



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:13 AM UTC

PDB ID : 8KHC / pdb_00008khc
EMDB ID : EMD-37240
Title : SARS-CoV-2 Omicron spike in complex with 5817 Fab
Authors : Cao, L.; Wang, X.
Deposited on : 2023-08-21
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

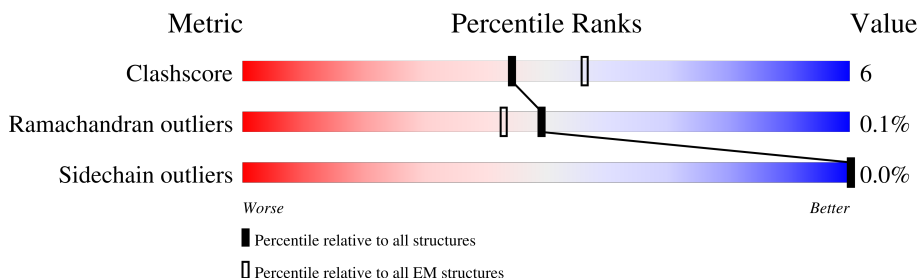
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1120	74% 17% 9%
1	B	1120	78% 13% 9%
1	C	1120	81% 11% 9%
2	F	125	79% 21%
2	H	125	79% 21%
3	G	108	81% 19%
3	J	108	80% 20%
4	D	2	100%
4	E	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27173 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1018	Total	C	N	O	S	0	0
			7729	4970	1282	1442	35		
1	B	1020	Total	C	N	O	S	0	0
			7738	4954	1289	1461	34		
1	C	1024	Total	C	N	O	S	0	0
			7642	4912	1267	1429	34		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	142	ASP	GLY	conflict	UNP P0DTC2
A	156	ASP	GLU	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	550	LYS	THR	conflict	UNP P0DTC2
A	617	GLY	ASP	conflict	UNP P0DTC2
A	658	TYR	HIS	conflict	UNP P0DTC2
A	767	LYS	ASN	conflict	UNP P0DTC2
A	799	TYR	ASP	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	859	LYS	ASN	conflict	UNP P0DTC2
A	957	HIS	GLN	conflict	UNP P0DTC2
A	972	LYS	ASN	conflict	UNP P0DTC2
A	984	PHE	LEU	conflict	UNP P0DTC2
A	989	PRO	LYS	conflict	UNP P0DTC2
A	990	PRO	VAL	conflict	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	142	ASP	GLY	conflict	UNP P0DTC2
B	156	ASP	GLU	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	550	LYS	THR	conflict	UNP P0DTC2
B	617	GLY	ASP	conflict	UNP P0DTC2
B	658	TYR	HIS	conflict	UNP P0DTC2
B	767	LYS	ASN	conflict	UNP P0DTC2
B	799	TYR	ASP	conflict	UNP P0DTC2
B	859	LYS	ASN	conflict	UNP P0DTC2
B	957	HIS	GLN	conflict	UNP P0DTC2
B	972	LYS	ASN	conflict	UNP P0DTC2
B	984	PHE	LEU	conflict	UNP P0DTC2
B	989	PRO	LYS	conflict	UNP P0DTC2
B	990	PRO	VAL	conflict	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	142	ASP	GLY	conflict	UNP P0DTC2
C	156	ASP	GLU	conflict	UNP P0DTC2
C	342	ASP	GLY	conflict	UNP P0DTC2
C	374	LEU	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	376	PRO	SER	conflict	UNP P0DTC2
C	378	PHE	SER	conflict	UNP P0DTC2
C	420	ASN	LYS	conflict	UNP P0DTC2
C	443	LYS	ASN	conflict	UNP P0DTC2
C	449	SER	GLY	conflict	UNP P0DTC2
C	480	ASN	SER	conflict	UNP P0DTC2
C	481	LYS	THR	conflict	UNP P0DTC2
C	487	ALA	GLU	conflict	UNP P0DTC2
C	496	ARG	GLN	conflict	UNP P0DTC2
C	499	SER	GLY	conflict	UNP P0DTC2
C	501	ARG	GLN	conflict	UNP P0DTC2
C	504	TYR	ASN	conflict	UNP P0DTC2
C	508	HIS	TYR	conflict	UNP P0DTC2
C	550	LYS	THR	conflict	UNP P0DTC2
C	617	GLY	ASP	conflict	UNP P0DTC2
C	658	TYR	HIS	conflict	UNP P0DTC2
C	767	LYS	ASN	conflict	UNP P0DTC2
C	799	TYR	ASP	conflict	UNP P0DTC2
C	859	LYS	ASN	conflict	UNP P0DTC2
C	957	HIS	GLN	conflict	UNP P0DTC2
C	972	LYS	ASN	conflict	UNP P0DTC2
C	984	PHE	LEU	conflict	UNP P0DTC2
C	989	PRO	LYS	conflict	UNP P0DTC2
C	990	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of 5817 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	125	Total	C	N	O	S	0	0
			917	577	149	184	7		
2	H	125	Total	C	N	O	S	0	0
			917	577	149	184	7		

- Molecule 3 is a protein called Light chain of 5817 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	108	Total	C	N	O	S	0	0
			806	497	141	166	2		
3	J	108	Total	C	N	O	S	0	0
			806	497	141	166	2		

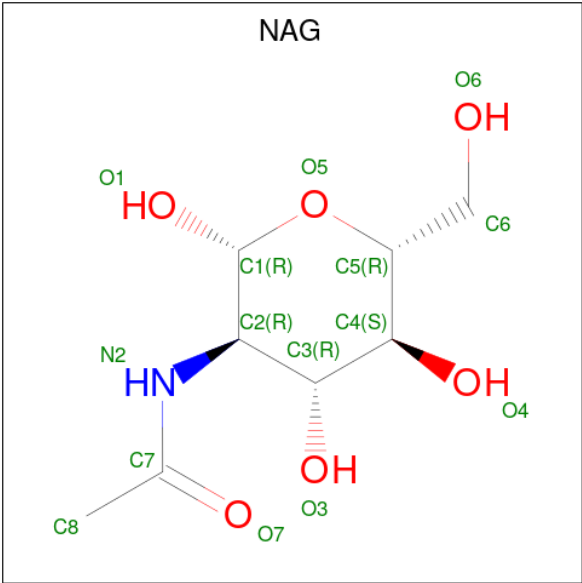
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

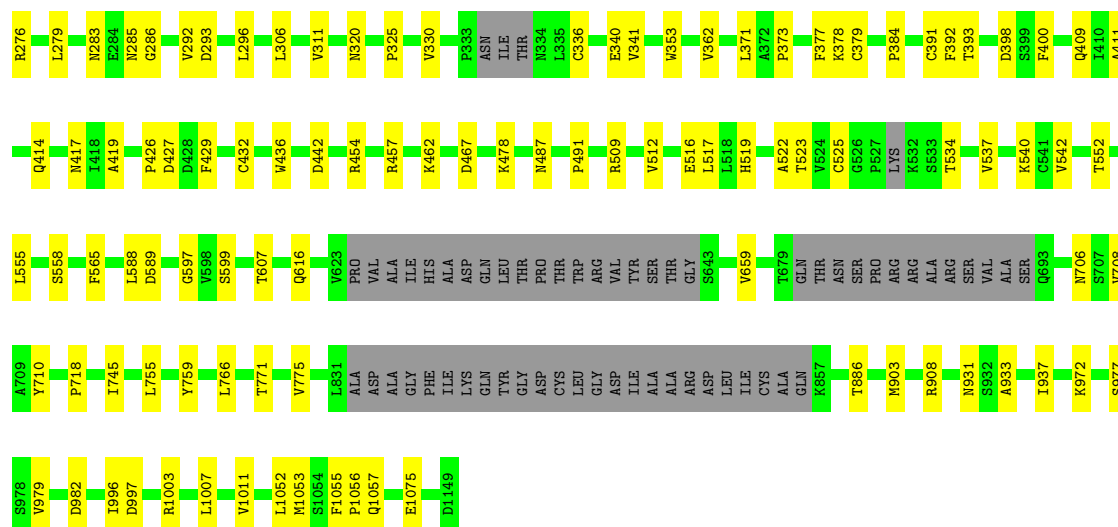
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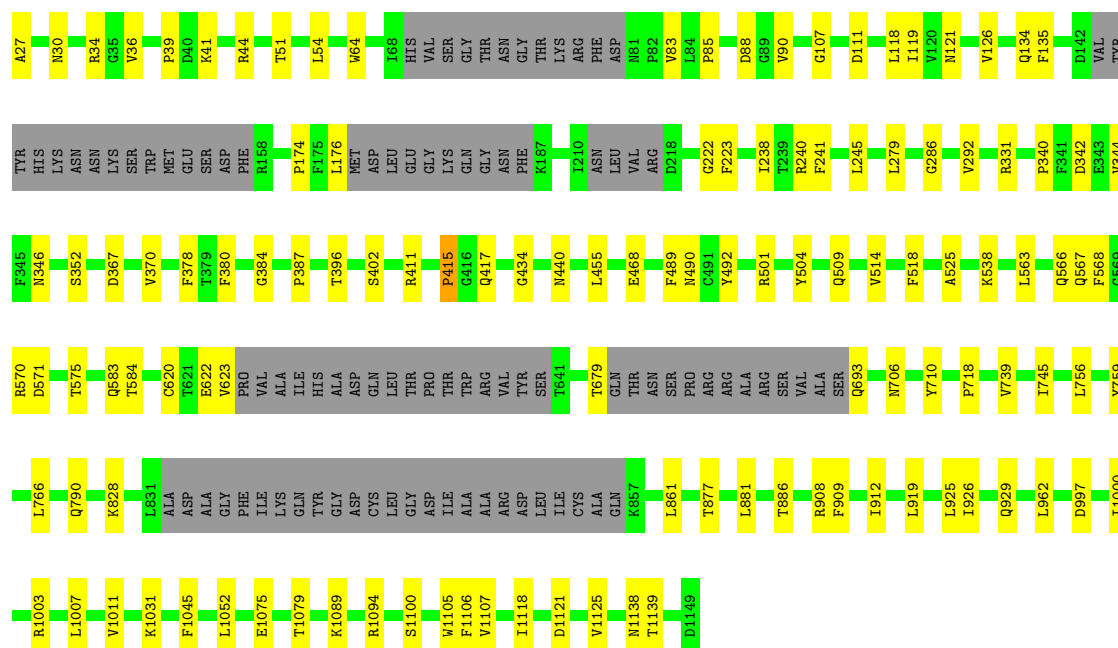
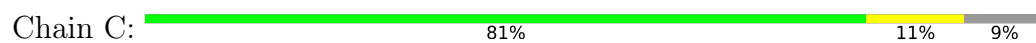
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is water.

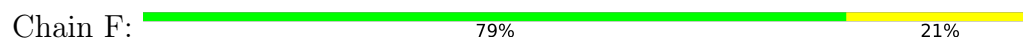
Mol	Chain	Residues	Atoms		AltConf
6	A	5	Total	O	0
			5	5	
6	B	4	Total	O	0
			4	4	
6	F	19	Total	O	0
			19	19	
6	G	6	Total	O	0
			6	6	
6	H	16	Total	O	0
			16	16	
6	J	8	Total	O	0
			8	8	



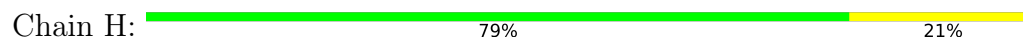
- Molecule 1: Spike glycoprotein



- Molecule 2: Heavy chain of 5817 Fab



- Molecule 2: Heavy chain of 5817 Fab





- Molecule 3: Light chain of 5817 Fab

Chain G: 81% 19%



- Molecule 3: Light chain of 5817 Fab

Chain J: 80% 20%



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

Chain D: 100%



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

Chain E: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5129	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/7911	0.35	0/10793
1	B	0.13	0/7918	0.34	0/10805
1	C	0.14	0/7823	0.36	1/10700 (0.0%)
2	F	0.11	0/934	0.30	0/1268
2	H	0.11	0/936	0.29	0/1274
3	G	0.08	0/822	0.28	0/1118
3	J	0.09	0/822	0.27	0/1118
All	All	0.13	0/27166	0.34	1/37076 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	PRO	CA-N-CD	-8.24	100.47	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	ASN	Peptide
1	A	620	CYS	Peptide

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	7729	0	7343	129	0
1	B	7738	0	7313	94	0
1	C	7642	0	7167	76	0
2	F	917	0	856	15	0
2	H	917	0	858	17	0
3	G	806	0	769	13	0
3	J	806	0	769	13	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	168	0	156	3	0
5	B	168	0	156	7	0
5	C	168	0	156	1	0
6	A	5	0	0	1	0
6	B	4	0	0	0	0
6	F	19	0	0	1	0
6	G	6	0	0	0	0
6	H	16	0	0	1	0
6	J	8	0	0	1	0
All	All	27173	0	25593	337	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 6.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:HB2	5:B:1303:NAG:HN2	1.47	0.79
1:A:201:PHE:HB3	1:A:232:LEU:HB2	1.66	0.76
1:A:402:ILE:HD11	1:A:418:ILE:HD13	1.69	0.73
1:A:384:PRO:HB3	1:C:490:ASN:HA	1.71	0.72
1:A:376:THR:HB	1:A:435:ALA:HB3	1.71	0.71
1:A:339:ASP:O	1:A:341:VAL:N	2.25	0.70
1:C:745:ILE:O	1:C:1003:ARG:NH1	2.24	0.69
1:B:745:ILE:O	1:B:1003:ARG:NH1	2.24	0.69
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:HH22	1:A:457:ARG:HD3	1.59	0.68
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.75	0.67
3:G:97:VAL:O	3:G:99:PHE:N	2.27	0.67
3:J:18:VAL:HB	3:J:74:ILE:HB	1.77	0.67
1:A:85:PRO:HA	1:A:240:ARG:HA	1.78	0.66
1:B:759:TYR:OH	1:B:997:ASP:OD1	2.14	0.66
3:J:97:VAL:O	3:J:99:PHE:N	2.24	0.65
1:A:398:ASP:HB3	1:A:512:VAL:HB	1.78	0.65
1:B:558:SER:HB3	1:B:589:ASP:HB2	1.77	0.65
1:A:1097:VAL:HG13	1:B:903:MET:HE1	1.78	0.64
1:B:931:ASN:HB3	5:B:1305:NAG:H61	1.79	0.64
1:A:41:LYS:HG2	1:A:228:PRO:HG3	1.80	0.64
1:B:908:ARG:NH1	1:B:1052:LEU:O	2.30	0.64
1:B:276:ARG:NH1	1:B:293:ASP:OD2	2.30	0.64
1:C:1107:VAL:HG23	1:C:1118:ILE:HG12	1.79	0.64
1:A:34:ARG:NE	1:A:191:GLU:OE2	2.31	0.64
1:A:378:LYS:HE3	1:A:380:TYR:HE1	1.63	0.63
1:A:986:ARG:NH1	1:C:384:GLY:O	2.31	0.63
1:A:790:GLN:OE1	1:C:706:ASN:ND2	2.32	0.63
1:B:127:VAL:HG22	1:B:171:VAL:HG22	1.81	0.63
1:C:54:LEU:HD21	1:C:88:ASP:HB3	1.81	0.63
1:A:886:THR:HG23	1:C:710:TYR:HB2	1.80	0.63
1:C:415:PRO:HD2	1:C:415:PRO:O	1.99	0.63
1:A:139:PRO:HB3	1:A:244:LEU:HD23	1.81	0.62
1:C:118:LEU:HD12	1:C:135:PHE:HE1	1.64	0.62
1:C:331:ARG:HH21	1:C:583:GLN:HB2	1.64	0.62
1:A:536:LEU:HD21	1:A:588:LEU:HD11	1.80	0.62
1:B:283:ASN:HD22	5:B:1303:NAG:H82	1.64	0.62
1:A:648:THR:HG23	1:A:673:ILE:HD12	1.82	0.62
1:B:66:HIS:O	1:B:80:ASP:N	2.33	0.61
1:A:498:ARG:HG3	1:A:500:THR:HG22	1.81	0.61
1:B:285:ASN:HB2	5:B:1303:NAG:N2	2.15	0.61
1:C:1094:ARG:NH1	1:C:1121:ASP:O	2.34	0.61
2:F:34:MET:HG2	2:F:74:ARG:HH21	1.64	0.61
1:A:403:ARG:HH21	1:A:505:HIS:HB3	1.65	0.61
1:B:409:GLN:NE2	1:B:417:ASN:O	2.34	0.61
1:B:710:TYR:HB2	1:C:886:THR:HG23	1.83	0.60
1:A:106:PHE:HD1	1:A:117:LEU:HD22	1.65	0.60
3:J:38:LYS:NZ	3:J:80:GLU:O	2.34	0.60
1:A:534:THR:HG22	1:A:535:ASN:H	1.65	0.60
1:A:457:ARG:HH21	1:A:460:ASN:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:VAL:HG23	1:A:593:CYS:HB3	1.83	0.59
1:C:861:LEU:HD13	1:C:962:LEU:HD22	1.82	0.59
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.84	0.59
1:B:398:ASP:HB3	1:B:512:VAL:HB	1.84	0.59
1:C:411:ARG:NH1	1:C:417:GLN:OE1	2.35	0.59
1:C:759:TYR:OH	1:C:997:ASP:OD1	2.21	0.59
3:J:82:GLU:HG3	3:J:106:THR:HA	1.83	0.59
1:C:766:LEU:HG	1:C:1011:VAL:HG21	1.84	0.58
1:B:105:ILE:HG23	1:B:244:LEU:HD21	1.84	0.58
1:C:402:SER:HB3	1:C:514:VAL:HG22	1.85	0.58
1:A:565:PHE:O	1:B:41:LYS:NZ	2.36	0.58
1:B:39:PRO:HD2	1:B:40:ASP:H	1.69	0.57
2:F:38:ARG:HG2	2:F:46:GLU:HB3	1.86	0.57
2:H:102:VAL:HG23	2:H:105:VAL:HG22	1.86	0.57
1:A:766:LEU:HD22	1:A:1011:VAL:HG21	1.85	0.57
1:A:371:LEU:HG	1:A:373:PRO:HD2	1.87	0.57
1:A:549:LEU:HD21	1:A:576:THR:HG21	1.86	0.57
1:C:107:GLY:H	1:C:238:ILE:HG23	1.70	0.57
1:B:371:LEU:HG	1:B:373:PRO:HD2	1.86	0.57
1:A:352:ALA:HA	1:A:466:ARG:HH22	1.70	0.56
1:A:331:ARG:HH21	1:A:536:LEU:HB2	1.70	0.56
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.86	0.56
1:B:379:CYS:HB3	1:B:432:CYS:HA	1.87	0.56
1:C:380:PHE:HE2	1:C:387:PRO:HB3	1.70	0.56
1:A:89:GLY:HA3	1:A:273:LEU:HB2	1.86	0.56
1:B:972:LYS:HE3	1:B:977:SER:HA	1.88	0.56
1:B:81:ASN:O	1:B:242:GLN:NE2	2.24	0.56
3:J:38:LYS:HB2	3:J:41:GLN:HB2	1.86	0.56
1:B:195:LYS:HD2	1:B:197:ILE:HG12	1.88	0.56
2:H:9:GLY:HA2	2:H:18:LEU:HD21	1.87	0.56
1:A:355:ARG:NH1	6:A:1401:HOH:O	2.30	0.56
1:A:355:ARG:HD2	1:A:396:TYR:HB3	1.87	0.56
1:B:766:LEU:HG	1:B:1011:VAL:HG21	1.88	0.56
3:G:38:LYS:HB2	3:G:41:GLN:HB2	1.88	0.55
1:A:433:VAL:HG12	1:A:512:VAL:HG13	1.88	0.55
1:A:457:ARG:NE	1:A:459:SER:O	2.35	0.55
2:H:20:LEU:HD13	2:H:85:MET:HE1	1.88	0.55
1:A:804:ASN:OD1	1:A:931:ASN:ND2	2.40	0.55
1:C:739:VAL:HG11	1:C:1007:LEU:HD11	1.89	0.55
3:J:97:VAL:C	3:J:99:PHE:H	2.14	0.55
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:GLU:OE1	1:B:519:HIS:ND1	2.39	0.55
1:A:354:ASN:ND2	2:H:55:ILE:O	2.40	0.54
1:A:908:ARG:NH1	1:A:1052:LEU:O	2.39	0.54
1:C:378:PHE:HE2	1:C:440:ASN:HB2	1.72	0.54
1:A:105:ILE:O	1:A:242:GLN:N	2.31	0.54
1:B:555:LEU:HD23	1:B:588:LEU:HD13	1.89	0.54
2:F:93:THR:HG22	2:F:125:VAL:H	1.71	0.54
1:A:293:ASP:O	1:A:300:SER:HB3	2.07	0.54
1:B:454:ARG:NH1	1:B:467:ASP:OD2	2.40	0.54
1:A:619:ASN:OD1	5:A:1309:NAG:N2	2.41	0.53
1:A:1107:VAL:HG23	1:A:1118:ILE:HG12	1.89	0.53
1:A:379:CYS:HB2	1:C:489:PHE:CD1	2.43	0.53
1:A:379:CYS:O	1:C:492:TYR:OH	2.20	0.53
1:A:393:THR:OG1	1:A:516:GLU:O	2.27	0.53
1:C:340:PRO:O	1:C:344:VAL:N	2.31	0.53
1:A:104:TRP:HA	1:A:243:THR:HA	1.89	0.53
1:A:105:ILE:HB	1:A:242:GLN:HB3	1.90	0.53
1:C:396:THR:HA	1:C:525:ALA:HA	1.91	0.53
3:G:82:GLU:HG3	3:G:106:THR:HA	1.90	0.53
1:C:83:VAL:HG11	1:C:240:ARG:HH11	1.73	0.53
2:H:15:GLY:H	2:H:88:LEU:HB2	1.73	0.53
1:B:279:LEU:HB3	1:B:292:VAL:HG22	1.90	0.53
1:A:421:TYR:HA	1:A:457:ARG:HH12	1.73	0.53
3:G:97:VAL:C	3:G:99:PHE:H	2.14	0.53
1:B:766:LEU:HD21	1:B:1007:LEU:HB3	1.91	0.53
1:C:679:THR:HA	1:C:693:GLN:HA	1.91	0.53
1:C:118:LEU:HD23	1:C:119:ILE:N	2.24	0.52
1:A:320:ASN:HD22	1:A:597:GLY:HA2	1.74	0.52
1:A:739:VAL:HG21	1:A:1007:LEU:HD11	1.90	0.52
1:B:210:ILE:HD12	1:B:220:PRO:HG3	1.91	0.52
1:C:908:ARG:NH1	1:C:1052:LEU:O	2.43	0.52
1:A:392:PHE:HD1	1:A:517:LEU:HD21	1.75	0.52
1:A:420:ASP:O	1:A:457:ARG:NH1	2.40	0.52
1:B:933:ALA:O	1:B:937:ILE:HG12	2.10	0.52
3:G:38:LYS:NZ	3:G:80:GLU:O	2.43	0.52
1:B:283:ASN:ND2	5:B:1303:NAG:H82	2.25	0.52
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.91	0.52
1:B:119:ILE:HG12	1:B:128:ILE:HG23	1.92	0.52
2:H:36:TRP:HD1	2:H:72:ILE:HD11	1.74	0.52
1:A:417:ASN:O	1:A:419:ALA:N	2.40	0.52
1:A:335:LEU:HD22	1:A:527:PRO:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:CYS:HB2	1:C:623:VAL:HA	1.91	0.51
1:A:297:ASP:OD1	1:A:300:SER:OG	2.26	0.51
1:B:336:CYS:SG	1:B:362:VAL:N	2.84	0.51
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.93	0.51
3:G:45:LEU:HD11	3:G:48:TYR:HB3	1.93	0.51
1:A:759:TYR:OH	1:A:997:ASP:OD1	2.23	0.51
1:A:117:LEU:HG	1:A:130:VAL:HG12	1.93	0.51
1:B:325:PRO:HG3	1:B:552:THR:HG21	1.93	0.51
2:H:50:ARG:NH1	2:H:112:ASP:OD2	2.42	0.51
1:A:386:LYS:HG2	1:A:389:ASP:HB3	1.92	0.51
1:B:442:ASP:HB2	1:B:509:ARG:HH21	1.76	0.50
1:C:1031:LYS:NZ	1:C:1045:PHE:O	2.44	0.50
1:A:367:VAL:HG23	1:A:368:LEU:HD12	1.92	0.50
1:B:411:ALA:HB3	1:B:414:GLN:HE22	1.76	0.50
1:A:458:LYS:NZ	1:A:474:GLN:O	2.36	0.50
1:A:1009:THR:O	1:A:1013:GLN:HG2	2.12	0.50
1:B:979:VAL:HG13	1:B:982:ASP:HB3	1.93	0.50
3:G:20:ILE:HB	3:G:72:LEU:HB3	1.94	0.50
1:B:393:THR:O	1:B:523:THR:OG1	2.30	0.50
1:B:409:GLN:HA	1:B:414:GLN:HE21	1.77	0.49
1:B:1053:MET:HE2	1:B:1055:PHE:CE1	2.47	0.49
2:F:104:ILE:HG13	2:F:104:ILE:O	2.11	0.49
1:A:86:PHE:N	1:A:239:THR:O	2.27	0.49
1:B:58:PHE:HB2	1:B:296:LEU:HD11	1.94	0.49
1:C:1138:ASN:OD1	1:C:1139:THR:N	2.44	0.49
1:A:92:PHE:HB3	1:A:194:PHE:HE1	1.76	0.49
1:B:718:PRO:HA	1:B:1075:GLU:HA	1.95	0.49
2:H:39:GLN:NE2	6:J:201:HOH:O	2.45	0.49
1:A:106:PHE:HB2	1:A:117:LEU:HD13	1.95	0.49
1:C:1106:PHE:HZ	5:C:1309:NAG:H82	1.78	0.49
1:A:718:PRO:HA	1:A:1075:GLU:HA	1.94	0.49
1:A:806:SER:HB2	5:A:1311:NAG:H5	1.94	0.49
1:C:34:ARG:NH1	1:C:222:GLY:O	2.46	0.49
1:C:342:ASP:OD1	1:C:346:ASN:ND2	2.45	0.49
6:F:205:HOH:O	3:G:37:GLN:NE2	2.45	0.49
1:A:351:TYR:CE1	1:A:452:LEU:HB2	2.48	0.48
1:C:27:ALA:HB1	1:C:64:TRP:HE3	1.78	0.48
1:A:299:LEU:HB2	1:A:611:VAL:HG21	1.95	0.48
1:A:106:PHE:CD1	1:A:117:LEU:HD22	2.48	0.48
1:A:293:ASP:OD1	1:A:294:CYS:N	2.46	0.48
1:A:534:THR:HG22	1:A:535:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:HE2	3:G:52:ASN:HD22	1.79	0.48
1:A:44:ARG:HA	1:C:571:ASP:HA	1.95	0.48
1:A:90:VAL:HG11	1:A:241:PHE:CE1	2.48	0.48
1:B:353:TRP:HB3	1:B:400:PHE:HB3	1.96	0.48
1:C:756:LEU:HD13	1:C:1000:ILE:HD12	1.95	0.48
1:A:745:ILE:O	1:A:1003:ARG:NH1	2.46	0.48
1:A:43:PHE:HB2	1:C:566:GLN:HB3	1.94	0.48
1:A:558:SER:HB3	1:A:587:ILE:HG13	1.96	0.48
1:C:718:PRO:HA	1:C:1075:GLU:HA	1.95	0.48
3:J:64:SER:OG	3:J:71:SER:OG	2.31	0.48
1:A:119:ILE:HG23	1:A:128:ILE:HG12	1.96	0.48
1:C:331:ARG:HH22	1:C:584:THR:HG23	1.79	0.47
1:A:57:PRO:HG3	1:A:274:GLN:HB2	1.97	0.47
1:B:88:ASP:O	1:B:273:LEU:HB2	2.14	0.47
1:A:117:LEU:HD21	1:A:119:ILE:HG13	1.97	0.47
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.96	0.47
1:B:659:VAL:HA	5:B:1307:NAG:H82	1.96	0.47
1:A:1129:CYS:HB2	1:A:1135:ILE:HD13	1.95	0.47
1:A:201:PHE:O	1:A:232:LEU:N	2.38	0.47
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.95	0.47
1:C:1105:TRP:HB2	1:C:1138:ASN:ND2	2.29	0.47
1:A:131:CYS:HA	1:A:166:CYS:CB	2.45	0.47
1:A:353:TRP:HB3	1:A:400:PHE:HB3	1.97	0.47
1:C:925:LEU:O	1:C:929:GLN:HG3	2.14	0.47
1:C:1079:THR:HG23	1:C:1100:SER:HB3	1.96	0.47
1:A:359:SER:OG	1:A:360:ASN:OD1	2.32	0.47
1:C:90:VAL:HG21	1:C:241:PHE:CE1	2.50	0.47
2:F:101:GLY:O	2:F:114:PHE:N	2.48	0.47
1:A:454:ARG:NH2	1:A:457:ARG:HH11	2.13	0.46
2:H:38:ARG:HG2	2:H:46:GLU:HB3	1.97	0.46
3:J:22:CYS:HB3	3:J:70:ALA:HB3	1.96	0.46
1:B:40:ASP:OD2	1:B:44:ARG:NH2	2.45	0.46
1:B:320:ASN:HA	1:B:597:GLY:HA2	1.97	0.46
1:C:622:GLU:N	1:C:622:GLU:OE2	2.49	0.46
1:A:58:PHE:CD2	1:A:293:ASP:HB2	2.51	0.46
1:B:417:ASN:O	1:B:419:ALA:N	2.44	0.46
1:C:440:ASN:ND2	1:C:509:GLN:OE1	2.35	0.46
2:F:38:ARG:HH22	2:F:92:ASP:HA	1.80	0.46
3:G:46:VAL:HG12	3:G:47:ILE:HG13	1.97	0.46
1:C:434:GLY:HA2	1:C:518:PHE:CE1	2.51	0.46
3:J:46:VAL:HG12	3:J:47:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLN:HG2	1:B:419:ALA:HB2	1.98	0.46
1:B:377:PHE:HE2	1:B:384:PRO:HB3	1.81	0.46
3:J:30:TYR:CG	3:J:90:ARG:HB2	2.51	0.46
1:A:34:ARG:O	1:A:56:LEU:HD23	2.16	0.45
1:A:1085:CYS:HB2	1:A:1129:CYS:HB2	1.88	0.45
2:F:7:SER:HB2	2:F:21:SER:HB2	1.98	0.45
1:A:379:CYS:SG	1:A:433:VAL:N	2.87	0.45
1:B:82:PRO:HG2	1:B:84:LEU:HD21	1.97	0.45
1:A:190:ARG:HG2	1:A:192:PHE:CZ	2.51	0.45
1:C:279:LEU:HB3	1:C:292:VAL:HB	1.98	0.45
1:B:771:THR:O	1:B:775:VAL:HG22	2.17	0.45
2:F:102:VAL:HG13	2:F:105:VAL:HG22	1.99	0.45
1:A:496:SER:O	1:A:498:ARG:NH1	2.50	0.45
2:F:9:GLY:HA2	2:F:18:LEU:HD21	1.99	0.45
1:B:1053:MET:HE2	1:B:1055:PHE:CZ	2.52	0.45
2:H:37:VAL:HG13	2:H:97:TYR:HB2	1.99	0.45
1:C:570:ARG:HA	1:C:575:THR:O	2.17	0.45
1:A:93:ALA:O	1:A:268:TYR:HB2	2.17	0.45
2:F:107:MET:SD	2:F:108:MET:N	2.90	0.45
1:B:607:THR:HG22	5:B:1309:NAG:H82	1.99	0.44
2:F:66:VAL:HA	2:F:69:ARG:HH11	1.82	0.44
1:A:516:GLU:OE1	1:A:519:HIS:ND1	2.50	0.44
2:H:101:GLY:O	2:H:114:PHE:N	2.51	0.44
1:B:80:ASP:O	1:B:268:TYR:OH	2.32	0.44
1:A:409:GLN:HA	1:A:414:GLN:HE21	1.81	0.44
1:A:421:TYR:HA	1:A:457:ARG:NH1	2.32	0.44
1:B:236:ILE:HG13	1:B:238:ILE:HG13	1.99	0.44
1:B:306:LEU:HD12	1:B:311:VAL:HG12	2.00	0.44
1:C:367:ASP:O	1:C:370:VAL:HG22	2.17	0.44
1:A:771:THR:O	1:A:775:VAL:HG23	2.17	0.44
1:A:909:PHE:CD2	1:A:919:LEU:HB2	2.53	0.44
1:A:976:ILE:HD12	1:A:986:ARG:NH2	2.33	0.44
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.52	0.44
1:B:565:PHE:HB2	1:C:41:LYS:NZ	2.32	0.44
5:A:1303:NAG:O3	1:C:468:GLU:OE2	2.28	0.44
2:F:29:PHE:CE2	2:F:81:LEU:HD21	2.51	0.44
2:F:119:GLN:HG2	2:F:120:GLY:N	2.31	0.44
1:B:241:PHE:CZ	1:B:270:VAL:HG11	2.53	0.44
1:B:708:VAL:HB	1:C:886:THR:HG21	1.99	0.44
1:A:348:ALA:HB2	2:H:55:ILE:HG21	2.00	0.43
1:A:644:ASN:OD1	1:A:645:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG11	1:B:175:PHE:CE2	2.53	0.43
1:C:121:ASN:HD21	1:C:176:LEU:H	1.65	0.43
3:G:18:VAL:HB	3:G:74:ILE:HB	2.00	0.43
1:A:58:PHE:HE2	1:A:278:PHE:CE2	2.36	0.43
1:B:283:ASN:OD1	1:B:286:GLY:N	2.51	0.43
1:B:393:THR:HG22	1:B:522:ALA:HA	2.00	0.43
1:B:537:VAL:HG21	1:B:540:LYS:HE2	2.01	0.43
2:H:33:TRP:N	6:H:204:HOH:O	2.46	0.43
2:H:106:VAL:H	3:J:48:TYR:HE1	1.66	0.43
1:B:91:TYR:HA	1:B:193:VAL:HG22	1.99	0.43
1:B:540:LYS:HG3	1:B:542:VAL:HG13	2.01	0.43
1:A:116:SER:HB2	1:A:135:PHE:CE2	2.54	0.43
3:J:51:ASN:OD1	3:J:51:ASN:N	2.52	0.43
1:C:563:LEU:HB2	1:C:566:GLN:HG2	2.01	0.43
1:C:909:PHE:CD2	1:C:919:LEU:HB2	2.54	0.43
1:A:994:VAL:O	1:A:998:ARG:HG3	2.19	0.43
1:A:600:VAL:HG13	1:A:611:VAL:HG13	2.01	0.42
1:A:829:VAL:HG13	1:A:1060:PRO:HG2	2.01	0.42
1:B:478:LYS:HG3	1:B:487:ASN:HD22	1.84	0.42
1:C:245:LEU:H	1:C:245:LEU:HD23	1.84	0.42
1:A:615:TYR:HE1	1:A:654:ILE:HD12	1.83	0.42
1:B:392:PHE:HD1	1:B:517:LEU:HD21	1.84	0.42
1:B:427:ASP:OD1	1:B:427:ASP:N	2.52	0.42
1:C:36:VAL:HG11	1:C:223:PHE:CZ	2.55	0.42
1:A:662:SER:HB3	1:A:701:SER:HB3	2.00	0.42
1:A:925:LEU:O	1:A:929:GLN:HG3	2.20	0.42
1:B:64:TRP:CD1	1:B:269:TYR:HE1	2.36	0.42
1:A:881:LEU:HD11	1:A:1055:PHE:HB3	2.01	0.42
1:B:1056:PRO:O	1:B:1057:GLN:NE2	2.45	0.42
1:A:320:ASN:ND2	1:A:597:GLY:HA2	2.33	0.42
1:C:111:ASP:HA	1:C:134:GLN:HA	2.01	0.42
1:C:352:SER:HB2	1:C:455:LEU:O	2.19	0.42
2:H:22:CYS:HB3	2:H:81:LEU:HB3	2.00	0.42
1:A:708:VAL:HG13	1:B:886:THR:HG21	2.01	0.42
1:B:41:LYS:HG2	1:B:41:LYS:O	2.20	0.42
1:B:457:ARG:NH1	1:B:467:ASP:OD1	2.53	0.42
3:J:10:VAL:HG12	3:J:12:VAL:HG23	2.02	0.42
1:A:84:LEU:HD13	1:A:270:VAL:HG11	2.02	0.42
1:A:570:ARG:HG3	1:B:42:VAL:HG11	2.02	0.42
1:A:974:GLY:O	1:A:998:ARG:NH1	2.53	0.41
1:C:501:ARG:NH1	1:C:504:TYR:OH	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:HG21	1:B:241:PHE:CE1	2.55	0.41
1:B:378:LYS:HB3	1:B:378:LYS:HE3	1.82	0.41
1:B:755:LEU:HD22	1:B:996:ILE:HG21	2.01	0.41
1:C:83:VAL:HG11	1:C:240:ARG:NH1	2.34	0.41
1:C:1089:LYS:HD2	1:C:1125:VAL:HG21	2.03	0.41
1:B:330:VAL:O	1:B:534:THR:N	2.53	0.41
1:C:39:PRO:HG3	1:C:51:THR:HG21	2.02	0.41
1:A:84:LEU:HB2	1:A:241:PHE:CZ	2.55	0.41
1:A:427:ASP:N	1:A:427:ASP:OD1	2.53	0.41
1:C:877:THR:O	1:C:881:LEU:HD23	2.20	0.41
1:C:909:PHE:HA	1:C:912:ILE:HG12	2.01	0.41
1:B:122:ASN:N	1:B:125:ASN:O	2.49	0.41
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.56	0.41
1:C:85:PRO:O	1:C:241:PHE:HE1	2.03	0.41
1:B:706:ASN:ND2	1:C:790:GLN:OE1	2.51	0.41
1:C:919:LEU:HD12	1:C:926:ILE:HD13	2.02	0.41
3:G:61:PHE:HD1	3:G:74:ILE:HG12	1.86	0.41
2:H:104:ILE:HG13	2:H:104:ILE:O	2.20	0.41
1:A:391:CYS:HA	1:A:525:CYS:CB	2.51	0.41
1:A:736:LYS:HE3	1:A:774:ALA:HB1	2.02	0.41
1:B:142:ASP:HB3	1:B:159:VAL:HG21	2.03	0.41
1:B:454:ARG:HE	1:B:491:PRO:HB2	1.85	0.41
1:C:44:ARG:O	1:C:286:GLY:HA2	2.21	0.41
1:C:828:LYS:HD3	1:C:828:LYS:HA	1.86	0.41
1:B:599:SER:OG	1:B:616:GLN:NE2	2.50	0.41
1:A:62:VAL:HB	1:A:270:VAL:O	2.20	0.40
1:A:130:VAL:O	1:A:130:VAL:HG23	2.21	0.40
1:A:805:PHE:HD1	1:A:808:ILE:HD11	1.86	0.40
1:C:107:GLY:HA2	1:C:238:ILE:HG12	2.03	0.40
1:C:538:LYS:C	1:C:538:LYS:HD2	2.46	0.40
1:A:393:THR:O	1:A:523:THR:OG1	2.39	0.40
1:B:340:GLU:HG2	1:B:341:VAL:N	2.36	0.40
1:C:567:GLN:HG3	1:C:568:PHE:HD1	1.86	0.40
1:A:457:ARG:HE	1:A:459:SER:C	2.28	0.40
1:B:436:TRP:CE2	1:B:509:ARG:HB2	2.56	0.40
2:F:34:MET:HG2	2:F:74:ARG:NH2	2.33	0.40
1:B:426:PRO:HG2	1:B:429:PHE:HB2	2.03	0.40
1:A:67:VAL:HG21	1:A:266:ALA:HB3	2.04	0.40
1:A:647:GLN:HA	1:A:652:CYS:HA	2.02	0.40
1:B:336:CYS:SG	1:B:362:VAL:HG22	2.61	0.40
3:G:90:ARG:HD2	3:G:97:VAL:HA	2.04	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 PDB entries followed by that with respect to all EM entries.

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	998/1120 (89%)	958 (96%)	39 (4%)	1 (0%)	48	80
1	B	1000/1120 (89%)	970 (97%)	30 (3%)	0	100	100
1	C	1008/1120 (90%)	973 (96%)	35 (4%)	0	100	100
2	F	120/125 (96%)	112 (93%)	8 (7%)	0	100	100
2	H	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
3	G	106/108 (98%)	101 (95%)	4 (4%)	1 (1%)	14	48
3	J	106/108 (98%)	101 (95%)	4 (4%)	1 (1%)	14	48
All	All	3461/3826 (90%)	3328 (96%)	130 (4%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	GLU
3	G	98	ILE
3	J	98	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	816/974 (84%)	816 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	822/974 (84%)	822 (100%)	0	100	100
1	C	792/974 (81%)	791 (100%)	1 (0%)	88	93
2	F	95/100 (95%)	95 (100%)	0	100	100
2	H	95/100 (95%)	95 (100%)	0	100	100
3	G	88/88 (100%)	88 (100%)	0	100	100
3	J	88/88 (100%)	88 (100%)	0	100	100
All	All	2796/3298 (85%)	2795 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	ASN
1	A	487	ASN
1	A	547	ASN
1	A	706	ASN
1	A	916	GLN
1	A	931	ASN
1	A	1067	HIS
1	B	87	ASN
1	B	125	ASN
1	B	409	GLN
1	B	448	ASN
1	B	487	ASN
1	B	995	GLN
1	B	1074	GLN
1	B	1104	HIS
1	B	1109	GLN
1	C	121	ASN
1	C	207	HIS
1	C	567	GLN
1	C	706	ASN
1	C	777	GLN
1	C	1074	GLN
1	C	1109	GLN

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Mol	Chain	Res	Type
3	G	6	GLN
3	G	52	ASN
3	J	6	GLN
3	J	36	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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.26	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	E	1	4,1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	E	2	4	14,14,15	0.22	0	17,19,21	0.45	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

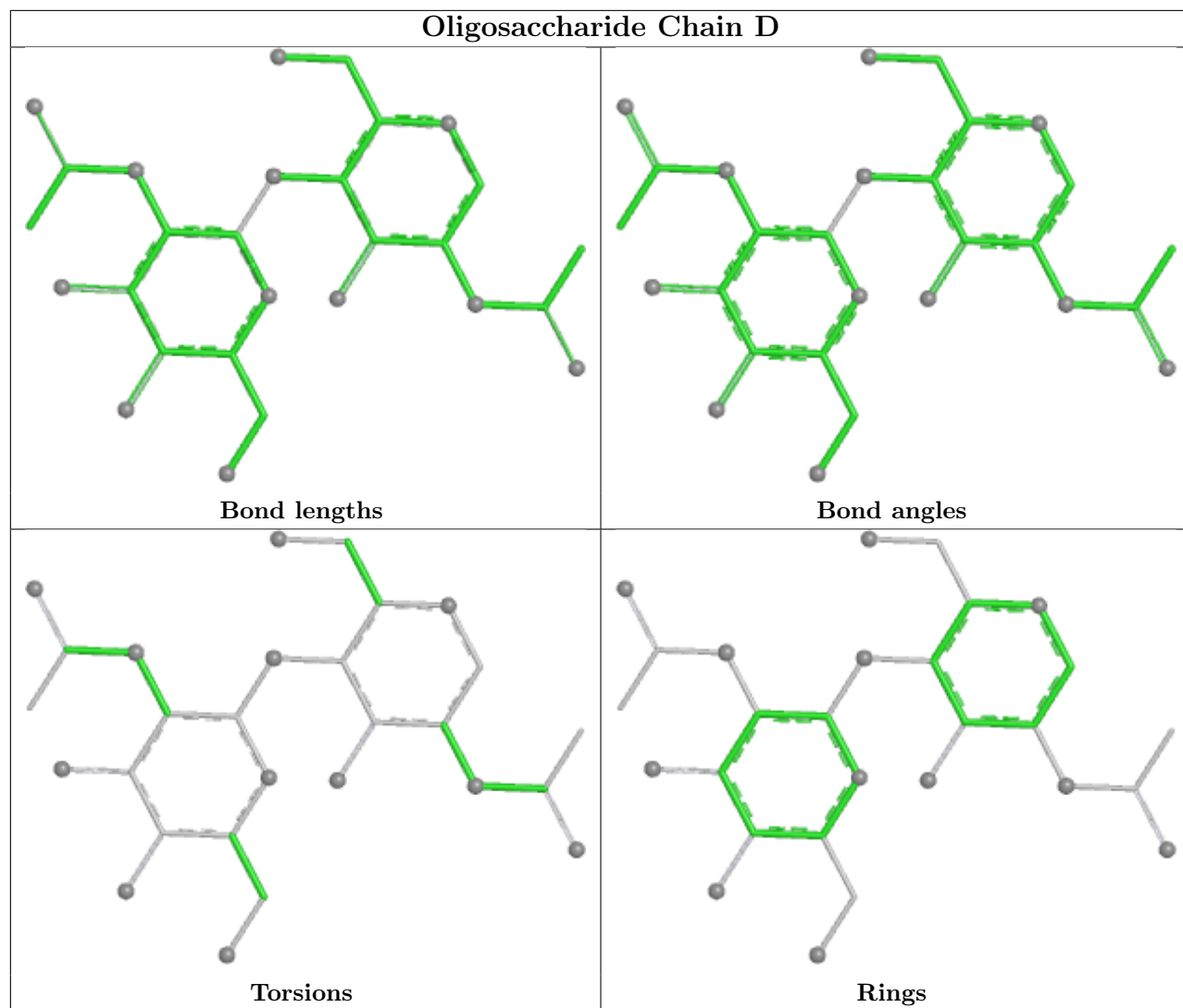
All (2) torsion outliers are listed below:

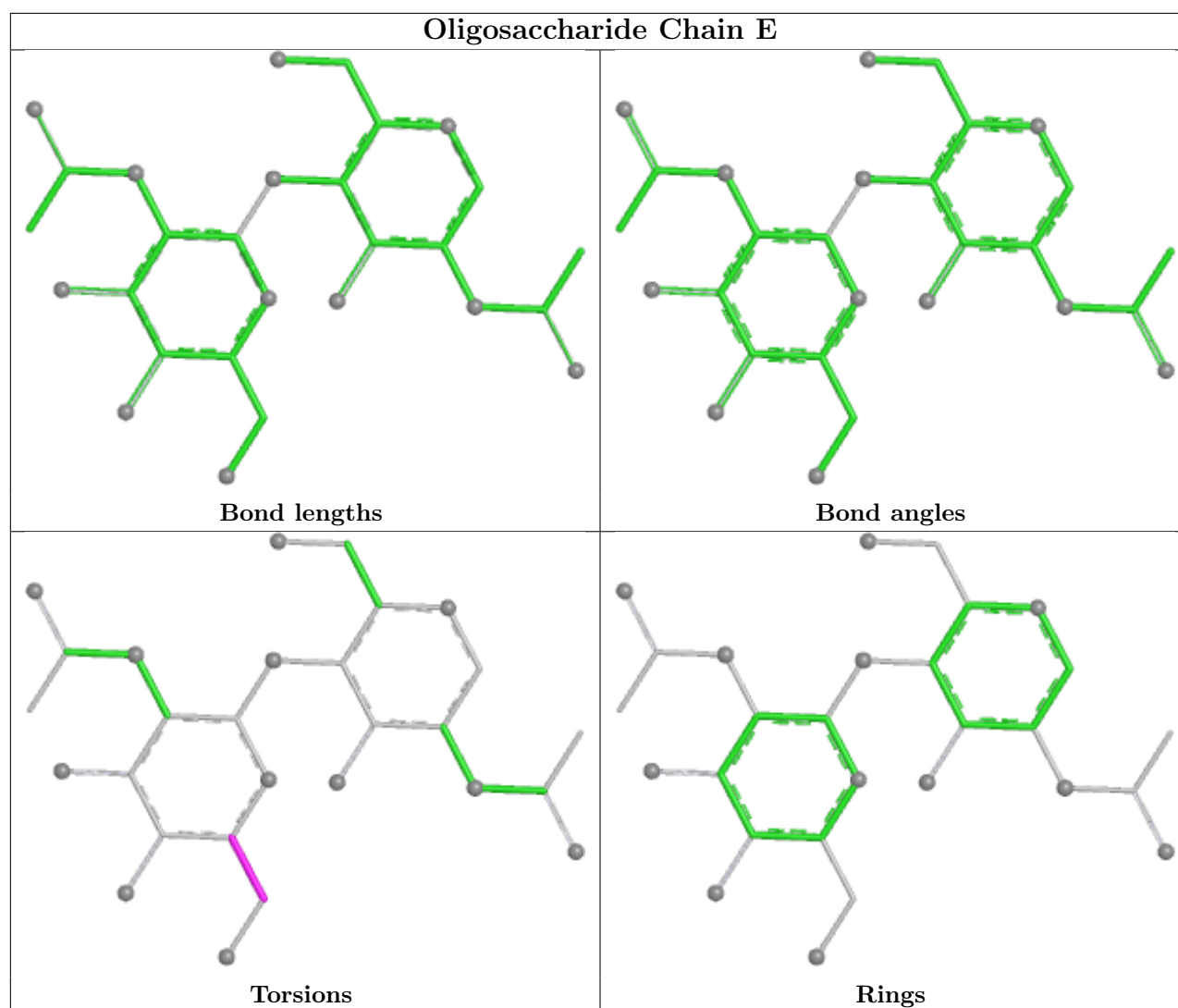
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	C	1301	1	14,14,15	0.47	0	17,19,21	0.46	0
5	NAG	A	1309	1	14,14,15	0.44	0	17,19,21	0.63	0
5	NAG	B	1311	1	14,14,15	0.29	0	17,19,21	0.55	0
5	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.60	0
5	NAG	B	1308	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	C	1304	1	14,14,15	0.30	0	17,19,21	0.45	0
5	NAG	B	1303	1	14,14,15	0.65	1 (7%)	17,19,21	0.72	1 (5%)
5	NAG	A	1311	1	14,14,15	0.60	0	17,19,21	0.88	1 (5%)
5	NAG	B	1309	1	14,14,15	0.19	0	17,19,21	0.38	0
5	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	C	1312	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.46	0
5	NAG	B	1304	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	A	1303	1	14,14,15	0.24	0	17,19,21	0.39	0
5	NAG	B	1306	1	14,14,15	0.24	0	17,19,21	0.51	0
5	NAG	A	1312	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	C	1308	1	14,14,15	0.36	0	17,19,21	0.52	0
5	NAG	C	1306	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	B	1302	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	B	1312	1	14,14,15	0.31	0	17,19,21	0.56	0
5	NAG	C	1310	1	14,14,15	0.27	0	17,19,21	0.51	0
5	NAG	C	1302	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.38	0
5	NAG	C	1311	1	14,14,15	0.23	0	17,19,21	0.53	0
5	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	C	1307	1	14,14,15	0.49	0	17,19,21	0.62	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	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1303	NAG	C1-C2	2.15	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1311	NAG	C1-O5-C5	2.95	116.14	112.19
5	B	1303	NAG	C1-O5-C5	2.50	115.54	112.19
5	C	1307	NAG	C1-O5-C5	2.08	114.98	112.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1309	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	A	1311	NAG	C4-C5-C6-O6
5	B	1312	NAG	O5-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	C	1311	NAG	C4-C5-C6-O6
5	B	1312	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1311	NAG	O5-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1311	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	A	1309	NAG	C3-C2-N2-C7
5	B	1311	NAG	C3-C2-N2-C7
5	B	1307	NAG	C4-C5-C6-O6
5	A	1309	NAG	C1-C2-N2-C7
5	B	1311	NAG	C1-C2-N2-C7
5	C	1308	NAG	C1-C2-N2-C7
5	C	1307	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1309	NAG	1	0
5	A	1309	NAG	1	0
5	B	1303	NAG	4	0
5	A	1311	NAG	1	0
5	B	1309	NAG	1	0
5	A	1303	NAG	1	0
5	B	1307	NAG	1	0
5	B	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	2
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	1:GLU	C	2:VAL	N	4.21
1	A	527:PRO	C	531:LYS	N	4.20
1	A	497:PHE	C	498:ARG	N	3.33
1	F	28:SER	C	29:PHE	N	3.27
1	B	497:PHE	C	498:ARG	N	3.17

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37240. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.