



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:32 AM UTC

PDB ID : 1MWA / pdb_00001mwa
Title : 2C/H-2KBM3/DEV8 ALLOGENEIC COMPLEX
Authors : Luz, J.G.; Huang, M.D.; Garcia, K.C.; Rudolph, M.G.; Teyton, L.; Wilson, I.A.
Deposited on : 2002-09-27
Resolution : 2.40 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

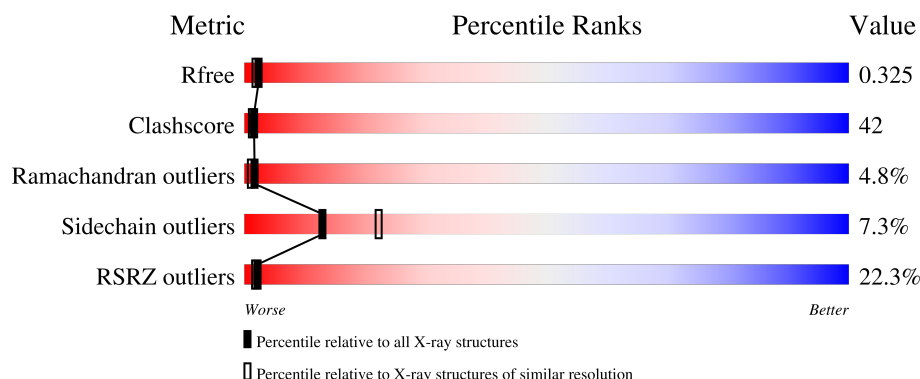
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	202	6% 53% 40% 6%
1	C	202	60% 32% 56% 11%
2	B	237	% 56% 37% 7%
2	D	237	70% 27% 62% 11%
3	H	275	55% 40% 5%

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Mol	Chain	Length	Quality of chain
3	I	275	
4	L	99	
4	M	99	
5	P	8	
5	Q	8	
6	E	2	
6	K	2	
7	F	3	
7	G	3	
7	J	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
6	NAG	K	1	X	-	-	-
7	NAG	F	1	-	-	X	-
7	NAG	J	1	-	-	X	-
9	NAG	B	808	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13973 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 2C T CELL RECEPTOR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			
1	C	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	SEE REMARK 999	GB 224220
A	165	ALA	LYS	SEE REMARK 999	GB 224220
C	127	ALA	GLN	SEE REMARK 999	GB 224220
C	165	ALA	LYS	SEE REMARK 999	GB 224220

- Molecule 2 is a protein called 2C T CELL RECEPTOR BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			
2	D	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	SEE REMARK 999	GB 1791255
B	?	-	ARG	SEE REMARK 999	GB 1791255
B	?	-	ALA	SEE REMARK 999	GB 1791255
B	105	THR	GLU	SEE REMARK 999	GB 1791255
B	106	LEU	GLN	SEE REMARK 999	GB 1791255
B	107	TYR	PHE	SEE REMARK 999	GB 1791255
B	110	ALA	PRO	SEE REMARK 999	GB 1791255
B	115	SER	THR	SEE REMARK 999	GB 1791255

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Chain	Residue	Modelled	Actual	Comment	Reference
D	97	GLY	GLN	SEE REMARK 999	GB 1791255
D	?	-	ARG	SEE REMARK 999	GB 1791255
D	?	-	ALA	SEE REMARK 999	GB 1791255
D	105	THR	GLU	SEE REMARK 999	GB 1791255
D	106	LEU	GLN	SEE REMARK 999	GB 1791255
D	107	TYR	PHE	SEE REMARK 999	GB 1791255
D	110	ALA	PRO	SEE REMARK 999	GB 1791255
D	115	SER	THR	SEE REMARK 999	GB 1791255

- Molecule 3 is a protein called H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	274	Total	C	N	O	S	0	0	0
			2225	1404	392	420	9			
3	I	274	Total	C	N	O	S	0	0	0
			2224	1404	392	419	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	77	SER	ASP	conflict	UNP P01901
H	89	ALA	LYS	conflict	UNP P01901
H	275	ARG	GLU	conflict	UNP P01901
I	77	SER	ASP	conflict	UNP P01901
I	89	ALA	LYS	conflict	UNP P01901
I	275	ARG	GLU	conflict	UNP P01901

- Molecule 4 is a protein called MICROGLOBULIN MHC LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
4	M	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 5 is a protein called DEV8.

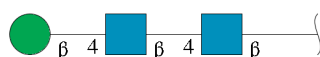
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	8	Total	C	N	O	0	0	0
			76	51	10	15			
5	Q	8	Total	C	N	O	0	0	0
			76	51	10	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



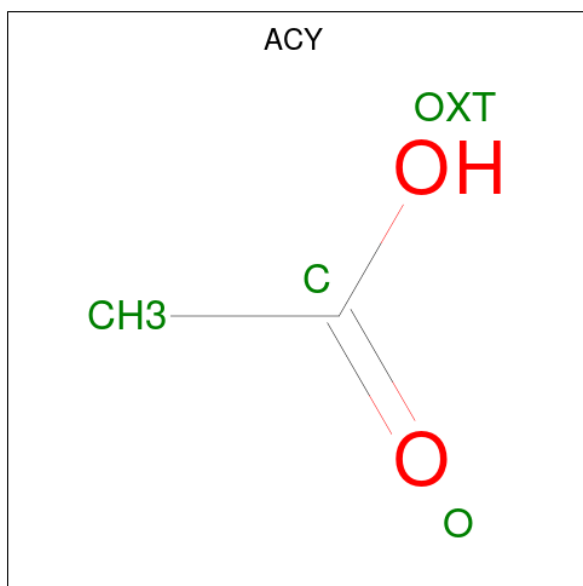
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	I	1	Total	C	O	0	0
			6	3	3		
8	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	106	Total	O	0	0
			106	106		
11	C	41	Total	O	0	0
			41	41		
11	B	118	Total	O	0	0
			118	118		
11	D	10	Total	O	0	0
			10	10		
11	H	183	Total	O	0	0
			183	183		
11	I	107	Total	O	0	0
			107	107		
11	L	62	Total	O	0	0
			62	62		
11	M	44	Total	O	0	0
			44	44		

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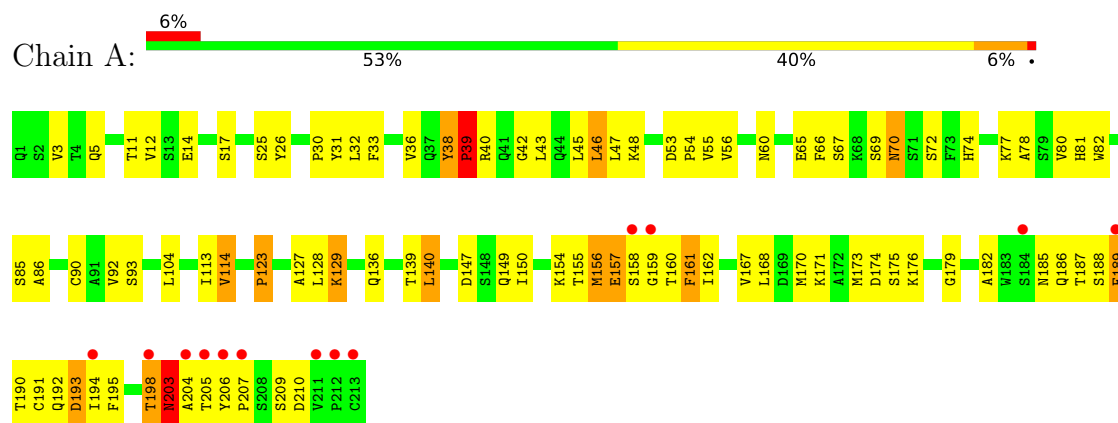
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	2	Total	O	0	0
			2	2		
11	Q	2	Total	O	0	0
			2	2		

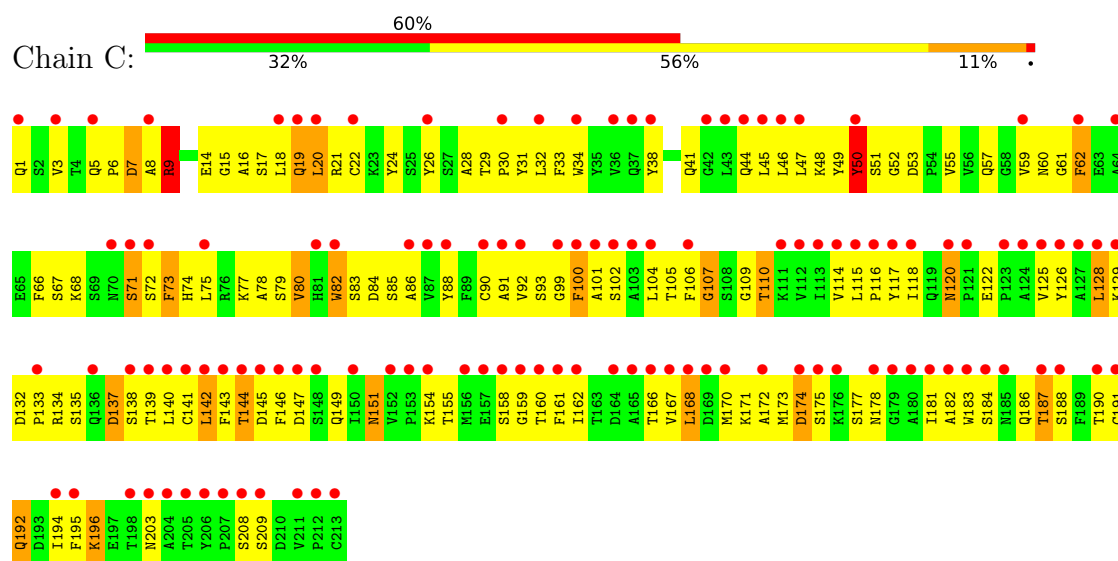
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

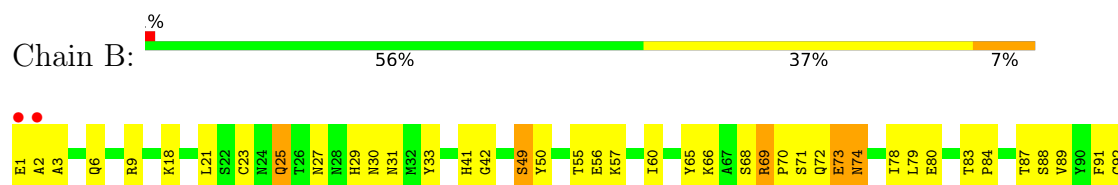
• Molecule 1: 2C T CELL RECEPTOR ALPHA CHAIN

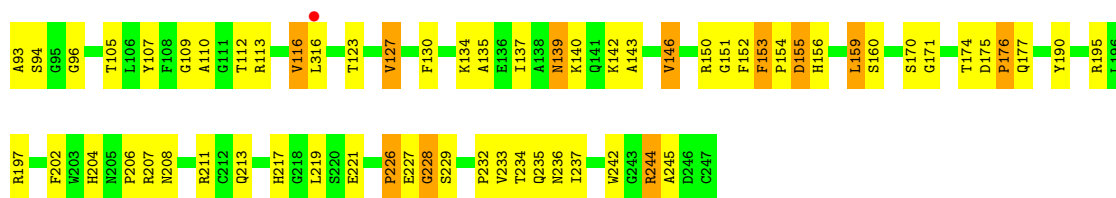


• Molecule 1: 2C T CELL RECEPTOR ALPHA CHAIN

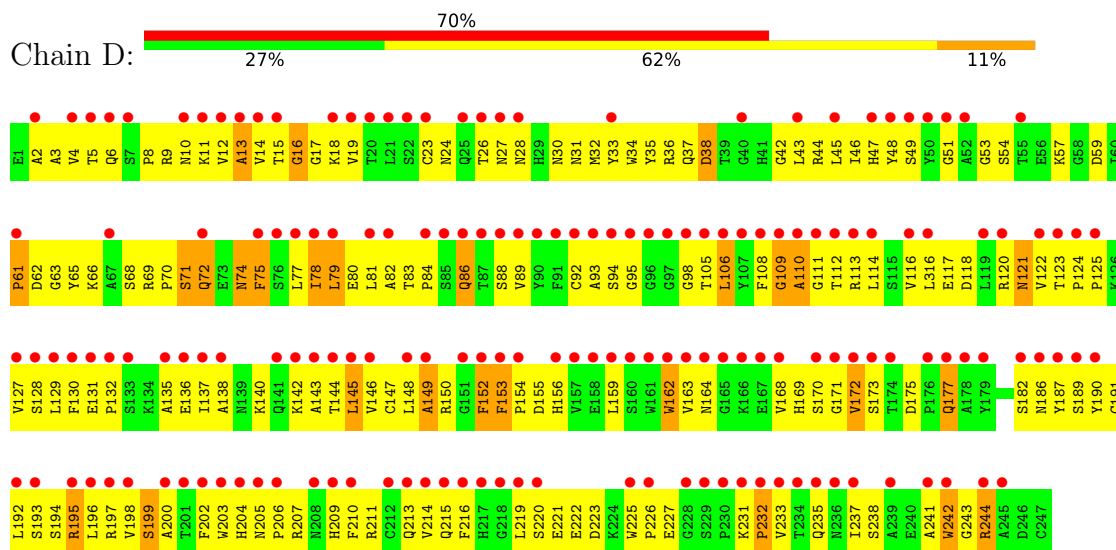


• Molecule 2: 2C T CELL RECEPTOR BETA CHAIN

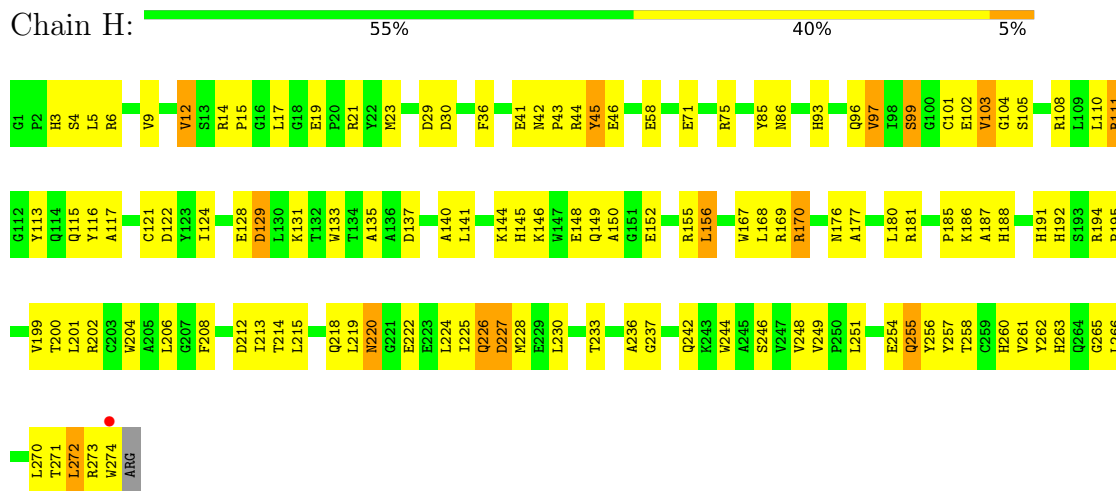




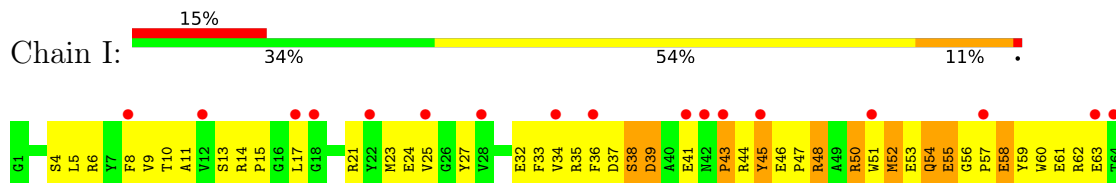
● Molecule 2: 2C T CELL RECEPTOR BETA CHAIN

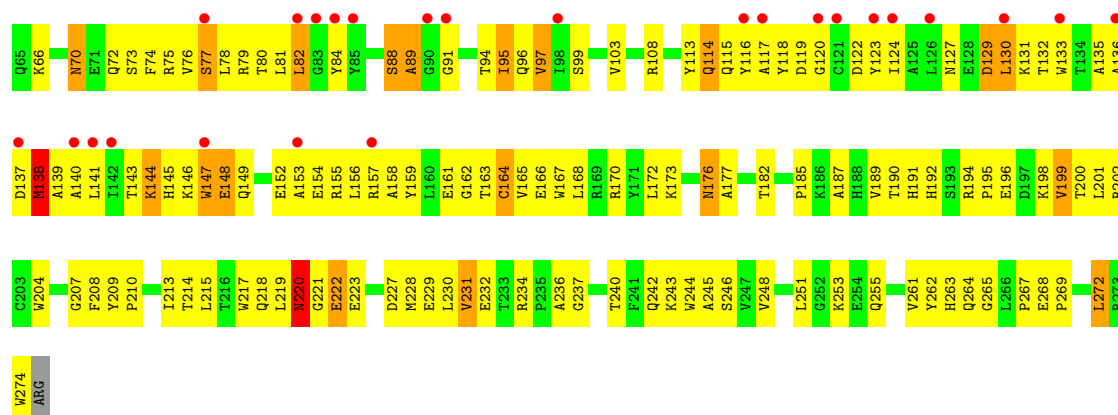


● Molecule 3: H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN



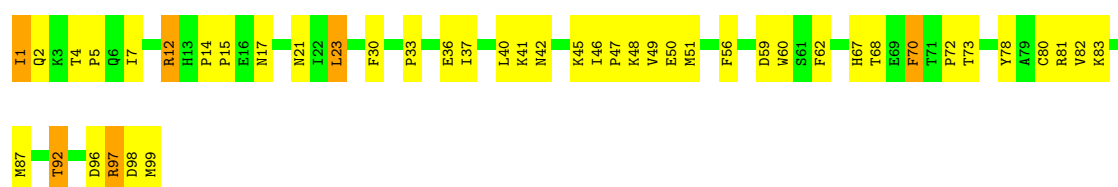
● Molecule 3: H-2KBM3 MHC CLASS I MOLECULE HEAVY CHAIN





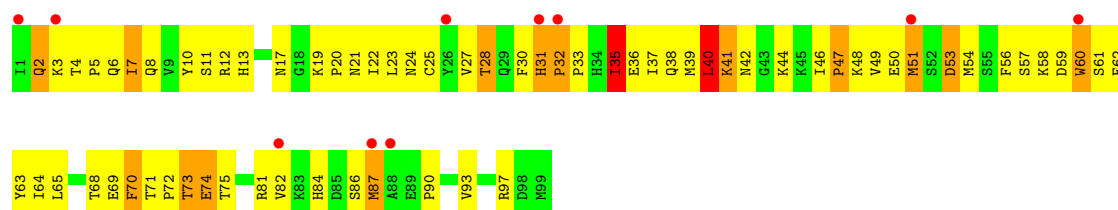
• Molecule 4: MICROGLOBULIN MHC LIGHT CHAIN

Chain L: 55% 39% 6%



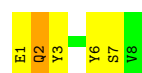
• Molecule 4: MICROGLOBULIN MHC LIGHT CHAIN

Chain M: 10% 31% 53% 14%



• Molecule 5: DEV8

Chain P: 38% 50% 12%



• Molecule 5: DEV8

Chain Q: 100% 62% 38%



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

NAG1
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

NAG1
NAG2

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

NAG1
NAG2
BMA3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	297.90Å 95.94Å 84.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.40 49.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.39-2.40) 99.5 (49.39-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.284 , 0.313 0.294 , 0.325	Depositor DCC
R_{free} test set	4781 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 93.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13973	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/1611	1.02	9/2193 (0.4%)
1	C	0.46	0/1611	0.87	3/2193 (0.1%)
2	B	0.56	2/1904 (0.1%)	1.01	12/2586 (0.5%)
2	D	0.41	1/1904 (0.1%)	0.82	2/2586 (0.1%)
3	H	0.52	0/2286	0.94	4/3106 (0.1%)
3	I	0.49	1/2285 (0.0%)	0.95	12/3105 (0.4%)
4	L	0.57	0/847	0.96	0/1148
4	M	0.43	0/847	1.01	6/1148 (0.5%)
5	P	0.45	0/78	0.98	0/102
5	Q	0.61	0/78	0.99	0/102
All	All	0.50	4/13451 (0.0%)	0.95	48/18269 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
3	I	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	220	ASN	C-N	-6.67	1.23	1.33
2	B	116	VAL	C-N	5.75	1.41	1.33
2	B	227	GLU	CA-C	-5.35	1.46	1.52
2	D	63	GLY	C-N	5.19	1.40	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	58	GLU	N-CA-C	-8.79	99.38	112.04
2	B	228	GLY	N-CA-C	-7.58	95.22	113.18
3	I	147	TRP	N-CA-C	-7.57	103.89	113.43
4	M	51	MET	N-CA-C	7.41	119.40	108.14
3	I	129	ASP	N-CA-C	-7.17	104.40	113.72
3	I	61	GLU	N-CA-C	-7.08	103.49	111.07
3	H	233	THR	N-CA-C	-6.85	101.04	110.35
3	I	97	VAL	N-CA-C	6.58	117.38	108.17
2	B	227	GLU	N-CA-C	6.34	118.94	108.99
1	C	68	LYS	N-CA-C	-6.32	104.83	112.54
1	A	5	GLN	CA-C-N	6.29	125.97	119.56
1	A	5	GLN	C-N-CA	6.29	125.97	119.56
2	B	151	GLY	N-CA-C	6.27	123.67	115.40
3	I	144	LYS	N-CA-C	-6.18	104.46	111.07
2	B	3	ALA	N-CA-C	6.12	119.33	110.28
3	I	77	SER	N-CA-C	-6.07	103.83	111.11
1	A	46	LEU	N-CA-C	-5.95	105.68	113.12
2	B	94	SER	N-CA-C	-5.95	100.49	109.95
4	M	35	ILE	N-CA-C	5.89	115.61	108.06
4	M	32	PRO	CA-C-N	5.83	125.38	119.19
4	M	32	PRO	C-N-CA	5.83	125.38	119.19
2	B	74	ASN	N-CA-C	5.80	118.22	109.23
3	I	138	MET	N-CA-C	-5.78	105.49	112.54
2	B	69	ARG	CA-C-N	5.74	125.86	119.32
2	B	69	ARG	C-N-CA	5.74	125.86	119.32
3	I	267	PRO	N-CA-C	-5.73	106.70	113.86
1	A	90	CYS	N-CA-C	-5.63	101.10	110.17
3	H	272	LEU	N-CA-C	5.52	117.91	108.90
2	D	38	ASP	N-CA-C	5.50	115.64	107.88
1	A	38	TYR	CA-C-N	5.47	126.68	119.84
1	A	38	TYR	C-N-CA	5.47	126.68	119.84
3	H	186	LYS	N-CA-C	-5.44	99.87	108.73
2	B	73	GLU	N-CA-C	5.34	117.86	111.71
1	C	107	GLY	N-CA-C	-5.34	104.25	112.85
2	D	195	ARG	N-CA-C	5.32	115.38	107.88
4	M	28	THR	N-CA-C	5.28	116.83	108.96
1	A	39	PRO	N-CA-C	5.26	123.31	112.47
4	M	2	GLN	N-CA-C	-5.25	99.61	110.80
1	A	60	ASN	N-CA-C	5.24	118.47	111.24
1	C	9	ARG	N-CA-C	-5.24	99.64	110.80
3	I	54	GLN	N-CA-C	-5.21	106.42	112.89
3	I	136	ALA	N-CA-C	-5.21	105.59	112.94
3	H	129	ASP	N-CA-C	-5.13	106.97	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	109	GLY	N-CA-C	-5.12	104.37	112.66
3	I	130	LEU	N-CA-C	-5.07	105.21	111.90
1	A	31	TYR	N-CA-C	-5.01	102.28	110.20
2	B	226	PRO	CA-C-N	-5.01	112.98	121.85
2	B	226	PRO	C-N-CA	-5.01	112.98	121.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	50	TYR	Peptide
3	I	220	ASN	Mainchain

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	1570	0	1503	93	0
1	C	1570	0	1503	155	1
2	B	1853	0	1761	103	0
2	D	1853	0	1763	236	0
3	H	2225	0	2115	123	0
3	I	2224	0	2113	251	0
4	L	821	0	796	37	0
4	M	821	0	796	107	0
5	P	76	0	70	8	0
5	Q	76	0	70	29	0
6	E	28	0	25	1	0
6	K	28	0	26	5	0
7	F	39	0	34	15	0
7	G	39	0	34	4	0
7	J	39	0	33	13	0
8	A	6	0	8	0	0
8	I	6	0	8	0	0
8	L	6	0	8	0	0
9	B	14	0	13	0	0
10	P	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	106	0	0	8	0
11	B	118	0	0	9	1
11	C	41	0	0	14	0
11	D	10	0	0	1	0
11	H	183	0	0	9	0
11	I	107	0	0	16	0
11	L	62	0	0	2	0
11	M	44	0	0	19	0
11	P	2	0	0	0	0
11	Q	2	0	0	0	0
All	All	13973	0	12682	1089	1

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 42.

All (1089) 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:236:ASN:HD21	7:J:1:NAG:C1	1.18	1.50
7:J:2:NAG:H61	7:J:3:BMA:C2	1.52	1.34
7:J:2:NAG:C6	7:J:3:BMA:H2	1.32	1.32
1:A:185:ASN:HD21	7:F:1:NAG:C2	1.53	1.20
1:A:185:ASN:ND2	7:F:1:NAG:C2	2.07	1.18
2:B:236:ASN:HD21	7:J:1:NAG:C2	1.57	1.15
2:B:9:ARG:HH12	2:B:110:ALA:HB3	1.12	1.13
3:H:180:LEU:CD1	6:K:2:NAG:H81	1.79	1.12
1:A:185:ASN:HD21	7:F:1:NAG:H2	1.07	1.09
3:H:177:ALA:HB3	11:H:924:HOH:O	1.52	1.09
3:I:78:LEU:HG	3:I:95:ILE:HD11	1.23	1.09
3:H:180:LEU:HD13	6:K:2:NAG:H81	1.12	1.08
2:D:4:VAL:H	2:D:109:GLY:HA3	1.21	1.06
3:H:9:VAL:HB	3:H:97:VAL:HG13	1.36	1.05
3:I:66:LYS:HB2	11:I:967:HOH:O	1.56	1.03
2:B:130:PHE:HB2	2:B:146:VAL:HG13	1.37	1.02
3:I:189:VAL:HG23	3:I:274:TRP:HD1	1.20	1.01
3:H:14:ARG:HB2	3:H:17:LEU:HB2	1.41	1.00
4:L:45:LYS:HE2	4:L:81:ARG:HH22	1.24	0.99
3:I:50:ARG:O	3:I:53:GLU:HG2	1.63	0.98
3:I:218:GLN:HB2	3:I:222:GLU:O	1.66	0.95
2:D:16:GLY:HA2	2:D:81:LEU:HA	1.48	0.94
1:A:185:ASN:ND2	7:F:1:NAG:H2	1.75	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:111:ARG:HG3	3:H:111:ARG:HH11	1.30	0.93
2:D:121:ASN:ND2	2:D:153:PHE:CE2	2.38	0.92
3:I:57:PRO:HA	3:I:60:TRP:HB2	1.51	0.92
1:A:185:ASN:CG	7:F:1:NAG:C1	2.44	0.91
4:M:2:GLN:HA	4:M:31:HIS:O	1.69	0.91
1:C:31:TYR:HB2	1:C:93:SER:HB3	1.51	0.91
3:I:145:HIS:HB3	3:I:149:GLN:NE2	1.86	0.90
4:M:31:HIS:HD1	4:M:32:PRO:HA	1.37	0.90
2:D:6:GLN:HE21	2:D:111:GLY:HA2	1.37	0.89
7:F:2:NAG:O3	7:F:3:BMA:O5	1.89	0.89
2:B:9:ARG:HH12	2:B:110:ALA:CB	1.84	0.89
3:I:234:ARG:HH11	4:M:8:GLN:NE2	1.71	0.88
2:B:204:HIS:HA	2:B:244:ARG:O	1.74	0.87
4:M:73:THR:HG22	4:M:75:THR:H	1.37	0.87
1:C:170:MET:H	1:C:175:SER:HB3	1.39	0.86
4:L:45:LYS:HE2	4:L:81:ARG:NH2	1.89	0.86
1:C:6:PRO:HB2	1:C:21:ARG:HE	1.38	0.86
1:C:155:THR:HG21	1:C:161:PHE:HA	1.55	0.86
5:Q:2:GLN:NE2	5:Q:3:TYR:H	1.73	0.86
3:H:180:LEU:HD13	6:K:2:NAG:C8	2.01	0.85
1:C:1:GLN:HE21	1:C:105:THR:HG23	1.42	0.85
6:K:1:NAG:H62	6:K:2:NAG:H82	1.59	0.84
2:D:46:ILE:HG22	2:D:47:HIS:ND1	1.91	0.84
3:H:104:GLY:HA3	11:H:836:HOH:O	1.76	0.84
1:C:45:LEU:HD12	1:C:46:LEU:N	1.93	0.83
4:M:37:ILE:HG22	4:M:82:VAL:HG12	1.59	0.83
3:I:77:SER:O	3:I:81:LEU:HG	1.78	0.83
3:I:131:LYS:HA	11:I:949:HOH:O	1.79	0.83
2:B:236:ASN:ND2	7:J:1:NAG:C2	2.32	0.82
3:I:11:ALA:HB3	3:I:95:ILE:HD12	1.60	0.82
2:D:14:VAL:HB	2:D:17:GLY:H	1.44	0.82
2:B:9:ARG:NH1	2:B:110:ALA:HB3	1.93	0.82
4:L:37:ILE:HD12	4:L:51:MET:HE1	1.61	0.82
1:C:18:LEU:HB3	1:C:77:LYS:HB3	1.61	0.82
3:I:253:LYS:HE3	11:I:971:HOH:O	1.78	0.82
1:C:9:ARG:O	1:C:9:ARG:HD3	1.80	0.81
2:D:164:ASN:ND2	2:D:209:HIS:HB3	1.95	0.81
5:Q:2:GLN:HE21	5:Q:3:TYR:H	1.26	0.81
3:I:194:ARG:HG3	3:I:195:PRO:HD2	1.60	0.81
1:A:194:ILE:HG23	1:A:195:PHE:HD1	1.44	0.80
2:D:68:SER:O	2:D:70:PRO:HD3	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:218:GLN:CB	3:I:222:GLU:O	2.29	0.80
3:I:48:ARG:HA	11:I:939:HOH:O	1.80	0.80
2:D:146:VAL:HG23	2:D:194:SER:O	1.81	0.80
3:I:185:PRO:HB3	3:I:208:PHE:HB3	1.64	0.80
2:B:236:ASN:CG	7:J:1:NAG:C1	2.55	0.79
4:M:63:TYR:HB3	11:M:281:HOH:O	1.83	0.78
4:M:7:ILE:HB	4:M:93:VAL:HG21	1.66	0.78
3:I:130:LEU:HB3	11:I:948:HOH:O	1.83	0.78
2:D:30:ASN:OD1	3:I:146:LYS:HE3	1.82	0.78
2:D:37:GLN:HB2	2:D:43:LEU:CD1	2.13	0.78
3:I:96:GLN:HG2	11:I:962:HOH:O	1.83	0.78
3:I:263:HIS:CD2	3:I:265:GLY:H	2.02	0.78
3:I:159:TYR:CE2	5:Q:3:TYR:HB2	2.18	0.78
2:D:9:ARG:HA	2:D:112:THR:HG22	1.65	0.78
3:I:182:THR:HG22	3:I:210:PRO:HD3	1.66	0.78
1:C:67:SER:OG	7:G:1:NAG:H82	1.84	0.77
1:A:53:ASP:OD2	1:A:55:VAL:HG22	1.84	0.77
2:D:4:VAL:H	2:D:109:GLY:CA	1.96	0.77
2:D:18:LYS:HA	2:D:80:GLU:HA	1.65	0.77
3:I:14:ARG:HH21	3:I:21:ARG:HD2	1.47	0.77
4:L:40:LEU:HD21	4:L:81:ARG:HH21	1.49	0.77
3:I:189:VAL:HG23	3:I:274:TRP:CD1	2.13	0.77
5:P:2:GLN:NE2	5:P:3:TYR:H	1.83	0.76
2:D:145:LEU:HD23	2:D:145:LEU:H	1.49	0.76
3:I:124:ILE:HB	3:I:140:ALA:HB1	1.67	0.76
1:C:8:ALA:HA	1:C:110:THR:HA	1.68	0.76
4:M:21:ASN:HB3	4:M:70:PHE:CE1	2.21	0.76
4:M:21:ASN:HD22	4:M:22:ILE:H	1.33	0.76
1:C:186:GLN:HG3	1:C:187:THR:H	1.51	0.76
1:A:185:ASN:ND2	7:F:1:NAG:O5	2.18	0.76
1:C:170:MET:HG2	1:C:171:LYS:H	1.50	0.75
3:I:147:TRP:HE1	5:Q:8:VAL:C	1.94	0.75
1:A:72:SER:HB2	1:A:74:HIS:CE1	2.21	0.75
7:F:2:NAG:C3	7:F:3:BMA:O5	2.35	0.75
1:C:20:LEU:HD23	1:C:20:LEU:H	1.50	0.75
1:A:81:HIS:HB2	11:A:937:HOH:O	1.86	0.75
1:C:132:ASP:HB3	1:C:135:SER:HB3	1.69	0.75
2:D:198:VAL:HB	2:D:202:PHE:HB3	1.67	0.75
7:F:1:NAG:HO4	7:F:2:NAG:C1	1.98	0.74
2:D:122:VAL:O	2:D:232:PRO:HG2	1.88	0.74
2:B:27:ASN:HB3	2:B:29:HIS:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:NE2	2:D:111:GLY:HA2	2.02	0.74
4:L:67:HIS:HD2	11:L:938:HOH:O	1.69	0.74
2:D:37:GLN:HA	2:D:43:LEU:HA	1.70	0.73
2:D:45:LEU:HD21	2:D:48:TYR:HD2	1.52	0.73
3:H:42:ASN:OD1	3:H:44:ARG:HD3	1.88	0.73
2:D:4:VAL:N	2:D:109:GLY:HA3	2.01	0.73
4:M:31:HIS:ND1	4:M:32:PRO:HA	2.02	0.73
2:D:18:LYS:HG3	2:D:80:GLU:HG3	1.71	0.73
3:H:219:LEU:O	3:H:220:ASN:ND2	2.22	0.73
3:I:145:HIS:HA	3:I:148:GLU:HB3	1.69	0.73
3:I:231:VAL:HG13	3:I:232:GLU:O	1.89	0.73
2:D:6:GLN:HE21	2:D:111:GLY:CA	2.02	0.72
1:C:53:ASP:OD1	1:C:55:VAL:HG22	1.89	0.72
3:H:249:VAL:CG2	3:H:254:GLU:HG3	2.20	0.72
2:D:32:MET:HG3	11:D:317:HOH:O	1.90	0.72
2:B:153:PHE:O	2:B:154:PRO:C	2.30	0.72
2:D:242:TRP:HB3	2:D:244:ARG:NH1	2.03	0.72
2:B:84:PRO:HA	2:B:116:VAL:HB	1.71	0.72
3:I:36:PHE:HE1	3:I:43:PRO:C	1.97	0.72
2:D:78:ILE:H	2:D:78:ILE:HD12	1.55	0.71
4:M:87:MET:HB2	11:M:375:HOH:O	1.91	0.71
1:C:20:LEU:HD11	1:C:75:LEU:HD23	1.73	0.71
1:C:26:TYR:HD2	1:C:28:ALA:H	1.36	0.71
3:H:237:GLY:HA3	11:L:931:HOH:O	1.91	0.71
1:C:80:VAL:HG23	1:C:80:VAL:O	1.91	0.71
2:D:83:THR:HG22	2:D:86:GLN:HG3	1.72	0.71
4:M:19:LYS:O	4:M:72:PRO:HD2	1.91	0.71
2:D:125:PRO:HG3	2:D:216:PHE:HB2	1.73	0.70
3:I:54:GLN:NE2	11:I:1000:HOH:O	2.24	0.70
3:H:249:VAL:HG21	3:H:254:GLU:HG3	1.73	0.70
3:I:194:ARG:NH1	3:I:248:VAL:HG11	2.06	0.70
1:C:170:MET:HE2	1:C:172:ALA:HB2	1.73	0.70
2:D:46:ILE:HG21	2:D:77:LEU:HD11	1.73	0.70
1:C:45:LEU:HD12	1:C:46:LEU:H	1.57	0.70
1:C:142:LEU:HD11	2:D:144:THR:HB	1.72	0.70
1:A:40:ARG:HD2	11:A:993:HOH:O	1.92	0.70
5:P:2:GLN:HA	5:P:2:GLN:HE21	1.57	0.70
6:K:1:NAG:C6	6:K:2:NAG:H82	2.22	0.70
1:C:166:THR:HB	2:D:173:SER:OG	1.91	0.69
1:C:115:LEU:HD22	1:C:115:LEU:H	1.57	0.69
3:H:6:ARG:NE	11:H:898:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLY:HA3	7:F:1:NAG:H82	1.74	0.69
2:D:152:PHE:O	2:D:189:SER:HA	1.92	0.69
5:Q:2:GLN:HE21	5:Q:3:TYR:N	1.90	0.69
3:H:14:ARG:HB2	3:H:17:LEU:CB	2.20	0.69
1:C:32:LEU:HD23	1:C:92:VAL:HG12	1.74	0.69
1:C:82:TRP:HA	1:C:114:VAL:HG13	1.73	0.69
2:D:61:PRO:HG2	2:D:62:ASP:H	1.57	0.69
3:H:111:ARG:HG3	3:H:111:ARG:NH1	2.07	0.69
3:I:215:LEU:HD23	3:I:261:VAL:HG13	1.74	0.69
1:A:77:LYS:HD3	1:A:80:VAL:HG12	1.76	0.69
1:C:3:VAL:HG21	1:C:90:CYS:O	1.92	0.69
1:C:82:TRP:HA	1:C:114:VAL:CG1	2.23	0.69
3:H:58:GLU:H	3:H:58:GLU:CD	2.00	0.69
3:I:230:LEU:HD12	3:I:245:ALA:HB2	1.73	0.68
3:I:46:GLU:HG3	3:I:47:PRO:HD2	1.75	0.68
4:M:12:ARG:HE	4:M:13:HIS:CE1	2.11	0.68
4:M:73:THR:CG2	4:M:75:THR:HG22	2.22	0.68
1:C:47:LEU:HD12	1:C:47:LEU:O	1.94	0.68
2:B:2:ALA:HA	2:B:27:ASN:OD1	1.94	0.67
4:M:69:GLU:HB2	11:M:599:HOH:O	1.93	0.67
4:M:21:ASN:HB3	4:M:70:PHE:HE1	1.59	0.67
4:M:87:MET:CB	11:M:375:HOH:O	2.41	0.67
1:A:67:SER:HB2	6:E:1:NAG:H82	1.76	0.67
2:D:244:ARG:HD2	2:D:244:ARG:N	2.10	0.67
2:D:13:ALA:HB3	2:D:116:VAL:HG12	1.75	0.67
1:C:6:PRO:HB2	1:C:21:ARG:NE	2.07	0.67
2:D:79:LEU:HD12	2:D:86:GLN:OE1	1.93	0.67
3:H:137:ASP:HB2	11:H:858:HOH:O	1.95	0.67
3:I:129:ASP:OD2	3:I:131:LYS:HB2	1.95	0.67
7:G:1:NAG:O3	7:G:2:NAG:O5	2.13	0.67
3:I:159:TYR:HA	3:I:163:THR:HB	1.75	0.67
4:L:82:VAL:HG23	4:L:87:MET:HE1	1.77	0.67
2:D:68:SER:OG	2:D:78:ILE:HD11	1.95	0.66
3:H:167:TRP:NE1	5:P:1:GLU:OE2	2.27	0.66
4:M:73:THR:HG21	4:M:75:THR:HG22	1.77	0.66
3:I:129:ASP:O	3:I:131:LYS:HG3	1.96	0.66
2:D:37:GLN:HA	2:D:42:GLY:O	1.95	0.66
3:H:41:GLU:HB3	11:H:864:HOH:O	1.95	0.66
3:H:41:GLU:O	3:H:43:PRO:HD3	1.95	0.66
3:I:116:TYR:HH	5:Q:5:PHE:HD2	1.44	0.66
3:H:219:LEU:HB3	3:H:224:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:SER:HB3	3:I:78:LEU:HD13	1.77	0.66
3:I:96:GLN:HG3	3:I:117:ALA:HB3	1.76	0.66
3:I:138:MET:HE3	3:I:141:LEU:HD22	1.77	0.66
5:Q:7:SER:O	5:Q:8:VAL:C	2.37	0.66
7:J:2:NAG:C6	7:J:3:BMA:C2	2.25	0.66
1:A:162:ILE:HB	11:A:941:HOH:O	1.95	0.66
1:A:150:ILE:HG13	11:A:940:HOH:O	1.96	0.66
3:I:4:SER:O	3:I:168:LEU:HD13	1.96	0.66
2:D:37:GLN:HB2	2:D:43:LEU:HD13	1.77	0.65
3:I:152:GLU:C	3:I:154:GLU:H	2.04	0.65
2:D:47:HIS:HE1	2:D:65:TYR:HB2	1.61	0.65
3:I:189:VAL:CG2	3:I:274:TRP:HD1	2.03	0.65
3:I:147:TRP:C	3:I:149:GLN:H	2.05	0.65
1:C:92:VAL:HG22	11:C:822:HOH:O	1.97	0.65
2:D:159:LEU:HD12	2:D:159:LEU:H	1.60	0.65
4:M:59:ASP:O	4:M:60:TRP:CD1	2.50	0.65
1:A:127:ALA:C	1:A:128:LEU:HD12	2.22	0.65
2:D:37:GLN:HB2	2:D:43:LEU:HD12	1.78	0.65
3:I:15:PRO:HG2	3:I:91:GLY:O	1.96	0.65
7:G:1:NAG:O3	7:G:2:NAG:H61	1.97	0.65
1:C:44:GLN:HG3	11:C:854:HOH:O	1.96	0.64
2:D:127:VAL:HG12	2:D:237:ILE:HG22	1.79	0.64
3:I:62:ARG:NH1	5:Q:1:GLU:OE1	2.30	0.64
4:M:36:GLU:HB3	11:M:657:HOH:O	1.97	0.64
2:D:3:ALA:HB1	2:D:109:GLY:HA2	1.79	0.64
3:I:123:TYR:CZ	3:I:140:ALA:HA	2.32	0.64
3:I:143:THR:HG23	5:Q:8:VAL:O	1.98	0.64
4:M:35:ILE:HG23	4:M:37:ILE:HG23	1.78	0.64
3:H:129:ASP:OD2	3:H:131:LYS:HB2	1.97	0.64
1:C:126:TYR:CE2	2:D:136:GLU:HB3	2.33	0.64
2:D:125:PRO:HD3	2:D:216:PHE:CD1	2.33	0.64
3:I:8:PHE:CD1	3:I:27:TYR:HD1	2.16	0.64
3:I:194:ARG:CG	3:I:195:PRO:HD2	2.28	0.64
5:P:2:GLN:HE21	5:P:3:TYR:H	1.43	0.64
3:I:94:THR:HG22	3:I:95:ILE:N	2.13	0.63
1:A:171:LYS:HE3	2:B:170:SER:HB2	1.80	0.63
11:I:962:HOH:O	4:M:62:PHE:HZ	1.81	0.63
2:B:236:ASN:ND2	7:J:1:NAG:O5	2.29	0.63
3:I:14:ARG:NH2	3:I:21:ARG:HD2	2.14	0.63
2:D:131:GLU:HB2	2:D:132:PRO:HD2	1.81	0.63
5:Q:2:GLN:HE21	5:Q:2:GLN:HA	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:ASN:CG	2:D:153:PHE:CD2	2.76	0.63
2:D:121:ASN:OD1	2:D:122:VAL:HG13	1.99	0.63
3:I:52:MET:HA	3:I:52:MET:HE2	1.80	0.63
4:M:44:LYS:O	4:M:44:LYS:HG3	1.98	0.63
3:H:144:LYS:O	3:H:148:GLU:HG3	1.98	0.63
1:C:32:LEU:HD12	1:C:49:TYR:HD2	1.64	0.63
3:H:129:ASP:O	3:H:131:LYS:HG3	1.99	0.63
3:I:217:TRP:HD1	3:I:228:MET:HE2	1.63	0.63
4:M:44:LYS:HE2	11:M:649:HOH:O	1.97	0.63
1:A:210:ASP:OD1	2:B:134:LYS:HE3	1.98	0.62
3:H:21:ARG:HE	3:H:23:MET:HE2	1.63	0.62
3:I:137:ASP:O	3:I:141:LEU:HD13	1.99	0.62
2:D:5:THR:HB	2:D:24:ASN:HB2	1.80	0.62
1:C:50:TYR:N	11:C:827:HOH:O	2.31	0.62
3:I:103:VAL:HG11	3:I:165:VAL:HG13	1.82	0.62
3:I:114:GLN:C	3:I:115:GLN:HG3	2.24	0.62
1:C:67:SER:O	1:C:71:SER:N	2.31	0.62
2:B:33:TYR:O	2:B:92:CYS:HA	1.99	0.62
4:M:5:PRO:HB3	4:M:30:PHE:HB3	1.81	0.62
4:M:48:LYS:O	4:M:68:THR:HG22	2.00	0.62
1:C:208:SER:HA	2:D:135:ALA:HB2	1.81	0.62
2:D:32:MET:HA	2:D:93:ALA:O	1.99	0.62
1:A:55:VAL:O	1:A:55:VAL:HG23	1.97	0.62
2:D:49:SER:CB	2:D:69:ARG:HE	2.12	0.62
4:M:13:HIS:H	4:M:21:ASN:HD21	1.46	0.62
7:J:2:NAG:H61	7:J:3:BMA:H2	0.63	0.62
1:A:33:PHE:CE1	1:A:104:LEU:HD22	2.35	0.62
1:C:22:CYS:H	1:C:74:HIS:CD2	2.18	0.62
3:H:111:ARG:HH11	3:H:111:ARG:CG	2.06	0.62
3:I:162:GLY:O	3:I:166:GLU:HG3	2.00	0.62
1:A:36:VAL:HG22	1:A:46:LEU:HD11	1.82	0.62
1:C:77:LYS:HD2	1:C:78:ALA:H	1.65	0.62
3:H:219:LEU:CB	3:H:224:LEU:HD21	2.30	0.62
2:B:142:LYS:HD3	2:B:197:ARG:HD3	1.80	0.62
2:D:37:GLN:C	2:D:37:GLN:NE2	2.58	0.62
1:A:40:ARG:HH11	2:B:113:ARG:HH22	1.48	0.61
1:C:142:LEU:HD23	1:C:181:ILE:HG12	1.82	0.61
1:C:3:VAL:HG13	1:C:107:GLY:CA	2.30	0.61
2:B:18:LYS:HD2	2:B:80:GLU:HA	1.82	0.61
1:C:128:LEU:HD23	1:C:128:LEU:N	2.15	0.61
3:H:135:ALA:HB1	3:H:140:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:41:LYS:O	4:M:42:ASN:HB2	1.99	0.61
2:D:242:TRP:HB3	2:D:244:ARG:HH12	1.65	0.61
1:A:191:CYS:HA	1:A:194:ILE:HG22	1.83	0.61
2:B:18:LYS:HE3	2:B:80:GLU:HG2	1.82	0.61
3:I:96:GLN:CG	3:I:117:ALA:HB3	2.30	0.61
3:I:145:HIS:O	3:I:149:GLN:HB2	2.00	0.61
7:F:2:NAG:O3	7:F:3:BMA:C1	2.49	0.61
1:A:158:SER:O	7:F:1:NAG:H82	2.01	0.61
1:C:17:SER:HA	11:C:820:HOH:O	2.00	0.61
3:I:62:ARG:NH1	3:I:63:GLU:OE2	2.34	0.61
3:I:96:GLN:NE2	4:M:31:HIS:NE2	2.47	0.61
2:D:124:PRO:HD3	2:D:232:PRO:HG3	1.82	0.61
4:M:2:GLN:HG3	4:M:2:GLN:O	2.00	0.61
2:B:27:ASN:HB3	2:B:29:HIS:ND1	2.15	0.61
3:H:191:HIS:HB2	3:H:274:TRP:NE1	2.15	0.61
2:D:13:ALA:HB2	2:D:19:VAL:HG21	1.83	0.61
2:D:74:ASN:O	2:D:75:PHE:HB2	2.01	0.61
3:I:144:LYS:HG2	3:I:148:GLU:OE2	2.01	0.61
1:C:32:LEU:HD12	1:C:49:TYR:CD2	2.36	0.60
1:C:66:PHE:CB	11:C:835:HOH:O	2.48	0.60
2:D:149:ALA:HB2	2:D:214:VAL:HG22	1.82	0.60
2:D:226:PRO:HG2	2:D:227:GLU:OE1	2.00	0.60
1:C:140:LEU:HB3	1:C:183:TRP:CB	2.31	0.60
2:D:6:GLN:HG3	2:D:111:GLY:N	2.17	0.60
1:C:140:LEU:HB3	1:C:183:TRP:HB3	1.83	0.60
2:B:57:LYS:HD2	11:B:896:HOH:O	2.01	0.60
4:M:11:SER:C	11:M:272:HOH:O	2.44	0.60
4:M:21:ASN:ND2	4:M:22:ILE:H	2.00	0.60
2:B:236:ASN:ND2	7:J:1:NAG:H2	2.14	0.60
2:D:23:CYS:HB3	2:D:75:PHE:O	2.02	0.60
1:C:45:LEU:HD13	11:C:825:HOH:O	2.01	0.60
2:B:130:PHE:HB2	2:B:146:VAL:CG1	2.23	0.60
2:B:236:ASN:OD1	7:J:1:NAG:C1	2.50	0.60
2:B:232:PRO:HA	11:B:884:HOH:O	2.01	0.60
3:I:209:TYR:HA	3:I:210:PRO:O	2.02	0.59
3:I:215:LEU:CD2	3:I:261:VAL:HG13	2.32	0.59
2:D:27:ASN:O	2:D:28:ASN:HB2	2.01	0.59
2:D:32:MET:HB3	2:D:75:PHE:CD2	2.37	0.59
3:I:130:LEU:N	3:I:130:LEU:HD22	2.18	0.59
2:B:211:ARG:NH2	2:B:213:GLN:OE1	2.35	0.59
1:C:20:LEU:HD23	1:C:20:LEU:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:135:ALA:HB1	3:I:137:ASP:CG	2.27	0.59
3:I:167:TRP:CG	5:Q:1:GLU:H3	2.21	0.59
3:I:189:VAL:HG13	3:I:272:LEU:HD12	1.83	0.59
2:D:242:TRP:HD1	2:D:243:GLY:H	1.49	0.59
3:I:228:MET:HE1	3:I:245:ALA:HB1	1.85	0.59
1:C:3:VAL:HG12	11:C:822:HOH:O	2.02	0.59
1:C:16:ALA:O	1:C:80:VAL:HG22	2.03	0.59
1:A:194:ILE:HG23	1:A:195:PHE:CD1	2.34	0.59
2:D:45:LEU:HD21	2:D:48:TYR:CD2	2.36	0.59
2:D:122:VAL:HA	2:D:153:PHE:HB3	1.85	0.59
3:I:35:ARG:HB3	3:I:48:ARG:CD	2.33	0.59
1:C:196:LYS:HB2	1:C:196:LYS:NZ	2.18	0.58
2:D:164:ASN:HD22	2:D:209:HIS:HB3	1.66	0.58
1:C:22:CYS:H	1:C:74:HIS:HD2	1.50	0.58
1:C:194:ILE:HG23	1:C:195:PHE:CD2	2.38	0.58
2:B:30:ASN:HD21	3:H:146:LYS:NZ	2.01	0.58
2:D:171:GLY:HA3	2:D:196:LEU:HD12	1.86	0.58
3:I:96:GLN:HB2	3:I:117:ALA:HB3	1.86	0.58
3:I:227:ASP:OD1	3:I:227:ASP:O	2.21	0.58
1:C:191:CYS:O	1:C:192:GLN:HG3	2.03	0.58
2:D:150:ARG:HG2	2:D:190:TYR:O	2.03	0.58
3:H:263:HIS:CD2	3:H:265:GLY:H	2.21	0.58
4:M:25:CYS:O	4:M:65:LEU:HD12	2.04	0.58
2:D:34:TRP:O	2:D:46:ILE:N	2.34	0.58
3:I:194:ARG:NH1	3:I:248:VAL:HG21	2.18	0.58
2:D:4:VAL:HG13	2:D:24:ASN:O	2.04	0.58
3:H:169:ARG:HH21	3:I:269:PRO:HD2	1.67	0.58
2:D:78:ILE:HD12	2:D:78:ILE:N	2.18	0.58
3:H:185:PRO:HB3	3:H:208:PHE:HB3	1.86	0.58
1:C:66:PHE:HB2	11:C:835:HOH:O	2.03	0.58
2:B:96:GLY:HA3	3:H:150:ALA:HB1	1.84	0.58
2:D:81:LEU:HD23	2:D:81:LEU:O	2.03	0.58
1:C:44:GLN:OE1	1:C:44:GLN:HA	2.03	0.58
2:D:3:ALA:HB1	2:D:109:GLY:CA	2.34	0.58
5:Q:6:TYR:O	5:Q:8:VAL:N	2.37	0.58
1:A:40:ARG:HH11	2:B:113:ARG:NH2	2.01	0.57
2:B:232:PRO:CA	11:B:884:HOH:O	2.51	0.57
2:D:153:PHE:HD1	2:D:187:TYR:O	1.85	0.57
2:D:128:SER:HB2	2:D:148:LEU:HD22	1.85	0.57
3:I:79:ARG:HB2	11:I:960:HOH:O	2.03	0.57
4:M:54:MET:SD	4:M:62:PHE:HD2	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:108:ARG:NH2	3:I:214:THR:OG1	2.37	0.57
5:P:2:GLN:HE21	5:P:2:GLN:CA	2.18	0.57
1:C:82:TRP:CH2	1:C:167:VAL:HG21	2.39	0.57
3:I:23:MET:HA	3:I:36:PHE:O	2.04	0.57
3:I:147:TRP:HB3	3:I:152:GLU:HB3	1.85	0.57
3:I:263:HIS:HD2	3:I:265:GLY:H	1.47	0.57
1:A:48:LYS:HD3	2:B:105:THR:CG2	2.35	0.57
1:C:142:LEU:HD22	1:C:143:PHE:N	2.18	0.57
2:B:25:GLN:OE1	2:B:27:ASN:HB2	2.05	0.57
3:I:45:TYR:HB3	3:I:60:TRP:CE3	2.39	0.57
3:I:194:ARG:HH12	3:I:248:VAL:HG21	1.70	0.57
4:M:73:THR:HG22	4:M:75:THR:N	2.14	0.57
1:C:168:LEU:HD23	1:C:168:LEU:N	2.19	0.57
4:M:21:ASN:C	4:M:22:ILE:HD12	2.29	0.57
1:A:185:ASN:HD21	7:F:1:NAG:C7	2.16	0.57
3:I:97:VAL:HG11	5:Q:5:PHE:CE2	2.39	0.57
3:I:234:ARG:HH11	4:M:8:GLN:HE21	1.50	0.57
1:C:170:MET:N	1:C:175:SER:HB3	2.17	0.57
2:D:35:TYR:HA	2:D:44:ARG:O	2.04	0.57
2:D:82:ALA:HB1	2:D:116:VAL:HG11	1.87	0.57
2:D:94:SER:O	2:D:106:LEU:HB3	2.05	0.57
2:D:137:ILE:HG12	2:D:137:ILE:O	2.05	0.57
2:D:150:ARG:HG3	2:D:191:CYS:HA	1.87	0.57
2:D:150:ARG:CG	2:D:191:CYS:HA	2.35	0.57
2:D:150:ARG:HD2	2:D:150:ARG:C	2.30	0.56
3:I:138:MET:HE3	3:I:141:LEU:CD2	2.35	0.56
4:M:2:GLN:HB3	4:M:32:PRO:HD3	1.87	0.56
1:A:206:TYR:HB3	2:B:135:ALA:HB1	1.86	0.56
3:I:135:ALA:HB1	3:I:137:ASP:OD2	2.05	0.56
1:A:156:MET:HB3	11:A:956:HOH:O	2.05	0.56
1:C:128:LEU:HD21	1:C:140:LEU:HG	1.86	0.56
3:I:62:ARG:HH12	5:Q:1:GLU:HB2	1.70	0.56
3:I:8:PHE:HB2	3:I:25:VAL:HG23	1.87	0.56
3:I:56:GLY:C	3:I:58:GLU:H	2.13	0.56
3:I:66:LYS:HG2	3:I:70:ASN:HD21	1.70	0.56
3:I:194:ARG:HH11	3:I:248:VAL:CG1	2.19	0.56
4:M:37:ILE:HG22	4:M:82:VAL:CG1	2.32	0.56
1:A:190:THR:CG2	1:A:192:GLN:HG2	2.36	0.56
1:C:33:PHE:HB2	11:C:832:HOH:O	2.05	0.56
3:I:6:ARG:NH1	4:M:58:LYS:HD3	2.20	0.56
1:A:150:ILE:HG23	11:A:940:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASN:ND2	1:C:122:GLU:OE1	2.35	0.56
1:C:129:LYS:HD2	1:C:129:LYS:N	2.21	0.56
2:D:53:GLY:HA2	2:D:69:ARG:HB3	1.87	0.56
1:A:14:GLU:OE2	1:A:81:HIS:HB3	2.05	0.56
2:B:69:ARG:HH12	2:B:72:GLN:C	2.14	0.56
3:I:38:SER:HA	3:I:43:PRO:HB3	1.88	0.56
3:I:124:ILE:HB	3:I:140:ALA:CB	2.34	0.56
3:I:185:PRO:CB	3:I:208:PHE:HB3	2.36	0.56
4:L:40:LEU:HD23	4:L:45:LYS:HA	1.86	0.56
1:C:91:ALA:HB3	11:C:832:HOH:O	2.06	0.56
2:B:18:LYS:CD	2:B:80:GLU:HA	2.36	0.55
2:D:142:LYS:HD3	2:D:197:ARG:CZ	2.36	0.55
3:I:24:GLU:O	3:I:35:ARG:HA	2.06	0.55
3:I:96:GLN:CB	3:I:117:ALA:HB3	2.36	0.55
3:I:167:TRP:CD1	5:Q:1:GLU:HG2	2.40	0.55
1:C:118:ILE:HD11	1:C:147:ASP:OD2	2.06	0.55
2:D:37:GLN:CA	2:D:43:LEU:HA	2.37	0.55
1:C:140:LEU:HB2	1:C:182:ALA:O	2.05	0.55
2:D:105:THR:O	2:D:105:THR:HG23	2.07	0.55
3:I:58:GLU:O	3:I:62:ARG:HB2	2.06	0.55
4:L:21:ASN:HB3	4:L:70:PHE:CE1	2.41	0.55
2:B:31:ASN:HD22	2:B:50:TYR:HA	1.70	0.55
2:D:19:VAL:O	2:D:79:LEU:HD23	2.06	0.55
3:H:225:ILE:HG23	3:H:226:GLN:NE2	2.22	0.55
4:M:49:VAL:HA	4:M:68:THR:CG2	2.36	0.55
2:B:221:GLU:CD	2:B:221:GLU:H	2.15	0.55
2:D:9:ARG:HA	2:D:112:THR:CG2	2.36	0.55
3:I:51:TRP:HZ3	3:I:52:MET:HE3	1.71	0.55
3:I:138:MET:O	3:I:141:LEU:HB2	2.06	0.55
3:I:140:ALA:O	3:I:144:LYS:N	2.40	0.55
1:A:186:GLN:HB3	1:A:189:PHE:HD2	1.71	0.55
3:I:23:MET:HB3	3:I:37:ASP:OD1	2.06	0.55
4:M:33:PRO:HB3	4:M:62:PHE:CE2	2.41	0.55
4:M:2:GLN:CB	4:M:32:PRO:HD3	2.37	0.55
2:D:186:ASN:O	2:D:186:ASN:ND2	2.40	0.55
3:H:192:HIS:CE1	4:L:98:ASP:HB3	2.42	0.55
3:H:202:ARG:HG3	3:H:246:SER:HB3	1.89	0.55
3:I:25:VAL:HG11	3:I:35:ARG:CZ	2.37	0.55
4:L:49:VAL:HG22	4:L:68:THR:CG2	2.37	0.55
4:M:69:GLU:O	4:M:70:PHE:HB3	2.06	0.55
5:Q:2:GLN:HE21	5:Q:2:GLN:CA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:HG23	1:A:191:CYS:N	2.21	0.55
2:B:153:PHE:O	2:B:155:ASP:N	2.40	0.55
2:D:225:TRP:CZ3	2:D:232:PRO:HD2	2.42	0.55
3:I:170:ARG:HG2	3:I:170:ARG:HH11	1.71	0.55
1:C:106:PHE:CD1	2:D:43:LEU:HD23	2.42	0.55
1:C:170:MET:HG2	1:C:171:LYS:N	2.21	0.55
2:D:77:LEU:HD23	2:D:77:LEU:C	2.32	0.55
2:D:316:LEU:HG	2:D:117:GLU:H	1.72	0.55
3:I:11:ALA:HA	3:I:21:ARG:O	2.07	0.55
3:I:202:ARG:HG2	3:I:204:TRP:NE1	2.22	0.55
7:J:2:NAG:H61	7:J:3:BMA:C3	2.33	0.55
2:B:68:SER:C	2:B:70:PRO:HD3	2.32	0.54
2:D:143:ALA:HB3	2:D:198:VAL:HG23	1.88	0.54
1:C:128:LEU:C	1:C:129:LYS:HD2	2.32	0.54
2:D:86:GLN:NE2	2:D:114:LEU:HD21	2.23	0.54
3:I:230:LEU:CD1	3:I:245:ALA:HB2	2.38	0.54
4:M:12:ARG:N	11:M:272:HOH:O	2.40	0.54
1:C:115:LEU:H	1:C:115:LEU:CD2	2.20	0.54
2:B:123:THR:O	2:B:152:PHE:HA	2.08	0.54
2:B:235:GLN:OE1	2:B:237:ILE:HD11	2.07	0.54
1:C:34:TRP:CH2	1:C:90:CYS:HB2	2.42	0.54
4:M:12:ARG:HE	4:M:13:HIS:HE1	1.54	0.54
1:A:158:SER:O	7:F:1:NAG:C8	2.56	0.54
2:B:228:GLY:O	2:B:229:SER:C	2.50	0.54
1:A:17:SER:HA	1:A:78:ALA:O	2.06	0.54
3:I:35:ARG:HB3	3:I:48:ARG:HD3	1.89	0.54
2:D:35:TYR:CD2	2:D:43:LEU:HG	2.43	0.54
2:D:164:ASN:HD22	2:D:164:ASN:N	2.04	0.54
3:H:271:THR:O	3:H:271:THR:HG23	2.08	0.54
3:I:152:GLU:C	3:I:154:GLU:N	2.66	0.54
4:M:6:GLN:O	4:M:27:VAL:HA	2.07	0.54
4:L:97:ARG:HG2	4:L:97:ARG:HH11	1.72	0.54
2:D:33:TYR:O	2:D:92:CYS:HA	2.08	0.53
2:D:123:THR:O	2:D:152:PHE:HB2	2.07	0.53
3:H:220:ASN:ND2	3:H:222:GLU:OE1	2.41	0.53
3:I:127:ASN:N	3:I:127:ASN:HD22	2.05	0.53
3:I:141:LEU:HA	3:I:144:LYS:HB3	1.91	0.53
3:I:207:GLY:HA2	3:I:240:THR:HB	1.89	0.53
2:D:198:VAL:HG21	2:D:203:TRP:HB2	1.90	0.53
3:I:37:ASP:C	3:I:39:ASP:H	2.16	0.53
1:A:36:VAL:HG21	1:A:46:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:117:ALA:HB2	4:M:60:TRP:CE3	2.43	0.53
2:D:127:VAL:HG23	2:D:148:LEU:O	2.08	0.53
3:I:17:LEU:N	3:I:17:LEU:HD22	2.23	0.53
4:M:7:ILE:HD12	4:M:7:ILE:N	2.23	0.53
4:M:62:PHE:HD1	11:M:247:HOH:O	1.89	0.53
1:C:38:TYR:HB2	1:C:41:GLN:HB2	1.91	0.53
2:D:171:GLY:HA3	2:D:196:LEU:CD1	2.37	0.53
2:D:171:GLY:O	2:D:172:VAL:C	2.51	0.53
3:I:155:ARG:O	3:I:155:ARG:HG2	2.08	0.53
4:M:49:VAL:HA	4:M:68:THR:HG22	1.91	0.53
1:C:168:LEU:HD21	1:C:178:ASN:O	2.09	0.53
2:D:124:PRO:HG3	2:D:235:GLN:HE22	1.73	0.53
3:H:152:GLU:OE1	3:H:155:ARG:NH1	2.39	0.53
1:C:172:ALA:C	1:C:174:ASP:H	2.17	0.53
2:D:242:TRP:CD1	2:D:243:GLY:H	2.26	0.53
3:I:41:GLU:N	3:I:41:GLU:OE2	2.41	0.53
3:I:272:LEU:N	3:I:272:LEU:HD23	2.24	0.53
4:M:28:THR:HB	11:M:281:HOH:O	2.07	0.52
1:A:25:SER:O	1:A:26:TYR:HB2	2.09	0.52
1:C:115:LEU:HD22	1:C:115:LEU:N	2.24	0.52
2:D:145:LEU:HD23	2:D:145:LEU:N	2.20	0.52
3:I:25:VAL:CG1	3:I:35:ARG:CZ	2.86	0.52
3:I:185:PRO:HB3	3:I:208:PHE:CB	2.38	0.52
2:D:86:GLN:HE21	2:D:114:LEU:HD21	1.75	0.52
3:H:133:TRP:HH2	3:H:156:LEU:HD12	1.73	0.52
1:A:38:TYR:HB3	1:A:39:PRO:HD2	1.90	0.52
1:A:139:THR:O	1:A:140:LEU:HB2	2.09	0.52
3:H:135:ALA:HB1	3:H:140:ALA:CB	2.40	0.52
4:M:56:PHE:HB2	4:M:61:SER:O	2.09	0.52
1:C:151:ASN:O	1:C:151:ASN:ND2	2.42	0.52
3:I:127:ASN:HB2	3:I:129:ASP:OD1	2.10	0.52
3:I:232:GLU:HB2	11:I:950:HOH:O	2.10	0.52
4:M:23:LEU:C	4:M:39:MET:HE1	2.34	0.52
2:D:121:ASN:OD1	2:D:122:VAL:N	2.42	0.52
3:I:237:GLY:HA3	11:M:248:HOH:O	2.09	0.52
11:B:812:HOH:O	3:H:146:LYS:HG3	2.09	0.52
2:D:83:THR:OG1	2:D:84:PRO:HD2	2.10	0.52
3:I:32:GLU:OE2	3:I:48:ARG:HG3	2.10	0.52
5:P:2:GLN:HE21	5:P:3:TYR:N	2.06	0.52
2:D:8:PRO:C	2:D:10:ASN:H	2.17	0.51
2:D:57:LYS:HD2	2:D:61:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ARG:HH12	2:D:72:GLN:HA	1.74	0.51
3:H:145:HIS:O	3:H:149:GLN:HG3	2.11	0.51
1:A:36:VAL:CG2	1:A:46:LEU:HD21	2.41	0.51
1:C:18:LEU:HD12	1:C:19:GLN:H	1.75	0.51
2:B:143:ALA:O	2:B:197:ARG:HA	2.10	0.51
2:B:159:LEU:HD12	2:B:160:SER:N	2.26	0.51
2:D:51:GLY:O	2:D:69:ARG:CZ	2.59	0.51
3:I:94:THR:HG22	3:I:95:ILE:H	1.75	0.51
1:A:147:ASP:OD2	1:A:149:GLN:HB2	2.10	0.51
4:L:7:ILE:HD11	4:L:82:VAL:CG2	2.40	0.51
4:M:12:ARG:HH21	4:M:13:HIS:HE1	1.58	0.51
5:Q:2:GLN:HG3	5:Q:3:TYR:O	2.10	0.51
2:B:156:HIS:HB2	2:B:217:HIS:HB2	1.92	0.51
2:D:31:ASN:HB2	2:D:95:GLY:O	2.10	0.51
3:I:194:ARG:HH11	3:I:248:VAL:HG11	1.75	0.51
1:A:36:VAL:HG23	1:A:46:LEU:HG	1.92	0.51
1:C:50:TYR:HB3	3:I:158:ALA:HB1	1.92	0.51
1:A:42:GLY:HA2	2:B:91:PHE:CE2	2.46	0.51
3:H:111:ARG:NH1	3:H:111:ARG:CG	2.67	0.51
3:I:10:THR:HA	3:I:95:ILE:O	2.10	0.51
2:B:31:ASN:HA	2:B:49:SER:O	2.11	0.51
2:B:68:SER:O	2:B:70:PRO:HD3	2.11	0.51
2:B:204:HIS:O	2:B:206:PRO:HD3	2.10	0.51
4:L:40:LEU:HD21	4:L:81:ARG:NH2	2.20	0.51
1:C:137:ASP:CG	1:C:138:SER:H	2.18	0.51
3:I:155:ARG:HH22	5:Q:4:LYS:HB3	1.75	0.51
3:I:196:GLU:HB3	11:I:992:HOH:O	2.11	0.51
1:C:110:THR:HG23	1:C:110:THR:O	2.11	0.51
2:D:159:LEU:HD12	2:D:159:LEU:N	2.26	0.51
3:H:180:LEU:O	3:H:181:ARG:C	2.53	0.51
3:I:11:ALA:O	3:I:95:ILE:HG13	2.10	0.51
4:M:53:ASP:O	4:M:64:ILE:HD12	2.11	0.50
1:A:157:GLU:HG2	1:A:158:SER:O	2.11	0.50
1:A:168:LEU:O	1:A:176:LYS:HA	2.10	0.50
1:C:168:LEU:HG	1:C:177:SER:HB3	1.93	0.50
2:D:77:LEU:HD23	2:D:79:LEU:HD22	1.92	0.50
2:D:220:SER:C	2:D:222:GLU:H	2.19	0.50
3:H:218:GLN:NE2	3:H:260:HIS:CE1	2.79	0.50
1:A:140:LEU:HA	1:A:182:ALA:O	2.12	0.50
2:D:3:ALA:HA	2:D:108:PHE:O	2.12	0.50
3:H:15:PRO:C	3:H:17:LEU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:242:GLN:HG2	11:I:912:HOH:O	2.11	0.50
1:A:173:MET:HG3	1:A:174:ASP:H	1.76	0.50
3:I:202:ARG:HD2	3:I:244:TRP:CD2	2.47	0.50
4:M:12:ARG:HB2	11:M:272:HOH:O	2.11	0.50
1:A:82:TRP:CZ2	1:A:167:VAL:HB	2.47	0.50
1:C:93:SER:HB2	1:C:104:LEU:HD23	1.93	0.50
2:B:153:PHE:HB3	2:B:154:PRO:CD	2.41	0.50
2:D:77:LEU:CD2	2:D:79:LEU:HD22	2.41	0.50
3:H:9:VAL:O	3:H:96:GLN:HA	2.11	0.50
3:I:170:ARG:O	3:I:173:LYS:HB3	2.11	0.50
1:A:54:PRO:O	1:A:65:GLU:HA	2.12	0.50
1:C:14:GLU:HG2	1:C:15:GLY:N	2.26	0.50
1:C:3:VAL:CG1	1:C:107:GLY:N	2.75	0.50
2:D:210:PHE:HB2	2:D:241:ALA:HB3	1.93	0.50
3:I:96:GLN:HB3	4:M:56:PHE:CZ	2.47	0.50
4:M:19:LYS:C	4:M:71:THR:HG23	2.37	0.50
2:D:6:GLN:HG2	2:D:110:ALA:HB3	1.93	0.50
2:D:152:PHE:N	2:D:152:PHE:CD1	2.80	0.50
3:H:202:ARG:HD3	3:H:244:TRP:CD2	2.46	0.50
4:M:12:ARG:CA	11:M:272:HOH:O	2.59	0.50
4:M:73:THR:HG22	4:M:74:GLU:N	2.27	0.50
2:D:140:LYS:CD	2:D:142:LYS:HB2	2.41	0.49
3:I:35:ARG:HB3	3:I:48:ARG:HE	1.76	0.49
3:I:148:GLU:O	3:I:149:GLN:HG3	2.12	0.49
4:M:2:GLN:CA	4:M:31:HIS:O	2.51	0.49
1:C:59:VAL:O	1:C:62:PHE:HD1	1.95	0.49
2:D:33:TYR:N	2:D:33:TYR:CD1	2.80	0.49
4:M:37:ILE:HD11	4:M:51:MET:HE1	1.92	0.49
4:M:73:THR:CG2	4:M:74:GLU:N	2.75	0.49
1:C:60:ASN:HB2	1:C:62:PHE:HE1	1.77	0.49
2:D:125:PRO:HB2	2:D:214:VAL:HG11	1.92	0.49
2:D:205:ASN:C	2:D:207:ARG:H	2.21	0.49
4:L:49:VAL:HA	4:L:68:THR:HG22	1.93	0.49
4:M:28:THR:HG22	4:M:63:TYR:HB2	1.92	0.49
1:C:53:ASP:C	1:C:55:VAL:H	2.21	0.49
2:B:93:ALA:HA	2:B:107:TYR:O	2.12	0.49
2:D:169:HIS:O	2:D:170:SER:HB2	2.13	0.49
3:H:169:ARG:NH2	3:I:269:PRO:HD2	2.27	0.49
3:H:215:LEU:HD22	3:H:261:VAL:HG22	1.95	0.49
4:M:4:THR:HG23	4:M:86:SER:OG	2.12	0.49
1:A:156:MET:SD	1:A:156:MET:N	2.82	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:LYS:HD2	2:D:12:VAL:H	1.77	0.49
3:I:56:GLY:O	3:I:59:TYR:HB3	2.12	0.49
3:I:116:TYR:OH	5:Q:5:PHE:HD2	1.95	0.49
3:I:9:VAL:HB	3:I:97:VAL:CG2	2.43	0.49
1:A:179:GLY:HA3	2:B:195:ARG:NH1	2.27	0.49
1:A:188:SER:O	1:A:189:PHE:HB2	2.12	0.49
1:C:160:THR:HG23	1:C:184:SER:HB3	1.94	0.49
2:B:78:ILE:HD12	2:B:78:ILE:N	2.28	0.49
2:D:49:SER:OG	2:D:69:ARG:NE	2.45	0.49
2:D:146:VAL:HG22	2:D:147:CYS:N	2.27	0.49
2:D:150:ARG:HB2	2:D:191:CYS:HA	1.94	0.49
2:D:175:ASP:HB2	2:D:192:LEU:HD12	1.94	0.49
4:M:51:MET:HE3	4:M:64:ILE:CD1	2.42	0.49
1:C:82:TRP:CD1	1:C:116:PRO:HD3	2.48	0.49
2:D:14:VAL:HB	2:D:17:GLY:N	2.19	0.49
3:I:9:VAL:O	3:I:96:GLN:HA	2.12	0.49
3:I:36:PHE:HB2	3:I:45:TYR:CD1	2.48	0.49
4:L:48:LYS:O	4:L:48:LYS:HG3	2.12	0.49
4:M:51:MET:HE3	4:M:64:ILE:HD11	1.94	0.49
2:B:152:PHE:CE1	2:B:190:TYR:HB2	2.48	0.49
1:A:92:VAL:HG22	1:A:93:SER:N	2.28	0.49
1:A:170:MET:HB2	1:A:175:SER:CB	2.43	0.49
2:B:66:LYS:NZ	2:B:80:GLU:OE2	2.35	0.49
2:D:79:LEU:HD12	2:D:86:GLN:CD	2.37	0.49
3:I:35:ARG:HB3	3:I:48:ARG:NE	2.28	0.49
1:C:3:VAL:HG13	1:C:107:GLY:N	2.28	0.48
1:C:60:ASN:CB	1:C:62:PHE:HE1	2.26	0.48
2:D:199:SER:HB2	2:D:202:PHE:CD2	2.48	0.48
3:H:97:VAL:HA	3:H:115:GLN:O	2.13	0.48
1:C:142:LEU:HD22	1:C:143:PHE:H	1.78	0.48
2:B:87:THR:O	2:B:88:SER:HB2	2.12	0.48
3:H:6:ARG:NH1	3:H:113:TYR:OH	2.44	0.48
3:I:9:VAL:HG11	3:I:74:PHE:CE1	2.48	0.48
3:I:15:PRO:O	3:I:17:LEU:HD22	2.13	0.48
3:I:32:GLU:OE1	3:I:35:ARG:NH2	2.44	0.48
4:M:3:LYS:O	4:M:30:PHE:HA	2.14	0.48
4:M:20:PRO:HG3	4:M:71:THR:OG1	2.13	0.48
3:H:9:VAL:HB	3:H:97:VAL:CG1	2.24	0.48
3:I:191:HIS:HB2	3:I:274:TRP:CZ2	2.48	0.48
4:M:46:ILE:HG23	4:M:47:PRO:HD2	1.95	0.48
2:B:25:GLN:HG2	2:B:27:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:VAL:HG23	2:D:225:TRP:HZ3	1.77	0.48
2:D:143:ALA:HB3	2:D:198:VAL:CG2	2.42	0.48
3:H:113:TYR:N	3:H:113:TYR:CD2	2.80	0.48
2:D:34:TRP:CD1	2:D:77:LEU:HB2	2.48	0.48
3:H:85:TYR:O	3:H:86:ASN:C	2.56	0.48
3:I:10:THR:HG22	3:I:23:MET:HG3	1.95	0.48
3:I:55:GLU:HB3	3:I:59:TYR:CD2	2.49	0.48
3:I:167:TRP:NE1	5:Q:1:GLU:OE2	2.46	0.48
1:C:55:VAL:HG23	1:C:55:VAL:O	2.14	0.48
2:B:316:LEU:N	2:B:316:LEU:HD12	2.29	0.48
2:D:173:SER:HB3	2:D:195:ARG:HG2	1.96	0.48
3:H:121:CYS:O	3:H:122:ASP:C	2.56	0.48
1:C:80:VAL:O	1:C:80:VAL:CG2	2.58	0.48
2:D:109:GLY:O	2:D:110:ALA:HB2	2.13	0.48
2:D:120:ARG:HB2	2:D:120:ARG:NH1	2.29	0.48
3:H:248:VAL:O	3:H:248:VAL:HG23	2.12	0.48
3:I:45:TYR:HB3	3:I:60:TRP:CZ3	2.49	0.48
4:M:51:MET:HE3	4:M:64:ILE:HG12	1.95	0.48
3:H:194:ARG:HG2	3:H:195:PRO:HD2	1.95	0.48
3:H:249:VAL:HG23	3:H:254:GLU:HG3	1.95	0.48
3:I:207:GLY:HA2	3:I:240:THR:CB	2.44	0.48
2:B:174:THR:O	2:B:175:ASP:C	2.57	0.48
2:D:79:LEU:HD23	2:D:79:LEU:N	2.29	0.48
2:D:216:PHE:HB3	2:D:235:GLN:O	2.13	0.48
3:H:199:VAL:HG21	3:H:251:LEU:HD13	1.95	0.48
3:I:209:TYR:HA	3:I:210:PRO:C	2.39	0.48
1:C:142:LEU:HD13	1:C:142:LEU:C	2.39	0.47
2:D:194:SER:C	2:D:195:ARG:HE	2.22	0.47
2:D:221:GLU:N	2:D:221:GLU:CD	2.72	0.47
3:H:271:THR:C	3:H:272:LEU:HD12	2.39	0.47
3:I:14:ARG:NH2	3:I:21:ARG:HB2	2.29	0.47
1:C:14:GLU:HA	1:C:114:VAL:HG23	1.96	0.47
3:I:116:TYR:O	3:I:122:ASP:HA	2.14	0.47
2:D:18:LYS:HG3	2:D:80:GLU:OE2	2.14	0.47
2:D:31:ASN:O	2:D:94:SER:HA	2.14	0.47
2:D:142:LYS:HD3	2:D:197:ARG:NH1	2.29	0.47
2:D:147:CYS:C	2:D:148:LEU:HD12	2.39	0.47
3:I:51:TRP:CZ3	3:I:52:MET:HG2	2.49	0.47
3:I:132:THR:HG22	3:I:133:TRP:N	2.29	0.47
2:B:30:ASN:HA	2:B:72:GLN:HE22	1.79	0.47
3:H:218:GLN:NE2	3:H:260:HIS:ND1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:130:LEU:N	3:I:130:LEU:CD2	2.77	0.47
4:L:17:ASN:HA	4:L:72:PRO:O	2.14	0.47
1:A:12:VAL:O	1:A:114:VAL:HA	2.14	0.47
2:B:159:LEU:HD12	2:B:159:LEU:C	2.39	0.47
2:D:46:ILE:HG22	2:D:47:HIS:CE1	2.49	0.47
5:Q:2:GLN:NE2	5:Q:2:GLN:HA	2.28	0.47
2:B:127:VAL:HG13	2:B:237:ILE:HG22	1.96	0.47
2:D:14:VAL:HG12	2:D:15:THR:H	1.78	0.47
3:I:13:SER:C	3:I:15:PRO:HD3	2.39	0.47
3:I:155:ARG:HH22	5:Q:4:LYS:CB	2.27	0.47
1:A:45:LEU:HD11	1:A:47:LEU:O	2.15	0.47
1:A:128:LEU:HD12	1:A:128:LEU:N	2.30	0.47
1:C:91:ALA:HB2	1:C:106:PHE:HA	1.97	0.47
2:B:69:ARG:NH1	2:B:71:SER:O	2.48	0.47
2:D:125:PRO:HD3	2:D:216:PHE:CG	2.50	0.47
2:D:142:LYS:HZ2	2:D:197:ARG:HD3	1.80	0.47
2:D:214:VAL:O	2:D:216:PHE:N	2.47	0.47
3:I:14:ARG:CZ	3:I:21:ARG:HB2	2.45	0.47
1:C:167:VAL:C	1:C:168:LEU:HD23	2.39	0.47
3:H:128:GLU:CD	11:H:913:HOH:O	2.58	0.47
3:H:236:ALA:O	4:L:12:ARG:HD3	2.15	0.47
3:I:44:ARG:HG2	3:I:44:ARG:HH11	1.79	0.47
3:I:143:THR:HG21	5:Q:8:VAL:CB	2.45	0.47
3:I:214:THR:HB	3:I:262:TYR:HB2	1.96	0.47
2:D:6:GLN:OE1	2:D:6:GLN:HA	2.15	0.47
3:I:222:GLU:HG3	3:I:223:GLU:H	1.80	0.47
1:A:207:PRO:C	1:A:209:SER:H	2.23	0.47
2:B:316:LEU:HD23	2:B:153:PHE:HE2	1.80	0.47
4:L:23:LEU:HD11	4:L:78:TYR:CB	2.45	0.47
4:L:23:LEU:HD11	4:L:78:TYR:HB3	1.97	0.47
4:M:30:PHE:O	4:M:31:HIS:HB2	2.14	0.47
1:C:48:LYS:C	11:C:827:HOH:O	2.58	0.46
1:C:50:TYR:HB3	3:I:158:ALA:CB	2.45	0.46
1:C:61:GLY:HA3	1:C:77:LYS:NZ	2.30	0.46
1:C:77:LYS:HE3	1:C:79:SER:H	1.81	0.46
1:C:93:SER:HB2	1:C:104:LEU:CD2	2.45	0.46
1:C:191:CYS:C	1:C:192:GLN:HG3	2.41	0.46
1:C:196:LYS:HB2	1:C:196:LYS:HZ1	1.78	0.46
3:H:266:LEU:HD13	3:H:270:LEU:HG	1.95	0.46
3:I:10:THR:CG2	3:I:23:MET:CG	2.93	0.46
3:I:79:ARG:HA	3:I:82:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HG3	2:B:170:SER:HB2	1.97	0.46
1:C:1:GLN:OE1	1:C:100:PHE:N	2.47	0.46
2:B:73:GLU:H	2:B:73:GLU:CD	2.24	0.46
2:D:8:PRO:C	2:D:10:ASN:N	2.73	0.46
3:H:21:ARG:NE	3:H:23:MET:HE2	2.30	0.46
3:I:4:SER:C	11:I:954:HOH:O	2.57	0.46
3:I:143:THR:OG1	5:Q:8:VAL:HB	2.16	0.46
2:B:233:VAL:HG22	2:B:234:THR:N	2.30	0.46
3:H:191:HIS:NE2	3:H:199:VAL:HG11	2.30	0.46
3:I:74:PHE:CZ	3:I:97:VAL:HG21	2.50	0.46
3:I:143:THR:O	3:I:143:THR:HG22	2.14	0.46
1:C:7:ASP:CG	1:C:110:THR:HB	2.40	0.46
3:H:152:GLU:CD	3:H:155:ARG:HH11	2.23	0.46
3:I:147:TRP:HZ2	5:Q:8:VAL:HA	1.81	0.46
4:M:31:HIS:HD1	4:M:32:PRO:CA	2.19	0.46
1:A:129:LYS:HB2	1:A:129:LYS:NZ	2.30	0.46
1:C:5:GLN:HB3	1:C:7:ASP:OD2	2.15	0.46
2:D:15:THR:HG22	2:D:15:THR:O	2.14	0.46
2:D:136:GLU:HB2	2:D:140:LYS:NZ	2.31	0.46
3:H:206:LEU:HD23	3:H:242:GLN:HB3	1.97	0.46
3:I:88:SER:O	3:I:89:ALA:O	2.34	0.46
3:I:164:CYS:O	3:I:165:VAL:C	2.58	0.46
1:A:154:LYS:C	1:A:162:ILE:HD12	2.40	0.46
1:C:29:THR:HG21	11:C:853:HOH:O	2.15	0.46
2:B:1:GLU:HB3	11:B:842:HOH:O	2.16	0.46
3:I:27:TYR:HE2	3:I:32:GLU:HB2	1.80	0.46
3:I:152:GLU:O	3:I:154:GLU:N	2.49	0.46
4:L:7:ILE:HD11	4:L:82:VAL:HG21	1.98	0.46
1:C:20:LEU:HD13	1:C:88:TYR:CG	2.50	0.46
1:C:47:LEU:HD12	1:C:47:LEU:C	2.41	0.46
1:C:146:PHE:CD1	1:C:146:PHE:C	2.93	0.46
2:D:14:VAL:C	2:D:16:GLY:H	2.23	0.46
2:D:175:ASP:HB2	2:D:192:LEU:CD1	2.45	0.46
3:I:187:ALA:HA	3:I:204:TRP:O	2.16	0.46
4:M:24:ASN:OD1	4:M:65:LEU:HD21	2.16	0.46
1:A:43:LEU:N	1:A:43:LEU:HD12	2.31	0.46
1:A:195:PHE:O	1:A:198:THR:HG23	2.16	0.46
3:H:191:HIS:HB2	3:H:274:TRP:CE2	2.51	0.46
3:I:94:THR:CG2	3:I:95:ILE:N	2.78	0.46
3:I:221:GLY:O	3:I:222:GLU:HB2	2.16	0.46
1:A:156:MET:HE3	11:A:956:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:HB2	1:C:41:GLN:CB	2.45	0.46
1:C:155:THR:CG2	1:C:161:PHE:HA	2.38	0.46
3:I:33:PHE:CA	3:I:48:ARG:HB2	2.45	0.46
2:B:236:ASN:HD21	7:J:1:NAG:H2	1.61	0.45
2:D:33:TYR:HB3	2:D:45:LEU:CD1	2.46	0.45
2:D:70:PRO:O	2:D:71:SER:CB	2.64	0.45
3:H:99:SER:HA	3:H:113:TYR:O	2.16	0.45
4:M:39:MET:O	4:M:46:ILE:HB	2.16	0.45
1:A:182:ALA:HB3	1:A:195:PHE:HE1	1.81	0.45
3:I:27:TYR:CE2	3:I:32:GLU:HB2	2.52	0.45
3:I:72:GLN:O	3:I:73:SER:C	2.57	0.45
3:I:194:ARG:NH1	3:I:248:VAL:CG1	2.74	0.45
2:B:21:LEU:HD22	2:B:112:THR:HG21	1.97	0.45
2:D:6:GLN:HE21	2:D:111:GLY:C	2.25	0.45
2:D:32:MET:SD	2:D:75:PHE:HB2	2.56	0.45
2:D:122:VAL:HA	2:D:154:PRO:HD3	1.98	0.45
3:I:81:LEU:O	3:I:82:LEU:C	2.58	0.45
2:B:23:CYS:O	2:B:74:ASN:HB2	2.17	0.45
1:C:24:TYR:OH	1:C:66:PHE:HE2	2.00	0.45
3:H:228:MET:HG2	3:H:246:SER:O	2.16	0.45
3:I:51:TRP:CZ3	3:I:52:MET:HE3	2.50	0.45
3:I:194:ARG:HB3	3:I:198:LYS:O	2.16	0.45
4:L:41:LYS:O	4:L:42:ASN:C	2.59	0.45
1:C:34:TRP:CZ3	1:C:90:CYS:HB2	2.51	0.45
1:C:167:VAL:O	2:D:173:SER:HB2	2.17	0.45
1:A:70:ASN:OD1	1:A:70:ASN:N	2.49	0.45
1:A:85:SER:O	1:A:86:ALA:HB2	2.17	0.45
2:D:121:ASN:CG	2:D:153:PHE:CE2	2.93	0.45
3:I:157:ARG:O	3:I:161:GLU:N	2.36	0.45
2:D:45:LEU:O	2:D:59:ASP:HB3	2.17	0.45
2:D:148:LEU:HD12	2:D:148:LEU:N	2.32	0.45
3:H:220:ASN:ND2	3:H:220:ASN:O	2.46	0.45
3:H:254:GLU:C	3:H:256:TYR:H	2.24	0.45
3:I:14:ARG:HB3	3:I:17:LEU:HB2	1.98	0.45
4:M:25:CYS:C	4:M:65:LEU:HD12	2.41	0.45
4:M:40:LEU:N	4:M:40:LEU:CD1	2.80	0.45
1:A:136:GLN:HA	1:A:136:GLN:NE2	2.32	0.45
1:A:168:LEU:HD11	2:B:171:GLY:O	2.17	0.45
1:C:1:GLN:HE21	1:C:105:THR:CG2	2.23	0.45
3:H:111:ARG:HD3	3:H:128:GLU:OE1	2.17	0.45
2:B:176:PRO:HG2	2:B:177:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ARG:HA	2:B:207:ARG:HE	1.81	0.45
2:D:127:VAL:HG13	2:D:127:VAL:O	2.17	0.45
2:D:140:LYS:HG3	2:D:142:LYS:H	1.82	0.45
2:D:162:TRP:HE1	2:D:213:GLN:CB	2.29	0.45
3:I:114:GLN:O	3:I:115:GLN:HG3	2.17	0.45
3:H:14:ARG:O	3:H:17:LEU:HB2	2.17	0.44
3:I:191:HIS:HB2	3:I:274:TRP:CE2	2.52	0.44
4:L:56:PHE:HA	4:L:62:PHE:HA	1.98	0.44
4:M:23:LEU:O	4:M:39:MET:HE1	2.17	0.44
11:C:826:HOH:O	3:H:220:ASN:HA	2.16	0.44
2:D:13:ALA:CB	2:D:19:VAL:HG21	2.45	0.44
2:D:125:PRO:HG2	2:D:237:ILE:HB	1.99	0.44
3:H:12:VAL:HA	3:H:93:HIS:O	2.17	0.44
3:H:133:TRP:CH2	3:H:156:LEU:HD12	2.50	0.44
2:D:175:ASP:O	2:D:192:LEU:HD11	2.17	0.44
2:D:200:ALA:C	2:D:202:PHE:H	2.25	0.44
3:I:47:PRO:CB	3:I:52:MET:HB3	2.48	0.44
3:I:80:THR:HG22	3:I:84:TYR:CE2	2.53	0.44
3:I:108:ARG:HG3	3:I:108:ARG:HH11	1.82	0.44
3:I:166:GLU:HG2	11:I:999:HOH:O	2.17	0.44
1:A:190:THR:HG23	1:A:192:GLN:HG2	1.99	0.44
3:H:105:SER:O	3:I:264:GLN:HA	2.18	0.44
3:I:5:LEU:HB2	3:I:168:LEU:HB2	1.98	0.44
3:I:56:GLY:C	3:I:58:GLU:N	2.75	0.44
1:C:51:SER:OG	1:C:52:GLY:N	2.50	0.44
3:H:29:ASP:O	3:H:30:ASP:HB2	2.18	0.44
3:I:33:PHE:O	3:I:52:MET:HG3	2.18	0.44
4:M:38:GLN:HE21	4:M:81:ARG:HB3	1.83	0.44
4:M:51:MET:CE	4:M:64:ILE:CD1	2.95	0.44
2:B:202:PHE:O	2:B:208:ASN:ND2	2.39	0.44
4:M:28:THR:CA	11:M:281:HOH:O	2.66	0.44
5:P:2:GLN:NE2	5:P:2:GLN:HA	2.30	0.44
4:M:12:ARG:H	4:M:21:ASN:ND2	2.15	0.44
1:C:170:MET:CE	1:C:172:ALA:HB2	2.46	0.44
2:D:32:MET:C	2:D:33:TYR:CD1	2.95	0.44
4:L:21:ASN:N	4:L:70:PHE:O	2.47	0.44
4:M:44:LYS:O	4:M:44:LYS:CG	2.65	0.44
1:A:48:LYS:HD3	2:B:105:THR:HG23	2.00	0.44
1:A:160:THR:HG22	1:A:161:PHE:N	2.33	0.44
2:D:72:GLN:HE21	2:D:72:GLN:HB2	1.54	0.44
3:H:103:VAL:HG13	3:H:168:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:51:MET:CE	4:M:64:ILE:HD11	2.47	0.44
1:C:82:TRP:CZ2	1:C:167:VAL:HG21	2.52	0.43
1:C:114:VAL:HG13	1:C:114:VAL:O	2.17	0.43
4:M:59:ASP:O	4:M:60:TRP:CG	2.71	0.43
1:A:40:ARG:O	1:A:40:ARG:CD	2.66	0.43
1:A:205:THR:HG22	1:A:205:THR:O	2.16	0.43
1:C:128:LEU:HD12	2:D:130:PHE:HB2	2.00	0.43
2:B:33:TYR:CD1	2:B:33:TYR:N	2.86	0.43
2:D:6:GLN:CG	2:D:110:ALA:HB3	2.48	0.43
2:D:18:LYS:CG	2:D:80:GLU:HG3	2.42	0.43
2:D:34:TRP:CH2	2:D:92:CYS:HB3	2.52	0.43
3:I:129:ASP:OD2	3:I:132:THR:N	2.51	0.43
4:L:1:ILE:HB	4:L:2:GLN:H	1.52	0.43
4:M:19:LYS:HD3	11:M:469:HOH:O	2.18	0.43
4:M:53:ASP:HB3	4:M:54:MET:H	1.59	0.43
4:M:84:HIS:ND1	4:M:86:SER:CB	2.81	0.43
7:G:1:NAG:HO3	7:G:2:NAG:H61	1.84	0.43
1:A:32:LEU:CD1	1:A:66:PHE:HD2	2.31	0.43
2:B:55:THR:O	2:B:56:GLU:HG3	2.18	0.43
2:B:127:VAL:HG13	2:B:237:ILE:CG2	2.48	0.43
2:B:153:PHE:CB	2:B:154:PRO:CD	2.96	0.43
2:D:82:ALA:CB	2:D:116:VAL:HG11	2.48	0.43
2:D:219:LEU:HB2	2:D:231:LYS:HZ3	1.83	0.43
3:H:3:HIS:HB3	3:H:29:ASP:OD1	2.18	0.43
1:C:151:ASN:HD22	1:C:151:ASN:N	2.15	0.43
3:H:187:ALA:HA	3:H:204:TRP:O	2.18	0.43
1:C:24:TYR:OH	1:C:71:SER:HA	2.19	0.43
2:D:129:LEU:C	2:D:129:LEU:HD23	2.44	0.43
2:D:163:VAL:HB	2:D:168:VAL:HG13	2.01	0.43
2:D:164:ASN:HD22	2:D:164:ASN:H	1.66	0.43
2:D:205:ASN:ND2	2:D:207:ARG:O	2.51	0.43
3:H:213:ILE:HG12	3:H:214:THR:H	1.83	0.43
3:I:214:THR:HA	11:I:983:HOH:O	2.17	0.43
3:I:236:ALA:O	4:M:24:ASN:ND2	2.51	0.43
4:L:96:ASP:HB3	4:L:99:MET:HB2	2.01	0.43
2:D:121:ASN:O	2:D:153:PHE:CB	2.67	0.43
2:D:199:SER:HB2	2:D:202:PHE:HD2	1.83	0.43
3:H:255:GLN:OE1	3:H:273:ARG:HD3	2.19	0.43
3:I:13:SER:HB3	3:I:78:LEU:CD1	2.48	0.43
3:I:143:THR:HG21	5:Q:8:VAL:HB	1.99	0.43
3:I:176:ASN:OD1	3:I:176:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:5:PRO:HB3	4:L:30:PHE:HB3	2.01	0.43
2:D:118:ASP:O	2:D:121:ASN:ND2	2.51	0.43
2:D:244:ARG:HD2	2:D:244:ARG:H	1.82	0.43
3:I:127:ASN:N	3:I:127:ASN:ND2	2.67	0.43
3:I:213:ILE:HG12	3:I:214:THR:N	2.34	0.43
4:L:49:VAL:HG22	4:L:68:THR:HG21	2.00	0.43
7:F:2:NAG:H3	7:F:3:BMA:O5	2.15	0.43
1:C:117:TYR:CD1	1:C:118:ILE:N	2.87	0.43
3:I:143:THR:CG2	5:Q:8:VAL:HB	2.49	0.43
4:L:14:PRO:HA	4:L:15:PRO:HD2	1.81	0.43
4:L:80:CYS:O	4:L:92:THR:HA	2.18	0.43
4:M:54:MET:HE3	4:M:54:MET:HA	2.00	0.43
2:D:2:ALA:HA	2:D:26:THR:OG1	2.19	0.43
2:D:140:LYS:HD2	2:D:142:LYS:HB2	2.01	0.43
3:H:110:LEU:O	3:H:111:ARG:HG2	2.19	0.43
3:I:163:THR:O	3:I:166:GLU:HB2	2.18	0.43
3:I:190:THR:OG1	3:I:192:HIS:HE1	2.01	0.43
2:B:245:ALA:HA	11:B:880:HOH:O	2.19	0.43
2:D:66:LYS:O	2:D:78:ILE:N	2.52	0.43
3:I:159:TYR:CZ	5:Q:3:TYR:HB2	2.53	0.43
4:M:97:ARG:HG3	11:M:121:HOH:O	2.18	0.43
1:C:72:SER:HB3	1:C:74:HIS:CD2	2.54	0.42
1:C:149:GLN:HA	1:C:149:GLN:NE2	2.33	0.42
2:D:94:SER:O	2:D:106:LEU:HD22	2.18	0.42
3:H:128:GLU:HG3	11:H:841:HOH:O	2.19	0.42
3:H:194:ARG:CG	3:H:195:PRO:HD2	2.49	0.42
3:H:272:LEU:HD12	3:H:272:LEU:N	2.34	0.42
3:I:147:TRP:C	3:I:149:GLN:N	2.73	0.42
1:C:82:TRP:C	1:C:84:ASP:H	2.27	0.42
1:C:85:SER:OG	1:C:114:VAL:HG12	2.19	0.42
1:C:170:MET:HB3	1:C:175:SER:OG	2.19	0.42
2:D:30:ASN:O	2:D:51:GLY:N	2.52	0.42
3:H:12:VAL:HG11	4:L:33:PRO:HG3	2.01	0.42
3:H:116:TYR:HB2	3:H:124:ILE:HG22	2.00	0.42
3:I:199:VAL:HG23	3:I:200:THR:N	2.33	0.42
3:I:219:LEU:O	3:I:220:ASN:C	2.62	0.42
4:M:7:ILE:CB	4:M:93:VAL:HG21	2.43	0.42
2:D:61:PRO:CG	2:D:62:ASP:H	2.30	0.42
2:D:89:VAL:HG13	2:D:113:ARG:HB3	2.00	0.42
2:D:127:VAL:HG11	2:D:238:SER:CA	2.49	0.42
2:D:193:SER:C	2:D:195:ARG:HH21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:169:ARG:HE	3:I:268:GLU:HB3	1.84	0.42
3:H:220:ASN:HD22	3:H:220:ASN:C	2.25	0.42
3:I:25:VAL:HA	3:I:34:VAL:O	2.18	0.42
3:H:117:ALA:HB2	4:L:60:TRP:CE2	2.54	0.42
3:I:234:ARG:HD2	4:M:10:TYR:CE2	2.54	0.42
3:I:234:ARG:HD3	4:M:8:GLN:HE22	1.83	0.42
4:M:12:ARG:CB	11:M:272:HOH:O	2.68	0.42
1:C:59:VAL:O	1:C:62:PHE:CD1	2.72	0.42
2:B:65:TYR:CE2	2:B:79:LEU:HD21	2.54	0.42
2:B:137:ILE:HG21	2:B:204:HIS:NE2	2.35	0.42
2:D:18:LYS:HG3	2:D:80:GLU:CG	2.47	0.42
2:D:33:TYR:HB3	2:D:45:LEU:HD11	2.00	0.42
2:D:121:ASN:OD1	2:D:153:PHE:CD2	2.72	0.42
3:H:21:ARG:NE	3:H:23:MET:CE	2.82	0.42
3:I:156:LEU:O	3:I:157:ARG:C	2.62	0.42
4:M:17:ASN:OD1	4:M:73:THR:C	2.63	0.42
3:I:176:ASN:O	3:I:177:ALA:C	2.61	0.42
1:C:114:VAL:O	1:C:114:VAL:HG22	2.19	0.42
2:D:31:ASN:HB3	2:D:33:TYR:OH	2.20	0.42
2:D:88:SER:OG	2:D:89:VAL:N	2.51	0.42
2:D:193:SER:OG	2:D:195:ARG:NH2	2.52	0.42
3:H:21:ARG:HE	3:H:23:MET:CE	2.31	0.42
3:I:263:HIS:HD2	3:I:265:GLY:N	2.15	0.42
4:M:12:ARG:H	4:M:21:ASN:HD21	1.65	0.42
2:B:69:ARG:NH1	2:B:72:GLN:O	2.41	0.42
2:B:142:LYS:CG	11:B:906:HOH:O	2.67	0.42
3:H:6:ARG:HG2	3:H:113:TYR:OH	2.20	0.42
3:H:170:ARG:NH1	11:H:832:HOH:O	2.53	0.42
3:I:33:PHE:C	3:I:48:ARG:HB2	2.44	0.42
3:I:80:THR:HG22	3:I:84:TYR:CZ	2.55	0.42
3:I:81:LEU:O	3:I:84:TYR:HB2	2.20	0.42
1:A:203:ASN:HB3	1:A:204:ALA:H	1.59	0.42
1:C:133:PRO:HB2	1:C:134:ARG:NH1	2.35	0.42
1:C:155:THR:HG21	1:C:160:THR:O	2.19	0.42
2:B:41:HIS:O	2:B:42:GLY:C	2.59	0.42
2:D:235:GLN:OE1	2:D:237:ILE:HD11	2.19	0.42
3:H:192:HIS:HB2	3:H:200:THR:HB	2.02	0.42
3:H:215:LEU:CD2	3:H:261:VAL:HG13	2.50	0.42
3:H:218:GLN:CD	3:H:260:HIS:CE1	2.98	0.42
4:L:36:GLU:HB3	4:L:83:LYS:HB3	2.02	0.42
1:A:55:VAL:O	1:A:55:VAL:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ALA:HB1	11:C:829:HOH:O	2.20	0.42
1:C:144:THR:HA	1:C:178:ASN:O	2.19	0.42
2:D:6:GLN:NE2	2:D:112:THR:HG23	2.35	0.42
2:D:121:ASN:O	2:D:153:PHE:HB2	2.20	0.42
2:D:182:SER:HB2	2:D:189:SER:HB2	2.02	0.42
2:D:219:LEU:HD13	2:D:223:ASP:OD1	2.20	0.42
3:I:118:TYR:C	3:I:120:GLY:N	2.78	0.42
4:L:7:ILE:HD11	4:L:82:VAL:HG22	2.02	0.42
1:A:11:THR:HA	1:A:113:ILE:O	2.20	0.41
1:C:106:PHE:CE1	2:D:43:LEU:HD23	2.55	0.41
2:B:2:ALA:HB2	11:H:871:HOH:O	2.19	0.41
3:H:230:LEU:HD23	3:H:230:LEU:O	2.19	0.41
3:I:48:ARG:HA	3:I:48:ARG:HH11	1.85	0.41
3:I:230:LEU:HG	3:I:243:LYS:HE3	2.02	0.41
4:M:31:HIS:HA	4:M:32:PRO:C	2.45	0.41
1:A:123:PRO:HG2	1:A:203:ASN:HB2	2.02	0.41
1:A:191:CYS:HA	1:A:194:ILE:CG2	2.48	0.41
1:C:1:GLN:HG3	1:C:105:THR:HG21	2.02	0.41
1:C:118:ILE:C	1:C:118:ILE:HD12	2.45	0.41
2:B:27:ASN:CB	2:B:29:HIS:ND1	2.81	0.41
2:B:83:THR:C	2:B:116:VAL:HG11	2.45	0.41
2:D:152:PHE:HD2	2:D:154:PRO:HD2	1.84	0.41
3:I:25:VAL:HG12	3:I:35:ARG:NE	2.35	0.41
3:I:234:ARG:HD3	4:M:8:GLN:NE2	2.34	0.41
4:M:21:ASN:N	4:M:70:PHE:O	2.48	0.41
1:C:161:PHE:O	1:C:162:ILE:HD13	2.21	0.41
2:D:68:SER:C	2:D:70:PRO:HD3	2.41	0.41
2:D:154:PRO:C	2:D:156:HIS:H	2.28	0.41
3:H:36:PHE:HB2	3:H:45:TYR:CD1	2.55	0.41
3:I:25:VAL:HG23	3:I:25:VAL:O	2.21	0.41
1:A:188:SER:O	1:A:189:PHE:CB	2.68	0.41
1:C:8:ALA:O	1:C:9:ARG:HB3	2.20	0.41
2:D:162:TRP:O	2:D:211:ARG:HB2	2.20	0.41
3:I:190:THR:OG1	3:I:202:ARG:HB3	2.21	0.41
1:A:40:ARG:HD2	1:A:40:ARG:O	2.20	0.41
1:A:140:LEU:HD23	1:A:140:LEU:C	2.45	0.41
1:A:191:CYS:O	1:A:194:ILE:HG22	2.21	0.41
2:D:74:ASN:HD22	2:D:74:ASN:HA	1.58	0.41
2:D:162:TRP:HB2	2:D:211:ARG:HB2	2.02	0.41
3:H:214:THR:HB	3:H:262:TYR:HB2	2.01	0.41
3:H:218:GLN:HB2	3:H:258:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:33:PHE:HA	3:I:48:ARG:HB2	2.03	0.41
3:I:76:VAL:O	3:I:77:SER:C	2.63	0.41
2:D:120:ARG:HB2	2:D:120:ARG:CZ	2.51	0.41
2:D:199:SER:O	2:D:202:PHE:HB2	2.21	0.41
3:I:8:PHE:CD1	3:I:27:TYR:CD1	3.04	0.41
3:I:45:TYR:HB3	3:I:60:TRP:HE3	1.85	0.41
4:M:84:HIS:ND1	4:M:86:SER:HB3	2.35	0.41
1:A:186:GLN:O	1:A:187:THR:C	2.63	0.41
1:C:77:LYS:HD2	1:C:78:ALA:N	2.33	0.41
1:C:144:THR:O	1:C:145:ASP:HB2	2.21	0.41
2:B:1:GLU:O	2:B:2:ALA:C	2.64	0.41
2:D:154:PRO:HG2	2:D:216:PHE:CZ	2.56	0.41
2:D:198:VAL:HG21	2:D:203:TRP:CB	2.50	0.41
3:H:4:SER:HA	3:H:101:CYS:O	2.21	0.41
4:M:40:LEU:N	4:M:40:LEU:HD12	2.35	0.41
2:B:152:PHE:CE1	2:B:190:TYR:CB	3.04	0.41
2:D:120:ARG:NH1	2:D:120:ARG:CB	2.84	0.41
3:I:96:GLN:OE1	4:M:56:PHE:CD1	2.74	0.41
4:L:46:ILE:HG23	4:L:47:PRO:HD2	2.03	0.41
4:M:28:THR:CB	11:M:281:HOH:O	2.65	0.41
1:A:186:GLN:HG2	11:A:976:HOH:O	2.21	0.41
2:D:137:ILE:HG13	2:D:204:HIS:NE2	2.36	0.41
2:D:153:PHE:H	2:D:154:PRO:CD	2.34	0.41
2:D:177:GLN:OE1	2:D:177:GLN:HA	2.20	0.41
3:H:176:ASN:OD1	3:H:177:ALA:N	2.54	0.41
3:H:249:VAL:HG12	3:H:257:TYR:CE2	2.55	0.41
3:H:271:THR:O	3:H:271:THR:CG2	2.69	0.41
3:I:78:LEU:O	3:I:82:LEU:HG	2.21	0.41
3:I:124:ILE:HD12	3:I:135:ALA:HB2	2.01	0.41
3:I:194:ARG:NH1	3:I:248:VAL:CG2	2.83	0.41
3:I:222:GLU:HG3	3:I:223:GLU:N	2.35	0.41
3:I:262:TYR:CD1	3:I:269:PRO:HB3	2.56	0.41
4:M:8:GLN:HG2	11:M:426:HOH:O	2.19	0.41
1:C:14:GLU:HA	1:C:114:VAL:CG2	2.50	0.41
1:C:57:GLN:HE22	3:H:256:TYR:HD1	1.65	0.41
1:C:196:LYS:NZ	1:C:196:LYS:CB	2.84	0.41
2:B:6:GLN:OE1	2:B:91:PHE:HA	2.20	0.41
2:B:88:SER:OG	2:B:89:VAL:N	2.54	0.41
2:B:211:ARG:NH1	11:B:869:HOH:O	2.43	0.41
3:H:71:GLU:OE2	3:H:75:ARG:NH2	2.53	0.41
3:H:201:LEU:HD11	3:H:254:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:156:LEU:HD23	3:I:156:LEU:HA	1.94	0.41
3:I:194:ARG:CG	3:I:195:PRO:CD	2.97	0.41
4:L:82:VAL:CG2	4:L:87:MET:HE1	2.49	0.41
1:A:188:SER:HB3	1:A:189:PHE:H	1.70	0.40
1:C:142:LEU:HD11	2:D:144:THR:CB	2.46	0.40
2:B:30:ASN:HB2	5:P:6:TYR:CE1	2.56	0.40
2:B:139:ASN:HD22	2:B:140:LYS:HG3	1.86	0.40
2:B:153:PHE:HB3	2:B:154:PRO:HD2	2.03	0.40
2:D:146:VAL:CG2	2:D:147:CYS:N	2.84	0.40
3:I:94:THR:CG2	3:I:95:ILE:H	2.33	0.40
4:M:51:MET:HE3	4:M:64:ILE:CG1	2.51	0.40
5:Q:2:GLN:HG3	5:Q:3:TYR:N	2.36	0.40
1:A:192:GLN:HG3	1:A:193:ASP:N	2.35	0.40
1:C:32:LEU:HD13	1:C:73:PHE:CD1	2.56	0.40
1:C:109:GLY:O	1:C:110:THR:HB	2.21	0.40
2:B:60:ILE:HG13	2:B:60:ILE:O	2.21	0.40
2:D:54:SER:H	2:D:69:ARG:CB	2.34	0.40
3:I:75:ARG:NH1	11:I:951:HOH:O	2.53	0.40
4:L:59:ASP:O	4:L:60:TRP:HB2	2.22	0.40
1:C:19:GLN:HE22	1:C:74:HIS:HB3	1.86	0.40
1:C:128:LEU:CD2	1:C:140:LEU:HG	2.49	0.40
3:H:102:GLU:HG3	3:H:113:TYR:HE2	1.85	0.40
3:I:36:PHE:HB2	3:I:45:TYR:HA	2.03	0.40
3:I:201:LEU:O	3:I:246:SER:CB	2.69	0.40
1:A:206:TYR:CB	2:B:135:ALA:HB1	2.50	0.40
1:C:82:TRP:HH2	1:C:167:VAL:HG21	1.83	0.40
2:B:6:GLN:HG2	2:B:92:CYS:SG	2.61	0.40
2:D:33:TYR:CD2	2:D:48:TYR:CB	3.05	0.40
2:D:36:ARG:O	2:D:36:ARG:HG2	2.20	0.40
2:D:205:ASN:O	2:D:207:ARG:N	2.54	0.40
3:H:141:LEU:O	3:H:145:HIS:CD2	2.75	0.40
3:H:185:PRO:HA	3:H:206:LEU:O	2.22	0.40
3:H:187:ALA:O	3:H:188:HIS:HB3	2.21	0.40
4:L:17:ASN:OD1	4:L:73:THR:O	2.39	0.40
1:A:81:HIS:O	1:A:114:VAL:HG11	2.21	0.40
1:C:140:LEU:N	1:C:140:LEU:HD23	2.36	0.40
2:B:142:LYS:HG2	11:B:906:HOH:O	2.21	0.40
2:D:34:TRP:CZ3	2:D:92:CYS:HB3	2.57	0.40
3:H:133:TRP:O	3:H:144:LYS:NZ	2.46	0.40
3:H:230:LEU:HD23	3:H:230:LEU:H	1.87	0.40
3:I:132:THR:HG22	3:I:133:TRP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:SER:CB	11:B:859:HOH:O[4_555]	1.98	0.22

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	200/202 (99%)	169 (84%)	24 (12%)	7 (4%)	3	2
1	C	200/202 (99%)	134 (67%)	43 (22%)	23 (12%)	0	0
2	B	235/237 (99%)	214 (91%)	17 (7%)	4 (2%)	7	10
2	D	235/237 (99%)	154 (66%)	62 (26%)	19 (8%)	1	0
3	H	272/275 (99%)	246 (90%)	23 (8%)	3 (1%)	11	18
3	I	272/275 (99%)	226 (83%)	34 (12%)	12 (4%)	2	1
4	L	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
4	M	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	0	0
5	P	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
5	Q	6/8 (75%)	5 (83%)	0	1 (17%)	0	0
All	All	1620/1642 (99%)	1319 (81%)	223 (14%)	78 (5%)	2	1

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	PRO
1	A	140	LEU
1	C	7	ASP
2	B	153	PHE
2	B	226	PRO
2	D	13	ALA
2	D	75	PHE

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Mol	Chain	Res	Type
2	D	172	VAL
3	H	226	GLN
3	I	89	ALA
4	M	41	LYS
1	C	50	TYR
1	C	73	PHE
1	C	82	TRP
1	C	83	SER
1	C	174	ASP
1	C	190	THR
1	C	203	ASN
2	D	61	PRO
2	D	71	SER
2	D	149	ALA
2	D	199	SER
2	D	215	GLN
4	M	60	TRP
5	P	7	SER
5	Q	7	SER
1	C	101	ALA
1	C	144	THR
1	C	154	LYS
1	C	158	SER
1	C	159	GLY
1	C	209	SER
2	D	16	GLY
2	D	121	ASN
2	D	155	ASP
3	I	139	ALA
3	I	153	ALA
3	I	164	CYS
3	I	176	ASN
3	I	222	GLU
4	M	47	PRO
4	M	50	GLU
4	M	57	SER
1	A	69	SER
1	A	203	ASN
1	C	110	THR
1	C	137	ASP
1	C	187	THR
2	B	155	ASP

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Mol	Chain	Res	Type
2	D	110	ALA
2	D	138	ALA
2	D	206	PRO
2	D	233	VAL
3	I	55	GLU
3	I	82	LEU
3	I	148	GLU
4	M	40	LEU
1	A	198	THR
1	C	86	ALA
1	C	173	MET
1	C	192	GLN
2	D	153	PHE
3	H	227	ASP
3	H	255	GLN
3	I	38	SER
3	I	119	ASP
4	M	31	HIS
4	M	90	PRO
1	A	123	PRO
1	A	189	PHE
1	C	80	VAL
1	C	99	GLY
2	D	98	GLY
2	B	176	PRO
2	D	109	GLY
3	I	43	PRO
1	C	125	VAL
2	D	232	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/176 (100%)	163 (93%)	13 (7%)	13	22
1	C	176/176 (100%)	160 (91%)	16 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	200/200 (100%)	190 (95%)	10 (5%)	22	38
2	D	200/200 (100%)	187 (94%)	13 (6%)	15	27
3	H	231/232 (100%)	217 (94%)	14 (6%)	17	30
3	I	230/232 (99%)	211 (92%)	19 (8%)	10	17
4	L	94/94 (100%)	86 (92%)	8 (8%)	10	16
4	M	94/94 (100%)	86 (92%)	8 (8%)	10	16
5	P	8/8 (100%)	7 (88%)	1 (12%)	4	6
5	Q	8/8 (100%)	6 (75%)	2 (25%)	0	1
All	All	1417/1420 (100%)	1313 (93%)	104 (7%)	13	22

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	30	PRO
1	A	39	PRO
1	A	56	VAL
1	A	70	ASN
1	A	114	VAL
1	A	129	LYS
1	A	155	THR
1	A	156	MET
1	A	157	GLU
1	A	161	PHE
1	A	193	ASP
1	A	203	ASN
1	C	9	ARG
1	C	19	GLN
1	C	20	LEU
1	C	30	PRO
1	C	62	PHE
1	C	71	SER
1	C	100	PHE
1	C	102	SER
1	C	120	ASN
1	C	128	LEU
1	C	139	THR
1	C	141	CYS
1	C	142	LEU

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Mol	Chain	Res	Type
1	C	151	ASN
1	C	168	LEU
1	C	196	LYS
2	B	25	GLN
2	B	49	SER
2	B	127	VAL
2	B	139	ASN
2	B	146	VAL
2	B	150	ARG
2	B	159	LEU
2	B	219	LEU
2	B	242	TRP
2	B	244	ARG
2	D	38	ASP
2	D	72	GLN
2	D	74	ASN
2	D	78	ILE
2	D	79	LEU
2	D	86	GLN
2	D	106	LEU
2	D	145	LEU
2	D	152	PHE
2	D	162	TRP
2	D	177	GLN
2	D	242	TRP
2	D	244	ARG
3	H	5	LEU
3	H	12	VAL
3	H	19	GLU
3	H	45	TYR
3	H	46	GLU
3	H	97	VAL
3	H	99	SER
3	H	103	VAL
3	H	111	ARG
3	H	156	LEU
3	H	170	ARG
3	H	212	ASP
3	H	220	ASN
3	H	227	ASP
3	I	39	ASP
3	I	45	TYR

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Mol	Chain	Res	Type
3	I	48	ARG
3	I	50	ARG
3	I	52	MET
3	I	70	ASN
3	I	88	SER
3	I	95	ILE
3	I	99	SER
3	I	113	TYR
3	I	114	GLN
3	I	138	MET
3	I	172	LEU
3	I	199	VAL
3	I	229	GLU
3	I	231	VAL
3	I	251	LEU
3	I	255	GLN
3	I	272	LEU
4	L	1	ILE
4	L	4	THR
4	L	12	ARG
4	L	23	LEU
4	L	50	GLU
4	L	70	PHE
4	L	92	THR
4	L	97	ARG
4	M	7	ILE
4	M	35	ILE
4	M	40	LEU
4	M	53	ASP
4	M	70	PHE
4	M	73	THR
4	M	74	GLU
4	M	87	MET
5	P	2	GLN
5	Q	2	GLN
5	Q	8	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	120	ASN

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Mol	Chain	Res	Type
1	A	136	GLN
1	A	185	ASN
1	A	186	GLN
1	A	203	ASN
1	C	19	GLN
1	C	74	HIS
1	C	149	GLN
1	C	151	ASN
1	C	203	ASN
2	B	30	ASN
2	B	31	ASN
2	B	37	GLN
2	B	47	HIS
2	B	72	GLN
2	B	121	ASN
2	B	139	ASN
2	B	236	ASN
2	D	6	GLN
2	D	10	ASN
2	D	25	GLN
2	D	37	GLN
2	D	74	ASN
2	D	86	GLN
2	D	139	ASN
2	D	164	ASN
2	D	186	ASN
2	D	215	GLN
2	D	235	GLN
3	H	54	GLN
3	H	115	GLN
3	H	127	ASN
3	H	145	HIS
3	H	174	ASN
3	H	188	HIS
3	H	218	GLN
3	H	220	ASN
3	H	226	GLN
3	H	263	HIS
3	I	42	ASN
3	I	54	GLN
3	I	70	ASN
3	I	72	GLN

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Mol	Chain	Res	Type
3	I	86	ASN
3	I	87	GLN
3	I	96	GLN
3	I	114	GLN
3	I	127	ASN
3	I	145	HIS
3	I	149	GLN
3	I	192	HIS
3	I	218	GLN
3	I	255	GLN
3	I	263	HIS
3	I	264	GLN
4	L	13	HIS
4	L	29	GLN
4	M	8	GLN
4	M	13	HIS
4	M	21	ASN
4	M	29	GLN
4	M	38	GLN
5	P	2	GLN
5	Q	2	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

13 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
6	NAG	E	1	1,6	14,14,15	1.07	0	17,19,21	1.81	2 (11%)
6	NAG	E	2	6	14,14,15	1.07	2 (14%)	17,19,21	1.84	5 (29%)
7	NAG	F	1	1,7	14,14,15	0.91	0	17,19,21	1.37	1 (5%)
7	NAG	F	2	7	14,14,15	0.61	0	17,19,21	1.16	1 (5%)
7	BMA	F	3	7	11,11,12	1.53	3 (27%)	15,15,17	2.64	6 (40%)
7	NAG	G	1	1,7	14,14,15	1.08	1 (7%)	17,19,21	1.62	3 (17%)
7	NAG	G	2	7	14,14,15	1.11	2 (14%)	17,19,21	2.29	4 (23%)
7	BMA	G	3	7	11,11,12	1.18	1 (9%)	15,15,17	0.96	0
7	NAG	J	1	7,2	14,14,15	1.00	0	17,19,21	1.67	3 (17%)
7	NAG	J	2	7	14,14,15	1.12	2 (14%)	17,19,21	2.17	5 (29%)
7	BMA	J	3	7	11,11,12	0.75	1 (9%)	15,15,17	1.52	3 (20%)
6	NAG	K	1	3,6	14,14,15	1.06	0	17,19,21	1.90	1 (5%)
6	NAG	K	2	6	14,14,15	0.61	0	17,19,21	1.06	2 (11%)

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
6	NAG	E	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	2	7	-	0/6/23/26	0/1/1/1
7	BMA	F	3	7	-	2/2/19/22	0/1/1/1
7	NAG	G	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	2/2/19/22	0/1/1/1
7	NAG	J	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3	BMA	O5-C5	-3.58	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	3	BMA	O5-C1	-3.13	1.38	1.43
7	J	2	NAG	O5-C1	-2.73	1.39	1.43
7	G	2	NAG	O5-C1	-2.63	1.39	1.43
6	E	2	NAG	O5-C1	-2.61	1.39	1.43
7	G	2	NAG	C1-C2	-2.37	1.49	1.52
7	J	2	NAG	O4-C4	-2.35	1.37	1.43
7	G	1	NAG	C2-N2	-2.19	1.42	1.46
7	F	3	BMA	O5-C1	-2.18	1.40	1.43
7	F	3	BMA	O2-C2	-2.09	1.38	1.43
6	E	2	NAG	C1-C2	2.09	1.55	1.52
7	J	3	BMA	O5-C1	-2.06	1.40	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	O5-C1-C2	-7.05	100.38	111.29
7	G	2	NAG	O5-C1-C2	-7.04	100.39	111.29
7	F	3	BMA	C1-O5-C5	6.83	121.34	112.19
6	E	1	NAG	O5-C1-C2	-6.22	101.67	111.29
7	J	2	NAG	O5-C1-C2	5.54	119.86	111.29
7	J	1	NAG	O5-C1-C2	-5.06	103.46	111.29
7	F	3	BMA	O2-C2-C3	4.86	120.22	110.15
7	G	1	NAG	O5-C1-C2	-4.68	104.05	111.29
7	F	1	NAG	O5-C1-C2	-4.62	104.14	111.29
7	J	2	NAG	O5-C5-C4	4.55	121.89	110.83
7	F	3	BMA	O2-C2-C1	-3.94	100.19	109.22
7	G	2	NAG	O6-C6-C5	-3.93	97.95	111.33
7	J	2	NAG	O4-C4-C3	-3.84	101.33	110.38
6	E	2	NAG	O5-C1-C2	3.66	116.95	111.29
7	J	1	NAG	O4-C4-C5	-3.44	100.86	109.32
7	J	3	BMA	O5-C1-C2	-3.40	102.67	110.79
6	E	2	NAG	O5-C5-C4	3.21	118.64	110.83
6	E	1	NAG	O4-C4-C3	3.15	117.79	110.38
7	J	3	BMA	C1-C2-C3	3.05	114.08	109.64
6	E	2	NAG	C1-C2-N2	3.05	115.23	110.43
7	G	2	NAG	O4-C4-C3	-3.00	103.30	110.38
6	E	2	NAG	C1-O5-C5	2.99	116.19	112.19
7	G	1	NAG	C3-C4-C5	2.81	115.32	110.23
7	G	2	NAG	O5-C5-C6	-2.67	102.47	107.66
7	J	2	NAG	O5-C5-C6	-2.48	102.83	107.66
7	F	2	NAG	O5-C1-C2	-2.46	107.49	111.29
7	G	1	NAG	C4-C3-C2	-2.29	107.66	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2	NAG	O5-C5-C6	-2.27	103.25	107.66
7	F	3	BMA	C1-C2-C3	2.25	112.92	109.64
7	F	3	BMA	O4-C4-C5	-2.15	104.04	109.32
6	K	2	NAG	O5-C1-C2	-2.14	107.97	111.29
7	F	3	BMA	O5-C1-C2	-2.14	105.69	110.79
7	J	3	BMA	C6-C5-C4	-2.09	107.89	113.02
7	J	2	NAG	C1-C2-N2	2.02	113.62	110.43
7	J	1	NAG	O4-C4-C3	2.02	115.13	110.38
6	K	2	NAG	C4-C3-C2	-2.01	108.06	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	K	1	NAG	C1

All (8) torsion outliers are listed below:

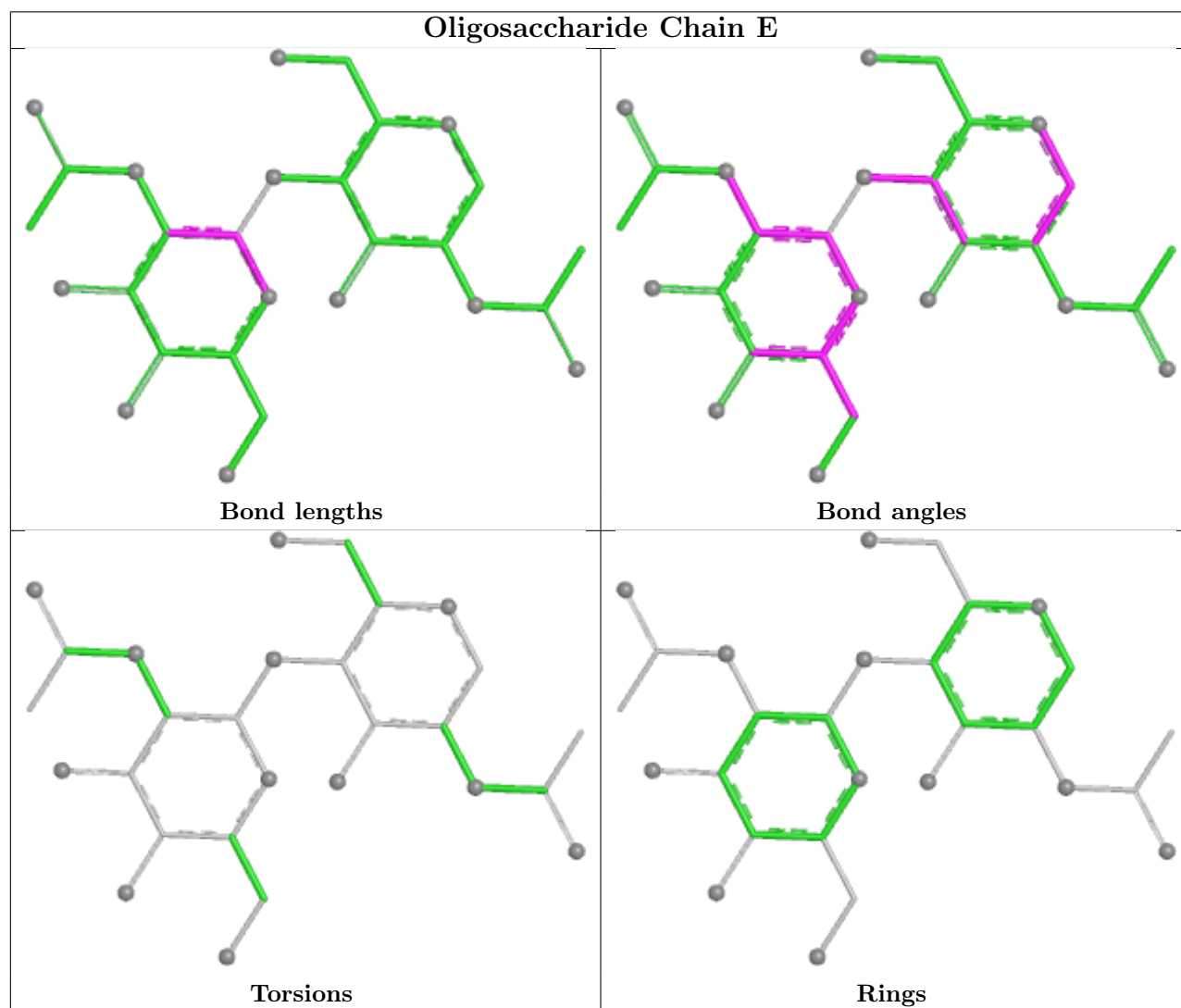
Mol	Chain	Res	Type	Atoms
7	G	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
7	G	3	BMA	O5-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	G	3	BMA	C4-C5-C6-O6
7	F	3	BMA	O5-C5-C6-O6
7	F	3	BMA	C4-C5-C6-O6

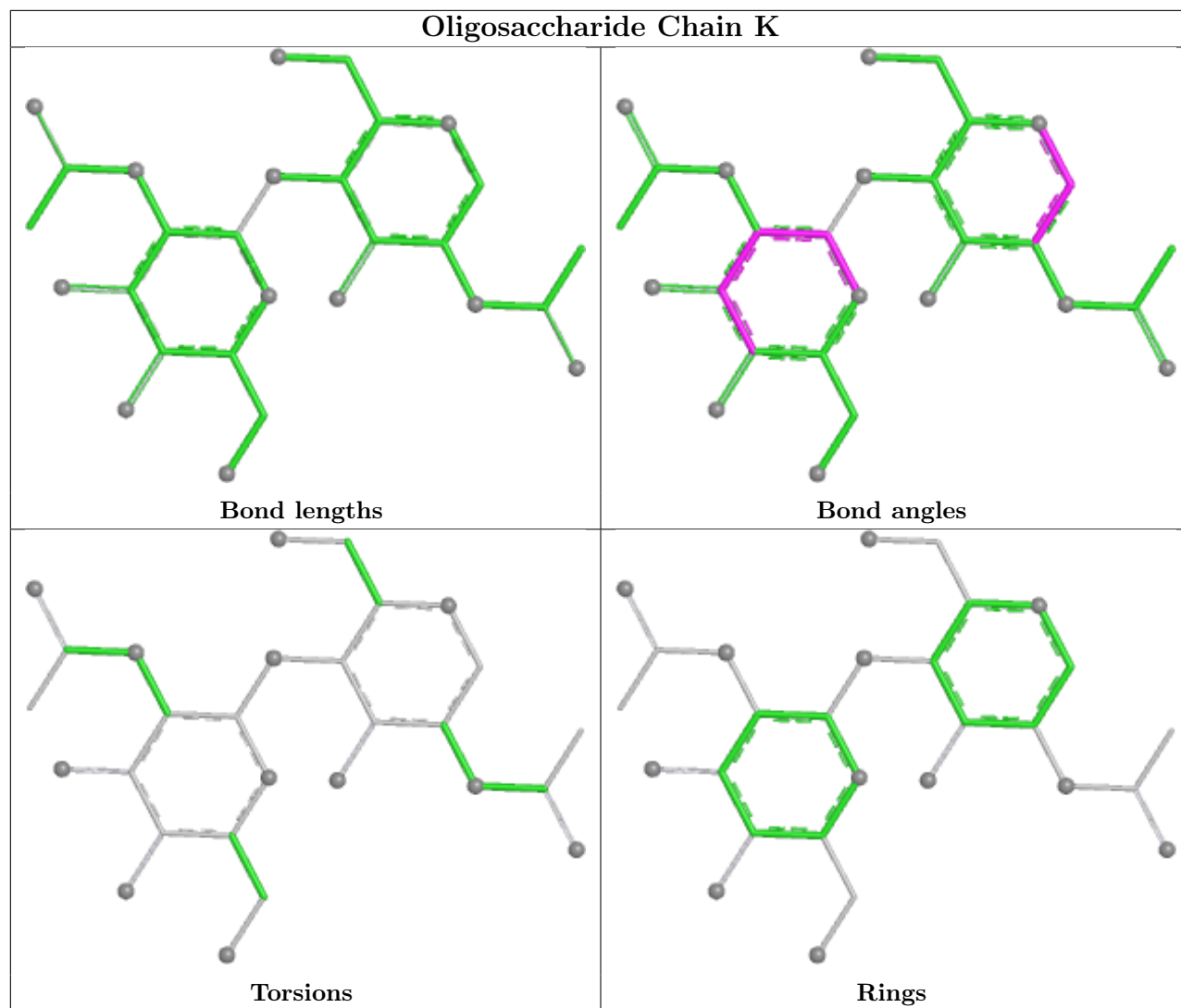
There are no ring outliers.

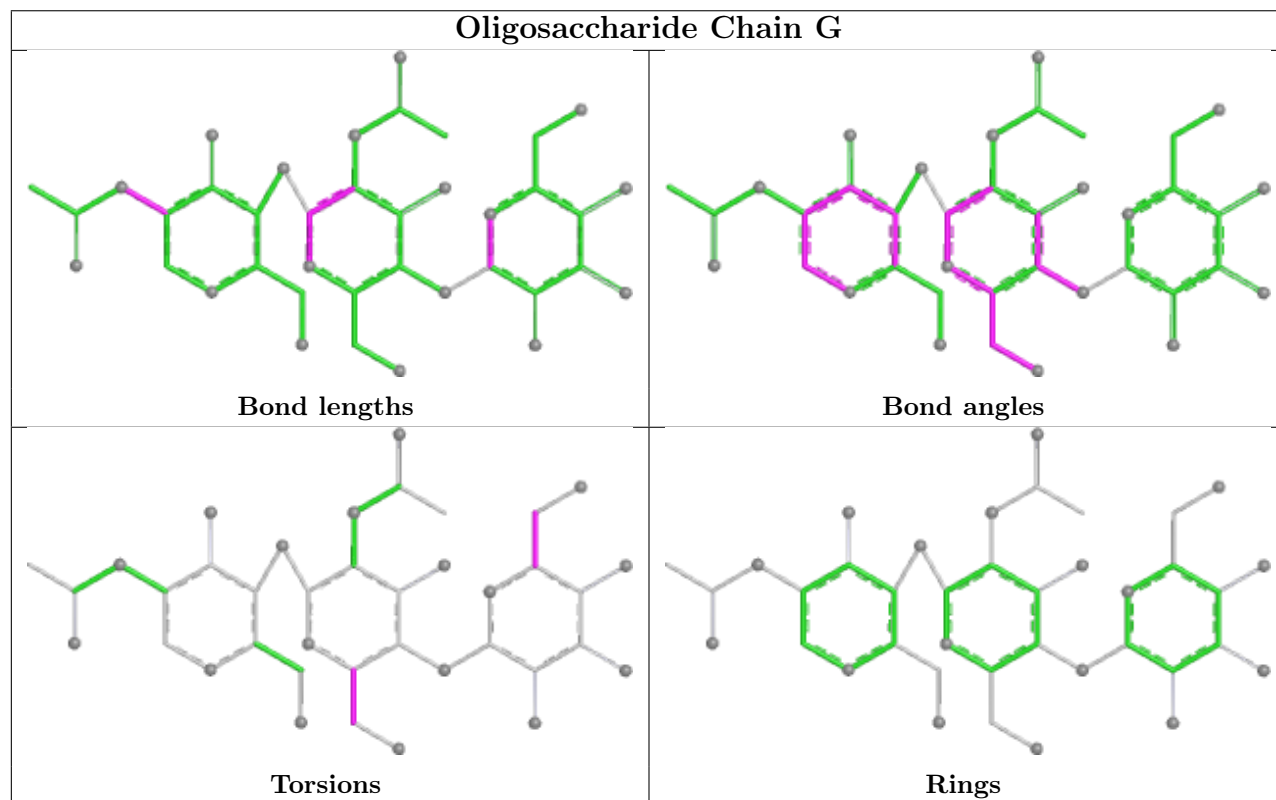
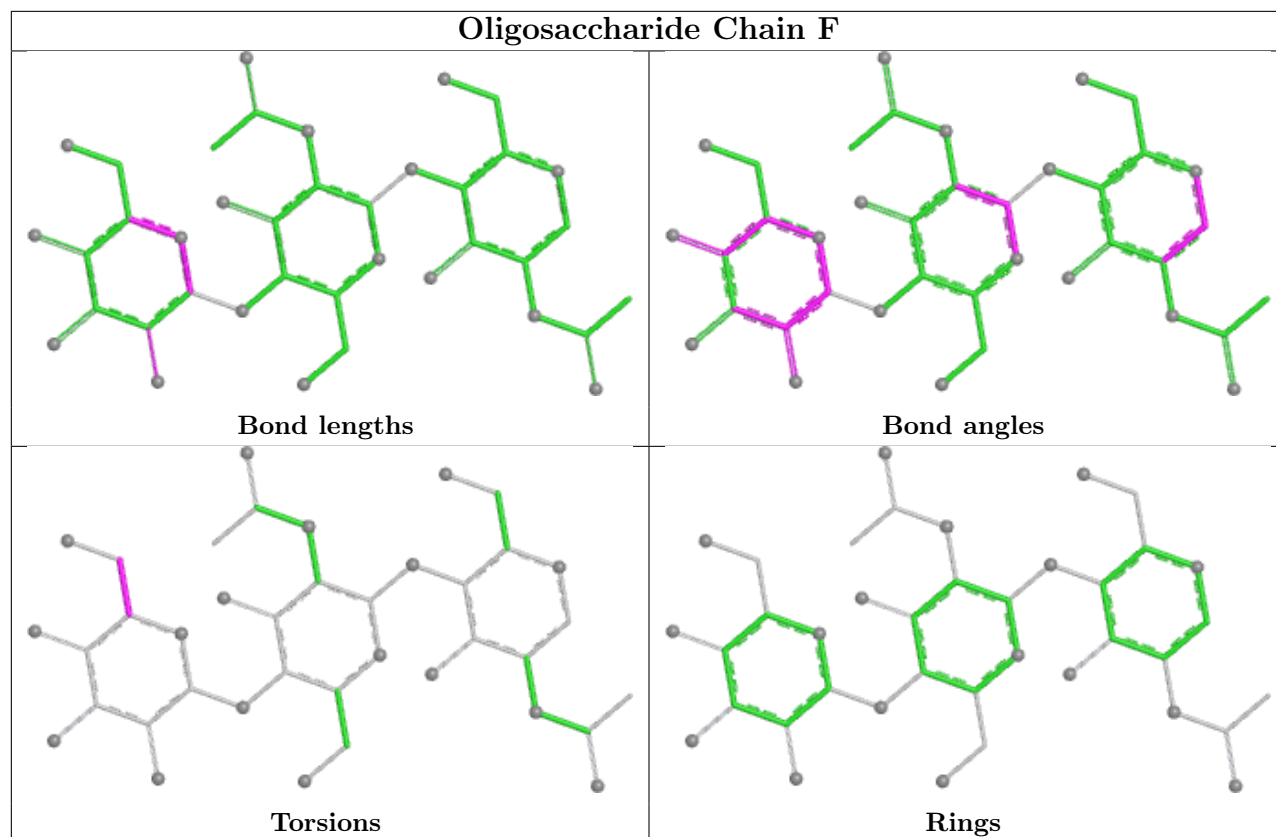
11 monomers are involved in 38 short contacts:

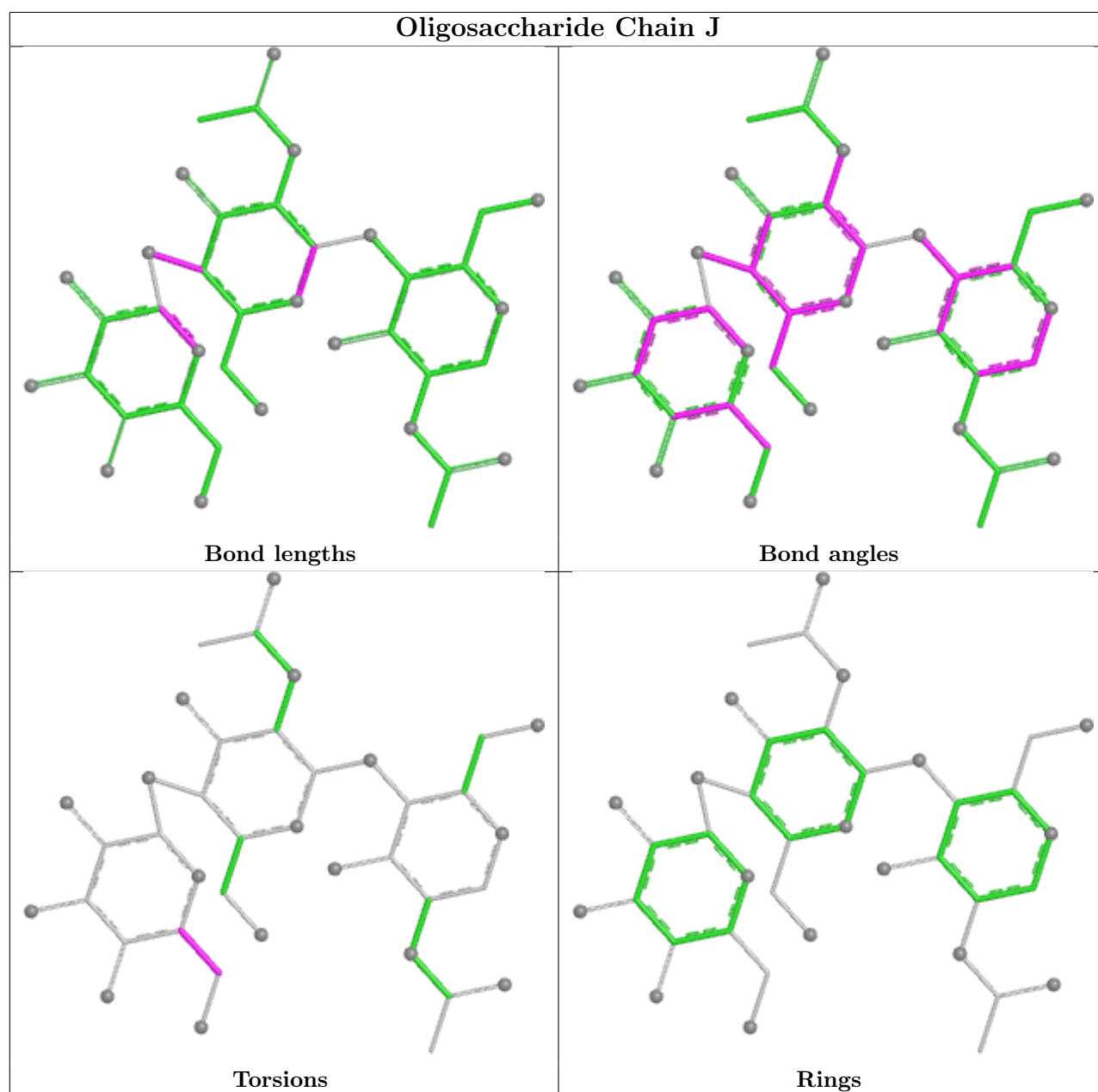
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	3	BMA	4	0
6	E	1	NAG	1	0
7	G	1	NAG	4	0
7	G	2	NAG	3	0
7	J	1	NAG	8	0
6	K	2	NAG	5	0
7	F	1	NAG	11	0
6	K	1	NAG	2	0
7	F	2	NAG	5	0
7	J	3	BMA	5	0
7	J	2	NAG	5	0

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](#)

5 ligands 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
8	GOL	A	902	-	5,5,5	0.29	0	5,5,5	0.77	0
10	ACY	P	1001	-	3,3,3	0.86	0	3,3,3	1.12	0
8	GOL	I	903	-	5,5,5	0.70	0	5,5,5	0.84	0
8	GOL	L	901	-	5,5,5	0.36	0	5,5,5	0.75	0
9	NAG	B	808	2	14,14,15	0.92	1 (7%)	17,19,21	1.73	1 (5%)

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
8	GOL	A	902	-	-	2/4/4/4	-
8	GOL	I	903	-	-	2/4/4/4	-
8	GOL	L	901	-	-	2/4/4/4	-
9	NAG	B	808	2	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	808	NAG	C2-N2	-2.20	1.42	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	808	NAG	O5-C1-C2	-5.98	102.03	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	B	808	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	902	GOL	C1-C2-C3-O3
8	I	903	GOL	C1-C2-C3-O3
8	L	901	GOL	C1-C2-C3-O3
8	A	902	GOL	O2-C2-C3-O3
8	I	903	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
8	L	901	GOL	O2-C2-C3-O3

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	202/202 (100%)	0.23	13 (6%) 25 22	4, 25, 74, 98	0
1	C	202/202 (100%)	2.32	121 (59%) 0 0	52, 82, 127, 136	0
2	B	237/237 (100%)	0.03	3 (1%) 75 71	14, 27, 47, 74	0
2	D	237/237 (100%)	2.71	167 (70%) 0 0	59, 113, 124, 141	0
3	H	274/275 (99%)	-0.14	1 (0%) 88 86	7, 23, 43, 54	0
3	I	274/275 (99%)	0.93	42 (15%) 5 4	15, 47, 70, 77	0
4	L	99/99 (100%)	-0.25	0 100 100	9, 21, 36, 44	0
4	M	99/99 (100%)	0.89	10 (10%) 12 9	32, 47, 61, 65	0
5	P	8/8 (100%)	-0.47	0 100 100	10, 14, 19, 19	0
5	Q	8/8 (100%)	3.50	8 (100%) 0 0	81, 84, 89, 91	0
All	All	1640/1642 (99%)	0.89	365 (22%) 2 2	4, 39, 122, 141	0

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	145	LEU	8.1
1	C	211	VAL	7.1
2	D	214	VAL	6.8
2	D	219	LEU	6.3
2	D	233	VAL	6.0
5	Q	8	VAL	6.0
2	D	218	GLY	5.8
2	D	196	LEU	5.7
2	D	137	ILE	5.4
3	I	123	TYR	5.4
2	D	4	VAL	5.3
2	D	161	TRP	5.2
2	D	14	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
2	D	93	ALA	5.0
2	D	97	GLY	5.0
2	D	91	PHE	4.9
1	C	146	PHE	4.9
1	C	176	LYS	4.8
2	D	128	SER	4.8
2	D	127	VAL	4.8
2	B	2	ALA	4.8
2	D	237	ILE	4.7
1	C	91	ALA	4.7
2	D	241	ALA	4.7
2	D	98	GLY	4.7
2	D	129	LEU	4.6
2	D	154	PRO	4.5
2	D	77	LEU	4.5
1	C	114	VAL	4.5
2	D	143	ALA	4.5
2	D	178	ALA	4.5
2	D	13	ALA	4.5
2	D	203	TRP	4.4
2	D	151	GLY	4.4
2	D	163	VAL	4.3
1	C	161	PHE	4.3
2	D	75	PHE	4.3
2	D	146	VAL	4.2
1	C	125	VAL	4.2
1	C	121	PRO	4.2
2	D	153	PHE	4.2
2	D	132	PRO	4.1
2	D	316	LEU	4.1
2	D	22	SER	4.0
2	D	234	THR	4.0
2	D	119	LEU	4.0
2	D	122	VAL	4.0
2	D	193	SER	4.0
2	D	210	PHE	4.0
2	D	144	THR	4.0
2	D	182	SER	3.9
5	Q	3	TYR	3.9
1	C	181	ILE	3.9
1	C	38	TYR	3.9
1	C	8	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	21	LEU	3.9
2	D	159	LEU	3.9
2	D	92	CYS	3.9
2	D	165	GLY	3.8
1	C	184	SER	3.8
5	Q	7	SER	3.8
1	C	112	VAL	3.8
1	C	123	PRO	3.8
1	C	102	SER	3.8
2	D	111	GLY	3.8
2	B	316	LEU	3.8
1	C	92	VAL	3.7
2	D	197	ARG	3.7
1	A	206	TYR	3.7
2	D	81	LEU	3.7
1	C	204	ALA	3.7
3	I	22	TYR	3.7
1	C	159	GLY	3.7
2	D	114	LEU	3.7
2	D	110	ALA	3.7
2	D	130	PHE	3.7
3	I	84	TYR	3.6
1	C	34	TRP	3.6
2	D	198	VAL	3.6
3	I	142	ILE	3.6
1	C	141	CYS	3.6
2	D	12	VAL	3.6
1	C	88	TYR	3.5
2	D	179	TYR	3.5
2	D	242	TRP	3.5
2	D	232	PRO	3.5
1	C	70	ASN	3.5
2	D	215	GLN	3.5
1	C	118	ILE	3.5
2	D	108	PHE	3.5
1	C	179	GLY	3.4
2	D	94	SER	3.4
1	C	32	LEU	3.4
1	A	212	PRO	3.4
3	I	124	ILE	3.4
1	C	168	LEU	3.4
1	C	169	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	235	GLN	3.4
1	C	142	LEU	3.4
1	C	152	VAL	3.4
2	D	245	ALA	3.4
3	I	136	ALA	3.4
1	A	205	THR	3.3
2	D	172	VAL	3.3
1	C	170	MET	3.3
1	A	207	PRO	3.3
1	C	59	VAL	3.3
2	D	228	GLY	3.3
2	D	208	ASN	3.3
2	D	157	VAL	3.3
1	C	148	SER	3.2
1	C	147	ASP	3.2
3	I	116	TYR	3.2
1	C	75	LEU	3.2
1	C	207	PRO	3.2
1	C	157	GLU	3.2
2	D	158	GLU	3.2
1	C	205	THR	3.2
2	D	142	LYS	3.2
2	D	231	LYS	3.2
5	Q	4	LYS	3.2
1	C	162	ILE	3.2
2	D	162	TRP	3.2
1	C	124	ALA	3.2
1	C	183	TRP	3.2
2	D	202	PHE	3.2
1	C	174	ASP	3.2
1	C	128	LEU	3.2
2	D	131	GLU	3.2
2	D	149	ALA	3.1
2	D	200	ALA	3.1
1	C	82	TRP	3.1
1	C	140	LEU	3.1
2	D	171	GLY	3.1
1	C	127	ALA	3.1
2	D	138	ALA	3.1
2	D	230	PRO	3.1
3	I	140	ALA	3.1
1	C	22	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	62	PHE	3.1
2	D	124	PRO	3.1
1	C	188	SER	3.1
1	C	43	LEU	3.1
1	C	208	SER	3.1
1	C	117	TYR	3.0
1	C	126	TYR	3.0
3	I	137	ASP	3.0
5	Q	5	PHE	3.0
1	A	184	SER	3.0
2	D	189	SER	3.0
1	C	178	ASN	3.0
1	C	99	GLY	3.0
1	C	129	LYS	3.0
4	M	82	VAL	3.0
2	D	72	GLN	3.0
2	D	209	HIS	3.0
2	D	206	PRO	3.0
2	D	50	TYR	3.0
2	D	148	LEU	3.0
2	D	167	GLU	2.9
3	I	64	THR	2.9
3	I	147	TRP	2.9
2	D	113	ARG	2.9
1	C	104	LEU	2.9
2	D	45	LEU	2.9
1	C	87	VAL	2.9
1	C	180	ALA	2.9
2	D	2	ALA	2.9
1	C	47	LEU	2.9
2	D	216	PHE	2.9
5	Q	1	GLU	2.9
1	C	187	THR	2.9
1	C	172	ALA	2.9
1	C	115	LEU	2.9
5	Q	6	TYR	2.9
1	C	212	PRO	2.9
2	D	225	TRP	2.9
1	A	189	PHE	2.9
2	D	187	TYR	2.9
1	A	159	GLY	2.9
2	D	160	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	M	3	LYS	2.8
1	C	139	THR	2.8
2	D	226	PRO	2.8
2	D	27	ASN	2.8
2	D	217	HIS	2.8
3	I	17	LEU	2.8
2	D	109	GLY	2.8
2	D	7	SER	2.8
2	D	236	ASN	2.8
1	C	86	ALA	2.8
3	I	82	LEU	2.8
2	D	152	PHE	2.8
1	C	101	ALA	2.8
1	C	144	THR	2.8
2	D	23	CYS	2.8
1	C	100	PHE	2.8
1	C	143	PHE	2.8
3	I	83	GLY	2.7
2	D	78	ILE	2.7
2	D	123	THR	2.7
2	D	174	THR	2.7
1	C	90	CYS	2.7
2	D	212	CYS	2.7
1	A	204	ALA	2.7
1	C	165	ALA	2.7
2	D	239	ALA	2.7
2	D	125	PRO	2.7
2	D	19	VAL	2.7
2	D	170	SER	2.7
2	D	173	SER	2.7
3	I	12	VAL	2.7
3	I	34	VAL	2.7
3	I	43	PRO	2.7
1	A	211	VAL	2.7
2	D	5	THR	2.7
2	D	6	GLN	2.7
1	C	30	PRO	2.6
3	I	130	LEU	2.6
1	C	158	SER	2.6
2	D	190	TYR	2.6
3	I	126	LEU	2.6
3	I	90	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	121	CYS	2.6
1	A	198	THR	2.6
3	I	153	ALA	2.6
1	C	206	TYR	2.6
2	D	11	LYS	2.6
2	D	18	LYS	2.6
1	C	45	LEU	2.6
2	D	116	VAL	2.6
1	C	182	ALA	2.6
2	D	133	SER	2.6
2	D	15	THR	2.6
2	D	176	PRO	2.5
1	C	37	GLN	2.5
1	C	103	ALA	2.5
2	D	105	THR	2.5
3	I	45	TYR	2.5
2	D	168	VAL	2.5
2	D	204	HIS	2.5
1	C	213	CYS	2.5
1	C	150	ILE	2.5
2	D	20	THR	2.5
2	D	112	THR	2.5
3	I	77	SER	2.5
1	C	191	CYS	2.5
2	B	1	GLU	2.5
3	I	85	TYR	2.5
1	C	20	LEU	2.5
1	C	195	PHE	2.5
2	D	195	ARG	2.5
2	D	220	SER	2.5
2	D	136	GLU	2.4
3	I	18	GLY	2.4
2	D	107	TYR	2.4
2	D	192	LEU	2.4
1	C	1	GLN	2.4
1	C	44	GLN	2.4
1	C	203	ASN	2.4
2	D	229	SER	2.4
1	C	46	LEU	2.4
2	D	156	HIS	2.4
2	D	89	VAL	2.4
1	C	166	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	133	PRO	2.4
1	C	19	GLN	2.4
2	D	48	TYR	2.4
2	D	90	TYR	2.4
3	I	51	TRP	2.4
1	C	160	THR	2.4
1	C	198	THR	2.4
1	C	167	VAL	2.4
2	D	205	ASN	2.4
3	H	274	TRP	2.4
3	I	120	GLY	2.3
2	D	43	LEU	2.3
2	D	10	ASN	2.3
2	D	67	ALA	2.3
2	D	201	THR	2.3
1	C	5	GLN	2.3
1	C	136	GLN	2.3
2	D	177	GLN	2.3
1	C	156	MET	2.3
3	I	25	VAL	2.3
1	C	72	SER	2.3
3	I	141	LEU	2.3
2	D	95	GLY	2.3
2	D	96	GLY	2.3
1	C	36	VAL	2.3
1	A	213	CYS	2.3
1	C	64	ALA	2.2
1	C	120	ASN	2.2
2	D	186	ASN	2.2
5	Q	2	GLN	2.2
1	C	18	LEU	2.2
2	D	49	SER	2.2
2	D	61	PRO	2.2
1	C	26	TYR	2.2
1	C	50	TYR	2.2
2	D	86	GLN	2.2
2	D	141	GLN	2.2
2	D	166	LYS	2.2
2	D	76	SER	2.2
2	D	88	SER	2.2
1	C	116	PRO	2.2
2	D	84	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
4	M	32	PRO	2.2
2	D	28	ASN	2.2
2	D	52	ALA	2.2
3	I	117	ALA	2.2
2	D	79	LEU	2.2
1	A	194	ILE	2.2
1	C	113	ILE	2.2
1	C	194	ILE	2.2
3	I	63	GLU	2.2
1	C	106	PHE	2.2
3	I	36	PHE	2.2
4	M	31	HIS	2.2
2	D	26	THR	2.2
1	C	71	SER	2.2
1	C	164	ASP	2.2
3	I	41	GLU	2.2
3	I	157	ARG	2.2
1	C	3	VAL	2.1
2	D	47	HIS	2.1
4	M	88	ALA	2.1
1	C	138	SER	2.1
2	D	85	SER	2.1
3	I	57	PRO	2.1
3	I	28	VAL	2.1
3	I	133	TRP	2.1
2	D	87	THR	2.1
4	M	26	TYR	2.1
1	C	209	SER	2.1
1	C	154	LYS	2.1
1	C	81	HIS	2.1
2	D	25	GLN	2.1
2	D	135	ALA	2.1
3	I	42	ASN	2.1
2	D	55	THR	2.1
1	C	153	PRO	2.1
2	D	82	ALA	2.1
4	M	60	TRP	2.1
1	C	42	GLY	2.1
3	I	91	GLY	2.1
1	C	190	THR	2.1
4	M	1	ILE	2.1
3	I	8	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	185	ASN	2.0
2	D	106	LEU	2.0
2	D	164	ASN	2.0
2	D	40	GLY	2.0
2	D	51	GLY	2.0
1	C	111	LYS	2.0
3	I	98	ILE	2.0
1	C	145	ASP	2.0
4	M	51	MET	2.0
2	D	213	GLN	2.0
2	D	120	ARG	2.0
2	D	244	ARG	2.0
4	M	87	MET	2.0
1	A	158	SER	2.0
1	C	175	SER	2.0
2	D	33	TYR	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.

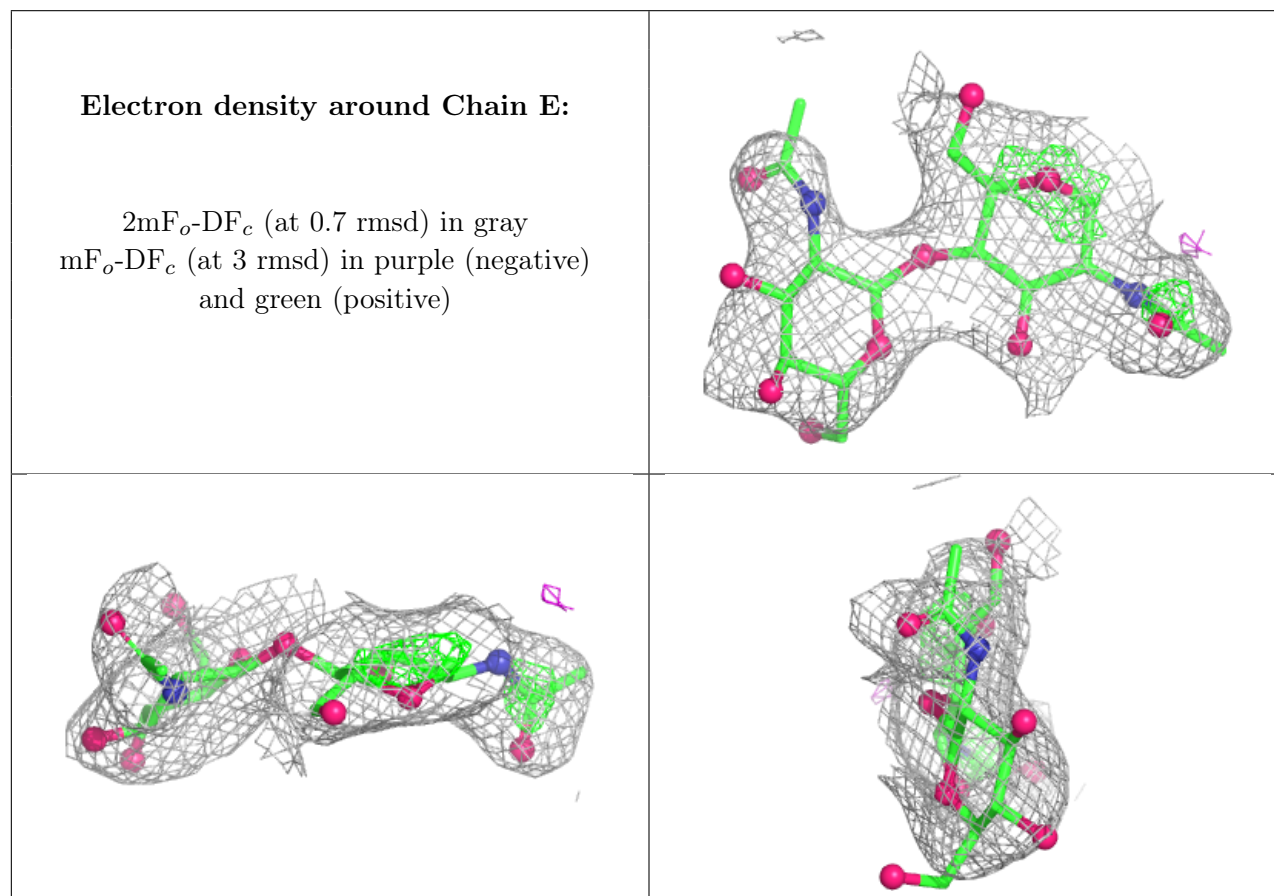
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	E	1	14/15	-	-	80,88,98,103	0
6	NAG	E	2	14/15	-	-	109,114,116,116	0
6	NAG	K	2	14/15	0.69	0.22	125,126,126,126	0
6	NAG	K	1	14/15	0.84	0.23	102,113,115,115	0
7	NAG	F	1	14/15	-	-	128,129,130,130	0
7	NAG	F	2	14/15	-	-	130,130,130,131	0
7	BMA	F	3	11/12	-	-	129,130,130,131	0
7	NAG	G	1	14/15	-	-	115,122,124,125	0
7	NAG	G	2	14/15	-	-	125,127,128,130	0
7	BMA	G	3	11/12	-	-	131,132,132,133	0
7	NAG	J	1	14/15	-	-	101,103,106,108	0
7	NAG	J	2	14/15	-	-	112,115,117,119	0

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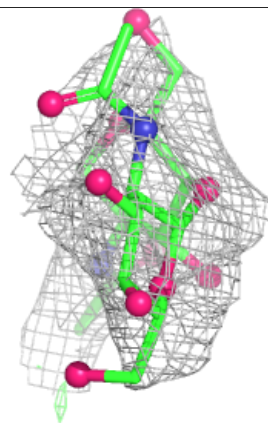
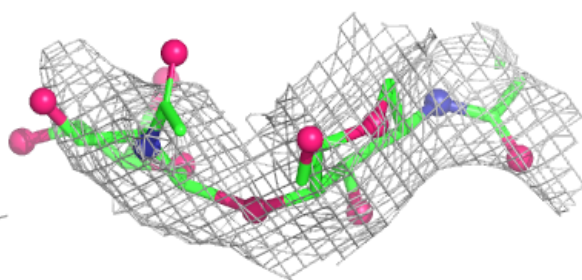
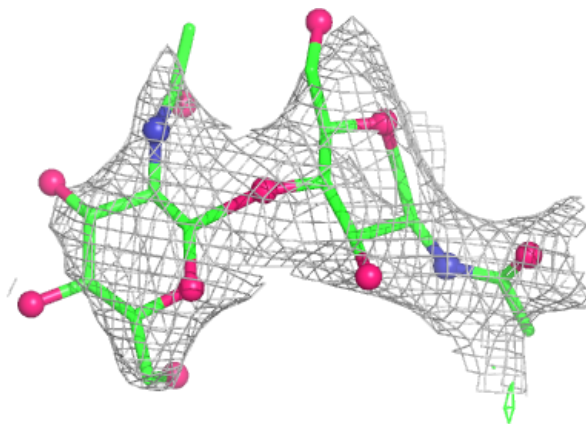
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BMA	J	3	11/12	-	-	121,123,124,124	0

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.

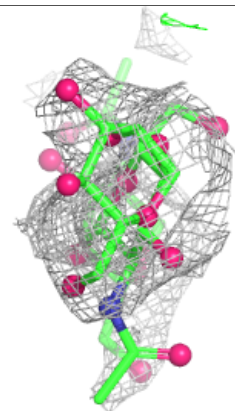
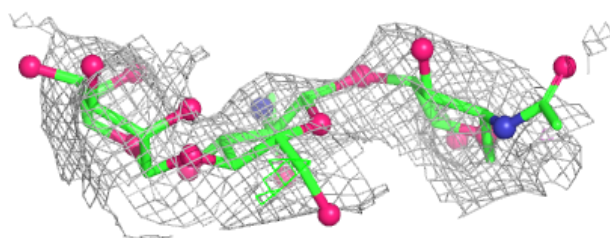
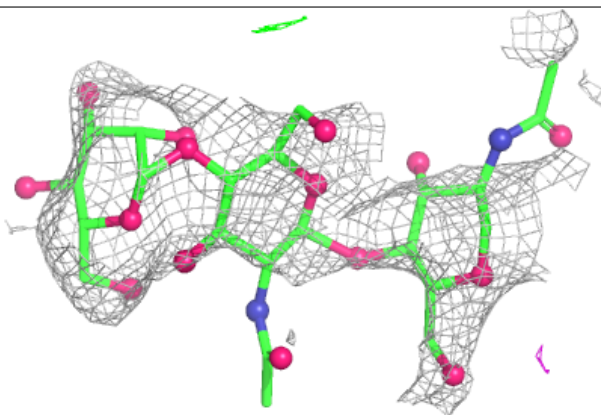


Electron density around Chain K:

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

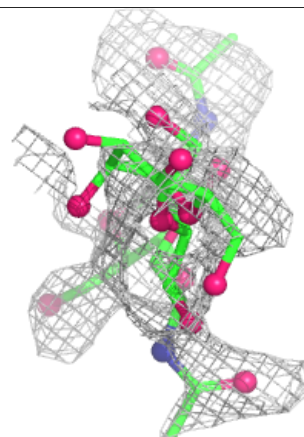
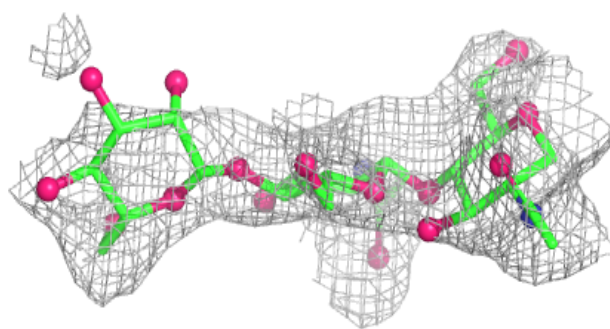
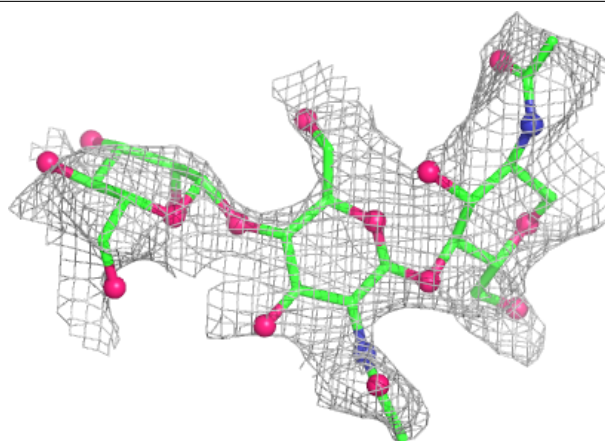
**Electron density around Chain F:**

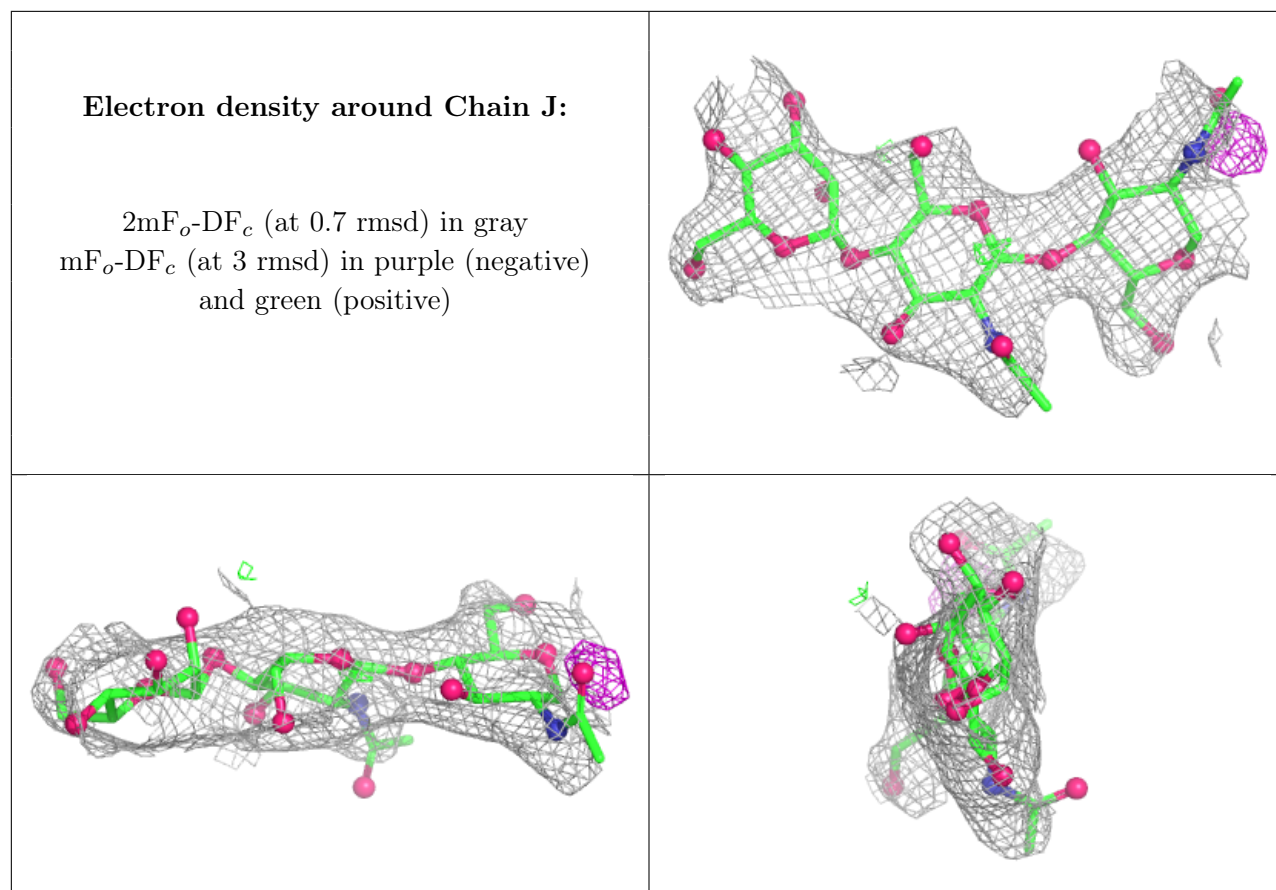
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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
9	NAG	B	808	14/15	0.62	0.16	91,103,104,105	0
8	GOL	I	903	6/6	0.69	0.21	101,102,102,102	0
10	ACY	P	1001	4/4	0.76	0.40	84,84,84,85	0
8	GOL	A	902	6/6	0.85	0.44	112,112,112,112	0
8	GOL	L	901	6/6	0.92	0.35	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.