



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 AM UTC

PDB ID : 4J4P / pdb_00004j4p
Title : The complex of human IgE-Fc with two bound Fab fragments
Authors : Drinkwater, N.; Sutton, B.J.
Deposited on : 2013-02-07
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

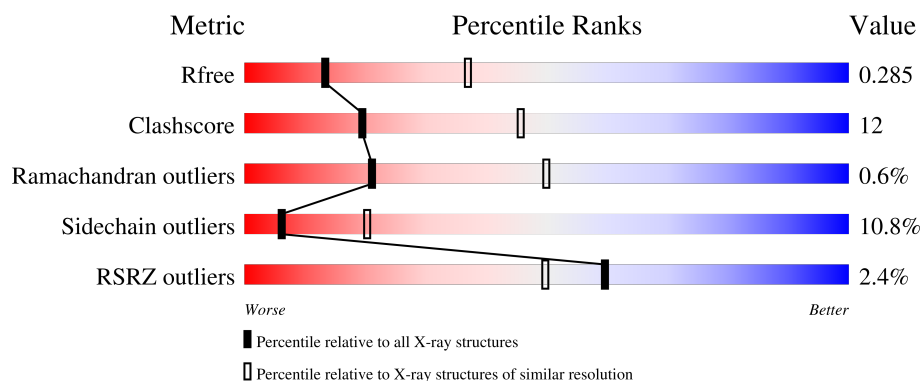
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	323	 2% 61% 33% . .
1	B	323	 % 64% 28% 6% .
2	C	249	 3% 58% 27% 5% 11%
2	H	249	 2% 55% 28% 6% . 10%
3	D	235	 5% 67% 22% . 9%

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Mol	Chain	Length	Quality of chain
3	L	235	% 59% 28% 9%
4	E	5	20% 60% 20%
4	F	5	80% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11702 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	6	0	0
			2461	1535	438	477	11			
1	B	317	Total	C	N	O	S	6	0	0
			2480	1548	441	480	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	engineered mutation	UNP P01854
A	371	GLN	ASN	engineered mutation	UNP P01854
B	265	GLN	ASN	engineered mutation	UNP P01854
B	371	GLN	ASN	engineered mutation	UNP P01854

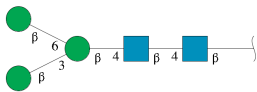
- Molecule 2 is a protein called Immunoglobulin G Fab Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1715	1081	288	339	7			
2	C	222	Total	C	N	O	S	6	0	0
			1701	1074	286	335	6			

- Molecule 3 is a protein called Immunoglobulin G Fab Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1591	993	262	332	4			
3	D	215	Total	C	N	O	S	0	0	0
			1591	993	262	332	4			

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



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

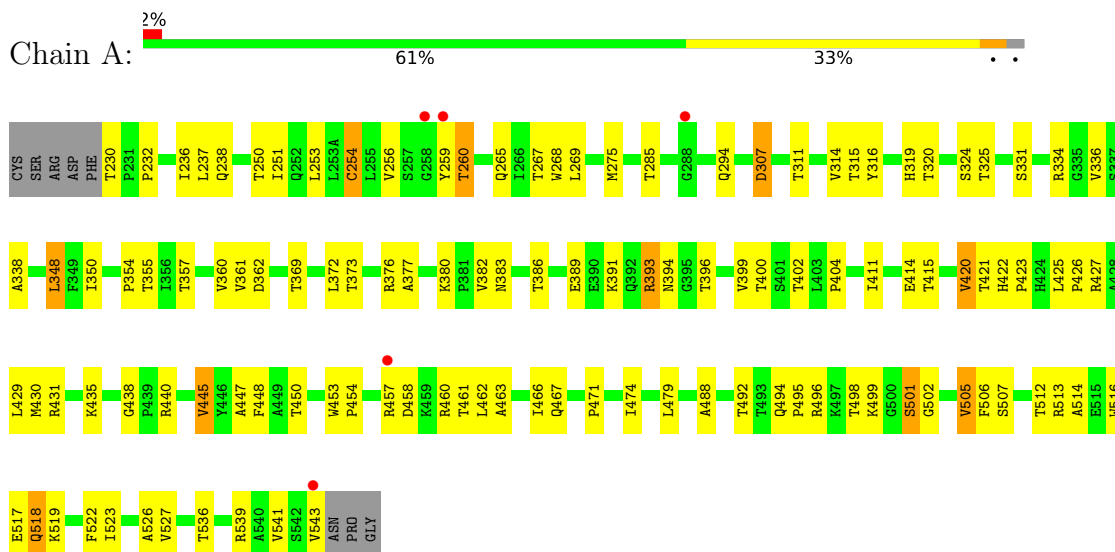
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	8	Total	O	0	0
			8	8		
5	H	9	Total	O	0	0
			9	9		
5	L	2	Total	O	0	0
			2	2		
5	C	5	Total	O	0	0
			5	5		
5	D	6	Total	O	0	0
			6	6		

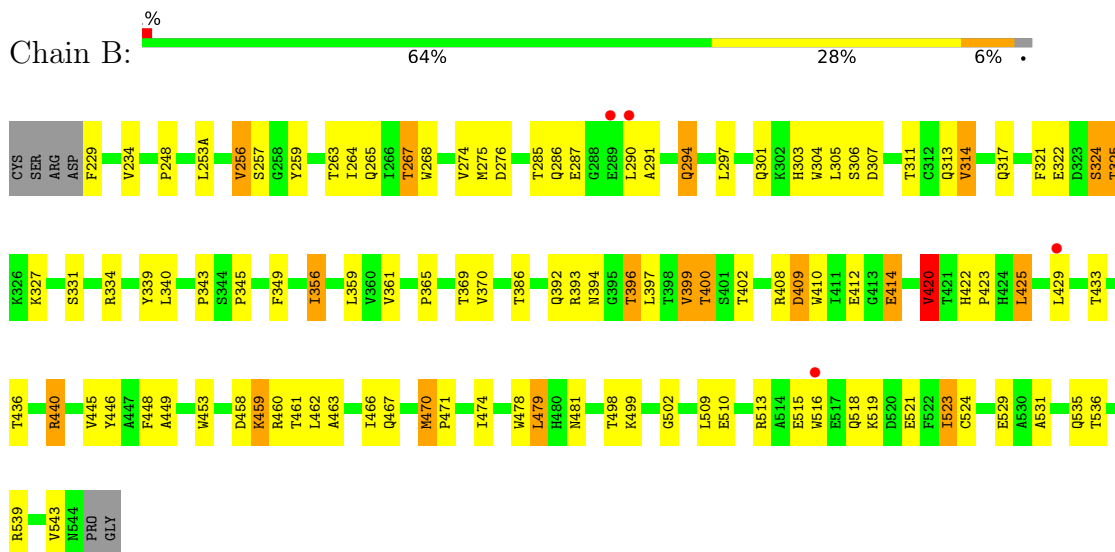
3 Residue-property plots

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: Ig epsilon chain C region

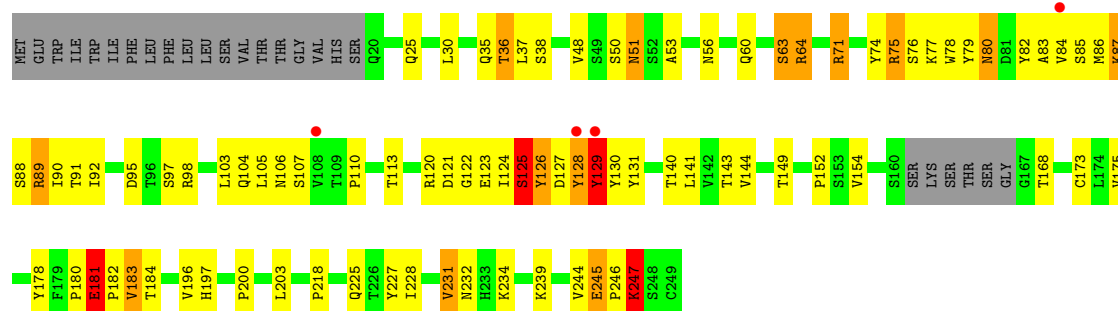


- Molecule 1: Ig epsilon chain C region

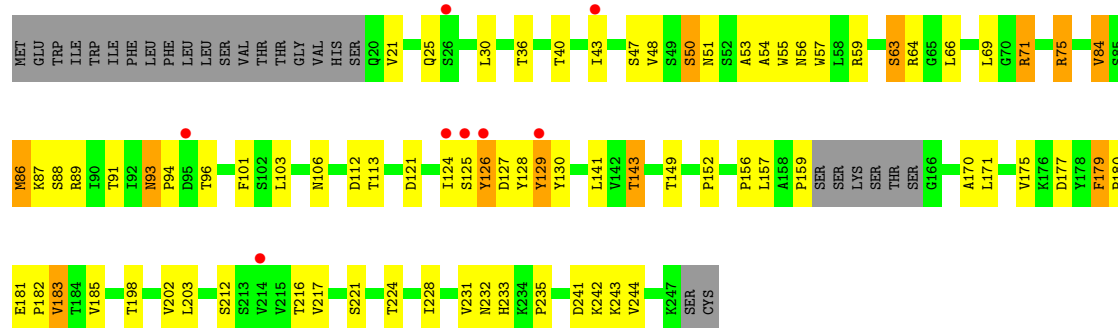


- Molecule 2: Immunoglobulin G Fab Fragment Heavy Chain

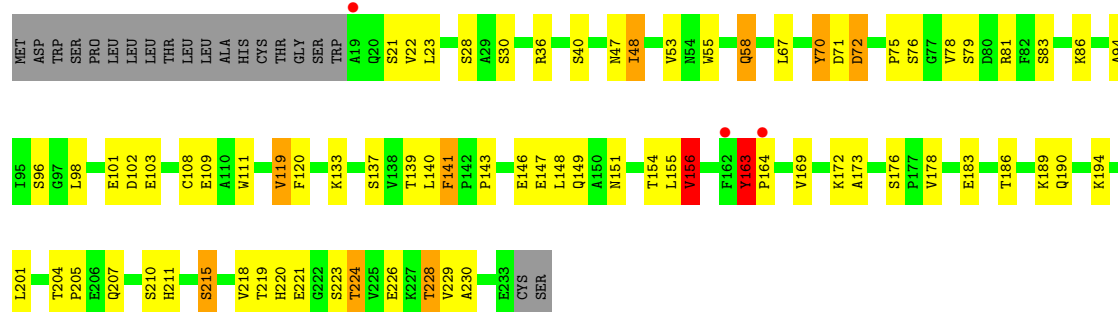




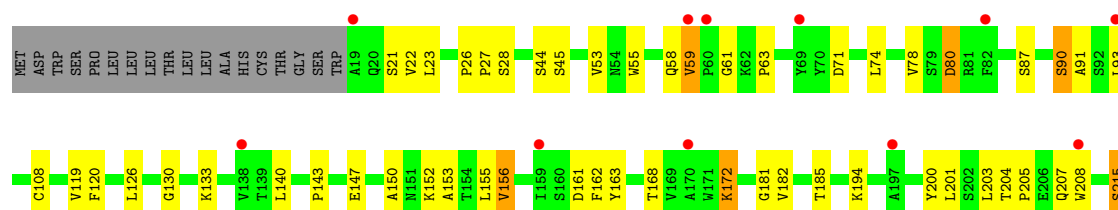
• Molecule 2: Immunoglobulin G Fab Fragment Heavy Chain

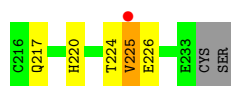


• Molecule 3: Immunoglobulin G Fab Fragment Light Chain



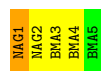
• Molecule 3: Immunoglobulin G Fab Fragment Light Chain





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

Chain E: 20% 60% 20%



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

Chain F: 80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.59Å 100.81Å 219.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.02 – 2.91 67.02 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.7 (67.02-2.91) 99.7 (67.02-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.236 , 0.284 0.238 , 0.285	Depositor DCC
R_{free} test set	2115 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11702	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: BMA, 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	0.64	0/2521	1.08	15/3436 (0.4%)
1	B	0.63	0/2541	1.05	13/3463 (0.4%)
2	C	0.63	0/1745	1.06	5/2383 (0.2%)
2	H	0.78	0/1759	1.22	12/2402 (0.5%)
3	D	0.57	1/1629 (0.1%)	1.03	9/2226 (0.4%)
3	L	0.71	0/1629	1.23	13/2226 (0.6%)
All	All	0.66	1/11824 (0.0%)	1.11	67/16136 (0.4%)

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
2	C	0	2
2	H	0	4
3	D	0	1
3	L	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	215	SER	CB-OG	7.37	1.56	1.42

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	84	VAL	N-CA-C	-11.91	94.22	109.58
3	L	141	PHE	CA-C-N	11.10	131.81	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	141	PHE	C-N-CA	11.10	131.81	120.38
3	L	163	TYR	CA-C-N	10.00	132.34	119.84
3	L	163	TYR	C-N-CA	10.00	132.34	119.84
2	H	234	LYS	CA-C-N	-9.47	108.00	119.84
2	H	234	LYS	C-N-CA	-9.47	108.00	119.84
1	B	467	GLN	N-CA-C	8.10	120.28	108.86
1	A	334	ARG	N-CA-C	-7.71	96.70	108.96
2	H	51	ASN	N-CA-C	-7.46	100.94	110.19
3	D	59	VAL	CA-C-N	7.36	127.40	119.89
3	D	59	VAL	C-N-CA	7.36	127.40	119.89
2	H	239	LYS	N-CA-C	7.17	122.91	113.30
2	C	93	ASN	CA-C-N	7.09	127.65	119.99
2	C	93	ASN	C-N-CA	7.09	127.65	119.99
2	H	48	VAL	CB-CA-C	-7.06	102.61	112.14
1	B	248	PRO	CA-C-N	6.97	127.27	119.32
1	B	248	PRO	C-N-CA	6.97	127.27	119.32
1	A	438	GLY	CA-C-N	6.97	128.55	119.84
1	A	438	GLY	C-N-CA	6.97	128.55	119.84
1	B	414	GLU	N-CA-C	6.58	124.82	110.80
2	H	128	TYR	CB-CA-C	-6.46	107.37	115.89
1	A	518	GLN	N-CA-C	-6.44	97.08	110.80
1	A	519	LYS	N-CA-C	-6.32	99.69	109.24
1	A	502	GLY	N-CA-C	6.27	120.73	111.76
3	D	63	PRO	CA-C-N	6.21	126.24	119.90
3	D	63	PRO	C-N-CA	6.21	126.24	119.90
1	B	420	VAL	N-CA-C	6.07	116.61	108.11
3	D	61	GLY	N-CA-C	-6.04	107.89	115.08
1	B	334	ARG	N-CA-C	-6.01	100.20	109.76
1	A	467	GLN	N-CA-C	5.96	118.76	109.52
1	B	459	LYS	N-CA-C	5.89	116.72	108.00
3	L	149	GLN	N-CA-C	-5.71	101.82	110.28
3	D	53	VAL	N-CA-C	5.69	116.68	108.48
3	L	223	SER	N-CA-C	5.67	118.19	109.07
3	L	72	ASP	N-CA-C	5.66	120.18	112.88
1	A	512	THR	N-CA-C	5.65	115.57	108.45
1	B	425	LEU	CA-C-N	5.65	124.84	118.97
1	B	425	LEU	C-N-CA	5.65	124.84	118.97
1	B	453	TRP	CA-C-N	5.59	125.54	119.78
1	B	453	TRP	C-N-CA	5.59	125.54	119.78
1	A	457	ARG	N-CA-C	-5.57	103.03	111.56
3	D	90	SER	N-CA-C	5.39	117.60	109.41
1	A	260	THR	CA-C-N	5.36	126.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	THR	C-N-CA	5.36	126.54	119.84
2	C	51	ASN	N-CA-C	-5.35	103.56	110.19
3	L	70	TYR	CA-C-N	-5.31	110.33	121.80
3	L	70	TYR	C-N-CA	-5.31	110.33	121.80
3	L	215	SER	N-CA-C	5.29	117.71	108.76
1	B	259	TYR	N-CA-C	5.24	117.15	109.24
3	L	156	VAL	N-CA-C	5.24	115.40	107.75
1	B	392	GLN	N-CA-C	5.23	117.61	110.55
2	H	89	ARG	N-CA-C	5.20	119.32	112.92
1	A	389	GLU	CB-CA-C	-5.18	102.80	110.62
3	D	120	PHE	N-CA-C	5.17	117.74	110.14
2	H	125	SER	N-CA-C	5.15	121.76	110.80
1	A	519	LYS	CA-C-N	-5.14	115.71	122.85
1	A	519	LYS	C-N-CA	-5.14	115.71	122.85
1	A	251	ILE	CB-CA-C	-5.12	104.74	111.25
3	L	204	THR	CA-C-N	5.10	124.82	119.82
3	L	204	THR	C-N-CA	5.10	124.82	119.82
2	C	106	ASN	N-CA-C	5.09	117.42	110.55
2	H	181	GLU	N-CA-C	5.08	117.84	108.69
3	D	130	GLY	N-CA-C	-5.07	108.24	115.64
2	H	245	GLU	CA-C-N	5.04	126.14	119.84
2	H	245	GLU	C-N-CA	5.04	126.14	119.84
2	C	177	ASP	N-CA-C	5.04	116.81	110.91

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	179	PHE	Peptide
2	C	181	GLU	Peptide
3	D	59	VAL	Peptide
2	H	124	ILE	Peptide
2	H	181	GLU	Peptide
2	H	247	LYS	Peptide
2	H	83	ALA	Peptide
3	L	163	TYR	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	2461	0	2408	60	0
1	B	2480	0	2423	61	0
2	C	1701	0	1648	39	0
2	H	1715	0	1660	47	0
3	D	1591	0	1530	30	0
3	L	1591	0	1530	42	0
4	E	61	0	52	2	0
4	F	61	0	52	2	0
5	A	11	0	0	0	0
5	B	8	0	0	0	0
5	C	5	0	0	0	0
5	D	6	0	0	0	0
5	H	9	0	0	0	0
5	L	2	0	0	1	0
All	All	11702	0	11303	266	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 12.

All (266) 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:232:PRO:HB3	1:A:259:TYR:HB3	1.58	0.86
2:H:125:SER:OG	2:H:126:TYR:N	2.09	0.81
1:B:460:ARG:HH22	1:B:543:VAL:HG21	1.45	0.81
3:L:133:LYS:HD2	3:L:221:GLU:HG3	1.63	0.79
3:L:172:LYS:HB2	3:L:215:SER:HB2	1.66	0.78
2:C:152:PRO:HD3	2:C:233:HIS:HD2	1.49	0.77
1:A:422:HIS:HB3	1:A:425:LEU:HD13	1.68	0.74
1:A:348:LEU:HD12	1:A:354:PRO:HB3	1.70	0.73
3:D:161:ASP:HA	3:D:194:LYS:HB3	1.68	0.73
1:B:393:ARG:O	2:C:71:ARG:NH2	2.22	0.72
1:B:370:VAL:HG11	1:B:399:VAL:HG11	1.69	0.72
1:A:488:ALA:O	1:B:499:LYS:NZ	2.23	0.72
2:H:168:THR:HB	2:H:218:PRO:HA	1.73	0.70
3:L:141:PHE:HB2	3:L:156:VAL:HG13	1.74	0.69
1:A:393:ARG:O	2:H:71:ARG:NH2	2.26	0.69
2:H:175:VAL:HG11	2:H:183:VAL:HG11	1.74	0.69
1:B:314:VAL:HG22	1:B:321:PHE:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TRP:HB3	1:A:275:MET:HE3	1.76	0.67
1:B:445:VAL:HG22	1:B:466:ILE:HG23	1.77	0.67
3:D:21:SER:OG	3:D:22:VAL:N	2.27	0.67
1:B:481:ASN:H	1:B:519:LYS:HZ1	1.43	0.66
2:C:30:LEU:HB2	2:C:180:PRO:HG3	1.77	0.66
2:C:221:SER:HB2	2:C:224:THR:HB	1.75	0.66
2:C:152:PRO:HD3	2:C:233:HIS:CD2	2.30	0.66
1:A:307:ASP:HB2	2:H:77:LYS:HD3	1.77	0.65
2:H:30:LEU:HB2	2:H:180:PRO:HG3	1.79	0.65
1:B:339:TYR:HD2	1:B:359:LEU:HD23	1.62	0.65
2:H:50:SER:OG	2:H:51:ASN:O	2.14	0.64
1:A:393:ARG:HG3	3:L:111:TRP:HB2	1.80	0.64
2:H:128:TYR:HD1	2:H:129:TYR:H	1.46	0.64
1:A:355:THR:HG22	1:A:404:PRO:HA	1.79	0.64
3:L:103:GLU:OE1	3:L:189:LYS:NZ	2.30	0.63
3:D:172:LYS:HE2	3:D:217:GLN:HB2	1.80	0.63
1:A:488:ALA:HB1	1:B:499:LYS:HZ1	1.64	0.63
3:L:207:GLN:HA	3:L:210:SER:HB3	1.79	0.63
2:H:53:ALA:O	2:H:75:ARG:NH2	2.31	0.62
1:B:436:THR:O	1:B:440:ARG:NH1	2.26	0.62
1:A:393:ARG:HD2	2:H:131:TYR:HB2	1.82	0.62
2:C:228:ILE:HG12	2:C:243:LYS:HB3	1.82	0.62
2:H:129:TYR:CD1	4:E:1:NAG:H62	2.34	0.61
3:D:80:ASP:OD1	3:D:80:ASP:N	2.32	0.61
3:D:203:LEU:HD21	3:D:208:TRP:HB2	1.81	0.61
2:H:35:GLN:HG2	2:H:36:THR:H	1.66	0.61
3:D:55:TRP:CZ3	3:D:108:CYS:HB3	2.35	0.61
1:B:394:ASN:OD1	1:B:396:THR:OG1	2.18	0.61
2:C:53:ALA:O	2:C:75:ARG:NH2	2.34	0.61
3:D:152:LYS:HA	3:D:205:PRO:HD3	1.82	0.60
2:H:120:ARG:NH1	2:H:122:GLY:HA3	2.17	0.60
2:H:113:THR:HG23	2:H:143:THR:HA	1.84	0.60
3:L:178:VAL:HG11	3:L:201:LEU:HD11	1.83	0.59
1:A:513:ARG:O	1:A:516:TRP:HB2	2.03	0.59
2:C:128:TYR:C	2:C:130:TYR:H	2.09	0.59
3:L:146:GLU:OE2	3:L:146:GLU:N	2.36	0.58
3:D:162:PHE:HB2	3:D:220:HIS:NE2	2.18	0.58
1:B:422:HIS:CD2	1:B:423:PRO:HD2	2.38	0.58
2:H:154:VAL:HG21	2:H:231:VAL:HG11	1.86	0.58
1:A:360:VAL:HG21	1:A:420:VAL:HG11	1.86	0.57
1:A:447:ALA:HB1	1:A:541:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:ASN:HD21	2:H:121:ASP:HB2	1.69	0.57
3:D:44:SER:OG	3:D:45:SER:N	2.37	0.57
3:D:143:PRO:HB3	3:D:153:ALA:HB1	1.87	0.57
3:D:23:LEU:HG	3:D:119:VAL:HG12	1.87	0.57
2:C:212:SER:HG	3:D:200:TYR:HH	1.53	0.57
1:A:236:ILE:O	1:A:237:LEU:HD23	2.04	0.56
2:C:113:THR:HG23	2:C:143:THR:HA	1.86	0.56
3:D:22:VAL:HB	3:D:119:VAL:HG13	1.87	0.56
1:A:394:ASN:O	2:H:75:ARG:NH1	2.39	0.56
2:H:128:TYR:C	2:H:130:TYR:H	2.13	0.56
1:A:265:GLN:NE2	1:A:315:THR:O	2.39	0.55
3:L:164:PRO:HD2	3:L:220:HIS:NE2	2.22	0.55
3:L:219:THR:HG23	3:L:224:THR:HG22	1.88	0.55
1:A:253:LEU:HD22	1:A:325:THR:HG21	1.88	0.55
2:C:84:VAL:HG22	2:C:87:LYS:HB3	1.87	0.55
2:H:225:GLN:NE2	2:H:227:TYR:OH	2.38	0.54
3:L:75:PRO:HG2	3:L:78:VAL:HG21	1.87	0.54
2:C:170:ALA:HB2	2:C:216:THR:HG22	1.89	0.54
1:A:420:VAL:HG22	1:A:429:LEU:HB2	1.88	0.54
3:L:79:SER:OG	3:L:81:ARG:HG3	2.07	0.54
1:A:435:LYS:HE3	1:A:440:ARG:HH21	1.72	0.54
1:A:488:ALA:HB1	1:B:499:LYS:NZ	2.23	0.54
1:B:515:GLU:HA	1:B:518:GLN:HB3	1.89	0.53
3:L:21:SER:HB3	3:L:120:PHE:O	2.09	0.53
3:L:81:ARG:HB3	3:L:96:SER:O	2.09	0.53
2:C:233:HIS:CE1	2:C:235:PRO:HG2	2.44	0.53
1:B:408:ARG:NH1	1:B:412:GLU:OE2	2.42	0.53
1:B:448:PHE:HB2	1:B:463:ALA:O	2.09	0.53
1:B:343:PRO:HD3	1:B:356:ILE:HG22	1.91	0.53
1:A:265:GLN:HB2	1:A:315:THR:HB	1.91	0.52
3:D:153:ALA:HB3	3:D:203:LEU:HD22	1.92	0.52
3:L:173:ALA:HB1	3:L:211:HIS:ND1	2.24	0.52
3:L:215:SER:OG	3:L:228:THR:HB	2.08	0.52
3:D:204:THR:O	3:D:207:GLN:N	2.42	0.52
2:H:86:MET:HE3	2:H:105:LEU:HD11	1.91	0.52
1:B:286:GLN:NE2	1:B:290:LEU:O	2.43	0.52
2:C:47:SER:O	2:C:50:SER:HB3	2.10	0.52
2:C:43:ILE:HD12	2:C:55:TRP:CH2	2.44	0.52
1:B:276:ASP:OD1	1:B:276:ASP:N	2.43	0.52
1:B:343:PRO:HD2	1:B:410:TRP:CZ2	2.45	0.52
2:H:110:PRO:HA	2:H:144:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:224:THR:HG22	3:D:225:VAL:H	1.74	0.52
1:B:268:TRP:HB3	1:B:275:MET:HE3	1.92	0.51
3:L:229:VAL:HG22	3:L:230:ALA:H	1.76	0.51
2:C:56:ASN:HD21	2:C:121:ASP:HB2	1.75	0.51
1:B:479:LEU:HB2	1:B:523:ILE:HG13	1.92	0.51
3:D:74:LEU:HG	3:D:78:VAL:HB	1.92	0.51
2:C:221:SER:CB	2:C:224:THR:HB	2.41	0.51
3:D:225:VAL:HG12	3:D:226:GLU:H	1.76	0.51
2:H:122:GLY:O	2:H:131:TYR:HA	2.11	0.51
1:B:267:THR:HG22	1:B:313:GLN:HB3	1.92	0.51
1:B:478:TRP:CZ3	1:B:524:CYS:HB2	2.45	0.51
1:A:494:GLN:O	1:A:496:ARG:HG3	2.10	0.51
3:L:71:ASP:OD1	3:L:86:LYS:HD3	2.11	0.51
1:A:372:LEU:HG	1:A:420:VAL:HG12	1.92	0.50
2:C:59:ARG:HB3	2:C:69:LEU:HD11	1.92	0.50
3:D:147:GLU:HA	3:D:150:ALA:HB3	1.92	0.50
2:C:55:TRP:HB3	2:C:101:PHE:CE2	2.47	0.50
2:H:129:TYR:CE1	4:E:1:NAG:H62	2.46	0.50
1:A:315:THR:HA	1:A:319:HIS:O	2.11	0.50
3:D:152:LYS:HB3	3:D:203:LEU:O	2.12	0.50
1:A:338:ALA:HB3	1:A:431:ARG:HE	1.75	0.49
3:L:36:ARG:HG3	3:L:96:SER:HA	1.94	0.49
1:B:331:SER:HB3	2:H:74:TYR:CE2	2.47	0.49
1:A:376:ARG:NE	1:A:414:GLU:OE2	2.38	0.49
1:B:460:ARG:HG3	1:B:461:THR:H	1.77	0.49
3:L:47:ASN:OD1	3:L:48:ILE:N	2.42	0.49
3:L:81:ARG:NH2	3:L:102:ASP:OD2	2.46	0.49
1:A:440:ARG:NH1	1:A:471:PRO:HD3	2.28	0.49
2:H:95:ASP:OD1	2:H:97:SER:HB3	2.13	0.48
1:B:313:GLN:HG3	1:B:322:GLU:HB3	1.94	0.48
1:B:446:TYR:CE2	1:B:448:PHE:HE1	2.31	0.48
1:B:340:LEU:HG	1:B:433:THR:HB	1.95	0.48
2:H:184:THR:OG1	2:H:232:ASN:OD1	2.30	0.48
2:C:185:VAL:HG22	2:C:231:VAL:HA	1.95	0.48
1:A:357:THR:HG23	1:A:402:THR:HG22	1.96	0.48
2:C:89:ARG:NH2	2:C:112:ASP:OD2	2.36	0.48
2:H:127:ASP:OD1	2:H:128:TYR:N	2.46	0.48
3:L:67:LEU:O	3:L:75:PRO:HD2	2.14	0.48
3:L:155:LEU:HB2	3:L:201:LEU:HB3	1.95	0.48
3:L:163:TYR:CD1	3:L:163:TYR:C	2.91	0.48
1:B:462:LEU:HD12	1:B:509:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HB3	1:A:427:ARG:O	2.13	0.48
3:L:22:VAL:HB	3:L:119:VAL:HG13	1.96	0.48
2:H:56:ASN:ND2	2:H:121:ASP:HB2	2.29	0.47
2:H:129:TYR:HD1	2:H:129:TYR:O	1.96	0.47
2:H:197:HIS:HD2	5:L:301:HOH:O	1.97	0.47
1:B:361:VAL:HG11	4:F:2:NAG:H2	1.95	0.47
2:H:63:SER:HB2	2:H:64:ARG:NE	2.30	0.47
2:H:77:LYS:HE3	2:H:79:TYR:CZ	2.50	0.47
1:A:479:LEU:HB2	1:A:523:ILE:HB	1.96	0.47
2:C:63:SER:HB2	2:C:64:ARG:HD2	1.96	0.47
3:L:169:VAL:HG22	3:L:218:VAL:HG12	1.97	0.47
2:C:124:ILE:O	2:C:125:SER:HB2	2.15	0.47
2:C:241:ASP:OD1	2:C:241:ASP:N	2.46	0.47
1:A:260:THR:HB	1:A:316:TYR:OH	2.15	0.46
1:A:448:PHE:N	1:A:541:VAL:HG21	2.30	0.46
2:H:129:TYR:CD1	2:H:129:TYR:C	2.93	0.46
1:A:362:ASP:HA	1:A:396:THR:HB	1.96	0.46
1:A:447:ALA:CB	1:A:541:VAL:HB	2.45	0.46
1:A:466:ILE:HD13	1:A:526:ALA:HB2	1.98	0.46
1:B:440:ARG:NE	1:B:529:GLU:OE1	2.34	0.46
1:B:531:ALA:HB3	1:B:535:GLN:C	2.39	0.46
2:H:203:LEU:HD12	2:H:203:LEU:O	2.15	0.46
1:B:359:LEU:HD12	1:B:400:THR:HG22	1.96	0.46
1:B:513:ARG:HA	1:B:516:TRP:HB2	1.98	0.46
3:L:53:VAL:O	3:L:70:TYR:O	2.33	0.46
2:H:227:TYR:O	2:H:244:VAL:HG22	2.15	0.46
3:L:164:PRO:HG2	3:L:221:GLU:CD	2.41	0.46
1:B:519:LYS:NZ	1:B:521:GLU:OE2	2.44	0.46
1:A:376:ARG:HD3	1:A:380:LYS:O	2.15	0.46
3:L:190:GLN:HG3	3:L:194:LYS:O	2.15	0.46
2:C:57:TRP:CD1	2:C:103:LEU:HB2	2.51	0.46
2:H:245:GLU:HA	2:H:246:PRO:HD2	1.74	0.45
3:L:55:TRP:CZ3	3:L:108:CYS:HB3	2.52	0.45
2:H:77:LYS:HG3	2:H:78:TRP:N	2.32	0.45
2:H:247:LYS:HD2	2:H:247:LYS:HA	1.63	0.45
2:C:159:PRO:HG3	2:C:171:LEU:HD23	1.97	0.45
1:A:382:VAL:HG23	1:A:383:ASN:O	2.16	0.45
1:A:450:THR:O	1:A:460:ARG:NH2	2.41	0.45
1:B:449:ALA:HA	1:B:462:LEU:HA	1.98	0.45
3:L:23:LEU:HG	3:L:119:VAL:HG12	1.98	0.45
3:L:155:LEU:HA	3:L:155:LEU:HD23	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:ASN:ND2	2:C:121:ASP:HB2	2.30	0.45
2:C:128:TYR:C	2:C:130:TYR:N	2.72	0.45
2:C:127:ASP:OD1	2:C:128:TYR:N	2.50	0.45
2:C:156:PRO:HD3	2:C:242:LYS:HG3	1.99	0.45
1:B:253(A):LEU:HD11	1:B:294:GLN:HG3	1.97	0.45
1:A:463:ALA:HB1	1:A:506:PHE:HE1	1.82	0.44
2:H:60:GLN:HE22	3:L:58:GLN:CD	2.25	0.44
3:L:143:PRO:HD3	3:L:155:LEU:CD2	2.47	0.44
1:B:345:PRO:HG2	1:B:474:ILE:CA	2.47	0.44
2:C:93:ASN:HA	2:C:94:PRO:HD3	1.86	0.44
1:A:425:LEU:HA	1:A:426:PRO:HD2	1.83	0.44
1:B:234:VAL:HG22	1:B:256:VAL:HG13	2.00	0.44
3:L:148:LEU:HG	3:L:205:PRO:HB3	1.98	0.44
3:D:90:SER:OG	3:D:91:ALA:N	2.50	0.44
2:C:84:VAL:HG22	2:C:87:LYS:CB	2.46	0.44
1:A:492:THR:HG23	1:A:507:SER:HB2	2.00	0.44
1:A:362:ASP:OD1	1:A:396:THR:HG21	2.18	0.44
2:H:82:TYR:HE1	2:H:92:ILE:HG13	1.81	0.44
2:C:183:VAL:HA	2:C:232:ASN:O	2.17	0.44
1:B:460:ARG:NH2	1:B:543:VAL:HG11	2.33	0.44
3:L:151:ASN:HA	3:L:205:PRO:HG3	1.98	0.44
2:C:129:TYR:CD1	2:C:129:TYR:C	2.95	0.44
1:B:311:THR:HA	1:B:324:SER:HB3	2.00	0.44
3:D:155:LEU:HD12	3:D:201:LEU:HD23	1.99	0.44
1:B:265:GLN:HE22	1:B:267:THR:HB	1.83	0.43
1:B:470:MET:HG3	1:B:471:PRO:HA	2.00	0.43
1:B:361:VAL:CG1	4:F:2:NAG:H83	2.49	0.43
2:H:37:LEU:HD12	2:H:38:SER:N	2.33	0.43
2:C:126:TYR:HB3	2:C:127:ASP:H	1.53	0.43
3:D:215:SER:HB2	3:D:226:GLU:CD	2.42	0.43
1:B:539:ARG:HA	1:B:539:ARG:HD3	1.77	0.43
1:A:377:ALA:HB2	1:A:415:THR:HB	1.99	0.43
1:B:229:PHE:CE1	1:B:317:GLN:HG3	2.54	0.43
3:D:26:PRO:HA	3:D:27:PRO:HD3	1.85	0.43
1:A:254:CYS:O	1:A:294:GLN:HA	2.18	0.43
3:L:147:GLU:OE2	3:L:154:THR:OG1	2.26	0.43
1:A:453:TRP:CD1	1:A:454:PRO:HD2	2.54	0.43
1:A:498:THR:HG21	1:A:501:SER:C	2.43	0.43
1:B:409:ASP:O	1:B:414:GLU:HB3	2.18	0.43
2:C:59:ARG:CZ	2:C:86:MET:HE1	2.49	0.43
3:D:55:TRP:CE2	3:D:93:LEU:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:181:GLY:O	3:D:201:LEU:HD12	2.19	0.43
2:H:85:SER:O	2:H:87:LYS:N	2.51	0.42
2:C:179:PHE:CD2	2:C:180:PRO:HD3	2.54	0.42
1:B:263:THR:C	1:B:264:ILE:HD12	2.45	0.42
3:D:23:LEU:HG	3:D:119:VAL:CG1	2.49	0.42
1:A:435:LYS:CE	1:A:440:ARG:HH21	2.33	0.42
1:B:301:GLN:O	1:B:305:LEU:HG	2.19	0.42
1:B:425:LEU:HD23	1:B:429:LEU:HD13	2.02	0.42
2:H:128:TYR:C	2:H:130:TYR:N	2.75	0.42
1:A:462:LEU:HD11	1:A:522:PHE:CD2	2.55	0.42
3:D:133:LYS:NZ	3:D:163:TYR:HD2	2.18	0.42
1:A:458:ASP:HB3	1:A:513:ARG:HG3	2.02	0.42
1:B:303:HIS:O	1:B:306:SER:HB2	2.20	0.42
1:B:365:PRO:HA	1:B:397:LEU:HB2	2.02	0.42
1:A:445:VAL:HG21	1:A:539:ARG:HB2	2.01	0.42
3:D:140:LEU:HD12	3:D:156:VAL:O	2.20	0.42
1:A:499:LYS:HB2	1:B:510:GLU:OE1	2.20	0.41
2:H:36:THR:HB	2:H:106:ASN:HA	2.01	0.41
3:L:83:SER:HB3	3:L:94:ALA:HB3	2.02	0.41
3:L:109:GLU:HB3	3:L:120:PHE:CD1	2.55	0.41
2:C:171:LEU:HD13	2:C:244:VAL:HG11	2.02	0.41
1:A:422:HIS:ND1	1:A:423:PRO:HD2	2.35	0.41
1:B:304:TRP:HH2	1:B:325:THR:CG2	2.32	0.41
2:H:152:PRO:HB3	2:H:178:TYR:HB3	2.01	0.41
3:D:152:LYS:HA	3:D:205:PRO:CD	2.50	0.41
1:A:499:LYS:HA	1:A:499:LYS:HD3	1.80	0.41
1:B:498:THR:HG23	1:B:502:GLY:O	2.20	0.41
1:B:458:ASP:O	1:B:459:LYS:HG2	2.21	0.41
2:C:54:ALA:N	2:C:121:ASP:O	2.50	0.41
1:A:495:PRO:HA	1:A:505:VAL:HG12	2.03	0.41
1:A:514:ALA:O	1:A:518:GLN:HG2	2.20	0.41
1:A:527:VAL:HG13	1:A:536:THR:HG22	2.03	0.41
1:B:349:PHE:CE2	1:B:529:GLU:HA	2.55	0.41
1:B:420:VAL:HG22	1:B:429:LEU:HB2	2.03	0.41
1:A:269:LEU:HB2	1:A:311:THR:HB	2.04	0.40
1:B:286:GLN:HG2	1:B:291:ALA:HB2	2.02	0.40
3:L:218:VAL:O	3:L:224:THR:HA	2.21	0.40
1:B:285:THR:HG22	1:B:287:GLU:HG3	2.02	0.40
2:H:129:TYR:CZ	2:H:130:TYR:HE1	2.39	0.40
1:A:314:VAL:O	1:A:320:THR:HA	2.22	0.40
1:A:435:LYS:HE3	1:A:435:LYS:HB2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:98:LEU:HD23	3:L:98:LEU:HA	1.87	0.40
2:H:80:ASN:HD22	2:H:80:ASN:HA	1.74	0.40
3:L:141:PHE:HB2	3:L:156:VAL:CG1	2.48	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	313/323 (97%)	299 (96%)	13 (4%)	1 (0%)	36	64
1	B	315/323 (98%)	298 (95%)	17 (5%)	0	100	100
2	C	218/249 (88%)	198 (91%)	18 (8%)	2 (1%)	14	40
2	H	220/249 (88%)	197 (90%)	17 (8%)	6 (3%)	4	15
3	D	213/235 (91%)	194 (91%)	19 (9%)	0	100	100
3	L	213/235 (91%)	199 (93%)	14 (7%)	0	100	100
All	All	1492/1614 (92%)	1385 (93%)	98 (7%)	9 (1%)	21	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	125	SER
2	H	182	PRO
2	H	183	VAL
2	C	182	PRO
2	C	183	VAL
2	H	76	SER
2	H	247	LYS
2	H	129	TYR
1	A	350	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/286 (98%)	248 (89%)	31 (11%)	6	19
1	B	281/286 (98%)	256 (91%)	25 (9%)	9	27
2	C	193/219 (88%)	167 (86%)	26 (14%)	4	11
2	H	196/219 (90%)	167 (85%)	29 (15%)	3	9
3	D	180/198 (91%)	168 (93%)	12 (7%)	15	41
3	L	180/198 (91%)	161 (89%)	19 (11%)	6	21
All	All	1309/1406 (93%)	1167 (89%)	142 (11%)	6	20

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	THR
1	A	238	GLN
1	A	250	THR
1	A	254	CYS
1	A	256	VAL
1	A	267	THR
1	A	285	THR
1	A	307	ASP
1	A	324	SER
1	A	331	SER
1	A	336	VAL
1	A	348	LEU
1	A	361	VAL
1	A	369	THR
1	A	373	THR
1	A	386	THR
1	A	391	LYS
1	A	393	ARG
1	A	399	VAL
1	A	400	THR
1	A	411	ILE
1	A	420	VAL

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Mol	Chain	Res	Type
1	A	421	THR
1	A	430	MET
1	A	445	VAL
1	A	461	THR
1	A	474	ILE
1	A	501	SER
1	A	505	VAL
1	A	517	GLU
1	A	543	VAL
1	B	256	VAL
1	B	257	SER
1	B	267	THR
1	B	274	VAL
1	B	294	GLN
1	B	297	LEU
1	B	307	ASP
1	B	314	VAL
1	B	324	SER
1	B	325	THR
1	B	327	LYS
1	B	356	ILE
1	B	369	THR
1	B	386	THR
1	B	396	THR
1	B	399	VAL
1	B	400	THR
1	B	402	THR
1	B	409	ASP
1	B	420	VAL
1	B	440	ARG
1	B	470	MET
1	B	479	LEU
1	B	523	ILE
1	B	536	THR
2	H	25	GLN
2	H	36	THR
2	H	63	SER
2	H	64	ARG
2	H	71	ARG
2	H	75	ARG
2	H	80	ASN
2	H	87	LYS

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Mol	Chain	Res	Type
2	H	88	SER
2	H	89	ARG
2	H	90	ILE
2	H	91	THR
2	H	98	ARG
2	H	103	LEU
2	H	104	GLN
2	H	107	SER
2	H	123	GLU
2	H	125	SER
2	H	126	TYR
2	H	129	TYR
2	H	140	THR
2	H	141	LEU
2	H	149	THR
2	H	173	CYS
2	H	181	GLU
2	H	196	VAL
2	H	200	PRO
2	H	228	ILE
2	H	231	VAL
3	L	28	SER
3	L	30	SER
3	L	40	SER
3	L	48	ILE
3	L	58	GLN
3	L	72	ASP
3	L	76	SER
3	L	101	GLU
3	L	119	VAL
3	L	137	SER
3	L	139	THR
3	L	140	LEU
3	L	156	VAL
3	L	176	SER
3	L	183	GLU
3	L	186	THR
3	L	224	THR
3	L	226	GLU
3	L	228	THR
2	C	21	VAL
2	C	25	GLN

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Mol	Chain	Res	Type
2	C	36	THR
2	C	40	THR
2	C	48	VAL
2	C	50	SER
2	C	63	SER
2	C	66	LEU
2	C	71	ARG
2	C	75	ARG
2	C	84	VAL
2	C	86	MET
2	C	88	SER
2	C	91	THR
2	C	96	THR
2	C	126	TYR
2	C	129	TYR
2	C	141	LEU
2	C	143	THR
2	C	149	THR
2	C	157	LEU
2	C	175	VAL
2	C	198	THR
2	C	202	VAL
2	C	203	LEU
2	C	217	VAL
3	D	28	SER
3	D	58	GLN
3	D	71	ASP
3	D	80	ASP
3	D	87	SER
3	D	126	LEU
3	D	156	VAL
3	D	168	THR
3	D	172	LYS
3	D	182	VAL
3	D	185	THR
3	D	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	383	ASN

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Mol	Chain	Res	Type
1	A	417	GLN
1	B	392	GLN
1	B	481	ASN
1	B	484	GLN
2	H	104	GLN
2	H	106	ASN
3	L	51	ASN
3	L	57	GLN
2	C	51	ASN
2	C	106	ASN
2	C	233	HIS
3	D	190	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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	E	1	4,1	14,14,15	0.57	0	17,19,21	2.41	6 (35%)
4	NAG	E	2	4	14,14,15	0.65	0	17,19,21	1.36	4 (23%)
4	BMA	E	3	4	11,11,12	0.70	0	15,15,17	2.07	5 (33%)
4	BMA	E	4	4	11,11,12	0.49	0	15,15,17	1.13	2 (13%)
4	BMA	E	5	4	11,11,12	0.59	0	15,15,17	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	4,1	14,14,15	1.07	1 (7%)	17,19,21	0.65	0
4	NAG	F	2	4	14,14,15	0.48	0	17,19,21	1.02	1 (5%)
4	BMA	F	3	4	11,11,12	1.70	3 (27%)	15,15,17	1.59	4 (26%)
4	BMA	F	4	4	11,11,12	1.51	3 (27%)	15,15,17	1.37	2 (13%)
4	BMA	F	5	4	11,11,12	1.47	2 (18%)	15,15,17	1.30	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
4	NAG	E	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	BMA	E	4	4	-	2/2/19/22	0/1/1/1
4	BMA	E	5	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	BMA	F	4	4	-	0/2/19/22	0/1/1/1
4	BMA	F	5	4	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	BMA	C4-C5	3.52	1.60	1.53
4	F	1	NAG	O5-C1	-3.50	1.37	1.43
4	F	4	BMA	C2-C3	2.89	1.56	1.52
4	F	3	BMA	C2-C3	2.83	1.56	1.52
4	F	4	BMA	C1-C2	2.67	1.58	1.52
4	F	5	BMA	C4-C3	2.53	1.58	1.52
4	F	4	BMA	C4-C3	2.43	1.58	1.52
4	F	3	BMA	O5-C5	2.35	1.48	1.43
4	F	3	BMA	O3-C3	2.24	1.48	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	7.76	122.58	112.19
4	E	3	BMA	O5-C5-C6	4.42	116.26	107.66
4	E	3	BMA	O3-C3-C2	4.17	118.57	110.05
4	F	3	BMA	O3-C3-C2	3.96	118.14	110.05
4	F	2	NAG	C1-O5-C5	3.73	117.18	112.19
4	F	5	BMA	C1-C2-C3	-3.54	104.48	109.64
4	F	4	BMA	C1-C2-C3	3.35	114.52	109.64
4	E	1	NAG	O4-C4-C5	-2.70	102.68	109.32
4	E	2	NAG	O5-C5-C6	2.69	112.90	107.66
4	E	4	BMA	C1-O5-C5	-2.61	108.69	112.19
4	E	2	NAG	C2-N2-C7	-2.57	119.45	122.90
4	F	4	BMA	C2-C3-C4	2.56	115.36	110.86
4	E	3	BMA	O4-C4-C5	-2.48	103.23	109.32
4	F	5	BMA	C3-C4-C5	2.44	114.65	110.23
4	F	3	BMA	C1-C2-C3	-2.40	106.15	109.64
4	E	1	NAG	C2-N2-C7	-2.36	119.73	122.90
4	E	4	BMA	O5-C5-C6	2.33	112.19	107.66
4	F	3	BMA	O5-C5-C6	2.32	112.19	107.66
4	E	1	NAG	O5-C5-C4	2.29	116.41	110.83
4	E	2	NAG	O5-C1-C2	-2.28	107.77	111.29
4	E	1	NAG	O4-C4-C3	2.24	115.66	110.38
4	E	3	BMA	O2-C2-C3	2.24	114.79	110.15
4	E	2	NAG	O3-C3-C2	-2.21	104.81	109.40
4	F	3	BMA	C3-C4-C5	-2.13	106.37	110.23
4	E	1	NAG	O3-C3-C2	-2.11	105.01	109.40
4	E	3	BMA	C1-O5-C5	-2.04	109.45	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	E	4	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	E	3	BMA	C4-C5-C6-O6

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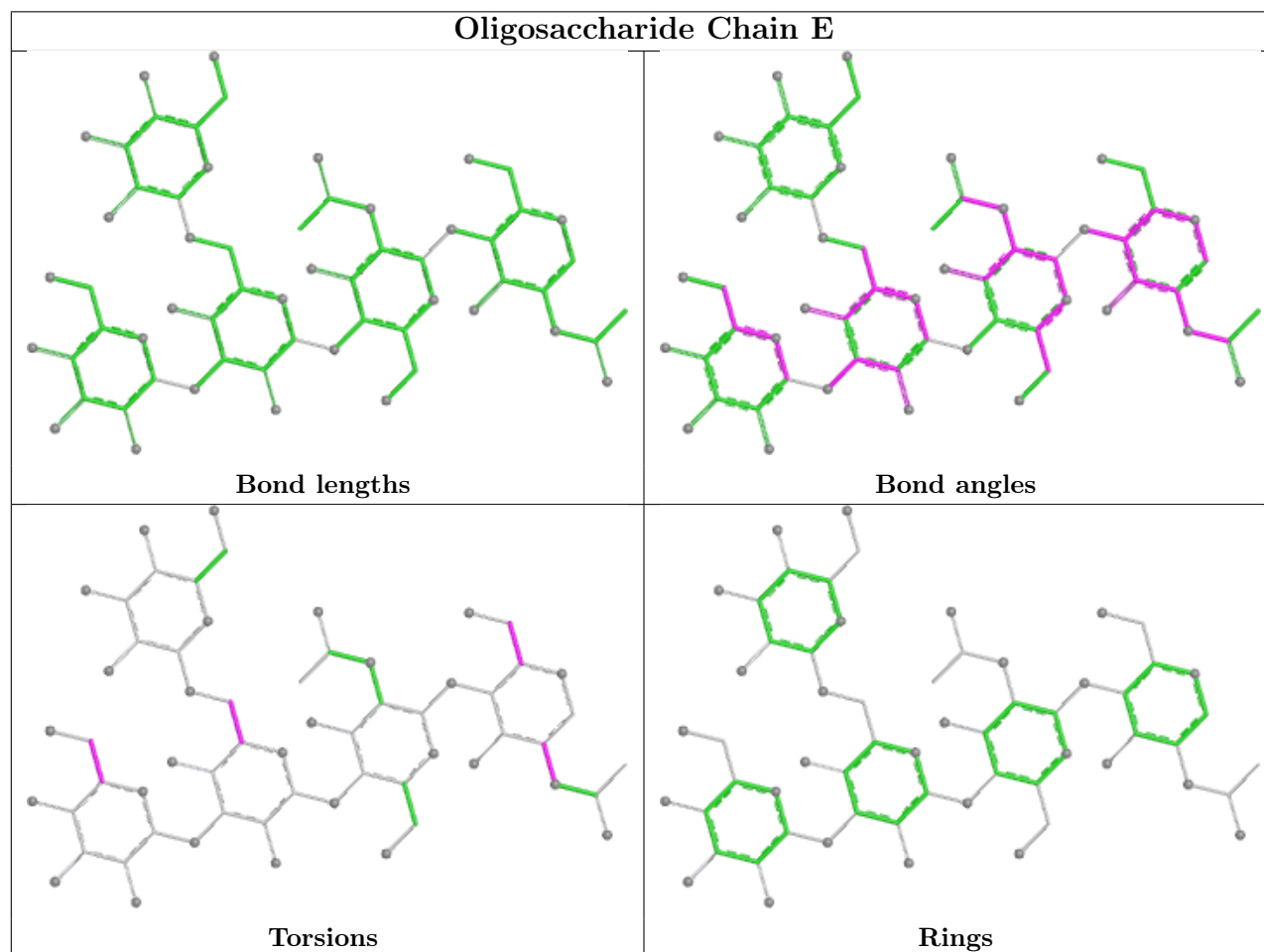
Mol	Chain	Res	Type	Atoms
4	E	4	BMA	C4-C5-C6-O6
4	E	1	NAG	C1-C2-N2-C7
4	E	3	BMA	O5-C5-C6-O6

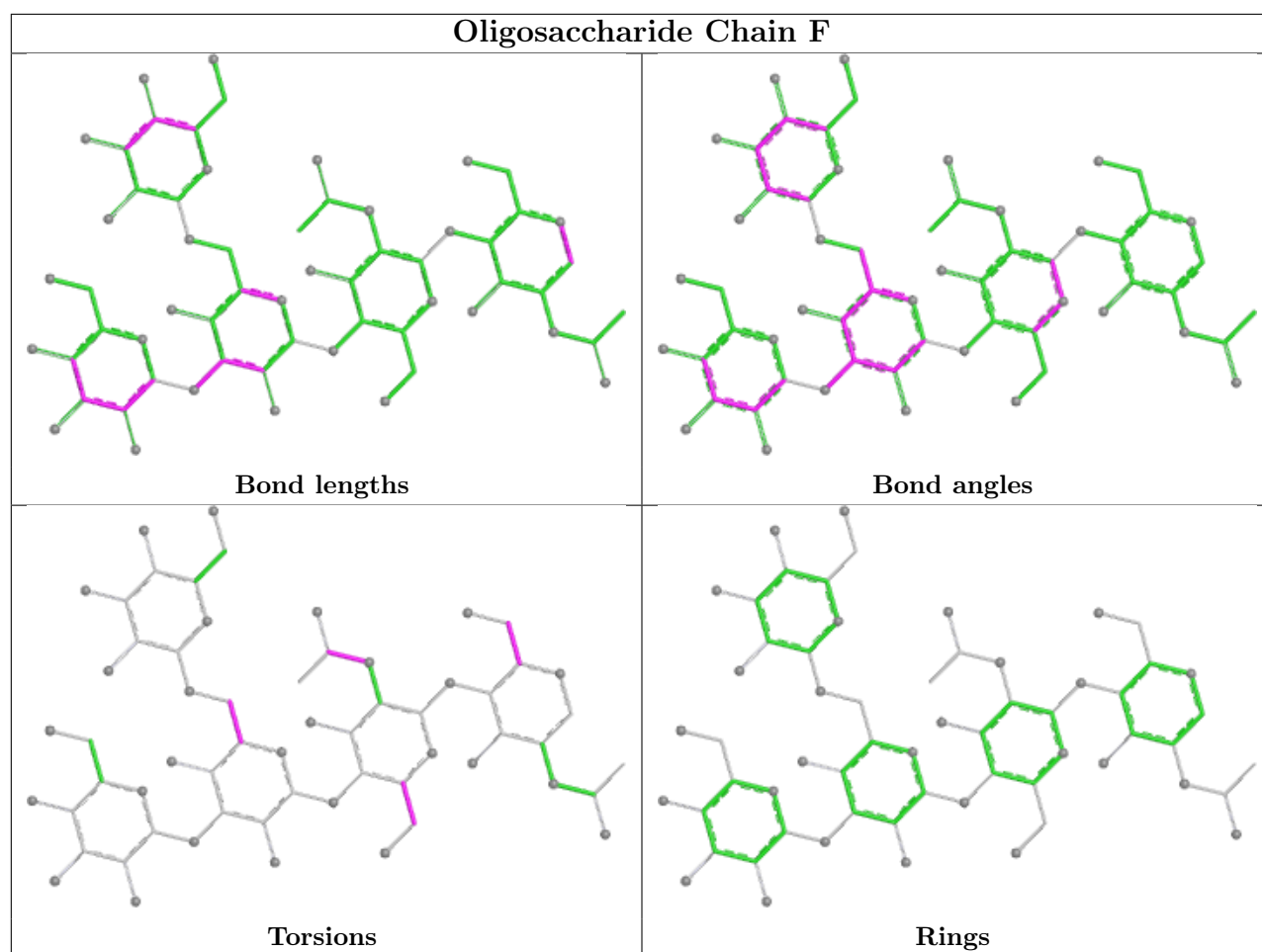
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	2	0
4	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](#)

There are no ligands in this entry.

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	315/323 (97%)	0.16	5 (1%) 70 62	42, 92, 132, 142	4 (1%)
1	B	317/323 (98%)	0.22	4 (1%) 75 67	43, 93, 164, 193	6 (1%)
2	C	222/249 (89%)	0.45	8 (3%) 46 37	47, 102, 214, 225	5 (2%)
2	H	224/249 (89%)	0.19	4 (1%) 67 59	50, 80, 159, 189	2 (0%)
3	D	215/235 (91%)	0.54	12 (5%) 30 23	64, 139, 199, 211	0
3	L	215/235 (91%)	0.24	3 (1%) 73 65	53, 85, 123, 159	0
All	All	1508/1614 (93%)	0.29	36 (2%) 59 50	42, 93, 186, 225	17 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	LEU	4.5
2	H	129	TYR	3.6
2	C	124	ILE	3.2
1	A	543	VAL	3.0
3	D	159	ILE	2.9
1	A	258	GLY	2.8
3	D	208	TRP	2.8
2	C	214	VAL	2.8
2	C	95	ASP	2.7
1	B	289	GLU	2.7
3	D	138	VAL	2.7
1	A	259	TYR	2.6
3	D	59	VAL	2.5
3	D	170	ALA	2.5
2	C	129	TYR	2.5
3	D	197	ALA	2.5
1	A	457	ARG	2.4
3	D	93	LEU	2.4
2	H	108	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	84	VAL	2.3
3	L	162	PHE	2.3
3	L	19	ALA	2.3
2	C	126	TYR	2.3
1	B	516	TRP	2.2
3	D	60	PRO	2.2
3	D	225	VAL	2.2
3	D	82	PHE	2.2
3	D	69	TYR	2.2
1	B	429	LEU	2.2
2	C	26	SER	2.2
2	C	125	SER	2.2
3	D	19	ALA	2.1
3	L	164	PRO	2.1
1	A	288	GLY	2.1
2	C	43	ILE	2.1
2	H	128	TYR	2.0

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

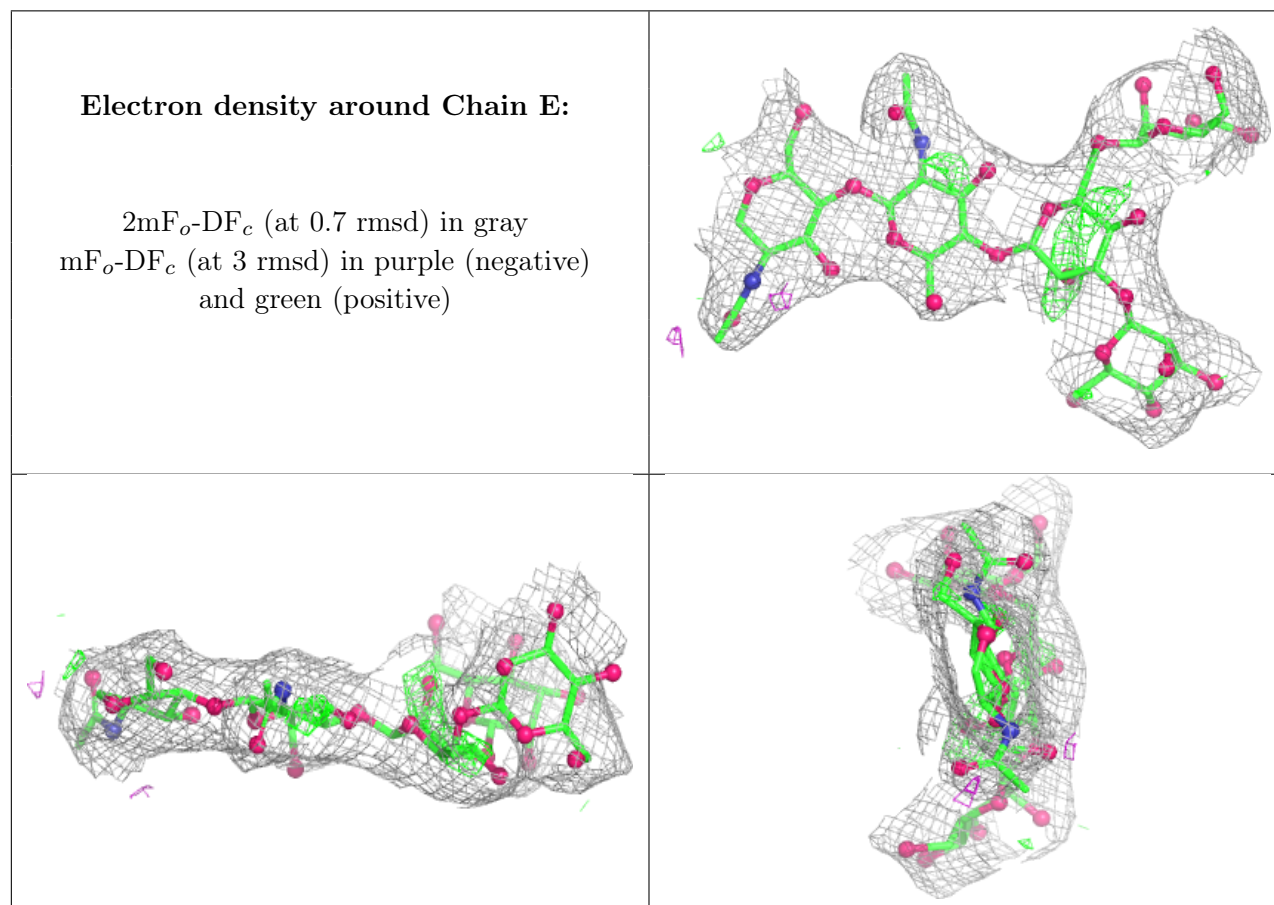
There are no non-standard protein/DNA/RNA residues in this entry.

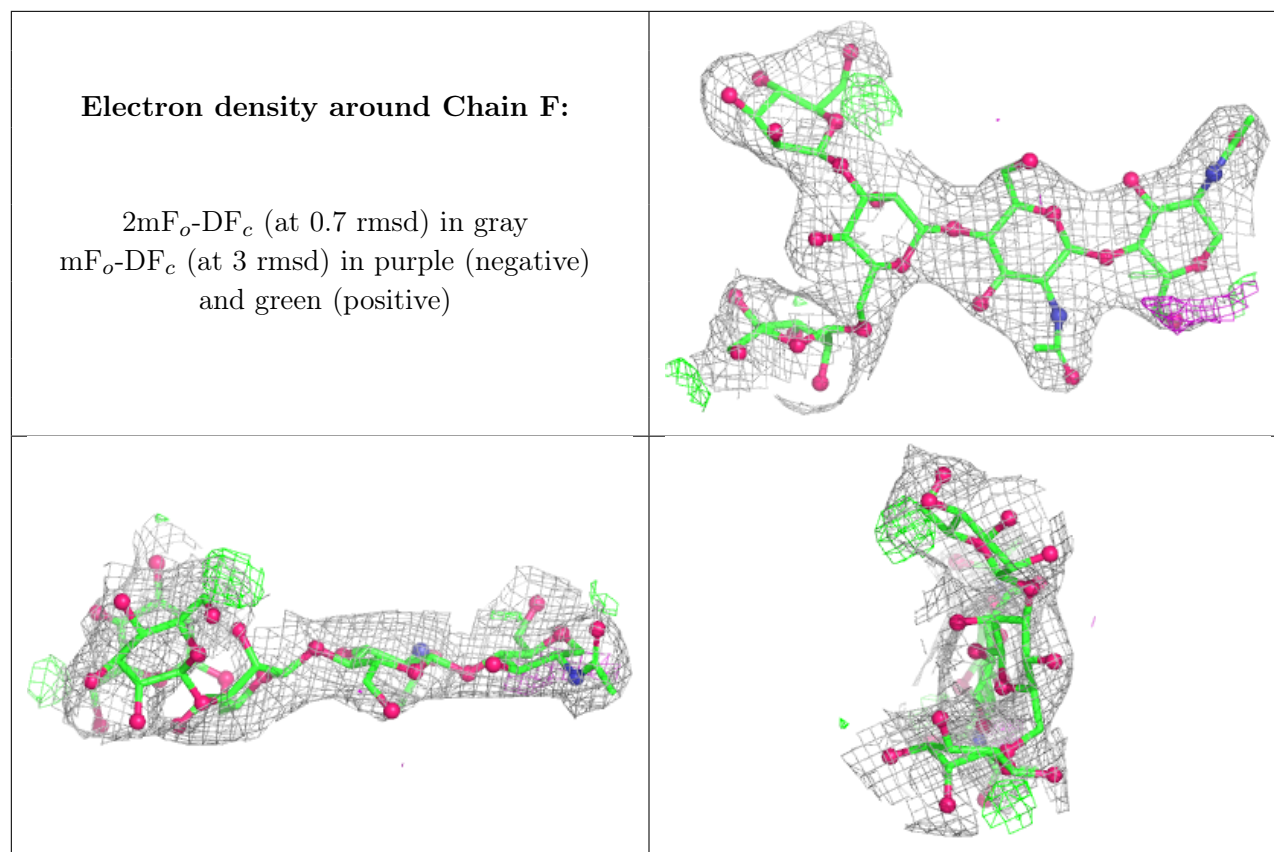
6.3 Carbohydrates ⓘ

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	E	1	14/15	-	-	70,76,82,86	0
4	NAG	E	2	14/15	-	-	79,85,89,90	0
4	BMA	E	3	11/12	-	-	97,101,112,115	0
4	BMA	E	4	11/12	-	-	120,131,135,138	0
4	BMA	E	5	11/12	-	-	117,126,139,140	0
4	NAG	F	1	14/15	-	-	80,92,96,102	0
4	NAG	F	2	14/15	-	-	94,101,105,107	0
4	BMA	F	3	11/12	-	-	110,114,120,123	0
4	BMA	F	4	11/12	-	-	129,132,140,142	0
4	BMA	F	5	11/12	-	-	117,127,129,129	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.