



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:21 PM UTC

PDB ID : 1A0H / pdb_00001a0h
Title : THE X-RAY CRYSTAL STRUCTURE OF PPACK-MEIZOTHROMBIN
DESF1: KRINGLE/THROMBIN AND CARBOHYDRATE/KRINGLE/TH
ROMBIN INTERACTIONS AND LOCATION OF THE LINKER CHAIN
Authors : Martin, P.D.; Malkowski, M.G.; Box, J.; Esmon, C.T.; Edwards, B.F.P.
Deposited on : 1997-11-30
Resolution : 3.20 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

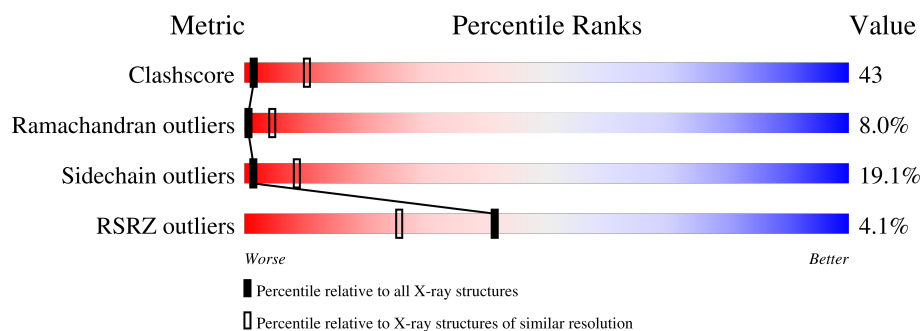
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	159	9% 41% 40% 16% .
1	D	159	12% 31% 45% 19% 5%
2	B	259	30% 53% 14% .
2	E	259	25% 51% 19% 5%
3	C	2	100%
3	F	2	50% 50%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6901 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 MEIZOTHROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1255	773	213	262	7			
1	D	159	Total	C	N	O	S	0	0	0
			1255	773	213	262	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	HIS	SER	conflict	UNP P00735
D	187	HIS	SER	conflict	UNP P00735

- Molecule 2 is a protein called MEIZOTHROMBIN.

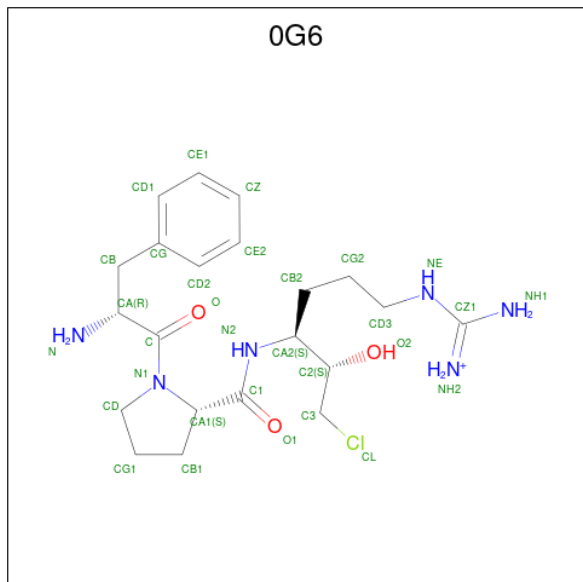
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			
2	E	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: $C_{21}H_{34}ClN_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			30	21	6	3		
4	E	1	Total	C	N	O	0	0
			30	21	6	3		

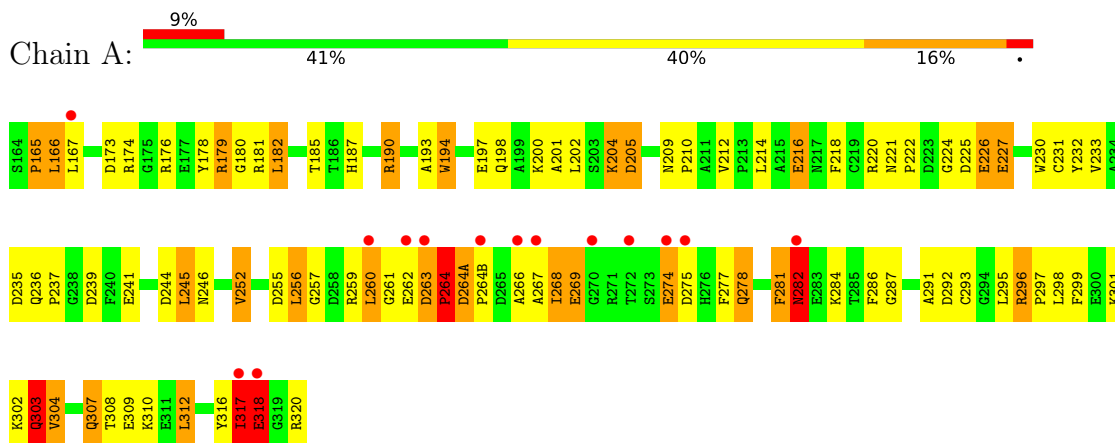
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	23	Total	O	0	0
			23	23		
5	D	16	Total	O	0	0
			16	16		
5	E	23	Total	O	0	0
			23	23		

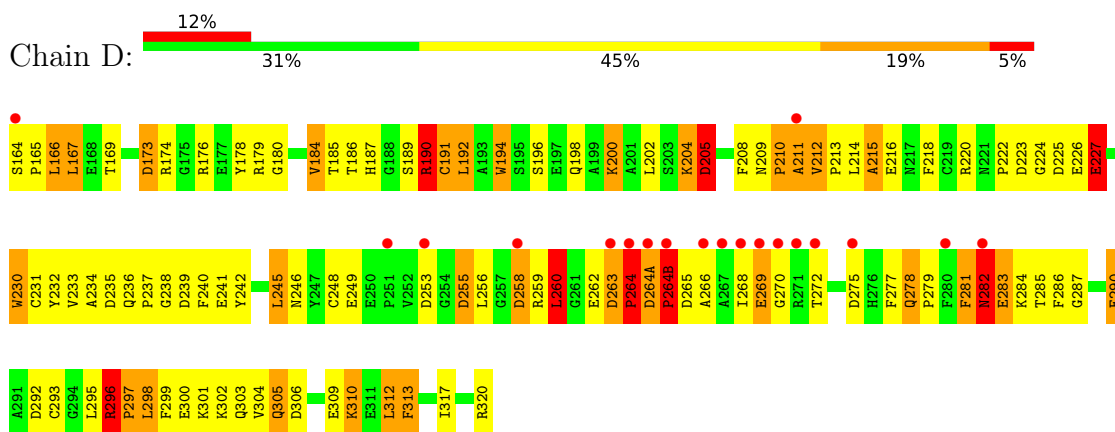
3 Residue-property plots

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.

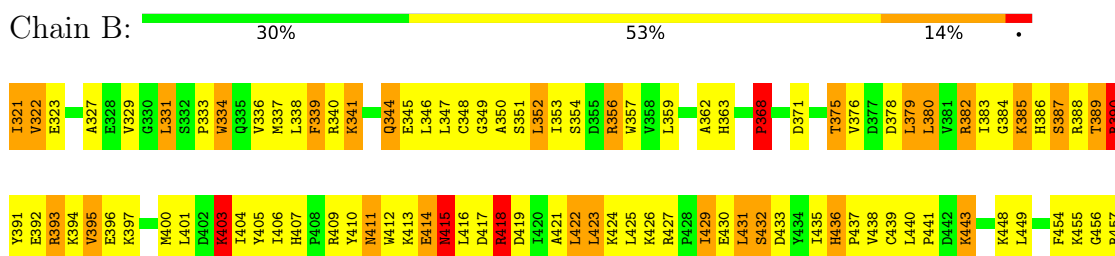
• Molecule 1: MEIZOTHROMBIN

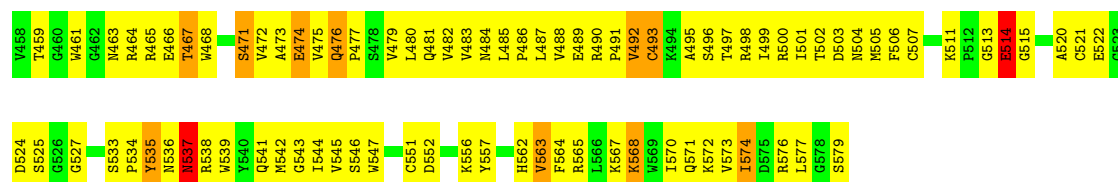


• Molecule 1: MEIZOTHROMBIN

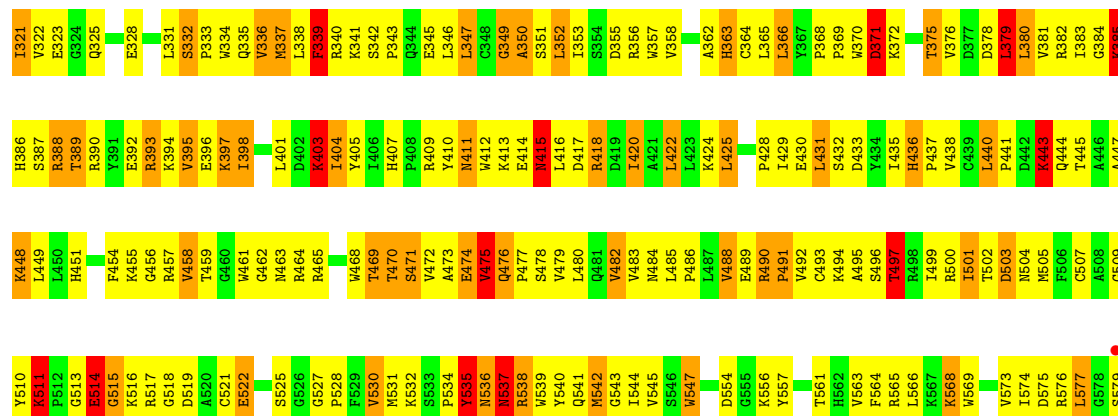


• Molecule 2: MEIZOTHROMBIN





• Molecule 2: MEIZOTHROMBIN



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	186.15Å 186.15Å 120.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 3.20 7.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	84.0 (7.00-3.20) 78.1 (7.00-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.12Å)	Xtriage
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.205 , 0.242 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 98.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6901	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: 0G6, 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	1.08	3/1285 (0.2%)	1.26	12/1739 (0.7%)
1	D	0.78	0/1285	1.30	21/1739 (1.2%)
2	B	0.86	1/2148 (0.0%)	1.35	22/2905 (0.8%)
2	E	0.87	1/2148 (0.0%)	1.41	36/2905 (1.2%)
All	All	0.90	5/6866 (0.1%)	1.34	91/9288 (1.0%)

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
2	E	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	ILE	CA-CB	25.25	1.91	1.54
1	A	317	ILE	CA-C	11.65	1.70	1.52
1	A	318	GLU	N-CA	6.08	1.54	1.46
2	E	501	ILE	CA-CB	-5.16	1.48	1.54
2	B	429	ILE	CA-CB	5.02	1.59	1.54

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	395	VAL	N-CA-C	13.63	123.57	112.12
2	B	395	VAL	N-CA-C	12.55	126.74	111.05
1	A	296	ARG	CA-C-N	11.21	130.90	119.24
1	A	296	ARG	C-N-CA	11.21	130.90	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	535	TYR	N-CA-C	-9.73	94.44	109.52
2	B	368	PRO	N-CA-C	9.25	121.99	110.70
1	D	263	ASP	CA-C-N	9.21	131.35	119.84
1	D	263	ASP	C-N-CA	9.21	131.35	119.84
2	B	341	LYS	N-CA-C	9.14	122.42	111.82
1	A	263	ASP	N-CA-C	8.50	122.44	110.20
2	E	332	SER	CA-C-N	7.89	127.55	119.82
2	E	332	SER	C-N-CA	7.89	127.55	119.82
2	E	463	ASN	N-CA-C	7.73	121.71	110.42
1	D	232	TYR	N-CA-C	-7.62	97.31	109.59
2	E	366	LEU	N-CA-C	7.62	120.83	108.34
2	B	414	GLU	N-CA-C	7.53	122.45	112.13
1	D	305	GLN	N-CA-C	7.42	121.46	110.48
2	B	403	LYS	N-CA-C	7.25	124.62	110.56
2	B	415	ASN	N-CA-C	7.24	118.96	110.41
2	B	514	GLU	N-CA-C	7.03	125.77	110.80
2	E	403	LYS	N-CA-C	6.97	125.65	110.80
2	B	574	ILE	N-CA-C	6.90	117.61	110.36
2	E	349	GLY	N-CA-C	-6.75	103.49	112.81
2	B	546	SER	N-CA-C	6.70	121.30	112.72
2	E	362	ALA	N-CA-C	6.49	118.35	111.28
2	B	356	ARG	N-CA-C	6.44	122.62	114.31
2	E	336	VAL	N-CA-C	6.43	118.05	107.24
1	D	264(B)	PRO	N-CA-C	-6.40	103.84	112.48
1	D	230	TRP	N-CA-C	6.37	116.97	108.38
2	B	429	ILE	N-CA-C	-6.36	103.02	110.21
1	D	264	PRO	N-CA-C	6.33	125.51	112.47
2	E	339	PHE	N-CA-C	6.31	119.30	109.52
1	A	281	PHE	N-CA-C	6.23	121.72	112.94
1	A	307	GLN	N-CA-C	6.21	124.02	110.80
1	D	208	PHE	N-CA-C	6.18	118.25	108.67
2	B	419	ASP	N-CA-C	-6.09	106.51	112.97
2	E	482	VAL	N-CA-C	6.03	117.44	108.46
2	B	376	VAL	N-CA-C	6.00	116.66	110.36
2	E	385	LYS	N-CA-C	5.99	118.62	110.35
1	A	263	ASP	CA-C-N	5.97	127.30	119.84
1	A	263	ASP	C-N-CA	5.97	127.30	119.84
2	E	398	ILE	CB-CA-C	-5.96	104.85	111.35
2	B	463	ASN	N-CA-C	5.94	118.67	110.35
1	D	233	VAL	N-CA-CB	-5.89	105.73	112.21
2	E	547	TRP	N-CA-C	5.89	117.17	108.86
1	A	231	CYS	CB-CA-C	-5.86	99.22	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	448	LYS	N-CA-C	5.82	117.43	111.14
2	E	473	ALA	N-CA-C	-5.80	104.86	111.07
2	E	505	MET	N-CA-C	-5.77	99.64	108.76
1	D	296	ARG	CA-C-N	5.74	127.02	119.84
1	D	296	ARG	C-N-CA	5.74	127.02	119.84
1	D	312	LEU	N-CA-C	-5.74	105.54	112.54
2	E	476	GLN	CA-C-N	5.72	126.99	119.84
2	E	476	GLN	C-N-CA	5.72	126.99	119.84
2	E	379	LEU	N-CA-C	5.70	118.75	109.24
1	D	282	ASN	N-CA-C	5.66	122.86	110.80
2	E	469	THR	N-CA-C	-5.66	103.89	112.04
1	D	227	GLU	N-CA-C	-5.65	104.17	113.50
1	D	189	SER	N-CA-C	5.60	118.02	109.95
2	E	364	CYS	N-CA-C	-5.50	104.80	112.45
2	E	511	LYS	CA-C-N	5.49	125.84	119.47
2	E	511	LYS	C-N-CA	5.49	125.84	119.47
1	A	282	ASN	N-CA-C	5.46	122.43	110.80
2	E	515	GLY	N-CA-C	5.44	123.45	115.08
2	B	448	LYS	N-CA-C	5.41	117.88	111.33
1	A	312	LEU	N-CA-C	-5.37	105.43	111.28
1	A	232	TYR	N-CA-C	-5.32	100.58	109.24
1	D	296	ARG	N-CA-C	5.31	119.05	109.44
2	E	538	ARG	N-CA-C	-5.30	102.34	110.14
1	A	182	LEU	CB-CG-CD2	-5.28	94.87	110.70
1	D	281	PHE	N-CA-C	5.28	122.21	113.50
1	D	194	TRP	N-CA-C	5.25	119.17	112.34
2	E	440	LEU	N-CA-C	-5.20	103.22	109.72
1	D	313	PHE	N-CA-C	5.17	117.71	111.40
2	B	476	GLN	CA-C-N	5.17	125.17	119.90
2	B	476	GLN	C-N-CA	5.17	125.17	119.90
2	B	385	LYS	N-CA-C	5.16	117.71	109.65
1	D	258	ASP	N-CA-C	5.16	119.06	112.87
2	E	384	GLY	N-CA-C	5.15	122.69	115.43
2	E	530	VAL	N-CA-C	5.13	116.11	108.46
2	B	543	GLY	N-CA-C	5.12	118.69	111.42
2	E	437	PRO	N-CA-C	5.12	119.34	111.57
2	E	514	GLU	N-CA-C	5.11	121.67	110.80
2	E	436	HIS	CA-C-N	-5.08	115.33	120.31
2	E	436	HIS	C-N-CA	-5.08	115.33	120.31
2	E	415	ASN	N-CA-C	5.05	119.17	112.30
2	B	334	TRP	N-CA-C	-5.05	106.53	113.30
2	E	497	THR	N-CA-C	5.04	116.73	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	436	HIS	CA-C-N	5.02	124.78	119.76
2	B	436	HIS	C-N-CA	5.02	124.78	119.76
1	D	224	GLY	N-CA-C	-5.01	106.24	114.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	540	TYR	Sidechain

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	1255	0	1127	89	0
1	D	1255	0	1127	122	0
2	B	2094	0	2095	200	0
2	E	2094	0	2095	232	0
3	C	28	0	25	0	0
3	F	28	0	25	2	0
4	B	30	0	31	3	0
4	E	30	0	31	4	0
5	A	25	0	0	2	0
5	B	23	0	0	3	1
5	D	16	0	0	3	0
5	E	23	0	0	0	1
All	All	6901	0	6556	577	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 43.

All (577) 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:317:ILE:CA	1:A:317:ILE:CB	1.91	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LEU:HA	5:D:62:HOH:O	1.59	1.02
1:D:165:PRO:HG2	1:D:166:LEU:HD13	1.43	1.01
2:B:397:LYS:HB3	2:B:429:ILE:HD11	1.45	0.98
1:A:227:GLU:HG3	2:B:500:ARG:HH11	1.24	0.98
2:B:382:ARG:NH1	2:B:385:LYS:HD2	1.79	0.96
2:E:397:LYS:HB3	2:E:429:ILE:HD11	1.51	0.93
2:B:322:VAL:HG11	2:B:552:ASP:HB2	1.51	0.92
1:D:306:ASP:HB3	1:D:309:GLU:HB2	1.48	0.91
1:D:202:LEU:HD21	1:D:235:ASP:O	1.68	0.90
2:E:338:LEU:HD21	2:E:379:LEU:HD23	1.53	0.89
1:A:182:LEU:HD11	2:E:369:PRO:O	1.73	0.88
1:D:227:GLU:HG3	2:E:500:ARG:HH11	1.37	0.88
1:A:227:GLU:HG3	2:B:500:ARG:NH1	1.91	0.86
2:B:483:VAL:HG13	2:B:485:LEU:HD13	1.57	0.85
2:E:403:LYS:HG3	2:E:405:TYR:CZ	2.10	0.85
1:D:194:TRP:HB3	1:D:214:LEU:HD13	1.59	0.84
2:E:365:LEU:HD13	2:E:404:ILE:HG23	1.59	0.83
2:E:416:LEU:HD11	4:E:1:OG6:HB21	1.60	0.83
2:B:388:ARG:HB3	2:B:461:TRP:CD1	2.15	0.82
5:B:64:HOH:O	1:D:166:LEU:HG	1.79	0.82
1:D:286:PHE:HD1	2:E:574:ILE:HD13	1.42	0.82
1:D:227:GLU:HG3	2:E:500:ARG:NH1	1.94	0.81
2:B:443:LYS:H	2:B:443:LYS:HD2	1.45	0.81
2:B:488:VAL:HG11	2:B:557:TYR:CE2	2.15	0.81
1:D:299:PHE:HA	1:D:304:VAL:CG1	2.10	0.81
2:E:536:ASN:ND2	2:E:538:ARG:HG3	1.95	0.81
2:E:490:ARG:HH21	2:E:494:LYS:HD2	1.47	0.80
2:B:382:ARG:HH12	2:B:385:LYS:HD2	1.48	0.78
1:D:302:LYS:O	1:D:302:LYS:HG2	1.84	0.77
2:E:322:VAL:HG22	2:E:464:ARG:O	1.85	0.77
2:E:445:THR:HA	2:E:448:LYS:HD2	1.67	0.76
2:B:417:ASP:O	2:B:418:ARG:HB2	1.86	0.76
1:D:204:LYS:O	1:D:205:ASP:HB2	1.85	0.76
2:B:479:VAL:HG23	2:B:480:LEU:O	1.86	0.75
1:A:179:ARG:HE	1:A:212:VAL:HG12	1.51	0.75
2:E:415:ASN:H	2:E:415:ASN:HD22	1.34	0.75
2:E:544:ILE:HB	2:E:561:THR:HB	1.68	0.75
2:B:464:ARG:HG2	2:B:477:PRO:HG3	1.69	0.75
2:E:447:ALA:O	2:E:451:HIS:HE1	1.70	0.74
2:E:357:TRP:CZ3	2:E:424:LYS:HB2	2.22	0.74
1:A:179:ARG:HG3	1:A:212:VAL:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:403:LYS:HD3	2:E:424:LYS:HD3	1.69	0.74
2:E:385:LYS:HZ2	2:E:385:LYS:HB3	1.51	0.74
1:A:227:GLU:HG3	2:B:500:ARG:HD2	1.69	0.74
1:A:260:LEU:HG	1:A:261:GLY:H	1.52	0.73
1:D:313:PHE:HZ	2:E:532:LYS:HE3	1.50	0.73
2:B:504:ASN:HB3	2:B:565:ARG:HD2	1.68	0.73
1:A:302:LYS:O	1:A:304:VAL:HG12	1.89	0.72
2:B:397:LYS:HD2	2:B:429:ILE:HD11	1.71	0.72
2:E:346:LEU:HD23	2:E:347:LEU:N	2.04	0.72
2:E:385:LYS:HB3	2:E:385:LYS:NZ	2.05	0.72
2:B:344:GLN:HE21	2:B:344:GLN:HA	1.54	0.72
1:A:166:LEU:HD22	1:A:166:LEU:H	1.53	0.72
2:B:352:LEU:HD22	2:B:354:SER:O	1.89	0.72
1:D:166:LEU:HD13	1:D:166:LEU:H	1.53	0.72
2:E:388:ARG:HB3	2:E:461:TRP:CD1	2.25	0.71
2:B:464:ARG:NH1	2:B:477:PRO:HA	2.06	0.70
2:E:451:HIS:HB2	2:E:454:PHE:CE2	2.26	0.70
1:A:167:LEU:HB3	5:A:31:HOH:O	1.91	0.70
1:D:190:ARG:H	1:D:190:ARG:HD2	1.56	0.70
2:B:397:LYS:HZ3	2:B:430:GLU:HB3	1.55	0.70
1:D:194:TRP:CZ3	1:D:222:PRO:HG3	2.27	0.70
2:E:403:LYS:HE3	2:E:405:TYR:OH	1.92	0.70
2:E:397:LYS:CB	2:E:429:ILE:HD11	2.22	0.70
2:B:339:PHE:HB2	2:B:345:GLU:O	1.91	0.69
1:D:286:PHE:CD1	2:E:574:ILE:HD13	2.25	0.69
1:D:200:LYS:HA	1:D:200:LYS:HE3	1.74	0.69
1:A:190:ARG:H	1:A:190:ARG:HD2	1.57	0.69
2:E:530:VAL:HG12	2:E:541:GLN:HA	1.75	0.69
1:D:299:PHE:HA	1:D:304:VAL:HG12	1.74	0.68
2:E:528:PRO:HB3	2:E:541:GLN:NE2	2.06	0.68
2:B:443:LYS:HD2	2:B:443:LYS:N	2.08	0.68
4:B:1:0G6:HD3	4:B:1:0G6:CD1	2.24	0.68
1:A:281:PHE:HB3	1:A:286:PHE:HB2	1.76	0.68
1:D:215:ALA:HB3	1:D:220:ARG:NH2	2.09	0.67
1:D:312:LEU:HD13	2:E:484:ASN:OD1	1.93	0.67
2:E:469:THR:OG1	2:E:470:THR:HG22	1.94	0.67
1:A:264(A):ASP:HB2	1:A:266:ALA:O	1.95	0.67
1:D:185:THR:HG21	1:D:241:GLU:HB2	1.75	0.67
2:E:489:GLU:O	2:E:492:VAL:HG12	1.95	0.67
1:D:198:GLN:CD	1:D:198:GLN:H	2.03	0.66
2:E:527:GLY:O	2:E:545:VAL:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:420:ILE:HG21	2:E:566:LEU:HD13	1.77	0.66
2:B:357:TRP:CH2	2:B:424:LYS:HD2	2.30	0.66
1:D:310:LYS:HB2	1:D:310:LYS:NZ	2.11	0.66
2:E:397:LYS:HE2	2:E:429:ILE:HG12	1.78	0.66
2:E:569:TRP:O	2:E:573:VAL:HG23	1.96	0.65
2:B:350:ALA:HB1	2:B:359:LEU:O	1.97	0.65
1:D:194:TRP:CH2	1:D:222:PRO:HG3	2.30	0.65
2:E:321:ILE:HD11	2:E:458:VAL:HG22	1.79	0.65
2:B:480:LEU:HD12	2:B:481:GLN:H	1.62	0.65
1:A:178:TYR:CZ	1:A:180:GLY:HA3	2.32	0.65
1:A:179:ARG:NE	1:A:212:VAL:HG12	2.11	0.65
2:B:415:ASN:HD21	2:B:500:ARG:NH2	1.95	0.65
2:B:385:LYS:HG2	2:B:396:GLU:HG2	1.79	0.64
1:A:286:PHE:HD1	2:B:574:ILE:HD13	1.61	0.64
2:E:411:ASN:HB2	2:E:417:ASP:HB3	1.79	0.64
1:A:236:GLN:HB3	1:A:237:PRO:HD2	1.79	0.64
1:D:253:ASP:HB3	2:E:490:ARG:NE	2.11	0.64
2:B:359:LEU:HD12	2:B:422:LEU:HD13	1.80	0.64
2:B:464:ARG:CZ	2:B:477:PRO:HA	2.28	0.64
2:E:410:TYR:CZ	2:E:412:TRP:HB3	2.33	0.64
2:B:390:ARG:O	2:B:390:ARG:HG3	1.97	0.63
2:B:500:ARG:HD3	5:B:47:HOH:O	1.97	0.63
2:E:403:LYS:HB2	2:E:424:LYS:HB3	1.80	0.63
2:E:355:ASP:OD2	2:E:428:PRO:HB3	1.97	0.63
2:E:489:GLU:H	2:E:489:GLU:CD	2.07	0.63
1:A:264:PRO:HG2	2:B:567:LYS:HG2	1.81	0.63
1:D:259:ARG:CZ	1:D:259:ARG:HA	2.28	0.63
2:E:370:TRP:O	2:E:371:ASP:HB2	1.99	0.63
1:D:309:GLU:OE2	2:E:532:LYS:HE2	1.99	0.63
2:B:502:THR:HG22	2:B:503:ASP:N	2.13	0.62
2:E:525:SER:HA	2:E:545:VAL:HB	1.82	0.62
2:B:344:GLN:HA	2:B:344:GLN:NE2	2.11	0.62
1:D:279:PRO:HA	1:D:290:GLU:OE2	2.00	0.62
2:E:342:SER:HA	2:E:343:PRO:C	2.24	0.62
2:B:497:THR:OG1	2:B:499:ILE:HG13	1.99	0.62
1:A:318:GLU:HG3	1:A:320:ARG:H	1.64	0.62
2:B:387:SER:C	2:B:389:THR:H	2.08	0.62
1:D:179:ARG:HG3	1:D:220:ARG:HH12	1.65	0.62
2:E:352:LEU:HD23	2:E:358:VAL:HG22	1.82	0.62
2:E:357:TRP:CE2	2:E:574:ILE:HG12	2.35	0.61
2:E:415:ASN:ND2	2:E:500:ARG:HH21	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:CB	1:A:317:ILE:N	2.62	0.61
2:E:403:LYS:NZ	2:E:403:LYS:HA	2.14	0.61
2:B:416:LEU:HD12	2:B:547:TRP:HB3	1.81	0.61
2:B:443:LYS:H	2:B:443:LYS:CD	2.11	0.61
2:E:321:ILE:N	2:E:462:GLY:O	2.33	0.61
2:E:492:VAL:O	2:E:495:ALA:HB3	2.00	0.61
1:D:263:ASP:CB	1:D:264:PRO:HD2	2.29	0.61
1:D:302:LYS:HD3	1:D:304:VAL:HG11	1.83	0.61
2:E:387:SER:HA	2:E:479:VAL:HA	1.81	0.61
2:E:397:LYS:HB3	2:E:429:ILE:CD1	2.27	0.61
2:E:457:ARG:HD2	2:E:482:VAL:CG2	2.31	0.61
1:A:178:TYR:O	1:A:212:VAL:HG21	2.01	0.60
2:B:466:GLU:HB2	2:B:551:CYS:HB2	1.84	0.60
2:E:379:LEU:HD12	2:E:379:LEU:N	2.16	0.60
1:A:274:GLU:HG2	1:A:275:ASP:N	2.15	0.60
1:A:259:ARG:HB2	2:B:565:ARG:HH22	1.67	0.60
5:A:6:HOH:O	2:B:568:LYS:HD3	2.02	0.60
2:E:407:HIS:HD2	2:E:409:ARG:H	1.49	0.60
2:E:411:ASN:OD1	2:E:414:GLU:HG2	2.02	0.60
2:B:363:HIS:CE1	2:B:525:SER:OG	2.54	0.60
2:B:431:LEU:HD12	2:B:435:ILE:O	2.02	0.60
2:B:394:LYS:HG3	2:B:395:VAL:HG23	1.84	0.59
1:D:263:ASP:HA	2:E:568:LYS:NZ	2.17	0.59
2:E:415:ASN:HD21	2:E:500:ARG:HH21	1.48	0.59
2:B:472:VAL:HG11	1:D:166:LEU:HA	1.83	0.59
2:E:356:ARG:O	2:E:425:LEU:HD22	2.01	0.59
2:E:441:PRO:HG3	2:E:542:MET:SD	2.43	0.59
1:D:282:ASN:HD21	1:D:284:LYS:HB3	1.66	0.59
2:B:340:ARG:HB3	2:B:347:LEU:HD11	1.84	0.59
2:B:409:ARG:CZ	2:B:418:ARG:HH22	2.16	0.59
1:D:194:TRP:CD2	1:D:214:LEU:HD22	2.37	0.59
2:B:490:ARG:O	2:B:493:CYS:HB2	2.02	0.59
2:E:331:LEU:HD23	2:E:331:LEU:O	2.03	0.59
2:E:379:LEU:HD12	2:E:379:LEU:H	1.68	0.59
1:D:279:PRO:HA	1:D:290:GLU:CD	2.27	0.59
2:B:441:PRO:HD3	2:B:541:GLN:O	2.03	0.58
2:E:485:LEU:HD12	2:E:509:GLY:HA2	1.84	0.58
2:B:341:LYS:HB3	2:B:380:LEU:HD22	1.84	0.58
2:B:438:VAL:HG22	2:B:439:CYS:H	1.68	0.58
2:E:518:GLY:O	2:E:519:ASP:HB2	2.03	0.58
1:D:297:PRO:HB2	1:D:298:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:385:LYS:HE2	2:E:392:GLU:HG3	1.84	0.58
2:E:456:GLY:O	2:E:484:ASN:HA	2.04	0.58
2:E:488:VAL:CG2	2:E:507:CYS:SG	2.91	0.58
1:D:313:PHE:CZ	2:E:532:LYS:HE3	2.36	0.58
1:A:174:ARG:HG2	1:A:226:GLU:O	2.04	0.58
2:B:334:TRP:O	2:B:351:SER:HA	2.03	0.58
1:D:264(A):ASP:HB2	1:D:266:ALA:O	2.04	0.58
2:B:488:VAL:HG11	2:B:557:TYR:CD2	2.38	0.57
2:E:322:VAL:HG12	2:E:323:GLU:HG2	1.84	0.57
1:A:267:ALA:O	1:A:268:ILE:HB	2.04	0.57
2:E:497:THR:OG1	2:E:499:ILE:HD12	2.04	0.57
1:D:281:PHE:HB3	1:D:286:PHE:CG	2.40	0.57
2:B:375:THR:O	2:B:378:ASP:HB2	2.04	0.57
2:B:431:LEU:HD11	2:B:437:PRO:HD3	1.87	0.57
2:B:487:LEU:HD21	2:B:506:PHE:CD1	2.40	0.57
2:E:414:GLU:HG3	2:E:415:ASN:H	1.69	0.57
1:A:287:GLY:HA2	2:B:356:ARG:NH1	2.19	0.56
2:B:339:PHE:HB2	2:B:346:LEU:HA	1.87	0.56
1:D:187:HIS:HB2	1:D:241:GLU:OE1	2.04	0.56
1:D:282:ASN:O	1:D:283:GLU:HB2	2.05	0.56
2:E:501:ILE:HG13	2:E:501:ILE:O	2.06	0.56
1:A:252:VAL:HB	1:A:259:ARG:HH21	1.70	0.56
1:D:298:LEU:HD12	1:D:298:LEU:N	2.21	0.56
2:E:445:THR:HA	2:E:448:LYS:CD	2.33	0.56
2:B:382:ARG:HG2	2:B:382:ARG:HH11	1.71	0.56
2:E:459:THR:HB	2:E:480:LEU:HD11	1.88	0.56
1:A:198:GLN:O	1:A:202:LEU:HD23	2.06	0.55
2:B:344:GLN:HE21	2:B:344:GLN:CA	2.18	0.55
1:D:185:THR:CG2	1:D:241:GLU:HB2	2.36	0.55
2:B:457:ARG:HD2	2:B:482:VAL:CG2	2.35	0.55
2:B:504:ASN:CB	2:B:565:ARG:HD2	2.33	0.55
2:B:527:GLY:O	2:B:545:VAL:HG23	2.06	0.55
2:B:411:ASN:OD1	2:B:414:GLU:HG2	2.06	0.55
2:B:415:ASN:HD22	2:B:415:ASN:H	1.52	0.55
2:B:465:ARG:H	2:B:475:VAL:CG2	2.19	0.55
2:B:502:THR:HG22	2:B:503:ASP:H	1.70	0.55
2:E:368:PRO:HD2	2:E:369:PRO:HD2	1.88	0.55
2:B:415:ASN:HD21	2:B:500:ARG:HH21	1.53	0.55
2:B:421:ALA:O	2:B:422:LEU:HB2	2.07	0.55
2:B:465:ARG:H	2:B:475:VAL:HG23	1.72	0.55
1:D:299:PHE:HA	1:D:304:VAL:HG13	1.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:337:MET:HE3	2:E:385:LYS:HD3	1.89	0.55
2:B:471:SER:O	2:B:474:GLU:HG2	2.07	0.55
2:E:397:LYS:NZ	2:E:430:GLU:HB3	2.22	0.55
1:D:164:SER:HB3	1:D:167:LEU:HB2	1.89	0.55
2:E:341:LYS:HZ2	2:E:380:LEU:HD22	1.71	0.55
2:E:574:ILE:HG22	2:E:575:ASP:N	2.20	0.55
2:E:368:PRO:HD2	2:E:412:TRP:CE3	2.42	0.55
2:B:341:LYS:HE2	2:B:380:LEU:HD22	1.89	0.54
2:E:471:SER:O	2:E:474:GLU:HG2	2.07	0.54
2:B:390:ARG:NH1	2:B:392:GLU:HG2	2.23	0.54
2:E:502:THR:HG22	2:E:503:ASP:N	2.22	0.54
2:E:510:TYR:CE2	2:E:516:LYS:HB2	2.42	0.54
2:B:357:TRP:CZ3	2:B:424:LYS:HB2	2.43	0.54
1:D:282:ASN:ND2	1:D:284:LYS:HB3	2.22	0.54
2:B:384:GLY:O	2:B:395:VAL:HG12	2.08	0.54
1:A:263:ASP:CB	1:A:264:PRO:HD2	2.37	0.54
1:A:286:PHE:CD1	2:B:574:ILE:HD13	2.43	0.54
2:B:327:ALA:O	2:B:386:HIS:HE1	1.90	0.54
2:B:382:ARG:HH11	2:B:385:LYS:HD2	1.68	0.54
2:B:387:SER:HB2	2:B:389:THR:O	2.08	0.54
1:D:230:TRP:HB3	1:D:242:TYR:HA	1.89	0.54
2:B:323:GLU:HG2	5:B:60:HOH:O	2.07	0.54
2:B:415:ASN:ND2	2:B:500:ARG:HH21	2.06	0.54
2:E:322:VAL:HG23	2:E:521:CYS:HB2	1.90	0.54
2:B:427:ARG:HG2	2:B:427:ARG:HH11	1.73	0.54
2:B:391:TYR:CE2	2:B:393:ARG:HA	2.43	0.54
1:D:196:SER:O	1:D:200:LYS:HB2	2.08	0.54
2:E:414:GLU:HG3	2:E:415:ASN:N	2.22	0.54
2:B:405:TYR:CD2	2:B:573:VAL:HG11	2.43	0.53
2:B:477:PRO:HB3	2:B:481:GLN:HG3	1.90	0.53
1:A:281:PHE:HB3	1:A:286:PHE:CB	2.38	0.53
1:D:215:ALA:HB3	1:D:220:ARG:CZ	2.37	0.53
2:E:340:ARG:NH1	2:E:343:PRO:HD2	2.24	0.53
2:B:337:MET:HE2	2:B:382:ARG:HD3	1.89	0.53
1:D:230:TRP:NE1	2:E:409:ARG:NH1	2.56	0.53
1:A:221:ASN:OD1	1:A:225:ASP:N	2.40	0.53
2:E:490:ARG:HB3	2:E:491:PRO:HD3	1.89	0.53
1:D:260:LEU:H	1:D:260:LEU:HD23	1.72	0.53
2:E:444:GLN:O	2:E:448:LYS:HG3	2.08	0.53
1:A:286:PHE:CE2	2:B:354:SER:HB3	2.44	0.53
1:D:296:ARG:HG3	1:D:300:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HG2	2:B:576:ARG:NH2	2.24	0.53
1:D:255:ASP:N	1:D:258:ASP:HB2	2.23	0.53
1:D:309:GLU:CD	2:E:532:LYS:HE2	2.34	0.53
2:E:405:TYR:HB2	2:E:422:LEU:HB3	1.89	0.52
2:E:510:TYR:CD2	2:E:516:LYS:HB2	2.43	0.52
1:D:320:ARG:HB3	1:D:320:ARG:CZ	2.38	0.52
2:B:534:PRO:HG2	2:B:535:TYR:CD1	2.44	0.52
2:E:351:SER:O	2:E:358:VAL:HG13	2.09	0.52
1:A:259:ARG:HB2	2:B:565:ARG:NH2	2.24	0.52
2:E:375:THR:O	2:E:378:ASP:HB2	2.09	0.52
2:E:431:LEU:HD13	2:E:435:ILE:O	2.09	0.52
2:E:339:PHE:HB2	2:E:345:GLU:O	2.10	0.52
1:D:165:PRO:HG2	1:D:166:LEU:CD1	2.29	0.52
1:D:223:ASP:OD2	1:D:225:ASP:HB2	2.09	0.52
1:A:165:PRO:HD2	1:A:166:LEU:HD22	1.92	0.52
2:B:362:ALA:HA	2:B:421:ALA:HB2	1.90	0.52
5:D:61:HOH:O	2:E:436:HIS:HE1	1.92	0.52
2:B:415:ASN:HD22	2:B:415:ASN:N	2.07	0.52
1:D:234:ALA:HB3	1:D:239:ASP:HB3	1.93	0.51
1:A:227:GLU:HG3	2:B:500:ARG:CD	2.40	0.51
1:A:260:LEU:HG	1:A:261:GLY:N	2.23	0.51
2:E:403:LYS:HG3	2:E:405:TYR:CE1	2.43	0.51
1:D:310:LYS:HB2	1:D:310:LYS:HZ2	1.76	0.51
1:A:259:ARG:HD2	2:B:503:ASP:OD1	2.11	0.51
1:D:230:TRP:CH2	2:E:409:ARG:HD2	2.46	0.51
2:E:368:PRO:CD	2:E:369:PRO:HD2	2.41	0.51
2:E:387:SER:C	2:E:389:THR:H	2.18	0.51
2:B:397:LYS:HD2	2:B:429:ILE:CD1	2.38	0.51
2:B:488:VAL:HG11	2:B:557:TYR:HE2	1.69	0.51
2:E:333:PRO:HB2	2:E:436:HIS:H	1.76	0.51
2:E:457:ARG:HG2	2:E:484:ASN:CG	2.36	0.51
2:B:357:TRP:HE3	2:B:423:LEU:O	1.94	0.51
1:D:226:GLU:HG3	5:D:74:HOH:O	2.09	0.51
2:E:403:LYS:HB2	2:E:424:LYS:CB	2.40	0.51
2:E:415:ASN:HD22	2:E:415:ASN:N	2.00	0.51
2:B:334:TRP:CG	2:B:438:VAL:HB	2.45	0.51
2:B:490:ARG:HA	2:B:493:CYS:HB2	1.93	0.51
1:D:263:ASP:HA	2:E:568:LYS:HZ2	1.76	0.51
2:E:534:PRO:HG2	2:E:535:TYR:CE1	2.45	0.51
1:A:198:GLN:N	1:A:198:GLN:OE1	2.44	0.51
2:B:340:ARG:HA	2:B:379:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:VAL:CG1	2:B:485:LEU:HD13	2.37	0.51
2:E:368:PRO:N	2:E:369:PRO:HD2	2.26	0.51
2:E:443:LYS:H	2:E:443:LYS:HD2	1.76	0.51
2:E:488:VAL:HG11	2:E:557:TYR:CD2	2.46	0.51
1:A:166:LEU:HD22	1:A:166:LEU:N	2.23	0.50
1:A:230:TRP:CH2	2:B:409:ARG:HD2	2.46	0.50
2:B:382:ARG:NH1	2:B:382:ARG:HG2	2.24	0.50
2:B:466:GLU:O	2:B:466:GLU:HG2	2.10	0.50
2:B:348:CYS:HB3	2:B:525:SER:O	2.11	0.50
2:B:414:GLU:HG3	2:B:415:ASN:ND2	2.26	0.50
1:D:173:ASP:HB3	1:D:176:ARG:HB2	1.93	0.50
2:E:379:LEU:N	2:E:379:LEU:CD1	2.74	0.50
2:B:409:ARG:NH1	2:B:418:ARG:NH2	2.60	0.50
2:E:457:ARG:HD2	2:E:482:VAL:HG21	1.91	0.50
2:E:535:TYR:O	2:E:537:ASN:N	2.44	0.50
1:A:187:HIS:HB2	1:A:241:GLU:OE1	2.12	0.50
1:D:218:PHE:O	1:D:220:ARG:HG2	2.12	0.50
1:A:187:HIS:HE1	2:B:413:LYS:HD3	1.76	0.50
1:A:214:LEU:HD21	1:A:222:PRO:HB3	1.94	0.50
1:A:218:PHE:HB2	1:A:220:ARG:NH1	2.27	0.50
1:A:292:ASP:HA	2:B:538:ARG:HH12	1.76	0.50
1:D:281:PHE:HB3	1:D:286:PHE:CB	2.42	0.50
2:E:385:LYS:HG2	2:E:396:GLU:HB3	1.93	0.50
2:E:407:HIS:CD2	2:E:409:ARG:H	2.29	0.50
1:D:264:PRO:HD3	2:E:568:LYS:HG3	1.93	0.50
2:E:544:ILE:HG13	2:E:563:VAL:HG22	1.93	0.50
1:A:202:LEU:HD21	1:A:235:ASP:O	2.12	0.50
1:A:298:LEU:HD11	2:B:433:ASP:HB3	1.93	0.50
2:E:394:LYS:HG3	2:E:395:VAL:HG23	1.94	0.49
2:B:427:ARG:HG2	2:B:427:ARG:NH1	2.27	0.49
1:D:218:PHE:HB2	1:D:220:ARG:HH21	1.76	0.49
2:E:403:LYS:HA	2:E:403:LYS:HZ3	1.77	0.49
2:E:532:LYS:HD2	2:E:539:TRP:CZ2	2.48	0.49
1:D:230:TRP:CZ2	2:E:409:ARG:HD2	2.48	0.49
2:E:385:LYS:NZ	2:E:386:HIS:H	2.11	0.49
2:E:416:LEU:HD11	4:E:1:OG6:CB1	2.38	0.49
1:D:263:ASP:HB3	1:D:264:PRO:HD2	1.93	0.49
2:E:465:ARG:HH22	2:E:468:TRP:HA	1.76	0.49
2:E:415:ASN:HD21	2:E:500:ARG:NH2	2.11	0.49
2:E:475:VAL:O	2:E:475:VAL:HG13	2.11	0.49
1:A:277:PHE:O	1:A:278:GLN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:ILE:HD11	2:B:563:VAL:CG2	2.43	0.49
2:B:322:VAL:HA	2:B:464:ARG:O	2.13	0.49
1:D:286:PHE:CE1	2:E:353:ILE:HD12	2.48	0.49
2:E:544:ILE:HG13	2:E:563:VAL:CG2	2.42	0.49
1:D:210:PRO:O	1:D:211:ALA:HB3	2.12	0.49
2:B:438:VAL:HG22	2:B:439:CYS:N	2.27	0.48
1:D:223:ASP:OD2	2:E:409:ARG:NH1	2.46	0.48
1:A:284:LYS:HG2	2:B:579:SER:HB2	1.95	0.48
2:E:443:LYS:HD2	2:E:443:LYS:N	2.28	0.48
2:E:556:LYS:C	2:E:557:TYR:CD1	2.91	0.48
2:B:397:LYS:CB	2:B:429:ILE:HD11	2.32	0.48
2:B:489:GLU:CD	2:B:489:GLU:H	2.21	0.48
2:E:557:TYR:CD1	2:E:557:TYR:N	2.81	0.48
2:B:321:ILE:HD12	2:B:524:ASP:OD2	2.13	0.48
2:E:493:CYS:O	2:E:496:SER:HB3	2.14	0.48
1:A:316:TYR:HD1	2:B:454:PHE:CD2	2.31	0.48
2:B:389:THR:O	2:B:390:ARG:HB3	2.13	0.48
2:E:397:LYS:HZ1	2:E:430:GLU:HB3	1.78	0.48
1:A:178:TYR:OH	1:A:180:GLY:HA3	2.13	0.48
2:E:336:VAL:HB	2:E:350:ALA:HB3	1.96	0.48
1:D:277:PHE:CZ	1:D:293:CYS:SG	3.07	0.48
1:A:200:LYS:HA	1:A:200:LYS:HD2	1.67	0.47
2:B:339:PHE:CB	2:B:346:LEU:HA	2.43	0.47
1:D:227:GLU:HG3	2:E:500:ARG:HD2	1.96	0.47
1:D:264(A):ASP:HB2	1:D:264(B):PRO:HD2	1.96	0.47
2:E:383:ILE:HG22	2:E:435:ILE:HG12	1.96	0.47
2:E:536:ASN:CG	2:E:538:ARG:HG3	2.38	0.47
1:A:298:LEU:N	1:A:298:LEU:HD12	2.29	0.47
1:D:259:ARG:HA	1:D:259:ARG:NE	2.29	0.47
2:E:444:GLN:OE1	2:E:448:LYS:HE3	2.14	0.47
2:B:388:ARG:HB3	2:B:461:TRP:CG	2.49	0.47
2:E:333:PRO:HB2	2:E:436:HIS:N	2.29	0.47
1:D:190:ARG:O	1:D:191:CYS:HB2	2.14	0.47
1:D:302:LYS:HD3	1:D:304:VAL:CG1	2.44	0.47
2:E:353:ILE:HG21	2:E:440:LEU:HD11	1.97	0.47
2:E:490:ARG:O	2:E:493:CYS:HB2	2.15	0.47
1:A:201:ALA:O	1:A:204:LYS:HB3	2.14	0.47
2:B:331:LEU:O	2:B:333:PRO:HD3	2.14	0.47
1:D:277:PHE:O	1:D:278:GLN:CB	2.62	0.47
2:E:414:GLU:HG3	2:E:415:ASN:ND2	2.30	0.47
2:E:418:ARG:O	2:E:420:ILE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:511:LYS:HG3	2:E:557:TYR:OH	2.15	0.47
2:E:521:CYS:SG	2:E:522:GLU:N	2.88	0.47
1:A:303:GLN:HE21	1:A:303:GLN:HA	1.80	0.47
2:B:387:SER:HA	2:B:479:VAL:HA	1.96	0.47
1:D:184:VAL:HG12	1:D:185:THR:H	1.78	0.47
1:D:230:TRP:CE2	2:E:409:ARG:NH1	2.82	0.47
1:D:260:LEU:HD23	1:D:260:LEU:N	2.29	0.47
1:A:308:THR:O	1:A:309:GLU:C	2.58	0.47
2:B:412:TRP:CZ3	2:B:413:LYS:HG2	2.49	0.47
2:B:331:LEU:C	2:B:331:LEU:HD23	2.40	0.46
2:B:368:PRO:HG2	2:B:412:TRP:CE2	2.50	0.46
2:B:511:LYS:HA	2:B:557:TYR:OH	2.16	0.46
2:E:547:TRP:C	4:E:1:OG6:HD31	2.39	0.46
1:A:187:HIS:CE1	2:B:413:LYS:HD3	2.51	0.46
2:B:363:HIS:HE1	2:B:525:SER:OG	1.99	0.46
2:B:455:LYS:HA	2:B:486:PRO:HA	1.98	0.46
2:B:511:LYS:HB2	2:B:514:GLU:OE2	2.16	0.46
1:A:182:LEU:CD1	2:E:369:PRO:O	2.55	0.46
1:A:293:CYS:C	2:B:439:CYS:SG	2.98	0.46
2:B:349:GLY:O	2:B:350:ALA:HB2	2.14	0.46
2:B:401:LEU:CD1	2:B:423:LEU:HG	2.45	0.46
2:E:488:VAL:HG22	2:E:507:CYS:SG	2.54	0.46
1:A:286:PHE:CE1	2:B:353:ILE:HD12	2.50	0.46
2:B:385:LYS:HE2	2:B:385:LYS:HB3	1.74	0.46
2:E:482:VAL:CG2	2:E:483:VAL:N	2.77	0.46
2:B:443:LYS:HA	2:B:564:PHE:CE1	2.50	0.46
2:B:533:SER:O	2:B:537:ASN:HA	2.15	0.46
1:A:277:PHE:CZ	1:A:293:CYS:SG	3.08	0.46
1:D:264(B):PRO:C	1:D:266:ALA:H	2.24	0.46
2:E:338:LEU:O	2:E:347:LEU:HB2	2.15	0.46
2:E:489:GLU:O	2:E:490:ARG:C	2.59	0.46
2:B:352:LEU:HG	2:B:383:ILE:HD13	1.99	0.45
2:B:341:LYS:HB3	2:B:341:LYS:HE2	1.64	0.45
2:B:498:ARG:NH2	2:E:494:LYS:HE3	2.31	0.45
2:B:537:ASN:HD22	2:B:537:ASN:C	2.25	0.45
2:E:447:ALA:O	2:E:451:HIS:CE1	2.60	0.45
2:B:513:GLY:O	2:B:515:GLY:N	2.49	0.45
1:D:296:ARG:NH1	2:E:331:LEU:HD23	2.32	0.45
1:A:282:ASN:OD1	1:A:282:ASN:C	2.59	0.45
2:B:488:VAL:CG2	2:B:507:CYS:SG	3.05	0.45
1:D:264:PRO:HD3	2:E:568:LYS:CG	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:ASN:O	1:D:283:GLU:CB	2.64	0.45
2:E:334:TRP:CG	2:E:438:VAL:HB	2.51	0.45
2:E:469:THR:OG1	2:E:470:THR:N	2.49	0.45
1:A:176:ARG:NH1	1:A:224:GLY:O	2.49	0.45
1:A:312:LEU:HD11	2:B:456:GLY:CA	2.46	0.45
2:B:387:SER:C	2:B:389:THR:N	2.73	0.45
2:B:400:MET:CE	2:B:426:LYS:HZ1	2.30	0.45
2:B:436:HIS:CD2	2:B:437:PRO:HD2	2.52	0.45
2:E:321:ILE:CD1	2:E:458:VAL:HG22	2.46	0.45
1:D:238:GLY:O	2:E:413:LYS:HE3	2.17	0.45
2:E:349:GLY:O	2:E:350:ALA:HB2	2.16	0.45
1:D:178:TYR:CE1	1:D:245:LEU:HD21	2.51	0.45
1:A:263:ASP:HB3	1:A:264:PRO:HD2	1.97	0.45
2:B:455:LYS:HG2	2:B:486:PRO:HB3	1.99	0.45
1:D:264(A):ASP:C	1:D:265:ASP:H	2.24	0.45
1:D:286:PHE:HD1	2:E:574:ILE:CD1	2.21	0.45
2:E:337:MET:HB3	2:E:382:ARG:HB2	1.99	0.45
2:B:502:THR:OG1	2:B:505:MET:HE3	2.17	0.45
1:A:282:ASN:HD21	1:A:284:LYS:HB3	1.80	0.44
2:E:366:LEU:HD12	2:E:372:LYS:O	2.17	0.44
2:E:458:VAL:CG1	2:E:483:VAL:HG13	2.47	0.44
2:E:333:PRO:HG2	2:E:334:TRP:CE3	2.52	0.44
2:E:511:LYS:HD3	2:E:514:GLU:OE2	2.17	0.44
2:E:577:LEU:HD22	2:E:577:LEU:HA	1.83	0.44
2:B:456:GLY:N	2:B:485:LEU:O	2.49	0.44
2:E:331:LEU:HD21	2:E:457:ARG:NH2	2.32	0.44
2:B:490:ARG:C	2:B:493:CYS:HB2	2.41	0.44
2:E:379:LEU:H	2:E:379:LEU:CD1	2.29	0.44
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.60	0.44
1:D:253:ASP:HB3	2:E:490:ARG:HE	1.79	0.44
1:D:296:ARG:NH2	1:D:306:ASP:HB2	2.33	0.44
2:B:396:GLU:O	2:B:397:LYS:HG2	2.17	0.44
1:D:264:PRO:HG3	2:E:568:LYS:HA	2.00	0.44
2:E:385:LYS:HZ3	2:E:386:HIS:H	1.66	0.44
1:D:178:TYR:CZ	1:D:180:GLY:HA3	2.53	0.44
2:E:366:LEU:HD11	3:F:1:NAG:H82	2.00	0.44
2:E:536:ASN:ND2	2:E:538:ARG:CG	2.76	0.44
1:A:218:PHE:HB2	1:A:220:ARG:HH12	1.83	0.44
2:B:490:ARG:N	2:B:491:PRO:CD	2.81	0.44
2:E:385:LYS:NZ	2:E:385:LYS:CB	2.74	0.44
1:A:281:PHE:HB3	1:A:286:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:ARG:NH1	2:B:418:ARG:HH22	2.16	0.44
2:B:489:GLU:HB2	2:B:492:VAL:HG12	2.00	0.44
1:D:253:ASP:HB3	2:E:490:ARG:CZ	2.48	0.44
2:E:414:GLU:HG3	2:E:415:ASN:HD22	1.83	0.44
2:E:458:VAL:HG13	2:E:483:VAL:HG13	2.00	0.44
1:A:178:TYR:CG	1:A:245:LEU:HD21	2.52	0.43
1:D:287:GLY:HA2	2:E:356:ARG:NH1	2.33	0.43
1:A:299:PHE:O	1:A:303:GLN:N	2.52	0.43
2:E:410:TYR:CE2	2:E:412:TRP:HB3	2.52	0.43
2:E:420:ILE:HG13	2:E:544:ILE:CD1	2.48	0.43
2:E:528:PRO:CB	2:E:541:GLN:NE2	2.79	0.43
2:B:511:LYS:HD2	2:B:557:TYR:OH	2.19	0.43
1:D:204:LYS:HD2	2:E:576:ARG:NH2	2.32	0.43
1:D:231:CYS:O	1:D:240:PHE:HB2	2.18	0.43
1:D:264(A):ASP:C	1:D:265:ASP:N	2.76	0.43
1:D:286:PHE:CD1	2:E:574:ILE:CD1	3.00	0.43
2:E:409:ARG:O	2:E:418:ARG:NH1	2.51	0.43
2:B:394:LYS:NZ	2:B:395:VAL:HA	2.33	0.43
1:D:295:LEU:HD12	2:E:538:ARG:HH21	1.83	0.43
1:A:312:LEU:HD11	2:B:456:GLY:HA2	2.00	0.43
2:B:363:HIS:CE1	2:B:525:SER:CB	3.02	0.43
2:B:471:SER:C	2:B:473:ALA:N	2.75	0.43
2:E:420:ILE:HG13	2:E:544:ILE:HD12	2.00	0.43
2:B:388:ARG:O	2:B:389:THR:HG23	2.18	0.43
2:B:387:SER:OG	2:B:390:ARG:HG2	2.19	0.43
2:B:443:LYS:HA	2:B:564:PHE:CZ	2.54	0.43
1:D:245:LEU:O	1:D:246:ASN:HB3	2.19	0.43
2:E:476:GLN:HA	2:E:477:PRO:HD3	1.89	0.43
1:D:296:ARG:HD2	1:D:299:PHE:CD1	2.54	0.43
2:E:381:VAL:O	2:E:398:ILE:HA	2.18	0.43
1:A:218:PHE:N	1:A:218:PHE:CD1	2.84	0.43
1:A:312:LEU:HD13	2:B:484:ASN:OD1	2.18	0.43
2:B:339:PHE:HD1	2:B:339:PHE:O	2.02	0.43
2:B:457:ARG:NH2	2:B:539:TRP:CH2	2.87	0.43
2:B:502:THR:CG2	2:B:503:ASP:N	2.81	0.43
2:B:567:LYS:HA	2:B:570:ILE:HD12	2.00	0.43
2:E:321:ILE:HG12	2:E:483:VAL:HG12	2.01	0.43
2:E:325:GLN:H	2:E:325:GLN:HG2	1.70	0.43
2:E:335:GLN:HG3	2:E:461:TRP:CH2	2.53	0.43
1:D:264:PRO:HD3	2:E:568:LYS:HE3	2.00	0.43
2:E:369:PRO:HD3	2:E:412:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:O	1:A:194:TRP:C	2.62	0.42
1:A:287:GLY:HA2	2:B:356:ARG:CZ	2.49	0.42
2:B:322:VAL:CG2	2:B:464:ARG:O	2.66	0.42
2:B:340:ARG:HD3	2:B:345:GLU:OE1	2.19	0.42
2:B:466:GLU:HG3	2:B:551:CYS:SG	2.59	0.42
2:E:387:SER:CB	2:E:479:VAL:HG12	2.49	0.42
2:E:449:LEU:O	2:E:531:MET:HE1	2.19	0.42
2:B:475:VAL:HG22	2:B:475:VAL:O	2.18	0.42
1:A:233:VAL:HB	1:A:239:ASP:O	2.19	0.42
2:B:339:PHE:CD1	2:B:339:PHE:C	2.98	0.42
2:B:472:VAL:O	2:B:472:VAL:HG22	2.19	0.42
1:D:204:LYS:HD2	2:E:576:ARG:HH22	1.85	0.42
2:E:379:LEU:HD13	2:E:401:LEU:HD12	2.02	0.42
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.71	0.42
2:E:528:PRO:HB2	2:E:541:GLN:HG3	2.01	0.42
2:B:403:LYS:HD2	2:B:403:LYS:N	2.33	0.42
1:D:234:ALA:HB3	1:D:239:ASP:CB	2.49	0.42
1:D:236:GLN:OE1	3:F:1:NAG:H3	2.19	0.42
2:E:472:VAL:O	2:E:472:VAL:HG22	2.20	0.42
2:E:568:LYS:HZ2	2:E:568:LYS:HB2	1.84	0.42
1:A:227:GLU:CG	2:B:500:ARG:NH1	2.72	0.42
2:B:467:THR:C	2:B:468:TRP:CE3	2.98	0.42
2:E:465:ARG:H	2:E:475:VAL:CG2	2.33	0.42
2:E:503:ASP:OD1	2:E:565:ARG:NE	2.53	0.42
1:A:245:LEU:O	1:A:246:ASN:HB3	2.20	0.42
2:B:476:GLN:HA	2:B:477:PRO:HD3	1.85	0.42
2:B:489:GLU:HB3	2:B:491:PRO:HD2	2.02	0.42
1:D:212:VAL:HB	1:D:213:PRO:HD2	2.01	0.42
2:B:362:ALA:HB1	2:B:406:ILE:HG23	2.01	0.42
2:E:363:HIS:CE1	4:E:1:OG6:H1	2.38	0.42
1:A:185:THR:HG21	1:A:241:GLU:HB2	2.02	0.41
1:A:286:PHE:CZ	2:B:354:SER:HB3	2.54	0.41
2:E:397:LYS:HE2	2:E:429:ILE:CG1	2.48	0.41
2:E:397:LYS:CG	2:E:429:ILE:HD11	2.50	0.41
2:E:543:GLY:HA2	2:E:561:THR:O	2.19	0.41
1:A:236:GLN:O	1:A:239:ASP:HB2	2.20	0.41
1:A:256:LEU:HB3	1:A:257:GLY:H	1.60	0.41
1:A:295:LEU:HB2	1:A:301:LYS:HE2	2.02	0.41
1:D:292:ASP:HB2	1:D:301:LYS:HZ1	1.85	0.41
2:E:337:MET:HE2	2:E:337:MET:HB2	1.85	0.41
1:D:184:VAL:HG12	1:D:185:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD12	1:D:262:GLU:OE2	2.20	0.41
2:E:341:LYS:HE3	2:E:380:LEU:HD13	2.03	0.41
2:E:388:ARG:C	2:E:389:THR:HG1	2.28	0.41
2:B:321:ILE:HD12	2:B:520:ALA:HA	2.01	0.41
2:B:416:LEU:HD11	4:B:1:OG6:HG2	2.00	0.41
2:B:357:TRP:CZ3	2:B:424:LYS:HD2	2.55	0.41
2:B:401:LEU:HD13	2:B:423:LEU:HG	2.02	0.41
1:D:281:PHE:HB2	1:D:290:GLU:OE1	2.21	0.41
2:E:338:LEU:CD2	2:E:379:LEU:HD23	2.39	0.41
2:E:449:LEU:O	2:E:454:PHE:HD2	2.03	0.41
2:B:521:CYS:O	4:B:1:OG6:HG31	2.20	0.41
2:E:356:ARG:C	2:E:425:LEU:HD22	2.45	0.41
2:E:435:ILE:O	2:E:435:ILE:HG22	2.20	0.41
2:E:404:ILE:O	2:E:405:TYR:HD1	2.03	0.41
2:E:513:GLY:O	2:E:515:GLY:N	2.54	0.41
1:D:236:GLN:HB3	1:D:237:PRO:HD2	2.03	0.41
1:D:284:LYS:HG2	2:E:579:SER:O	2.21	0.41
2:B:321:ILE:CD1	2:B:520:ALA:HA	2.51	0.41
2:B:504:ASN:C	2:B:562:HIS:HB2	2.45	0.41
2:E:403:LYS:HA	2:E:403:LYS:HZ2	1.86	0.41
2:E:405:TYR:HD2	2:E:573:VAL:HG12	1.86	0.41
1:A:298:LEU:HD12	1:A:298:LEU:H	1.86	0.41
2:B:407:HIS:HD2	2:B:409:ARG:H	1.69	0.41
2:B:496:SER:OG	2:B:556:LYS:HA	2.21	0.41
2:E:332:SER:HA	2:E:333:PRO:HD2	1.82	0.41
2:E:375:THR:O	2:E:379:LEU:HD12	2.21	0.41
1:A:166:LEU:H	1:A:166:LEU:CD2	2.27	0.40
2:B:336:VAL:HG12	2:B:337:MET:N	2.37	0.40
1:A:296:ARG:HA	1:A:297:PRO:HD3	1.81	0.40
2:B:568:LYS:O	2:B:572:LYS:HG3	2.22	0.40
1:D:284:LYS:C	1:D:284:LYS:HD2	2.46	0.40
2:E:363:HIS:CE1	2:E:525:SER:OG	2.74	0.40
2:E:387:SER:O	2:E:389:THR:N	2.54	0.40
2:E:532:LYS:NZ	2:E:537:ASN:HB2	2.36	0.40
1:D:263:ASP:HB2	2:E:564:PHE:CZ	2.55	0.40
2:E:455:LYS:HG2	2:E:486:PRO:HB3	2.03	0.40
2:B:477:PRO:HB3	2:B:481:GLN:CG	2.50	0.40
1:D:269:GLU:HB3	1:D:272:THR:HG21	2.03	0.40
1:D:309:GLU:HG2	1:D:313:PHE:CE2	2.57	0.40
2:E:482:VAL:HG22	2:E:483:VAL:N	2.37	0.40
2:B:432:SER:OG	2:B:433:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:LYS:N	2:B:443:LYS:CD	2.79	0.40
2:B:457:ARG:HD2	2:B:482:VAL:HG21	2.04	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)
5:B:78:HOH:O	5:E:40:HOH:O[3_545]	0.44	1.76

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	157/159 (99%)	108 (69%)	30 (19%)	19 (12%)	0	1
1	D	157/159 (99%)	96 (61%)	42 (27%)	19 (12%)	0	1
2	B	257/259 (99%)	204 (79%)	40 (16%)	13 (5%)	1	13
2	E	257/259 (99%)	203 (79%)	39 (15%)	15 (6%)	1	10
All	All	828/836 (99%)	611 (74%)	151 (18%)	66 (8%)	1	4

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	205	ASP
1	A	210	PRO
1	A	255	ASP
1	A	264	PRO
2	B	331	LEU
2	B	390	ARG
2	B	393	ARG

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Mol	Chain	Res	Type
2	B	411	ASN
2	B	514	GLU
1	D	169	THR
1	D	190	ARG
1	D	205	ASP
1	D	210	PRO
1	D	260	LEU
1	D	264	PRO
1	D	268	ILE
1	D	278	GLN
2	E	388	ARG
2	E	390	ARG
2	E	475	VAL
2	E	514	GLU
2	E	536	ASN
2	E	537	ASN
1	A	262	GLU
1	A	307	GLN
2	B	422	LEU
2	B	471	SER
2	B	537	ASN
1	D	167	LEU
1	D	215	ALA
1	D	248	CYS
1	D	270	GLY
1	D	275	ASP
1	D	290	GLU
2	E	371	ASP
2	E	411	ASN
2	E	471	SER
1	A	173	ASP
1	A	260	LEU
1	A	291	ALA
2	B	495	ALA
1	D	204	LYS
2	E	393	ARG
2	E	443	LYS
1	A	216	GLU
1	A	268	ILE
1	A	278	GLN
2	B	418	ARG
2	B	474	GLU

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Mol	Chain	Res	Type
1	D	191	CYS
1	D	255	ASP
2	E	474	GLU
1	A	194	TRP
1	A	204	LYS
1	A	269	GLU
1	A	303	GLN
1	A	318	GLU
2	B	536	ASN
1	D	173	ASP
1	D	211	ALA
2	E	350	ALA
2	E	363	HIS
2	E	404	ILE
2	B	404	ILE
1	A	165	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	133/133 (100%)	110 (83%)	23 (17%)	2	10
1	D	133/133 (100%)	103 (77%)	30 (23%)	1	5
2	B	226/226 (100%)	186 (82%)	40 (18%)	2	10
2	E	226/226 (100%)	182 (80%)	44 (20%)	1	8
All	All	718/718 (100%)	581 (81%)	137 (19%)	1	9

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	LEU
1	A	179	ARG
1	A	181	ARG
1	A	197	GLU
1	A	205	ASP

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Mol	Chain	Res	Type
1	A	209	ASN
1	A	216	GLU
1	A	226	GLU
1	A	227	GLU
1	A	244	ASP
1	A	245	LEU
1	A	252	VAL
1	A	256	LEU
1	A	264	PRO
1	A	264(A)	ASP
1	A	264(B)	PRO
1	A	269	GLU
1	A	274	GLU
1	A	282	ASN
1	A	303	GLN
1	A	304	VAL
1	A	310	LYS
1	A	317	ILE
2	B	321	ILE
2	B	322	VAL
2	B	329	VAL
2	B	338	LEU
2	B	339	PHE
2	B	344	GLN
2	B	352	LEU
2	B	368	PRO
2	B	371	ASP
2	B	375	THR
2	B	379	LEU
2	B	380	LEU
2	B	382	ARG
2	B	387	SER
2	B	389	THR
2	B	390	ARG
2	B	403	LYS
2	B	410	TYR
2	B	415	ASN
2	B	418	ARG
2	B	423	LEU
2	B	425	LEU
2	B	431	LEU
2	B	432	SER

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Mol	Chain	Res	Type
2	B	440	LEU
2	B	443	LYS
2	B	449	LEU
2	B	459	THR
2	B	467	THR
2	B	492	VAL
2	B	493	CYS
2	B	501	ILE
2	B	522	GLU
2	B	535	TYR
2	B	537	ASN
2	B	542	MET
2	B	563	VAL
2	B	568	LYS
2	B	571	GLN
2	B	577	LEU
1	D	166	LEU
1	D	174	ARG
1	D	184	VAL
1	D	186	THR
1	D	190	ARG
1	D	192	LEU
1	D	200	LYS
1	D	205	ASP
1	D	209	ASN
1	D	212	VAL
1	D	216	GLU
1	D	227	GLU
1	D	245	LEU
1	D	249	GLU
1	D	256	LEU
1	D	260	LEU
1	D	264	PRO
1	D	264(A)	ASP
1	D	264(B)	PRO
1	D	269	GLU
1	D	282	ASN
1	D	283	GLU
1	D	285	THR
1	D	296	ARG
1	D	297	PRO
1	D	298	LEU

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Mol	Chain	Res	Type
1	D	303	GLN
1	D	305	GLN
1	D	310	LYS
1	D	317	ILE
2	E	321	ILE
2	E	328	GLU
2	E	337	MET
2	E	339	PHE
2	E	347	LEU
2	E	352	LEU
2	E	371	ASP
2	E	375	THR
2	E	376	VAL
2	E	379	LEU
2	E	380	LEU
2	E	385	LYS
2	E	389	THR
2	E	393	ARG
2	E	397	LYS
2	E	403	LYS
2	E	415	ASN
2	E	418	ARG
2	E	420	ILE
2	E	422	LEU
2	E	425	LEU
2	E	431	LEU
2	E	432	SER
2	E	433	ASP
2	E	443	LYS
2	E	458	VAL
2	E	470	THR
2	E	475	VAL
2	E	478	SER
2	E	488	VAL
2	E	490	ARG
2	E	491	PRO
2	E	497	THR
2	E	503	ASP
2	E	504	ASN
2	E	511	LYS
2	E	517	ARG
2	E	522	GLU

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Mol	Chain	Res	Type
2	E	535	TYR
2	E	537	ASN
2	E	542	MET
2	E	554	ASP
2	E	568	LYS
2	E	577	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
2	B	344	GLN
2	B	386	HIS
2	B	407	HIS
2	B	415	ASN
2	B	476	GLN
1	D	246	ASN
1	D	303	GLN
1	D	305	GLN
1	D	307	GLN
2	E	386	HIS
2	E	407	HIS
2	E	415	ASN
2	E	436	HIS
2	E	451	HIS
2	E	481	GLN
2	E	536	ASN
2	E	541	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	$\# Z > 2$
3	NAG	C	1	3,2	14,14,15	0.68	0	17,19,21	1.00	1 (5%)
3	NAG	C	2	3	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
3	NAG	F	1	3,2	14,14,15	0.55	0	17,19,21	0.74	1 (5%)
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.78	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
3	NAG	C	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	-2.37	119.73	122.90
3	C	1	NAG	C2-N2-C7	-2.34	119.77	122.90
3	F	1	NAG	C2-N2-C7	-2.11	120.07	122.90
3	F	2	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

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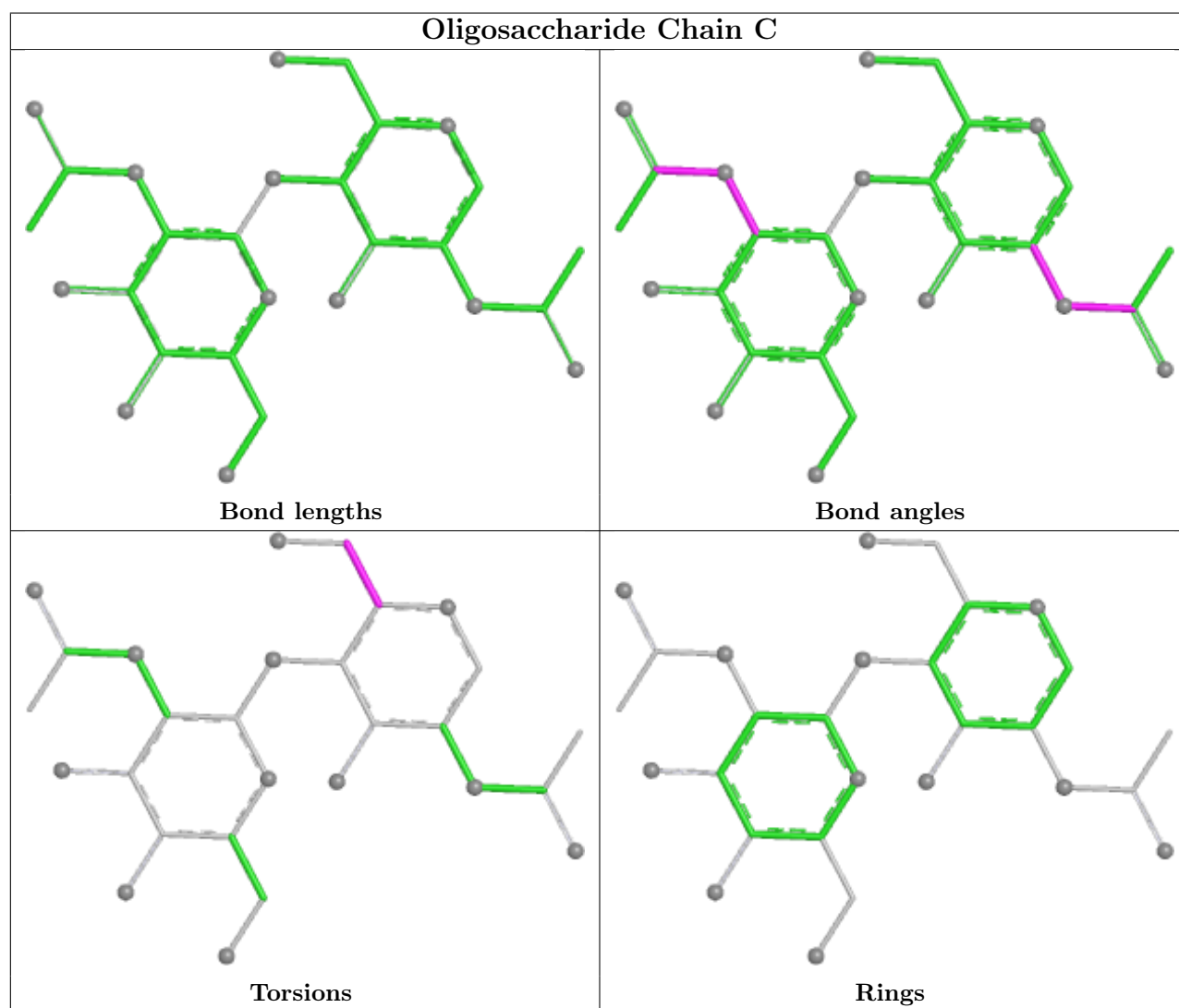
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6

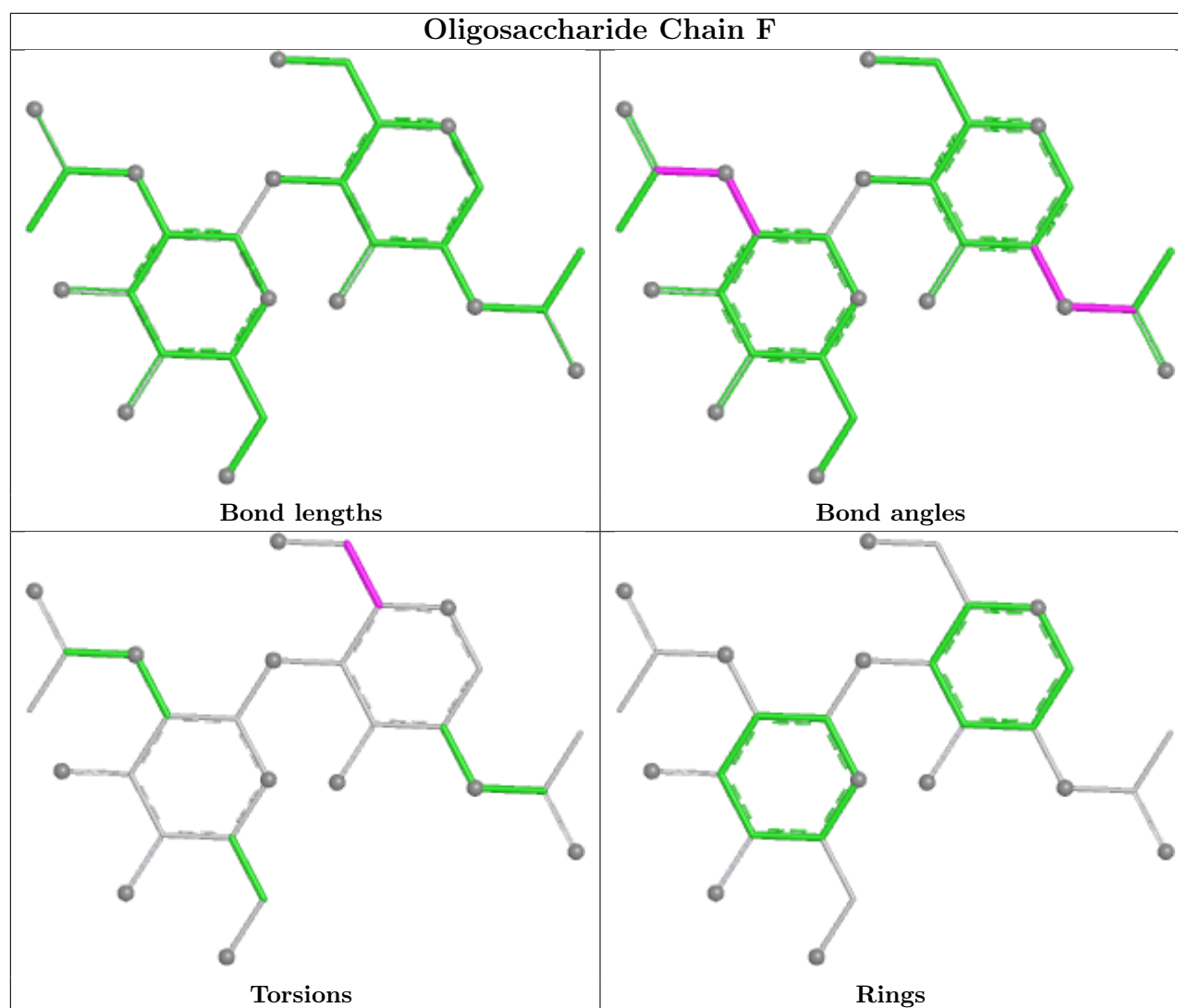
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	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	$\# Z > 2$
4	0G6	B	1	2	30,31,32	0.85	0	37,41,42	0.82	1 (2%)
4	0G6	E	1	2	30,31,32	0.63	1 (3%)	37,41,42	0.77	1 (2%)

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
4	0G6	B	1	2	-	4/31/41/43	0/2/2/2
4	0G6	E	1	2	-	0/31/41/43	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	0G6	O2-C2	-2.21	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	0G6	C1-CA1-N1	-3.04	104.21	112.50
4	B	1	0G6	CB2-CA2-N2	2.25	113.22	110.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	0G6	NE-CD3-CG2-CB2
4	B	1	0G6	C2-CA2-CB2-CG2
4	B	1	0G6	N2-CA2-CB2-CG2
4	B	1	0G6	CA2-CB2-CG2-CD3

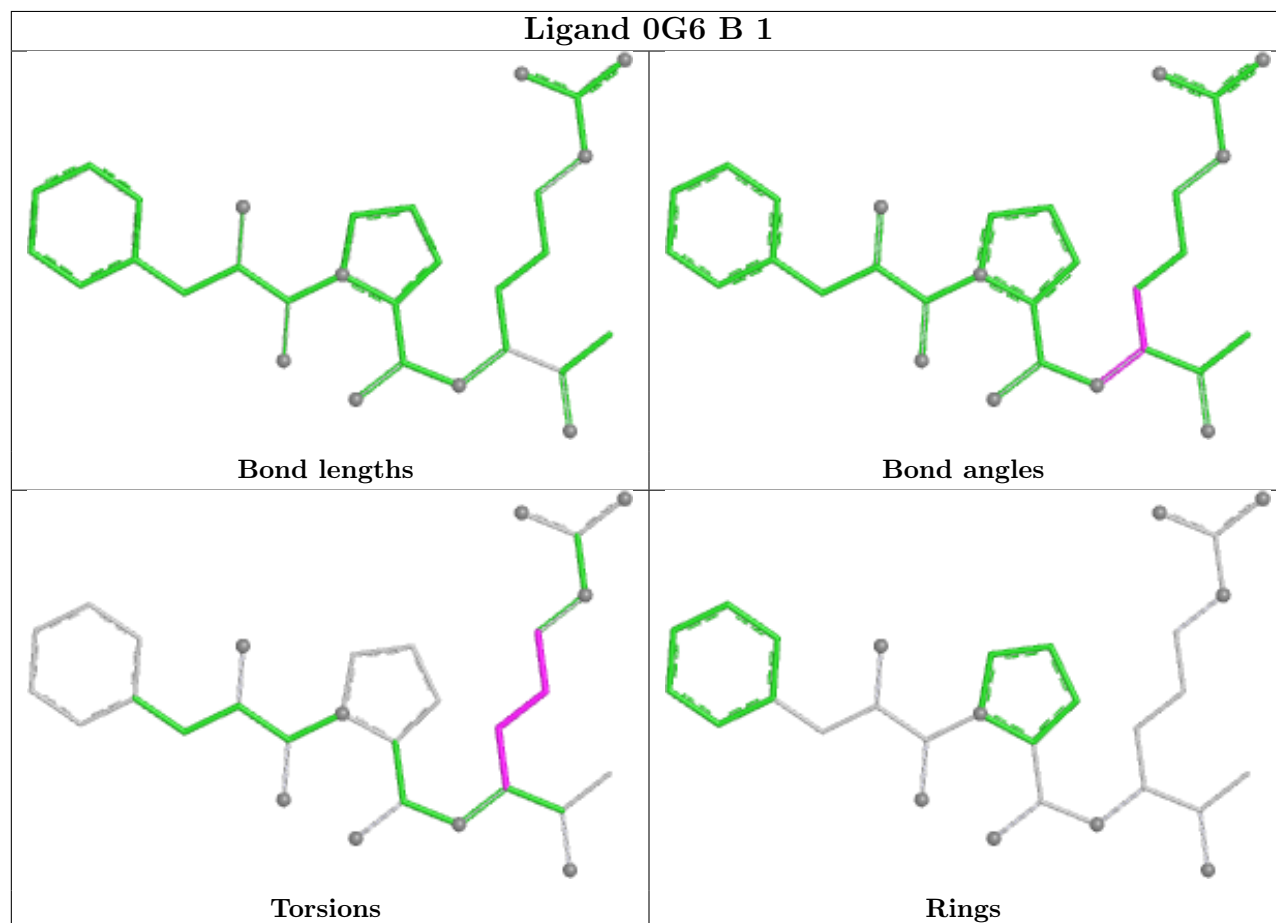
There are no ring outliers.

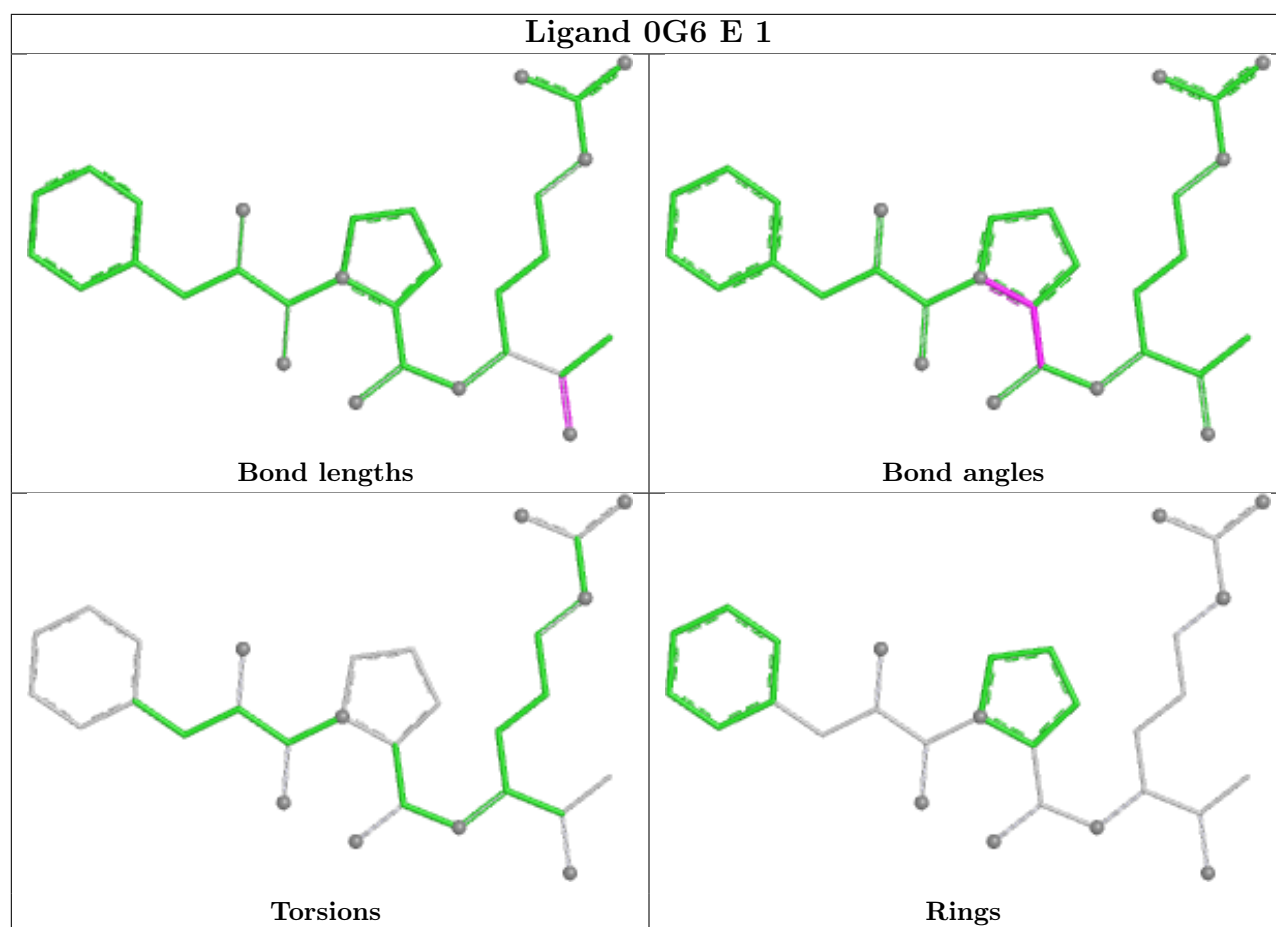
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	0G6	3	0
4	E	1	0G6	4	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	159/159 (100%)	0.22	14 (8%) 15 10	3, 40, 99, 100	0
1	D	159/159 (100%)	0.23	19 (11%) 9 6	4, 42, 100, 100	0
2	B	259/259 (100%)	-0.77	0 100 100	2, 11, 42, 97	0
2	E	259/259 (100%)	-0.74	1 (0%) 88 79	2, 15, 43, 92	0
All	All	836/836 (100%)	-0.38	34 (4%) 41 25	2, 19, 96, 100	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	GLU	5.4
1	D	263	ASP	4.3
1	A	266	ALA	4.3
1	A	317	ILE	4.1
1	D	282	ASN	3.9
1	A	272	THR	3.8
1	D	272	THR	3.8
1	D	164	SER	3.6
1	A	260	LEU	3.6
1	D	267	ALA	3.3
1	D	253	ASP	3.1
1	D	270	GLY	2.9
1	D	268	ILE	2.8
1	A	270	GLY	2.7
1	D	264	PRO	2.6
1	D	258	ASP	2.5
1	A	282	ASN	2.5
1	D	264(B)	PRO	2.5
1	D	271	ARG	2.4
1	A	264(B)	PRO	2.4
1	D	275	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	167	LEU	2.3
1	D	264(A)	ASP	2.3
1	A	263	ASP	2.3
1	D	280	PHE	2.2
1	D	266	ALA	2.2
1	D	211	ALA	2.2
1	D	251	PRO	2.2
1	D	269	GLU	2.1
2	E	579	SER	2.1
1	A	318	GLU	2.1
1	A	267	ALA	2.0
1	A	275	ASP	2.0
1	A	262	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

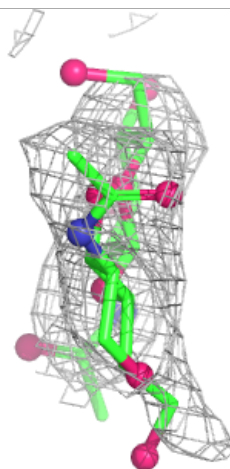
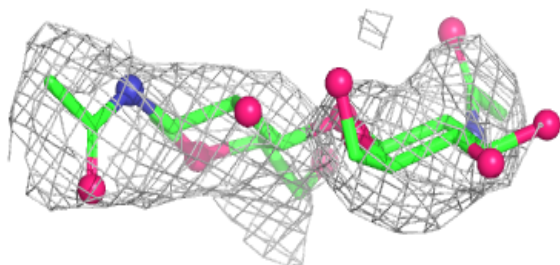
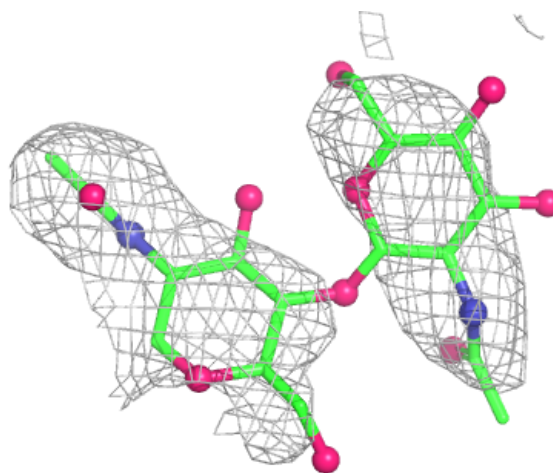
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

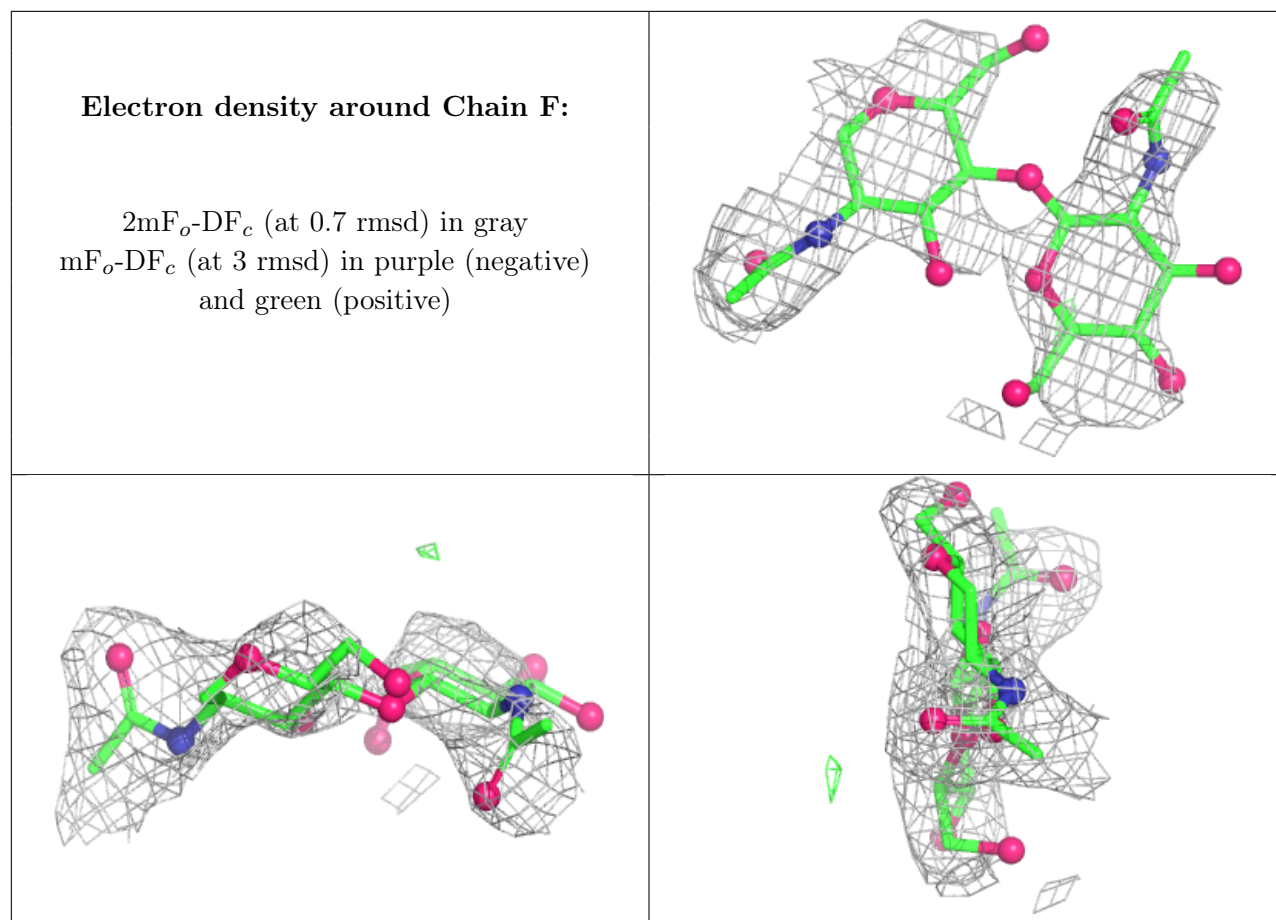
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	43,50,64,75	0
3	NAG	C	2	14/15	-	-	68,72,82,82	0
3	NAG	F	2	14/15	0.75	0.12	69,74,82,83	0
3	NAG	F	1	14/15	0.82	0.13	42,49,66,72	0

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 C:

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





6.4 Ligands [i](#)

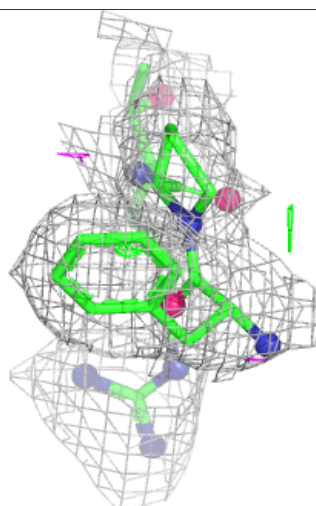
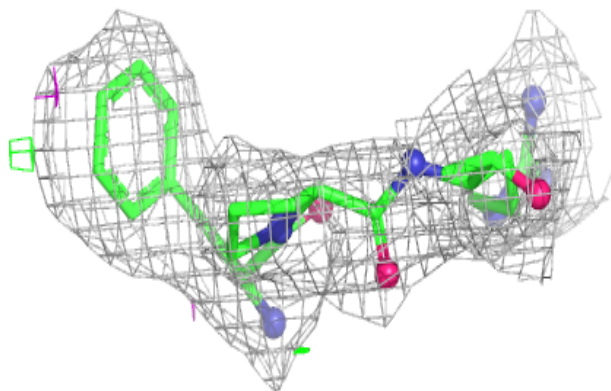
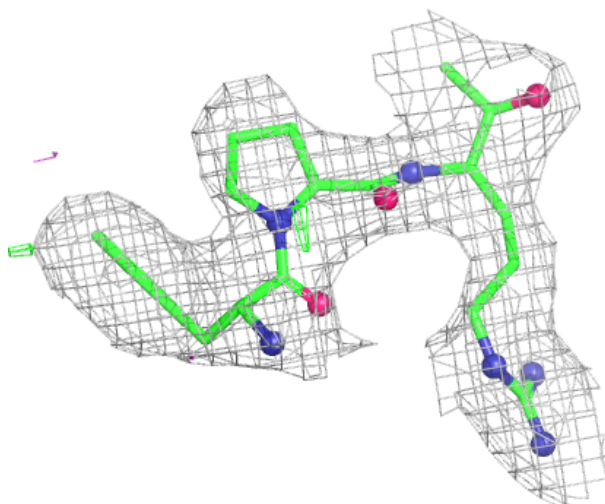
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
4	OG6	B	1	30/31	0.96	0.07	2,9,19,26	0
4	OG6	E	1	30/31	0.97	0.06	2,5,18,20	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.

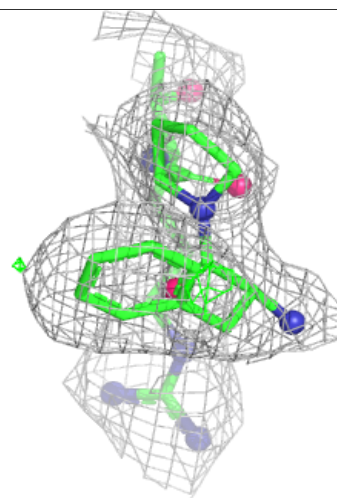
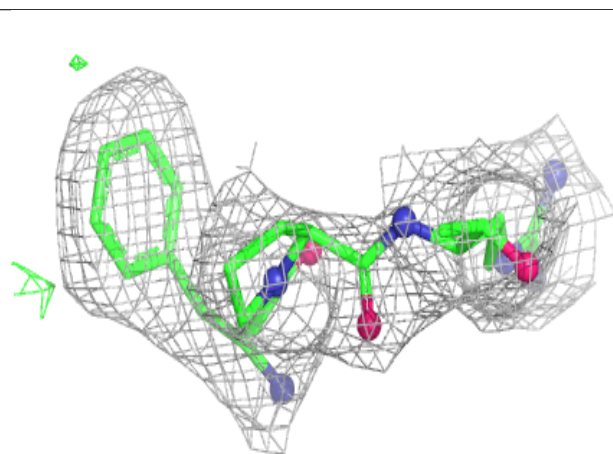
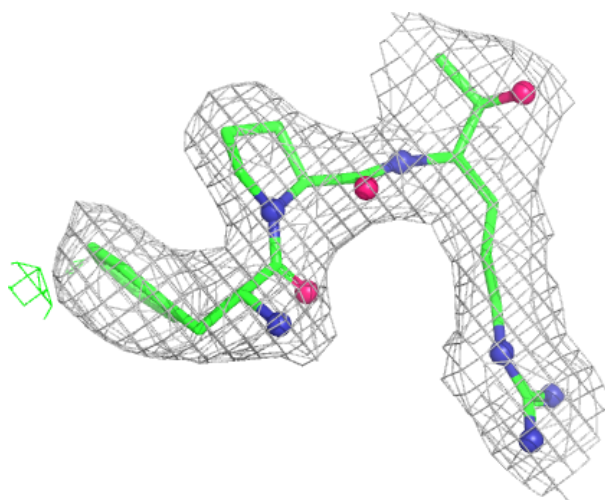
Electron density around 0G6 B 1:

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



Electron density around 0G6 E 1:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.