ARG:HB3	1:D:612:LEU:HD23	1.92	0.51
1:B:429:TYR:CE2	1:B:455:LEU:HD13	2.45	0.51
1:C:433:HIS:HD2	1:C:457:SER:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:GLN:CD	1:B:627:ARG:HA	2.31	0.51
1:D:165:TYR:CE1	1:D:189:ARG:HD2	2.45	0.51
1:A:158:LYS:HD3	1:A:279:ARG:NH1	2.26	0.51
1:B:343:ASN:CG	1:B:356:TRP:HB2	2.31	0.51
1:D:138:GLU:CB	2:F:1:NAG:H83	2.41	0.51
1:A:328:ARG:HH21	1:A:333:LYS:HG2	1.76	0.50
1:A:597:TYR:CE1	1:A:601:LEU:HD11	2.46	0.50
1:D:139:GLY:C	2:F:1:NAG:H82	2.31	0.50
1:A:319:PHE:CZ	1:A:321:GLN:HB2	2.47	0.50
1:B:420:ALA:O	1:B:423:ARG:HB3	2.10	0.50
1:D:540:ASN:O	1:D:543:ARG:HG2	2.12	0.50
1:C:325:PHE:CD2	1:C:342:ARG:HB2	2.47	0.50
2:E:1:NAG:H3	2:E:1:NAG:O7	2.12	0.50
1:A:605:ARG:HB3	1:A:611:PRO:O	2.12	0.50
1:B:584:GLN:HG2	1:B:586:SER:H	1.76	0.50
1:A:319:PHE:O	1:A:320:LYS:HD3	2.11	0.50
1:C:117:PRO:HA	1:C:625:LEU:HD21	1.92	0.50
1:D:177:HIS:O	1:D:178:ARG:HB3	2.12	0.50
1:A:633:CYS:HA	1:A:653:TYR:OH	2.12	0.50
1:C:125:VAL:O	1:C:567:VAL:HG13	2.11	0.50
1:C:567:VAL:HG12	1:C:568:MET:N	2.27	0.50
1:A:241:THR:O	1:A:243:THR:HG23	2.12	0.50
1:B:420:ALA:O	1:B:424:ILE:HG13	2.12	0.50
1:D:468:HIS:O	1:D:472:GLN:HG3	2.12	0.50
1:D:597:TYR:CZ	1:D:601:LEU:HD11	2.47	0.50
1:B:412:CYS:HA	1:B:415:LYS:HD2	1.94	0.49
1:B:552:SER:HA	1:B:559:VAL:HG22	1.93	0.49
1:D:343:ASN:ND2	1:D:356:TRP:HB2	2.28	0.49
1:A:262:PHE:N	1:A:262:PHE:CD1	2.78	0.49
1:B:377:ARG:HA	1:B:385:ARG:O	2.12	0.49
1:B:287:PHE:CD2	1:B:299:PRO:HG3	2.46	0.49
1:B:616:GLN:HB3	1:B:627:ARG:HG2	1.93	0.49
1:C:639:ARG:HB3	1:C:641:PHE:CE1	2.48	0.49
1:C:702:TYR:O	1:C:706:GLN:HG2	2.13	0.49
1:A:183:MET:N	1:A:184:GLY:CA	2.71	0.49
1:C:604:PHE:CZ	1:C:613:VAL:HB	2.47	0.49
1:D:425:PHE:CE2	1:D:430:ASN:HA	2.47	0.49
1:B:501:ILE:O	1:B:501:ILE:HG13	2.12	0.49
1:B:212:LYS:HE2	1:B:219:GLU:OE2	2.13	0.49
1:B:114:TYR:HA	1:B:574:VAL:O	2.13	0.49
1:B:617:LEU:HD12	1:B:622:GLU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LYS:HZ1	1:C:192:VAL:HG22	1.77	0.49
1:D:501:ILE:HG13	1:D:501:ILE:O	2.13	0.49
1:A:285:ASP:HB2	1:A:311:HIS:HB3	1.93	0.48
1:B:511:ASN:O	1:B:515:ARG:HG2	2.13	0.48
1:C:287:PHE:CD2	1:C:299:PRO:HG3	2.48	0.48
1:A:311:HIS:CG	1:A:312:THR:N	2.81	0.48
1:C:304:ARG:HB3	1:C:305:GLU:OE1	2.12	0.48
1:C:494:ARG:HG2	1:C:495:ILE:N	2.27	0.48
1:B:543:ARG:O	1:B:547:PRO:HG3	2.13	0.48
1:C:597:TYR:CE2	1:C:601:LEU:HD21	2.49	0.48
1:A:386:PHE:HB2	1:A:395:PHE:HB2	1.95	0.48
1:B:106:ALA:HA	1:B:643:PHE:CE2	2.49	0.48
1:D:119:PRO:HG3	1:D:561:ALA:CA	2.43	0.48
1:C:531:LEU:O	1:C:535:GLU:HG2	2.13	0.48
1:C:253:LYS:HA	1:C:268:THR:HG21	1.95	0.48
1:D:412:CYS:HA	1:D:415:LYS:NZ	2.29	0.48
1:D:551:ALA:HB2	1:D:568:MET:SD	2.53	0.48
1:A:286:GLU:HA	1:A:297:MET:O	2.13	0.48
1:B:305:GLU:HG2	1:B:305:GLU:O	2.14	0.48
1:D:377:ARG:HH21	1:D:454:PRO:HG3	1.78	0.48
1:D:507:GLN:HG3	1:D:511:ASN:OD1	2.14	0.48
1:D:647:TYR:CE2	1:D:661:ARG:HG2	2.49	0.48
1:B:166:LYS:HE3	1:B:207:CYS:SG	2.54	0.48
1:D:300:PHE:O	1:D:307:SER:HB2	2.14	0.48
1:D:377:ARG:HA	1:D:385:ARG:O	2.13	0.48
1:A:172:GLN:HB3	1:A:184:GLY:HA2	1.95	0.48
1:A:234:LEU:HD23	1:A:249:THR:HG23	1.96	0.48
1:C:105:LYS:HG3	1:C:582:ILE:HG22	1.95	0.48
1:D:599:ARG:NH2	1:D:619:GLU:HG2	2.29	0.48
1:A:199:ASP:O	1:A:203:ALA:HB3	2.14	0.47
1:B:304:ARG:HG2	1:A:320:LYS:NZ	2.29	0.47
1:C:205:GLY:HA3	1:C:328:ARG:NH1	2.29	0.47
1:C:559:VAL:HG12	1:C:572:THR:HA	1.97	0.47
1:A:619:GLU:O	1:A:622:GLU:HB2	2.15	0.47
1:C:311:HIS:CG	1:C:312:THR:N	2.83	0.47
1:A:559:VAL:HA	1:A:573:CYS:H	1.80	0.47
1:D:434:ILE:HG23	1:D:458:ASN:HD21	1.80	0.47
1:D:596:CYS:O	1:D:630:ILE:HG23	2.13	0.47
1:B:360:ARG:HE	1:B:409:LEU:HD23	1.79	0.47
1:B:433:HIS:HA	1:B:457:SER:HA	1.97	0.47
1:C:158:LYS:HD3	1:C:279:ARG:HH12	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:GLN:HG3	1:C:624:ARG:HD2	1.96	0.47
1:D:106:ALA:HA	1:D:658:GLN:OE1	2.13	0.47
1:D:360:ARG:N	1:D:361:PRO:HD2	2.30	0.47
1:A:172:GLN:HG2	1:A:183:MET:CE	2.45	0.47
1:A:519:ASP:O	1:A:523:ARG:HG3	2.14	0.47
1:B:115:VAL:HB	1:B:623:LEU:HB2	1.96	0.47
1:B:264:ARG:HG3	1:B:265[A]:TYR:H	1.79	0.47
1:B:259:VAL:HG13	1:B:260:GLU:N	2.30	0.47
1:B:105:LYS:HE3	1:B:579:ASP:O	2.15	0.47
1:B:119:PRO:HG3	1:B:561:ALA:CA	2.44	0.47
1:A:583:VAL:HA	1:A:602:VAL:HG12	1.97	0.47
1:B:115:VAL:HG23	1:B:623:LEU:O	2.15	0.47
1:C:116:CYS:HB3	1:C:560:SER:CB	2.43	0.47
1:C:598:SER:HB3	1:C:631:GLU:HG2	1.97	0.47
1:A:113:PHE:O	1:A:575:PRO:HA	2.15	0.46
1:B:194:PHE:HE1	1:B:344:LEU:HD13	1.79	0.46
1:B:114:TYR:O	1:B:622:GLU:HA	2.15	0.46
1:C:599:ARG:NH1	1:C:617:LEU:HG	2.25	0.46
1:A:222:ALA:HB1	1:A:267:THR:HG21	1.96	0.46
1:C:543:ARG:HB3	1:C:550:ILE:HG21	1.97	0.46
1:D:138:GLU:HB2	2:F:1:NAG:H83	1.98	0.46
1:D:690:THR:OG1	1:D:693:GLU:HG3	2.14	0.46
1:D:174:TRP:CZ3	1:D:176:GLY:HA3	2.51	0.46
1:D:572:THR:HG22	1:D:573:CYS:H	1.80	0.46
1:C:166:LYS:NZ	1:C:192:VAL:HG22	2.31	0.46
1:D:167:ASP:OD2	1:D:189:ARG:HG2	2.14	0.46
1:B:589:ILE:HG12	1:B:597:TYR:CE1	2.51	0.46
1:C:199:ASP:O	1:C:203:ALA:HB3	2.14	0.46
1:C:548:ASN:HB3	1:C:622:GLU:OE2	2.15	0.46
1:D:113:PHE:O	1:D:575:PRO:HA	2.15	0.46
1:A:548:ASN:OD1	1:A:560:SER:HA	2.15	0.46
1:A:559:VAL:HG12	1:A:572:THR:HA	1.97	0.46
1:B:601:LEU:HD13	1:B:627:ARG:NH1	2.30	0.46
1:A:124:VAL:HG12	1:A:569:ALA:HA	1.98	0.46
1:B:250:THR:HB	1:B:270:ASN:CB	2.45	0.46
1:B:581:VAL:HG22	1:B:604:PHE:HB3	1.97	0.46
1:C:190:ALA:HA	1:C:191:PRO:HD3	1.77	0.46
1:D:601:LEU:HA	1:D:616:GLN:HA	1.97	0.46
1:B:202:ASN:O	1:B:328:ARG:HB3	2.16	0.46
1:B:248:HIS:HA	1:B:271:CYS:O	2.16	0.46
1:B:270:ASN:O	1:B:272:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASP:O	1:C:333:LYS:HA	2.16	0.46
1:C:157:TYR:CD1	1:C:363:VAL:HG12	2.51	0.46
1:D:457:SER:O	1:D:458:ASN:HB2	2.16	0.46
1:A:520:MET:O	1:A:524:VAL:HG23	2.16	0.45
1:B:646:GLY:HA3	1:B:659:LEU:O	2.17	0.45
1:C:285:ASP:HA	1:C:298:SER:HB2	1.97	0.45
1:C:140:GLN:HE21	1:C:378:SER:HB2	1.80	0.45
1:D:252:LEU:N	1:D:252:LEU:HD23	2.31	0.45
1:D:440:GLN:NE2	1:D:471:GLU:HB3	2.32	0.45
1:C:147:ALA:HA	1:C:451:ALA:O	2.16	0.45
1:C:224:HIS:HB2	1:C:269:VAL:HB	1.97	0.45
1:C:319:PHE:CZ	1:C:321:GLN:HB2	2.51	0.45
1:D:498:THR:HG21	1:D:503:PHE:CE2	2.50	0.45
1:D:616:GLN:CD	1:D:627:ARG:HA	2.36	0.45
1:B:657:HIS:HD2	1:B:659:LEU:HG	1.81	0.45
1:C:502:GLU:HG3	1:C:503:PHE:N	2.31	0.45
1:D:584:GLN:CG	1:D:601:LEU:HB2	2.45	0.45
1:B:164:TYR:HD1	1:B:351:THR:O	2.00	0.45
1:C:425:PHE:CZ	1:C:430:ASN:HA	2.51	0.45
1:A:701:ASP:OD1	1:A:704:GLU:HG3	2.16	0.45
1:A:236:PRO:HA	1:A:246:GLY:O	2.17	0.45
1:A:202:ASN:OD1	1:A:327:ALA:HA	2.16	0.45
1:A:343:ASN:C	1:A:344:LEU:HD12	2.37	0.45
1:D:164:TYR:HE1	1:D:353:ALA:HB3	1.81	0.45
1:D:408:ASP:OD1	1:D:409:LEU:HG	2.16	0.45
1:D:394:THR:N	1:D:508:PHE:HB2	2.32	0.45
1:A:162:THR:HA	1:A:275:GLU:HA	1.99	0.45
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.51	0.45
1:C:567:VAL:CG1	1:C:568:MET:N	2.80	0.45
1:A:314:TYR:CE1	1:A:345:LEU:HD21	2.52	0.45
1:B:194:PHE:CD1	1:B:320:LYS:HD2	2.51	0.45
1:B:378:SER:O	1:B:385:ARG:N	2.50	0.45
1:C:327:ALA:H	1:C:336:ALA:HB3	1.81	0.45
1:C:407:VAL:HA	1:C:493:GLU:O	2.17	0.45
1:A:328:ARG:HE	1:A:333:LYS:HA	1.82	0.45
1:C:325:PHE:O	1:C:339:PRO:HA	2.16	0.45
1:C:340:THR:HG21	1:C:355:ASP:OD2	2.17	0.45
1:D:207:CYS:HB3	1:D:249:THR:HG21	1.98	0.45
1:B:259:VAL:HG22	1:B:260:GLU:N	2.23	0.44
1:B:443:LEU:HD12	1:B:448:PHE:O	2.17	0.44
1:C:342:ARG:HD2	1:C:354:TRP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:HE3	1:A:277:ASP:OD1	2.17	0.44
1:A:200:LYS:HE3	1:A:208:ARG:CZ	2.48	0.44
1:B:202:ASN:O	1:B:328:ARG:HD3	2.18	0.44
1:C:115:VAL:O	1:C:117:PRO:HD3	2.17	0.44
1:C:605:ARG:HG2	1:C:611:PRO:O	2.16	0.44
1:B:297:MET:HE1	1:B:319:PHE:HB2	1.99	0.44
1:B:328:ARG:HG3	1:B:335:ARG:HB3	1.99	0.44
1:B:212:LYS:HE2	1:B:219:GLU:CD	2.38	0.44
1:B:587:MET:HB2	1:B:653:TYR:HB3	1.99	0.44
1:D:191:PRO:HG3	1:D:350:PHE:N	2.32	0.44
1:A:125:VAL:O	1:A:567:VAL:HG13	2.18	0.44
1:A:635:VAL:HG12	1:A:636:GLY:N	2.32	0.44
1:B:147:ALA:HA	1:B:451:ALA:O	2.17	0.44
1:B:175:PHE:CE1	1:B:258:ARG:HA	2.53	0.44
1:D:659:LEU:HB2	1:D:663:ASP:OD1	2.17	0.44
1:C:186:PHE:CZ	1:C:188:ASP:HB2	2.52	0.44
1:C:406:ARG:HG2	1:C:406:ARG:O	2.17	0.44
1:A:166:LYS:NZ	1:A:192:VAL:HG22	2.33	0.44
1:B:343:ASN:OD1	1:B:356:TRP:HB2	2.18	0.44
1:C:116:CYS:CB	1:C:560:SER:HB2	2.45	0.44
1:B:583:VAL:HG22	1:B:584:GLN:N	2.33	0.44
1:C:600:PRO:O	1:C:616:GLN:HB2	2.18	0.44
1:D:250:THR:HB	1:D:270:ASN:HB2	2.00	0.44
1:D:375:MET:O	1:D:452:TYR:HE1	2.01	0.44
1:B:116:CYS:HB2	1:B:622:GLU:CD	2.39	0.43
1:C:279:ARG:O	1:C:288:VAL:HG22	2.18	0.43
1:D:433:HIS:HA	1:D:456:LEU:O	2.17	0.43
1:A:332:THR:O	1:A:333:LYS:HB2	2.18	0.43
1:B:145:GLY:HA2	1:B:455:LEU:HD12	2.00	0.43
1:C:235:LYS:HG2	1:C:248:HIS:O	2.18	0.43
1:D:280:SER:HB2	1:D:287:PHE:CB	2.47	0.43
1:A:181:GLN:HG2	1:A:182:PHE:O	2.17	0.43
1:B:175:PHE:HD1	1:B:258:ARG:HH11	1.66	0.43
1:C:209:SER:HB2	1:C:224:HIS:HB3	2.00	0.43
1:A:250:THR:HG22	1:A:251:ASP:N	2.34	0.43
1:B:168:VAL:HA	1:B:268:THR:O	2.18	0.43
1:C:434:ILE:HD12	1:C:434:ILE:O	2.18	0.43
1:A:384:PHE:CE2	1:A:399:LEU:HA	2.54	0.43
1:A:382:GLY:HA2	1:A:399:LEU:HD11	2.00	0.43
1:B:265[B]:TYR:C	1:B:265[B]:TYR:CD1	2.91	0.43
1:C:170:VAL:HA	1:C:266:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:VAL:HG12	1:C:572:THR:HG23	2.00	0.43
1:C:635:VAL:HG22	1:C:636:GLY:H	1.83	0.43
1:A:402:TYR:HA	1:A:403:PRO:HD3	1.72	0.43
1:B:156:PRO:O	1:B:158:LYS:HG3	2.18	0.43
1:C:384:PHE:O	1:C:396:THR:HA	2.19	0.43
1:A:172:GLN:HG2	1:A:183:MET:HE2	2.00	0.43
1:C:193:PRO:O	1:C:197:VAL:HG23	2.18	0.43
1:A:574:VAL:HA	1:A:575:PRO:HD3	1.86	0.43
1:B:106:ALA:HA	1:B:643:PHE:HE2	1.83	0.43
1:C:327:ALA:H	1:C:336:ALA:CB	2.32	0.43
1:D:327:ALA:HB3	1:D:336:ALA:HB2	2.00	0.43
1:B:110:ASP:OD1	1:B:645:GLY:HA3	2.18	0.43
1:B:175:PHE:CD1	1:B:258:ARG:HD2	2.54	0.43
1:B:616:GLN:NE2	1:B:629:ALA:HB3	2.33	0.43
1:C:113:PHE:CD1	1:C:581:VAL:HG21	2.54	0.43
1:A:276:VAL:HB	1:A:290:ALA:HB3	2.01	0.42
1:C:105:LYS:HB3	1:C:106:ALA:H	1.51	0.42
1:C:406:ARG:HG2	1:C:493:GLU:HB3	2.00	0.42
1:C:435:LYS:HD2	1:C:453:GLN:CD	2.40	0.42
1:C:104:ILE:O	1:C:582:ILE:HB	2.19	0.42
1:D:392:SER:HA	1:D:508:PHE:CZ	2.54	0.42
1:D:616:GLN:HE22	1:D:629:ALA:H	1.65	0.42
1:D:106:ALA:HB2	1:D:643:PHE:CZ	2.54	0.42
1:A:236:PRO:HA	1:A:247:TRP:CD1	2.54	0.42
1:A:256:PRO:HG3	1:A:266:GLY:N	2.35	0.42
1:C:319:PHE:O	1:C:320:LYS:HD3	2.20	0.42
1:C:458:ASN:HA	1:C:461:ALA:HB2	2.02	0.42
1:A:402:TYR:OH	1:A:495:ILE:HD11	2.19	0.42
1:B:225:ARG:HD2	1:B:254:TYR:CD1	2.53	0.42
1:B:408:ASP:OD1	1:B:409:LEU:HG	2.20	0.42
1:B:574:VAL:HA	1:B:575:PRO:HD3	1.88	0.42
1:C:619:GLU:O	1:C:622:GLU:HB3	2.19	0.42
1:D:234:LEU:HD23	1:D:249:THR:HG23	2.00	0.42
1:A:369:TRP:CD2	1:A:370:GLN:HG2	2.55	0.42
1:C:304:ARG:NH1	5:C:2001:MRY:HAA2	2.35	0.42
1:C:629:ALA:C	1:C:630:ILE:HD12	2.39	0.42
1:D:343:ASN:O	1:D:353:ALA:HA	2.20	0.42
1:D:144:GLU:HA	1:D:376:LEU:HD23	2.01	0.42
1:D:113:PHE:CD2	1:D:623:LEU:HD21	2.55	0.42
1:A:166:LYS:HG2	1:A:271:CYS:HA	2.00	0.42
1:A:298:SER:CB	1:A:310:GLU:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HB2	1:A:452:TYR:HD1	1.85	0.42
1:C:148:VAL:HB	1:C:451:ALA:HB3	2.01	0.42
1:D:155:ALA:HA	1:D:156:PRO:HD3	1.82	0.42
1:C:276:VAL:HB	1:C:290:ALA:HB3	2.00	0.42
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.90	0.42
1:C:589:ILE:HG22	1:C:592:ARG:H	1.84	0.42
1:D:616:GLN:NE2	1:D:629:ALA:HB3	2.35	0.42
1:D:617:LEU:HD12	1:D:622:GLU:O	2.20	0.42
1:A:127:PHE:HA	1:A:127:PHE:HD2	1.75	0.42
1:A:196:GLU:O	1:A:200:LYS:HB2	2.19	0.42
1:A:587:MET:O	1:A:596:CYS:HB3	2.19	0.42
1:C:237:ALA:HA	1:C:248:HIS:CD2	2.53	0.42
1:D:175:PHE:CD1	1:D:258:ARG:HD2	2.54	0.42
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.74	0.42
1:C:157:TYR:HB2	1:C:284:TYR:CE2	2.55	0.42
1:C:604:PHE:O	1:C:612:LEU:HA	2.19	0.42
1:D:397:THR:HG22	1:D:444:ALA:HA	2.01	0.42
1:D:511:ASN:O	1:D:515:ARG:HG2	2.19	0.42
1:B:392:SER:HA	1:B:508:PHE:CE2	2.55	0.42
1:C:130:PRO:HB3	1:C:533:ASN:HB3	2.02	0.42
1:D:589:ILE:HG12	1:D:597:TYR:CE1	2.54	0.42
1:B:402:TYR:HA	1:B:403:PRO:HD3	1.89	0.41
1:B:492:VAL:HG12	1:B:493:GLU:N	2.35	0.41
1:C:280:SER:HB2	1:C:287:PHE:HB3	2.02	0.41
1:C:119:PRO:HG3	1:C:560:SER:O	2.20	0.41
1:C:606:TYR:HD2	1:C:613:VAL:HG21	1.81	0.41
1:A:671:ILE:N	1:A:671:ILE:HD12	2.35	0.41
1:B:637:HIS:CE1	1:B:639:ARG:HD2	2.54	0.41
1:C:233:GLU:O	1:C:249:THR:HG22	2.18	0.41
1:C:425:PHE:O	1:C:430:ASN:HB3	2.20	0.41
1:C:433:HIS:HA	1:C:456:LEU:O	2.20	0.41
1:C:557:ARG:HG3	1:C:559:VAL:HG13	2.02	0.41
1:A:528:TRP:O	1:A:532:GLN:HG2	2.20	0.41
1:B:120:THR:O	1:B:121:GLY:C	2.59	0.41
1:B:288:VAL:HG12	1:B:294:PHE:HA	2.02	0.41
1:B:359:LYS:O	1:B:363:VAL:HG22	2.19	0.41
1:C:248:HIS:HE1	6:C:733:HOH:O	2.02	0.41
1:C:402:TYR:HA	1:C:403:PRO:HD3	1.79	0.41
1:C:558:ARG:NH2	1:C:622:GLU:HB2	2.36	0.41
1:A:248:HIS:HA	1:A:271:CYS:O	2.21	0.41
1:C:129:GLN:HB3	1:C:130:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:PRO:HA	1:C:350:PHE:HA	2.02	0.41
1:C:298:SER:HB3	1:C:310:GLU:HB3	2.02	0.41
1:D:572:THR:HG22	1:D:573:CYS:N	2.35	0.41
1:B:514:GLN:O	1:B:517:VAL:HG22	2.21	0.41
1:B:659:LEU:HB3	1:B:663:ASP:OD1	2.20	0.41
1:D:146:ILE:HD11	1:D:429:TYR:CD1	2.55	0.41
1:A:604:PHE:O	1:A:613:VAL:N	2.49	0.41
1:D:145:GLY:HA3	1:D:452:TYR:CZ	2.55	0.41
1:A:384:PHE:O	1:A:396:THR:HA	2.20	0.41
1:B:411:ASP:HB3	1:B:415:LYS:HE3	2.02	0.41
1:D:190:ALA:HA	1:D:191:PRO:HD3	1.87	0.41
1:D:420:ALA:O	1:D:424:ILE:HG13	2.21	0.41
1:D:605:ARG:HH11	1:D:609:GLN:HA	1.85	0.41
2:E:1:NAG:C3	2:E:1:NAG:O7	2.69	0.41
1:B:133:CYS:HA	1:B:134:PRO:HD3	1.91	0.41
1:C:282:TYR:CG	1:C:283:PRO:HA	2.56	0.41
1:C:519:ASP:O	1:C:523:ARG:HG3	2.21	0.41
1:D:647:TYR:HE2	1:D:661:ARG:HG2	1.86	0.41
1:A:152:GLU:HG2	1:A:153:ASN:N	2.36	0.41
1:B:264:ARG:HG3	1:B:265[B]:TYR:H	1.84	0.41
1:B:368:LYS:NZ	1:B:368:LYS:HB3	2.35	0.41
1:B:401:GLU:HB3	1:B:402:TYR:H	1.75	0.41
1:C:326:TYR:HD1	1:C:336:ALA:O	2.04	0.41
1:C:539:TRP:HA	1:C:542:ALA:HB3	2.03	0.41
1:D:639:ARG:HB3	1:D:641:PHE:CZ	2.55	0.41
1:B:122:ALA:HA	1:B:123:THR:HA	1.66	0.41
1:C:690:THR:OG1	1:C:693:GLU:HG3	2.21	0.41
1:A:302:GLY:O	1:A:307:SER:HB2	2.21	0.41
1:A:441:TYR:HB3	1:A:449:LEU:HD11	2.02	0.41
1:B:555:VAL:HG12	1:B:555:VAL:O	2.21	0.41
1:B:332:THR:C	1:B:334:ALA:H	2.24	0.40
1:C:321:GLN:NE2	1:C:341:THR:HG22	2.36	0.40
1:C:641:PHE:HB2	1:C:648:VAL:HG13	2.03	0.40
1:D:116:CYS:HB3	1:D:560:SER:HB3	2.03	0.40
1:D:175:PHE:CE1	1:D:258:ARG:HA	2.55	0.40
1:B:392:SER:HA	1:B:508:PHE:CZ	2.56	0.40
1:C:347:THR:N	1:C:350:PHE:O	2.54	0.40
1:C:568:MET:HE3	1:C:568:MET:HB2	1.85	0.40
1:D:114:TYR:HB3	1:D:573:CYS:HB3	2.04	0.40
1:D:174:TRP:CH2	1:D:176:GLY:HA3	2.56	0.40
1:D:659:LEU:N	1:D:659:LEU:HD23	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HE3	1:A:208:ARG:NH1	2.36	0.40
1:A:549:ALA:O	1:A:553:VAL:HG12	2.22	0.40
1:C:340:THR:HG22	1:C:341:THR:N	2.36	0.40
1:D:200:LYS:HB3	1:D:206:VAL:HG23	2.04	0.40
1:A:224:HIS:HB2	1:A:269:VAL:HB	2.02	0.40
1:B:224:HIS:CD2	1:B:225:ARG:HG2	2.56	0.40
1:B:303:TYR:O	1:A:317:ASP:HB3	2.21	0.40
1:B:157:TYR:CD1	1:B:363:VAL:HG12	2.57	0.40
1:C:250:THR:HG22	1:C:251:ASP:N	2.36	0.40
1:C:343:ASN:O	1:C:353:ALA:HA	2.21	0.40
1:C:215:ARG:NH2	1:C:349:LYS:HG2	2.37	0.40
1:C:601:LEU:HA	1:C:616:GLN:HA	2.03	0.40
1:C:304:ARG:HD3	1:C:356:TRP:CZ3	2.57	0.40
1:C:597:TYR:HA	1:C:630:ILE:HA	2.04	0.40
1:D:175:PHE:HB2	1:D:259:VAL:O	2.21	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	603/703 (86%)	543 (90%)	56 (9%)	4 (1%)	22	52
1	B	590/703 (84%)	523 (89%)	64 (11%)	3 (0%)	29	59
1	C	595/703 (85%)	532 (89%)	58 (10%)	5 (1%)	19	48
1	D	601/703 (86%)	548 (91%)	52 (9%)	1 (0%)	47	76
All	All	2389/2812 (85%)	2146 (90%)	230 (10%)	13 (0%)	29	59

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	VAL
1	B	413	ILE
1	A	238	ASN
1	C	429	TYR
1	B	106	ALA
1	D	315	ALA
1	A	134	PRO
1	A	264	ARG
1	A	699	LEU
1	C	390	ALA
1	C	413	ILE
1	C	134	PRO
1	C	139	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	517/593 (87%)	505 (98%)	12 (2%)	50	79
1	B	509/593 (86%)	501 (98%)	8 (2%)	62	85
1	C	506/593 (85%)	501 (99%)	5 (1%)	76	91
1	D	514/593 (87%)	509 (99%)	5 (1%)	76	91
All	All	2046/2372 (86%)	2016 (98%)	30 (2%)	65	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	113	PHE
1	B	135	THR
1	B	141	ASN
1	B	143	THR
1	B	264	ARG
1	B	293	ASP
1	B	606	TYR
1	B	625	LEU
1	A	127	PHE

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Mol	Chain	Res	Type
1	A	141	ASN
1	A	170	VAL
1	A	185	ILE
1	A	186	PHE
1	A	262	PHE
1	A	323	ASP
1	A	331	THR
1	A	397	THR
1	A	401	GLU
1	A	464	TYR
1	A	502	GLU
1	C	141	ASN
1	C	263	HIS
1	C	265	TYR
1	C	270	ASN
1	C	631	GLU
1	D	294	PHE
1	D	340	THR
1	D	384	PHE
1	D	546	ASN
1	D	625	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	453	GLN
1	B	709	ASN
1	A	440	GLN
1	A	620	ASN
1	C	140	GLN
1	C	270	ASN
1	C	433	HIS
1	C	468	HIS
1	D	472	GLN

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	E	1	1,2	14,14,15	0.62	0	17,19,21	1.09	1 (5%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.70	0
2	NAG	F	1	1,2	14,14,15	0.55	0	17,19,21	1.46	4 (23%)
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.84	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	1,2	1/1/5/7	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	-3.44	118.00	122.90
2	F	1	NAG	C1-O5-C5	2.54	115.63	112.19
2	F	1	NAG	O7-C7-C8	-2.45	117.51	122.06
2	E	1	NAG	C2-N2-C7	2.41	126.34	122.90
2	F	1	NAG	O7-C7-N2	2.28	126.15	121.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	NAG	C1

All (7) torsion outliers are listed below:

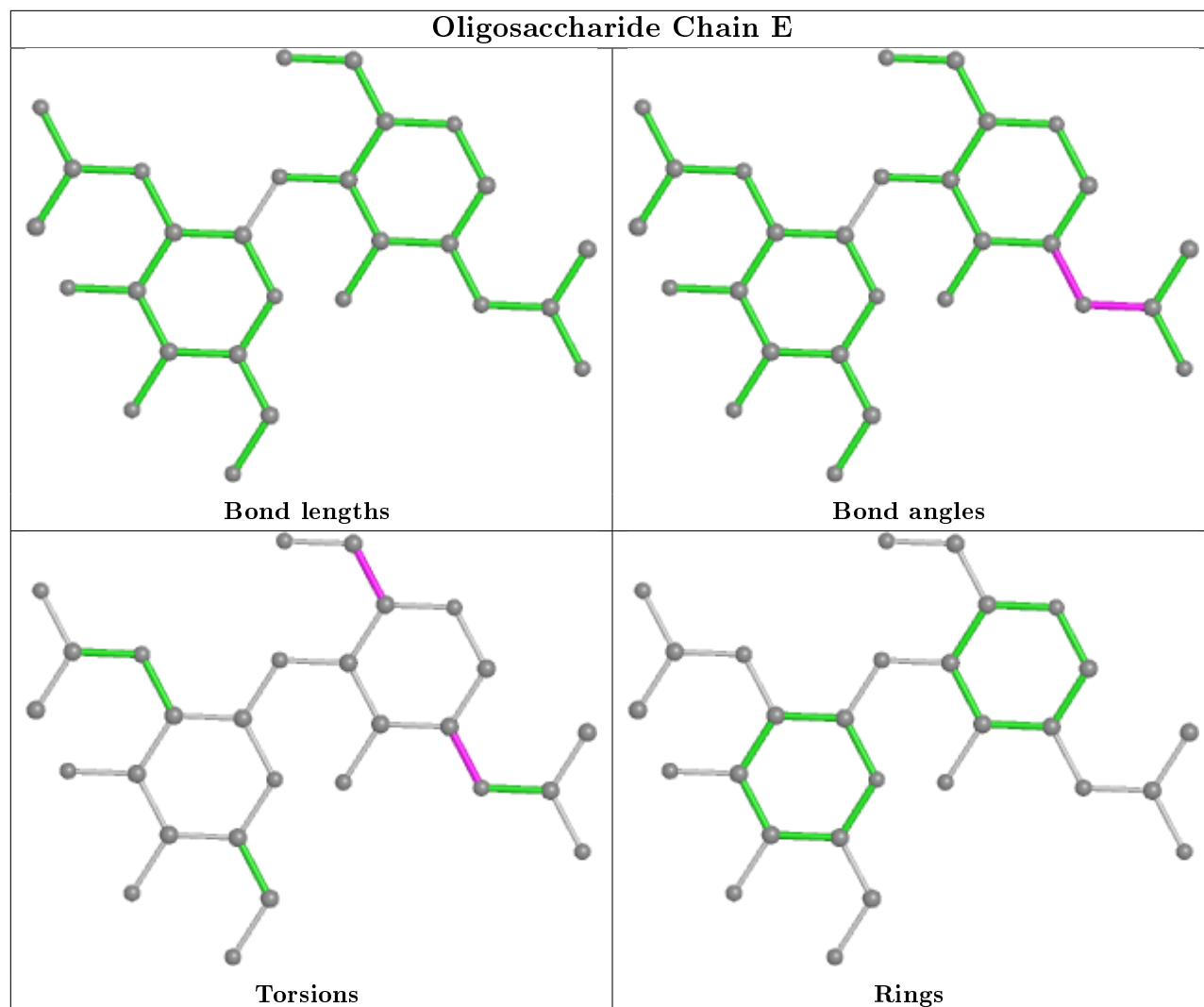
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C1-C2-N2-C7

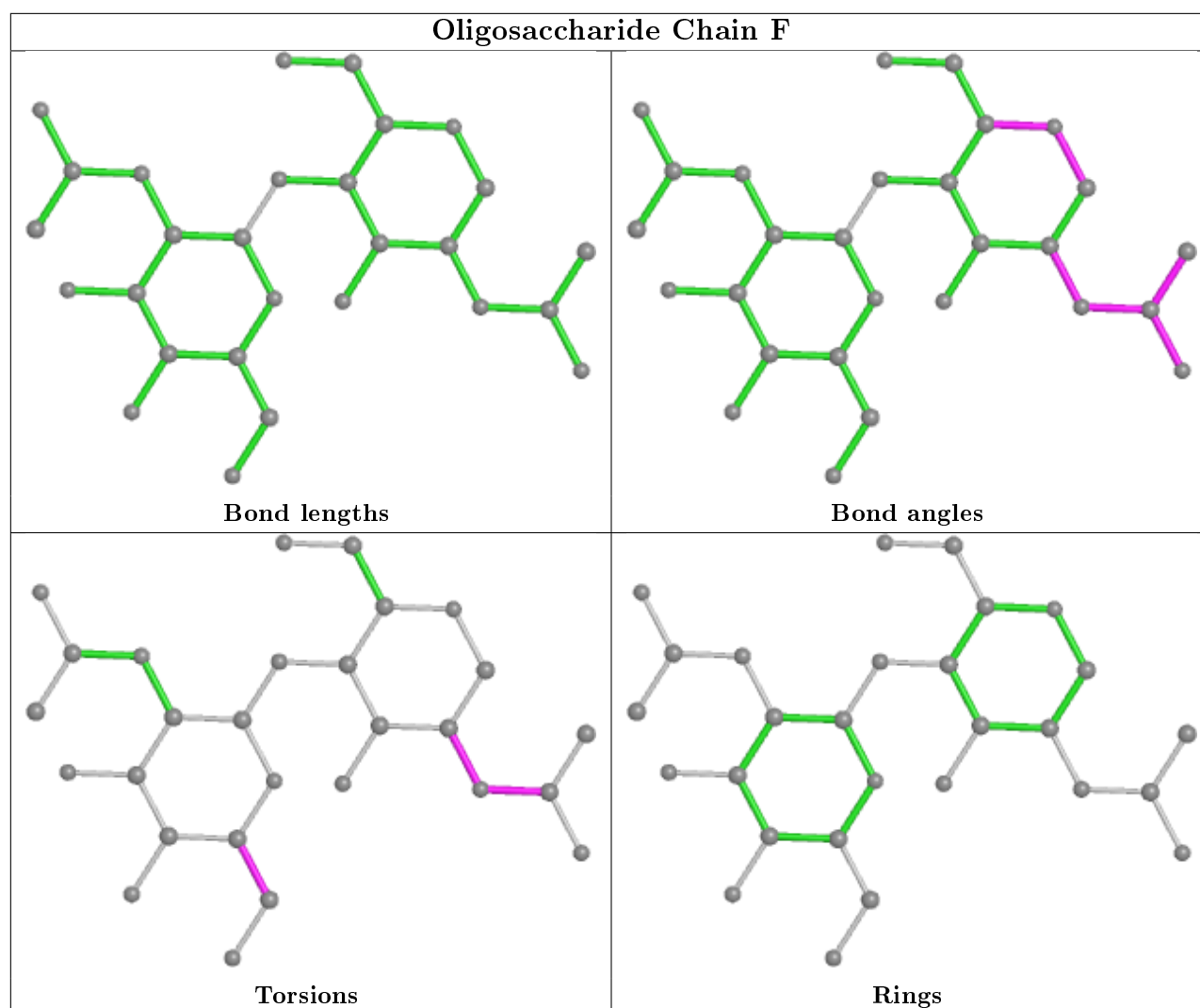
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	3	0
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](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
5	MRY	C	2001	-	7,7,7	0.38	0	8,8,8	0.34	0
3	NAG	C	1674	1	14,14,15	0.53	0	17,19,21	0.63	0
3	NAG	A	1674	1	14,14,15	0.52	0	17,19,21	0.64	0
3	NAG	A	1141	1	14,14,15	0.51	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1398	1	14,14,15	0.55	0	17,19,21	0.64	0
3	NAG	C	1141	1	14,14,15	0.54	0	17,19,21	0.62	0
3	NAG	D	1398	1	14,14,15	0.56	0	17,19,21	0.59	0
3	NAG	C	1430	1	14,14,15	0.48	0	17,19,21	1.16	1 (5%)
3	NAG	B	1430	1	14,14,15	0.59	0	17,19,21	1.30	2 (11%)
3	NAG	A	1430	1	14,14,15	0.56	0	17,19,21	0.92	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
5	MRY	C	2001	-	-	0/8/8/8	-
3	NAG	C	1674	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1674	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1141	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1398	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1141	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1398	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1430	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1430	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1430	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1430	NAG	C1-O5-C5	3.27	116.63	112.19
3	B	1430	NAG	O5-C1-C2	3.19	116.33	111.29
3	B	1430	NAG	C1-O5-C5	2.82	116.02	112.19
3	A	1430	NAG	C1-O5-C5	2.36	115.39	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1141	NAG	C3-C2-N2-C7
3	C	1141	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	1141	NAG	O7-C7-N2-C2
3	D	1398	NAG	C3-C2-N2-C7
3	D	1398	NAG	C8-C7-N2-C2
3	D	1398	NAG	O7-C7-N2-C2
3	B	1430	NAG	C3-C2-N2-C7
3	B	1430	NAG	C8-C7-N2-C2
3	B	1430	NAG	O7-C7-N2-C2
3	A	1141	NAG	C4-C5-C6-O6
3	A	1430	NAG	C8-C7-N2-C2
3	A	1141	NAG	O5-C5-C6-O6
3	A	1430	NAG	O7-C7-N2-C2
3	B	1430	NAG	O5-C5-C6-O6
3	C	1141	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2001	MRY	1	0

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	606/703 (86%)	0.48	42 (6%) 16 13	20, 66, 145, 550	0
1	B	597/703 (84%)	0.70	52 (8%) 10 7	23, 71, 174, 550	0
1	C	601/703 (85%)	0.60	53 (8%) 10 7	20, 76, 176, 550	0
1	D	606/703 (86%)	0.58	45 (7%) 14 11	22, 65, 151, 550	0
All	All	2410/2812 (85%)	0.59	192 (7%) 12 9	20, 69, 164, 550	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	PRO	23.9
1	C	595	ALA	22.8
1	D	600	PRO	16.5
1	B	612	LEU	15.9
1	D	604	PHE	14.1
1	B	640	TYR	13.9
1	B	577	ALA	13.8
1	D	603	SER	13.1
1	C	111	ALA	13.1
1	B	578	ALA	12.5
1	B	579	ASP	12.4
1	D	599	ARG	11.9
1	B	581	VAL	11.2
1	D	613	VAL	11.1
1	B	580	ASN	11.1
1	C	623	LEU	10.9
1	D	597	TYR	10.8
1	B	599	ARG	10.7
1	A	595	ALA	10.5
1	B	593	PRO	10.4
1	C	653	TYR	10.4

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Mol	Chain	Res	Type	RSRZ
1	C	594	GLY	10.3
1	D	612	LEU	10.1
1	B	604	PHE	10.1
1	A	111	ALA	10.0
1	B	597	TYR	9.6
1	D	402	TYR	9.5
1	D	581	VAL	9.4
1	A	623	LEU	9.3
1	B	402	TYR	9.2
1	B	455	LEU	9.1
1	C	433	HIS	8.9
1	A	594	GLY	8.9
1	A	433	HIS	8.7
1	C	672	ASP	8.6
1	B	613	VAL	8.5
1	B	150	PHE	8.2
1	D	578	ALA	8.1
1	C	648	VAL	7.7
1	C	601	LEU	7.5
1	A	629	ALA	7.2
1	A	443	LEU	7.1
1	B	636	GLY	6.9
1	D	640	TYR	6.6
1	B	218	LEU	6.4
1	D	455	LEU	6.2
1	A	653	TYR	5.9
1	C	319	PHE	5.7
1	B	453	GLN	5.7
1	D	591	SER	5.6
1	A	672	ASP	5.5
1	D	233	GLU	5.3
1	C	588	ARG	5.2
1	B	456	LEU	5.1
1	C	583	VAL	5.1
1	A	648	VAL	5.1
1	D	439	PRO	5.1
1	B	591	SER	5.1
1	C	159	PHE	5.0
1	C	108	ASN	5.0
1	B	643	PHE	5.0
1	B	564	LEU	4.9
1	D	593	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	601	LEU	4.6
1	C	606	TYR	4.6
1	D	579	ASP	4.6
1	D	218	LEU	4.6
1	B	611	PRO	4.6
1	B	587	MET	4.4
1	D	577	ALA	4.4
1	A	222	ALA	4.3
1	B	717	ALA	4.3
1	D	492	VAL	4.2
1	D	235	LYS	4.2
1	B	567	VAL	4.1
1	C	223	PHE	4.1
1	C	575	PRO	4.1
1	C	471	GLU	4.0
1	D	150	PHE	4.0
1	A	223	PHE	4.0
1	D	522	GLY	4.0
1	A	588	ARG	4.0
1	A	319	PHE	3.9
1	A	112	ASN	3.8
1	B	403	PRO	3.8
1	C	629	ALA	3.7
1	B	592	ARG	3.6
1	D	636	GLY	3.6
1	C	214	VAL	3.6
1	B	650	PHE	3.5
1	B	719	ILE	3.5
1	B	265[A]	TYR	3.4
1	A	471	GLU	3.4
1	B	305	GLU	3.4
1	D	437	GLY	3.4
1	C	432	THR	3.3
1	C	109	THR	3.2
1	D	473	SER	3.2
1	A	661	ARG	3.2
1	C	635	VAL	3.2
1	A	575	PRO	3.2
1	C	624	ARG	3.1
1	D	265[A]	TYR	3.1
1	C	615	GLY	3.0
1	C	164	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	163	MET	3.0
1	B	345	LEU	2.9
1	C	107	GLU	2.9
1	D	650	PHE	2.9
1	D	453	GLN	2.9
1	C	582	ILE	2.9
1	C	256	PRO	2.8
1	C	449	LEU	2.8
1	B	560	SER	2.8
1	A	582	ILE	2.7
1	D	456	LEU	2.7
1	C	658	GLN	2.7
1	A	649	TYR	2.7
1	D	182	PHE	2.7
1	A	262	PHE	2.7
1	B	448	PHE	2.7
1	C	314	TYR	2.7
1	B	434	ILE	2.6
1	C	110	ASP	2.6
1	D	584	GLN	2.6
1	B	396	THR	2.6
1	C	404	LEU	2.6
1	D	121	GLY	2.5
1	B	437	GLY	2.5
1	A	224	HIS	2.5
1	A	449	LEU	2.5
1	A	110	ASP	2.5
1	C	657	HIS	2.5
1	D	643	PHE	2.5
1	B	659	LEU	2.5
1	B	553	VAL	2.5
1	B	602	VAL	2.5
1	A	108	ASN	2.5
1	C	523	ARG	2.5
1	B	539	TRP	2.5
1	B	568	MET	2.4
1	B	718	ASP	2.4
1	C	596	CYS	2.4
1	A	265[A]	TYR	2.4
1	C	495	ILE	2.4
1	B	121	GLY	2.4
1	D	638	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	606	TYR	2.4
1	B	174	TRP	2.3
1	A	495	ILE	2.3
1	A	465	VAL	2.3
1	C	435	LYS	2.3
1	B	161	ALA	2.3
1	C	442	TYR	2.3
1	B	583	VAL	2.3
1	A	119	PRO	2.3
1	A	163	MET	2.3
1	C	659	LEU	2.2
1	A	397	THR	2.2
1	D	724	HIS	2.2
1	C	638	ARG	2.2
1	A	272	ILE	2.2
1	C	467	GLU	2.2
1	A	256	PRO	2.2
1	A	450	ILE	2.2
1	C	608	ASP	2.2
1	D	725	ALA	2.2
1	C	447	GLY	2.1
1	C	500	SER	2.1
1	D	174	TRP	2.1
1	D	477	PRO	2.1
1	A	498	THR	2.1
1	D	107	GLU	2.1
1	D	108	ASN	2.1
1	A	473	SER	2.1
1	D	467	GLU	2.1
1	A	192	VAL	2.1
1	C	492	VAL	2.1
1	B	113	PHE	2.1
1	D	592	ARG	2.1
1	C	263	HIS	2.1
1	A	109	THR	2.1
1	C	431	ALA	2.1
1	C	105	LYS	2.1
1	C	412	CYS	2.0
1	A	494	ARG	2.0
1	D	582	ILE	2.0
1	B	594	GLY	2.0
1	B	269	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	222	ALA	2.0
1	A	625	LEU	2.0
1	A	659	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](#)

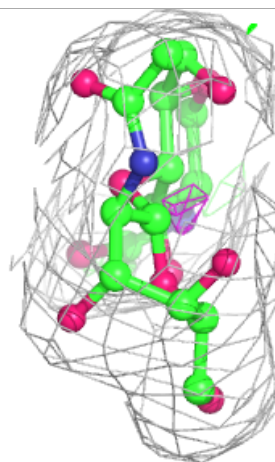
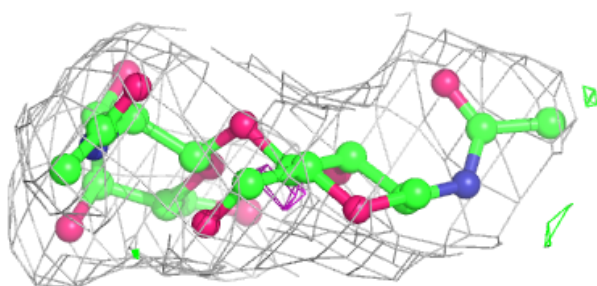
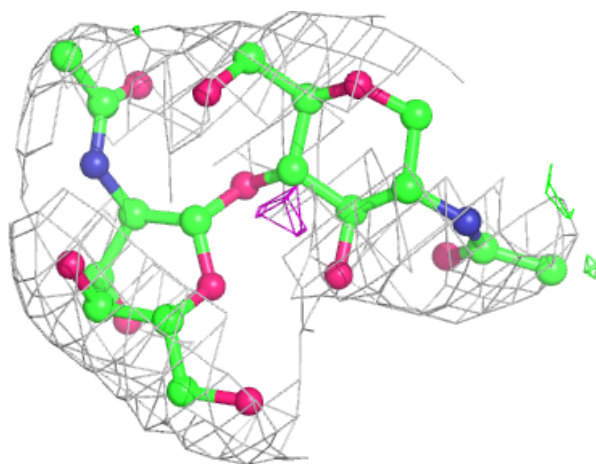
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

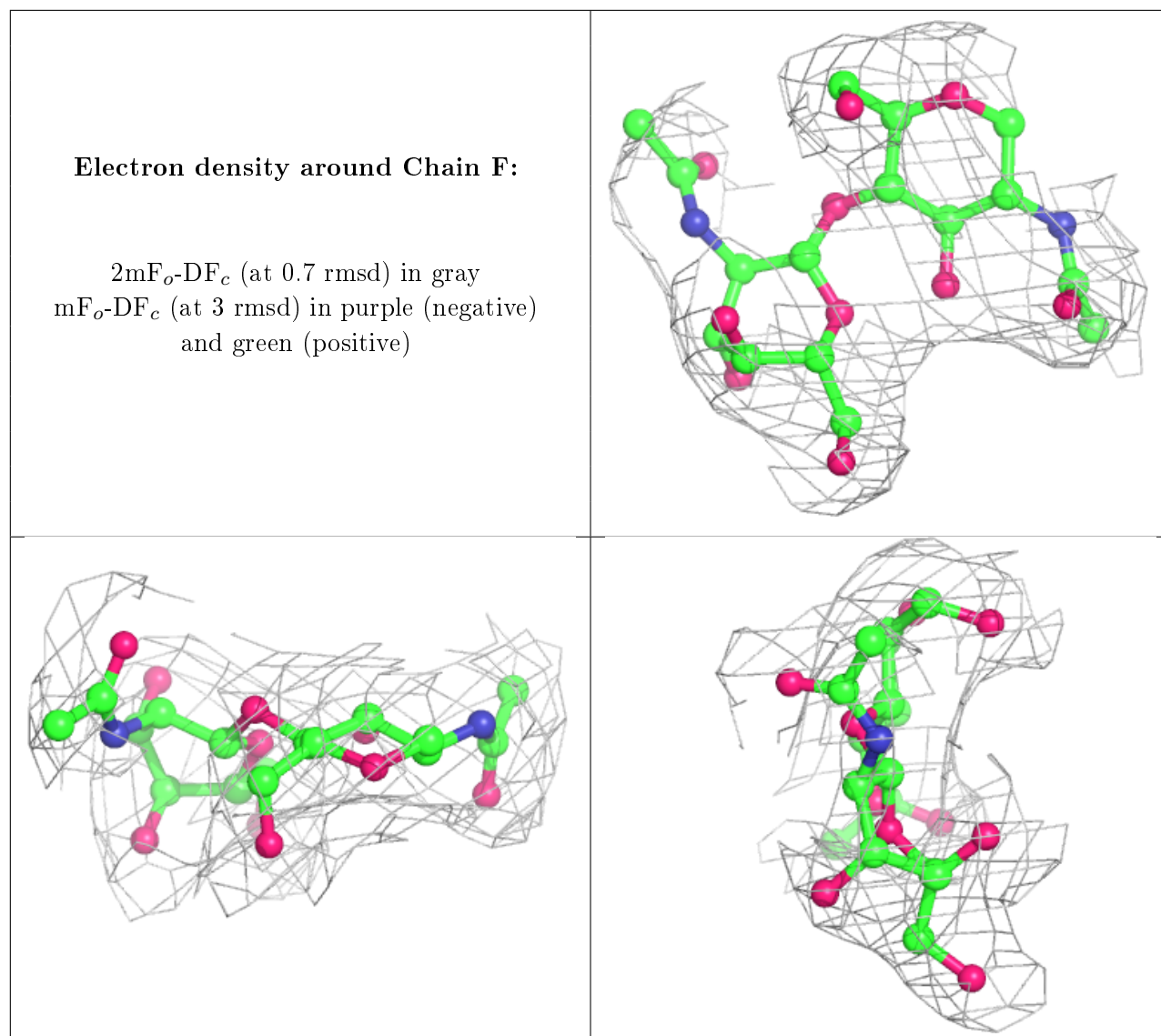
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	1	14/15	0.91	0.10	104,104,104,104	0
2	NAG	F	2	14/15	0.92	0.14	91,91,91,91	0
2	NAG	E	2	14/15	0.94	0.09	89,89,89,89	0
2	NAG	F	1	14/15	0.96	0.12	77,77,77,77	0

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)





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	NAG	C	1141	14/15	0.81	0.26	113,113,113,113	0
3	NAG	A	1430	14/15	0.81	0.18	118,118,118,118	0
3	NAG	C	1430	14/15	0.84	0.17	117,117,117,117	0
3	NAG	B	1430	14/15	0.85	0.20	117,117,117,117	0
3	NAG	D	1398	14/15	0.88	0.16	87,87,87,87	0
4	CL	A	2	1/1	0.89	0.11	78,78,78,78	0
3	NAG	C	1674	14/15	0.89	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	1398	14/15	0.90	0.14	92,92,92,92	0
4	CL	D	1	1/1	0.90	0.15	59,59,59,59	0
3	NAG	A	1674	14/15	0.92	0.14	89,89,89,89	0
3	NAG	A	1141	14/15	0.94	0.25	120,120,120,120	0
5	MRY	C	2001	8/8	0.95	0.17	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.