



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:05 AM UTC

PDB ID : 1RE3 / pdb_00001re3
Title : Crystal Structure of Fragment D of BbetaD398A Fibrinogen with the Peptide
Ligand Gly-His-Arg-Pro-Amide
Authors : Kostelansky, M.S.; Betts, L.; Gorkun, O.V.; Lord, S.T.
Deposited on : 2003-11-06
Resolution : 2.45 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

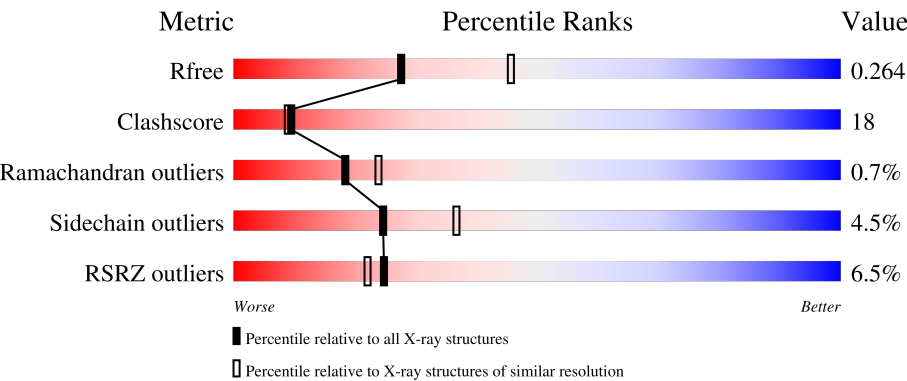
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	66	20% 41% 48% 9%
1	D	66	8% 53% 32% 11% 5%
2	B	313	6% 65% 26% 6%
2	E	313	6% 62% 27% 6%
3	C	311	5% 70% 20% 7%

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Mol	Chain	Length	Quality of chain
3	F	311	 5% 63% 27% 6%
4	G	4	 75% 25%
4	H	4	 75% 25%
5	I	2	 100%
5	J	2	 50% 50%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10794 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 Fibrinogen alpha/alpha-E chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	60	Total	C	N	O	S	0	0	0
			490	300	94	93	3			
1	D	63	Total	C	N	O	S	0	0	0
			516	317	99	97	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	294	Total	C	N	O	S	0	0	0
			2359	1474	417	446	22			
2	E	301	Total	C	N	O	S	0	0	0
			2410	1505	426	457	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	398	ALA	ASP	engineered mutation	UNP P02675
E	398	ALA	ASP	engineered mutation	UNP P02675

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2312	1468	390	443	11			
3	F	291	Total	C	N	O	S	0	0	0
			2336	1481	395	449	11			

- Molecule 4 is a protein called GHRP peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			33	19	9	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			33	19	9	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	2	Total	Ca	0	0
			2	2		
6	E	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		
7	B	63	Total	O	0	0
			63	63		
7	C	54	Total	O	0	0
			54	54		
7	D	9	Total	O	0	0
			9	9		
7	E	63	Total	O	0	0
			63	63		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	50	Total 50	O 50	0	0
7	G	1	Total 1	O 1	0	0
7	H	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

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.

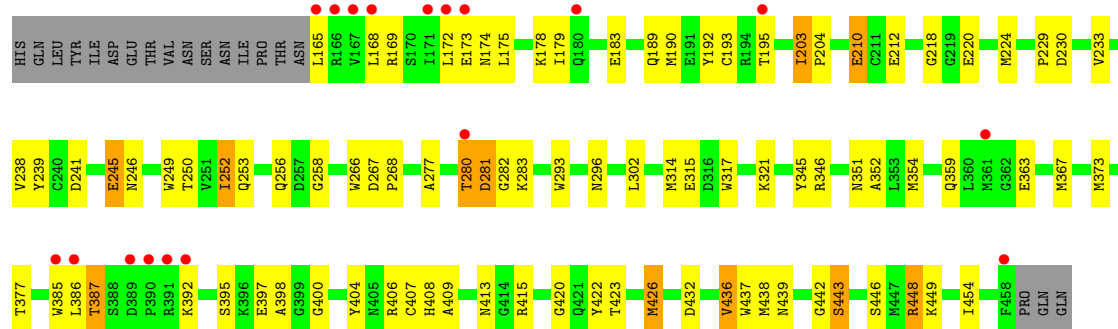
- Molecule 1: Fibrinogen alpha/alpha-E chain



- Molecule 1: Fibrinogen alpha/alpha-E chain

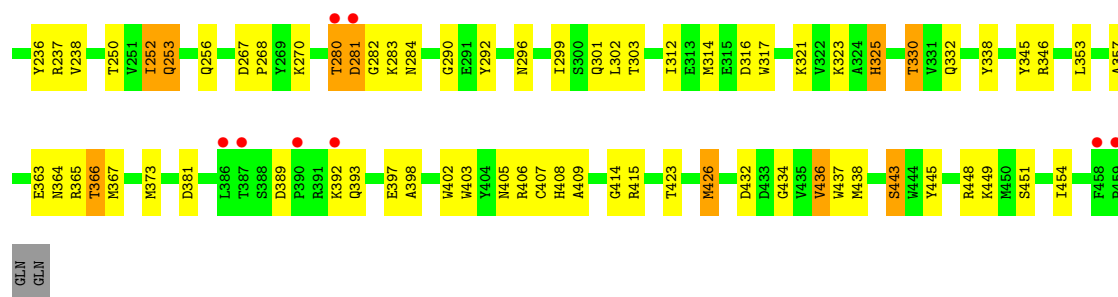


- Molecule 2: Fibrinogen beta chain

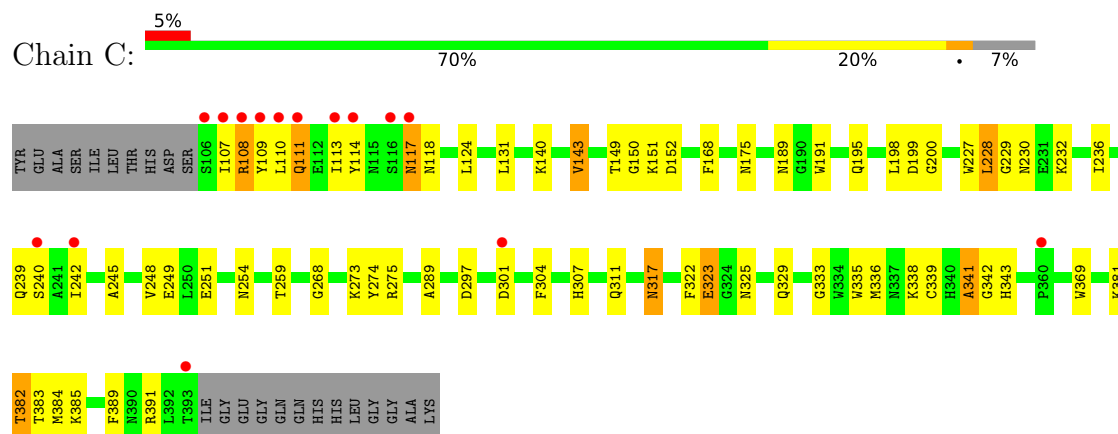


- Molecule 2: Fibrinogen beta chain

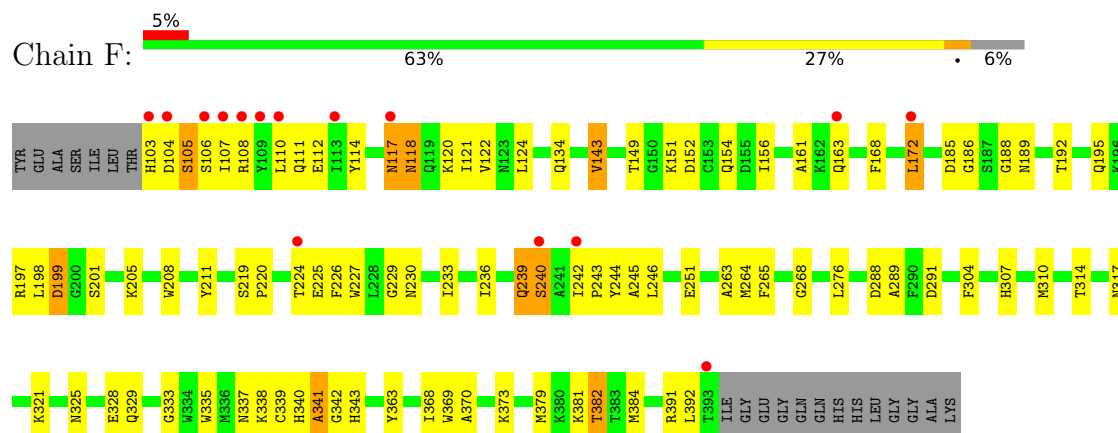




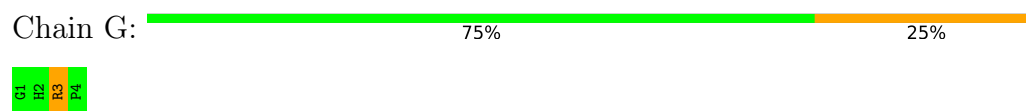
• Molecule 3: Fibrinogen gamma chain



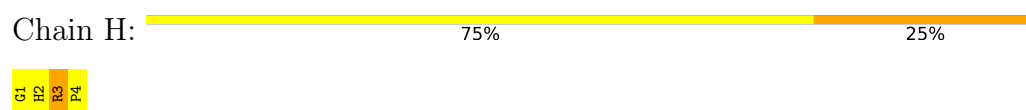
• Molecule 3: Fibrinogen gamma chain



• Molecule 4: GHRP peptide



• Molecule 4: GHRP peptide



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50%  50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.51Å 147.66Å 229.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.98 – 2.45 17.98 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.3 (17.98-2.45) 98.0 (17.98-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.46Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.263 0.223 , 0.264	Depositor DCC
R_{free} test set	3443 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10794	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, CA

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	0.35	0/491	0.90	0/655
1	D	0.41	0/517	0.91	1/687 (0.1%)
2	B	0.42	0/2419	0.94	7/3264 (0.2%)
2	E	0.44	0/2472	0.98	18/3339 (0.5%)
3	C	0.41	0/2376	0.93	5/3213 (0.2%)
3	F	0.39	0/2401	0.92	9/3247 (0.3%)
4	G	0.55	0/34	0.60	0/43
4	H	0.55	0/34	0.85	0/43
All	All	0.41	0/10744	0.94	40/14491 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	ILE	N-CA-C	11.83	118.80	108.63
2	E	409	ALA	N-CA-C	-9.56	101.97	114.31
3	C	228	LEU	N-CA-C	-8.18	99.78	110.33
2	B	409	ALA	N-CA-C	-8.09	103.93	113.88
2	E	203	ILE	N-CA-C	7.76	115.30	108.63
3	C	341	ALA	N-CA-C	-7.46	105.08	114.56
2	E	436	VAL	N-CA-C	7.33	120.33	108.97
2	B	436	VAL	N-CA-C	7.28	119.95	108.89
1	D	183	LYS	N-CA-C	-6.86	103.03	111.40
3	C	111	GLN	N-CA-C	-6.80	105.11	113.41
2	E	166	ARG	N-CA-C	-6.77	104.64	113.17
3	F	105	SER	N-CA-C	-6.56	105.39	113.19
2	B	408	HIS	N-CA-C	6.51	118.76	108.79
3	F	201	SER	N-CA-C	6.46	118.40	111.36
2	E	443	SER	N-CA-C	6.44	120.87	112.89
2	E	228	GLN	CA-C-N	6.41	125.91	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	228	GLN	C-N-CA	6.41	125.91	119.24
2	E	211	CYS	N-CA-C	6.38	119.05	111.71
2	B	426	MET	N-CA-C	-6.32	106.16	114.31
3	F	199	ASP	N-CA-C	-6.29	99.88	108.38
3	F	341	ALA	N-CA-C	-6.24	106.30	114.04
3	F	268	GLY	CA-C-N	5.91	125.88	120.21
3	F	268	GLY	C-N-CA	5.91	125.88	120.21
2	E	280	THR	N-CA-C	-5.88	100.91	110.20
2	E	194	ARG	N-CA-C	-5.82	106.03	113.01
2	E	290	GLY	N-CA-C	-5.72	104.91	112.81
2	B	443	SER	N-CA-C	5.61	119.85	112.89
2	E	292	TYR	N-CA-C	5.54	116.55	108.14
3	F	368	ILE	N-CA-C	5.40	117.56	109.20
2	E	426	MET	N-CA-C	-5.36	107.29	113.88
2	E	408	HIS	N-CA-C	5.35	116.98	108.79
2	E	163	THR	N-CA-C	-5.31	105.49	111.28
3	C	297	ASP	N-CA-C	5.29	117.46	111.11
3	F	120	LYS	N-CA-C	-5.27	105.61	111.36
2	E	353	LEU	N-CA-C	5.24	116.99	111.28
3	C	333	GLY	N-CA-C	-5.14	101.00	113.18
2	E	221	THR	N-CA-C	5.12	118.15	109.76
3	F	226	PHE	N-CA-C	5.09	115.93	107.73
2	E	197	CYS	N-CA-C	-5.08	103.69	110.55
2	B	448	ARG	N-CA-C	-5.04	106.29	112.90

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	490	0	508	40	0
1	D	516	0	543	41	0
2	B	2359	0	2232	80	0
2	E	2410	0	2281	94	0
3	C	2312	0	2165	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2336	0	2181	80	0
4	G	33	0	32	7	0
4	H	33	0	32	9	0
5	I	28	0	25	1	0
5	J	28	0	25	1	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	63	0	0	2	0
7	C	54	0	0	2	0
7	D	9	0	0	0	0
7	E	63	0	0	3	0
7	F	50	0	0	1	0
7	G	1	0	0	1	0
7	H	2	0	0	1	0
All	All	10794	0	10024	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (369) 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)
3:F:172:LEU:HD12	3:F:172:LEU:H	1.20	1.06
3:C:329:GLN:NE2	4:G:3:ARG:HH11	1.64	0.95
2:E:373:MET:HE2	2:E:405:ASN:HA	1.49	0.94
2:E:166:ARG:H	2:E:166:ARG:HD3	1.39	0.88
3:C:117:ASN:HD22	3:C:118:ASN:N	1.74	0.84
3:C:108:ARG:H	3:C:108:ARG:HD2	1.43	0.84
1:A:169:LEU:H	2:B:189:GLN:HE22	1.25	0.83
2:E:179:ILE:HD12	3:F:117:ASN:HB2	1.60	0.83
3:F:329:GLN:NE2	4:H:3:ARG:HH11	1.77	0.82
3:F:307:HIS:HE1	3:F:341:ALA:H	1.28	0.81
1:A:175:LEU:H	1:A:175:LEU:HD23	1.47	0.79
3:C:149:THR:HG23	3:C:168:PHE:O	1.83	0.79
3:F:149:THR:HG22	3:F:168:PHE:O	1.83	0.78
3:F:172:LEU:H	3:F:172:LEU:CD1	1.97	0.77
2:E:423:THR:H	2:E:426:MET:HE3	1.51	0.75
1:D:133:ILE:HD12	1:D:133:ILE:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:THR:N	2:E:426:MET:HE3	2.02	0.75
2:B:363:GLU:HG2	2:B:367:MET:HE3	1.68	0.74
2:E:281:ASP:OD1	2:E:282:GLY:N	2.20	0.73
2:E:364:ASN:HA	2:E:367:MET:HE3	1.70	0.73
2:B:438:MET:HE3	2:B:443:SER:HB3	1.71	0.73
2:E:230:ASP:O	2:E:233:VAL:HG22	1.89	0.72
3:F:219:SER:OG	3:F:224:THR:HG22	1.90	0.72
3:F:329:GLN:HE21	4:H:3:ARG:NH1	1.89	0.71
1:D:129:LYS:HD2	1:D:129:LYS:O	1.91	0.71
1:A:153:ASP:O	1:A:157:LYS:HG2	1.91	0.71
2:E:252:ILE:HD13	2:E:454:ILE:HG12	1.73	0.71
2:E:168:LEU:O	2:E:172:LEU:HD23	1.91	0.70
3:C:108:ARG:HD2	3:C:108:ARG:N	2.07	0.69
1:D:176:LYS:HA	1:D:176:LYS:HE2	1.74	0.69
1:A:178:TYR:O	1:A:182:GLN:HG2	1.93	0.69
3:F:239:GLN:O	3:F:240:SER:HB3	1.92	0.69
3:C:329:GLN:HE21	4:G:3:ARG:HH11	1.41	0.69
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.57	0.68
2:E:161:ILE:HD13	2:E:161:ILE:H	1.58	0.68
3:C:240:SER:OG	3:C:242:ILE:HG12	1.94	0.68
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.92	0.68
2:B:230:ASP:O	2:B:233:VAL:HG22	1.93	0.68
3:C:149:THR:HG21	7:C:433:HOH:O	1.94	0.68
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.93	0.68
3:F:172:LEU:HD12	3:F:172:LEU:N	2.02	0.67
3:F:329:GLN:NE2	4:H:3:ARG:NH1	2.40	0.67
3:F:307:HIS:CE1	3:F:341:ALA:H	2.12	0.67
1:D:139:ASN:HB3	3:F:114:TYR:CE2	2.29	0.67
3:C:149:THR:HG22	3:C:150:GLY:N	2.09	0.67
1:D:133:ILE:HD12	1:D:133:ILE:N	2.09	0.67
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.40	0.67
2:E:179:ILE:CD1	3:F:117:ASN:HB2	2.24	0.67
2:B:386:LEU:O	2:B:387:THR:HB	1.94	0.66
3:C:195:GLN:OE1	3:C:382:THR:HG22	1.95	0.66
3:C:307:HIS:HE1	3:C:342:GLY:H	1.44	0.66
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.60	0.65
3:C:329:GLN:NE2	4:G:3:ARG:NH1	2.41	0.65
2:B:385:TRP:HA	2:B:406:ARG:HD3	1.79	0.65
1:A:131:GLN:HE21	1:A:132:HIS:HB2	1.63	0.64
1:A:181:GLN:HE21	2:B:174:ASN:ND2	1.95	0.64
2:E:166:ARG:H	2:E:166:ARG:CD	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.80	0.63
2:B:229:PRO:HD2	2:B:233:VAL:HG21	1.80	0.63
2:E:167:VAL:O	2:E:171:ILE:HG12	1.99	0.63
3:F:325:ASN:HD22	3:F:325:ASN:C	2.06	0.63
1:A:181:GLN:HE21	2:B:174:ASN:HD22	1.46	0.63
3:C:323:GLU:H	3:C:323:GLU:CD	2.05	0.63
2:E:161:ILE:N	2:E:162:PRO:HD2	2.13	0.62
3:F:310:MET:HE1	3:F:321:LYS:HE3	1.81	0.62
1:A:175:LEU:H	1:A:175:LEU:CD2	2.13	0.62
2:B:363:GLU:O	2:B:367:MET:HG2	1.99	0.62
1:D:137:GLN:NE2	1:D:189:ILE:HG23	2.14	0.62
1:D:144:LEU:HD13	1:D:182:GLN:HB3	1.82	0.62
2:E:448:ARG:HH11	2:E:448:ARG:HG2	1.65	0.62
1:A:139:ASN:HB3	3:C:114:TYR:CE2	2.35	0.61
1:A:166:SER:HB3	2:B:195:THR:HG23	1.82	0.61
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.35	0.61
3:F:329:GLN:HE21	4:H:3:ARG:HH11	1.43	0.61
3:C:329:GLN:HE22	4:G:3:ARG:HH11	1.44	0.61
3:C:117:ASN:HD22	3:C:117:ASN:C	2.06	0.61
1:D:169:LEU:H	2:E:189:GLN:NE2	1.98	0.61
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	1.98	0.61
2:B:359:GLN:NE2	2:B:442:GLY:HA2	2.16	0.60
3:C:329:GLN:HE21	4:G:3:ARG:NH1	1.98	0.60
2:E:280:THR:O	2:E:281:ASP:C	2.45	0.60
2:E:389:ASP:HB3	2:E:392:LYS:HD2	1.84	0.60
3:C:249:GLU:HB2	3:C:383:THR:HB	1.84	0.60
1:D:136:LEU:O	1:D:140:VAL:HG13	2.02	0.59
2:E:363:GLU:HA	2:E:366:THR:HG23	1.84	0.59
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.68	0.59
2:B:363:GLU:HG2	2:B:367:MET:CE	2.32	0.59
2:B:165:LEU:N	2:B:165:LEU:HD12	2.18	0.59
3:C:109:TYR:HD1	3:C:110:LEU:HD12	1.67	0.59
3:C:307:HIS:HE1	3:C:341:ALA:H	1.51	0.59
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.37	0.59
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.84	0.58
3:F:104:ASP:C	3:F:106:SER:H	2.10	0.58
1:D:189:ILE:HG22	1:D:189:ILE:O	2.04	0.58
1:A:131:GLN:NE2	1:A:132:HIS:H	2.01	0.58
3:C:149:THR:HG22	3:C:150:GLY:H	1.68	0.57
3:F:117:ASN:C	3:F:117:ASN:HD22	2.12	0.57
3:F:185:ASP:OD2	3:F:189:ASN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ASN:O	2:B:178:LYS:HG2	2.04	0.57
3:C:338:LYS:N	3:C:339:CYS:HA	2.18	0.57
2:E:438:MET:HE3	2:E:443:SER:HB3	1.85	0.57
1:A:144:LEU:HD23	2:B:175:LEU:HD21	1.87	0.57
1:A:185:LEU:O	1:A:189:ILE:HG13	2.05	0.57
1:D:169:LEU:H	2:E:189:GLN:HE22	1.52	0.57
2:B:230:ASP:HB3	2:B:233:VAL:HG13	1.87	0.57
2:E:238:VAL:HG21	2:E:250:THR:HG23	1.86	0.57
3:F:117:ASN:O	3:F:121:ILE:HG13	2.05	0.56
2:B:245:GLU:O	2:B:246:ASN:HB2	2.05	0.56
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.40	0.56
1:A:133:ILE:HA	1:A:136:LEU:HB3	1.87	0.56
1:D:188:VAL:HG11	2:E:165:LEU:HG	1.87	0.56
5:I:1:NAG:H62	5:I:2:NAG:O5	2.06	0.56
2:E:159:SER:HA	2:E:162:PRO:HG3	1.87	0.56
2:B:423:THR:OG1	2:B:426:MET:HE3	2.06	0.56
1:A:140:VAL:HG21	2:B:168:LEU:HD11	1.87	0.56
3:C:307:HIS:CE1	3:C:342:GLY:H	2.22	0.56
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.87	0.55
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.88	0.55
2:E:174:ASN:HD21	2:E:178:LYS:NZ	2.03	0.55
2:B:302:LEU:HD13	2:B:454:ILE:HD11	1.87	0.55
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.70	0.55
2:B:406:ARG:N	2:B:407:CYS:HA	2.22	0.55
1:A:133:ILE:HD12	2:B:165:LEU:HD22	1.88	0.55
1:A:136:LEU:HD13	1:A:136:LEU:O	2.05	0.55
3:C:307:HIS:CE1	3:C:341:ALA:H	2.25	0.55
3:F:338:LYS:N	3:F:339:CYS:HA	2.21	0.55
3:C:242:ILE:HG13	3:C:242:ILE:O	2.07	0.55
2:E:389:ASP:OD2	2:E:392:LYS:HE3	2.07	0.55
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.88	0.55
1:A:136:LEU:HD13	1:A:136:LEU:C	2.31	0.55
1:D:135:LEU:HD13	1:D:135:LEU:C	2.31	0.54
3:F:117:ASN:HD22	3:F:118:ASN:N	2.05	0.54
1:A:140:VAL:HG11	2:B:172:LEU:HD21	1.89	0.54
3:C:189:ASN:OD1	3:C:391:ARG:HG3	2.07	0.54
3:F:163:GLN:CD	3:F:163:GLN:H	2.15	0.54
3:F:199:ASP:O	3:F:225:GLU:OE2	2.26	0.54
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.88	0.54
1:D:133:ILE:H	1:D:133:ILE:CD1	2.17	0.54
2:E:162:PRO:HA	2:E:165:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:GLY:HA2	7:C:419:HOH:O	2.07	0.54
2:E:160:ASN:C	2:E:162:PRO:HD2	2.33	0.54
2:E:224:MET:CE	2:E:237:ARG:HD3	2.38	0.54
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.73	0.54
3:F:325:ASN:ND2	3:F:328:GLU:H	2.06	0.54
1:D:131:GLN:N	1:D:131:GLN:CD	2.66	0.54
1:D:135:LEU:HD13	1:D:135:LEU:O	2.09	0.53
1:D:185:LEU:O	1:D:189:ILE:HG13	2.09	0.53
1:D:165:CYS:HB3	2:E:193:CYS:HA	1.89	0.53
2:B:238:VAL:HG21	2:B:250:THR:CG2	2.39	0.53
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.44	0.53
1:D:136:LEU:HD21	3:F:111:GLN:HG2	1.91	0.53
2:E:224:MET:HE2	2:E:237:ARG:HD3	1.91	0.53
3:F:195:GLN:OE1	3:F:382:THR:CG2	2.56	0.52
3:C:107:ILE:HD12	3:C:108:ARG:NH2	2.24	0.52
3:F:211:TYR:CE2	3:F:333:GLY:HA3	2.45	0.52
2:E:323:LYS:NZ	2:E:325:HIS:HD2	2.08	0.52
2:E:230:ASP:OD2	2:E:233:VAL:HG13	2.09	0.52
3:C:323:GLU:CD	3:C:323:GLU:N	2.68	0.52
2:E:161:ILE:N	2:E:162:PRO:CD	2.71	0.52
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.45	0.52
3:F:151:LYS:HD2	3:F:172:LEU:HD11	1.91	0.51
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.92	0.51
2:E:162:PRO:O	2:E:165:LEU:HB2	2.10	0.51
3:C:322:PHE:CZ	4:G:3:ARG:HG2	2.46	0.51
2:E:160:ASN:HD22	2:E:160:ASN:N	2.08	0.51
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.92	0.51
2:B:169:ARG:O	2:B:173:GLU:HG2	2.11	0.51
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.93	0.51
2:B:172:LEU:HB3	3:C:113:ILE:HG22	1.93	0.51
2:E:201:CYS:O	3:F:143:VAL:HG21	2.11	0.51
3:F:276:LEU:HD23	3:F:276:LEU:C	2.35	0.51
1:A:167:ARG:HD3	2:B:192:TYR:CE1	2.46	0.50
2:E:229:PRO:CB	2:E:301:GLN:HE22	2.24	0.50
3:C:325:ASN:C	3:C:325:ASN:HD22	2.19	0.50
1:A:175:LEU:HD23	1:A:175:LEU:N	2.22	0.50
3:F:118:ASN:O	3:F:122:VAL:HG23	2.11	0.50
2:B:252:ILE:HD13	2:B:454:ILE:HG12	1.94	0.50
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.11	0.50
2:B:224:MET:HE3	2:B:277:ALA:HB3	1.94	0.49
1:D:131:GLN:CD	1:D:131:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:N	2:E:407:CYS:HA	2.27	0.49
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.78	0.49
2:E:161:ILE:H	2:E:161:ILE:CD1	2.23	0.49
3:F:104:ASP:C	3:F:106:SER:N	2.67	0.49
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.94	0.49
1:A:169:LEU:H	2:B:189:GLN:NE2	2.01	0.49
2:B:359:GLN:HE22	2:B:442:GLY:HA2	1.76	0.49
1:D:135:LEU:HD13	1:D:139:ASN:ND2	2.27	0.49
1:A:186:GLU:CD	1:A:189:ILE:HD12	2.38	0.49
3:F:245:ALA:HB1	3:F:392:LEU:HD11	1.94	0.49
1:D:133:ILE:O	1:D:137:GLN:HG2	2.13	0.49
4:G:3:ARG:NH2	7:G:40:HOH:O	2.41	0.49
2:B:398:ALA:O	2:B:415:ARG:HD3	2.13	0.48
2:E:398:ALA:O	2:E:415:ARG:HD3	2.13	0.48
3:F:172:LEU:CD1	3:F:239:GLN:HE21	2.26	0.48
3:F:205:LYS:HD2	7:F:439:HOH:O	2.13	0.48
2:B:218:GLY:O	2:B:220:GLU:HG3	2.13	0.48
2:E:332:GLN:O	2:E:338:TYR:HA	2.13	0.48
2:B:204:PRO:HG2	2:B:224:MET:O	2.12	0.48
2:B:385:TRP:CD1	2:B:406:ARG:HD2	2.48	0.48
3:F:208:TRP:HA	3:F:314:THR:HG21	1.95	0.48
2:B:386:LEU:O	2:B:387:THR:CB	2.59	0.48
2:B:422:TYR:OH	2:B:432:ASP:HB2	2.14	0.48
2:E:314:MET:HA	2:E:449:LYS:O	2.12	0.48
3:F:108:ARG:O	3:F:112:GLU:HG3	2.14	0.48
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.95	0.48
1:D:129:LYS:HG2	3:F:107:ILE:HD12	1.95	0.48
2:E:168:LEU:HD12	2:E:168:LEU:H	1.79	0.48
3:C:307:HIS:HD2	3:C:335:TRP:O	1.95	0.48
2:E:281:ASP:OD1	2:E:283:LYS:HD3	2.13	0.47
3:F:307:HIS:HD2	3:F:335:TRP:O	1.97	0.47
1:A:131:GLN:O	1:A:134:GLN:HG2	2.14	0.47
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.80	0.47
3:F:103:HIS:CE1	3:F:105:SER:HB3	2.50	0.47
1:A:140:VAL:CG1	2:B:172:LEU:HD21	2.45	0.47
2:B:351:ASN:HD22	2:B:351:ASN:C	2.22	0.47
3:C:389:PHE:C	3:C:391:ARG:H	2.22	0.47
2:B:238:VAL:HG22	2:B:239:TYR:N	2.30	0.47
2:E:202:ASN:HD22	2:E:284:ASN:HB2	1.79	0.47
2:B:351:ASN:ND2	2:B:354:MET:H	2.11	0.47
3:C:117:ASN:HD22	3:C:118:ASN:H	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:ASN:C	3:C:117:ASN:ND2	2.69	0.47
3:C:149:THR:CG2	3:C:150:GLY:N	2.77	0.47
2:E:414:GLY:HA3	2:E:434:GLY:O	2.15	0.47
1:A:155:ASP:HB2	1:A:173:VAL:HG21	1.96	0.47
2:B:179:ILE:HD12	3:C:117:ASN:HB2	1.97	0.47
2:B:281:ASP:OD1	2:B:282:GLY:N	2.38	0.47
2:E:226:LEU:HD12	2:E:236:TYR:C	2.40	0.47
2:B:280:THR:O	2:B:281:ASP:C	2.57	0.46
1:A:165:CYS:HB3	2:B:193:CYS:HA	1.97	0.46
2:E:325:HIS:O	2:E:345:TYR:HA	2.15	0.46
1:D:137:GLN:HE21	1:D:189:ILE:HG23	1.78	0.46
4:H:3:ARG:NH2	7:H:5:HOH:O	2.48	0.46
3:C:275:ARG:HA	3:C:311:GLN:HA	1.97	0.46
2:E:166:ARG:HD3	2:E:166:ARG:N	2.16	0.46
2:E:436:VAL:CG1	2:E:437:TRP:N	2.79	0.46
2:B:436:VAL:CG1	2:B:437:TRP:N	2.78	0.46
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.14	0.46
2:E:330:THR:HG22	7:E:477:HOH:O	2.16	0.46
3:F:104:ASP:HB2	3:F:107:ILE:HD12	1.97	0.46
7:E:474:HOH:O	3:F:143:VAL:CG2	2.63	0.46
3:F:118:ASN:HD22	3:F:118:ASN:HA	1.53	0.46
1:A:186:GLU:C	1:A:188:VAL:H	2.23	0.46
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.90	0.46
3:F:373:LYS:HG3	3:F:379:MET:HE1	1.96	0.46
3:C:107:ILE:HB	3:C:108:ARG:NE	2.31	0.45
2:E:161:ILE:HD13	2:E:161:ILE:N	2.29	0.45
2:B:245:GLU:O	2:B:246:ASN:CB	2.65	0.45
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.52	0.45
2:B:175:LEU:O	2:B:178:LYS:HB2	2.17	0.45
2:B:280:THR:O	2:B:282:GLY:N	2.49	0.45
2:E:161:ILE:HD13	2:E:162:PRO:HD3	1.99	0.45
3:F:340:HIS:CE1	4:H:1:GLY:N	2.85	0.45
3:F:289:ALA:HB3	3:F:369:TRP:CE2	2.51	0.45
1:A:180:ASP:O	1:A:184:GLN:CB	2.64	0.45
2:E:281:ASP:CG	2:E:282:GLY:H	2.16	0.45
4:H:2:HIS:CD2	4:H:4:PRO:HD3	2.51	0.45
2:E:357:ALA:O	2:E:365:ARG:HG3	2.17	0.45
1:A:188:VAL:HG12	1:A:188:VAL:O	2.17	0.45
2:E:381:ASP:HB2	2:E:393:GLN:HE21	1.82	0.45
3:F:152:ASP:OD2	3:F:244:TYR:OH	2.33	0.45
1:D:166:SER:HB3	2:E:195:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:ASN:N	2:E:160:ASN:ND2	2.64	0.44
3:F:152:ASP:C	3:F:152:ASP:OD1	2.60	0.44
3:F:340:HIS:ND1	3:F:343:HIS:HB2	2.32	0.44
3:C:198:LEU:HD12	3:C:199:ASP:N	2.32	0.44
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.33	0.44
3:F:195:GLN:HB3	3:F:384:MET:HB2	1.99	0.44
1:A:176:LYS:HA	1:A:179:GLU:OE1	2.17	0.44
2:B:258:GLY:HA2	7:B:500:HOH:O	2.17	0.44
2:B:367:MET:HE2	2:B:406:ARG:NH2	2.32	0.44
1:D:179:GLU:O	1:D:183:LYS:HG3	2.17	0.44
2:E:389:ASP:CG	2:E:392:LYS:HG3	2.43	0.44
3:F:197:ARG:HB2	3:F:382:THR:HB	1.99	0.44
3:F:363:TYR:HB3	4:H:3:ARG:NH2	2.32	0.44
2:B:283:LYS:N	2:B:283:LYS:HD2	2.33	0.44
2:E:159:SER:HA	2:E:162:PRO:CG	2.48	0.44
1:A:137:GLN:O	1:A:140:VAL:HG22	2.18	0.44
3:C:273:LYS:HE2	3:C:317:ASN:HD21	1.83	0.44
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.99	0.44
1:A:180:ASP:O	1:A:184:GLN:HB2	2.17	0.44
2:B:190:MET:HE1	3:C:131:LEU:HA	1.98	0.44
2:B:420:GLY:HA2	2:B:446:SER:O	2.18	0.44
3:C:114:TYR:CD1	3:C:114:TYR:C	2.95	0.44
2:B:345:TYR:CG	2:B:346:ARG:N	2.86	0.43
2:E:299:ILE:O	2:E:303:THR:HG23	2.18	0.43
2:B:397:GLU:O	2:B:398:ALA:HB3	2.18	0.43
3:F:307:HIS:CE1	3:F:342:GLY:H	2.37	0.43
1:D:132:HIS:O	1:D:136:LEU:HB2	2.18	0.43
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.53	0.43
2:B:385:TRP:CH2	2:B:392:LYS:HB3	2.53	0.43
3:C:117:ASN:ND2	3:C:118:ASN:N	2.56	0.43
1:D:178:TYR:O	1:D:182:GLN:HG2	2.19	0.43
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.17	0.43
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.66	0.43
3:C:236:ILE:O	3:C:239:GLN:HG2	2.18	0.43
3:C:336:MET:HE1	3:C:343:HIS:NE2	2.34	0.43
1:D:136:LEU:HD22	1:D:136:LEU:HA	1.84	0.43
7:E:530:HOH:O	3:F:220:PRO:HD2	2.18	0.43
1:D:140:VAL:HG11	2:E:172:LEU:HD21	1.99	0.42
1:D:151:GLU:HG2	1:D:173:VAL:HG13	2.01	0.42
2:E:253:GLN:NE2	2:E:451:SER:HA	2.34	0.42
1:D:181:GLN:OE1	2:E:174:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:SER:HB2	2:B:404:TYR:CE2	2.54	0.42
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.85	0.42
3:C:389:PHE:C	3:C:391:ARG:N	2.76	0.42
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.20	0.42
2:B:314:MET:HE1	2:B:437:TRP:CE3	2.54	0.42
2:B:367:MET:HB2	2:B:406:ARG:HB3	2.01	0.42
3:C:113:ILE:HG22	3:C:113:ILE:O	2.18	0.42
3:F:192:THR:HG21	3:F:236:ILE:HD13	2.00	0.42
1:A:151:GLU:CG	1:A:173:VAL:HG13	2.50	0.42
3:C:108:ARG:N	3:C:108:ARG:CD	2.73	0.42
1:D:185:LEU:HG	1:D:189:ILE:HD11	2.01	0.42
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.19	0.42
2:E:397:GLU:O	2:E:398:ALA:HB3	2.19	0.42
3:C:227:TRP:C	3:C:228:LEU:O	2.60	0.42
3:F:340:HIS:CE1	3:F:343:HIS:HB2	2.54	0.42
3:F:189:ASN:OD1	3:F:391:ARG:HG3	2.20	0.42
3:C:268:GLY:O	3:C:274:TYR:HA	2.20	0.42
2:E:163:THR:C	2:E:165:LEU:H	2.28	0.42
2:E:174:ASN:HD21	2:E:178:LYS:HZ3	1.66	0.42
3:F:186:GLY:C	3:F:188:GLY:H	2.28	0.42
5:J:2:NAG:H83	5:J:2:NAG:H3	2.02	0.42
2:E:229:PRO:HB3	2:E:301:GLN:HE22	1.84	0.41
3:F:105:SER:HA	3:F:108:ARG:NE	2.35	0.41
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.55	0.41
3:F:172:LEU:HD13	3:F:239:GLN:HB2	2.01	0.41
3:F:329:GLN:HE22	4:H:3:ARG:HH11	1.63	0.41
2:E:312:ILE:HA	2:E:451:SER:O	2.21	0.41
2:B:317:TRP:CE3	2:B:448:ARG:HD3	2.56	0.41
3:C:229:GLY:H	3:C:232:LYS:HD2	1.85	0.41
3:C:248:VAL:O	3:C:259:THR:HA	2.20	0.41
2:E:389:ASP:HB3	2:E:392:LYS:CD	2.50	0.41
1:A:144:LEU:HD23	2:B:175:LEU:HD11	2.03	0.41
2:E:367:MET:HB2	2:E:406:ARG:HB2	2.03	0.41
2:B:266:TRP:HA	2:B:377:THR:HG21	2.02	0.41
2:E:345:TYR:CG	2:E:346:ARG:N	2.88	0.41
2:E:402:TRP:CG	2:E:403:TRP:N	2.89	0.41
2:B:400:GLY:HA3	2:B:413:ASN:O	2.21	0.41
3:C:230:ASN:HD22	3:C:230:ASN:HA	1.67	0.41
1:D:151:GLU:CG	1:D:173:VAL:HG13	2.51	0.41
2:E:167:VAL:HG22	2:E:168:LEU:HD12	2.03	0.41
2:E:174:ASN:ND2	2:E:178:LYS:HZ3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:106:SER:O	3:F:110:LEU:HD13	2.21	0.41
3:F:143:VAL:O	3:F:143:VAL:HG23	2.21	0.41
3:F:242:ILE:HA	3:F:243:PRO:HD2	1.95	0.41
3:F:304:PHE:O	3:F:337:ASN:HB3	2.20	0.41
7:B:473:HOH:O	3:C:143:VAL:HG22	2.21	0.41
3:C:152:ASP:OD1	3:C:152:ASP:C	2.64	0.41
1:D:140:VAL:CG1	2:E:172:LEU:HD21	2.51	0.41
3:C:245:ALA:HB2	3:C:389:PHE:HD1	1.86	0.40
2:E:448:ARG:HG2	2:E:448:ARG:NH1	2.33	0.40
3:F:152:ASP:OD1	3:F:154:GLN:N	2.55	0.40
1:D:150:LEU:HD21	3:F:124:LEU:HD23	2.02	0.40
2:E:253:GLN:C	2:E:253:GLN:HE21	2.29	0.40
3:F:263:ALA:HB1	3:F:264:MET:HE2	2.03	0.40
2:B:373:MET:HA	2:B:373:MET:HE3	2.03	0.40
2:E:238:VAL:HG21	2:E:250:THR:CG2	2.50	0.40
2:E:432:ASP:O	2:E:432:ASP:CG	2.64	0.40
1:A:186:GLU:OE1	1:A:189:ILE:HD12	2.22	0.40
2:B:229:PRO:HD2	2:B:233:VAL:CG2	2.49	0.40
3:C:304:PHE:CD1	3:C:338:LYS:HE3	2.57	0.40
1:D:134:GLN:H	1:D:134:GLN:HG2	1.74	0.40
3:F:229:GLY:O	3:F:233:ILE:HG13	2.21	0.40
1:A:166:SER:CB	2:B:195:THR:HG23	2.49	0.40
2:B:230:ASP:H	2:B:233:VAL:HG22	1.86	0.40
2:B:352:ALA:HB2	2:B:439:ASN:ND2	2.37	0.40
3:F:156:ILE:HG22	3:F:161:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/66 (88%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	61/66 (92%)	58 (95%)	2 (3%)	1 (2%)	7	7
2	B	292/313 (93%)	272 (93%)	17 (6%)	3 (1%)	12	14
2	E	299/313 (96%)	278 (93%)	18 (6%)	3 (1%)	12	14
3	C	286/311 (92%)	271 (95%)	15 (5%)	0	100	100
3	F	289/311 (93%)	272 (94%)	15 (5%)	2 (1%)	18	24
4	G	2/4 (50%)	2 (100%)	0	0	100	100
4	H	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1289/1388 (93%)	1208 (94%)	72 (6%)	9 (1%)	18	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	281	ASP
2	B	387	THR
2	E	281	ASP
3	F	240	SER
2	B	256	GLN
2	E	160	ASN
2	E	256	GLN
3	F	370	ALA
1	D	189	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	55/61 (90%)	53 (96%)	2 (4%)	31	45
1	D	58/61 (95%)	53 (91%)	5 (9%)	10	11
2	B	251/270 (93%)	245 (98%)	6 (2%)	43	58
2	E	258/270 (96%)	243 (94%)	15 (6%)	18	27
3	C	242/259 (93%)	231 (96%)	11 (4%)	24	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	245/259 (95%)	236 (96%)	9 (4%)	30	44
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1115/1186 (94%)	1065 (96%)	50 (4%)	24	37

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	175	LEU
2	B	210	GLU
2	B	245	GLU
2	B	252	ILE
2	B	253	GLN
2	B	280	THR
2	B	321	LYS
3	C	108	ARG
3	C	111	GLN
3	C	117	ASN
3	C	140	LYS
3	C	143	VAL
3	C	175	ASN
3	C	254	ASN
3	C	301	ASP
3	C	317	ASN
3	C	323	GLU
3	C	382	THR
1	D	133	ILE
1	D	134	GLN
1	D	136	LEU
1	D	140	VAL
1	D	176	LYS
2	E	161	ILE
2	E	166	ARG
2	E	180	GLN
2	E	195	THR
2	E	196	PRO
2	E	210	GLU
2	E	224	MET
2	E	230	ASP
2	E	233	VAL

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Mol	Chain	Res	Type
2	E	252	ILE
2	E	253	GLN
2	E	321	LYS
2	E	325	HIS
2	E	330	THR
2	E	366	THR
3	F	117	ASN
3	F	118	ASN
3	F	134	GLN
3	F	143	VAL
3	F	172	LEU
3	F	198	LEU
3	F	239	GLN
3	F	317	ASN
3	F	382	THR
4	G	3	ARG
4	H	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	134	GLN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
2	B	180	GLN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	332	GLN
2	B	339	GLN
2	B	351	ASN
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	118	ASN
3	C	130	GLN
3	C	136	GLN

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Mol	Chain	Res	Type
3	C	146	HIS
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	329	GLN
1	D	137	GLN
1	D	139	ASN
1	D	181	GLN
1	D	184	GLN
2	E	160	ASN
2	E	164	ASN
2	E	174	ASN
2	E	180	GLN
2	E	189	GLN
2	E	202	ASN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	332	GLN
2	E	339	GLN
2	E	351	ASN
2	E	393	GLN
2	E	408	HIS
2	E	429	HIS
2	E	439	ASN
3	F	103	HIS
3	F	111	GLN
3	F	117	ASN
3	F	118	ASN
3	F	130	GLN
3	F	136	GLN
3	F	177	GLN
3	F	230	ASN

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Mol	Chain	Res	Type
3	F	239	GLN
3	F	254	ASN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN
4	G	2	HIS

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](#)

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	$\# Z > 2$
5	NAG	I	1	2,5	14,14,15	0.71	0	17,19,21	1.27	2 (11%)
5	NAG	I	2	5	14,14,15	0.61	0	17,19,21	0.65	1 (5%)
5	NAG	J	1	2,5	14,14,15	0.62	0	17,19,21	0.79	0
5	NAG	J	2	5	14,14,15	0.67	0	17,19,21	0.57	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
5	NAG	I	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	J	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	NAG	C4-C3-C2	2.91	115.28	111.02
5	I	1	NAG	C3-C4-C5	2.46	114.70	110.23
5	I	2	NAG	C2-N2-C7	-2.07	120.13	122.90

There are no chirality outliers.

All (15) torsion outliers are listed below:

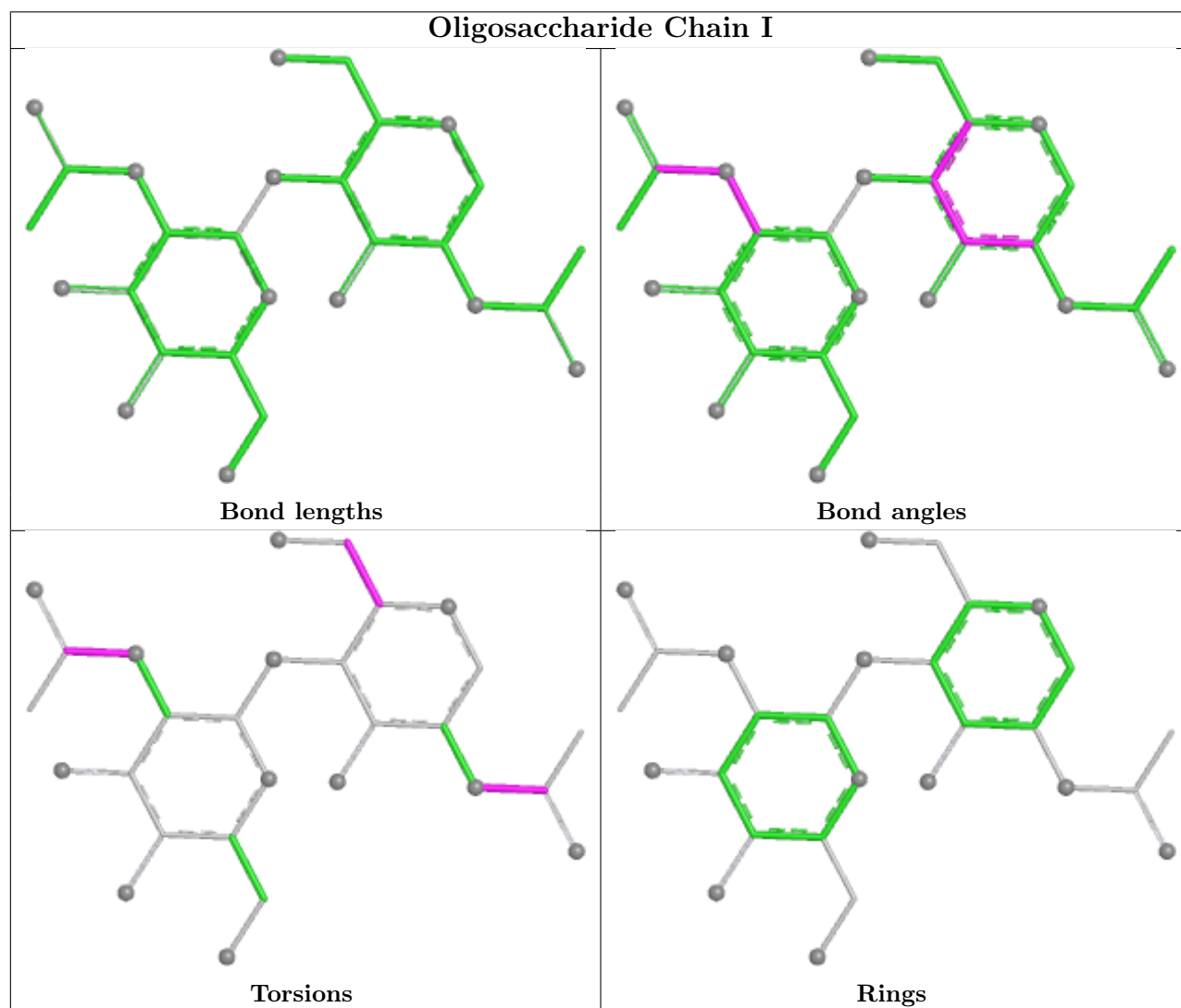
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C3-C2-N2-C7
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	J	1	NAG	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6

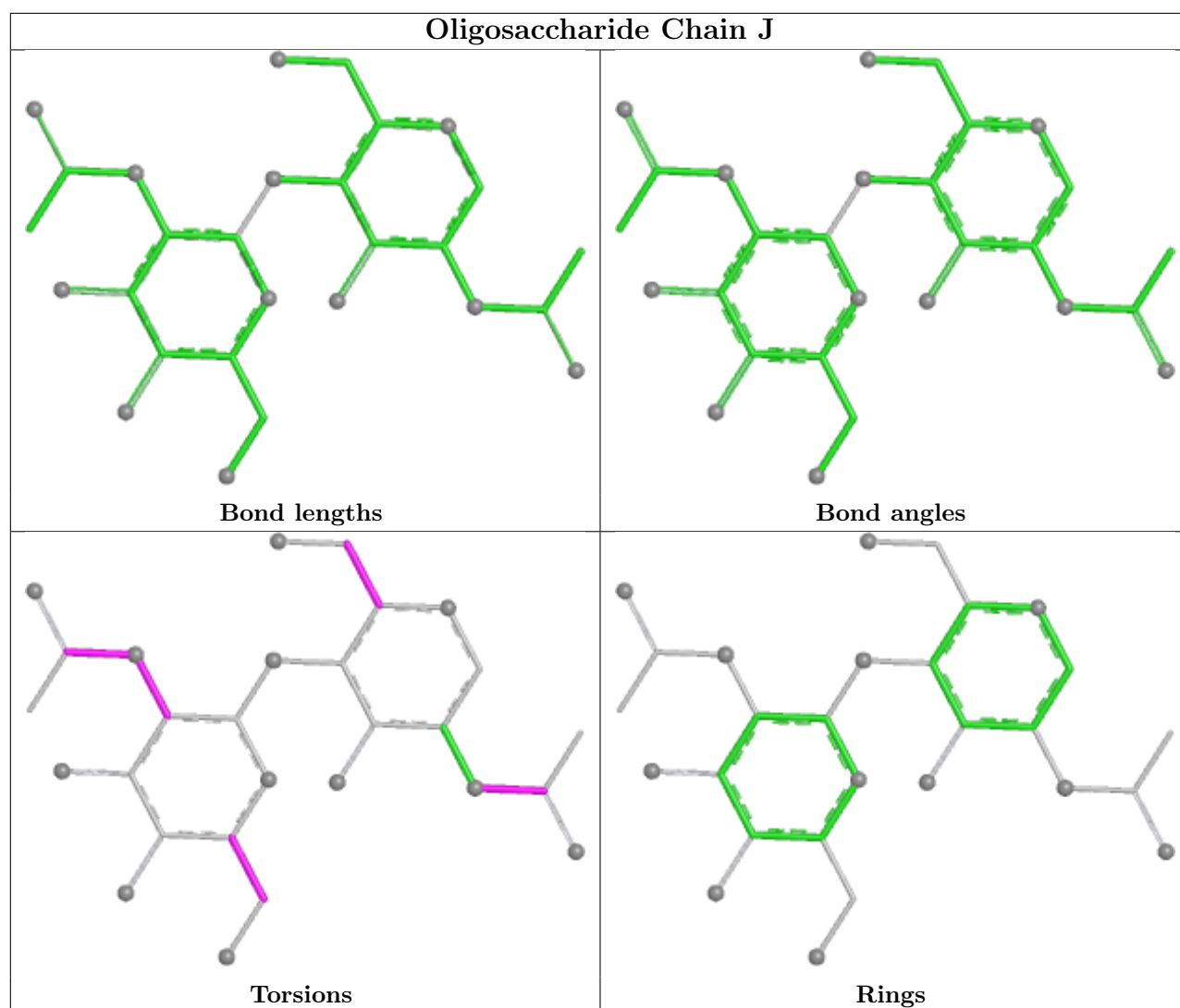
There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2	NAG	1	0
5	I	1	NAG	1	0
5	I	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 ⓘ

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	60/66 (90%)	1.10	13 (21%)	2 2	32, 73, 110, 113	0
1	D	63/66 (95%)	0.32	5 (7%)	18 16	27, 45, 93, 99	0
2	B	294/313 (93%)	-0.00	18 (6%)	27 24	20, 33, 84, 114	0
2	E	301/313 (96%)	-0.08	19 (6%)	26 23	22, 33, 73, 112	0
3	C	288/311 (92%)	-0.18	15 (5%)	33 30	19, 30, 65, 115	0
3	F	291/311 (93%)	-0.02	15 (5%)	33 30	21, 35, 58, 108	0
4	G	4/4 (100%)	0.47	0	100 100	33, 35, 46, 50	0
4	H	4/4 (100%)	0.39	0	100 100	25, 31, 34, 46	0
All	All	1305/1388 (94%)	0.01	85 (6%)	25 22	19, 34, 87, 115	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130	VAL	6.2
1	A	190	ALA	6.1
2	B	165	LEU	5.4
2	B	167	VAL	5.0
2	E	459	PRO	4.9
1	D	129	LYS	4.7
3	C	107	ILE	4.7
3	F	393	THR	4.6
2	B	458	PHE	4.6
3	C	113	ILE	4.2
1	A	135	LEU	4.2
2	B	391	ARG	4.1
2	E	161	ILE	4.1
3	C	109	TYR	4.0
2	E	165	LEU	3.8
3	F	103	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	389	ASP	3.7
2	E	159	SER	3.6
2	B	166	ARG	3.6
3	C	110	LEU	3.5
3	F	242	ILE	3.4
2	E	162	PRO	3.4
2	E	163	THR	3.4
3	F	107	ILE	3.3
3	F	109	TYR	3.3
2	B	385	TRP	3.3
2	B	392	LYS	3.3
1	A	133	ILE	3.2
1	A	131	GLN	3.2
3	C	106	SER	3.2
3	F	117	ASN	3.1
2	B	390	PRO	3.0
2	B	168	LEU	3.0
3	C	117	ASN	3.0
3	F	113	ILE	3.0
2	E	281	ASP	2.9
2	E	160	ASN	2.9
2	B	280	THR	2.8
2	E	233	VAL	2.8
2	E	386	LEU	2.8
3	F	163	GLN	2.8
1	A	132	HIS	2.8
2	E	458	PHE	2.7
2	B	361	MET	2.7
3	F	104	ASP	2.7
2	E	390	PRO	2.7
2	E	164	ASN	2.7
1	D	190	ALA	2.6
2	B	171	ILE	2.5
3	C	114	TYR	2.5
1	A	136	LEU	2.5
2	B	195	THR	2.5
3	C	108	ARG	2.4
3	C	393	THR	2.4
3	C	242	ILE	2.4
3	F	106	SER	2.3
3	C	360	PRO	2.3
1	A	137	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	110	LEU	2.3
2	E	230	ASP	2.3
1	A	134	GLN	2.3
1	A	175	LEU	2.3
2	B	386	LEU	2.3
1	A	183	LYS	2.3
1	A	182	GLN	2.2
3	F	224	THR	2.2
1	D	189	ILE	2.2
3	C	116	SER	2.2
1	A	140	VAL	2.2
2	B	172	LEU	2.2
3	C	240	SER	2.2
2	B	173	GLU	2.2
1	D	131	GLN	2.1
3	F	108	ARG	2.1
3	C	301	ASP	2.1
2	E	392	LYS	2.1
1	A	181	GLN	2.1
2	E	387	THR	2.1
2	E	167	VAL	2.1
2	B	180	GLN	2.0
3	C	111	GLN	2.0
2	E	168	LEU	2.0
3	F	172	LEU	2.0
2	E	280	THR	2.0
3	F	240	SER	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
5	NAG	I	2	14/15	0.29	0.22	110,112,113,113	0

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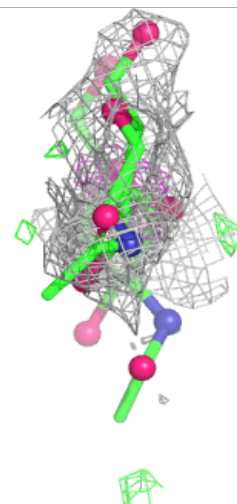
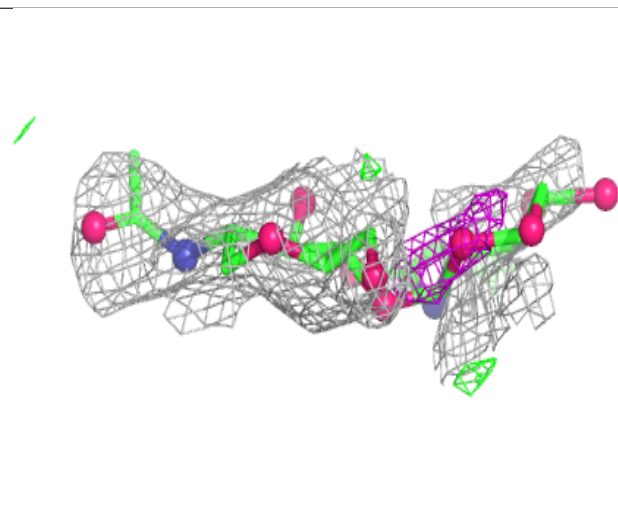
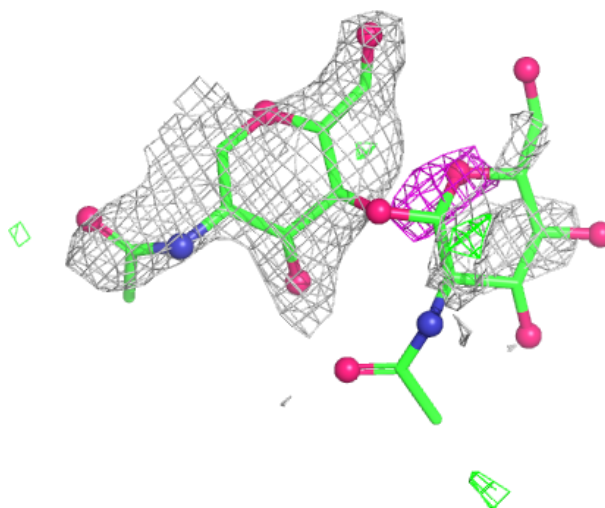
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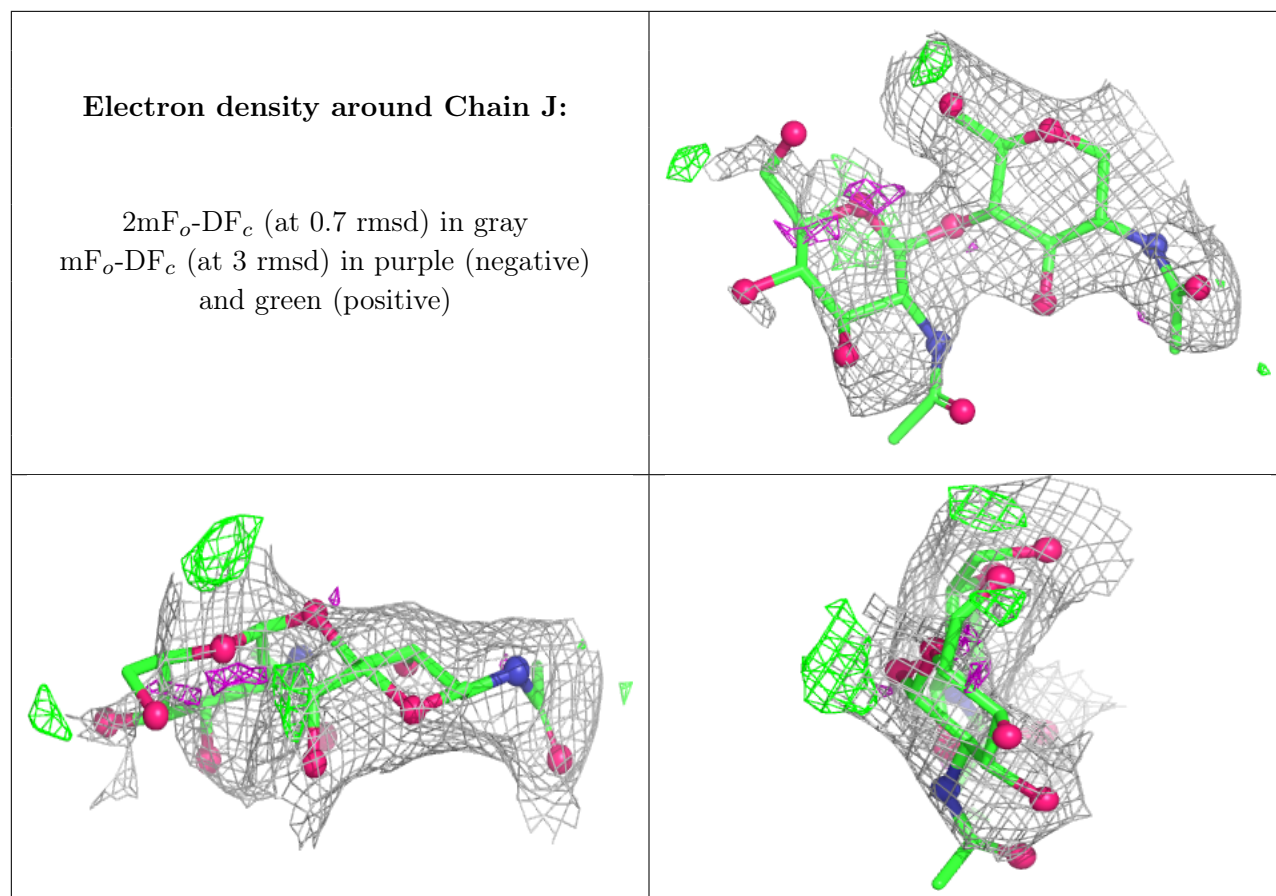
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	J	2	14/15	0.46	0.18	79,84,87,88	0
5	NAG	I	1	14/15	0.51	0.18	93,96,99,105	0
5	NAG	J	1	14/15	0.72	0.13	56,61,66,74	0

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

Electron density around Chain I:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	E	472	1/1	0.94	0.04	46,46,46,46	0
6	CA	C	407	1/1	0.95	0.04	32,32,32,32	0
6	CA	B	472	1/1	0.95	0.06	44,44,44,44	0
6	CA	C	408	1/1	0.97	0.04	31,31,31,31	0
6	CA	F	407	1/1	0.99	0.02	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.