



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:39 PM UTC

PDB ID : 2PMV / pdb_00002pmv
Title : Crystal Structure of Human Intrinsic Factor- Cobalamin Complex at 2.6 Å Resolution
Authors : Mathews, F.S.; Gordon, M.M.; Chen, Z.; Rajashankar, K.R.; Ealick, S.E.; Alpers, D.H.; Sukumar, N.
Deposited on : 2007-04-23
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:

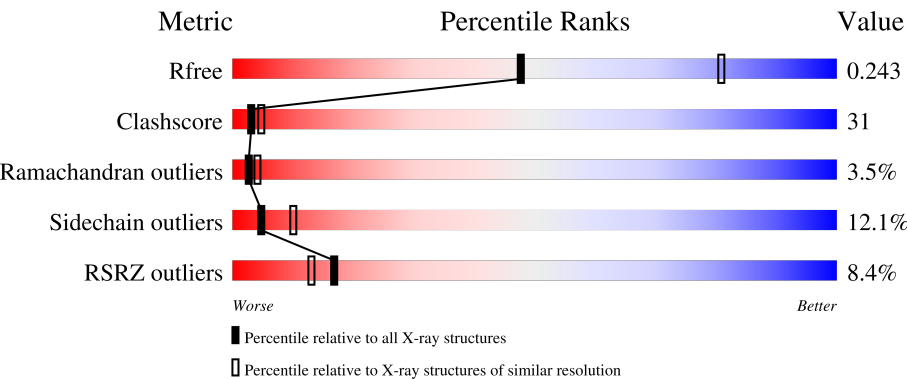
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	399	8% 49% 31% 12% • 5%
1	B	399	3% 38% 21% 6% • 33%
1	C	399	13% 46% 35% 11% • 5%
1	D	399	3% 38% 22% 5% • 33%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10457 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 Gastric intrinsic factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	3	0	0
			2871	1820	475	557	19			
1	B	267	Total	C	N	O	S	0	0	0
			2009	1268	332	392	17			
1	C	378	Total	C	N	O	S	5	0	0
			2871	1820	475	557	19			
1	D	267	Total	C	N	O	S	0	0	0
			2009	1268	332	392	17			

There are 4 discrepancies between the modelled and reference sequences:

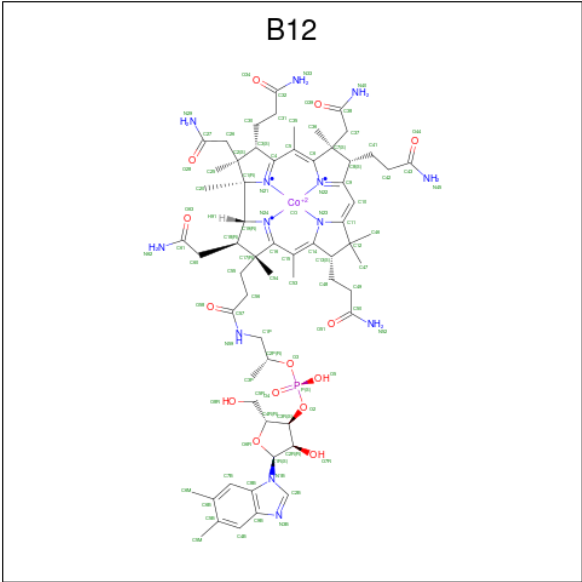
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIS	GLN	conflict	UNP P27352
B	73	HIS	GLN	conflict	UNP P27352
C	73	HIS	GLN	conflict	UNP P27352
D	73	HIS	GLN	conflict	UNP P27352

- Molecule 2 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
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

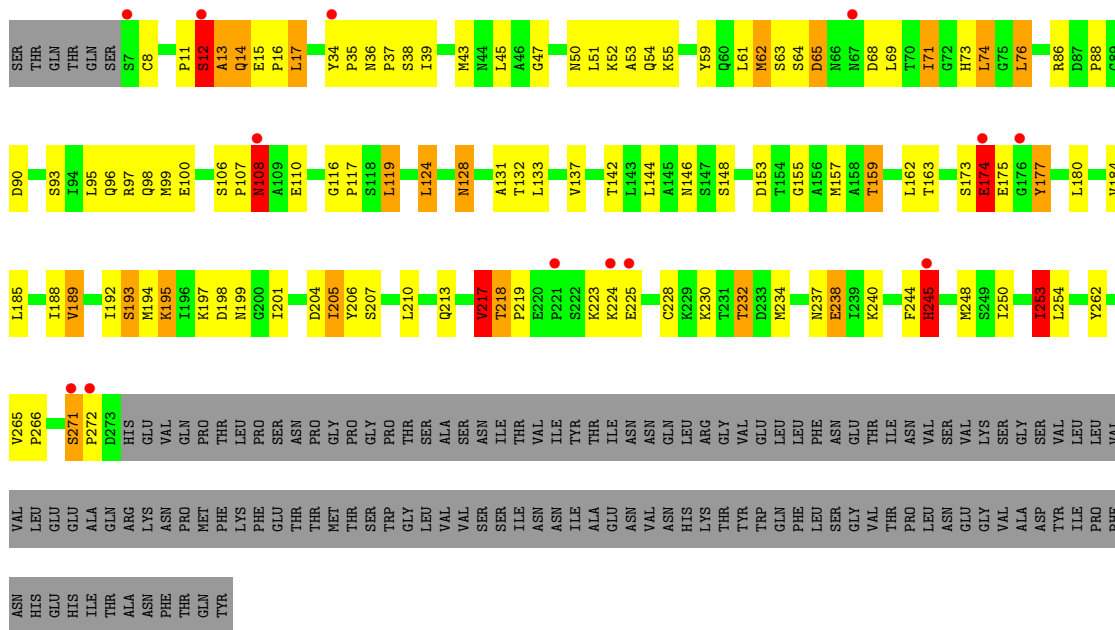
- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	100	Total	O	0	0
			100	100		
4	C	129	Total	O	0	0
			129	129		
4	D	95	Total	O	0	0
			95	95		



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

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.10Å 67.30Å 147.70Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	37.53 – 2.60 37.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.4 (37.53-2.60) 93.3 (37.53-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.249 0.205 , 0.243	Depositor DCC
R_{free} test set	1678 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10457	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: B12, 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	0.76	3/2925 (0.1%)	1.34	42/3978 (1.1%)
1	B	0.74	2/2044 (0.1%)	1.16	18/2775 (0.6%)
1	C	0.79	4/2925 (0.1%)	1.32	39/3978 (1.0%)
1	D	0.71	1/2044 (0.0%)	1.16	16/2775 (0.6%)
All	All	0.76	10/9938 (0.1%)	1.26	115/13506 (0.9%)

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	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	LYS	CB-CG	-7.74	1.29	1.52
1	A	265	VAL	CA-CB	7.51	1.57	1.54
1	D	51	LEU	C-N	-7.42	1.23	1.33
1	C	52	LYS	CA-CB	-7.41	1.41	1.53
1	C	52	LYS	CG-CD	-7.15	1.30	1.52
1	B	51	LEU	C-N	-6.16	1.24	1.33
1	B	52	LYS	C-N	-6.15	1.25	1.33
1	A	174	GLU	CA-C	6.07	1.61	1.52
1	C	51	LEU	C-N	-6.00	1.25	1.33
1	A	175	GLU	CB-CG	-5.71	1.35	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	LEU	N-CA-C	24.51	142.05	108.23
1	A	304	LEU	N-CA-C	24.00	141.36	108.23
1	A	321	SER	N-CA-C	-14.94	78.97	110.80
1	A	175	GLU	N-CA-CB	-14.64	87.12	110.11
1	C	321	SER	N-CA-C	-13.38	82.29	110.80
1	A	290	SER	N-CA-C	12.96	138.40	110.80
1	C	290	SER	N-CA-C	12.85	138.17	110.80
1	A	175	GLU	CA-CB-CG	10.83	135.76	114.10
1	D	195	LYS	N-CA-C	-10.78	97.37	114.09
1	A	195	LYS	N-CA-C	-10.66	97.61	113.61
1	C	195	LYS	N-CA-C	-10.48	97.33	113.89
1	B	195	LYS	N-CA-C	-10.28	98.16	114.09
1	C	322	GLY	N-CA-C	-10.01	89.47	113.18
1	C	52	LYS	CB-CA-C	-9.59	95.76	110.90
1	C	52	LYS	CD-CE-NZ	-9.31	82.11	111.90
1	A	52	LYS	CD-CE-NZ	-9.14	82.66	111.90
1	D	193	SER	N-CA-C	-9.01	98.64	110.53
1	D	253	ILE	CB-CA-C	-8.98	103.16	111.06
1	C	175	GLU	N-CA-C	8.82	122.85	109.62
1	B	253	ILE	CB-CA-C	-8.77	103.34	111.06
1	A	271	SER	CA-C-N	8.73	128.80	119.90
1	A	271	SER	C-N-CA	8.73	128.80	119.90
1	B	193	SER	N-CA-C	-8.65	99.11	110.53
1	C	271	SER	CA-C-N	8.34	128.41	119.90
1	C	271	SER	C-N-CA	8.34	128.41	119.90
1	A	175	GLU	CB-CG-CD	-8.26	98.56	112.60
1	A	193	SER	N-CA-C	-7.99	99.96	110.43
1	A	174	GLU	O-C-N	-7.78	109.84	121.89
1	C	175	GLU	CB-CA-C	-7.75	100.49	112.12
1	C	52	LYS	CB-CG-CD	-7.65	93.70	111.30
1	D	177	TYR	N-CA-C	-7.50	103.19	111.36
1	C	193	SER	N-CA-C	-7.34	100.81	110.43
1	B	217	VAL	N-CA-C	7.17	121.81	113.42
1	B	177	TYR	N-CA-C	-7.13	103.58	111.36
1	B	224	LYS	N-CA-C	-7.13	99.27	109.96
1	A	150	PHE	N-CA-C	7.01	120.54	110.10
1	C	304	LEU	CA-CB-CG	-6.83	92.38	116.30
1	D	271	SER	CA-C-N	6.79	128.33	119.84
1	D	271	SER	C-N-CA	6.79	128.33	119.84
1	A	385	ILE	CA-C-N	6.62	126.58	119.76
1	A	385	ILE	C-N-CA	6.62	126.58	119.76
1	B	271	SER	CA-C-N	6.59	128.07	119.84
1	B	271	SER	C-N-CA	6.59	128.07	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	217	VAL	N-CA-C	6.39	120.90	113.42
1	C	320	LYS	N-CA-C	6.37	124.37	110.80
1	A	304	LEU	CA-CB-CG	-6.34	94.12	116.30
1	A	322	GLY	N-CA-C	-6.34	98.16	113.18
1	C	253	ILE	CB-CA-C	-6.27	105.54	111.06
1	D	245	HIS	N-CA-C	-6.21	106.33	114.04
1	C	192	ILE	N-CA-C	-6.17	104.73	110.53
1	D	224	LYS	N-CA-C	-6.17	100.71	109.96
1	C	217	VAL	N-CA-C	6.13	119.54	113.53
1	B	245	HIS	N-CA-C	-6.13	106.44	114.04
1	C	73	HIS	N-CA-C	-6.10	104.32	110.97
1	A	73	HIS	N-CA-C	-6.09	104.33	110.97
1	C	289	THR	CA-C-N	-6.09	109.91	121.54
1	C	289	THR	C-N-CA	-6.09	109.91	121.54
1	B	174	GLU	CA-CB-CG	-6.05	102.00	114.10
1	B	14	GLN	N-CA-C	-6.03	105.96	113.38
1	C	385	ILE	CA-C-N	5.99	125.93	119.76
1	C	385	ILE	C-N-CA	5.99	125.93	119.76
1	D	62	MET	N-CA-C	-5.98	102.07	110.50
1	C	304	LEU	CB-CA-C	-5.97	101.56	113.80
1	C	150	PHE	N-CA-C	5.94	118.61	110.24
1	B	62	MET	N-CA-C	-5.93	102.14	110.50
1	C	292	SER	N-CA-C	5.90	123.36	110.80
1	C	14	GLN	N-CA-C	-5.89	106.07	113.72
1	C	47	GLY	N-CA-C	-5.85	99.31	113.18
1	A	175	GLU	N-CA-C	5.76	117.29	109.11
1	C	305	ARG	N-CA-C	-5.75	98.56	110.80
1	A	320	LYS	N-CA-C	5.74	123.02	110.80
1	C	357	ASN	N-CA-C	5.71	119.45	111.74
1	A	305	ARG	N-CA-C	-5.70	98.66	110.80
1	C	91	LYS	N-CA-C	5.67	118.19	111.33
1	A	253	ILE	CB-CA-C	-5.65	106.09	111.06
1	D	88	PRO	N-CA-C	-5.63	106.05	113.65
1	A	304	LEU	CA-C-N	5.62	132.27	121.54
1	A	304	LEU	C-N-CA	5.62	132.27	121.54
1	D	14	GLN	N-CA-C	-5.62	106.47	113.38
1	D	73	HIS	N-CA-C	-5.61	105.07	111.07
1	C	175	GLU	CA-C-O	-5.60	115.41	122.63
1	A	177	TYR	N-CA-C	-5.54	105.14	111.07
1	A	203	GLY	N-CA-C	-5.54	100.05	113.18
1	B	34	TYR	CA-C-N	5.53	126.75	119.84
1	B	34	TYR	C-N-CA	5.53	126.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ILE	CB-CA-C	-5.49	104.72	112.14
1	B	174	GLU	CB-CG-CD	5.44	121.84	112.60
1	A	173	SER	N-CA-C	-5.41	100.78	109.39
1	A	290	SER	O-C-N	5.38	129.75	122.59
1	C	175	GLU	CA-CB-CG	5.36	124.82	114.10
1	D	52	LYS	N-CA-C	-5.35	105.11	111.69
1	A	205	ILE	CB-CA-C	-5.33	104.95	112.14
1	D	47	GLY	N-CA-C	-5.32	100.58	113.18
1	A	217	VAL	N-CA-CB	-5.32	104.94	112.12
1	C	321	SER	O-C-N	-5.30	115.55	122.59
1	A	91	LYS	N-CA-C	5.28	117.04	111.28
1	B	73	HIS	N-CA-C	-5.26	105.23	110.97
1	A	289	THR	CA-C-N	-5.25	111.51	121.54
1	A	289	THR	C-N-CA	-5.25	111.51	121.54
1	B	174	GLU	N-CA-C	5.25	121.99	110.80
1	A	301	ASN	N-CA-C	5.25	116.63	109.18
1	A	217	VAL	N-CA-C	5.24	118.66	113.53
1	A	357	ASN	N-CA-C	5.18	118.73	111.74
1	C	177	TYR	N-CA-C	-5.17	105.54	111.07
1	D	225	GLU	N-CA-C	5.17	118.49	110.17
1	C	174	GLU	N-CA-C	5.16	119.26	112.25
1	B	88	PRO	N-CA-C	-5.13	107.17	113.84
1	A	192	ILE	N-CA-C	-5.11	105.73	110.53
1	A	14	GLN	N-CA-C	-5.11	107.08	113.72
1	A	292	SER	N-CA-C	5.10	121.66	110.80
1	C	290	SER	CA-C-N	5.08	131.25	121.54
1	C	290	SER	C-N-CA	5.08	131.25	121.54
1	A	290	SER	CA-C-N	5.03	131.15	121.54
1	A	290	SER	C-N-CA	5.03	131.15	121.54
1	A	100	GLU	N-CA-C	-5.03	106.98	113.01

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLU	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	2871	0	2861	217	1
1	B	2009	0	2043	101	0
1	C	2871	0	2861	226	1
1	D	2009	0	2043	87	0
2	E	28	0	25	1	0
2	F	28	0	25	2	0
3	A	91	0	87	10	0
3	C	91	0	87	1	0
4	A	135	0	0	8	0
4	B	100	0	0	15	0
4	C	129	0	0	12	0
4	D	95	0	0	9	0
All	All	10457	0	10032	630	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 31.

All (630) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:OE1	1:A:177:TYR:CE1	1.89	1.24
1:C:305:ARG:O	1:C:307:VAL:N	1.80	1.14
1:A:333:GLN:HE21	1:A:340:LYS:HB2	1.09	1.13
1:C:304:LEU:CD1	1:C:305:ARG:HG3	1.77	1.13
1:C:302:ASN:HD22	1:C:303:GLN:N	1.46	1.12
1:C:292:SER:HB2	1:C:319:VAL:HA	1.30	1.10
1:A:305:ARG:O	1:A:307:VAL:N	1.85	1.07
1:A:304:LEU:HD13	1:A:305:ARG:H	1.05	1.06
1:C:333:GLN:HE21	1:C:340:LYS:HB2	1.12	1.06
1:A:292:SER:HB2	1:A:319:VAL:HA	1.33	1.05
1:C:304:LEU:HD13	1:C:305:ARG:N	1.75	0.99
1:C:133:LEU:HD22	1:C:177:TYR:CD2	1.98	0.97
1:C:304:LEU:HD13	1:C:305:ARG:HG3	1.43	0.96
1:A:304:LEU:CD1	1:A:305:ARG:H	1.78	0.96
1:C:292:SER:CB	1:C:319:VAL:HA	1.95	0.95
1:C:302:ASN:HD22	1:C:303:GLN:H	1.10	0.95
1:A:107:PRO:HD3	1:C:107:PRO:HB3	1.48	0.95
1:A:292:SER:CB	1:A:319:VAL:HA	1.95	0.95
1:A:289:THR:HG22	1:A:289:THR:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG23	1:A:313:GLU:HG3	1.46	0.95
1:A:304:LEU:HD13	1:A:305:ARG:N	1.81	0.94
1:C:299:THR:HG23	1:C:313:GLU:HG3	1.49	0.94
1:C:304:LEU:HD13	1:C:305:ARG:H	1.29	0.94
1:C:310:LEU:HD21	1:C:356:ASN:HD22	1.33	0.93
1:A:310:LEU:HD21	1:A:356:ASN:HD22	1.32	0.92
1:D:250:ILE:HA	1:D:253:ILE:HD11	1.50	0.91
1:C:304:LEU:CD1	1:C:305:ARG:H	1.82	0.91
1:C:304:LEU:H	1:C:309:LEU:CD2	1.83	0.91
1:C:133:LEU:HD22	1:C:177:TYR:HD2	1.32	0.90
1:D:199:ASN:HD21	1:D:201:ILE:HD12	1.38	0.89
1:B:12:SER:HA	1:B:15:GLU:HG3	1.55	0.89
1:C:304:LEU:H	1:C:309:LEU:HD21	1.36	0.88
1:C:14:GLN:HE21	1:C:14:GLN:HA	1.37	0.88
1:D:12:SER:HA	1:D:15:GLU:HG3	1.55	0.87
1:A:310:LEU:HD21	1:A:356:ASN:ND2	1.89	0.87
1:A:370:PHE:H	3:A:1001:B12:H402	1.21	0.86
1:A:333:GLN:NE2	1:A:340:LYS:HB2	1.91	0.86
1:B:199:ASN:HD21	1:B:201:ILE:HD12	1.38	0.86
1:C:175:GLU:OE1	1:C:177:TYR:CE1	2.28	0.86
1:C:310:LEU:HD21	1:C:356:ASN:ND2	1.90	0.86
1:A:107:PRO:CD	1:C:107:PRO:HB3	2.06	0.86
1:B:250:ILE:HA	1:B:253:ILE:HD11	1.55	0.86
1:A:304:LEU:CD1	1:A:305:ARG:HG3	2.07	0.85
1:A:133:LEU:HD13	1:A:177:TYR:HE2	1.41	0.84
1:A:322:GLY:O	1:A:323:SER:C	2.19	0.84
1:A:304:LEU:H	1:A:309:LEU:HD21	1.42	0.84
1:A:175:GLU:OE1	1:A:177:TYR:HE1	1.59	0.84
1:A:14:GLN:HE21	1:A:14:GLN:HA	1.42	0.83
1:C:185:LEU:O	1:C:189:VAL:HG23	1.78	0.83
1:A:185:LEU:O	1:A:189:VAL:HG23	1.79	0.82
1:A:133:LEU:HD22	1:A:177:TYR:CD2	2.15	0.82
1:C:333:GLN:NE2	1:C:340:LYS:HB2	1.94	0.82
1:A:133:LEU:HD13	1:A:177:TYR:CE2	2.15	0.82
1:D:155:GLY:O	1:D:159:THR:HG23	1.79	0.82
1:A:305:ARG:C	1:A:307:VAL:H	1.89	0.81
1:B:155:GLY:O	1:B:159:THR:HG23	1.81	0.81
1:A:304:LEU:H	1:A:309:LEU:CD2	1.93	0.81
1:C:336:ASN:C	1:C:338:MET:H	1.89	0.81
3:A:1001:B12:H401	3:A:1001:B12:H8	1.46	0.81
1:C:340:LYS:NZ	1:C:357:ASN:HD22	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:CD1	1:C:305:ARG:CG	2.58	0.80
1:A:299:THR:HG23	1:A:313:GLU:CG	2.11	0.80
1:A:335:LYS:C	1:A:337:PRO:HD3	2.06	0.79
1:C:335:LYS:C	1:C:337:PRO:HD3	2.06	0.79
1:A:183:GLN:HG2	1:C:179:SER:OG	1.83	0.79
1:C:302:ASN:ND2	1:C:303:GLN:N	2.29	0.79
1:C:340:LYS:HZ1	1:C:357:ASN:HD22	1.28	0.78
1:A:340:LYS:NZ	1:A:357:ASN:HD22	1.81	0.78
1:C:322:GLY:O	1:C:323:SER:C	2.26	0.78
1:A:50:ASN:C	1:A:50:ASN:HD22	1.90	0.78
1:B:50:ASN:C	1:B:50:ASN:HD22	1.91	0.78
1:A:336:ASN:C	1:A:338:MET:H	1.91	0.78
1:C:17:LEU:HD21	1:C:240:LYS:HG2	1.66	0.77
1:A:304:LEU:HD13	1:A:305:ARG:HG3	1.66	0.77
1:A:290:SER:OG	1:A:291:ALA:N	2.17	0.77
1:A:304:LEU:HD13	1:A:305:ARG:CG	2.15	0.77
1:C:299:THR:HG23	1:C:313:GLU:CG	2.13	0.77
1:A:151:ASN:ND2	1:A:154:THR:H	1.82	0.76
1:A:178:ARG:NH1	4:A:1018:HOH:O	2.18	0.76
1:C:305:ARG:C	1:C:307:VAL:H	1.91	0.76
1:C:303:GLN:O	1:C:304:LEU:HD23	1.86	0.75
1:A:271:SER:N	1:A:272:PRO:HD3	2.01	0.75
1:C:50:ASN:C	1:C:50:ASN:HD22	1.94	0.75
1:C:151:ASN:ND2	1:C:154:THR:H	1.85	0.75
1:B:193:SER:O	1:B:194:MET:HG2	1.85	0.75
1:C:290:SER:OG	1:C:291:ALA:N	2.14	0.74
1:B:163:THR:HG21	1:B:217:VAL:HG13	1.67	0.74
1:D:36:ASN:C	1:D:36:ASN:HD22	1.96	0.74
1:D:163:THR:HG21	1:D:217:VAL:HG13	1.67	0.74
1:C:360:GLU:O	1:C:366:THR:HG23	1.87	0.74
1:C:336:ASN:O	1:C:338:MET:N	2.21	0.73
1:A:355:ILE:O	1:A:358:ILE:HG23	1.88	0.73
1:A:289:THR:O	1:A:289:THR:CG2	2.37	0.73
1:C:175:GLU:CD	1:C:177:TYR:HE1	1.96	0.73
1:B:36:ASN:C	1:B:36:ASN:HD22	1.97	0.72
1:C:294:ILE:HD13	1:C:388:ASN:HA	1.71	0.72
1:C:176:GLY:HA2	4:C:1199:HOH:O	1.89	0.72
1:C:304:LEU:HD13	1:C:305:ARG:CG	2.20	0.72
1:A:304:LEU:CD1	1:A:305:ARG:CG	2.67	0.71
1:C:361:ASN:HD21	1:C:363:ASN:HB2	1.55	0.71
1:A:360:GLU:O	1:A:366:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ASN:HD21	1:C:52:LYS:HB2	1.55	0.71
1:A:340:LYS:HZ1	1:A:357:ASN:HD22	1.37	0.71
1:C:271:SER:N	1:C:272:PRO:HD3	2.06	0.70
1:A:300:ILE:HD13	1:A:339:PHE:HD2	1.56	0.70
1:A:319:VAL:HG22	1:A:323:SER:OG	1.92	0.70
1:C:332:ALA:HB1	1:C:339:PHE:CZ	2.26	0.70
1:A:336:ASN:O	1:A:338:MET:N	2.23	0.69
1:D:173:SER:O	1:D:175:GLU:N	2.21	0.69
1:C:175:GLU:OE1	1:C:177:TYR:HE1	1.74	0.69
1:A:332:ALA:HB1	1:A:339:PHE:CZ	2.28	0.69
1:C:128:ASN:C	1:C:128:ASN:HD22	2.00	0.69
1:A:304:LEU:HD13	1:A:305:ARG:CB	2.23	0.68
1:A:304:LEU:HD11	1:A:305:ARG:HG3	1.76	0.68
1:A:299:THR:HG23	1:A:313:GLU:CD	2.19	0.68
1:D:193:SER:O	1:D:194:MET:HG2	1.94	0.68
1:A:133:LEU:HD22	1:A:177:TYR:HD2	1.56	0.68
1:D:50:ASN:HD22	1:D:50:ASN:C	2.02	0.68
1:D:155:GLY:O	1:D:159:THR:CG2	2.42	0.68
1:A:294:ILE:HD13	1:A:388:ASN:HA	1.76	0.67
1:C:245:HIS:HB3	4:C:1186:HOH:O	1.94	0.67
1:A:213:GLN:HE21	1:A:261:THR:HB	1.60	0.67
1:B:144:LEU:HD13	1:B:184:VAL:HG22	1.76	0.67
1:A:50:ASN:ND2	1:A:53:ALA:H	1.92	0.67
1:C:299:THR:HG23	1:C:313:GLU:CD	2.19	0.67
1:C:303:GLN:O	1:C:304:LEU:CG	2.43	0.66
1:D:17:LEU:HD21	1:D:240:LYS:HG3	1.76	0.66
1:A:107:PRO:HD3	1:C:107:PRO:CB	2.22	0.66
1:B:146:ASN:HD21	1:B:148:SER:HB3	1.61	0.65
1:C:193:SER:O	1:C:194:MET:HG2	1.96	0.65
1:C:355:ILE:O	1:C:358:ILE:HG23	1.96	0.65
1:A:213:GLN:NE2	1:A:262:TYR:H	1.95	0.65
1:A:361:ASN:HD21	1:A:363:ASN:HB2	1.62	0.65
1:B:244:PHE:CE2	1:B:253:ILE:HG12	2.32	0.65
1:B:93:SER:O	1:B:97:ARG:HG3	1.97	0.65
1:A:128:ASN:C	1:A:128:ASN:HD22	2.04	0.64
1:C:155:GLY:O	1:C:159:THR:CG2	2.45	0.64
1:A:193:SER:O	1:A:194:MET:HG2	1.98	0.64
1:B:173:SER:O	1:B:175:GLU:N	2.28	0.64
1:A:303:GLN:O	1:A:304:LEU:HD23	1.98	0.63
1:C:299:THR:HB	1:C:393:THR:HG23	1.80	0.63
1:D:250:ILE:HA	1:D:253:ILE:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD21	1:A:240:LYS:HG2	1.80	0.63
1:C:213:GLN:HE22	1:C:262:TYR:H	1.45	0.63
1:D:76:LEU:HD13	1:D:119:LEU:HG	1.80	0.63
1:C:300:ILE:HD13	1:C:339:PHE:HD2	1.62	0.63
1:A:216:SER:HB3	4:A:1109:HOH:O	1.99	0.63
1:D:144:LEU:HB3	4:D:422:HOH:O	1.98	0.63
1:C:155:GLY:O	1:C:159:THR:HG22	1.98	0.63
1:D:144:LEU:HD13	1:D:184:VAL:HG22	1.81	0.63
1:C:303:GLN:O	1:C:304:LEU:CD2	2.47	0.62
1:A:319:VAL:HG22	1:A:323:SER:CB	2.29	0.62
1:B:245:HIS:HB2	4:B:484:HOH:O	1.99	0.62
1:C:17:LEU:HD21	1:C:240:LYS:CG	2.29	0.62
1:C:228:CYS:O	1:C:232:THR:HG22	1.99	0.62
1:C:295:THR:HA	1:C:316:ASN:O	2.00	0.62
1:C:319:VAL:HG22	1:C:323:SER:OG	1.98	0.62
1:A:69:LEU:HD22	1:A:73:HIS:HB3	1.80	0.62
1:A:299:THR:CG2	1:A:313:GLU:CD	2.73	0.62
1:C:294:ILE:CD1	1:C:388:ASN:HA	2.30	0.62
1:A:213:GLN:HE22	1:A:262:TYR:H	1.46	0.62
1:B:228:CYS:O	1:B:232:THR:HG22	2.00	0.62
1:C:76:LEU:HD13	1:C:119:LEU:HG	1.81	0.62
1:C:310:LEU:O	1:C:311:PHE:HB2	2.00	0.61
1:B:43:MET:HE2	1:B:54:GLN:HB2	1.80	0.61
1:B:64:SER:O	1:B:65:ASP:C	2.43	0.61
1:C:50:ASN:C	1:C:50:ASN:ND2	2.58	0.61
1:C:308:GLU:O	1:C:308:GLU:HG3	2.00	0.61
1:C:365:LYS:HG3	1:C:399:TYR:CE1	2.35	0.61
1:C:213:GLN:NE2	1:C:262:TYR:H	1.99	0.61
1:A:310:LEU:O	1:A:311:PHE:HB2	2.00	0.61
1:A:365:LYS:HG3	1:A:399:TYR:CE1	2.35	0.61
1:A:163:THR:HG21	1:A:217:VAL:HG13	1.81	0.61
1:C:304:LEU:HD11	1:C:305:ARG:HG3	1.76	0.61
1:C:358:ILE:HG12	1:C:358:ILE:O	2.00	0.61
1:A:336:ASN:C	1:A:338:MET:N	2.59	0.61
1:C:151:ASN:HD22	1:C:154:THR:H	1.47	0.60
1:C:213:GLN:HE21	1:C:261:THR:HB	1.65	0.60
1:A:304:LEU:HD11	1:A:305:ARG:HD2	1.82	0.60
1:B:163:THR:HG21	1:B:217:VAL:CG1	2.31	0.60
1:C:361:ASN:ND2	1:C:363:ASN:H	1.99	0.60
1:B:205:ILE:HG13	1:B:206:TYR:CE2	2.36	0.60
1:D:163:THR:HG21	1:D:217:VAL:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLY:N	1:C:174:GLU:OE1	2.34	0.60
1:A:17:LEU:HD21	1:A:240:LYS:CG	2.31	0.60
1:C:336:ASN:N	1:C:337:PRO:HD3	2.16	0.60
1:A:238:GLU:HG3	1:A:243:LYS:HG3	1.81	0.60
1:D:106:SER:OG	1:D:107:PRO:HD2	2.02	0.59
1:D:228:CYS:O	1:D:232:THR:HG22	2.02	0.59
1:C:240:LYS:HE3	4:C:1142:HOH:O	2.02	0.59
1:A:303:GLN:O	1:A:304:LEU:CG	2.50	0.59
1:C:199:ASN:O	1:C:230:LYS:HE3	2.03	0.59
1:D:110:GLU:OE1	1:D:110:GLU:N	2.34	0.59
1:D:128:ASN:HD22	1:D:128:ASN:C	2.08	0.59
1:B:174:GLU:HB3	4:B:474:HOH:O	2.02	0.59
1:A:341:PHE:HB2	1:A:354:SER:O	2.03	0.59
1:D:8:CYS:HB2	1:D:232:THR:HG21	1.84	0.58
1:D:93:SER:O	1:D:97:ARG:HG3	2.03	0.58
1:D:119:LEU:HD13	1:D:157:MET:SD	2.43	0.58
1:A:175:GLU:OE1	1:A:177:TYR:CD1	2.53	0.58
1:B:8:CYS:HB2	1:B:232:THR:HG21	1.85	0.58
1:A:370:PHE:N	3:A:1001:B12:H402	1.97	0.58
1:B:159:THR:HG22	1:B:188:ILE:HG21	1.84	0.58
1:B:250:ILE:HA	1:B:253:ILE:CD1	2.28	0.58
1:C:197:LYS:HE3	4:C:1121:HOH:O	2.03	0.58
1:C:303:GLN:O	1:C:304:LEU:HG	2.04	0.58
1:D:137:VAL:HG21	1:D:177:TYR:CE1	2.39	0.58
1:C:305:ARG:HH12	1:C:364:HIS:CG	2.22	0.58
1:C:340:LYS:NZ	1:C:357:ASN:ND2	2.51	0.58
1:C:299:THR:OG1	1:C:391:HIS:NE2	2.35	0.58
1:D:64:SER:O	1:D:65:ASP:C	2.46	0.58
1:D:146:ASN:HD21	1:D:148:SER:HB3	1.69	0.58
1:D:205:ILE:HG13	1:D:206:TYR:CE2	2.37	0.58
1:B:50:ASN:C	1:B:50:ASN:ND2	2.62	0.58
1:A:208:THR:O	1:A:212:MET:HG3	2.03	0.58
1:A:340:LYS:NZ	1:A:357:ASN:ND2	2.52	0.58
1:B:76:LEU:HD13	1:B:119:LEU:HG	1.85	0.57
1:C:138:ARG:HD2	4:C:1107:HOH:O	2.03	0.57
1:A:295:THR:HA	1:A:316:ASN:O	2.04	0.57
1:A:294:ILE:CD1	1:A:388:ASN:HA	2.34	0.57
1:A:358:ILE:HG12	1:A:358:ILE:O	2.03	0.57
1:A:361:ASN:ND2	1:A:363:ASN:H	2.02	0.57
1:A:76:LEU:HD13	1:A:119:LEU:HG	1.86	0.57
1:C:305:ARG:HH12	1:C:364:HIS:HB3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:CG2	1:C:313:GLU:CD	2.77	0.57
1:A:336:ASN:N	1:A:337:PRO:HD3	2.19	0.57
1:A:300:ILE:HD13	1:A:339:PHE:CD2	2.39	0.56
1:A:175:GLU:HB2	1:C:223:LYS:HZ2	1.70	0.56
1:B:184:VAL:O	1:B:188:ILE:HG13	2.05	0.56
1:C:95:LEU:HD23	1:C:124:LEU:HD13	1.87	0.56
1:A:171:VAL:HG11	1:B:54:GLN:HG2	1.88	0.56
1:A:170:PRO:HB2	1:A:173:SER:HB3	1.88	0.56
1:C:304:LEU:CD1	1:C:305:ARG:N	2.50	0.56
1:A:50:ASN:C	1:A:50:ASN:ND2	2.57	0.56
1:B:224:LYS:HE2	4:B:475:HOH:O	2.06	0.56
1:A:155:GLY:O	1:A:159:THR:CG2	2.54	0.56
1:C:238:GLU:HG3	1:C:243:LYS:HG3	1.86	0.56
1:C:361:ASN:C	1:C:361:ASN:HD22	2.14	0.56
1:D:128:ASN:ND2	1:D:131:ALA:H	2.03	0.56
1:D:244:PHE:CE2	1:D:253:ILE:HG12	2.40	0.56
1:C:341:PHE:HB2	1:C:354:SER:O	2.06	0.56
1:B:17:LEU:HD21	1:B:240:LYS:HG3	1.87	0.55
1:C:50:ASN:ND2	1:C:53:ALA:H	2.04	0.55
1:C:69:LEU:HD22	1:C:73:HIS:HB3	1.87	0.55
1:C:110:GLU:OE1	1:C:110:GLU:N	2.39	0.55
1:D:184:VAL:O	1:D:188:ILE:HG13	2.06	0.55
1:A:189:VAL:HG22	1:A:218:THR:HG21	1.89	0.55
1:A:228:CYS:O	1:A:232:THR:HG22	2.06	0.55
1:B:14:GLN:O	1:B:17:LEU:HB2	2.06	0.55
1:D:106:SER:OG	1:D:107:PRO:CD	2.54	0.55
1:A:303:GLN:O	1:A:304:LEU:HG	2.06	0.55
1:B:137:VAL:HG21	1:B:177:TYR:CE1	2.42	0.55
1:C:340:LYS:HZ1	1:C:357:ASN:ND2	2.00	0.55
1:A:265:VAL:HB	1:A:266:PRO:HD3	1.88	0.55
1:B:91:LYS:HE2	4:B:426:HOH:O	2.06	0.55
1:C:337:PRO:C	1:C:339:PHE:H	2.14	0.55
1:C:163:THR:HG21	1:C:217:VAL:HG13	1.88	0.55
1:A:172:GLY:N	1:A:174:GLU:OE1	2.39	0.55
1:C:302:ASN:ND2	1:C:303:GLN:H	1.92	0.55
1:C:19:ASN:HA	4:C:1106:HOH:O	2.05	0.55
1:A:334:ARG:C	1:A:336:ASN:N	2.63	0.55
1:A:334:ARG:C	1:A:336:ASN:H	2.15	0.54
1:A:199:ASN:O	1:A:230:LYS:HE3	2.08	0.54
1:A:386:PRO:HA	4:A:1103:HOH:O	2.07	0.54
1:C:319:VAL:HG22	1:C:323:SER:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:GLU:HB2	1:C:354:SER:HB3	1.90	0.54
1:C:199:ASN:C	1:C:230:LYS:HE3	2.32	0.54
1:A:337:PRO:C	1:A:339:PHE:H	2.15	0.54
1:B:155:GLY:O	1:B:159:THR:CG2	2.54	0.54
1:C:371:LEU:HD23	1:C:371:LEU:N	2.22	0.54
1:A:175:GLU:HB2	1:C:223:LYS:NZ	2.22	0.54
1:A:307:VAL:O	1:A:308:GLU:HB3	2.08	0.54
1:B:71:ILE:CD1	1:B:99:MET:SD	2.96	0.54
1:B:238:GLU:HA	1:B:238:GLU:OE1	2.06	0.54
1:C:302:ASN:HD22	1:C:302:ASN:C	2.04	0.54
1:C:305:ARG:NH1	1:C:364:HIS:HB3	2.22	0.54
1:D:95:LEU:HD23	1:D:124:LEU:HD13	1.89	0.54
1:A:201:ILE:HA	1:A:234:MET:HE2	1.90	0.53
1:A:310:LEU:CD2	1:A:356:ASN:HD22	2.14	0.53
1:A:360:GLU:O	1:A:366:THR:CG2	2.55	0.53
1:A:361:ASN:C	1:A:361:ASN:HD22	2.16	0.53
1:C:300:ILE:HD13	1:C:339:PHE:CD2	2.43	0.53
1:C:310:LEU:CD2	1:C:356:ASN:HD22	2.14	0.53
1:A:79:MET:HG2	1:A:126:GLN:HE22	1.73	0.53
1:A:303:GLN:O	1:A:304:LEU:CD2	2.57	0.53
1:C:174:GLU:HG3	4:D:441:HOH:O	2.09	0.53
1:C:220:GLU:HB2	4:C:1213:HOH:O	2.08	0.53
1:C:310:LEU:CD2	1:C:356:ASN:ND2	2.70	0.53
1:D:272:PRO:HD2	4:D:463:HOH:O	2.06	0.53
1:B:241:GLN:HG3	4:B:413:HOH:O	2.07	0.53
1:C:304:LEU:H	1:C:309:LEU:HD22	1.68	0.53
1:C:133:LEU:HD22	1:C:177:TYR:CE2	2.41	0.53
1:C:302:ASN:O	1:C:303:GLN:HG3	2.09	0.53
1:A:26:GLU:CD	1:A:43:MET:HE3	2.34	0.53
1:C:265:VAL:HB	1:C:266:PRO:HD3	1.90	0.53
1:A:133:LEU:CD2	1:A:177:TYR:HD2	2.22	0.53
1:C:40:LEU:HD23	1:C:80:ALA:HB1	1.91	0.53
1:B:71:ILE:HD11	1:B:99:MET:SD	2.49	0.52
1:C:258:LYS:NZ	4:C:1106:HOH:O	2.40	0.52
1:B:106:SER:OG	1:B:107:PRO:HD2	2.09	0.52
1:B:248:MET:HE1	4:B:412:HOH:O	2.08	0.52
1:C:171:VAL:O	1:D:86:ARG:NH2	2.35	0.52
1:C:315:ILE:O	1:C:335:LYS:NZ	2.42	0.52
1:A:151:ASN:HD22	1:A:154:THR:H	1.54	0.52
1:A:299:THR:HB	1:A:393:THR:HG23	1.90	0.52
1:B:218:THR:HG22	1:B:219:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:HG22	1:A:323:SER:HB2	1.91	0.52
1:B:245:HIS:CB	4:B:484:HOH:O	2.57	0.52
1:C:34:TYR:HA	4:C:1111:HOH:O	2.10	0.52
1:A:95:LEU:HD23	1:A:124:LEU:HD13	1.91	0.52
1:C:205:ILE:HD12	1:C:206:TYR:CZ	2.45	0.52
1:C:304:LEU:N	1:C:309:LEU:CD2	2.64	0.52
1:A:199:ASN:C	1:A:230:LYS:HE3	2.35	0.52
1:A:371:LEU:N	1:A:371:LEU:HD23	2.25	0.52
1:C:332:ALA:HB1	1:C:339:PHE:HZ	1.70	0.52
1:C:208:THR:O	1:C:212:MET:HG3	2.10	0.52
1:A:66:ASN:ND2	1:A:90:ASP:OD2	2.42	0.51
1:A:304:LEU:N	1:A:309:LEU:CD2	2.69	0.51
1:B:199:ASN:O	1:B:234:MET:HG2	2.10	0.51
1:C:334:ARG:C	1:C:336:ASN:N	2.65	0.51
1:A:304:LEU:CD1	1:A:305:ARG:HD2	2.39	0.51
1:C:336:ASN:C	1:C:338:MET:N	2.57	0.51
1:A:266:PRO:HB2	1:A:267:GLN:NE2	2.26	0.51
1:A:304:LEU:HD11	1:A:305:ARG:CG	2.39	0.51
1:A:299:THR:OG1	1:A:391:HIS:NE2	2.41	0.51
1:B:106:SER:OG	1:B:107:PRO:CD	2.59	0.51
1:C:133:LEU:HD13	1:C:177:TYR:CE2	2.46	0.51
1:A:340:LYS:HZ1	1:A:357:ASN:ND2	2.08	0.51
1:A:355:ILE:HB	1:A:368:TRP:CZ2	2.46	0.51
1:A:311:PHE:CZ	4:A:1094:HOH:O	2.55	0.51
1:B:36:ASN:ND2	1:B:38:SER:H	2.09	0.50
1:D:14:GLN:O	1:D:17:LEU:HB2	2.10	0.50
1:D:43:MET:HE2	1:D:54:GLN:HB2	1.93	0.50
1:A:96:GLN:O	1:A:100:GLU:HG3	2.10	0.50
1:A:339:PHE:CG	1:A:339:PHE:O	2.64	0.50
1:A:183:GLN:CG	1:C:179:SER:OG	2.56	0.50
1:A:151:ASN:HD22	1:A:154:THR:CB	2.24	0.50
1:C:8:CYS:HB2	1:C:232:THR:HG21	1.94	0.50
1:C:14:GLN:HA	1:C:14:GLN:NE2	2.18	0.50
1:C:50:ASN:ND2	1:C:52:LYS:H	2.09	0.50
1:D:237:ASN:HA	1:D:240:LYS:HE3	1.94	0.50
1:A:297:ILE:HD12	1:A:391:HIS:HB2	1.94	0.50
1:C:298:TYR:CZ	1:C:329:LEU:HD22	2.47	0.50
1:C:334:ARG:C	1:C:336:ASN:H	2.19	0.50
1:A:304:LEU:HD13	1:A:305:ARG:CA	2.42	0.50
1:A:390:GLU:CB	4:A:1103:HOH:O	2.59	0.50
1:C:296:VAL:HG12	1:C:390:GLU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:THR:HG22	1:C:353:SER:HB3	1.93	0.50
1:D:157:MET:CE	1:D:210:LEU:HD13	2.42	0.50
1:A:110:GLU:OE1	1:A:110:GLU:N	2.44	0.50
1:B:128:ASN:C	1:B:128:ASN:HD22	2.19	0.50
1:C:290:SER:OG	1:C:331:GLU:OE2	2.23	0.50
1:C:339:PHE:CG	1:C:339:PHE:O	2.65	0.49
1:C:304:LEU:HD12	1:C:305:ARG:HD2	1.94	0.49
1:A:296:VAL:HG12	1:A:390:GLU:O	2.13	0.49
1:A:298:TYR:CZ	1:A:329:LEU:HD22	2.47	0.49
4:A:1074:HOH:O	1:C:141:LYS:HE2	2.12	0.49
1:C:175:GLU:CD	1:C:177:TYR:CE1	2.81	0.49
1:C:189:VAL:HG22	1:C:218:THR:HG21	1.94	0.49
1:C:355:ILE:HB	1:C:368:TRP:CZ2	2.47	0.49
1:A:305:ARG:HH12	1:A:364:HIS:CG	2.30	0.49
1:A:310:LEU:CD2	1:A:356:ASN:ND2	2.71	0.49
1:D:106:SER:C	1:D:108:ASN:H	2.21	0.49
1:A:304:LEU:H	1:A:309:LEU:HD22	1.75	0.49
1:A:315:ILE:O	1:A:335:LYS:NZ	2.45	0.49
1:B:95:LEU:HD23	1:B:124:LEU:HD13	1.94	0.49
1:B:204:ASP:C	1:B:204:ASP:OD1	2.55	0.49
1:C:66:ASN:ND2	1:C:90:ASP:OD2	2.45	0.49
1:C:325:LEU:O	1:C:325:LEU:HD13	2.12	0.49
1:D:36:ASN:C	1:D:36:ASN:ND2	2.66	0.49
1:D:90:ASP:HB2	4:D:420:HOH:O	2.12	0.49
1:B:12:SER:HA	1:B:15:GLU:CG	2.35	0.49
1:A:305:ARG:C	1:A:307:VAL:N	2.56	0.49
1:A:344:THR:HG22	1:A:353:SER:HB3	1.93	0.49
1:D:96:GLN:O	1:D:100:GLU:HG3	2.13	0.49
1:A:305:ARG:HH12	1:A:364:HIS:HB3	1.77	0.48
1:A:340:LYS:HZ3	1:A:357:ASN:HD22	1.61	0.48
1:B:50:ASN:ND2	1:B:53:ALA:H	2.11	0.48
1:A:189:VAL:CG2	1:A:218:THR:HG21	2.43	0.48
1:B:212:MET:HE2	4:B:442:HOH:O	2.13	0.48
1:C:172:GLY:C	1:C:174:GLU:HG2	2.38	0.48
1:D:204:ASP:OD1	1:D:204:ASP:C	2.56	0.48
1:C:335:LYS:HB2	1:C:337:PRO:HD3	1.95	0.48
1:A:332:ALA:HB1	1:A:339:PHE:HZ	1.74	0.48
1:B:119:LEU:HD13	1:B:157:MET:SD	2.54	0.48
1:C:201:ILE:HA	1:C:234:MET:HE2	1.96	0.48
1:A:213:GLN:NE2	1:A:261:THR:HB	2.28	0.48
1:A:342:GLU:HB2	1:A:354:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:HD13	1:C:305:ARG:CA	2.41	0.48
1:A:175:GLU:HG3	1:C:223:LYS:CG	2.44	0.48
1:A:322:GLY:O	1:A:324:VAL:N	2.47	0.48
1:D:12:SER:HA	1:D:15:GLU:CG	2.37	0.48
1:D:250:ILE:O	1:D:253:ILE:HD12	2.13	0.48
1:A:159:THR:HG22	1:A:188:ILE:HG21	1.95	0.48
1:C:155:GLY:O	1:C:159:THR:HG23	2.14	0.48
1:D:159:THR:HG22	1:D:188:ILE:HG21	1.95	0.48
1:C:294:ILE:HD13	1:C:388:ASN:CA	2.44	0.48
1:A:133:LEU:HD22	1:A:177:TYR:CE2	2.49	0.47
1:A:302:ASN:HD22	1:A:309:LEU:HA	1.79	0.47
1:B:205:ILE:HG13	1:B:206:TYR:CD2	2.49	0.47
1:D:36:ASN:ND2	1:D:38:SER:H	2.11	0.47
1:A:40:LEU:HD23	1:A:80:ALA:HB1	1.95	0.47
1:C:198:ASP:O	1:C:230:LYS:HE2	2.14	0.47
1:D:55:LYS:HE3	1:D:59:TYR:CZ	2.49	0.47
1:A:155:GLY:O	1:A:159:THR:HG22	2.14	0.47
1:B:52:LYS:HG2	4:B:430:HOH:O	2.14	0.47
1:B:106:SER:C	1:B:108:ASN:H	2.21	0.47
1:C:56:LEU:O	1:C:60:GLN:HG3	2.15	0.47
1:D:218:THR:HG22	1:D:219:PRO:HD2	1.96	0.47
1:C:185:LEU:HD22	1:C:218:THR:HG22	1.96	0.47
1:D:238:GLU:OE1	1:D:238:GLU:HA	2.13	0.47
1:A:271:SER:H	1:A:272:PRO:HD3	1.79	0.47
1:B:213:GLN:NE2	1:B:262:TYR:H	2.11	0.47
1:A:50:ASN:ND2	1:A:52:LYS:H	2.13	0.47
1:A:172:GLY:C	1:A:174:GLU:HG2	2.40	0.47
1:A:302:ASN:O	1:A:303:GLN:HG3	2.14	0.47
1:A:322:GLY:H	1:A:385:ILE:HG23	1.80	0.47
3:A:1001:B12:H8	3:A:1001:B12:N40	2.18	0.47
1:D:205:ILE:HG21	1:D:238:GLU:HG2	1.96	0.47
1:B:237:ASN:HA	1:B:240:LYS:HE3	1.97	0.47
1:A:155:GLY:O	1:A:159:THR:HG23	2.14	0.47
1:C:322:GLY:O	1:C:324:VAL:N	2.47	0.47
1:A:194:MET:O	1:A:194:MET:HG3	2.15	0.47
1:C:172:GLY:O	1:C:174:GLU:HG2	2.15	0.47
1:B:157:MET:CE	1:B:210:LEU:HD13	2.45	0.46
1:C:361:ASN:ND2	1:C:363:ASN:HB2	2.27	0.46
1:C:308:GLU:O	1:C:308:GLU:CG	2.61	0.46
1:D:194:MET:O	1:D:194:MET:HG3	2.14	0.46
1:A:220:GLU:OE1	1:A:221:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:CD1	1:A:305:ARG:CD	2.94	0.46
1:C:128:ASN:ND2	1:C:131:ALA:H	2.13	0.46
1:A:175:GLU:HG3	1:C:223:LYS:HG3	1.98	0.46
1:B:36:ASN:C	1:B:36:ASN:ND2	2.68	0.46
1:B:36:ASN:HD21	1:B:38:SER:HB2	1.81	0.46
1:C:305:ARG:C	1:C:307:VAL:N	2.55	0.46
1:C:305:ARG:HH12	1:C:364:HIS:CB	2.26	0.46
1:D:192:ILE:O	1:D:195:LYS:HB2	2.16	0.46
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.16	0.46
1:A:335:LYS:HB2	1:A:337:PRO:HD3	1.97	0.46
1:C:79:MET:HG2	1:C:126:GLN:HE22	1.81	0.46
1:C:303:GLN:C	1:C:304:LEU:HD23	2.39	0.46
1:A:297:ILE:H	1:A:297:ILE:HG13	1.48	0.46
1:B:198:ASP:O	1:B:230:LYS:HE3	2.15	0.46
1:C:151:ASN:HD22	1:C:154:THR:CB	2.28	0.46
1:C:192:ILE:O	1:C:195:LYS:HB2	2.15	0.46
3:C:1002:B12:H361	3:C:1002:B12:H411	1.60	0.46
1:D:144:LEU:HD12	1:D:144:LEU:HA	1.80	0.46
4:C:1216:HOH:O	2:F:1:NAG:H83	2.15	0.46
1:D:71:ILE:CD1	1:D:99:MET:SD	3.04	0.46
1:A:304:LEU:HD11	1:A:305:ARG:CD	2.44	0.46
1:B:114:PHE:C	1:B:117:PRO:HD2	2.41	0.46
1:B:192:ILE:O	1:B:195:LYS:HB2	2.16	0.46
1:C:213:GLN:NE2	1:C:261:THR:HB	2.29	0.46
2:F:1:NAG:H61	2:F:2:NAG:HN2	1.81	0.46
1:B:144:LEU:HD12	1:B:144:LEU:HA	1.82	0.45
1:B:205:ILE:H	1:B:205:ILE:HG12	1.57	0.45
1:C:266:PRO:HB2	1:C:267:GLN:NE2	2.31	0.45
1:D:50:ASN:C	1:D:50:ASN:ND2	2.71	0.45
1:A:304:LEU:C	1:A:304:LEU:HD22	2.41	0.45
1:B:110:GLU:OE1	1:B:110:GLU:N	2.44	0.45
1:B:205:ILE:HG21	1:B:238:GLU:HG2	1.98	0.45
1:C:361:ASN:ND2	1:C:361:ASN:C	2.72	0.45
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.81	0.45
1:A:273:ASP:CG	1:B:178:ARG:HH21	2.25	0.45
1:D:15:GLU:N	1:D:16:PRO:CD	2.79	0.45
1:D:62:MET:O	1:D:63:SER:CB	2.63	0.45
1:D:98:GLN:HG2	4:D:411:HOH:O	2.17	0.45
1:D:153:ASP:OD1	1:D:207:SER:HB2	2.16	0.45
1:A:192:ILE:O	1:A:195:LYS:HB2	2.16	0.45
1:D:71:ILE:HD11	1:D:99:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:O	1:A:60:GLN:HG3	2.16	0.45
1:C:313:GLU:N	1:C:313:GLU:OE1	2.49	0.45
1:A:141:LYS:NZ	1:C:187:ASP:OD1	2.30	0.45
1:A:361:ASN:ND2	1:A:361:ASN:C	2.73	0.45
1:B:223:LYS:HD3	1:B:223:LYS:C	2.42	0.45
1:C:11:PRO:O	1:C:13:ALA:N	2.49	0.45
1:C:95:LEU:HD11	1:C:120:ALA:HB1	1.98	0.45
1:C:159:THR:HG22	1:C:188:ILE:HG21	1.99	0.45
1:B:193:SER:O	1:B:194:MET:CG	2.61	0.45
1:B:213:GLN:HE22	1:B:262:TYR:H	1.65	0.45
1:C:104:PRO:HG3	1:C:142:THR:CG2	2.47	0.45
1:D:248:MET:HE1	4:D:404:HOH:O	2.15	0.45
1:A:87:ASP:HA	1:A:88:PRO:HD3	1.79	0.45
1:B:90:ASP:HB2	4:B:466:HOH:O	2.16	0.45
1:A:133:LEU:HB2	1:A:134:PRO:HD3	1.99	0.44
1:C:291:ALA:C	1:C:292:SER:OG	2.58	0.44
1:D:11:PRO:O	1:D:13:ALA:N	2.50	0.44
1:D:39:ILE:O	1:D:43:MET:HG2	2.17	0.44
1:D:174:GLU:H	1:D:174:GLU:HG2	1.40	0.44
1:D:205:ILE:CG2	1:D:238:GLU:HG2	2.47	0.44
1:A:344:THR:CG2	1:A:353:SER:HB3	2.47	0.44
1:C:336:ASN:N	1:C:337:PRO:CD	2.80	0.44
1:D:213:GLN:NE2	1:D:262:TYR:H	2.15	0.44
2:E:1:NAG:H61	2:E:2:NAG:HN2	1.82	0.44
1:A:305:ARG:NH1	1:A:364:HIS:HB3	2.32	0.44
1:C:307:VAL:O	1:C:308:GLU:HB3	2.17	0.44
1:A:291:ALA:C	1:A:292:SER:OG	2.59	0.44
1:B:271:SER:N	1:B:272:PRO:HD3	2.32	0.44
1:A:325:LEU:HD13	1:A:325:LEU:O	2.17	0.44
1:C:15:GLU:N	1:C:16:PRO:CD	2.81	0.44
1:C:303:GLN:HA	1:C:309:LEU:HD22	1.99	0.44
1:C:360:GLU:O	1:C:366:THR:CG2	2.61	0.44
1:B:55:LYS:HE3	1:B:59:TYR:CZ	2.52	0.44
1:C:96:GLN:O	1:C:100:GLU:HG3	2.17	0.44
1:C:344:THR:CG2	1:C:353:SER:HB3	2.48	0.44
3:A:1001:B12:H533	3:A:1001:B12:H482	1.99	0.44
1:B:133:LEU:HA	1:B:165:MET:HE2	2.00	0.44
1:C:148:SER:HB3	1:C:149:PRO:HD2	1.99	0.44
1:C:229:LYS:HA	1:C:232:THR:CG2	2.48	0.44
1:C:240:LYS:CE	4:C:1142:HOH:O	2.61	0.44
1:C:303:GLN:OE1	4:C:1220:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:GLN:HG3	1:C:340:LYS:HB2	2.00	0.44
1:A:8:CYS:HB2	1:A:232:THR:HG21	1.99	0.43
1:B:11:PRO:O	1:B:13:ALA:N	2.51	0.43
1:B:69:LEU:HD22	1:B:73:HIS:HB3	2.00	0.43
1:B:157:MET:HE2	1:B:210:LEU:HD13	2.00	0.43
1:C:133:LEU:HB2	1:C:134:PRO:HD3	2.00	0.43
1:D:69:LEU:HD12	1:D:74:LEU:HD13	2.00	0.43
1:D:205:ILE:HG13	1:D:206:TYR:CD2	2.54	0.43
1:D:223:LYS:HD3	1:D:223:LYS:C	2.42	0.43
1:C:335:LYS:CB	1:C:337:PRO:HD3	2.49	0.43
1:C:323:SER:O	1:C:324:VAL:O	2.36	0.43
1:D:271:SER:N	1:D:272:PRO:HD3	2.32	0.43
1:D:34:TYR:HA	1:D:35:PRO:HD3	1.88	0.43
1:C:271:SER:H	1:C:272:PRO:HD3	1.81	0.43
1:C:292:SER:O	1:C:293:ASN:OD1	2.36	0.43
1:A:229:LYS:HA	1:A:232:THR:CG2	2.48	0.43
1:C:189:VAL:CG2	1:C:218:THR:HG21	2.49	0.43
1:A:104:PRO:HG3	1:A:142:THR:CG2	2.49	0.43
1:A:290:SER:O	1:A:291:ALA:O	2.36	0.43
1:B:217:VAL:HG11	1:B:263:LEU:HD11	2.00	0.43
1:C:362:VAL:HG23	1:C:399:TYR:OH	2.19	0.43
1:D:36:ASN:HD22	1:D:37:PRO:N	2.15	0.43
1:D:50:ASN:ND2	1:D:53:ALA:H	2.17	0.43
1:C:87:ASP:HA	1:C:88:PRO:HD3	1.80	0.43
1:C:371:LEU:N	1:C:371:LEU:CD2	2.81	0.43
1:D:198:ASP:O	1:D:230:LYS:HE3	2.18	0.43
1:D:205:ILE:HG12	4:D:477:HOH:O	2.17	0.43
1:A:114:PHE:CZ	1:A:142:THR:HG22	2.54	0.42
1:B:210:LEU:HB2	4:B:470:HOH:O	2.19	0.42
1:C:319:VAL:HG22	1:C:323:SER:HB2	2.00	0.42
1:C:290:SER:CB	1:C:331:GLU:OE2	2.67	0.42
1:D:124:LEU:HB3	1:D:132:THR:OG1	2.20	0.42
1:B:228:CYS:O	1:B:232:THR:CG2	2.65	0.42
1:C:133:LEU:HB3	1:C:177:TYR:HE2	1.85	0.42
1:D:128:ASN:C	1:D:128:ASN:ND2	2.75	0.42
1:A:95:LEU:HD23	1:A:124:LEU:CD1	2.49	0.42
1:A:304:LEU:CG	1:A:305:ARG:N	2.82	0.42
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.88	0.42
1:B:225:GLU:HG2	4:B:454:HOH:O	2.18	0.42
1:C:89:GLY:O	1:C:90:ASP:C	2.62	0.42
1:B:185:LEU:O	1:B:189:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:LEU:HD12	1:C:162:LEU:HA	1.85	0.42
1:A:27:ASN:HB3	4:A:1136:HOH:O	2.18	0.42
3:A:1001:B12:H362	3:A:1001:B12:H351	2.02	0.42
1:C:290:SER:O	1:C:291:ALA:O	2.37	0.42
1:A:99:MET:HB3	1:A:135:ILE:HD13	2.02	0.42
1:B:108:ASN:HD22	1:B:108:ASN:HA	1.69	0.42
1:B:153:ASP:OD1	1:B:207:SER:HB2	2.20	0.42
1:B:212:MET:HB3	4:B:442:HOH:O	2.18	0.42
1:B:221:PRO:HB2	4:B:454:HOH:O	2.20	0.42
1:A:195:LYS:HD3	1:A:195:LYS:HA	1.92	0.42
1:A:298:TYR:CE2	1:A:329:LEU:HD22	2.54	0.42
1:B:224:LYS:HB3	4:B:489:HOH:O	2.19	0.42
1:D:11:PRO:HG2	1:D:14:GLN:HG2	2.02	0.42
1:D:185:LEU:O	1:D:189:VAL:HG22	2.19	0.42
1:A:114:PHE:CD1	1:A:143:LEU:HD13	2.54	0.42
1:A:313:GLU:OE1	1:A:313:GLU:N	2.53	0.42
1:D:116:GLY:N	1:D:117:PRO:CD	2.82	0.42
1:A:266:PRO:HB2	1:A:267:GLN:HE22	1.85	0.41
1:B:205:ILE:CG2	1:B:238:GLU:HG2	2.49	0.41
1:C:333:GLN:HG3	1:C:340:LYS:CB	2.50	0.41
1:C:337:PRO:C	1:C:339:PHE:N	2.78	0.41
1:B:163:THR:O	1:B:164:CYS:C	2.63	0.41
1:D:228:CYS:O	1:D:232:THR:CG2	2.68	0.41
1:A:151:ASN:HD21	1:A:153:ASP:HB2	1.85	0.41
1:C:50:ASN:HD22	1:C:52:LYS:H	1.68	0.41
1:D:199:ASN:O	1:D:234:MET:HG2	2.20	0.41
1:A:52:LYS:HE3	1:A:52:LYS:HB2	1.44	0.41
1:A:127:LYS:HD3	1:A:127:LYS:HA	1.79	0.41
1:A:292:SER:O	1:A:293:ASN:OD1	2.37	0.41
1:A:325:LEU:O	1:A:325:LEU:HD22	2.19	0.41
1:A:362:VAL:HG23	1:A:399:TYR:OH	2.20	0.41
1:B:119:LEU:HD13	1:B:157:MET:HG2	2.03	0.41
1:C:26:GLU:CD	1:C:43:MET:HE3	2.45	0.41
1:C:375:THR:HA	1:C:376:PRO:HD3	1.89	0.41
1:A:12:SER:O	1:A:13:ALA:HB2	2.20	0.41
1:A:95:LEU:HD11	1:A:120:ALA:HB1	2.02	0.41
1:A:336:ASN:N	1:A:337:PRO:CD	2.84	0.41
1:B:36:ASN:HD22	1:B:38:SER:H	1.69	0.41
1:C:127:LYS:HA	1:C:127:LYS:HD3	1.83	0.41
1:A:367:TYR:CD1	1:A:399:TYR:HD2	2.39	0.41
3:A:1001:B12:H351	3:A:1001:B12:C36	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:HIS:HB3	4:A:1127:HOH:O	2.20	0.41
1:C:325:LEU:N	1:C:384:TYR:O	2.50	0.41
3:A:1001:B12:C6	3:A:1001:B12:H4B	2.50	0.41
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.88	0.41
1:B:227:ASN:ND2	1:B:230:LYS:HB2	2.35	0.41
1:C:304:LEU:HB3	1:C:305:ARG:H	1.36	0.41
1:C:369:GLN:HE21	1:C:397:THR:HG21	1.86	0.41
1:A:323:SER:C	1:A:324:VAL:O	2.63	0.41
1:A:324:VAL:HG11	1:A:382:ALA:O	2.21	0.41
3:A:1001:B12:H472	3:A:1001:B12:H481	1.83	0.41
1:B:96:GLN:O	1:B:100:GLU:HG3	2.20	0.41
1:B:173:SER:O	1:B:175:GLU:HG2	2.21	0.41
1:B:223:LYS:HD3	1:B:223:LYS:O	2.21	0.41
1:C:337:PRO:O	1:C:339:PHE:N	2.54	0.41
1:D:213:GLN:HE22	1:D:262:TYR:H	1.69	0.41
1:A:198:ASP:O	1:A:230:LYS:HE2	2.21	0.41
1:A:303:GLN:HE21	1:A:303:GLN:HB2	1.60	0.41
1:B:69:LEU:HD12	1:B:74:LEU:HD13	2.03	0.41
1:C:325:LEU:HD23	1:C:386:PRO:CG	2.51	0.41
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.83	0.40
1:C:169:ILE:HB	4:D:407:HOH:O	2.20	0.40
1:C:304:LEU:N	1:C:309:LEU:HD22	2.33	0.40
1:A:15:GLU:N	1:A:16:PRO:CD	2.85	0.40
1:A:201:ILE:CA	1:A:234:MET:HE2	2.51	0.40
1:A:371:LEU:HD12	1:A:374:VAL:O	2.21	0.40
1:B:15:GLU:N	1:B:16:PRO:CD	2.83	0.40
1:D:110:GLU:O	1:D:110:GLU:HG2	2.21	0.40
1:D:245:HIS:HB2	4:D:465:HOH:O	2.22	0.40
1:D:265:VAL:HB	1:D:266:PRO:HD3	2.03	0.40
3:A:1001:B12:H552	3:A:1001:B12:H531	2.03	0.40
1:B:194:MET:O	1:B:194:MET:HG3	2.21	0.40
1:C:81:LEU:HD23	1:C:81:LEU:HA	1.83	0.40
1:C:112:SER:HA	1:C:154:THR:OG1	2.21	0.40
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.96	0.40
1:A:193:SER:O	1:A:194:MET:CG	2.68	0.40
1:C:99:MET:HB3	1:C:135:ILE:HD13	2.04	0.40
1:C:323:SER:C	1:C:324:VAL:O	2.65	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:A:241:GLN:O	1:C:52:LYS:NZ[1_655]	1.87	0.33

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	374/399 (94%)	333 (89%)	24 (6%)	17 (4%)	2	2
1	B	265/399 (66%)	240 (91%)	20 (8%)	5 (2%)	6	13
1	C	374/399 (94%)	334 (89%)	22 (6%)	18 (5%)	2	2
1	D	265/399 (66%)	243 (92%)	17 (6%)	5 (2%)	6	13
All	All	1278/1596 (80%)	1150 (90%)	83 (6%)	45 (4%)	3	4

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ALA
1	A	291	ALA
1	A	306	GLY
1	A	311	PHE
1	A	320	LYS
1	A	321	SER
1	A	324	VAL
1	A	388	ASN
1	B	12	SER
1	B	13	ALA
1	B	108	ASN
1	B	174	GLU
1	C	13	ALA
1	C	291	ALA
1	C	305	ARG
1	C	306	GLY
1	C	311	PHE

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Mol	Chain	Res	Type
1	C	320	LYS
1	C	321	SER
1	C	324	VAL
1	C	388	ASN
1	D	13	ALA
1	D	108	ASN
1	D	174	GLU
1	A	307	VAL
1	A	323	SER
1	A	361	ASN
1	B	65	ASP
1	C	307	VAL
1	C	323	SER
1	D	12	SER
1	D	65	ASP
1	A	292	SER
1	A	305	ARG
1	A	338	MET
1	C	292	SER
1	C	338	MET
1	C	361	ASN
1	A	90	ASP
1	A	336	ASN
1	C	12	SER
1	C	90	ASP
1	C	336	ASN
1	A	319	VAL
1	C	319	VAL

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	322/349 (92%)	284 (88%)	38 (12%)	5	10
1	B	229/349 (66%)	203 (89%)	26 (11%)	5	11
1	C	322/349 (92%)	281 (87%)	41 (13%)	4	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	229/349 (66%)	201 (88%)	28 (12%)	5	10
All	All	1102/1396 (79%)	969 (88%)	133 (12%)	5	10

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	24	LEU
1	A	50	ASN
1	A	52	LYS
1	A	74	LEU
1	A	76	LEU
1	A	101	ASN
1	A	119	LEU
1	A	124	LEU
1	A	159	THR
1	A	162	LEU
1	A	180	LEU
1	A	194	MET
1	A	216	SER
1	A	217	VAL
1	A	218	THR
1	A	232	THR
1	A	238	GLU
1	A	254	LEU
1	A	273	ASP
1	A	292	SER
1	A	294	ILE
1	A	295	THR
1	A	296	VAL
1	A	297	ILE
1	A	299	THR
1	A	303	GLN
1	A	304	LEU
1	A	308	GLU
1	A	313	GLU
1	A	319	VAL
1	A	323	SER
1	A	345	MET
1	A	350	LEU
1	A	357	ASN
1	A	358	ILE

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Mol	Chain	Res	Type
1	A	371	LEU
1	A	377	LEU
1	B	12	SER
1	B	17	LEU
1	B	45	LEU
1	B	50	ASN
1	B	61	LEU
1	B	71	ILE
1	B	74	LEU
1	B	76	LEU
1	B	108	ASN
1	B	119	LEU
1	B	124	LEU
1	B	133	LEU
1	B	142	THR
1	B	159	THR
1	B	162	LEU
1	B	180	LEU
1	B	189	VAL
1	B	197	LYS
1	B	205	ILE
1	B	217	VAL
1	B	218	THR
1	B	232	THR
1	B	238	GLU
1	B	245	HIS
1	B	253	ILE
1	B	254	LEU
1	C	14	GLN
1	C	24	LEU
1	C	50	ASN
1	C	52	LYS
1	C	74	LEU
1	C	76	LEU
1	C	101	ASN
1	C	119	LEU
1	C	121	ILE
1	C	124	LEU
1	C	128	ASN
1	C	159	THR
1	C	162	LEU
1	C	180	LEU

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Mol	Chain	Res	Type
1	C	194	MET
1	C	205	ILE
1	C	216	SER
1	C	217	VAL
1	C	218	THR
1	C	232	THR
1	C	238	GLU
1	C	254	LEU
1	C	273	ASP
1	C	292	SER
1	C	294	ILE
1	C	295	THR
1	C	296	VAL
1	C	297	ILE
1	C	299	THR
1	C	302	ASN
1	C	303	GLN
1	C	304	LEU
1	C	313	GLU
1	C	319	VAL
1	C	323	SER
1	C	345	MET
1	C	350	LEU
1	C	357	ASN
1	C	358	ILE
1	C	371	LEU
1	C	377	LEU
1	D	12	SER
1	D	17	LEU
1	D	45	LEU
1	D	61	LEU
1	D	68	ASP
1	D	71	ILE
1	D	74	LEU
1	D	76	LEU
1	D	108	ASN
1	D	119	LEU
1	D	124	LEU
1	D	128	ASN
1	D	133	LEU
1	D	142	THR
1	D	159	THR

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Mol	Chain	Res	Type
1	D	162	LEU
1	D	174	GLU
1	D	180	LEU
1	D	189	VAL
1	D	197	LYS
1	D	205	ILE
1	D	217	VAL
1	D	218	THR
1	D	232	THR
1	D	238	GLU
1	D	245	HIS
1	D	253	ILE
1	D	254	LEU

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	14	GLN
1	A	50	ASN
1	A	66	ASN
1	A	67	ASN
1	A	98	GLN
1	A	108	ASN
1	A	126	GLN
1	A	128	ASN
1	A	151	ASN
1	A	213	GLN
1	A	245	HIS
1	A	267	GLN
1	A	302	ASN
1	A	303	GLN
1	A	333	GLN
1	A	356	ASN
1	A	357	ASN
1	A	361	ASN
1	A	363	ASN
1	A	398	GLN
1	B	27	ASN
1	B	36	ASN
1	B	50	ASN
1	B	67	ASN
1	B	98	GLN

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Mol	Chain	Res	Type
1	B	108	ASN
1	B	126	GLN
1	B	128	ASN
1	B	146	ASN
1	B	213	GLN
1	B	246	ASN
1	B	267	GLN
1	C	14	GLN
1	C	19	ASN
1	C	50	ASN
1	C	66	ASN
1	C	67	ASN
1	C	98	GLN
1	C	126	GLN
1	C	128	ASN
1	C	151	ASN
1	C	183	GLN
1	C	213	GLN
1	C	245	HIS
1	C	267	GLN
1	C	302	ASN
1	C	303	GLN
1	C	333	GLN
1	C	356	ASN
1	C	357	ASN
1	C	361	ASN
1	C	363	ASN
1	C	398	GLN
1	D	27	ASN
1	D	36	ASN
1	D	50	ASN
1	D	67	ASN
1	D	98	GLN
1	D	108	ASN
1	D	126	GLN
1	D	128	ASN
1	D	146	ASN
1	D	213	GLN
1	D	246	ASN
1	D	267	GLN

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	1.38	2 (14%)	17,19,21	1.93	4 (23%)
2	NAG	E	2	2	14,14,15	1.40	2 (14%)	17,19,21	1.40	3 (17%)
2	NAG	F	1	2,1	14,14,15	1.77	4 (28%)	17,19,21	2.05	4 (23%)
2	NAG	F	2	2	14,14,15	1.22	2 (14%)	17,19,21	1.33	3 (17%)

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
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	C1-C2	4.10	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	3.13	1.56	1.52
2	E	2	NAG	C4-C5	2.84	1.59	1.53
2	F	1	NAG	C4-C5	2.82	1.59	1.53
2	F	2	NAG	C4-C5	2.47	1.58	1.53
2	F	1	NAG	C2-N2	2.42	1.50	1.46
2	E	1	NAG	C4-C5	2.32	1.58	1.53
2	E	2	NAG	O5-C5	2.30	1.47	1.43
2	F	2	NAG	O5-C5	2.26	1.47	1.43
2	F	1	NAG	O5-C5	2.03	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	5.08	129.71	122.90
2	E	1	NAG	C2-N2-C7	4.66	129.14	122.90
2	F	1	NAG	C8-C7-N2	4.29	123.23	116.12
2	E	1	NAG	C8-C7-N2	4.18	123.05	116.12
2	F	1	NAG	O7-C7-C8	-3.74	115.40	122.05
2	E	1	NAG	O7-C7-C8	-3.42	115.96	122.05
2	F	1	NAG	C4-C3-C2	-2.91	106.75	111.02
2	E	1	NAG	C4-C3-C2	-2.82	106.89	111.02
2	E	2	NAG	C1-O5-C5	-2.75	108.51	112.19
2	F	2	NAG	C2-N2-C7	2.59	126.37	122.90
2	E	2	NAG	C2-N2-C7	2.59	126.37	122.90
2	F	2	NAG	C1-O5-C5	-2.40	108.97	112.19
2	F	2	NAG	C1-C2-N2	-2.28	106.85	110.43
2	E	2	NAG	C1-C2-N2	-2.13	107.08	110.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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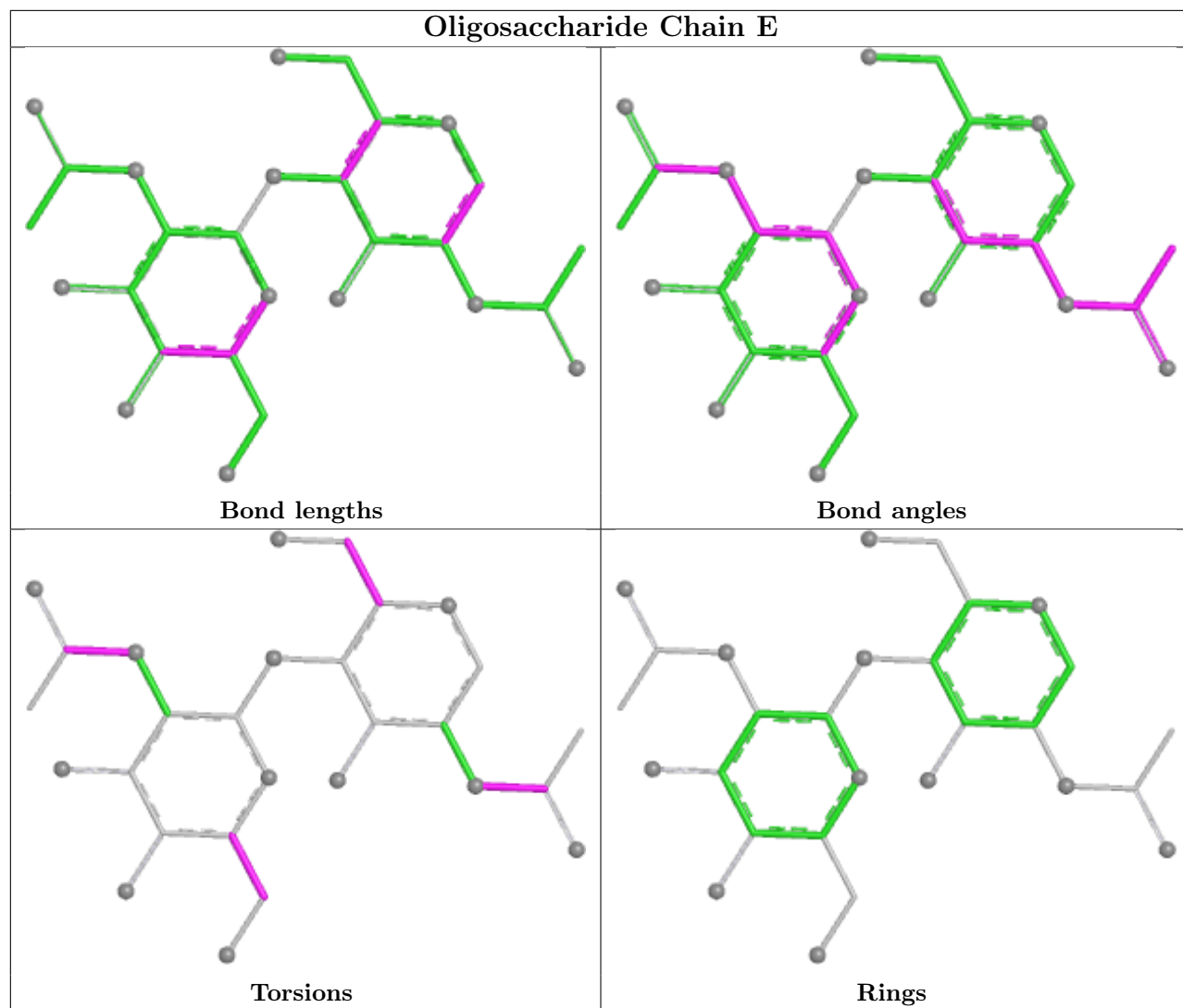
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

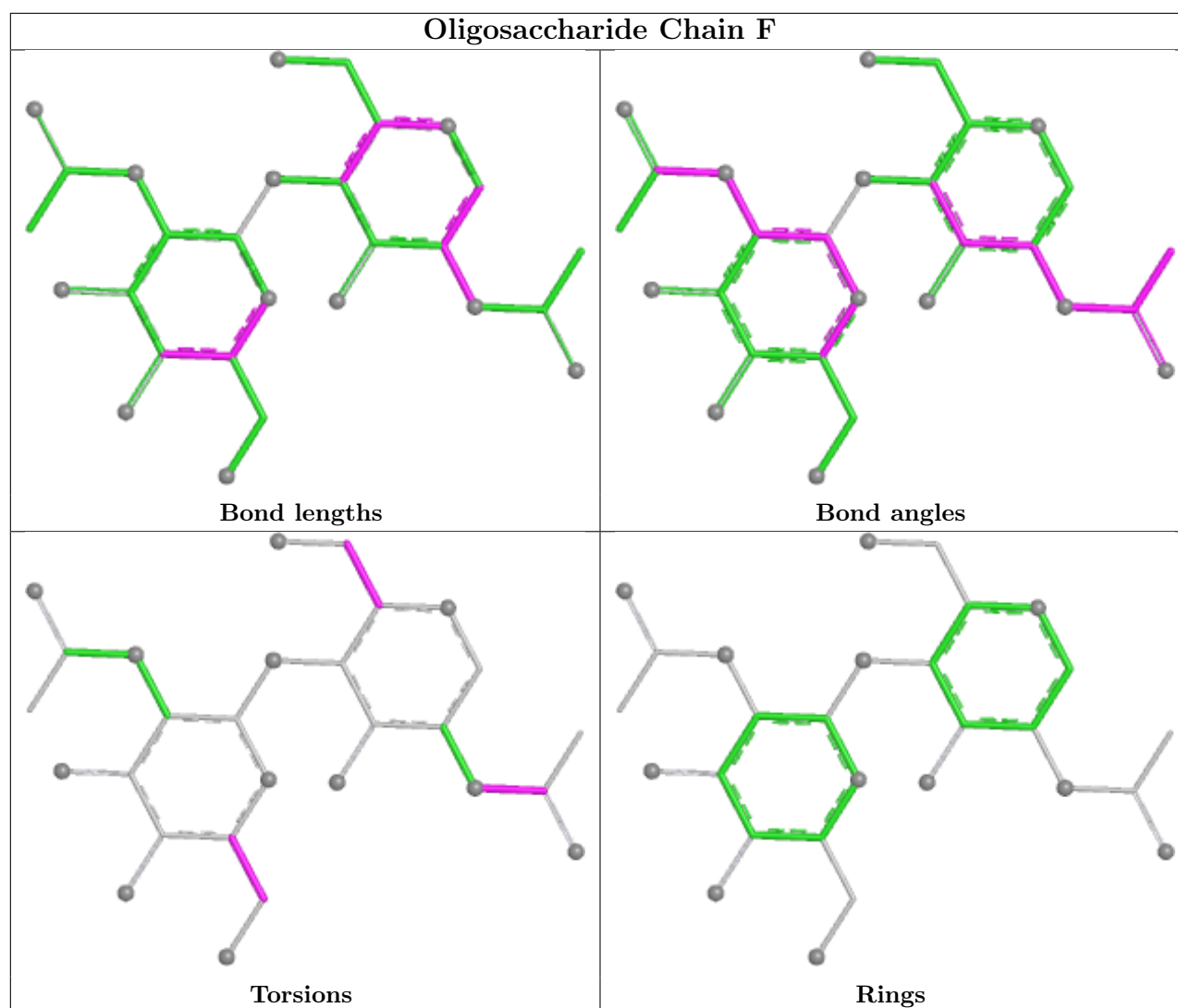
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	F	1	NAG	2	0
2	E	1	NAG	1	0
2	F	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	B12	A	1001	-	94,101,101	1.80	26 (27%)	149,166,166	1.35	22 (14%)
3	B12	C	1002	-	94,101,101	1.75	18 (19%)	149,166,166	1.33	20 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B12	A	1001	-	-	10/56/223/223	0/3/11/11
3	B12	C	1002	-	-	5/56/223/223	0/3/11/11

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	B12	C14-N23	5.08	1.41	1.35
3	C	1002	B12	C7B-C6B	4.85	1.46	1.39
3	A	1001	B12	C14-N23	4.42	1.41	1.35
3	A	1001	B12	C7B-C6B	4.33	1.45	1.39
3	A	1001	B12	C11-N23	4.24	1.44	1.36
3	C	1002	B12	C41-C8	4.22	1.64	1.54
3	A	1001	B12	C6B-C5B	3.99	1.50	1.40
3	A	1001	B12	C30-C3	3.84	1.63	1.54
3	C	1002	B12	C30-C3	3.84	1.63	1.54
3	C	1002	B12	C19-N24	3.82	1.54	1.49
3	C	1002	B12	C6B-C5B	3.69	1.49	1.40
3	A	1001	B12	C19-N24	3.56	1.54	1.49
3	A	1001	B12	C1-C2	3.55	1.67	1.58
3	C	1002	B12	C2R-C3R	-3.46	1.45	1.53
3	C	1002	B12	C9-N22	3.43	1.39	1.30
3	A	1001	B12	C2R-C3R	-3.41	1.45	1.53
3	C	1002	B12	C11-N23	3.32	1.43	1.36
3	C	1002	B12	C36-C7	3.27	1.59	1.54
3	A	1001	B12	C41-C8	3.22	1.61	1.54
3	C	1002	B12	O58-C57	3.18	1.29	1.23
3	A	1001	B12	C9-N22	3.18	1.38	1.30
3	A	1001	B12	O6R-C4R	3.06	1.51	1.45
3	A	1001	B12	C8B-C9B	3.06	1.45	1.40
3	A	1001	B12	O58-C57	2.87	1.28	1.23
3	A	1001	B12	C36-C7	2.85	1.59	1.54
3	C	1002	B12	C8B-C9B	2.81	1.44	1.40
3	C	1002	B12	C54-C17	2.77	1.59	1.54
3	C	1002	B12	C12-C11	2.76	1.56	1.52
3	A	1001	B12	C12-C11	2.62	1.56	1.52
3	C	1002	B12	C35-C5	2.61	1.56	1.50
3	A	1001	B12	C8B-N1B	-2.59	1.34	1.39
3	C	1002	B12	C6-C5	2.45	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	B12	C6-C5	2.32	1.42	1.36
3	A	1001	B12	C2B-N1B	2.31	1.41	1.37
3	A	1001	B12	C54-C17	2.30	1.58	1.54
3	A	1001	B12	C35-C5	2.23	1.55	1.50
3	A	1001	B12	O44-C43	2.23	1.30	1.23
3	A	1001	B12	C2R-C1R	2.20	1.60	1.53
3	A	1001	B12	C48-C13	2.19	1.59	1.54
3	C	1002	B12	C16-C15	2.14	1.50	1.44
3	A	1001	B12	C17-C16	2.12	1.59	1.54
3	A	1001	B12	P-O4	-2.08	1.43	1.50
3	C	1002	B12	P-O4	-2.01	1.43	1.50
3	A	1001	B12	C16-C15	2.01	1.50	1.44

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	B12	C60-C18-C17	4.05	126.91	115.82
3	A	1001	B12	C12-C13-C14	3.86	108.60	102.26
3	C	1002	B12	C12-C13-C14	3.75	108.43	102.26
3	A	1001	B12	C60-C18-C17	3.72	125.99	115.82
3	A	1001	B12	C41-C8-C9	3.65	117.56	111.19
3	C	1002	B12	C41-C8-C9	3.59	117.45	111.19
3	A	1001	B12	C37-C7-C8	-3.43	99.32	108.37
3	A	1001	B12	C47-C12-C46	-3.38	103.81	109.41
3	C	1002	B12	C42-C41-C8	3.13	123.51	114.65
3	A	1001	B12	C2-C3-C4	3.04	105.06	101.64
3	C	1002	B12	C7B-C8B-C9B	-3.01	118.86	122.47
3	C	1002	B12	C47-C12-C46	-2.94	104.53	109.41
3	C	1002	B12	C41-C8-C7	-2.94	106.09	114.19
3	C	1002	B12	C37-C7-C8	-2.90	100.71	108.37
3	A	1001	B12	C47-C12-C13	2.74	123.83	112.74
3	A	1001	B12	C41-C8-C7	-2.71	106.72	114.19
3	A	1001	B12	C49-C48-C13	2.61	122.06	114.65
3	A	1001	B12	C42-C41-C8	2.60	122.01	114.65
3	A	1001	B12	C20-C1-N21	-2.59	105.97	110.26
3	C	1002	B12	O58-C57-C56	-2.59	117.33	122.02
3	C	1002	B12	C9-N22-C6	2.54	108.34	105.28
3	C	1002	B12	C48-C13-C12	-2.53	109.28	116.52
3	A	1001	B12	C7B-C8B-C9B	-2.52	119.46	122.47
3	A	1001	B12	C48-C13-C12	-2.47	109.47	116.52
3	A	1001	B12	C2R-C3R-C4R	2.45	107.52	103.24
3	C	1002	B12	C18-C60-C61	2.41	120.16	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	B12	C9-N22-C6	2.41	108.17	105.28
3	A	1001	B12	O58-C57-C56	-2.41	117.66	122.02
3	A	1001	B12	C8-C7-C6	2.34	104.89	100.92
3	C	1002	B12	C2-C3-C4	2.32	104.25	101.64
3	C	1002	B12	C8-C7-C6	2.30	104.83	100.92
3	C	1002	B12	C7B-C8B-N1B	2.26	135.85	131.39
3	C	1002	B12	C20-C1-N21	-2.25	106.54	110.26
3	C	1002	B12	C8B-N1B-C1R	2.22	129.16	125.41
3	C	1002	B12	C47-C12-C13	2.17	121.55	112.74
3	A	1001	B12	C3R-C2R-C1R	2.11	104.54	99.89
3	C	1002	B12	C55-C17-C18	-2.11	107.10	111.12
3	A	1001	B12	C9B-N3B-C2B	-2.08	101.85	104.40
3	A	1001	B12	C15-C16-N24	-2.08	119.47	122.42
3	A	1001	B12	C47-C12-C11	2.05	117.41	110.08
3	C	1002	B12	C1-C19-C18	-2.04	118.60	121.90
3	A	1001	B12	C46-C12-C13	-2.02	104.55	112.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

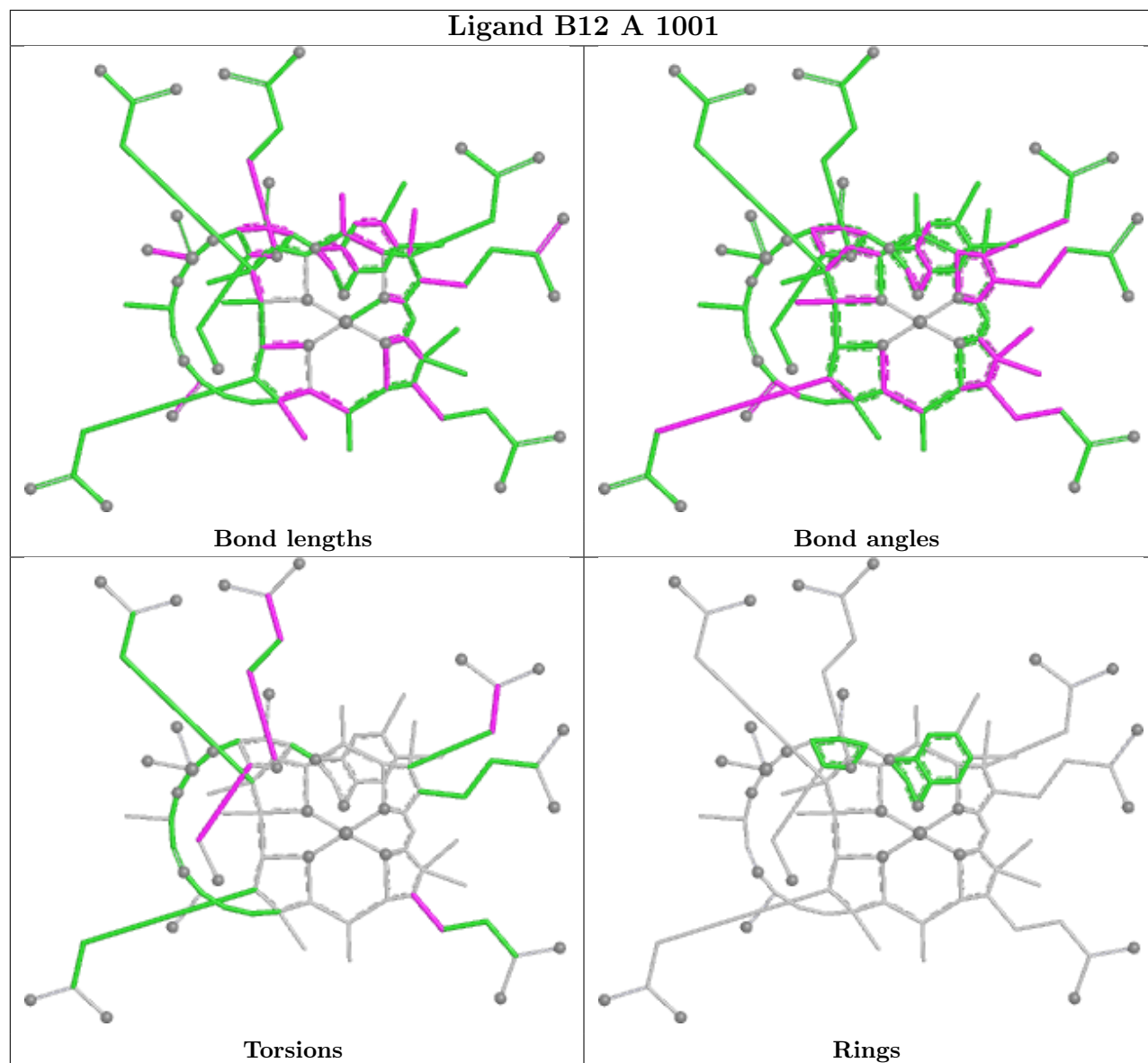
Mol	Chain	Res	Type	Atoms
3	A	1001	B12	C3R-C4R-C5R-O8R
3	A	1001	B12	O6R-C4R-C5R-O8R
3	C	1002	B12	C3R-C4R-C5R-O8R
3	C	1002	B12	O6R-C4R-C5R-O8R
3	A	1001	B12	C7-C37-C38-N40
3	A	1001	B12	C7-C37-C38-O39
3	A	1001	B12	C4-C3-C30-C31
3	A	1001	B12	C2-C3-C30-C31
3	C	1002	B12	C14-C13-C48-C49
3	C	1002	B12	C12-C13-C48-C49
3	C	1002	B12	C30-C31-C32-N33
3	A	1001	B12	C12-C13-C48-C49
3	A	1001	B12	C14-C13-C48-C49
3	A	1001	B12	C30-C31-C32-N33
3	A	1001	B12	C30-C31-C32-O34

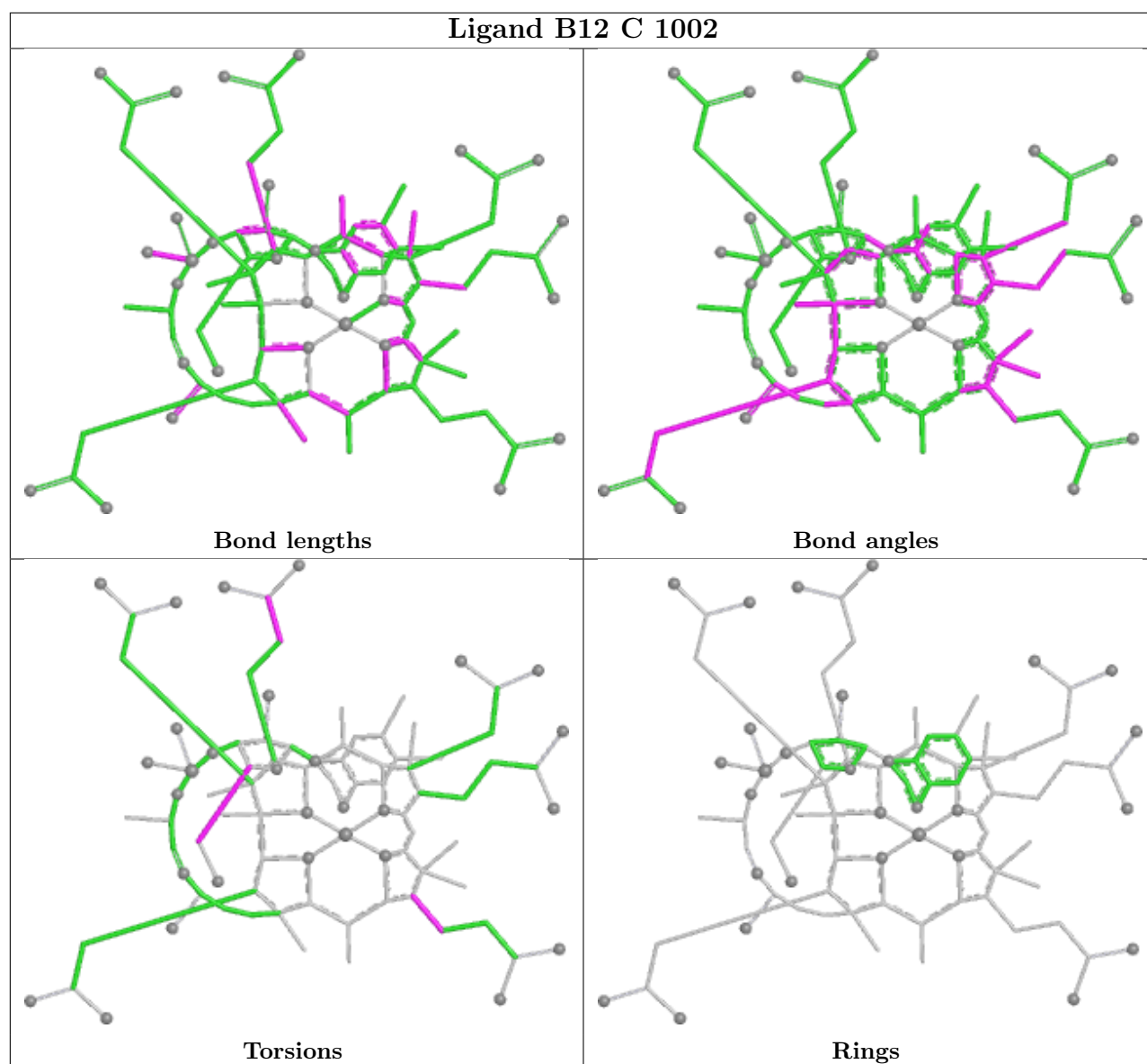
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	B12	10	0
3	C	1002	B12	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	378/399 (94%)	0.27	33 (8%) 16 12	29, 49, 97, 99	1 (0%)
1	B	267/399 (66%)	0.07	10 (3%) 45 39	31, 48, 85, 99	0
1	C	378/399 (94%)	0.52	52 (13%) 6 5	30, 52, 99, 99	2 (0%)
1	D	267/399 (66%)	0.01	13 (4%) 35 29	30, 46, 81, 99	0
All	All	1290/1596 (80%)	0.25	108 (8%) 17 13	29, 49, 97, 99	3 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	ALA	5.9
1	A	304	LEU	5.7
1	C	321	SER	5.4
1	C	322	GLY	5.4
1	C	306	GLY	5.2
1	C	307	VAL	5.1
1	A	292	SER	5.1
1	A	321	SER	4.9
1	A	307	VAL	4.4
1	C	336	ASN	4.3
1	A	312	ASN	4.1
1	A	322	GLY	3.9
1	A	290	SER	3.8
1	C	323	SER	3.8
1	D	224	LYS	3.8
1	C	304	LEU	3.7
1	C	332	ALA	3.7
1	C	311	PHE	3.7
1	C	12	SER	3.7
1	D	174	GLU	3.7
1	C	295	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	174	GLU	3.5
1	C	272	PRO	3.5
1	A	336	ASN	3.5
1	C	175	GLU	3.5
1	C	291	ALA	3.4
1	D	108	ASN	3.4
1	D	272	PRO	3.4
1	A	315	ILE	3.3
1	C	221	PRO	3.3
1	C	303	GLN	3.3
1	A	317	VAL	3.2
1	C	11	PRO	3.1
1	C	390	GLU	3.1
1	C	298	TYR	3.1
1	B	271	SER	3.1
1	B	108	ASN	3.0
1	B	272	PRO	3.0
1	A	303	GLN	3.0
1	D	245	HIS	3.0
1	C	370	PHE	3.0
1	A	7	SER	2.9
1	C	173	SER	2.9
1	A	27	ASN	2.9
1	A	176	GLY	2.9
1	C	14	GLN	2.8
1	B	34	TYR	2.8
1	A	323	SER	2.8
1	C	324	VAL	2.8
1	A	173	SER	2.8
1	C	237	ASN	2.8
1	A	314	THR	2.8
1	A	297	ILE	2.7
1	B	174	GLU	2.7
1	A	335	LYS	2.7
1	C	223	LYS	2.7
1	C	374	VAL	2.7
1	C	33	ALA	2.6
1	C	273	ASP	2.6
1	A	311	PHE	2.6
1	B	64	SER	2.6
1	C	10	VAL	2.6
1	A	313	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	7	SER	2.5
1	C	305	ARG	2.5
1	C	297	ILE	2.4
1	D	225	GLU	2.4
1	C	337	PRO	2.4
1	C	338	MET	2.4
1	A	306	GLY	2.4
1	C	292	SER	2.4
1	D	12	SER	2.4
1	C	16	PRO	2.4
1	D	221	PRO	2.4
1	C	289	THR	2.4
1	B	33	ALA	2.3
1	C	296	VAL	2.3
1	A	339	PHE	2.3
1	D	176	GLY	2.3
1	A	295	THR	2.3
1	C	310	LEU	2.3
1	C	339	PHE	2.3
1	D	7	SER	2.2
1	A	319	VAL	2.2
1	C	335	LYS	2.2
1	B	245	HIS	2.2
1	A	318	SER	2.2
1	B	173	SER	2.2
1	C	290	SER	2.2
1	C	300	ILE	2.2
1	A	272	PRO	2.1
1	A	228	CYS	2.1
1	C	194	MET	2.1
1	C	9	SER	2.1
1	A	175	GLU	2.1
1	C	366	THR	2.1
1	C	312	ASN	2.1
1	C	308	GLU	2.0
1	D	271	SER	2.0
1	B	221	PRO	2.0
1	C	389	HIS	2.0
1	D	67	ASN	2.0
1	C	319	VAL	2.0
1	D	34	TYR	2.0
1	A	308	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	341	PHE	2.0
1	A	310	LEU	2.0
1	C	315	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

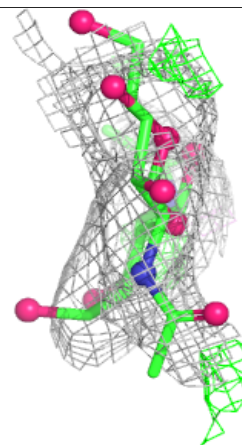
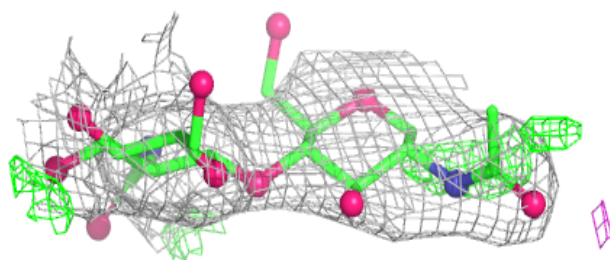
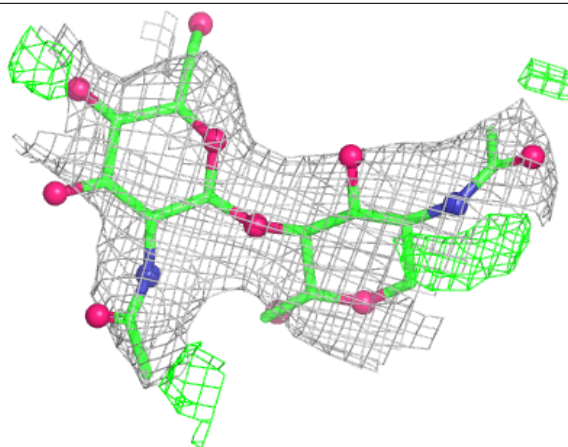
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

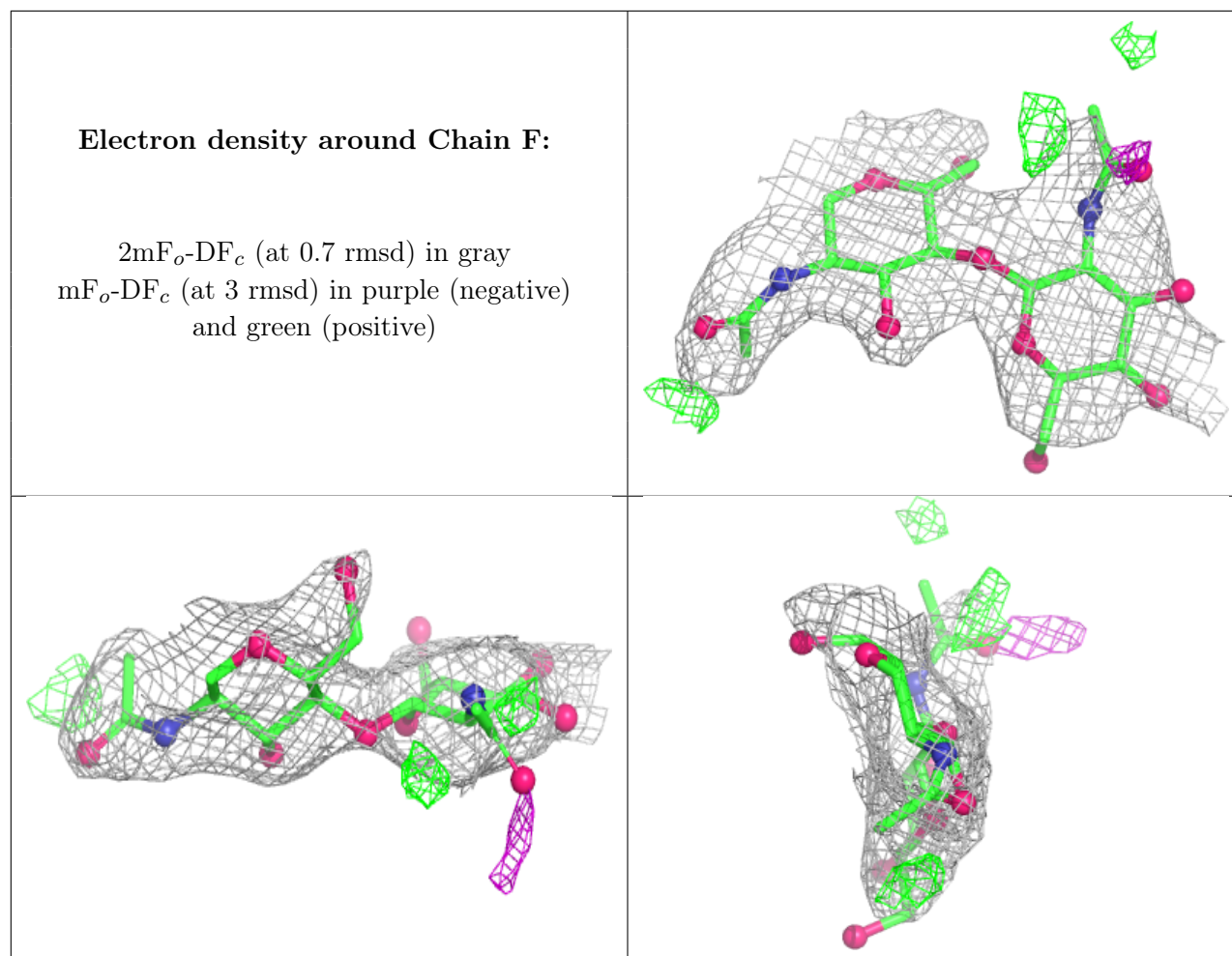
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	2	14/15	0.65	0.18	97,99,99,99	0
2	NAG	F	2	14/15	0.67	0.18	95,98,99,99	0
2	NAG	F	1	14/15	0.82	0.16	86,87,91,94	0
2	NAG	E	1	14/15	0.85	0.18	94,97,99,99	0

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 E:

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





6.4 Ligands [i](#)

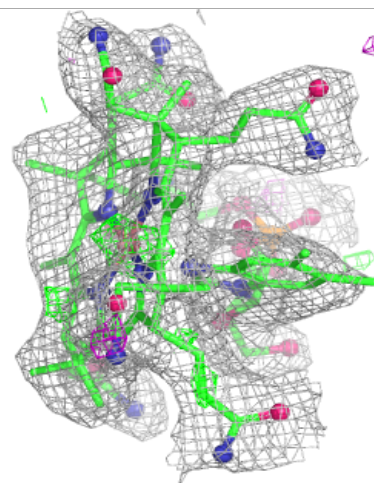
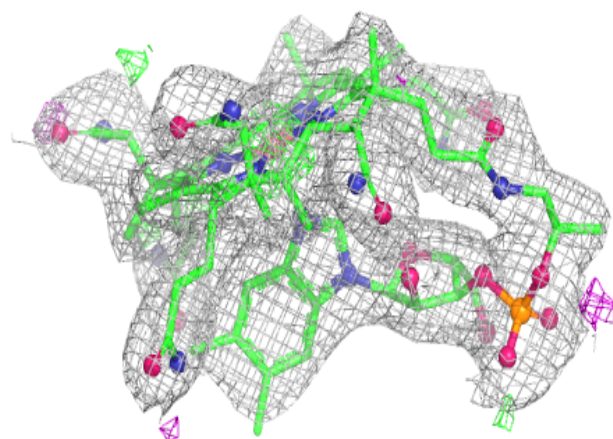
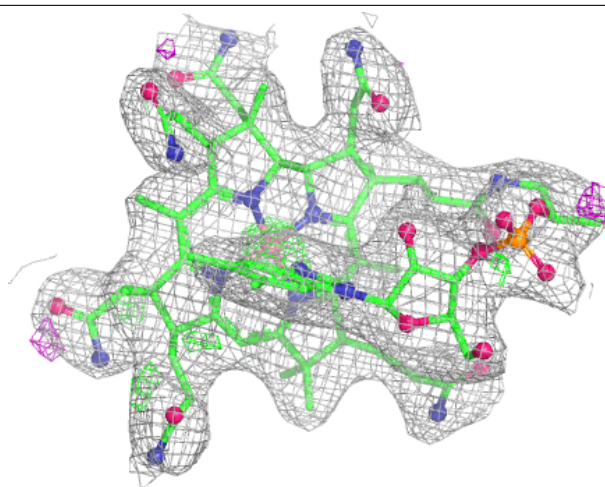
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	B12	A	1001	91/91	0.95	0.09	30,41,53,68	0
3	B12	C	1002	91/91	0.95	0.09	37,47,60,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

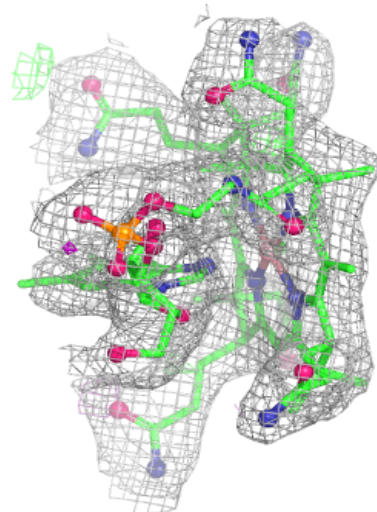
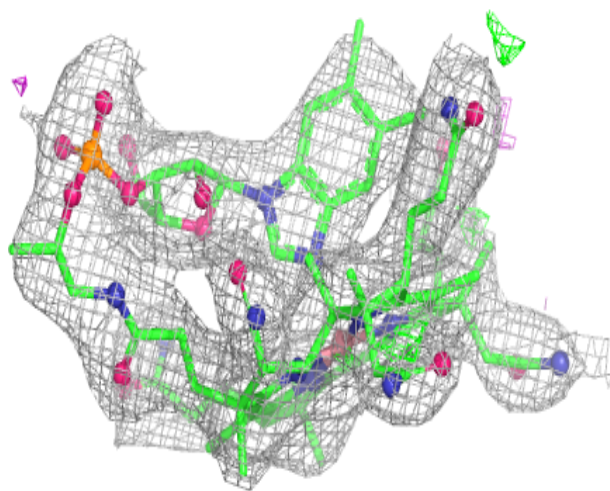
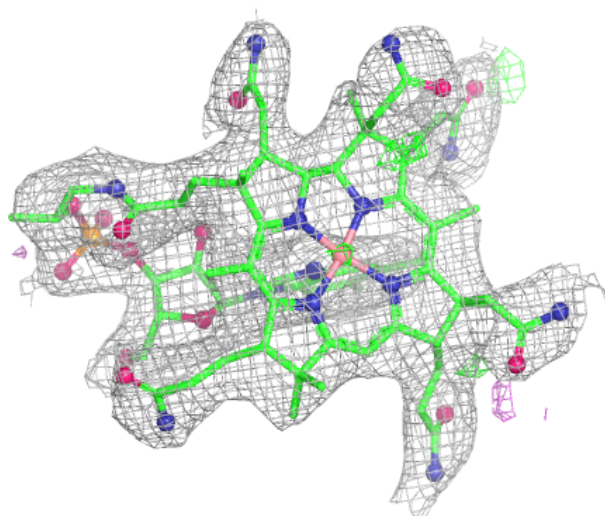
Electron density around B12 A 1001:

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



Electron density around B12 C 1002:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.