



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:45 PM UTC

PDB ID : 3BVH / pdb_00003bvh
Title : Crystal Structure of Recombinant gammaD364A Fibrinogen Fragment D with the Peptide Ligand Gly-Pro-Arg-Pro-Amide
Authors : Bowley, S.R.; Merenbloom, B.K.; Betts, L.; Okumura, N.; Heroux, A.; Gorkun, O.V.; Lord, S.T.
Deposited on : 2008-01-07
Resolution : 2.60 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

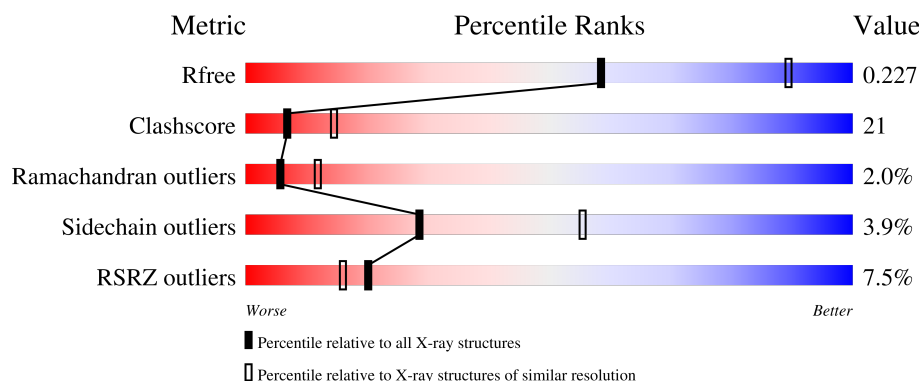
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	62	
1	D	62	
2	B	298	
2	E	298	
3	C	293	

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Mol	Chain	Length	Quality of chain
3	F	293	
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	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11144 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	62	Total	C	N	O	S	0	0	0
			507	311	97	96	3			
1	D	62	Total	C	N	O	S	0	0	0
			507	311	97	96	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2393	1494	422	455	22			
2	E	298	Total	C	N	O	S	0	0	0
			2393	1494	422	455	22			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	293	Total	C	N	O	S	0	0	0
			2349	1490	397	451	11			
3	F	293	Total	C	N	O	S	0	0	0
			2349	1490	397	451	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	364	ALA	ASP	engineered mutation	UNP P02679
F	364	ALA	ASP	engineered mutation	UNP P02679

- Molecule 4 is a protein called 4-mer peptide GPRP.

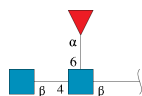
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			

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

- 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	0	0	0
			38	22	2	14			
5	L	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	1	Total	Ca	0	0
			1	1		
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	24	Total	O	0	0
			24	24		
7	B	169	Total	O	0	0
			169	169		
7	C	105	Total	O	0	0
			105	105		

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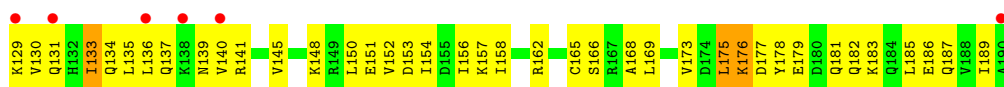
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	16	Total 16	O 16	0	0
7	E	92	Total 92	O 92	0	0
7	F	39	Total 39	O 39	0	0
7	I	1	Total 1	O 1	0	0

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.

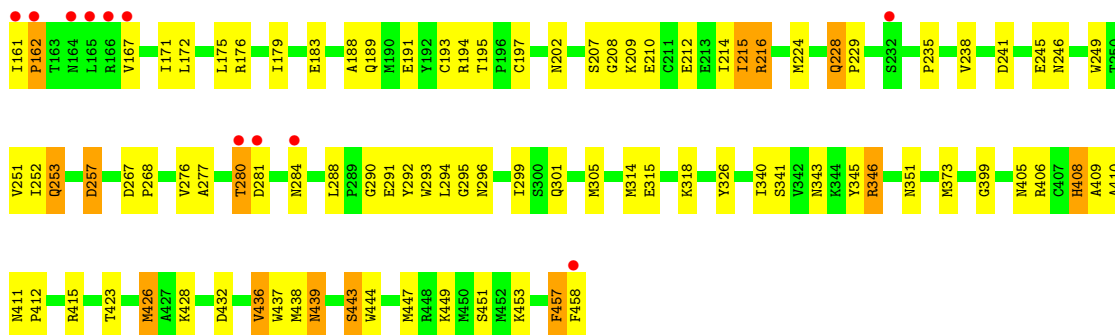
- Molecule 1: Fibrinogen alpha chain



- Molecule 1: Fibrinogen alpha chain

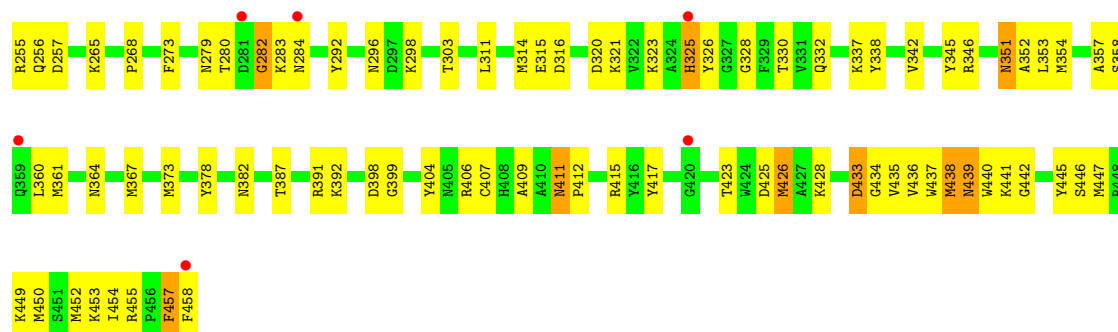


- Molecule 2: Fibrinogen beta chain

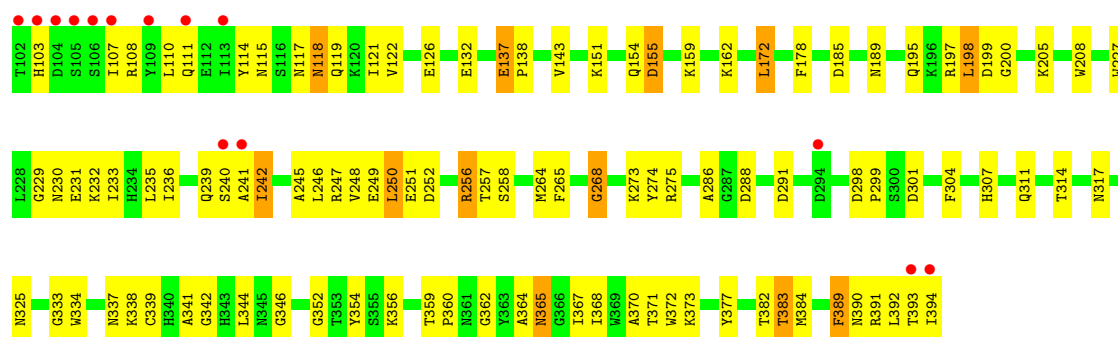


- Molecule 2: Fibrinogen beta chain

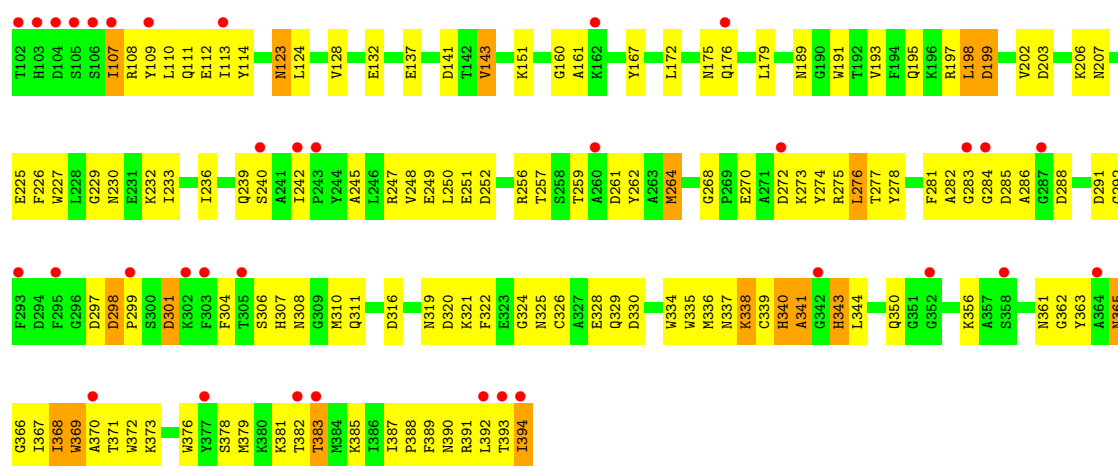




• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain



• Molecule 4: 4-mer peptide GPRP

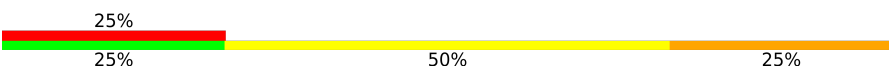


- Molecule 4: 4-mer peptide GPRP

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: 4-mer peptide GPRP

Chain H:  25% 25% 50% 25%

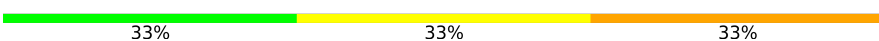


- Molecule 4: 4-mer peptide GPRP

Chain J:  75% 25%

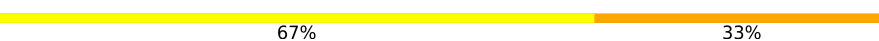


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 33% 33%



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

Chain L:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.84Å 94.91Å 225.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	48.1 (50.00-2.60) 92.6 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.260 0.222 , 0.227	Depositor DCC
R_{free} test set	3353 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.33% 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: FUC, CA, 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	0.41	0/508	0.86	0/676
1	D	0.40	0/508	0.83	1/676 (0.1%)
2	B	0.48	0/2454	0.99	11/3312 (0.3%)
2	E	0.40	0/2454	0.95	10/3312 (0.3%)
3	C	0.44	0/2414	0.92	9/3264 (0.3%)
3	F	0.36	0/2414	0.82	5/3264 (0.2%)
4	G	0.56	0/31	0.93	0/40
4	H	0.69	0/31	1.07	0/40
4	I	0.62	0/31	0.89	0/40
4	J	0.66	0/31	0.99	0/40
All	All	0.42	0/10876	0.92	36/14664 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	399	GLY	N-CA-C	9.73	128.79	114.10
2	B	409	ALA	N-CA-C	-8.85	103.00	113.88
2	E	409	ALA	N-CA-C	-8.62	103.19	114.31
2	E	203	ILE	N-CA-C	7.36	116.73	108.05
2	B	436	VAL	N-CA-C	7.09	119.96	108.97
2	B	257	ASP	N-CA-C	-6.89	98.56	108.07
3	C	268	GLY	CA-C-N	6.86	126.82	120.03
3	C	268	GLY	C-N-CA	6.86	126.82	120.03
2	B	194	ARG	N-CA-C	-6.78	104.82	113.23
2	B	444	TRP	N-CA-C	6.36	119.76	112.57
3	C	389	PHE	N-CA-C	6.32	118.17	111.28
2	B	197	CYS	N-CA-C	-6.27	101.24	110.52
2	E	411	ASN	CA-C-N	6.16	125.84	119.56
2	E	411	ASN	C-N-CA	6.16	125.84	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	426	MET	N-CA-C	-6.12	105.84	113.55
2	B	426	MET	N-CA-C	-6.07	106.20	113.97
3	C	137	GLU	CA-C-N	5.98	126.44	120.52
3	C	137	GLU	C-N-CA	5.98	126.44	120.52
3	F	341	ALA	N-CA-C	-5.90	105.92	114.12
3	F	368	ILE	N-CA-C	5.79	117.45	109.46
3	F	340	HIS	N-CA-C	5.78	117.04	108.60
2	E	279	ASN	N-CA-C	5.74	118.56	110.23
3	C	342	GLY	N-CA-C	-5.64	99.80	113.18
3	F	268	GLY	CA-C-N	5.64	125.61	120.03
3	F	268	GLY	C-N-CA	5.64	125.61	120.03
2	B	443	SER	N-CA-C	5.59	118.30	111.82
2	E	194	ARG	N-CA-C	-5.57	106.44	113.18
3	C	368	ILE	N-CA-C	5.52	117.59	108.99
2	E	197	CYS	N-CA-C	-5.39	102.54	110.52
2	B	408	HIS	N-CA-C	5.38	117.02	108.79
2	B	290	GLY	N-CA-C	-5.33	104.97	112.60
1	D	131	GLN	N-CA-C	-5.23	106.85	113.18
3	C	155	ASP	N-CA-C	-5.16	105.66	111.28
2	E	282	GLY	N-CA-C	-5.16	108.22	114.92
2	E	433	ASP	N-CA-C	-5.14	103.25	110.50
3	C	370	ALA	N-CA-C	5.13	117.28	111.02

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	507	0	530	44	0
1	D	507	0	530	35	0
2	B	2393	0	2262	73	0
2	E	2393	0	2261	104	0
3	C	2349	0	2200	78	0
3	F	2349	0	2200	125	0
4	G	30	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	30	0	32	4	0
4	I	30	0	32	0	0
4	J	30	0	32	1	0
5	K	38	0	34	5	0
5	L	38	0	35	7	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	24	0	0	1	0
7	B	169	0	0	3	0
7	C	105	0	0	2	0
7	D	16	0	0	0	0
7	E	92	0	0	2	0
7	F	39	0	0	0	0
7	I	1	0	0	0	0
All	All	11144	0	10180	443	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 21.

All (443) 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)
2:B:373:MET:HE2	2:B:405:ASN:HA	1.39	1.02
3:C:172:LEU:H	3:C:239:GLN:HE21	1.11	0.97
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.25	0.96
2:B:439:ASN:H	2:B:439:ASN:HD22	1.16	0.91
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.53	0.88
2:B:280:THR:HG23	2:B:288:LEU:HG	1.55	0.86
1:A:130:VAL:HG12	1:A:134:GLN:HE21	1.44	0.83
3:C:365:ASN:HD22	3:C:365:ASN:H	1.25	0.82
3:C:189:ASN:ND2	3:C:391:ARG:HE	1.78	0.82
1:A:157:LYS:HE3	3:C:132:GLU:OE2	1.81	0.80
2:B:439:ASN:HD22	2:B:439:ASN:N	1.80	0.80
2:B:228:GLN:HG3	2:B:235:PRO:HG3	1.65	0.79
2:E:315:GLU:OE1	2:E:321:LYS:HE2	1.83	0.79
3:F:189:ASN:ND2	3:F:391:ARG:HE	1.79	0.79
3:C:241:ALA:O	3:C:242:ILE:HG13	1.83	0.78
2:E:202:ASN:ND2	2:E:284:ASN:HB2	1.98	0.78
2:E:423:THR:N	2:E:426:MET:HE3	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:O	1:A:182:GLN:HG3	1.85	0.77
3:F:197:ARG:HB2	3:F:382:THR:HB	1.68	0.75
2:E:252:ILE:HD12	2:E:454:ILE:HG23	1.67	0.75
2:E:346:ARG:O	2:E:346:ARG:HG3	1.86	0.74
2:E:361:MET:HB2	5:L:1:NAG:O7	1.87	0.74
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.23	0.73
2:E:323:LYS:NZ	2:E:325:HIS:HD2	1.86	0.73
2:B:295:GLY:O	2:B:299:ILE:HG12	1.88	0.73
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.69	0.72
3:F:107:ILE:HD13	3:F:107:ILE:O	1.89	0.72
2:B:161:ILE:N	2:B:162:PRO:HD2	2.05	0.72
3:F:240:SER:O	3:F:242:ILE:HG13	1.90	0.72
3:F:252:ASP:OD2	3:F:256:ARG:HB2	1.89	0.72
3:F:288:ASP:OD2	3:F:291:ASP:HB2	1.89	0.72
3:C:189:ASN:HD22	3:C:391:ARG:HE	1.35	0.72
3:C:172:LEU:H	3:C:239:GLN:NE2	1.87	0.71
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.90	0.71
1:D:150:LEU:O	1:D:154:ILE:HG12	1.91	0.70
3:F:373:LYS:HG3	3:F:379:MET:HE1	1.72	0.70
3:F:249:GLU:HB2	3:F:383:THR:CG2	2.22	0.69
2:B:423:THR:N	2:B:426:MET:HE3	2.06	0.69
2:E:423:THR:H	2:E:426:MET:HE3	1.58	0.69
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.58	0.68
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.76	0.68
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.08	0.67
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.09	0.67
3:C:338:LYS:N	3:C:339:CYS:HA	2.10	0.66
3:F:273:LYS:HB2	3:F:311:GLN:HB3	1.77	0.66
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.31	0.66
2:E:202:ASN:HD22	2:E:284:ASN:HD22	1.44	0.65
3:C:365:ASN:HD22	3:C:365:ASN:N	1.94	0.65
2:E:351:ASN:C	2:E:351:ASN:HD22	2.04	0.65
3:F:245:ALA:HB2	3:F:389:PHE:HD1	1.62	0.65
1:D:133:ILE:O	1:D:137:GLN:HG3	1.97	0.64
3:F:326:CYS:HB3	3:F:336:MET:HE3	1.79	0.64
1:A:137:GLN:NE2	1:A:189:ILE:HA	2.12	0.64
2:E:323:LYS:HZ1	2:E:325:HIS:HD2	1.45	0.64
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.79	0.64
1:D:135:LEU:HG	1:D:139:ASN:HD21	1.64	0.63
5:L:1:NAG:C6	5:L:3:FUC:C1	2.76	0.63
1:A:166:SER:HB3	2:B:195:THR:OG1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:351:ASN:ND2	2:E:354:MET:H	1.97	0.63
1:D:177:ASP:O	1:D:181:GLN:HG3	1.99	0.62
3:F:124:LEU:O	3:F:128:VAL:HG23	2.00	0.62
2:B:252:ILE:HB	2:B:299:ILE:CD1	2.28	0.62
2:B:423:THR:H	2:B:426:MET:HE3	1.64	0.62
2:B:439:ASN:N	2:B:439:ASN:ND2	2.48	0.62
2:E:441:LYS:HG3	2:E:447:MET:HE1	1.81	0.62
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.00	0.62
2:E:434:GLY:O	2:E:436:VAL:N	2.33	0.62
1:A:141:ARG:O	1:A:145:VAL:HG23	1.99	0.61
2:B:176:ARG:HG3	3:C:117:ASN:HD21	1.65	0.61
3:F:276:LEU:HD12	3:F:277:THR:N	2.14	0.61
3:F:393:THR:O	3:F:394:ILE:HG22	2.00	0.61
3:F:203:ASP:O	3:F:206:LYS:HE2	2.00	0.61
2:E:168:LEU:HB3	3:F:110:LEU:HD13	1.81	0.61
4:H:3:ARG:O	4:H:4:PRO:C	2.43	0.61
1:A:135:LEU:HG	1:A:139:ASN:HD21	1.65	0.61
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.83	0.61
2:E:352:ALA:HB2	2:E:439:ASN:ND2	2.15	0.61
1:A:150:LEU:O	1:A:154:ILE:HD13	2.00	0.61
7:B:502:HOH:O	5:K:2:NAG:H2	2.00	0.61
3:F:151:LYS:NZ	3:F:172:LEU:HD21	2.16	0.61
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.01	0.60
3:C:189:ASN:ND2	3:C:391:ARG:HG3	2.15	0.60
3:F:175:ASN:HB3	3:F:176:GLN:HE21	1.65	0.60
1:A:169:LEU:H	2:B:189:GLN:NE2	1.98	0.60
3:C:365:ASN:H	3:C:365:ASN:ND2	1.99	0.60
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.35	0.60
4:H:3:ARG:HB3	4:H:4:PRO:HD2	1.83	0.60
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.02	0.60
2:E:166:ARG:HG3	7:E:483:HOH:O	2.01	0.60
2:E:172:LEU:HD13	3:F:113:ILE:HG13	1.84	0.60
3:F:232:LYS:O	3:F:236:ILE:HG13	2.01	0.60
1:A:133:ILE:HD13	1:A:133:ILE:C	2.26	0.60
2:E:212:GLU:O	2:E:216:ARG:HG3	2.01	0.60
1:A:185:LEU:HD13	1:A:185:LEU:O	2.01	0.59
2:B:346:ARG:O	2:B:346:ARG:HG3	2.02	0.59
3:F:123:ASN:N	3:F:123:ASN:HD22	2.00	0.59
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.37	0.59
2:B:188:ALA:O	2:B:191:GLU:HB3	2.02	0.59
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:LEU:CB	3:F:110:LEU:HD13	2.33	0.59
1:A:133:ILE:HD13	1:A:133:ILE:O	2.02	0.59
2:B:457:PHE:O	2:B:458:PHE:HB2	2.03	0.59
2:E:244:THR:HG22	2:E:245:GLU:HG2	1.82	0.59
2:E:316:ASP:OD2	2:E:320:ASP:HB2	2.03	0.59
3:F:338:LYS:N	3:F:339:CYS:HA	2.16	0.59
3:F:340:HIS:CE1	3:F:368:ILE:HD11	2.39	0.58
2:B:176:ARG:HG3	3:C:117:ASN:ND2	2.19	0.58
3:C:119:GLN:HA	3:C:119:GLN:HE21	1.67	0.58
2:E:326:TYR:CE2	2:E:353:LEU:HD12	2.38	0.58
2:E:282:GLY:C	2:E:283:LYS:HD2	2.28	0.58
2:E:351:ASN:HD21	2:E:354:MET:H	1.52	0.58
2:E:364:ASN:HA	2:E:367:MET:HE3	1.85	0.58
5:L:1:NAG:H4	5:L:2:NAG:HN2	1.69	0.58
2:E:360:LEU:HD11	4:H:2:PRO:HD3	1.84	0.58
2:E:162:PRO:HG2	2:E:163:THR:H	1.69	0.58
3:F:297:ASP:O	3:F:298:ASP:HB2	2.03	0.58
2:B:167:VAL:O	2:B:171:ILE:HG12	2.04	0.57
2:B:252:ILE:HB	2:B:299:ILE:HD11	1.87	0.57
1:D:164:SER:HB3	3:F:137:GLU:O	2.04	0.57
5:K:1:NAG:H4	5:K:2:NAG:HN2	1.69	0.57
3:C:393:THR:O	3:C:393:THR:HG22	2.04	0.57
4:J:4:PRO:HG3	5:K:1:NAG:H62	1.86	0.57
3:C:248:VAL:HG12	3:C:250:LEU:HD13	1.86	0.57
2:E:202:ASN:HD22	2:E:284:ASN:HB2	1.66	0.57
1:D:144:LEU:HD13	1:D:182:GLN:HG2	1.86	0.56
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.71	0.56
1:D:130:VAL:O	1:D:133:ILE:HG22	2.05	0.56
3:F:325:ASN:HD22	3:F:325:ASN:C	2.13	0.56
1:D:141:ARG:O	1:D:145:VAL:HG23	2.05	0.56
2:E:406:ARG:O	2:E:406:ARG:HG2	2.05	0.56
1:A:186:GLU:OE1	1:A:189:ILE:HD12	2.05	0.55
3:F:151:LYS:HZ3	3:F:172:LEU:HD21	1.72	0.55
3:F:247:ARG:HH22	3:F:392:LEU:HD11	1.72	0.55
3:C:304:PHE:O	3:C:337:ASN:HB3	2.07	0.55
3:C:307:HIS:CE1	3:C:341:ALA:H	2.24	0.55
2:E:387:THR:HG21	2:E:392:LYS:O	2.06	0.55
1:A:135:LEU:HG	1:A:139:ASN:ND2	2.22	0.55
2:E:417:TYR:HB2	2:E:446:SER:HB3	1.89	0.55
3:F:325:ASN:CG	3:F:328:GLU:HB2	2.32	0.55
1:D:169:LEU:H	2:E:189:GLN:NE2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:161:ILE:N	2:E:162:PRO:HD2	2.23	0.54
1:A:148:LYS:HE3	1:A:175:LEU:CD1	2.37	0.54
1:A:177:ASP:O	1:A:181:GLN:HG3	2.08	0.54
2:E:252:ILE:HD13	2:E:452:MET:O	2.07	0.54
3:F:264:MET:O	3:F:278:TYR:HA	2.06	0.54
3:F:297:ASP:HB2	3:F:301:ASP:OD2	2.06	0.54
1:A:136:LEU:HD11	3:C:111:GLN:HG2	1.88	0.54
2:E:330:THR:HG22	7:E:477:HOH:O	2.08	0.54
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.89	0.54
2:B:228:GLN:HG3	2:B:235:PRO:CG	2.36	0.54
1:A:175:LEU:O	1:A:179:GLU:HG3	2.07	0.54
1:D:132:HIS:O	1:D:136:LEU:HG	2.07	0.54
2:E:411:ASN:N	2:E:412:PRO:HD3	2.23	0.54
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.73	0.54
3:F:350:GLN:HA	3:F:350:GLN:NE2	2.22	0.54
3:C:151:LYS:HE2	3:C:172:LEU:HD13	1.89	0.54
3:F:248:VAL:O	3:F:259:THR:HA	2.07	0.54
1:D:129:LYS:HA	1:D:132:HIS:HD2	1.72	0.53
3:F:389:PHE:C	3:F:391:ARG:H	2.16	0.53
2:E:212:GLU:OE1	2:E:455:ARG:HD2	2.07	0.53
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.72	0.53
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.09	0.53
3:C:390:ASN:O	3:C:394:ILE:HA	2.07	0.53
2:E:169:ARG:HA	3:F:110:LEU:HD22	1.91	0.53
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.43	0.53
3:C:317:ASN:HD22	3:C:317:ASN:C	2.16	0.53
3:C:338:LYS:O	3:C:338:LYS:HG2	2.08	0.53
3:F:247:ARG:HH21	3:F:392:LEU:HD21	1.72	0.53
2:E:215:ILE:HD13	2:E:215:ILE:O	2.09	0.53
2:E:328:GLY:O	2:E:342:VAL:HA	2.09	0.53
3:F:229:GLY:O	3:F:233:ILE:HG13	2.08	0.53
3:C:354:TYR:OH	3:C:364:ALA:HB1	2.09	0.53
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.74	0.53
3:F:321:LYS:O	3:F:338:LYS:HB2	2.08	0.53
1:A:185:LEU:O	1:A:189:ILE:HG13	2.09	0.53
1:D:176:LYS:HB2	1:D:176:LYS:HZ3	1.73	0.53
2:B:228:GLN:CG	2:B:235:PRO:HG3	2.37	0.52
3:C:273:LYS:HB2	3:C:311:GLN:HB3	1.92	0.52
1:A:169:LEU:H	2:B:189:GLN:HE22	1.56	0.52
2:B:253:GLN:NE2	2:B:451:SER:HA	2.25	0.52
3:F:361:ASN:N	3:F:361:ASN:HD22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.44	0.52
2:B:202:ASN:HD22	2:B:284:ASN:HD22	1.58	0.52
3:F:350:GLN:HA	3:F:350:GLN:HE21	1.75	0.52
2:B:280:THR:CG2	2:B:288:LEU:HG	2.34	0.52
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.45	0.52
2:E:252:ILE:HD13	2:E:252:ILE:H	1.75	0.51
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.45	0.51
3:C:197:ARG:HB2	3:C:382:THR:HB	1.92	0.51
3:C:229:GLY:O	3:C:233:ILE:HG13	2.10	0.51
3:F:322:PHE:CZ	3:F:324:GLY:HA3	2.46	0.51
2:B:251:VAL:HG22	2:B:453:LYS:HG2	1.91	0.51
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.25	0.51
2:E:351:ASN:C	2:E:351:ASN:ND2	2.68	0.51
3:C:189:ASN:HD22	3:C:391:ARG:HG3	1.76	0.51
3:C:352:GLY:O	3:C:377:TYR:HA	2.09	0.51
2:E:180:GLN:HA	2:E:183:GLU:OE1	2.10	0.51
1:D:175:LEU:H	1:D:175:LEU:HD22	1.76	0.51
2:E:445:TYR:HD1	2:E:447:MET:HE2	1.75	0.51
3:F:189:ASN:HD21	3:F:391:ARG:HE	1.55	0.51
3:C:122:VAL:O	3:C:126:GLU:HG3	2.10	0.51
1:A:136:LEU:O	1:A:140:VAL:HG13	2.10	0.51
2:E:311:LEU:HD23	2:E:453:LYS:HD2	1.91	0.51
2:E:332:GLN:O	2:E:338:TYR:HA	2.10	0.51
3:F:365:ASN:HD22	3:F:366:GLY:N	2.08	0.51
3:F:251:GLU:CD	3:F:381:LYS:HD2	2.36	0.51
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.11	0.50
3:C:307:HIS:HE1	3:C:341:ALA:H	1.59	0.50
1:D:154:ILE:O	1:D:158:ILE:HG12	2.11	0.50
4:G:3:ARG:HA	4:G:3:ARG:HE	1.76	0.50
1:D:134:GLN:O	1:D:138:LYS:HG3	2.12	0.50
3:F:247:ARG:NH2	3:F:392:LEU:HD21	2.27	0.50
3:C:298:ASP:HB3	3:C:301:ASP:OD1	2.12	0.50
3:F:108:ARG:O	3:F:112:GLU:HG3	2.11	0.50
1:A:136:LEU:HD11	3:C:111:GLN:CG	2.41	0.50
3:C:286:ALA:O	3:C:372:TRP:HB2	2.12	0.49
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.94	0.49
2:B:175:LEU:O	2:B:179:ILE:HG13	2.12	0.49
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.74	0.49
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.93	0.49
2:E:361:MET:CB	5:L:1:NAG:H81	2.42	0.49
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.59	0.49
2:B:410:ALA:C	2:B:412:PRO:HD3	2.38	0.49
2:E:311:LEU:HB3	2:E:453:LYS:HG3	1.93	0.49
3:F:310:MET:HB2	3:F:335:TRP:HB3	1.94	0.49
2:E:280:THR:HB	2:E:283:LYS:HG2	1.93	0.49
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.78	0.49
1:D:135:LEU:HG	1:D:139:ASN:ND2	2.26	0.49
2:E:373:MET:HE2	2:E:404:TYR:O	2.13	0.49
3:F:276:LEU:HD12	3:F:276:LEU:C	2.38	0.49
2:B:257:ASP:O	2:B:291:GLU:OE2	2.30	0.49
2:B:294:LEU:HB3	2:B:299:ILE:HD11	1.93	0.49
3:C:208:TRP:HA	3:C:314:THR:HG21	1.95	0.49
2:E:219:GLY:O	2:E:242:MET:HE3	2.12	0.49
2:B:179:ILE:O	2:B:183:GLU:HG3	2.12	0.49
3:C:117:ASN:O	3:C:121:ILE:HG13	2.13	0.49
3:C:200:GLY:HA2	7:C:409:HOH:O	2.12	0.48
3:F:273:LYS:CB	3:F:311:GLN:HB3	2.43	0.48
1:A:185:LEU:HD13	1:A:185:LEU:C	2.38	0.48
3:C:247:ARG:NH2	3:C:392:LEU:HD11	2.27	0.48
1:A:162:ARG:CZ	7:A:196:HOH:O	2.61	0.48
3:C:268:GLY:O	3:C:274:TYR:HA	2.12	0.48
2:B:438:MET:HE3	2:B:443:SER:OG	2.12	0.48
2:B:212:GLU:O	2:B:215:ILE:HG22	2.13	0.48
1:D:180:ASP:O	1:D:184:GLN:HB2	2.14	0.48
3:F:249:GLU:HG2	3:F:259:THR:HG22	1.94	0.48
1:D:169:LEU:H	2:E:189:GLN:HE22	1.60	0.48
3:C:298:ASP:OD1	3:C:299:PRO:HD2	2.13	0.48
5:K:1:NAG:H4	5:K:2:NAG:N2	2.28	0.48
2:B:423:THR:OG1	2:B:426:MET:HE3	2.13	0.48
3:C:155:ASP:O	3:C:159:LYS:HG3	2.14	0.47
2:E:187:SER:O	2:E:191:GLU:HG3	2.14	0.47
2:E:265:LYS:HE3	2:E:378:TYR:OH	2.13	0.47
3:F:370:ALA:C	3:F:372:TRP:H	2.22	0.47
5:K:1:NAG:O3	5:K:2:NAG:H82	2.14	0.47
1:A:183:LYS:O	1:A:187:GLN:HG3	2.14	0.47
3:F:307:HIS:CE1	3:F:341:ALA:H	2.31	0.47
5:L:1:NAG:O3	5:L:2:NAG:H82	2.14	0.47
1:A:130:VAL:HA	1:A:133:ILE:HG22	1.96	0.47
3:F:141:ASP:OD1	3:F:143:VAL:HG13	2.15	0.47
3:C:231:GLU:O	3:C:235:LEU:HG	2.15	0.47
3:F:338:LYS:O	3:F:338:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ASP:O	1:D:157:LYS:HG2	2.15	0.47
3:F:307:HIS:HD2	3:F:335:TRP:O	1.97	0.47
3:F:356:LYS:HG3	3:F:362:GLY:O	2.15	0.47
2:B:229:PRO:CB	2:B:301:GLN:HE22	2.27	0.47
2:E:361:MET:HB3	5:L:1:NAG:H81	1.96	0.47
3:C:275:ARG:HA	3:C:311:GLN:HA	1.98	0.46
2:E:439:ASN:HD22	2:E:439:ASN:H	1.64	0.46
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.50	0.46
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.30	0.46
2:E:346:ARG:O	2:E:346:ARG:CG	2.58	0.46
2:B:406:ARG:O	2:B:406:ARG:HG2	2.15	0.46
2:E:174:ASN:O	2:E:178:LYS:HG3	2.16	0.46
2:E:345:TYR:CE2	2:E:351:ASN:HB2	2.50	0.46
1:A:151:GLU:HG2	1:A:173:VAL:HG13	1.97	0.46
3:C:103:HIS:O	3:C:107:ILE:HG22	2.16	0.46
2:B:161:ILE:N	2:B:162:PRO:CD	2.76	0.46
1:A:176:LYS:HA	1:A:179:GLU:OE1	2.16	0.45
2:B:212:GLU:OE2	2:B:216:ARG:HD2	2.16	0.45
3:C:154:GLN:OE1	3:C:391:ARG:HG2	2.15	0.45
3:C:249:GLU:CB	3:C:383:THR:HG23	2.42	0.45
2:E:417:TYR:HB2	2:E:446:SER:CB	2.45	0.45
1:D:136:LEU:O	1:D:140:VAL:HG22	2.17	0.45
3:F:365:ASN:HD22	3:F:365:ASN:C	2.23	0.45
2:E:191:GLU:HG2	2:E:194:ARG:HH21	1.82	0.45
3:F:239:GLN:HB3	3:F:242:ILE:HD12	1.98	0.45
2:E:315:GLU:HB3	2:E:449:LYS:HB2	1.98	0.45
3:F:284:GLY:C	3:F:286:ALA:H	2.24	0.45
2:B:408:HIS:CD2	2:B:408:HIS:C	2.95	0.45
3:C:344:LEU:HD12	3:C:384:MET:SD	2.57	0.45
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.14	0.45
2:B:224:MET:HE3	2:B:277:ALA:HB3	1.99	0.45
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.99	0.45
3:C:393:THR:O	3:C:394:ILE:OXT	2.35	0.45
2:E:441:LYS:CG	2:E:447:MET:HE1	2.47	0.45
3:F:167:TYR:O	3:F:179:LEU:HD12	2.17	0.45
1:A:185:LEU:CD1	1:A:189:ILE:HD11	2.47	0.44
2:B:340:ILE:HG12	2:B:341:SER:N	2.31	0.44
3:F:387:ILE:HD11	3:F:391:ARG:HG2	1.99	0.44
2:E:436:VAL:CG1	2:E:437:TRP:N	2.79	0.44
3:F:262:TYR:CE2	3:F:288:ASP:OD1	2.71	0.44
3:C:118:ASN:HB3	7:C:480:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:247:ARG:NH2	3:F:392:LEU:HD11	2.32	0.44
2:B:428:LYS:HE3	2:B:428:LYS:HB2	1.81	0.44
2:E:236:TYR:CD2	2:E:298:LYS:HE2	2.52	0.44
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.16	0.44
2:B:439:ASN:H	2:B:439:ASN:ND2	1.94	0.44
2:E:433:ASP:OD1	2:E:433:ASP:O	2.36	0.44
3:F:325:ASN:O	3:F:328:GLU:HB3	2.17	0.44
3:C:325:ASN:C	3:C:325:ASN:HD22	2.24	0.44
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.18	0.44
2:E:406:ARG:N	2:E:407:CYS:HA	2.32	0.44
2:B:432:ASP:CB	2:B:443:SER:HB3	2.48	0.44
3:C:189:ASN:HD22	3:C:391:ARG:NE	2.11	0.44
1:A:148:LYS:HE3	1:A:175:LEU:HD12	1.98	0.44
2:E:358:SER:C	2:E:360:LEU:H	2.25	0.44
3:C:239:GLN:O	3:C:240:SER:C	2.61	0.43
1:D:148:LYS:O	1:D:152:VAL:HG23	2.17	0.43
1:D:175:LEU:HD22	1:D:175:LEU:N	2.33	0.43
2:E:209:LYS:C	2:E:210:GLU:HG3	2.43	0.43
1:A:129:LYS:C	1:A:131:GLN:H	2.26	0.43
3:F:207:ASN:HB2	3:F:316:ASP:OD2	2.17	0.43
1:A:137:GLN:CG	1:A:189:ILE:HG12	2.48	0.43
1:D:147:MET:HG3	2:E:175:LEU:HD22	2.00	0.43
2:B:207:SER:C	2:B:214:ILE:CD1	2.91	0.43
3:F:172:LEU:H	3:F:239:GLN:HE21	1.64	0.43
3:F:276:LEU:HD23	3:F:335:TRP:CD2	2.54	0.43
2:E:273:PHE:O	2:E:292:TYR:HB2	2.18	0.43
3:F:330:ASP:HB3	3:F:343:HIS:HE1	1.84	0.43
5:L:1:NAG:H4	5:L:2:NAG:N2	2.28	0.43
3:C:391:ARG:HD2	3:C:391:ARG:HA	1.83	0.43
2:E:391:ARG:HG3	2:E:391:ARG:HH11	1.84	0.43
3:F:239:GLN:CB	3:F:242:ILE:HD12	2.49	0.43
3:F:350:GLN:HE21	3:F:350:GLN:CA	2.30	0.43
1:A:129:LYS:C	1:A:131:GLN:N	2.77	0.43
2:B:345:TYR:CE2	2:B:351:ASN:HB2	2.54	0.43
3:C:333:GLY:O	3:C:334:TRP:HB2	2.19	0.43
2:B:436:VAL:CG1	2:B:437:TRP:N	2.82	0.43
3:C:356:LYS:HG3	3:C:362:GLY:O	2.19	0.43
2:E:169:ARG:HB2	3:F:110:LEU:HD21	2.00	0.43
2:E:178:LYS:O	2:E:182:LEU:HG	2.19	0.43
3:F:365:ASN:C	3:F:365:ASN:ND2	2.76	0.43
3:C:185:ASP:OD1	3:C:185:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:ALA:HB2	3:C:389:PHE:HD1	1.84	0.42
3:F:251:GLU:CG	3:F:257:THR:HG22	2.49	0.42
1:D:183:LYS:O	1:D:187:GLN:HG3	2.19	0.42
1:D:185:LEU:HD13	1:D:185:LEU:C	2.44	0.42
3:F:109:TYR:C	3:F:111:GLN:H	2.26	0.42
3:F:322:PHE:CE2	3:F:324:GLY:HA3	2.55	0.42
2:E:161:ILE:N	2:E:162:PRO:CD	2.82	0.42
3:F:334:TRP:CD1	3:F:335:TRP:H	2.38	0.42
3:F:387:ILE:HG13	3:F:388:PRO:HD2	2.01	0.42
2:B:208:GLY:N	2:B:214:ILE:HD11	2.35	0.42
3:C:197:ARG:CZ	3:C:367:ILE:HD11	2.50	0.42
1:D:150:LEU:HD21	3:F:124:LEU:HD23	2.02	0.42
2:E:440:TRP:CE3	2:E:441:LYS:HG2	2.53	0.42
3:F:363:TYR:HE1	4:G:4:PRO:HD2	1.84	0.42
3:F:387:ILE:O	3:F:388:PRO:C	2.61	0.42
1:A:137:GLN:HE22	1:A:189:ILE:HA	1.81	0.42
1:A:153:ASP:O	1:A:157:LYS:HG2	2.19	0.42
2:B:209:LYS:HD3	2:B:305:MET:HE1	2.02	0.42
2:B:423:THR:O	2:B:426:MET:HB2	2.20	0.42
2:B:432:ASP:HB3	2:B:443:SER:HB3	2.01	0.42
3:C:346:GLY:O	3:C:367:ILE:HD11	2.20	0.42
3:C:359:THR:HA	3:C:360:PRO:HD3	1.92	0.42
3:F:250:LEU:HD21	3:F:369:TRP:CG	2.54	0.42
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.54	0.42
1:A:152:VAL:O	1:A:156:ILE:HG12	2.20	0.42
1:D:169:LEU:C	1:D:169:LEU:HD13	2.45	0.42
3:F:307:HIS:O	3:F:308:ASN:C	2.62	0.42
3:F:320:ASP:OD1	3:F:322:PHE:HB3	2.19	0.42
3:F:367:ILE:O	3:F:378:SER:HA	2.20	0.42
2:B:436:VAL:HG12	2:B:437:TRP:N	2.34	0.42
3:C:107:ILE:HG23	3:C:108:ARG:N	2.34	0.42
2:E:265:LYS:O	2:E:268:PRO:HD2	2.19	0.42
3:F:261:ASP:HB2	3:F:282:ALA:HB3	2.01	0.42
2:E:202:ASN:HD21	2:E:284:ASN:HB2	1.82	0.42
2:E:265:LYS:C	2:E:268:PRO:HD2	2.45	0.42
2:E:345:TYR:CG	2:E:351:ASN:HB2	2.55	0.42
3:F:160:GLY:O	3:F:161:ALA:C	2.62	0.42
3:F:389:PHE:O	3:F:391:ARG:N	2.49	0.42
3:C:114:TYR:CD2	3:C:115:ASN:ND2	2.88	0.42
3:C:137:GLU:HA	3:C:138:PRO:HD3	1.84	0.42
2:E:438:MET:HA	2:E:442:GLY:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:272:ASP:OD2	3:F:275:ARG:NE	2.52	0.42
3:F:304:PHE:O	3:F:337:ASN:HB3	2.20	0.42
3:F:304:PHE:HB3	3:F:338:LYS:HB3	2.02	0.42
2:B:411:ASN:N	2:B:412:PRO:HD3	2.35	0.41
3:F:276:LEU:HD23	3:F:335:TRP:CG	2.55	0.41
3:F:325:ASN:C	3:F:325:ASN:ND2	2.77	0.41
3:F:387:ILE:CG1	3:F:388:PRO:HD2	2.50	0.41
3:F:393:THR:O	3:F:394:ILE:OXT	2.37	0.41
1:A:131:GLN:HA	1:A:131:GLN:NE2	2.34	0.41
1:D:157:LYS:HE3	3:F:132:GLU:OE2	2.19	0.41
2:E:296:ASN:HB3	2:E:338:TYR:CD1	2.55	0.41
2:E:303:THR:HB	2:E:330:THR:HA	2.02	0.41
2:E:337:LYS:HG2	2:E:382:ASN:ND2	2.35	0.41
1:D:136:LEU:HD21	3:F:111:GLN:HG2	2.02	0.41
2:E:428:LYS:HB2	2:E:428:LYS:HE3	1.86	0.41
3:F:334:TRP:CG	3:F:335:TRP:H	2.39	0.41
1:A:150:LEU:HG	1:A:154:ILE:HD13	2.02	0.41
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.69	0.41
3:C:232:LYS:O	3:C:236:ILE:HG13	2.19	0.41
3:C:246:LEU:HD22	3:C:265:PHE:CE1	2.56	0.41
2:E:181:LYS:O	2:E:184:SER:HB2	2.20	0.41
3:F:248:VAL:HG12	3:F:250:LEU:CD1	2.50	0.41
3:F:329:GLN:OE1	4:G:3:ARG:HD3	2.20	0.41
2:B:318:LYS:HD2	7:B:597:HOH:O	2.20	0.41
1:A:130:VAL:HG12	1:A:130:VAL:O	2.21	0.41
3:F:356:LYS:HA	3:F:376:TRP:CZ3	2.56	0.41
3:C:258:SER:OG	3:C:286:ALA:HB2	2.21	0.41
2:E:457:PHE:O	2:E:458:PHE:HB2	2.21	0.41
3:F:193:VAL:HG12	3:F:226:PHE:CZ	2.55	0.41
3:F:198:LEU:O	3:F:199:ASP:HB3	2.20	0.41
2:B:415:ARG:HD3	7:B:490:HOH:O	2.20	0.41
1:D:187:GLN:O	1:D:189:ILE:N	2.43	0.41
2:E:438:MET:HA	2:E:442:GLY:O	2.21	0.41
3:F:123:ASN:N	3:F:123:ASN:ND2	2.69	0.41
3:F:370:ALA:O	3:F:372:TRP:N	2.53	0.41
3:C:373:LYS:HD3	3:C:373:LYS:HA	1.90	0.41
3:F:361:ASN:N	3:F:361:ASN:ND2	2.68	0.41
2:B:326:TYR:OH	2:B:351:ASN:ND2	2.53	0.40
2:E:175:LEU:O	2:E:176:ARG:C	2.64	0.40
2:E:280:THR:HB	2:E:283:LYS:CG	2.51	0.40
3:F:281:PHE:C	3:F:283:GLY:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLU:O	2:B:246:ASN:HB2	2.21	0.40
3:F:298:ASP:CG	3:F:299:PRO:HD2	2.46	0.40
2:B:172:LEU:CD1	3:C:110:LEU:HB3	2.51	0.40
2:B:343:ASN:OD1	2:B:343:ASN:C	2.65	0.40
2:B:405:ASN:HB3	2:B:406:ARG:H	1.62	0.40
1:D:149:ARG:HG3	2:E:425:ASP:O	2.22	0.40
2:E:212:GLU:O	2:E:215:ILE:HG22	2.21	0.40
2:E:255:ARG:N	2:E:450:MET:O	2.51	0.40
3:F:202:VAL:HG21	3:F:225:GLU:O	2.20	0.40
4:H:3:ARG:HD3	4:H:3:ARG:HA	1.84	0.40
1:A:165:CYS:HB3	2:B:193:CYS:HA	2.04	0.40
2:B:276:VAL:HA	2:B:292:TYR:CD1	2.56	0.40
2:E:415:ARG:O	2:E:434:GLY:HA2	2.21	0.40
3:F:109:TYR:C	3:F:111:GLN:N	2.80	0.40
3:F:250:LEU:HD12	3:F:250:LEU:N	2.36	0.40
3:F:292:GLY:H	3:F:306:SER:HA	1.86	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	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
1	D	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	7	15
2	B	296/298 (99%)	275 (93%)	18 (6%)	3 (1%)	12	28
2	E	296/298 (99%)	267 (90%)	20 (7%)	9 (3%)	3	6
3	C	291/293 (99%)	267 (92%)	19 (6%)	5 (2%)	7	15
3	F	291/293 (99%)	253 (87%)	30 (10%)	8 (3%)	4	7
4	G	2/4 (50%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	2/4 (50%)	2 (100%)	0	0	100	100
4	I	2/4 (50%)	2 (100%)	0	0	100	100
4	J	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
All	All	1302/1322 (98%)	1182 (91%)	94 (7%)	26 (2%)	6	12

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	162	PRO
2	E	457	PHE
3	F	199	ASP
3	C	198	LEU
1	D	188	VAL
2	E	162	PRO
2	E	399	GLY
2	E	435	VAL
3	F	371	THR
3	F	390	ASN
2	B	281	ASP
2	B	457	PHE
3	C	371	THR
2	E	256	GLN
2	E	438	MET
3	F	198	LEU
3	F	338	LYS
2	E	439	ASN
3	F	285	ASP
3	F	369	TRP
3	C	199	ASP
3	C	172	LEU
3	C	242	ILE
2	E	257	ASP
2	E	351	ASN
3	F	298	ASP

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	57/57 (100%)	54 (95%)	3 (5%)	20	43
1	D	57/57 (100%)	54 (95%)	3 (5%)	20	43
2	B	256/256 (100%)	246 (96%)	10 (4%)	28	55
2	E	256/256 (100%)	250 (98%)	6 (2%)	44	71
3	C	246/246 (100%)	236 (96%)	10 (4%)	27	54
3	F	246/246 (100%)	236 (96%)	10 (4%)	27	54
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	I	3/3 (100%)	3 (100%)	0	100	100
4	J	3/3 (100%)	3 (100%)	0	100	100
All	All	1130/1130 (100%)	1086 (96%)	44 (4%)	28	55

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

Mol	Chain	Res	Type
1	A	133	ILE
1	A	175	LEU
1	A	176	LYS
2	B	210	GLU
2	B	215	ILE
2	B	216	ARG
2	B	228	GLN
2	B	238	VAL
2	B	253	GLN
2	B	280	THR
2	B	346	ARG
2	B	439	ASN
2	B	447	MET
3	C	118	ASN
3	C	143	VAL
3	C	162	LYS
3	C	198	LEU
3	C	205	LYS
3	C	250	LEU
3	C	256	ARG
3	C	264	MET
3	C	365	ASN

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Mol	Chain	Res	Type
3	C	383	THR
1	D	144	LEU
1	D	164	SER
1	D	176	LYS
2	E	210	GLU
2	E	215	ILE
2	E	233	VAL
2	E	252	ILE
2	E	253	GLN
2	E	325	HIS
3	F	107	ILE
3	F	123	ASN
3	F	143	VAL
3	F	264	MET
3	F	276	LEU
3	F	301	ASP
3	F	343	HIS
3	F	365	ASN
3	F	383	THR
3	F	394	ILE
4	G	3	ARG
4	H	4	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	134	GLN
1	A	137	GLN
1	A	139	ASN
1	A	143	GLN
1	A	181	GLN
1	A	184	GLN
1	A	187	GLN
2	B	189	GLN
2	B	202	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

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Mol	Chain	Res	Type
2	B	351	ASN
2	B	393	GLN
2	B	408	HIS
2	B	421	GLN
2	B	429	HIS
2	B	439	ASN
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	119	GLN
3	C	134	GLN
3	C	136	GLN
3	C	146	HIS
3	C	176	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	350	GLN
3	C	365	ASN
1	D	132	HIS
1	D	139	ASN
1	D	181	GLN
1	D	182	GLN
1	D	187	GLN
2	E	164	ASN
2	E	189	GLN
2	E	202	ASN
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	339	GLN
2	E	351	ASN
2	E	382	ASN
2	E	408	HIS
2	E	421	GLN

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Mol	Chain	Res	Type
2	E	429	HIS
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	123	ASN
3	F	136	GLN
3	F	176	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	350	GLN
3	F	361	ASN
3	F	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	K	1	2,5	14,14,15	0.68	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	2	5	14,14,15	0.82	1 (7%)	17,19,21	0.87	1 (5%)
5	FUC	K	3	5	10,10,11	0.45	0	14,14,16	0.38	0
5	NAG	L	1	2,5	14,14,15	0.68	0	17,19,21	0.86	0
5	NAG	L	2	5	14,14,15	0.81	1 (7%)	17,19,21	0.87	1 (5%)
5	FUC	L	3	5	10,10,11	0.45	0	14,14,16	0.38	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	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	5/6/23/26	0/1/1/1
5	FUC	K	3	5	-	-	0/1/1/1
5	NAG	L	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	L	2	5	-	5/6/23/26	0/1/1/1
5	FUC	L	3	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	NAG	C1-C2	2.27	1.55	1.52
5	K	2	NAG	C1-C2	2.24	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	2	NAG	C2-N2-C7	-2.14	120.04	122.90
5	K	2	NAG	C2-N2-C7	-2.13	120.05	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
5	L	2	NAG	C3-C2-N2-C7
5	L	2	NAG	C8-C7-N2-C2

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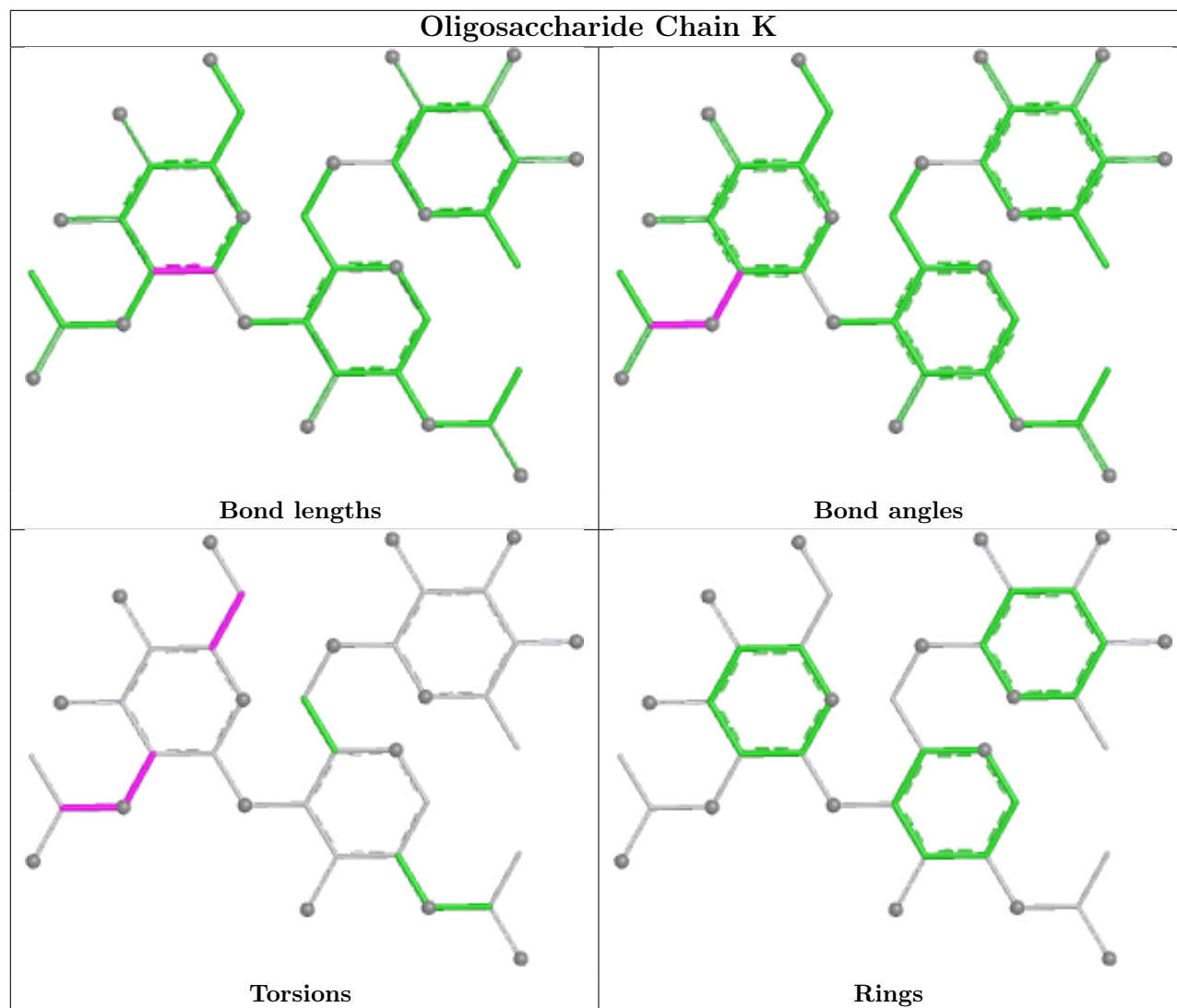
Mol	Chain	Res	Type	Atoms
5	L	2	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
5	L	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
5	L	2	NAG	C4-C5-C6-O6

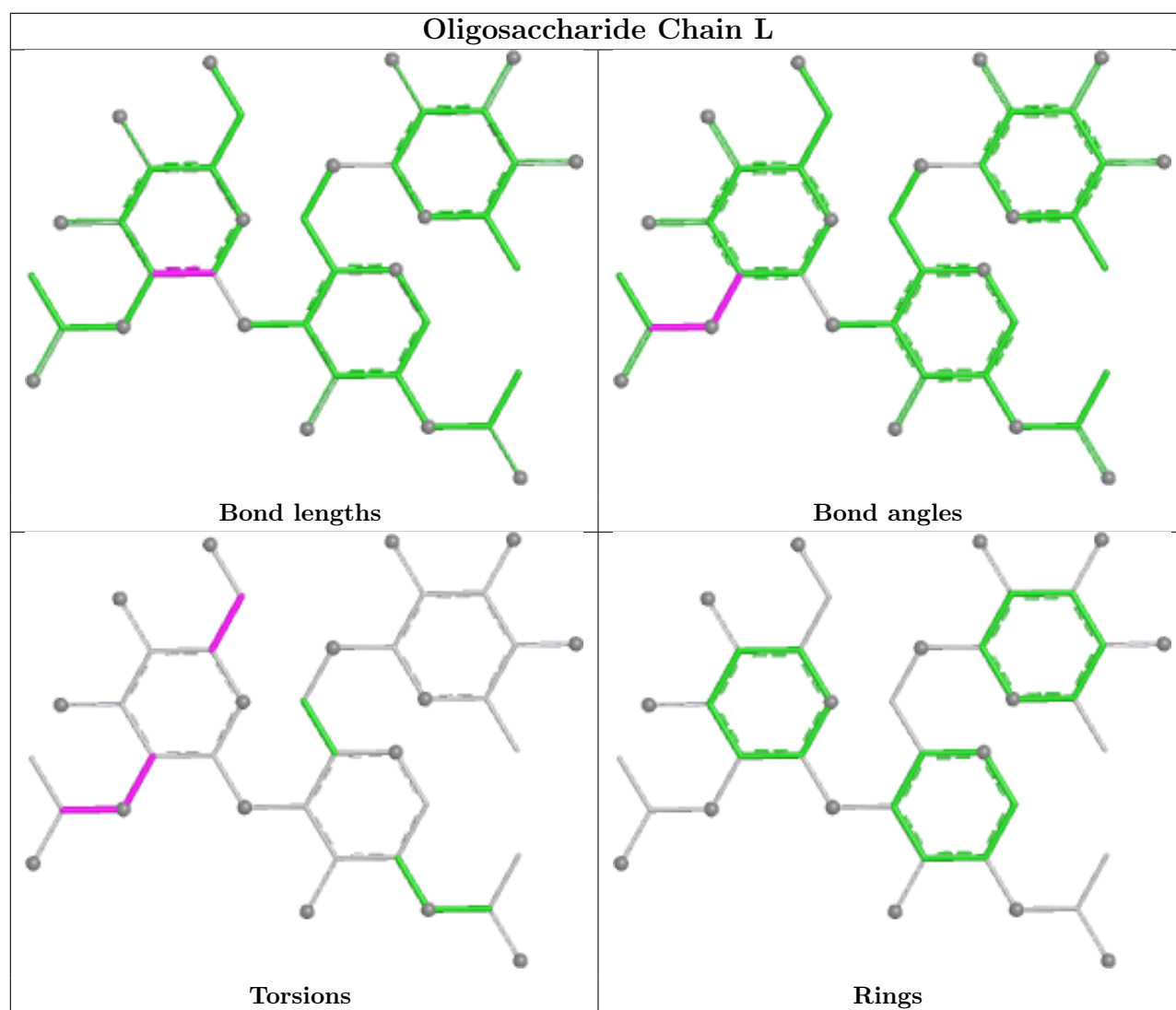
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	4	0
5	K	2	NAG	4	0
5	L	2	NAG	3	0
5	L	1	NAG	7	0
5	L	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	62/62 (100%)	0.63	6 (9%) 13 10	22, 49, 94, 108	0
1	D	62/62 (100%)	0.97	13 (20%) 2 2	24, 60, 99, 101	0
2	B	298/298 (100%)	-0.10	11 (3%) 45 39	10, 24, 61, 98	0
2	E	298/298 (100%)	0.37	18 (6%) 27 22	19, 39, 68, 97	0
3	C	293/293 (100%)	0.17	14 (4%) 35 30	16, 32, 67, 111	0
3	F	293/293 (100%)	0.90	35 (11%) 9 7	29, 52, 86, 116	0
4	G	4/4 (100%)	2.25	1 (25%) 2 1	85, 87, 87, 92	0
4	H	4/4 (100%)	1.09	1 (25%) 2 1	52, 59, 59, 63	0
4	I	4/4 (100%)	0.28	0 100 100	34, 34, 36, 46	0
4	J	4/4 (100%)	-0.15	0 100 100	25, 25, 28, 35	0
All	All	1322/1322 (100%)	0.38	99 (7%) 20 16	10, 37, 86, 116	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	394	ILE	7.0
3	C	394	ILE	5.8
2	E	161	ILE	5.6
2	E	168	LEU	4.8
2	E	162	PRO	4.5
3	F	102	THR	4.4
2	B	162	PRO	4.3
2	E	164	ASN	4.3
3	C	393	THR	4.2
3	C	107	ILE	4.1
4	G	1	GLY	4.0
3	F	107	ILE	3.9
3	F	104	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	190	ALA	3.8
2	E	166	ARG	3.8
3	F	393	THR	3.7
2	B	281	ASP	3.6
3	F	299	PRO	3.5
2	B	161	ILE	3.4
1	D	189	ILE	3.3
1	D	135	LEU	3.3
1	A	129	LYS	3.3
3	F	109	TYR	3.3
3	F	260	ALA	3.2
3	C	102	THR	3.2
1	D	173	VAL	3.1
3	C	113	ILE	3.1
3	C	240	SER	3.1
3	F	105	SER	3.1
1	A	140	VAL	3.1
3	C	109	TYR	3.0
2	E	281	ASP	2.9
2	B	232	SER	2.9
2	B	280	THR	2.9
1	A	190	ALA	2.9
3	F	352	GLY	2.8
3	F	295	PHE	2.8
3	F	302	LYS	2.8
3	C	241	ALA	2.8
1	D	129	LYS	2.7
2	E	165	LEU	2.7
3	F	272	ASP	2.7
2	B	458	PHE	2.7
3	F	103	HIS	2.7
3	F	392	LEU	2.7
2	E	458	PHE	2.7
2	E	163	THR	2.7
3	F	383	THR	2.7
2	E	177	SER	2.6
3	F	240	SER	2.6
3	F	242	ILE	2.6
2	E	180	GLN	2.6
3	F	364	ALA	2.6
3	F	370	ALA	2.6
3	C	111	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	283	GLY	2.5
1	D	140	VAL	2.5
2	B	284	ASN	2.4
2	E	359	GLN	2.4
3	F	382	THR	2.4
3	F	342	GLY	2.4
2	E	284	ASN	2.4
1	A	138	LYS	2.4
1	D	186	GLU	2.3
3	F	303	PHE	2.3
3	F	113	ILE	2.3
1	D	130	VAL	2.3
3	C	294	ASP	2.3
4	H	4	PRO	2.3
1	D	133	ILE	2.2
3	F	176	GLN	2.2
3	F	284	GLY	2.2
2	B	165	LEU	2.2
2	E	233	VAL	2.2
2	E	184	SER	2.2
2	E	172	LEU	2.2
3	F	162	LYS	2.2
2	E	420	GLY	2.2
3	F	287	GLY	2.2
3	F	293	PHE	2.2
2	B	166	ARG	2.2
3	C	103	HIS	2.2
1	D	184	GLN	2.1
2	B	164	ASN	2.1
3	F	106	SER	2.1
3	C	105	SER	2.1
3	F	243	PRO	2.1
1	D	131	GLN	2.1
1	A	136	LEU	2.1
3	F	377	TYR	2.1
2	E	325	HIS	2.1
1	D	178	TYR	2.1
3	F	358	SER	2.0
3	F	305	THR	2.0
1	A	131	GLN	2.0
2	B	167	VAL	2.0
3	C	104	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	106	SER	2.0
1	D	188	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

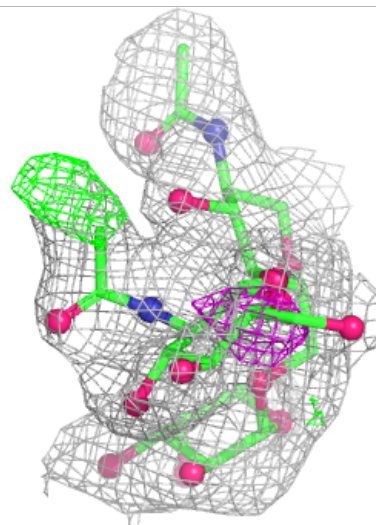
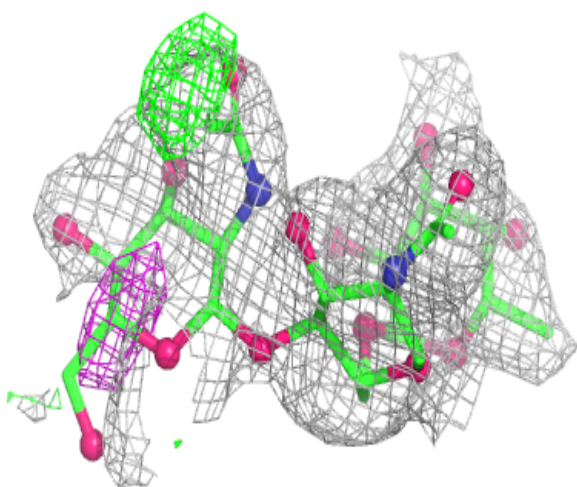
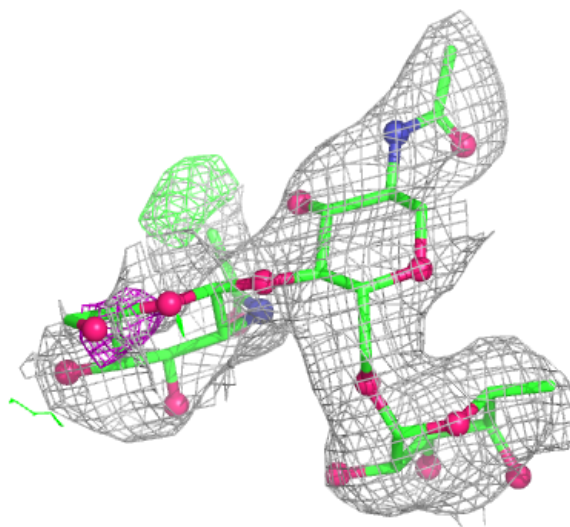
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

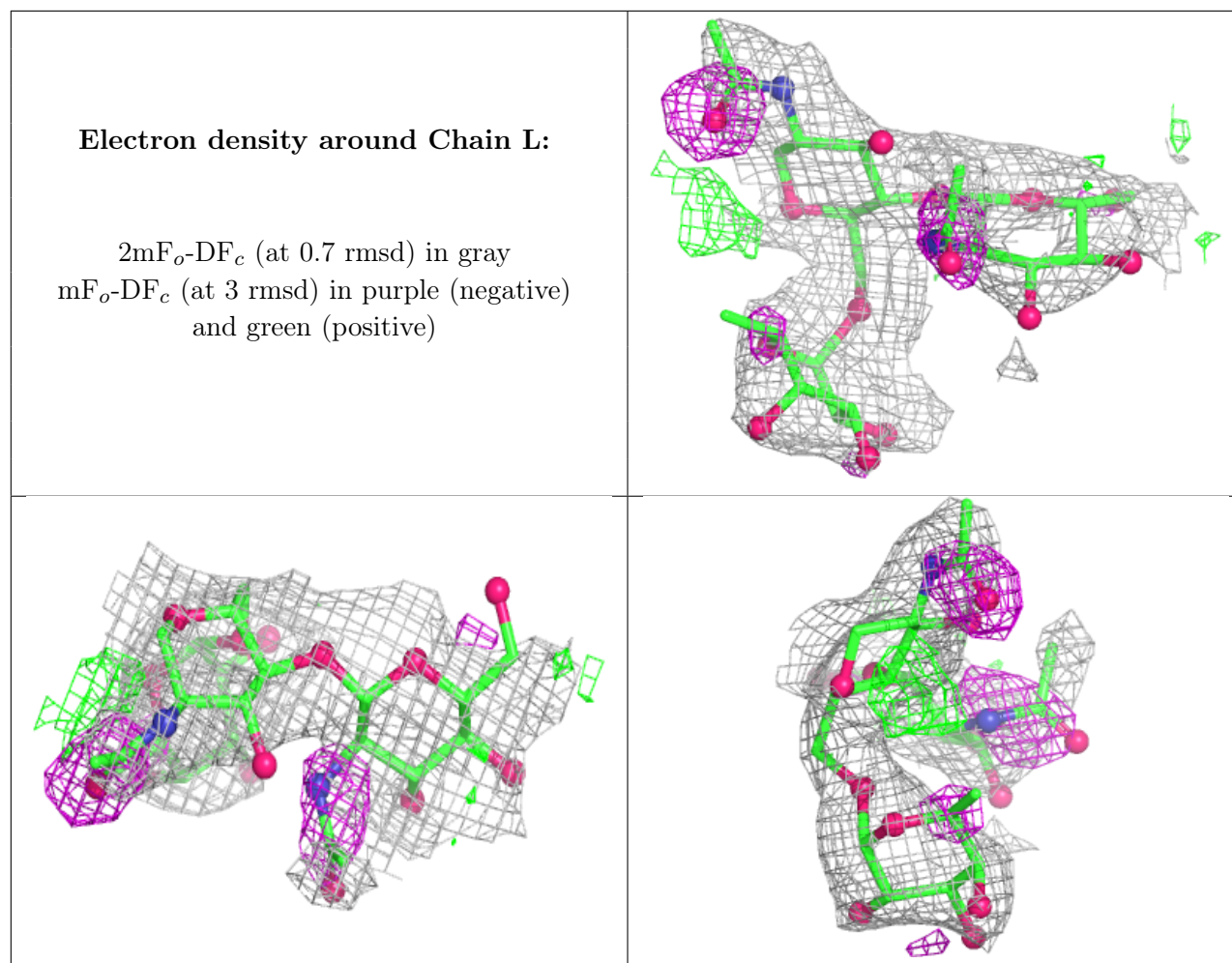
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	L	2	14/15	0.23	0.23	68,71,75,77	0
5	NAG	K	2	14/15	0.47	0.20	68,71,75,77	0
5	NAG	L	1	14/15	0.65	0.16	42,51,56,63	0
5	FUC	L	3	10/11	0.68	0.16	57,59,60,61	0
5	FUC	K	3	10/11	0.76	0.14	57,59,60,61	0
5	NAG	K	1	14/15	0.88	0.10	42,51,56,63	0

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	1	1/1	0.92	0.12	49,49,49,49	0
6	CA	F	1	1/1	0.96	0.06	51,51,51,51	0
6	CA	C	1	1/1	0.98	0.03	31,31,31,31	0
6	CA	B	1	1/1	0.99	0.04	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.