



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:44 PM UTC

PDB ID : 2OYI / pdb_00002oyi
Title : Crystal Structure of Fragment D of gammaD298,301A Fibrinogen with the Peptide Ligand Gly-Pro-Arg-Pro-Amide
Authors : Kostelansky, M.S.; Gorkun, O.V.; Lord, S.T.
Deposited on : 2007-02-22
Resolution : 2.70 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

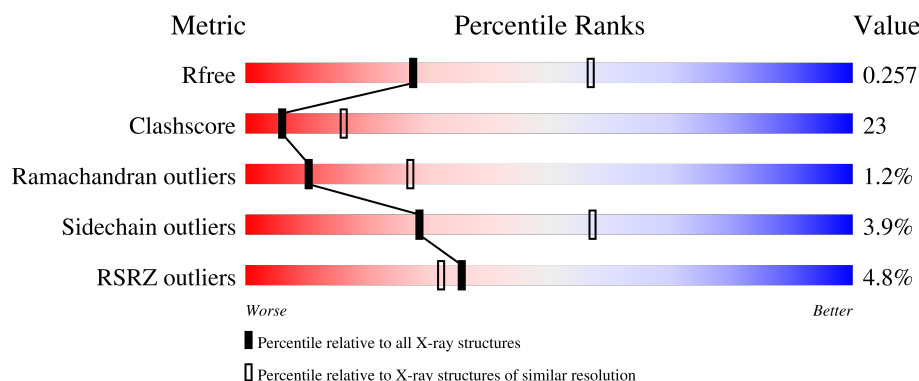
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
1	D	66	
2	B	313	
2	E	313	
3	C	311	

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Mol	Chain	Length	Quality of chain
3	F	311	
4	G	4	
4	H	4	
4	I	4	
4	J	4	
5	K	3	
5	L	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	L	1	-	-	X	-
5	FUC	L	3	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10784 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	0	0
			530	327	100	100	3			
1	D	56	Total	C	N	O	S	0	0	0
			458	280	87	88	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	301	Total	C	N	O	S	0	0	0
			2414	1505	427	460	22			
2	E	294	Total	C	N	O	S	0	0	0
			2362	1475	417	448	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	299	Total	C	N	O	S	0	0	0
			2393	1521	403	458	11			
3	F	285	Total	C	N	O	S	0	0	0
			2277	1448	384	434	11			

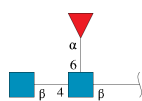
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	298	ALA	ASP	engineered mutation	UNP P02679
C	301	ALA	ASP	engineered mutation	UNP P02679
F	298	ALA	ASP	engineered mutation	UNP P02679
F	301	ALA	ASP	engineered mutation	UNP P02679

- Molecule 4 is a protein called GPRP Peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	4	Total C N O 30 18 7 5	0	0	0
4	H	4	Total C N O 30 18 7 5	0	0	0
4	I	4	Total C N O 30 18 7 5	0	0	0
4	J	4	Total C N O 30 18 7 5	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	K	3	Total C N O 38 22 2 14	0	0	0
5	L	3	Total C N O 38 22 2 14	0	0	0

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	27	Total O 27 27	0	0
7	C	18	Total O 18 18	0	0

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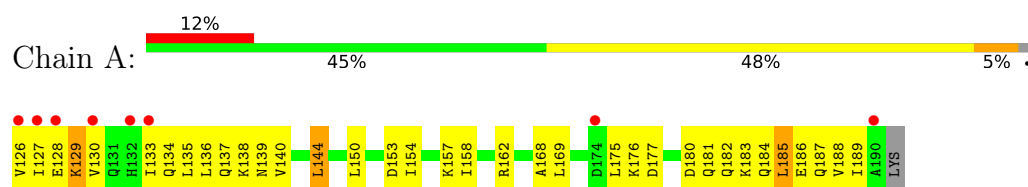
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	5	Total 5	O 5	0	0
7	E	63	Total 63	O 63	0	0
7	F	33	Total 33	O 33	0	0
7	I	1	Total 1	O 1	0	0

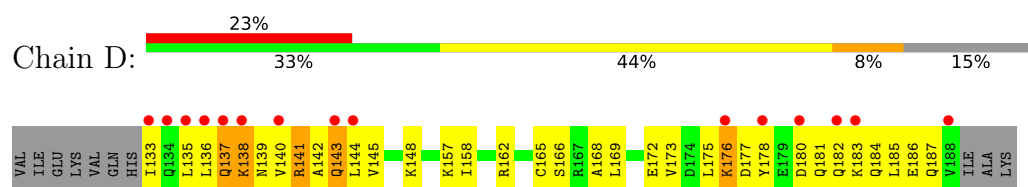
3 Residue-property plots [i](#)

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.

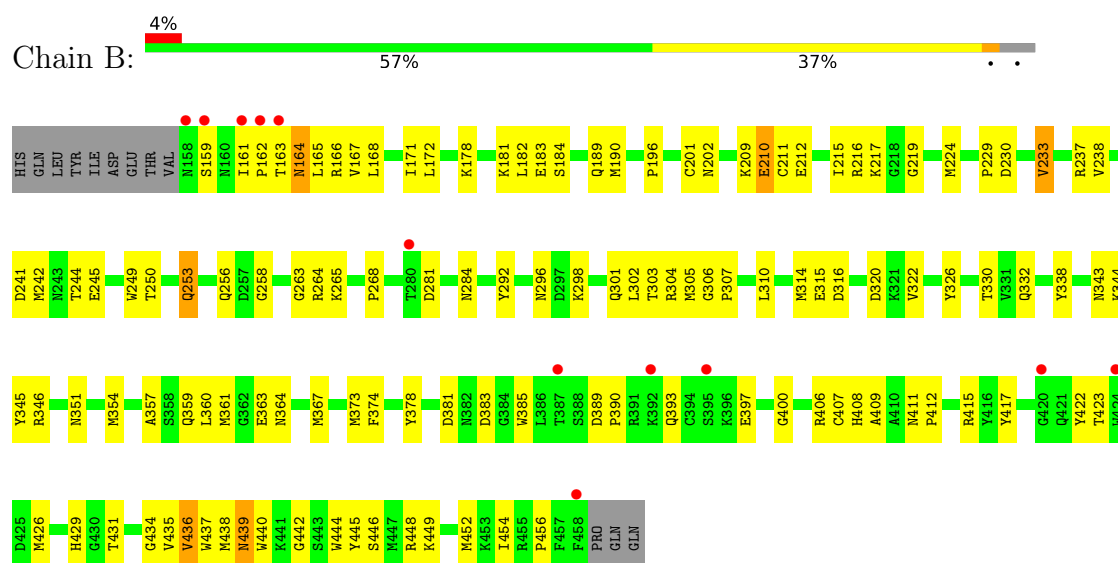
- Molecule 1: Fibrinogen alpha chain



- Molecule 1: Fibrinogen alpha chain



- Molecule 2: Fibrinogen beta chain



- Molecule 2: Fibrinogen beta chain





- Molecule 4: GPRP Peptide



- Molecule 4: GPRP Peptide



- Molecule 4: GPRP Peptide



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.99Å 94.04Å 226.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.97 – 2.70 17.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (17.97-2.70) 98.1 (17.97-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.70Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.256 0.218 , 0.257	Depositor DCC
R_{free} test set	2634 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.0	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	0.92	EDS
Total number of atoms	10784	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.96% 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: CA, NAG, FUC

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	0.38	0/531	0.82	0/709
1	D	0.37	0/458	0.89	2/610 (0.3%)
2	B	0.40	0/2475	0.93	4/3342 (0.1%)
2	E	0.44	0/2422	0.97	8/3268 (0.2%)
3	C	0.38	0/2459	0.86	6/3327 (0.2%)
3	F	0.42	0/2340	0.90	2/3165 (0.1%)
4	G	0.51	0/31	0.93	0/40
4	H	0.51	0/31	0.87	0/40
4	I	0.70	0/31	0.94	0/40
4	J	0.72	0/31	0.97	0/40
All	All	0.41	0/10809	0.91	22/14581 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	409	ALA	N-CA-C	-10.38	101.17	114.04
2	B	409	ALA	N-CA-C	-9.51	102.04	114.31
2	E	399	GLY	N-CA-C	9.47	128.73	114.61
2	E	194	ARG	N-CA-C	-6.96	104.78	113.28
1	D	143	GLN	N-CA-C	-6.72	105.71	114.04
3	C	341	ALA	N-CA-C	-6.70	105.73	114.04
1	D	141	ARG	N-CA-C	-6.27	105.48	113.01
2	E	197	CYS	N-CA-C	-6.12	102.29	110.55
2	E	444	TRP	N-CA-C	5.98	120.38	112.25
3	C	368	ILE	N-CA-C	5.69	117.31	109.46
3	C	303	PHE	N-CA-C	5.65	122.83	110.80
3	C	298	ALA	CA-C-N	5.61	125.13	119.19
3	C	298	ALA	C-N-CA	5.61	125.13	119.19
2	B	448	ARG	N-CA-C	-5.60	106.58	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	340	HIS	N-CA-C	5.57	117.31	108.79
2	B	436	VAL	N-CA-C	5.53	117.55	108.97
2	E	436	VAL	N-CA-C	5.51	117.34	108.85
3	F	341	ALA	N-CA-C	-5.50	107.22	114.31
2	B	292	TYR	N-CA-C	5.38	116.31	108.14
2	E	448	ARG	N-CA-C	-5.17	106.12	112.90
2	E	388	SER	N-CA-C	-5.11	107.01	114.12
3	F	298	ALA	N-CA-C	5.07	114.65	108.11

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	530	0	556	50	0
1	D	458	0	477	47	0
2	B	2414	0	2279	122	0
2	E	2362	0	2231	97	0
3	C	2393	0	2248	88	0
3	F	2277	0	2140	110	0
4	G	30	0	32	4	0
4	H	30	0	32	6	0
4	I	30	0	32	4	0
4	J	30	0	32	4	0
5	K	38	0	34	5	0
5	L	38	0	34	11	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	3	0	0	0	0
7	B	27	0	0	4	0
7	C	18	0	0	3	0
7	D	5	0	0	0	0
7	E	63	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	33	0	0	2	0
7	I	1	0	0	0	0
All	All	10784	0	10127	471	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 23.

All (471) 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)
5:L:1:NAG:H62	5:L:2:NAG:H2	1.30	1.11
2:B:397:GLU:HB3	2:B:431:THR:HG21	1.40	1.04
1:A:188:VAL:HG11	2:B:167:VAL:HG21	1.35	1.03
2:E:165:LEU:HD11	2:E:168:LEU:HD22	1.49	0.94
4:G:3:ARG:HG3	4:G:4:PRO:HD2	1.51	0.91
3:F:172:LEU:H	3:F:239:GLN:HE21	1.15	0.88
2:B:423:THR:H	2:B:426:MET:HE3	1.38	0.86
3:C:322:PHE:CZ	4:G:3:ARG:HG2	2.10	0.86
5:L:1:NAG:H61	5:L:3:FUC:H5	1.54	0.85
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.26	0.82
2:E:168:LEU:HD21	3:F:110:LEU:HB2	1.60	0.82
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.62	0.82
1:A:176:LYS:HE2	1:A:180:ASP:OD1	1.79	0.82
3:F:119:GLN:HE21	3:F:119:GLN:HA	1.45	0.81
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.44	0.81
3:C:393:THR:O	3:C:394:ILE:HG22	1.80	0.80
2:E:168:LEU:O	2:E:172:LEU:HB2	1.82	0.79
2:B:345:TYR:HB2	2:B:354:MET:HE3	1.64	0.78
3:F:307:HIS:HE1	3:F:341:ALA:H	1.32	0.78
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.49	0.77
2:B:415:ARG:O	2:B:434:GLY:HA2	1.84	0.77
1:A:130:VAL:O	1:A:134:GLN:HG3	1.85	0.76
1:D:185:LEU:HD13	1:D:185:LEU:O	1.86	0.76
2:E:321:LYS:HB3	2:E:321:LYS:HZ3	1.51	0.75
2:E:423:THR:N	2:E:426:MET:HE3	2.02	0.74
5:L:1:NAG:C6	5:L:2:NAG:H2	2.15	0.73
2:E:191:GLU:HG2	2:E:194:ARG:HH11	1.53	0.73
2:E:172:LEU:HB3	3:F:113:ILE:HG21	1.69	0.72
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.05	0.72
1:A:188:VAL:HG11	2:B:167:VAL:CG2	2.17	0.71
1:A:128:GLU:HG2	1:A:129:LYS:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:THR:N	2:B:426:MET:HE3	2.05	0.71
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.71	0.71
3:C:365:ASN:HD22	3:C:365:ASN:H	1.37	0.70
3:F:254:ASN:HB2	3:F:256:ARG:HH21	1.56	0.70
1:D:178:TYR:O	1:D:182:GLN:HG3	1.91	0.70
2:B:351:ASN:ND2	2:B:354:MET:H	1.90	0.70
2:B:163:THR:HA	2:B:166:ARG:HD2	1.74	0.70
5:L:1:NAG:H61	5:L:3:FUC:H3	1.74	0.70
1:D:140:VAL:HG11	2:E:172:LEU:HD11	1.74	0.69
3:F:241:ALA:O	3:F:242:ILE:HG12	1.91	0.69
1:A:188:VAL:CG1	2:B:167:VAL:HG21	2.17	0.69
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.75	0.69
2:B:351:ASN:HD22	2:B:351:ASN:C	2.00	0.69
2:E:321:LYS:HB3	2:E:321:LYS:NZ	2.09	0.68
4:H:4:PRO:HG3	5:K:1:NAG:H62	1.76	0.68
3:F:263:ALA:HB1	3:F:264:MET:HE2	1.76	0.68
2:B:202:ASN:HD22	2:B:284:ASN:HD22	1.40	0.68
2:B:212:GLU:HG3	2:B:216:ARG:HH11	1.59	0.68
2:B:351:ASN:HD21	2:B:354:MET:H	1.41	0.68
5:L:1:NAG:H61	5:L:3:FUC:C5	2.23	0.68
1:A:127:ILE:HG12	1:A:128:GLU:H	1.59	0.67
1:D:157:LYS:HE2	3:F:132:GLU:OE2	1.94	0.67
2:B:230:ASP:O	2:B:233:VAL:HG22	1.94	0.67
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.08	0.67
3:C:254:ASN:HD22	3:C:256:ARG:HH12	1.41	0.66
2:E:190:MET:HE3	3:F:131:LEU:HA	1.76	0.66
2:E:438:MET:HE3	2:E:443:SER:OG	1.94	0.66
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.78	0.66
1:A:185:LEU:HD22	1:A:189:ILE:HD11	1.78	0.66
2:B:316:ASP:HB2	2:B:445:TYR:OH	1.95	0.66
1:D:173:VAL:HG12	1:D:175:LEU:HD22	1.76	0.66
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.78	0.66
2:B:359:GLN:O	2:B:360:LEU:HD23	1.96	0.65
2:E:210:GLU:OE1	2:E:212:GLU:HB3	1.97	0.65
3:C:261:ASP:OD2	3:C:392:LEU:HD21	1.96	0.65
3:C:307:HIS:HE1	3:C:341:ALA:H	1.43	0.65
3:C:241:ALA:O	3:C:243:PRO:HD3	1.97	0.65
3:C:307:HIS:CE1	3:C:341:ALA:H	2.15	0.65
1:D:138:LYS:H	1:D:138:LYS:HD3	1.63	0.64
2:E:212:GLU:O	2:E:215:ILE:HG22	1.96	0.64
3:F:307:HIS:CE1	3:F:341:ALA:H	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:LEU:HD13	3:F:113:ILE:HD12	1.79	0.64
3:C:247:ARG:NH2	3:C:392:LEU:HD11	2.12	0.63
3:F:365:ASN:HD22	3:F:365:ASN:H	1.45	0.63
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.98	0.63
3:F:172:LEU:N	3:F:239:GLN:HE21	1.92	0.63
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.62	0.63
3:F:338:LYS:N	3:F:339:CYS:HA	2.13	0.63
2:B:439:ASN:H	2:B:439:ASN:HD22	1.47	0.62
1:D:169:LEU:H	2:E:189:GLN:NE2	1.96	0.62
1:A:128:GLU:HG2	1:A:129:LYS:H	1.63	0.62
1:A:157:LYS:HE3	3:C:132:GLU:OE2	1.99	0.62
2:B:343:ASN:OD1	2:B:344:LYS:HE2	1.99	0.62
3:F:321:LYS:O	3:F:338:LYS:HD3	1.98	0.62
1:A:127:ILE:HG22	1:A:130:VAL:HG23	1.81	0.62
3:C:338:LYS:N	3:C:339:CYS:HA	2.13	0.62
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.63	0.62
1:D:157:LYS:HD3	3:F:132:GLU:HG3	1.82	0.62
2:E:346:ARG:HG3	2:E:346:ARG:HH11	1.64	0.61
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.00	0.61
3:F:389:PHE:C	3:F:391:ARG:H	2.08	0.61
1:A:133:ILE:O	1:A:137:GLN:HG3	2.00	0.61
4:I:3:ARG:HG3	4:I:4:PRO:HD2	1.82	0.61
1:A:127:ILE:HG12	1:A:128:GLU:OE2	2.00	0.61
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.66	0.60
2:B:345:TYR:CG	2:B:346:ARG:N	2.69	0.60
3:F:118:ASN:O	3:F:122:VAL:HG23	2.01	0.60
2:B:367:MET:HE2	2:B:406:ARG:HD3	1.83	0.60
3:C:252:ASP:OD2	3:C:256:ARG:HB2	2.01	0.60
2:E:245:GLU:OE2	2:E:323:LYS:NZ	2.33	0.60
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.65	0.60
2:B:397:GLU:OE1	4:H:3:ARG:NH1	2.34	0.60
1:D:176:LYS:HG3	1:D:180:ASP:OD2	2.01	0.60
2:B:209:LYS:HD2	2:B:305:MET:HE1	1.84	0.59
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.37	0.59
1:A:144:LEU:HD13	1:A:182:GLN:HG2	1.84	0.59
7:E:476:HOH:O	3:F:138:PRO:HG3	2.02	0.59
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.38	0.59
1:D:185:LEU:HB2	2:E:171:ILE:CD1	2.32	0.59
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.68	0.58
2:E:253:GLN:NE2	2:E:451:SER:HA	2.18	0.58
3:C:197:ARG:HG2	3:C:382:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:ND2	2:B:284:ASN:HD22	2.01	0.58
3:F:172:LEU:HD22	3:F:239:GLN:NE2	2.18	0.58
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.85	0.58
2:E:423:THR:H	2:E:426:MET:HE3	1.67	0.58
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.17	0.58
1:A:126:VAL:HG13	1:A:126:VAL:O	2.03	0.58
1:A:127:ILE:CG2	1:A:130:VAL:H	2.16	0.58
3:F:192:THR:HG23	3:F:386:ILE:HG13	1.86	0.58
2:E:168:LEU:CD2	3:F:110:LEU:HB2	2.33	0.57
1:A:169:LEU:H	2:B:189:GLN:HE22	1.51	0.57
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.70	0.57
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.86	0.57
5:L:1:NAG:H61	5:L:3:FUC:C3	2.34	0.57
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.52	0.57
3:C:365:ASN:H	3:C:365:ASN:ND2	2.03	0.57
1:D:136:LEU:O	1:D:139:ASN:N	2.38	0.57
1:D:143:GLN:HE22	3:F:117:ASN:HB2	1.69	0.57
3:F:276:LEU:HD23	3:F:276:LEU:C	2.30	0.57
1:A:185:LEU:HD22	1:A:189:ILE:CD1	2.35	0.56
2:E:408:HIS:C	2:E:408:HIS:CD2	2.83	0.56
5:L:1:NAG:H62	5:L:2:NAG:C2	2.20	0.56
3:F:322:PHE:CZ	4:I:3:ARG:HG2	2.41	0.56
3:F:205:LYS:NZ	3:F:205:LYS:HB3	2.21	0.56
3:C:325:ASN:C	3:C:325:ASN:HD22	2.14	0.56
2:E:165:LEU:CD1	2:E:168:LEU:HD22	2.31	0.56
2:E:283:LYS:HE2	2:E:283:LYS:HA	1.88	0.55
3:F:200:GLY:HA2	7:F:409:HOH:O	2.05	0.55
3:F:268:GLY:O	3:F:274:TYR:HA	2.05	0.55
2:B:165:LEU:HD21	3:C:107:ILE:HD13	1.89	0.55
3:C:288:ASP:O	3:C:371:THR:HG21	2.07	0.55
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.71	0.55
3:F:224:THR:HG23	7:F:413:HOH:O	2.07	0.55
3:F:291:ASP:O	3:F:302:LYS:HD2	2.07	0.55
1:A:127:ILE:HG22	1:A:130:VAL:CG2	2.37	0.55
2:B:422:TYR:O	2:B:444:TRP:HB3	2.07	0.55
2:B:201:CYS:O	3:C:143:VAL:HG11	2.07	0.54
3:C:387:ILE:HG12	3:C:388:PRO:HD2	1.89	0.54
3:F:206:LYS:HD2	3:F:210:GLN:CD	2.31	0.54
2:B:201:CYS:C	3:C:143:VAL:HG11	2.31	0.54
2:B:345:TYR:CB	2:B:354:MET:HE3	2.37	0.54
1:A:181:GLN:OE1	2:B:171:ILE:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:ASN:ND2	2:B:351:ASN:C	2.63	0.54
2:B:212:GLU:HG3	2:B:216:ARG:NH1	2.23	0.54
1:A:177:ASP:O	1:A:181:GLN:HG3	2.07	0.54
3:C:273:LYS:HB2	3:C:311:GLN:HB3	1.89	0.54
2:B:161:ILE:H	2:B:161:ILE:HD12	1.73	0.54
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.42	0.54
3:C:365:ASN:HD22	3:C:365:ASN:N	2.00	0.54
1:D:136:LEU:O	1:D:137:GLN:C	2.51	0.54
2:E:280:THR:HB	2:E:283:LYS:HG3	1.89	0.53
3:F:254:ASN:HD22	3:F:256:ARG:NH2	2.07	0.53
2:E:327:GLY:HA3	2:E:344:LYS:HE2	1.90	0.53
3:F:393:THR:O	3:F:394:ILE:C	2.51	0.53
3:C:307:HIS:HE1	3:C:342:GLY:H	1.57	0.53
2:E:439:ASN:HD22	2:E:439:ASN:H	1.56	0.53
3:C:103:HIS:O	3:C:107:ILE:HG12	2.09	0.53
2:B:244:THR:HG22	2:B:245:GLU:HG3	1.90	0.53
2:B:438:MET:HA	2:B:442:GLY:O	2.08	0.53
3:F:179:LEU:HD23	3:F:218:LEU:HD12	1.91	0.53
3:F:264:MET:HE1	3:F:389:PHE:CD2	2.44	0.53
3:F:325:ASN:HD22	3:F:325:ASN:C	2.17	0.53
1:A:127:ILE:HG22	1:A:130:VAL:H	1.72	0.53
3:C:172:LEU:HD12	3:C:239:GLN:HB3	1.90	0.53
1:D:135:LEU:HD13	1:D:135:LEU:C	2.34	0.53
3:F:307:HIS:HD2	3:F:335:TRP:O	1.91	0.53
1:D:136:LEU:O	1:D:139:ASN:HB3	2.09	0.53
2:E:176:ARG:HB2	3:F:117:ASN:HD21	1.74	0.53
1:A:130:VAL:O	1:A:133:ILE:HG22	2.09	0.52
3:F:254:ASN:CB	3:F:256:ARG:HH21	2.20	0.52
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.08	0.52
2:B:439:ASN:HD22	2:B:439:ASN:N	2.07	0.52
3:F:192:THR:HG23	3:F:386:ILE:CG1	2.39	0.52
1:A:169:LEU:H	2:B:189:GLN:NE2	2.08	0.52
2:B:268:PRO:HG2	7:B:466:HOH:O	2.09	0.52
2:E:230:ASP:OD2	2:E:232:SER:HB2	2.09	0.52
2:B:172:LEU:HB3	3:C:113:ILE:CD1	2.39	0.52
1:D:169:LEU:H	2:E:189:GLN:HE22	1.58	0.52
1:D:180:ASP:O	1:D:184:GLN:HG3	2.09	0.52
2:B:422:TYR:HA	2:B:426:MET:HE1	1.92	0.52
2:B:178:LYS:HA	2:B:178:LYS:HE2	1.91	0.52
2:B:224:MET:HE1	7:C:412:HOH:O	2.09	0.52
3:C:172:LEU:H	3:C:239:GLN:HE21	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ARG:O	1:D:145:VAL:HG23	2.10	0.52
3:F:254:ASN:HD22	3:F:256:ARG:HH21	1.57	0.52
2:B:364:ASN:OD1	4:H:4:PRO:HB3	2.10	0.52
1:D:140:VAL:C	1:D:142:ALA:N	2.68	0.52
1:D:183:LYS:O	1:D:186:GLU:HB2	2.09	0.52
2:E:167:VAL:HA	2:E:170:SER:HB3	1.91	0.52
3:F:365:ASN:H	3:F:365:ASN:ND2	2.09	0.52
3:C:292:GLY:HA2	3:C:305:THR:O	2.10	0.51
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.91	0.51
3:F:217:HIS:HB2	3:F:224:THR:HG21	1.92	0.51
2:E:216:ARG:HH12	2:E:458:PHE:HZ	1.58	0.51
2:E:238:VAL:HG21	2:E:250:THR:CG2	2.40	0.51
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.23	0.51
2:B:316:ASP:OD2	2:B:320:ASP:HB2	2.11	0.51
3:C:96:TYR:O	3:C:97:GLU:HB2	2.10	0.51
3:C:124:LEU:O	3:C:128:VAL:HG23	2.10	0.51
2:E:346:ARG:HG3	2:E:346:ARG:NH1	2.25	0.51
3:F:192:THR:CG2	3:F:386:ILE:HG13	2.41	0.51
1:A:136:LEU:HD13	3:C:110:LEU:HD12	1.93	0.51
2:E:238:VAL:HG21	2:E:250:THR:HG23	1.92	0.51
2:E:332:GLN:O	2:E:338:TYR:HA	2.11	0.51
2:E:395:SER:HA	2:E:404:TYR:CE2	2.45	0.51
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.93	0.51
2:B:202:ASN:HD22	2:B:284:ASN:ND2	2.09	0.51
2:B:229:PRO:HB3	2:B:301:GLN:HE22	1.76	0.51
2:B:357:ALA:HB3	2:B:360:LEU:HD12	1.93	0.51
1:D:166:SER:HB3	2:E:195:THR:HB	1.93	0.51
2:E:280:THR:O	2:E:281:ASP:C	2.54	0.50
3:C:172:LEU:HG	3:C:239:GLN:HE21	1.77	0.50
2:E:191:GLU:HA	2:E:194:ARG:HD3	1.93	0.50
3:F:273:LYS:HB2	3:F:311:GLN:HB3	1.92	0.50
3:C:307:HIS:CE1	3:C:342:GLY:H	2.29	0.50
1:D:186:GLU:O	1:D:187:GLN:HG3	2.11	0.50
1:A:182:GLN:O	1:A:186:GLU:HG2	2.12	0.50
2:B:303:THR:HB	2:B:330:THR:HA	1.93	0.50
2:E:172:LEU:HD13	3:F:113:ILE:HB	1.94	0.50
2:E:176:ARG:CB	3:F:117:ASN:HD21	2.24	0.50
1:D:136:LEU:HD21	3:F:111:GLN:OE1	2.11	0.50
1:D:140:VAL:C	1:D:142:ALA:H	2.18	0.50
2:B:364:ASN:HD22	5:K:1:NAG:C7	2.24	0.50
1:D:185:LEU:HB2	2:E:171:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:303:THR:HB	2:E:330:THR:HA	1.92	0.50
3:F:239:GLN:O	3:F:240:SER:C	2.54	0.50
2:B:265:LYS:HD3	2:B:378:TYR:CE1	2.47	0.50
2:B:351:ASN:CG	2:B:354:MET:HB2	2.37	0.49
3:F:119:GLN:NE2	3:F:119:GLN:CA	2.74	0.49
2:B:361:MET:O	5:K:1:NAG:H81	2.12	0.49
3:F:172:LEU:H	3:F:239:GLN:NE2	1.97	0.49
2:B:265:LYS:HD3	2:B:378:TYR:CZ	2.47	0.49
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.95	0.49
3:F:389:PHE:C	3:F:391:ARG:N	2.71	0.49
5:L:1:NAG:C6	5:L:3:FUC:H5	2.34	0.49
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.48	0.49
3:F:155:ASP:O	3:F:159:LYS:HG3	2.13	0.49
1:A:139:ASN:HB3	3:C:114:TYR:CE1	2.47	0.49
3:F:197:ARG:HB2	3:F:382:THR:HB	1.95	0.49
2:E:271:GLN:HE21	2:E:271:GLN:HA	1.78	0.49
3:F:254:ASN:ND2	3:F:256:ARG:HH21	2.11	0.49
4:G:3:ARG:CG	4:G:4:PRO:HD2	2.35	0.48
5:L:1:NAG:C6	5:L:3:FUC:H3	2.41	0.48
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.95	0.48
1:D:144:LEU:CD2	1:D:182:GLN:HG2	2.42	0.48
2:E:165:LEU:HG	2:E:165:LEU:O	2.13	0.48
2:E:167:VAL:HG12	2:E:167:VAL:O	2.12	0.48
2:E:321:LYS:NZ	2:E:321:LYS:CB	2.76	0.48
3:F:365:ASN:HD22	3:F:365:ASN:N	2.06	0.48
2:E:176:ARG:HD2	2:E:176:ARG:C	2.37	0.48
2:E:385:TRP:CZ2	4:J:3:ARG:HG2	2.48	0.48
2:B:161:ILE:HD12	2:B:161:ILE:N	2.28	0.48
2:B:217:LYS:HB3	3:C:213:GLU:HG3	1.95	0.48
3:F:254:ASN:ND2	3:F:256:ARG:NH2	2.61	0.48
1:A:153:ASP:O	1:A:157:LYS:HG2	2.14	0.48
3:F:295:PHE:CD2	4:I:2:PRO:HD3	2.48	0.48
3:C:263:ALA:HB1	3:C:264:MET:CE	2.43	0.48
3:C:138:PRO:HG3	7:C:413:HOH:O	2.14	0.48
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.95	0.48
3:C:258:SER:HA	3:C:285:ASP:OD2	2.13	0.48
1:D:144:LEU:HD23	1:D:144:LEU:O	2.13	0.48
1:A:175:LEU:N	1:A:175:LEU:HD22	2.28	0.47
3:C:294:ASP:C	3:C:296:GLY:H	2.22	0.47
2:B:364:ASN:ND2	5:K:1:NAG:C7	2.77	0.47
1:A:127:ILE:HG22	1:A:130:VAL:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD22	1:D:182:GLN:HG2	1.95	0.47
2:E:172:LEU:O	3:F:113:ILE:HG22	2.14	0.47
2:E:201:CYS:O	3:F:143:VAL:HG21	2.14	0.47
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.12	0.47
2:E:266:TRP:HA	2:E:377:THR:HG21	1.97	0.47
3:C:153:CYS:HB2	3:C:192:THR:OG1	2.15	0.47
2:E:431:THR:HG21	4:J:3:ARG:HH12	1.79	0.47
1:A:154:ILE:HD12	2:B:182:LEU:HD13	1.97	0.47
2:B:172:LEU:HB3	3:C:113:ILE:HD11	1.97	0.47
2:B:332:GLN:O	2:B:338:TYR:HA	2.14	0.47
2:B:363:GLU:O	2:B:367:MET:HG2	2.14	0.47
3:F:205:LYS:HB3	3:F:205:LYS:HZ3	1.78	0.47
1:A:127:ILE:HG12	1:A:128:GLU:CD	2.40	0.47
2:B:159:SER:C	2:B:162:PRO:HD2	2.40	0.47
2:B:298:LYS:HG3	7:B:480:HOH:O	2.14	0.47
2:E:406:ARG:N	2:E:407:CYS:HA	2.27	0.47
2:B:258:GLY:HA2	7:B:462:HOH:O	2.15	0.47
3:C:363:TYR:HB3	4:G:3:ARG:NH2	2.30	0.47
1:A:183:LYS:O	1:A:187:GLN:HG3	2.15	0.47
2:B:253:GLN:HB3	2:B:452:MET:HB2	1.96	0.47
2:B:383:ASP:OD1	2:B:383:ASP:C	2.57	0.47
2:B:393:GLN:O	2:B:397:GLU:HG3	2.14	0.47
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.29	0.46
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.97	0.46
2:B:434:GLY:O	2:B:436:VAL:N	2.47	0.46
3:C:373:LYS:HB2	3:C:379:MET:HE1	1.96	0.46
2:E:236:TYR:CD2	2:E:298:LYS:HE2	2.49	0.46
1:A:162:ARG:NH1	1:A:162:ARG:HG2	2.30	0.46
2:B:162:PRO:HG2	3:C:97:GLU:OE1	2.15	0.46
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.51	0.46
1:D:162:ARG:NH1	1:D:162:ARG:HG2	2.30	0.46
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.97	0.46
5:L:2:NAG:C1	5:L:2:NAG:H83	2.45	0.46
2:B:351:ASN:HD21	2:B:354:MET:N	2.12	0.46
3:C:261:ASP:CB	3:C:282:ALA:HB3	2.45	0.46
3:C:292:GLY:O	3:C:302:LYS:HD2	2.16	0.46
3:C:307:HIS:HD2	3:C:335:TRP:O	1.99	0.46
1:D:166:SER:N	2:E:195:THR:O	2.46	0.46
1:A:181:GLN:O	1:A:184:GLN:HB3	2.15	0.46
2:B:381:ASP:HB2	2:B:393:GLN:OE1	2.16	0.46
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:O	2:E:406:ARG:HG2	2.16	0.46
3:F:292:GLY:C	3:F:302:LYS:HD3	2.41	0.46
2:B:164:ASN:HD22	2:B:164:ASN:HA	1.60	0.45
3:C:97:GLU:OE2	3:C:97:GLU:HA	2.15	0.45
2:B:408:HIS:O	4:H:1:GLY:N	2.39	0.45
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.16	0.45
2:B:181:LYS:O	2:B:184:SER:HB2	2.16	0.45
3:C:344:LEU:HD23	3:C:344:LEU:N	2.31	0.45
2:E:172:LEU:HD22	3:F:113:ILE:HB	1.98	0.45
3:F:234:HIS:NE2	3:F:269:PRO:HB3	2.31	0.45
1:A:127:ILE:HG22	1:A:130:VAL:HB	1.99	0.45
1:D:143:GLN:HB2	3:F:114:TYR:CE1	2.52	0.45
2:E:351:ASN:C	2:E:351:ASN:HD22	2.23	0.45
3:C:96:TYR:CG	3:C:97:GLU:N	2.85	0.45
1:D:140:VAL:HA	3:F:114:TYR:CE1	2.51	0.45
3:F:231:GLU:O	3:F:235:LEU:HG	2.15	0.45
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.98	0.45
3:F:230:ASN:HB3	3:F:274:TYR:CG	2.52	0.45
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.85	0.45
2:E:238:VAL:HG22	2:E:239:TYR:N	2.32	0.45
2:B:389:ASP:HA	2:B:390:PRO:HD2	1.84	0.45
2:E:385:TRP:CE2	4:J:3:ARG:HG2	2.52	0.45
3:F:121:ILE:O	3:F:125:LYS:HG3	2.17	0.45
2:B:211:CYS:SG	2:B:250:THR:HA	2.57	0.44
3:F:229:GLY:O	3:F:233:ILE:HG13	2.17	0.44
3:C:123:ASN:O	3:C:126:GLU:HB2	2.18	0.44
3:C:300:SER:O	3:C:301:ALA:C	2.60	0.44
3:F:172:LEU:HD22	3:F:239:GLN:HE21	1.82	0.44
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.99	0.44
2:E:397:GLU:OE1	4:J:3:ARG:NH1	2.51	0.44
2:B:212:GLU:O	2:B:215:ILE:HG22	2.17	0.44
3:C:206:LYS:HB3	3:C:210:GLN:HB2	1.98	0.44
3:C:259:THR:O	3:C:286:ALA:HB3	2.17	0.44
1:D:133:ILE:C	1:D:135:LEU:H	2.26	0.44
2:E:436:VAL:CG1	2:E:437:TRP:N	2.81	0.44
3:F:248:VAL:HG13	3:F:344:LEU:HD11	1.99	0.44
5:L:2:NAG:O7	5:L:2:NAG:O4	2.32	0.44
2:B:212:GLU:OE2	2:B:216:ARG:HD3	2.17	0.44
2:E:172:LEU:HB3	3:F:113:ILE:CG2	2.43	0.44
3:F:310:MET:HA	3:F:310:MET:HE2	1.99	0.44
2:B:224:MET:CE	2:B:237:ARG:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:HD21	2:B:284:ASN:HB2	1.78	0.44
2:E:279:ASN:O	2:E:281:ASP:N	2.51	0.43
3:F:110:LEU:N	3:F:110:LEU:HD23	2.33	0.43
3:F:322:PHE:HD1	3:F:338:LYS:HD2	1.83	0.43
4:I:3:ARG:CG	4:I:4:PRO:HD2	2.45	0.43
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.80	0.43
3:C:203:ASP:O	3:C:206:LYS:HE3	2.18	0.43
3:F:365:ASN:ND2	3:F:365:ASN:N	2.66	0.43
2:B:182:LEU:HB3	3:C:124:LEU:HD21	2.01	0.43
3:F:206:LYS:HB3	3:F:210:GLN:HB2	1.99	0.43
2:B:310:LEU:HB3	2:B:326:TYR:HB2	1.99	0.43
3:C:317:ASN:C	3:C:317:ASN:HD22	2.26	0.43
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.16	0.43
1:D:137:GLN:O	1:D:140:VAL:HG22	2.18	0.43
4:H:3:ARG:HA	4:H:3:ARG:HD3	1.86	0.43
2:B:190:MET:HE3	3:C:131:LEU:HA	2.01	0.43
3:F:249:GLU:CB	3:F:383:THR:HG23	2.45	0.43
2:B:306:GLY:O	2:B:307:PRO:C	2.58	0.43
1:D:177:ASP:O	1:D:181:GLN:HG3	2.18	0.43
2:E:179:ILE:O	2:E:183:GLU:HB2	2.19	0.43
2:B:161:ILE:H	2:B:161:ILE:CD1	2.31	0.43
1:D:143:GLN:HB2	3:F:114:TYR:HE1	1.84	0.43
2:E:165:LEU:HD21	3:F:110:LEU:HD12	2.00	0.43
3:F:387:ILE:CD1	3:F:391:ARG:HG2	2.48	0.43
2:B:385:TRP:CZ3	4:H:3:ARG:HG3	2.54	0.43
3:F:364:ASP:HB3	3:F:375:ARG:HG3	2.01	0.43
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.31	0.42
2:B:253:GLN:C	2:B:253:GLN:HE21	2.26	0.42
3:C:263:ALA:HB1	3:C:264:MET:HE2	2.00	0.42
2:E:218:GLY:HA3	3:F:210:GLN:HG2	2.01	0.42
2:E:351:ASN:ND2	2:E:354:MET:H	2.17	0.42
2:E:422:TYR:HA	2:E:426:MET:CE	2.49	0.42
3:F:221:THR:O	3:F:223:THR:HG23	2.19	0.42
3:F:320:ASP:HB3	3:F:336:MET:HB2	2.00	0.42
1:A:185:LEU:HD22	1:A:189:ILE:CG1	2.49	0.42
2:B:373:MET:HE3	2:B:374:PHE:H	1.83	0.42
3:F:206:LYS:HD2	3:F:210:GLN:OE1	2.19	0.42
1:A:189:ILE:O	1:A:189:ILE:HG22	2.18	0.42
1:D:176:LYS:C	1:D:178:TYR:N	2.75	0.42
3:F:217:HIS:O	3:F:224:THR:CG2	2.67	0.42
1:A:127:ILE:CG2	1:A:130:VAL:HG23	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:GLU:HG3	3:C:257:THR:HG22	2.02	0.42
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.55	0.42
1:A:134:GLN:O	1:A:138:LYS:HG3	2.19	0.42
2:B:264:ARG:HB3	7:B:466:HOH:O	2.19	0.42
1:D:168:ALA:HA	2:E:189:GLN:NE2	2.24	0.42
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.55	0.42
5:K:1:NAG:H4	5:K:3:FUC:H5	2.02	0.42
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
3:C:143:VAL:HA	7:C:419:HOH:O	2.19	0.42
2:E:253:GLN:HB3	2:E:452:MET:HB2	2.01	0.42
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.84	0.42
2:E:212:GLU:HB2	2:E:456:PRO:HD2	2.02	0.42
2:B:411:ASN:N	2:B:412:PRO:HD3	2.35	0.42
3:C:160:GLY:O	3:C:161:ALA:C	2.63	0.42
2:E:169:ARG:O	2:E:173:GLU:HB2	2.19	0.42
1:D:165:CYS:HB3	2:E:193:CYS:HA	2.02	0.41
2:E:306:GLY:O	2:E:307:PRO:C	2.63	0.41
2:E:411:ASN:N	2:E:412:PRO:HD3	2.36	0.41
3:C:197:ARG:HG2	3:C:382:THR:CG2	2.50	0.41
2:E:271:GLN:HA	2:E:271:GLN:NE2	2.34	0.41
2:E:389:ASP:HA	2:E:390:PRO:HD2	1.94	0.41
3:F:273:LYS:HE3	3:F:319:ASN:ND2	2.35	0.41
2:B:212:GLU:HB2	2:B:456:PRO:HD2	2.02	0.41
2:B:406:ARG:N	2:B:407:CYS:HA	2.33	0.41
2:B:434:GLY:O	2:B:436:VAL:HG23	2.20	0.41
3:C:113:ILE:HG13	3:C:114:TYR:N	2.34	0.41
1:D:139:ASN:O	1:D:142:ALA:HB3	2.20	0.41
3:F:124:LEU:O	3:F:127:LYS:HB3	2.20	0.41
1:A:150:LEU:HD21	3:C:124:LEU:HD23	2.03	0.41
2:B:161:ILE:N	2:B:162:PRO:CD	2.83	0.41
3:C:261:ASP:HB3	3:C:282:ALA:HB3	2.02	0.41
3:C:286:ALA:O	3:C:372:TRP:HB2	2.20	0.41
3:C:365:ASN:ND2	3:C:365:ASN:N	2.61	0.41
2:E:245:GLU:O	2:E:246:ASN:HB2	2.19	0.41
2:B:183:GLU:HG2	3:C:124:LEU:HD13	2.03	0.41
1:D:148:LYS:HE3	1:D:175:LEU:HD12	2.01	0.41
1:D:162:ARG:HG2	1:D:162:ARG:HH11	1.85	0.41
2:B:217:LYS:CB	3:C:213:GLU:HG3	2.51	0.41
3:C:141:ASP:OD1	3:C:143:VAL:HG13	2.20	0.41
1:A:185:LEU:HD22	1:A:189:ILE:HG13	2.02	0.41
2:B:322:VAL:HG11	2:B:440:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:LEU:O	3:C:134:GLN:HB2	2.20	0.41
2:E:253:GLN:HE22	2:E:451:SER:HA	1.84	0.41
2:B:315:GLU:HA	2:B:320:ASP:O	2.20	0.41
2:B:263:GLY:HA2	2:B:400:GLY:HA2	2.03	0.41
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.56	0.41
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.56	0.41
3:F:197:ARG:HD3	3:F:204:PHE:CZ	2.55	0.41
2:B:168:LEU:HB3	3:C:110:LEU:HD13	2.02	0.41
3:C:196:LYS:HD2	3:C:383:THR:HB	2.02	0.41
2:E:410:ALA:C	2:E:412:PRO:HD3	2.46	0.41
3:F:249:GLU:C	3:F:250:LEU:HD13	2.46	0.41
3:C:266:LYS:HE3	3:C:266:LYS:HB2	1.82	0.40
3:C:393:THR:O	3:C:393:THR:HG22	2.21	0.40
2:E:234:LYS:HA	2:E:235:PRO:HD3	1.95	0.40
3:F:344:LEU:HA	3:F:367:ILE:HG23	2.03	0.40
2:B:429:HIS:C	2:B:431:THR:H	2.29	0.40
3:C:275:ARG:NH2	3:C:311:GLN:HE21	2.19	0.40
2:E:357:ALA:HB3	2:E:360:LEU:CD1	2.51	0.40
3:F:307:HIS:CE1	3:F:342:GLY:H	2.39	0.40
1:A:133:ILE:HD11	2:B:164:ASN:HB3	2.02	0.40
2:B:172:LEU:CB	3:C:113:ILE:HD11	2.51	0.40
2:B:302:LEU:HD13	2:B:454:ILE:HD11	2.04	0.40
2:B:219:GLY:O	2:B:242:MET:HE3	2.22	0.40
1:D:180:ASP:C	1:D:182:GLN:N	2.79	0.40
1:D:186:GLU:C	1:D:187:GLN:HG3	2.46	0.40
3:F:304:PHE:O	3:F:337:ASN:HB3	2.21	0.40
3:F:391:ARG:HD2	3:F:391:ARG:HA	1.89	0.40
1:A:158:ILE:HG23	2:B:189:GLN:NE2	2.33	0.40
2:B:417:TYR:HB2	2:B:446:SER:HB3	2.03	0.40
3:F:315:TRP:CZ3	3:F:316:ASP:HB3	2.56	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	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
1	D	54/66 (82%)	44 (82%)	9 (17%)	1 (2%)	6	17
2	B	299/313 (96%)	266 (89%)	30 (10%)	3 (1%)	12	32
2	E	292/313 (93%)	268 (92%)	21 (7%)	3 (1%)	12	32
3	C	297/311 (96%)	269 (91%)	23 (8%)	5 (2%)	7	19
3	F	283/311 (91%)	262 (93%)	17 (6%)	4 (1%)	9	23
4	G	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	I	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	J	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1296/1396 (93%)	1173 (90%)	107 (8%)	16 (1%)	10	27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	435	VAL
3	C	97	GLU
3	C	301	ALA
1	D	137	GLN
2	E	281	ASP
3	F	241	ALA
2	B	281	ASP
3	C	198	LEU
3	F	240	SER
2	B	256	GLN
2	E	256	GLN
3	F	199	ASP
2	E	280	THR
3	F	390	ASN
3	C	241	ALA
3	C	303	PHE

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	60/61 (98%)	57 (95%)	3 (5%)	22	48
1	D	52/61 (85%)	49 (94%)	3 (6%)	18	42
2	B	259/271 (96%)	251 (97%)	8 (3%)	35	65
2	E	252/271 (93%)	244 (97%)	8 (3%)	34	64
3	C	250/257 (97%)	242 (97%)	8 (3%)	34	64
3	F	237/257 (92%)	226 (95%)	11 (5%)	24	51
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	H	3/3 (100%)	3 (100%)	0	100	100
4	I	3/3 (100%)	2 (67%)	1 (33%)	0	1
4	J	3/3 (100%)	2 (67%)	1 (33%)	0	1
All	All	1122/1190 (94%)	1078 (96%)	44 (4%)	28	57

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LYS
1	A	144	LEU
1	A	185	LEU
2	B	164	ASN
2	B	196	PRO
2	B	210	GLU
2	B	233	VAL
2	B	238	VAL
2	B	253	GLN
2	B	304	ARG
2	B	439	ASN
3	C	104	ASP
3	C	118	ASN
3	C	143	VAL
3	C	250	LEU
3	C	302	LYS
3	C	365	ASN
3	C	382	THR
3	C	383	THR
1	D	138	LYS
1	D	172	GLU
1	D	176	LYS

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Mol	Chain	Res	Type
2	E	190	MET
2	E	210	GLU
2	E	224	MET
2	E	253	GLN
2	E	267	ASP
2	E	280	THR
2	E	321	LYS
2	E	348	THR
3	F	113	ILE
3	F	143	VAL
3	F	172	LEU
3	F	176	GLN
3	F	205	LYS
3	F	250	LEU
3	F	302	LYS
3	F	317	ASN
3	F	365	ASN
3	F	382	THR
3	F	383	THR
4	G	3	ARG
4	I	3	ARG
4	J	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	139	ASN
1	A	181	GLN
1	A	187	GLN
2	B	160	ASN
2	B	164	ASN
2	B	189	GLN
2	B	202	ASN
2	B	243	ASN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	296	ASN
2	B	301	GLN
2	B	339	GLN
2	B	351	ASN

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Mol	Chain	Res	Type
2	B	382	ASN
2	B	421	GLN
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	136	GLN
3	C	163	GLN
3	C	176	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	311	GLN
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN
3	C	361	ASN
3	C	365	ASN
1	D	143	GLN
1	D	187	GLN
2	E	189	GLN
2	E	202	ASN
2	E	243	ASN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	429	HIS
2	E	439	ASN
3	F	115	ASN
3	F	117	ASN
3	F	118	ASN
3	F	119	GLN
3	F	123	ASN

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Mol	Chain	Res	Type
3	F	136	GLN
3	F	144	GLN
3	F	146	HIS
3	F	176	GLN
3	F	230	ASN
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	365	ASN

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](#)

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	$\# Z > 2$
5	NAG	K	1	2,5	14,14,15	0.70	0	17,19,21	0.77	1 (5%)
5	NAG	K	2	5	14,14,15	0.69	0	17,19,21	0.64	0
5	FUC	K	3	5	10,10,11	0.61	0	14,14,16	0.36	0
5	NAG	L	1	2,5	14,14,15	0.62	0	17,19,21	1.32	3 (17%)
5	NAG	L	2	5	14,14,15	0.77	0	17,19,21	0.76	0
5	FUC	L	3	5	10,10,11	0.60	0	14,14,16	0.70	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	K	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	4/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1	NAG	C2-N2-C7	-2.63	119.37	122.90
5	L	1	NAG	C3-C4-C5	2.54	114.84	110.23
5	L	1	NAG	O5-C1-C2	-2.35	107.66	111.29
5	K	1	NAG	C2-N2-C7	-2.29	119.83	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

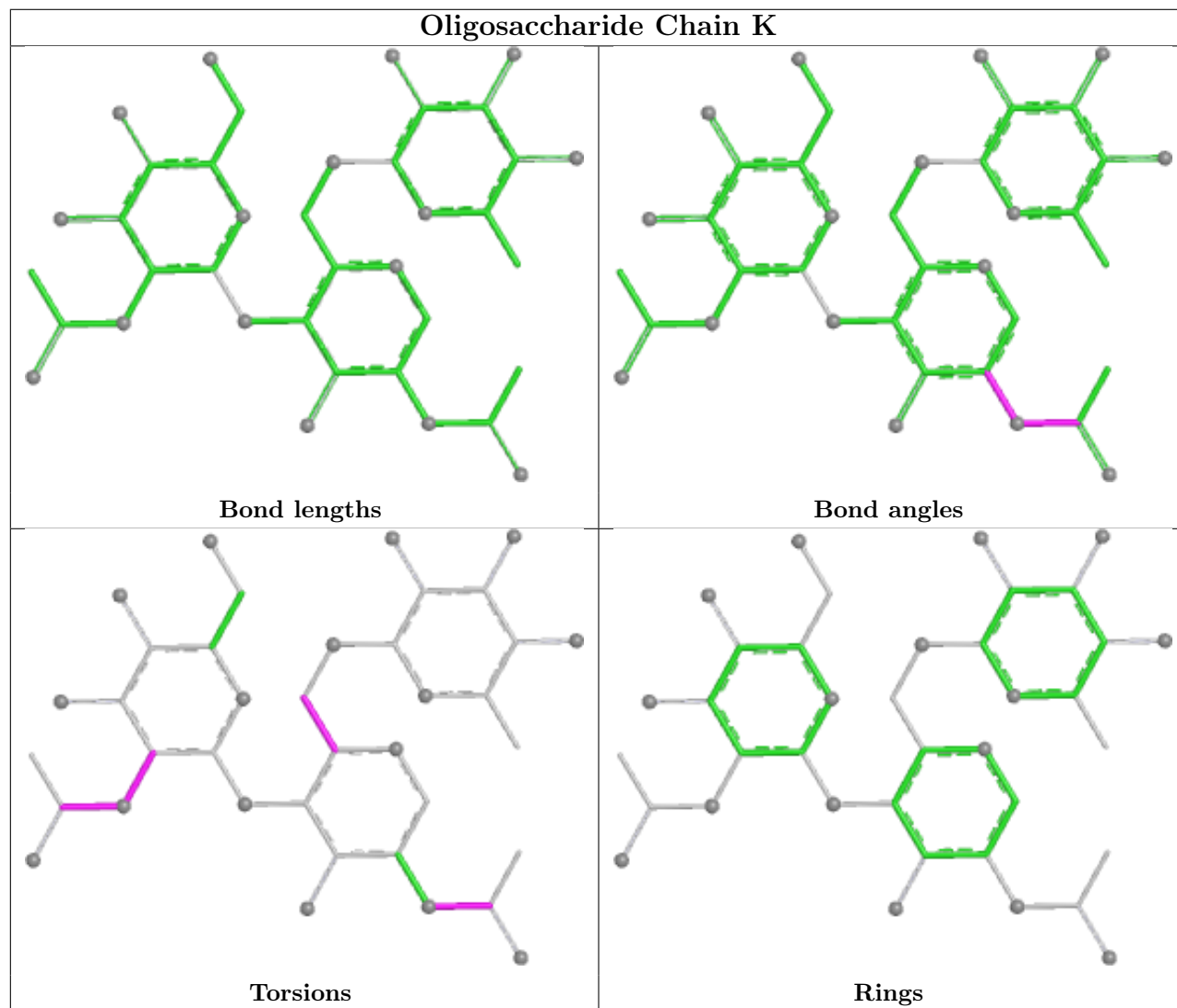
Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C1-C2-N2-C7
5	L	2	NAG	C8-C7-N2-C2
5	L	2	NAG	O7-C7-N2-C2
5	L	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C1-C2-N2-C7
5	K	2	NAG	C3-C2-N2-C7
5	K	1	NAG	O5-C5-C6-O6

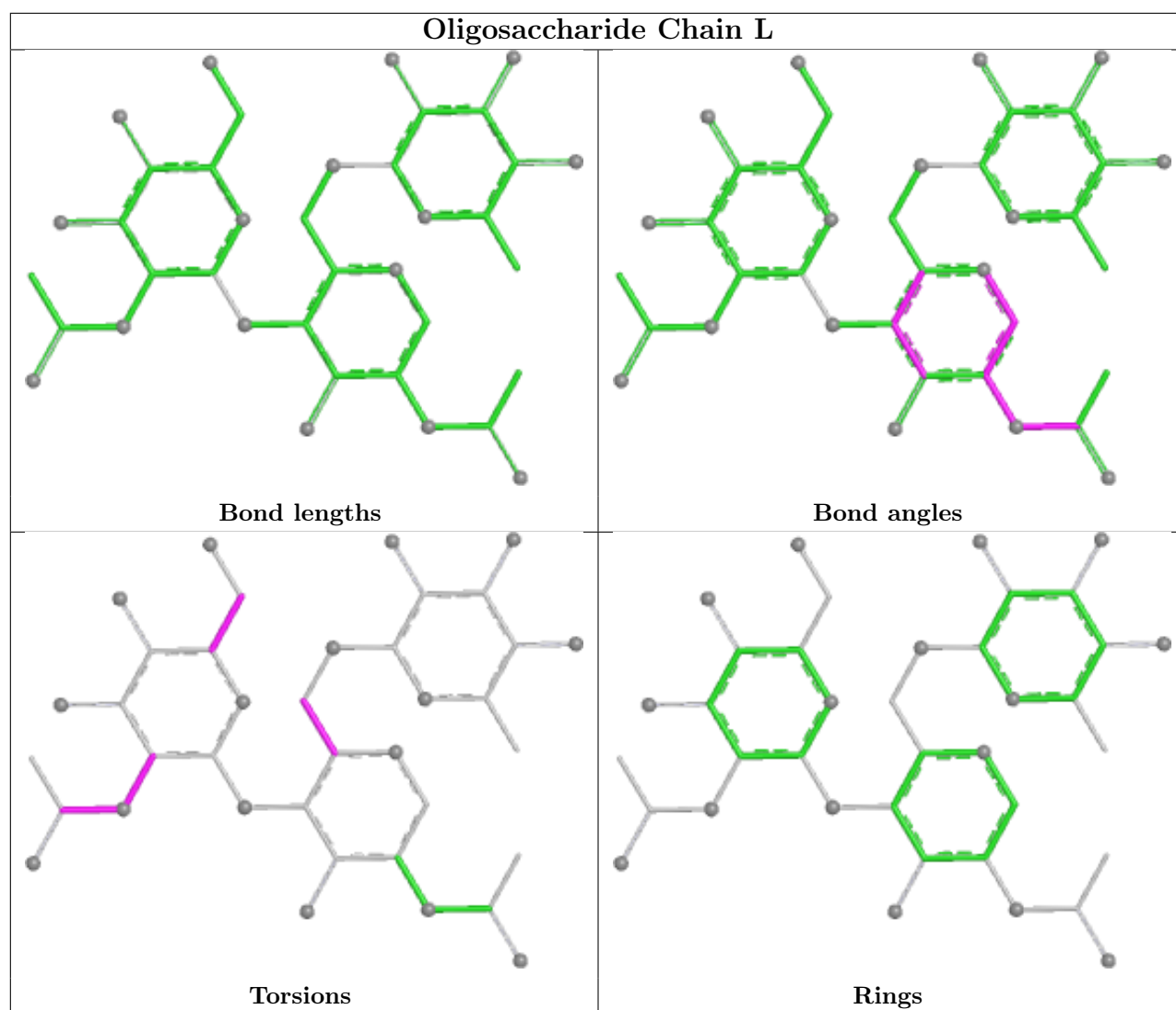
There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	3	FUC	6	0
5	L	2	NAG	5	0
5	K	1	NAG	5	0
5	L	1	NAG	9	0
5	K	3	FUC	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 4 ligands modelled in this entry, 4 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	65/66 (98%)	0.61	8 (12%) 8 7	24, 57, 85, 99	0
1	D	56/66 (84%)	1.06	15 (26%) 1 1	24, 68, 110, 115	0
2	B	301/313 (96%)	0.11	12 (3%) 42 38	22, 41, 69, 96	0
2	E	294/313 (93%)	-0.34	9 (3%) 51 48	13, 26, 64, 105	0
3	C	299/311 (96%)	0.03	6 (2%) 65 62	25, 44, 70, 86	0
3	F	285/311 (91%)	-0.19	11 (3%) 43 39	16, 30, 66, 113	0
4	G	4/4 (100%)	1.36	1 (25%) 2 1	63, 64, 65, 70	0
4	H	4/4 (100%)	1.37	1 (25%) 2 1	62, 62, 65, 66	0
4	I	4/4 (100%)	0.03	0 100 100	36, 38, 40, 43	0
4	J	4/4 (100%)	-0.20	0 100 100	34, 37, 38, 41	0
All	All	1316/1396 (94%)	-0.00	63 (4%) 35 32	13, 37, 80, 115	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	113	ILE	5.4
1	A	190	ALA	5.3
1	D	188	VAL	5.3
3	F	110	LEU	5.0
1	D	133	ILE	4.5
1	D	140	VAL	4.2
1	D	135	LEU	3.8
1	A	174	ASP	3.6
2	E	458	PHE	3.5
3	F	393	THR	3.4
1	D	136	LEU	3.4
2	B	458	PHE	3.3
1	D	138	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	394	ILE	3.2
1	A	126	VAL	3.1
3	F	116	SER	3.0
2	B	158	ASN	3.0
2	E	167	VAL	2.9
3	F	120	LYS	2.9
2	B	162	PRO	2.8
3	C	96	TYR	2.8
2	B	387	THR	2.8
1	D	137	GLN	2.8
2	E	165	LEU	2.7
1	A	132	HIS	2.7
2	E	280	THR	2.7
3	F	114	TYR	2.6
3	C	240	SER	2.6
1	D	134	GLN	2.6
3	F	115	ASN	2.6
2	B	420	GLY	2.6
1	D	183	LYS	2.5
3	F	240	SER	2.5
1	D	182	GLN	2.5
3	C	394	ILE	2.5
4	H	2	PRO	2.5
1	A	133	ILE	2.4
1	A	128	GLU	2.4
1	D	180	ASP	2.4
1	A	127	ILE	2.3
2	B	161	ILE	2.3
1	D	144	LEU	2.3
3	C	393	THR	2.3
3	F	123	ASN	2.3
2	B	280	THR	2.3
1	D	143	GLN	2.2
2	B	392	LYS	2.2
2	B	159	SER	2.2
2	E	232	SER	2.2
1	A	130	VAL	2.2
2	E	171	ILE	2.2
1	D	178	TYR	2.2
3	C	242	ILE	2.2
2	E	174	ASN	2.1
2	B	395	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	163	THR	2.1
2	E	168	LEU	2.1
3	F	297	ASP	2.1
3	C	301	ALA	2.1
2	E	176	ARG	2.0
1	D	176	LYS	2.0
4	G	4	PRO	2.0
2	B	424	TRP	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](#)

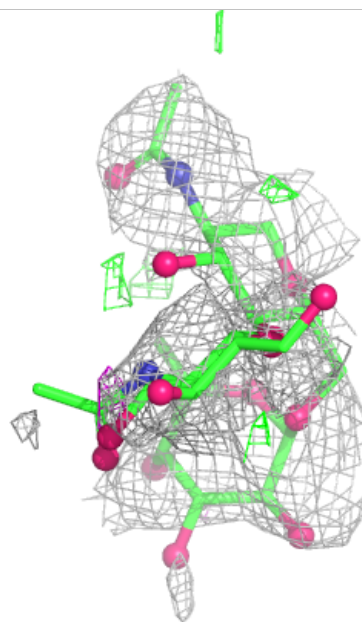
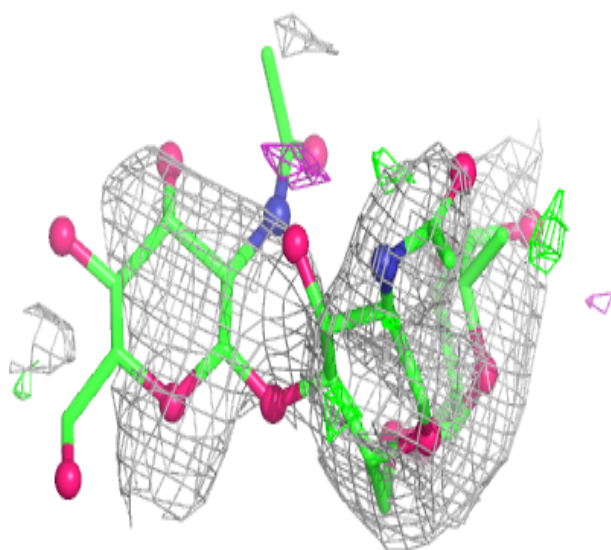
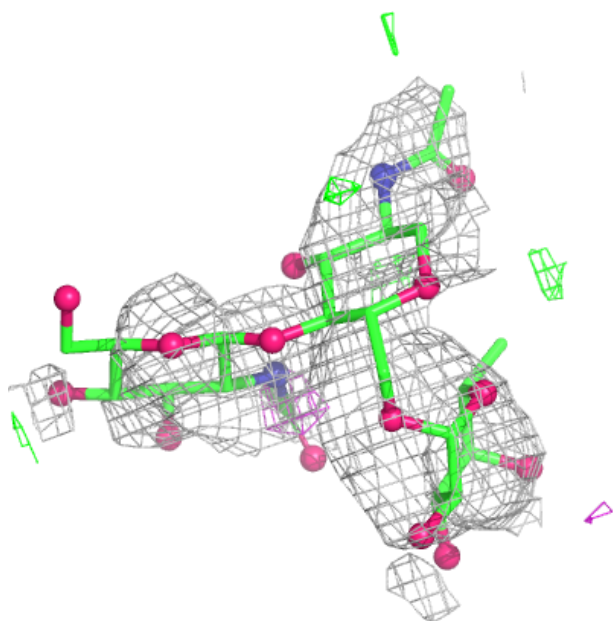
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

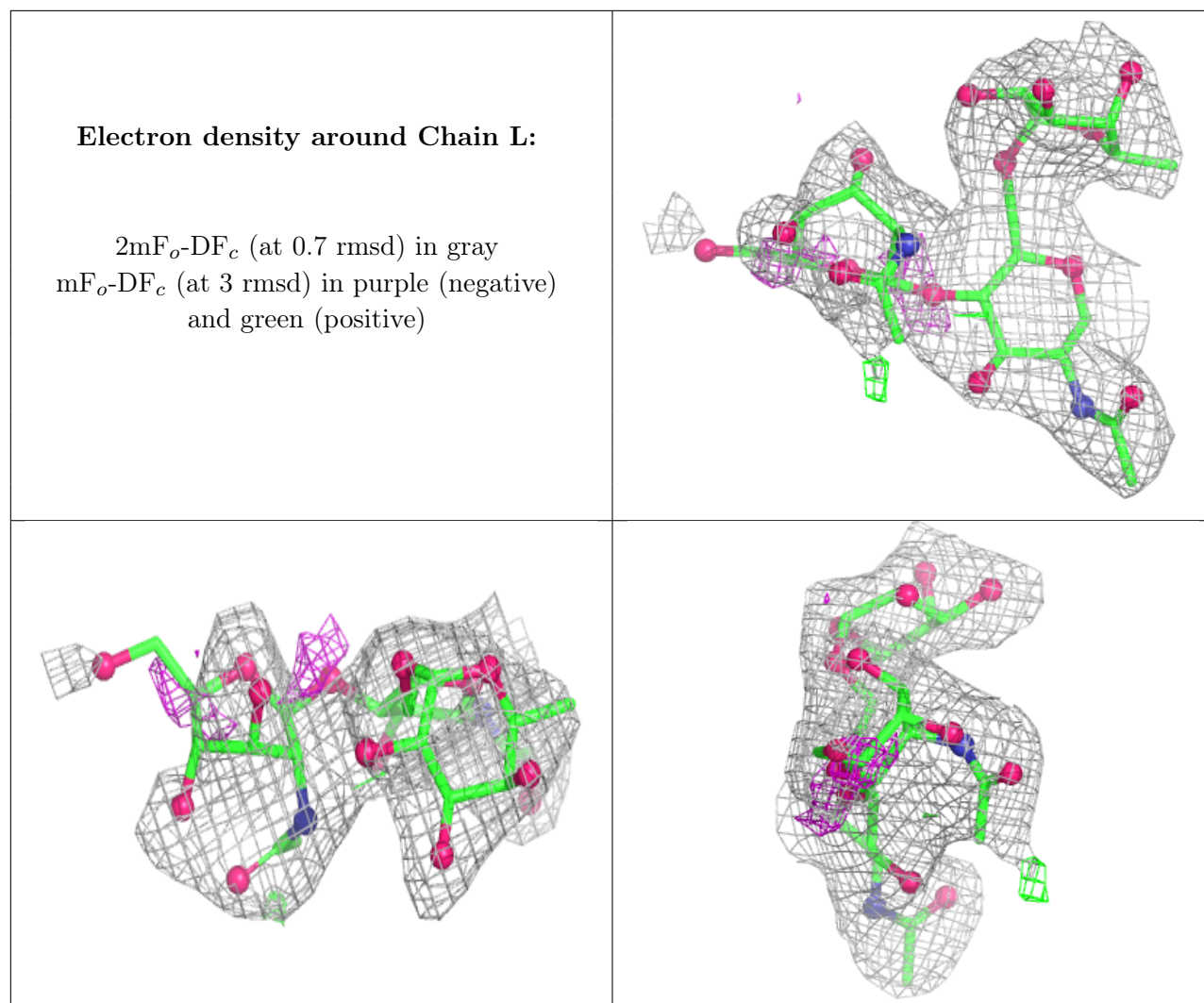
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	K	2	14/15	0.37	0.20	105,106,108,109	0
5	FUC	K	3	10/11	0.48	0.18	101,103,103,103	0
5	NAG	K	1	14/15	0.63	0.19	91,95,100,102	0
5	NAG	L	2	14/15	0.67	0.17	69,72,77,78	0
5	NAG	L	1	14/15	0.84	0.11	48,56,61,67	0
5	FUC	L	3	10/11	0.86	0.10	62,63,63,64	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 K:

$2mF_o-DF_c$ (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	2	1/1	0.94	0.08	29,29,29,29	0
6	CA	F	1	1/1	0.97	0.03	29,29,29,29	0
6	CA	B	2	1/1	0.98	0.05	54,54,54,54	0
6	CA	C	1	1/1	0.98	0.04	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.