



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:27 PM UTC

PDB ID : 2AJF / pdb_00002ajf
Title : Structure of SARS coronavirus spike receptor-binding domain complexed with its receptor
Authors : Li, F.; Li, W.; Farzan, M.; Harrison, S.C.
Deposited on : 2005-08-01
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

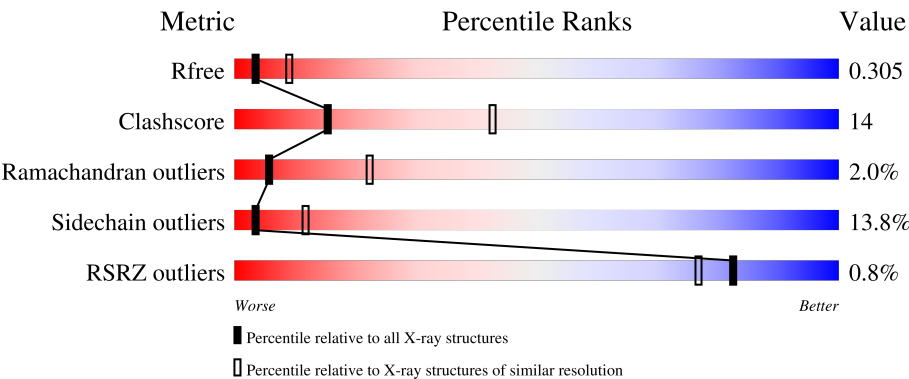
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	597	
1	B	597	
2	E	180	
2	F	180	
3	C	3	

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Mol	Chain	Length	Quality of chain
3	D	3	33% 33% 33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12777 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.

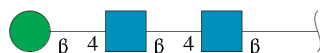
- Molecule 1 is a protein called Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			
1	B	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			

- Molecule 2 is a protein called SARS-coronavirus spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	174	Total	C	N	O	S	0	0	0
			1403	909	228	259	7			
2	F	174	Total	C	N	O	S	0	0	0
			1403	909	228	259	7			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

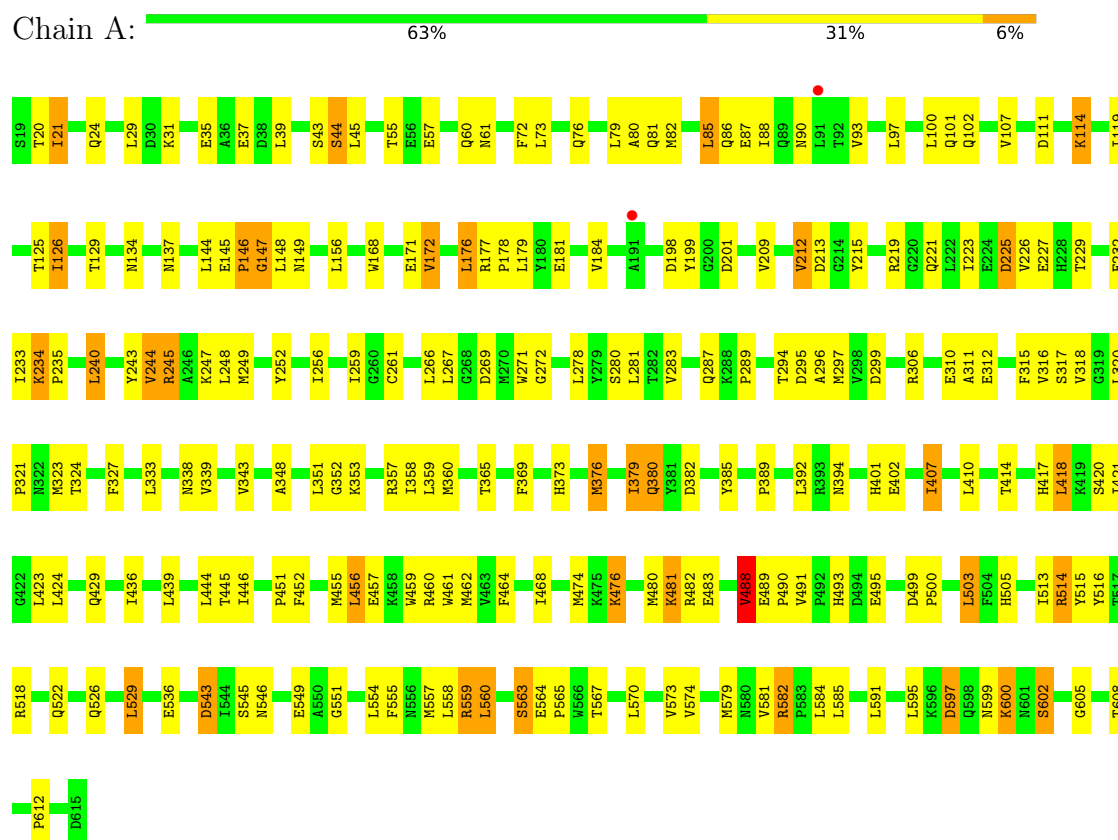
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	36	Total	O	0	0
			36	36		
7	B	24	Total	O	0	0
			24	24		
7	E	4	Total	O	0	0
			4	4		
7	F	1	Total	O	0	0
			1	1		

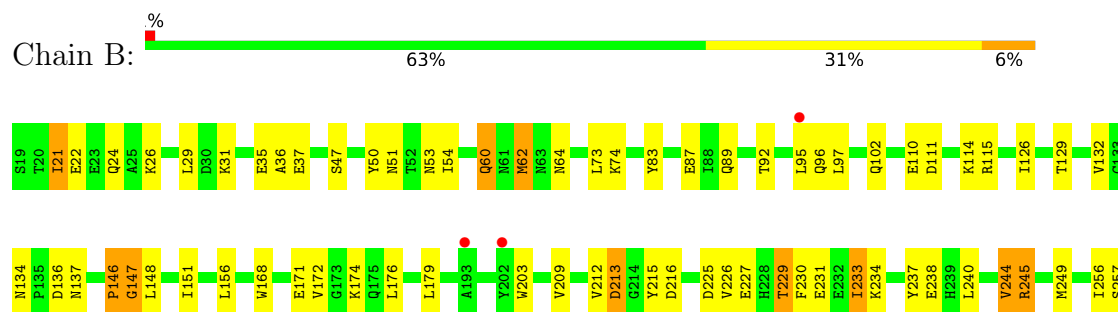
3 Residue-property plots

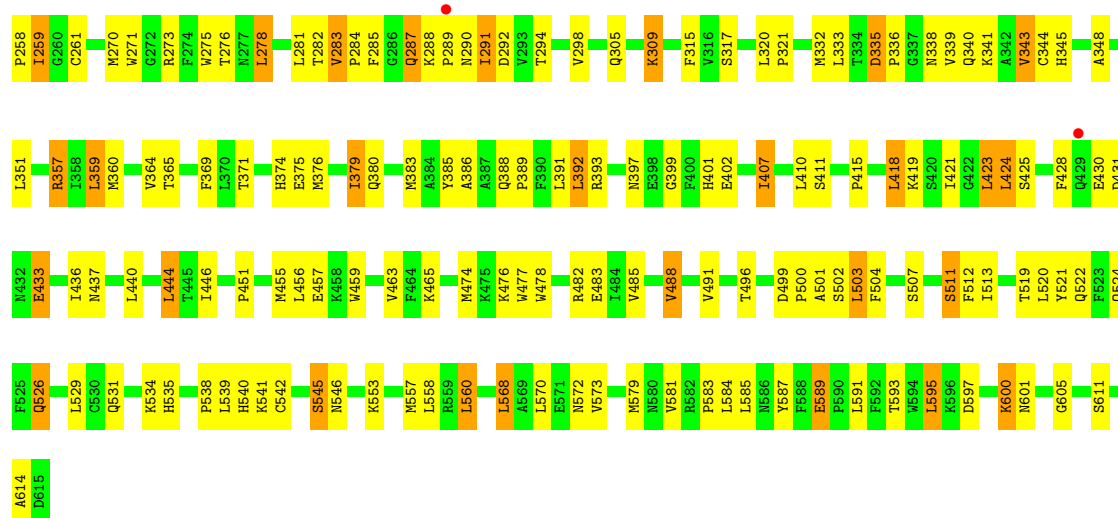
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2)

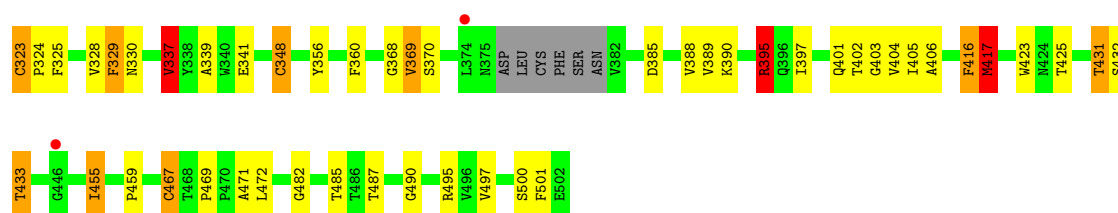


- Molecule 1: Angiotensin-converting enzyme-Related Carboxypeptidase (Ace2)

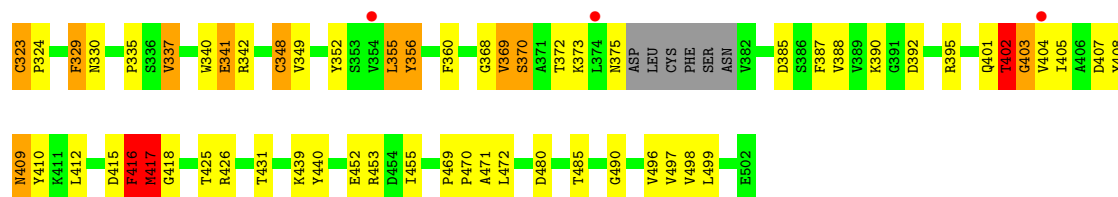




• Molecule 2: SARS-coronavirus spike protein



• Molecule 2: SARS-coronavirus spike protein



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.30Å 119.43Å 113.24Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	47.40 – 2.90 47.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.4 (47.40-2.90) 90.5 (47.40-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.218 , 0.275 (Not available) , 0.305	Depositor DCC
R_{free} test set	2449 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.57	0/5007	0.94	7/6803 (0.1%)
1	B	0.54	0/5007	0.89	6/6803 (0.1%)
2	E	0.56	0/1448	0.90	5/1972 (0.3%)
2	F	0.54	0/1448	0.89	4/1972 (0.2%)
All	All	0.55	0/12910	0.91	22/17550 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	LEU	N-CA-C	-8.96	97.22	110.48
1	B	425	SER	CA-C-N	7.17	127.50	119.32
1	B	425	SER	C-N-CA	7.17	127.50	119.32
1	A	240	LEU	N-CA-C	-7.11	103.46	111.07
2	E	417	MET	N-CA-C	6.98	118.79	108.60
1	B	369	PHE	N-CA-C	-6.17	104.19	111.03
2	F	417	MET	N-CA-C	6.08	118.31	109.07
2	E	360	PHE	N-CA-C	-5.92	106.22	113.50
1	A	536	GLU	N-CA-C	5.88	118.82	111.24
1	B	283	VAL	CA-C-N	5.66	124.86	118.97
1	B	283	VAL	C-N-CA	5.66	124.86	118.97
1	A	283	VAL	CA-C-N	5.45	124.90	119.24
1	A	283	VAL	C-N-CA	5.45	124.90	119.24
1	A	488	VAL	N-CA-C	5.30	115.60	108.17
2	F	330	ASN	N-CA-C	-5.23	106.14	112.88
1	A	488	VAL	CB-CA-C	-5.20	103.08	110.83
2	E	501	PHE	N-CA-C	5.17	117.14	107.99
2	E	337	VAL	CB-CA-C	-5.16	105.36	111.97
1	A	352	GLY	N-CA-C	-5.13	107.07	111.95
2	F	360	PHE	N-CA-C	-5.13	107.19	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	403	GLY	N-CA-C	5.08	118.55	111.19
2	E	455	ILE	N-CA-C	-5.05	107.37	112.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4870	0	4639	137	0
1	B	4870	0	4641	138	0
2	E	1403	0	1326	27	0
2	F	1403	0	1325	34	0
3	C	39	0	34	0	0
3	D	39	0	34	1	0
4	A	42	0	39	2	0
4	B	14	0	13	0	0
4	E	14	0	13	0	0
4	F	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
7	A	36	0	0	3	0
7	B	24	0	0	3	0
7	E	4	0	0	0	0
7	F	1	0	0	0	0
All	All	12777	0	12077	335	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 14.

All (335) 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:320:LEU:HD13	1:A:380:GLN:HG2	1.36	1.05
1:A:261:CYS:HB2	1:A:488:VAL:CG2	1.93	0.97
1:B:245:ARG:HG2	1:B:245:ARG:HH21	1.32	0.94
1:A:261:CYS:HB2	1:A:488:VAL:HG22	1.48	0.94
2:F:335:PRO:HG3	2:F:341:GLU:HG2	1.49	0.93
1:B:589:GLU:OE1	1:B:589:GLU:HA	1.69	0.91
1:B:407:ILE:HD11	1:B:522:GLN:O	1.71	0.91
1:B:371:THR:OG1	7:B:801:HOH:O	1.88	0.89
1:A:348:ALA:HB1	1:A:379:ILE:HD12	1.53	0.89
2:E:329:PHE:HD1	2:E:329:PHE:H	1.20	0.87
1:A:348:ALA:HB1	1:A:379:ILE:CD1	2.06	0.85
1:B:411:SER:OG	7:B:802:HOH:O	1.94	0.84
2:F:469:PRO:HA	2:F:471:ALA:H	1.41	0.84
1:B:261:CYS:HB2	1:B:488:VAL:HG22	1.62	0.82
1:B:21:ILE:HA	1:B:24:GLN:HE21	1.45	0.80
1:A:229:THR:HG23	1:A:516:TYR:OH	1.84	0.78
2:E:329:PHE:HB3	2:E:497:VAL:HG21	1.63	0.78
2:F:417:MET:HA	2:F:417:MET:HE2	1.66	0.78
1:B:320:LEU:HD13	1:B:380:GLN:HG2	1.68	0.75
1:B:380:GLN:HA	1:B:383:MET:HE3	1.69	0.74
1:A:493:HIS:HD2	1:A:499:ASP:OD1	1.73	0.72
1:A:310:GLU:HG2	1:A:421:ILE:HD11	1.72	0.72
1:B:457:GLU:HG2	1:B:512:PHE:HB3	1.72	0.71
1:B:209:VAL:HG23	1:B:216:ASP:HA	1.73	0.70
1:B:24:GLN:HG3	1:B:83:TYR:HE2	1.57	0.70
1:B:294:THR:O	1:B:298:VAL:HG23	1.94	0.68
1:B:520:LEU:HD22	1:B:579:MET:HE3	1.75	0.68
1:B:47:SER:HA	1:B:62:MET:HG2	1.73	0.68
1:A:320:LEU:CD1	1:A:380:GLN:HG2	2.20	0.67
1:B:132:VAL:HG12	1:B:171:GLU:HG3	1.75	0.67
1:B:111:ASP:O	1:B:115:ARG:HB3	1.93	0.67
1:B:315:PHE:HB2	7:B:805:HOH:O	1.93	0.67
1:A:529:LEU:HD21	1:A:554:LEU:HD13	1.77	0.67
1:A:126:ILE:HD11	1:A:176:LEU:HD22	1.77	0.66
1:B:168:TRP:O	1:B:172:VAL:HG22	1.94	0.66
1:B:240:LEU:O	1:B:244:VAL:HG13	1.95	0.66
1:A:248:LEU:HD21	1:A:278:LEU:HD23	1.77	0.66
1:B:440:LEU:HD13	1:B:444:LEU:CD2	2.25	0.66
1:B:379:ILE:HG22	1:B:383:MET:HE2	1.77	0.65
1:B:524:GLN:HE22	1:B:579:MET:HA	1.61	0.65
1:B:245:ARG:HH21	1:B:245:ARG:CG	2.08	0.65
1:A:597:ASP:O	1:A:600:LYS:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:HB3	1:A:518:ARG:HD2	1.77	0.65
2:F:323:CYS:N	2:F:348:CYS:SG	2.70	0.65
1:A:261:CYS:HB2	1:A:488:VAL:HG23	1.79	0.64
1:B:126:ILE:HA	1:B:129:THR:HG22	1.80	0.64
1:A:229:THR:OG1	1:A:581:VAL:HB	1.98	0.63
1:B:419:LYS:HD2	1:B:428:PHE:HB3	1.80	0.63
1:A:225:ASP:O	1:A:229:THR:HG22	1.99	0.63
1:A:320:LEU:HD13	1:A:380:GLN:CG	2.23	0.62
1:B:526:GLN:HE21	1:B:526:GLN:HA	1.64	0.62
1:A:248:LEU:HD21	1:A:278:LEU:CD2	2.28	0.62
2:F:403:GLY:HA2	2:F:407:ASP:CG	2.24	0.61
1:B:553:LYS:HE3	1:B:573:VAL:O	2.00	0.61
2:E:329:PHE:HD1	2:E:329:PHE:N	1.96	0.61
1:A:462:MET:HE3	1:A:468:ILE:HD11	1.82	0.61
2:E:395:ARG:HH11	2:E:395:ARG:HB2	1.65	0.61
1:A:72:PHE:O	1:A:76:GLN:HG2	2.01	0.60
1:A:455:MET:HE2	1:A:481:LYS:HG2	1.82	0.60
1:B:379:ILE:CG2	1:B:383:MET:HE2	2.31	0.60
1:B:499:ASP:N	1:B:500:PRO:HD2	2.17	0.60
1:A:296:ALA:HA	1:A:299:ASP:HB2	1.85	0.59
1:B:351:LEU:HD11	1:B:357:ARG:HD3	1.84	0.59
1:B:360:MET:HE1	1:B:371:THR:HB	1.84	0.59
1:A:269:ASP:OD2	1:A:272:GLY:N	2.31	0.59
1:B:338:ASN:C	1:B:340:GLN:H	2.09	0.59
2:E:323:CYS:N	2:E:348:CYS:SG	2.76	0.59
1:B:294:THR:HG23	1:B:365:THR:HA	1.84	0.58
2:F:469:PRO:HA	2:F:471:ALA:N	2.15	0.58
1:A:223:ILE:O	1:A:227:GLU:HG3	2.03	0.58
1:B:21:ILE:HA	1:B:24:GLN:NE2	2.18	0.58
1:B:51:ASN:HD22	1:B:343:VAL:HG11	1.68	0.58
1:A:233:ILE:HD11	1:A:584:LEU:HD23	1.86	0.57
2:E:325:PHE:HB3	2:E:329:PHE:HE1	1.70	0.56
2:F:323:CYS:HB2	2:F:324:PRO:HD3	1.87	0.56
1:B:134:ASN:HB3	1:B:137:ASN:HB3	1.87	0.56
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.87	0.56
1:B:176:LEU:HA	1:B:179:LEU:HD12	1.87	0.56
1:B:290:ASN:OD1	1:B:292:ASP:HB3	2.06	0.56
1:A:245:ARG:NH2	7:A:803:HOH:O	2.40	0.55
1:A:418:LEU:HB3	1:A:424:LEU:HB2	1.88	0.55
1:B:288:LYS:HB3	1:B:289:PRO:HD2	1.88	0.55
1:B:540:HIS:HA	1:B:587:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:TYR:O	1:B:522:GLN:C	2.49	0.55
2:F:418:GLY:HA3	2:F:499:LEU:O	2.07	0.55
1:B:433:GLU:O	1:B:437:ASN:OD1	2.24	0.54
1:A:146:PRO:O	1:A:148:LEU:N	2.40	0.54
1:B:348:ALA:HB1	1:B:379:ILE:HD13	1.90	0.54
1:A:144:LEU:HA	1:A:148:LEU:HB3	1.90	0.54
1:B:459:TRP:O	1:B:463:VAL:HG23	2.08	0.54
1:A:267:LEU:HD13	7:A:804:HOH:O	2.08	0.54
1:A:181:GLU:O	1:A:184:VAL:HG22	2.08	0.54
1:A:499:ASP:N	1:A:500:PRO:HD2	2.23	0.53
1:B:557:MET:HA	1:B:560:LEU:HD22	1.89	0.53
1:B:597:ASP:O	1:B:600:LYS:HD2	2.08	0.53
1:A:134:ASN:HB3	1:A:137:ASN:H	1.73	0.53
1:A:489:GLU:O	1:A:489:GLU:HG2	2.08	0.53
1:B:386:ALA:HA	1:B:393:ARG:HD3	1.91	0.53
1:A:455:MET:CE	1:A:481:LYS:HG2	2.39	0.53
1:A:407:ILE:HD13	1:A:407:ILE:N	2.22	0.53
1:B:520:LEU:HD22	1:B:579:MET:CE	2.39	0.53
1:B:389:PRO:HG2	1:B:392:LEU:HB2	1.91	0.53
1:B:611:SER:HB2	1:B:614:ALA:HB3	1.89	0.53
1:A:457:GLU:HA	1:A:457:GLU:OE1	2.08	0.53
1:A:245:ARG:NH1	1:A:605:GLY:O	2.42	0.52
1:A:490:PRO:HA	1:A:612:PRO:HG2	1.92	0.52
1:B:315:PHE:CE2	1:B:376:MET:HG2	2.44	0.52
1:A:420:SER:HB2	4:A:703:NAG:H61	1.91	0.52
2:F:455:ILE:HG22	2:F:455:ILE:O	2.10	0.52
1:B:146:PRO:O	1:B:148:LEU:N	2.43	0.52
1:B:538:PRO:HB2	1:B:540:HIS:CE1	2.45	0.52
2:E:417:MET:HE2	2:E:417:MET:HA	1.92	0.51
2:F:385:ASP:HB2	2:F:498:VAL:HB	1.92	0.51
2:E:425:THR:HG21	2:E:495:ARG:HD2	1.92	0.51
2:E:403:GLY:O	2:E:405:ILE:N	2.43	0.51
1:B:407:ILE:HG23	1:B:526:GLN:NE2	2.25	0.51
1:B:440:LEU:HD13	1:B:444:LEU:HD22	1.93	0.50
1:A:297:MET:HE1	1:A:369:PHE:HB2	1.94	0.50
1:A:85:LEU:HB3	1:A:101:GLN:HE22	1.77	0.50
1:A:379:ILE:O	1:A:382:ASP:HB2	2.12	0.50
1:A:573:VAL:HG23	1:A:574:VAL:HG13	1.92	0.50
1:B:51:ASN:ND2	1:B:343:VAL:HG11	2.26	0.50
2:F:403:GLY:O	2:F:405:ILE:N	2.45	0.50
1:A:560:LEU:O	1:A:563:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LEU:C	1:A:456:LEU:HD13	2.36	0.50
1:A:201:ASP:O	1:A:219:ARG:HD2	2.12	0.50
1:A:229:THR:HG23	1:A:516:TYR:HH	1.74	0.50
1:A:414:THR:O	1:A:418:LEU:HD22	2.12	0.50
2:E:337:VAL:HG22	2:E:389:VAL:HG12	1.93	0.50
1:A:21:ILE:HA	1:A:24:GLN:HE21	1.77	0.49
1:B:407:ILE:HG23	1:B:526:GLN:HE22	1.76	0.49
2:F:402:THR:HG23	3:D:3:BMA:H4	1.94	0.49
1:B:21:ILE:HA	1:B:24:GLN:HG2	1.93	0.49
1:A:233:ILE:HD11	1:A:584:LEU:CD2	2.42	0.49
1:A:474:MET:HE1	1:A:499:ASP:H	1.77	0.49
1:B:261:CYS:CB	1:B:488:VAL:HG22	2.40	0.49
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.94	0.49
1:A:402:GLU:OE2	1:A:402:GLU:HA	2.12	0.49
1:A:526:GLN:HE21	1:A:526:GLN:HA	1.77	0.49
1:A:505:HIS:CD2	1:A:505:HIS:H	2.31	0.49
1:B:36:ALA:O	1:B:37:GLU:C	2.55	0.49
1:B:348:ALA:HB1	1:B:379:ILE:CD1	2.43	0.49
2:E:329:PHE:N	2:E:329:PHE:CD1	2.68	0.49
1:B:225:ASP:O	1:B:229:THR:HB	2.13	0.49
1:B:31:LYS:HE3	1:B:35:GLU:OE1	2.13	0.48
2:E:337:VAL:CG2	2:E:389:VAL:HG12	2.43	0.48
1:A:229:THR:HG21	1:A:579:MET:HE3	1.95	0.48
1:B:203:TRP:CZ3	1:B:511:SER:HA	2.49	0.48
1:B:320:LEU:HD13	1:B:380:GLN:CG	2.39	0.48
1:A:338:ASN:HD22	1:A:339:VAL:HG23	1.77	0.48
1:B:388:GLN:HE21	1:B:388:GLN:HA	1.77	0.48
2:E:459:PRO:HB2	2:E:467:CYS:HB3	1.96	0.48
2:F:342:ARG:HG3	2:F:385:ASP:OD1	2.14	0.48
2:F:323:CYS:HB2	2:F:324:PRO:CD	2.44	0.48
2:F:349:VAL:HA	2:F:375:ASN:C	2.38	0.48
1:B:332:MET:HE2	1:B:336:PRO:HG3	1.96	0.48
1:B:320:LEU:HB3	1:B:321:PRO:HD2	1.95	0.48
1:A:80:ALA:C	1:A:82:MET:H	2.22	0.47
2:F:329:PHE:HZ	2:F:355:LEU:HD23	1.79	0.47
2:F:409:ASN:OD1	2:F:440:TYR:HB2	2.14	0.47
1:A:351:LEU:HD12	1:A:351:LEU:N	2.28	0.47
1:A:323:MET:HE3	1:A:376:MET:SD	2.54	0.47
1:A:351:LEU:HD11	1:A:357:ARG:HG2	1.96	0.47
1:A:55:THR:HG22	1:A:57:GLU:H	1.79	0.47
1:B:520:LEU:HD21	1:B:581:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:341:GLU:O	2:E:385:ASP:HA	2.15	0.47
2:E:395:ARG:HH11	2:E:395:ARG:CB	2.27	0.47
2:F:329:PHE:HB3	2:F:497:VAL:HG21	1.96	0.47
1:A:599:ASN:HA	1:A:602:SER:HB2	1.97	0.47
1:B:375:GLU:OE1	1:B:375:GLU:HA	2.13	0.47
1:B:231:GLU:OE1	1:B:234:LYS:HE2	2.15	0.47
1:A:245:ARG:HG2	7:A:803:HOH:O	2.13	0.47
1:B:305:GLN:O	1:B:309:LYS:HB2	2.14	0.47
1:B:440:LEU:O	1:B:444:LEU:HD22	2.15	0.47
1:B:245:ARG:HG2	1:B:245:ARG:NH2	2.13	0.47
2:F:356:TYR:OH	2:F:370:SER:O	2.33	0.46
1:A:324:THR:O	1:A:327:PHE:HB3	2.16	0.46
1:B:397:ASN:C	1:B:399:GLY:H	2.22	0.46
1:B:415:PRO:O	1:B:419:LYS:HB2	2.15	0.46
1:A:244:VAL:O	1:A:245:ARG:C	2.57	0.46
2:F:390:LYS:HG2	2:F:490:GLY:O	2.15	0.46
1:B:50:TYR:HE1	1:B:54:ILE:HG23	1.81	0.46
1:A:389:PRO:HG2	1:A:392:LEU:HD22	1.98	0.46
1:B:47:SER:HA	1:B:62:MET:CG	2.41	0.46
1:B:501:ALA:O	1:B:507:SER:HB3	2.16	0.46
1:A:199:TYR:HB3	1:A:464:PHE:CD1	2.51	0.45
1:A:457:GLU:HG3	1:A:513:ILE:HB	1.98	0.45
1:B:237:TYR:CE2	1:B:451:PRO:HG2	2.52	0.45
2:E:390:LYS:HG2	2:E:490:GLY:O	2.16	0.45
1:A:212:VAL:O	1:A:213:ASP:C	2.60	0.45
1:A:407:ILE:HD11	1:A:522:GLN:O	2.15	0.45
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.76	0.45
1:B:53:ASN:HD22	1:B:340:GLN:HG3	1.81	0.45
1:B:245:ARG:NH1	1:B:605:GLY:O	2.49	0.45
1:A:85:LEU:C	1:A:87:GLU:H	2.25	0.45
1:A:597:ASP:HA	1:A:600:LYS:NZ	2.30	0.45
1:B:359:LEU:HD13	1:B:359:LEU:C	2.42	0.45
2:F:392:ASP:O	2:F:395:ARG:HD3	2.17	0.45
1:B:60:GLN:O	1:B:64:ASN:HB2	2.16	0.45
1:A:168:TRP:O	1:A:172:VAL:HG22	2.17	0.45
1:A:252:TYR:CD2	1:A:266:LEU:HD13	2.51	0.45
1:A:111:ASP:HA	1:A:114:LYS:HB2	1.97	0.44
1:B:257:SER:OG	1:B:259:ILE:HD13	2.17	0.44
1:B:275:TRP:O	1:B:278:LEU:HB2	2.17	0.44
1:B:336:PRO:HB2	1:B:340:GLN:HB3	1.99	0.44
2:E:324:PRO:HD3	2:E:348:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:ASP:O	2:E:497:VAL:HA	2.17	0.44
1:B:233:ILE:HD11	1:B:584:LEU:HD22	2.00	0.44
2:E:455:ILE:O	2:E:455:ILE:CG2	2.65	0.44
2:F:452:GLU:HG2	2:F:453:ARG:H	1.81	0.44
1:A:215:TYR:HB3	1:A:567:THR:OG1	2.17	0.44
1:A:417:HIS:CE1	1:A:545:SER:OG	2.71	0.44
1:B:374:HIS:CD2	1:B:374:HIS:C	2.95	0.44
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.90	0.44
1:A:315:PHE:C	1:A:317:SER:N	2.72	0.44
1:A:461:TRP:CH2	1:A:513:ILE:HD12	2.53	0.44
1:A:499:ASP:HB3	6:A:705:CL:CL	2.54	0.44
1:B:526:GLN:HA	1:B:526:GLN:NE2	2.32	0.44
2:E:469:PRO:HA	2:E:471:ALA:N	2.32	0.44
1:B:430:GLU:O	1:B:431:ASP:C	2.61	0.44
2:E:339:ALA:HA	2:E:455:ILE:HD11	2.00	0.44
1:A:353:LYS:HD2	2:E:487:THR:HG21	2.00	0.44
1:A:514:ARG:HG2	1:A:515:TYR:N	2.33	0.44
2:F:408:TYR:C	2:F:409:ASN:HD22	2.25	0.44
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.83	0.44
1:A:199:TYR:HD2	1:A:464:PHE:CE1	2.35	0.44
1:B:374:HIS:NE2	1:B:402:GLU:OE1	2.46	0.44
1:A:21:ILE:HD11	1:A:87:GLU:O	2.18	0.43
2:F:415:ASP:O	2:F:416:PHE:C	2.61	0.43
1:A:555:PHE:O	1:A:559:ARG:HG2	2.18	0.43
1:B:168:TRP:CD1	1:B:502:SER:OG	2.71	0.43
1:B:456:LEU:HD23	1:B:512:PHE:CE1	2.53	0.43
2:F:352:TYR:HD1	2:F:372:THR:HG23	1.83	0.43
1:A:543:ASP:OD1	1:A:543:ASP:C	2.61	0.43
1:B:410:LEU:HD22	1:B:522:GLN:HE21	1.83	0.43
1:A:177:ARG:NH1	1:A:495:GLU:HB3	2.34	0.43
1:B:289:PRO:O	1:B:290:ASN:C	2.60	0.43
1:B:539:LEU:HD23	1:B:587:TYR:HB2	2.01	0.43
1:B:600:LYS:HG2	1:B:601:ASN:ND2	2.33	0.43
2:F:410:TYR:HE2	2:F:412:LEU:HD13	1.83	0.43
1:B:344:CYS:O	1:B:345:HIS:C	2.60	0.43
1:A:327:PHE:HE2	1:A:358:ILE:HG13	1.82	0.43
1:A:474:MET:CE	1:A:499:ASP:H	2.31	0.43
1:B:249:MET:HG2	1:B:256:ILE:HB	1.99	0.43
1:B:568:LEU:HD22	1:B:572:ASN:HD21	1.84	0.43
1:A:243:TYR:CZ	1:A:247:LYS:HE3	2.54	0.43
2:E:324:PRO:O	2:E:328:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:HA	1:A:24:GLN:NE2	2.34	0.43
1:A:146:PRO:HB2	1:A:147:GLY:H	1.63	0.43
1:B:213:ASP:C	1:B:215:TYR:H	2.26	0.43
1:B:513:ILE:HD12	1:B:513:ILE:HA	1.92	0.43
2:E:431:THR:C	2:E:433:THR:N	2.75	0.43
1:A:226:VAL:HG21	1:A:513:ILE:HD11	2.01	0.43
1:B:457:GLU:CG	1:B:512:PHE:HB3	2.44	0.43
1:A:97:LEU:O	1:A:101:GLN:HG2	2.18	0.43
1:B:291:ILE:O	1:B:291:ILE:CG2	2.67	0.43
1:A:31:LYS:NZ	1:A:76:GLN:OE1	2.51	0.42
1:A:318:VAL:O	1:A:551:GLY:HA3	2.19	0.42
1:A:482:ARG:HD3	1:A:608:THR:O	2.19	0.42
1:A:591:LEU:HG	1:A:595:LEU:HD13	2.01	0.42
2:E:403:GLY:O	2:E:406:ALA:N	2.51	0.42
2:F:329:PHE:CD1	2:F:329:PHE:N	2.87	0.42
1:A:126:ILE:HD11	1:A:176:LEU:CD2	2.47	0.42
1:A:555:PHE:HA	1:A:558:LEU:HB2	2.01	0.42
1:A:564:GLU:HB3	1:A:565:PRO:CD	2.49	0.42
1:B:335:ASP:HA	1:B:336:PRO:HD3	1.89	0.42
1:B:359:LEU:C	1:B:359:LEU:CD1	2.92	0.42
1:A:516:TYR:CD2	1:A:516:TYR:C	2.97	0.42
1:A:80:ALA:C	1:A:82:MET:N	2.75	0.42
2:F:410:TYR:CE2	2:F:412:LEU:HD13	2.55	0.42
1:B:270:MET:HB3	1:B:271:TRP:CE3	2.55	0.42
1:A:35:GLU:OE1	1:A:72:PHE:HE1	2.03	0.42
1:A:245:ARG:HG2	1:A:245:ARG:HH21	1.83	0.42
1:B:285:PHE:C	1:B:287:GLN:H	2.28	0.42
1:B:388:GLN:HB3	1:B:389:PRO:HD2	2.02	0.42
2:F:337:VAL:HA	2:F:387:PHE:HB2	2.02	0.42
2:F:340:TRP:CD1	2:F:340:TRP:H	2.37	0.42
1:A:407:ILE:N	1:A:407:ILE:CD1	2.78	0.42
1:B:230:PHE:O	1:B:231:GLU:C	2.61	0.42
1:A:296:ALA:HA	1:A:299:ASP:CB	2.48	0.42
1:A:321:PRO:HD2	1:A:380:GLN:OE1	2.19	0.42
1:A:327:PHE:CE2	1:A:358:ILE:HG13	2.55	0.42
1:B:557:MET:HG2	1:B:573:VAL:HG21	2.02	0.42
1:A:459:TRP:N	1:A:480:MET:HE1	2.35	0.42
1:B:111:ASP:O	1:B:115:ARG:CB	2.65	0.42
1:A:43:SER:O	1:A:44:SER:C	2.63	0.41
1:A:311:ALA:HA	1:A:373:HIS:NE2	2.34	0.41
1:B:96:GLN:HG2	1:B:392:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HD12	1:A:407:ILE:HA	1.57	0.41
1:B:418:LEU:O	1:B:423:LEU:O	2.38	0.41
1:B:591:LEU:HG	1:B:595:LEU:HD22	2.02	0.41
1:A:119:ILE:HG23	1:A:179:LEU:HB3	2.02	0.41
1:A:232:GLU:HB2	1:A:581:VAL:HG11	2.01	0.41
1:A:312:GLU:N	1:A:376:MET:HE1	2.35	0.41
1:B:257:SER:HA	1:B:258:PRO:HD3	1.87	0.41
1:B:281:LEU:HD12	1:B:282:THR:HG23	2.01	0.41
1:B:47:SER:HB2	1:B:62:MET:HE3	2.02	0.41
2:F:395:ARG:HH11	2:F:395:ARG:HB2	1.86	0.41
1:B:455:MET:HE1	1:B:477:TRP:CE3	2.56	0.41
2:F:439:LYS:HG2	2:F:480:ASP:OD1	2.20	0.41
1:B:146:PRO:HB2	1:B:147:GLY:H	1.67	0.41
2:F:387:PHE:CE1	2:F:496:VAL:HB	2.56	0.41
1:A:134:ASN:HB2	1:A:137:ASN:O	2.21	0.41
1:A:145:GLU:HA	1:A:146:PRO:HA	1.81	0.41
1:A:233:ILE:O	1:A:234:LYS:C	2.64	0.41
1:A:306:ARG:O	1:A:310:GLU:HB2	2.20	0.41
1:A:315:PHE:C	1:A:317:SER:H	2.28	0.41
1:A:451:PRO:O	1:A:452:PHE:C	2.63	0.41
1:A:456:LEU:C	1:A:456:LEU:CD1	2.94	0.41
1:A:468:ILE:HD12	1:A:476:LYS:HG3	2.02	0.41
1:A:582:ARG:HE	1:A:582:ARG:HB2	1.45	0.41
1:B:51:ASN:HD22	1:B:343:VAL:CG1	2.32	0.41
1:B:499:ASP:N	1:B:500:PRO:CD	2.84	0.41
1:B:545:SER:O	1:B:546:ASN:HB2	2.20	0.41
2:E:431:THR:O	2:E:432:SER:C	2.64	0.41
2:F:409:ASN:HD22	2:F:409:ASN:N	2.19	0.41
1:A:234:LYS:O	1:A:235:PRO:C	2.63	0.41
1:A:249:MET:HG2	1:A:256:ILE:HB	2.03	0.41
1:B:174:LYS:HA	1:B:496:THR:O	2.20	0.41
1:B:421:ILE:HD13	1:B:421:ILE:HA	1.90	0.41
1:B:474:MET:HE1	1:B:499:ASP:CG	2.46	0.41
1:A:271:TRP:CD2	1:A:503:LEU:HD23	2.56	0.40
1:B:53:ASN:ND2	1:B:340:GLN:HE21	2.19	0.40
1:B:478:TRP:O	1:B:482:ARG:HG3	2.21	0.40
1:B:534:LYS:HA	1:B:534:LYS:HD3	1.96	0.40
1:B:535:HIS:CE1	1:B:542:CYS:HA	2.56	0.40
1:A:420:SER:HB2	4:A:703:NAG:C6	2.51	0.40
1:B:22:GLU:HG2	1:B:26:LYS:HE3	2.03	0.40
1:B:226:VAL:O	1:B:229:THR:HG22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HA	1:B:284:PRO:HD3	1.90	0.40
1:B:503:LEU:HD23	1:B:504:PHE:H	1.86	0.40
1:A:178:PRO:O	1:A:181:GLU:HB2	2.21	0.40
1:A:156:LEU:HD21	1:A:281:LEU:HD11	2.02	0.40
1:A:261:CYS:CB	1:A:488:VAL:HG22	2.36	0.40
2:E:397:ILE:N	2:E:397:ILE:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	595/597 (100%)	536 (90%)	55 (9%)	4 (1%)	18	48
1	B	595/597 (100%)	529 (89%)	56 (9%)	10 (2%)	7	26
2	E	170/180 (94%)	137 (81%)	24 (14%)	9 (5%)	1	5
2	F	170/180 (94%)	143 (84%)	19 (11%)	8 (5%)	2	7
All	All	1530/1554 (98%)	1345 (88%)	154 (10%)	31 (2%)	6	22

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
1	B	146	PRO
2	E	402	THR
2	E	404	VAL
2	E	416	PHE
1	A	147	GLY
1	B	87	GLU
1	B	110	GLU
1	B	147	GLY

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Mol	Chain	Res	Type
1	B	339	VAL
1	B	519	THR
2	F	370	SER
2	F	402	THR
2	F	404	VAL
1	B	407	ILE
1	B	424	LEU
2	E	395	ARG
2	F	416	PHE
1	B	213	ASP
1	A	86	GLN
2	E	368	GLY
2	E	369	VAL
2	E	370	SER
2	F	369	VAL
2	F	401	GLN
2	E	401	GLN
2	F	368	GLY
1	A	289	PRO
2	E	482	GLY
1	B	364	VAL
2	F	470	PRO

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	527/527 (100%)	445 (84%)	82 (16%)	2	9
1	B	527/527 (100%)	458 (87%)	69 (13%)	4	13
2	E	152/158 (96%)	134 (88%)	18 (12%)	5	17
2	F	152/158 (96%)	133 (88%)	19 (12%)	4	15
All	All	1358/1370 (99%)	1170 (86%)	188 (14%)	3	12

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	21	ILE
1	A	29	LEU
1	A	37	GLU
1	A	39	LEU
1	A	44	SER
1	A	45	LEU
1	A	60	GLN
1	A	61	ASN
1	A	73	LEU
1	A	79	LEU
1	A	81	GLN
1	A	85	LEU
1	A	88	ILE
1	A	102	GLN
1	A	107	VAL
1	A	114	LYS
1	A	125	THR
1	A	126	ILE
1	A	129	THR
1	A	149	ASN
1	A	171	GLU
1	A	172	VAL
1	A	176	LEU
1	A	198	ASP
1	A	209	VAL
1	A	212	VAL
1	A	221	GLN
1	A	225	ASP
1	A	234	LYS
1	A	240	LEU
1	A	244	VAL
1	A	245	ARG
1	A	259	ILE
1	A	280	SER
1	A	287	GLN
1	A	294	THR
1	A	295	ASP
1	A	316	VAL
1	A	333	LEU
1	A	343	VAL
1	A	359	LEU
1	A	360	MET

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Mol	Chain	Res	Type
1	A	365	THR
1	A	376	MET
1	A	379	ILE
1	A	380	GLN
1	A	385	TYR
1	A	394	ASN
1	A	401	HIS
1	A	407	ILE
1	A	410	LEU
1	A	418	LEU
1	A	429	GLN
1	A	436	ILE
1	A	439	LEU
1	A	444	LEU
1	A	445	THR
1	A	446	ILE
1	A	456	LEU
1	A	460	ARG
1	A	476	LYS
1	A	481	LYS
1	A	483	GLU
1	A	488	VAL
1	A	491	VAL
1	A	503	LEU
1	A	514	ARG
1	A	529	LEU
1	A	543	ASP
1	A	546	ASN
1	A	549	GLU
1	A	557	MET
1	A	559	ARG
1	A	560	LEU
1	A	563	SER
1	A	570	LEU
1	A	582	ARG
1	A	585	LEU
1	A	597	ASP
1	A	600	LYS
1	A	602	SER
1	B	21	ILE
1	B	29	LEU
1	B	60	GLN

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Mol	Chain	Res	Type
1	B	62	MET
1	B	73	LEU
1	B	74	LYS
1	B	89	GLN
1	B	92	THR
1	B	95	LEU
1	B	97	LEU
1	B	102	GLN
1	B	114	LYS
1	B	136	ASP
1	B	151	ILE
1	B	156	LEU
1	B	212	VAL
1	B	227	GLU
1	B	229	THR
1	B	233	ILE
1	B	238	GLU
1	B	244	VAL
1	B	245	ARG
1	B	259	ILE
1	B	273	ARG
1	B	276	THR
1	B	278	LEU
1	B	287	GLN
1	B	291	ILE
1	B	309	LYS
1	B	317	SER
1	B	333	LEU
1	B	335	ASP
1	B	341	LYS
1	B	343	VAL
1	B	357	ARG
1	B	359	LEU
1	B	379	ILE
1	B	385	TYR
1	B	391	LEU
1	B	392	LEU
1	B	401	HIS
1	B	418	LEU
1	B	424	LEU
1	B	433	GLU
1	B	436	ILE

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Mol	Chain	Res	Type
1	B	444	LEU
1	B	446	ILE
1	B	465	LYS
1	B	476	LYS
1	B	483	GLU
1	B	485	VAL
1	B	488	VAL
1	B	491	VAL
1	B	503	LEU
1	B	511	SER
1	B	526	GLN
1	B	529	LEU
1	B	531	GLN
1	B	541	LYS
1	B	545	SER
1	B	558	LEU
1	B	560	LEU
1	B	568	LEU
1	B	570	LEU
1	B	585	LEU
1	B	589	GLU
1	B	593	THR
1	B	595	LEU
1	B	600	LYS
2	E	323	CYS
2	E	329	PHE
2	E	330	ASN
2	E	337	VAL
2	E	348	CYS
2	E	356	TYR
2	E	369	VAL
2	E	388	VAL
2	E	395	ARG
2	E	416	PHE
2	E	417	MET
2	E	423	TRP
2	E	431	THR
2	E	433	THR
2	E	467	CYS
2	E	472	LEU
2	E	485	THR
2	E	500	SER

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Mol	Chain	Res	Type
2	F	323	CYS
2	F	329	PHE
2	F	337	VAL
2	F	341	GLU
2	F	348	CYS
2	F	355	LEU
2	F	356	TYR
2	F	369	VAL
2	F	373	LYS
2	F	388	VAL
2	F	402	THR
2	F	409	ASN
2	F	416	PHE
2	F	417	MET
2	F	425	THR
2	F	426	ARG
2	F	431	THR
2	F	472	LEU
2	F	485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	ASN
1	A	101	GLN
1	A	137	ASN
1	A	154	ASN
1	A	277	ASN
1	A	287	GLN
1	A	338	ASN
1	A	442	GLN
1	A	472	GLN
1	A	493	HIS
1	A	505	HIS
1	A	526	GLN
1	A	552	GLN
1	A	586	ASN
1	B	24	GLN
1	B	33	ASN
1	B	42	GLN
1	B	49	ASN

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Mol	Chain	Res	Type
1	B	51	ASN
1	B	53	ASN
1	B	60	GLN
1	B	102	GLN
1	B	134	ASN
1	B	154	ASN
1	B	175	GLN
1	B	373	HIS
1	B	388	GLN
1	B	442	GLN
1	B	493	HIS
1	B	505	HIS
1	B	508	ASN
1	B	524	GLN
1	B	526	GLN
1	B	535	HIS
1	B	552	GLN
1	B	556	ASN
1	B	586	ASN
1	B	601	ASN
2	E	375	ASN
2	E	473	ASN
2	F	473	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	1,3	14,14,15	0.48	0	17,19,21	2.06	5 (29%)
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	2.65	3 (17%)
3	BMA	C	3	3	11,11,12	0.61	0	15,15,17	1.09	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.54	0	17,19,21	0.77	0
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	1.08	2 (11%)
3	BMA	D	3	3	11,11,12	0.61	0	15,15,17	1.23	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	9.05	124.32	112.19
3	C	1	NAG	C1-O5-C5	5.97	120.18	112.19
3	C	2	NAG	O5-C1-C2	4.37	118.06	111.29
3	C	3	BMA	C1-O5-C5	3.14	116.39	112.19
3	D	3	BMA	C1-O5-C5	2.67	115.77	112.19
3	D	3	BMA	C1-C2-C3	2.66	113.52	109.64
3	C	2	NAG	O5-C5-C4	2.40	116.67	110.83
3	C	1	NAG	O7-C7-C8	-2.38	117.82	122.05
3	D	2	NAG	C3-C4-C5	-2.33	106.01	110.23
3	C	1	NAG	C2-N2-C7	2.31	126.00	122.90
3	C	1	NAG	O5-C5-C4	2.16	116.09	110.83
3	C	1	NAG	C3-C4-C5	2.11	114.06	110.23
3	D	2	NAG	O5-C5-C6	2.06	111.67	107.66

There are no chirality outliers.

All (17) torsion outliers are listed below:

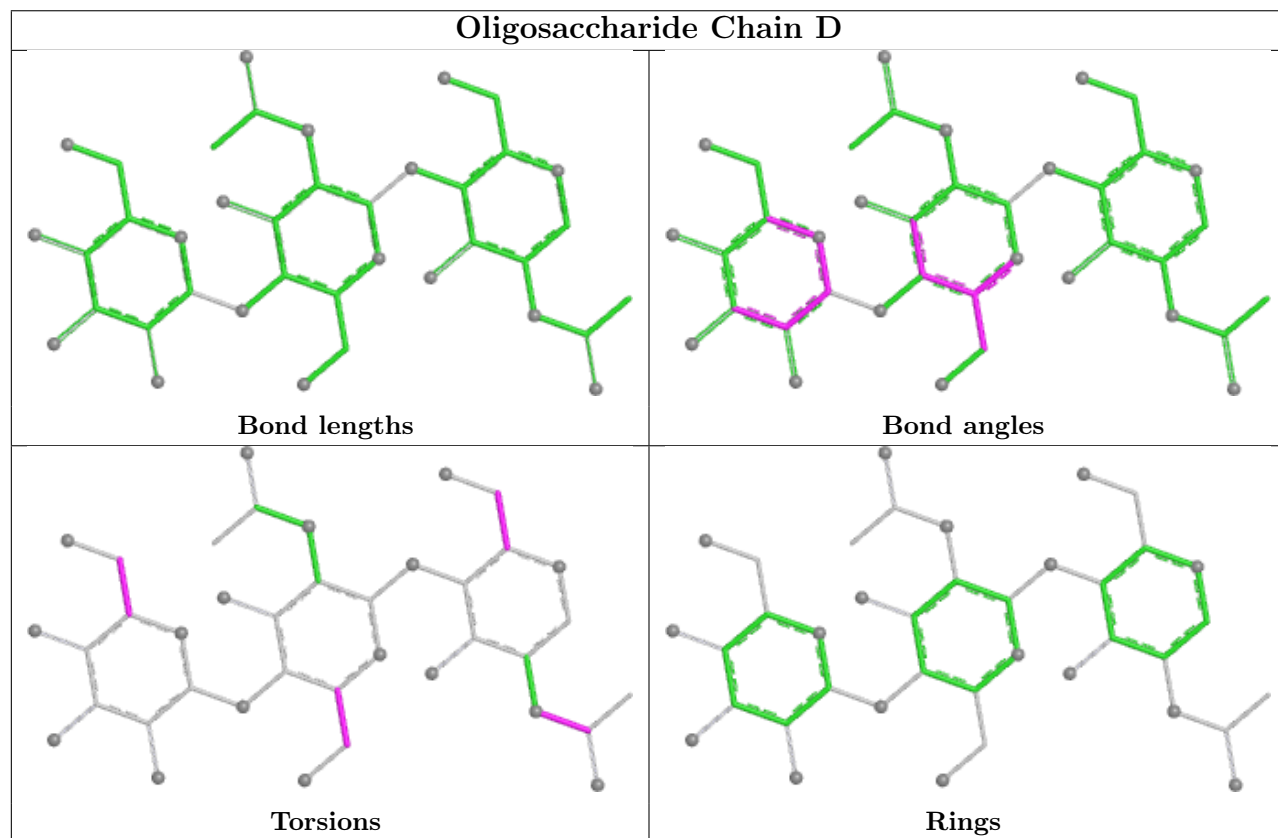
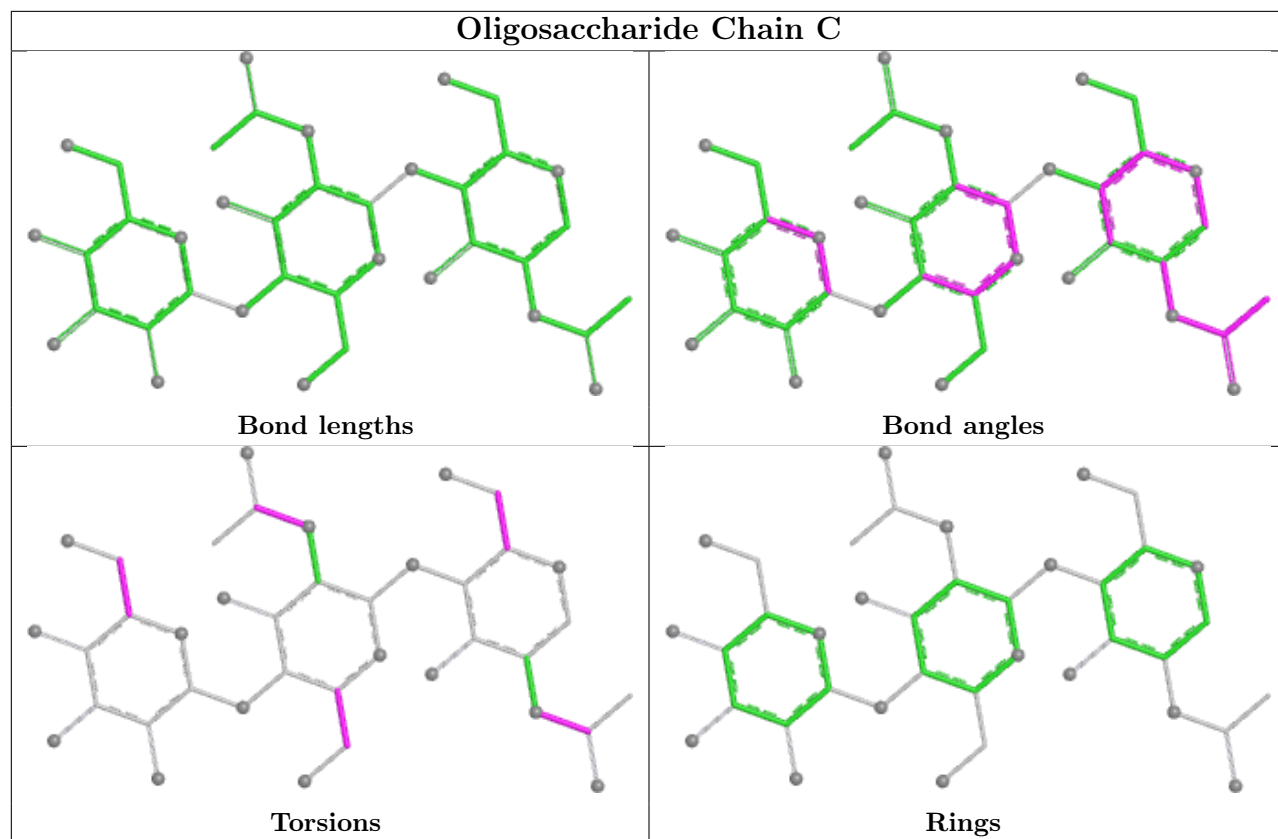
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	1	0

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



5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	703	1	14,14,15	0.74	0	17,19,21	1.81	4 (23%)
4	NAG	A	702	1	14,14,15	0.58	0	17,19,21	1.83	1 (5%)
4	NAG	E	601	2	14,14,15	0.51	0	17,19,21	1.40	2 (11%)
4	NAG	B	701	1	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
4	NAG	A	701	1	14,14,15	0.49	0	17,19,21	1.39	2 (11%)
4	NAG	F	601	2	14,14,15	0.51	0	17,19,21	2.24	4 (23%)

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	A	703	1	-	2/6/23/26	0/1/1/1
4	NAG	A	702	1	-	3/6/23/26	0/1/1/1
4	NAG	E	601	2	-	2/6/23/26	0/1/1/1
4	NAG	B	701	1	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	4/6/23/26	0/1/1/1
4	NAG	F	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	NAG	C1-O5-C5	6.29	120.62	112.19
4	F	601	NAG	C1-O5-C5	5.89	120.08	112.19
4	A	701	NAG	C1-O5-C5	4.39	118.07	112.19
4	F	601	NAG	C4-C3-C2	-4.33	104.67	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	601	NAG	C2-N2-C7	-4.19	117.29	122.90
4	A	703	NAG	C4-C3-C2	-3.95	105.23	111.02
4	A	703	NAG	C1-O5-C5	3.56	116.95	112.19
4	E	601	NAG	C1-O5-C5	3.49	116.86	112.19
4	A	703	NAG	C3-C4-C5	-3.41	104.06	110.23
4	E	601	NAG	O7-C7-C8	-2.31	117.94	122.05
4	B	701	NAG	C1-O5-C5	2.29	115.26	112.19
4	F	601	NAG	C1-C2-N2	2.26	113.99	110.43
4	A	701	NAG	O5-C1-C2	2.19	114.68	111.29
4	A	703	NAG	C1-C2-N2	2.17	113.86	110.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	NAG	O7-C7-N2-C2
4	A	702	NAG	C8-C7-N2-C2
4	A	702	NAG	O7-C7-N2-C2
4	A	701	NAG	C8-C7-N2-C2
4	A	703	NAG	O5-C5-C6-O6
4	B	701	NAG	C8-C7-N2-C2
4	B	701	NAG	O7-C7-N2-C2
4	A	701	NAG	C4-C5-C6-O6
4	A	701	NAG	O5-C5-C6-O6
4	A	703	NAG	C4-C5-C6-O6
4	A	702	NAG	O5-C5-C6-O6
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	NAG	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	597/597 (100%)	-0.01	2 (0%) 90 87	56, 82, 123, 147	0
1	B	597/597 (100%)	0.14	5 (0%) 82 77	56, 82, 123, 148	0
2	E	174/180 (96%)	0.24	2 (1%) 78 71	75, 96, 142, 153	0
2	F	174/180 (96%)	0.38	3 (1%) 69 61	76, 96, 142, 152	0
All	All	1542/1554 (99%)	0.12	12 (0%) 82 77	56, 88, 131, 153	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	PRO	2.8
2	E	374	LEU	2.7
1	B	193	ALA	2.7
2	F	354	VAL	2.6
1	B	202	TYR	2.6
1	A	91	LEU	2.5
1	A	191	ALA	2.3
2	E	446	GLY	2.3
1	B	429	GLN	2.3
1	B	95	LEU	2.2
2	F	374	LEU	2.1
2	F	404	VAL	2.0

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

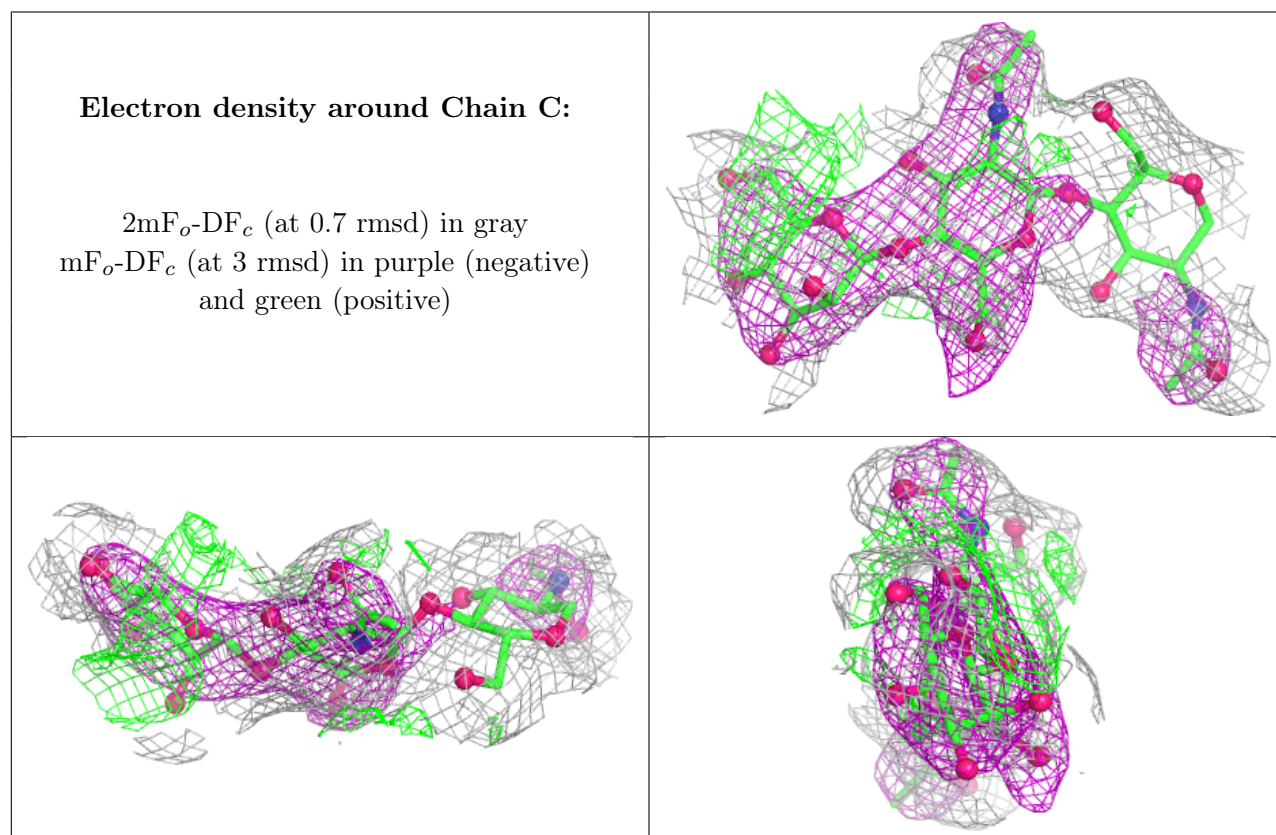
There are no non-standard protein/DNA/RNA residues in this entry.

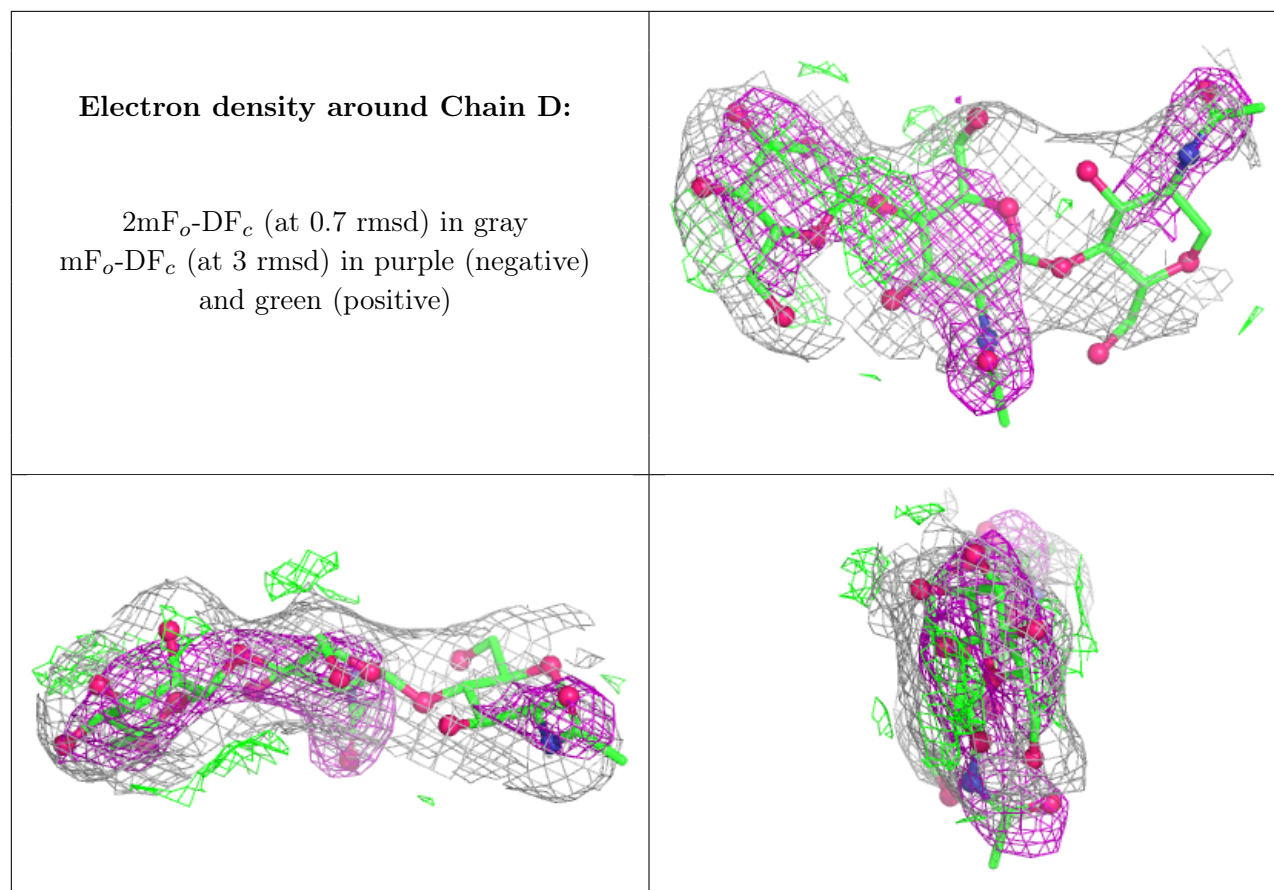
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	-	-	79,86,89,93	0
3	NAG	C	2	14/15	-	-	70,75,77,79	0
3	BMA	C	3	11/12	-	-	79,80,81,81	0
3	NAG	D	1	14/15	-	-	93,99,100,102	0
3	NAG	D	2	14/15	-	-	87,90,91,91	0
3	BMA	D	3	11/12	-	-	83,84,84,85	0

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	701	14/15	0.29	0.18	88,89,90,90	0
4	NAG	E	601	14/15	0.34	0.18	108,109,112,113	0
4	NAG	F	601	14/15	0.41	0.20	106,107,108,108	0
4	NAG	A	703	14/15	0.56	0.16	72,74,77,78	0
4	NAG	B	701	14/15	0.59	0.16	72,74,76,77	0
4	NAG	A	702	14/15	0.65	0.14	75,77,78,78	0
6	CL	B	703	1/1	0.80	0.18	115,115,115,115	0
6	CL	A	705	1/1	0.93	0.18	74,74,74,74	0
5	ZN	B	702	1/1	0.99	0.09	84,84,84,84	0
5	ZN	A	704	1/1	1.00	0.10	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.