



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 1MAA / pdb_00001maa
Title : MOUSE ACETYLCHOLINESTERASE CATALYTIC DOMAIN, GLYCOSYLATED PROTEIN
Authors : Bourne, Y.; Taylor, P.; Bougis, P.E.; Marchot, P.
Deposited on : 1998-11-04
Resolution : 2.90 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

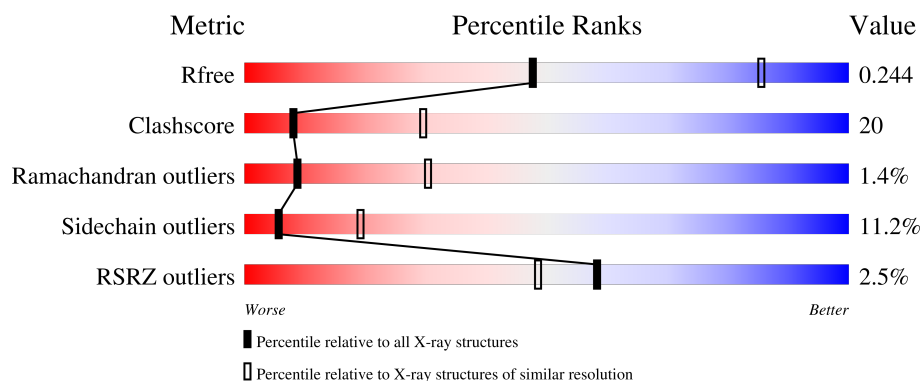
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



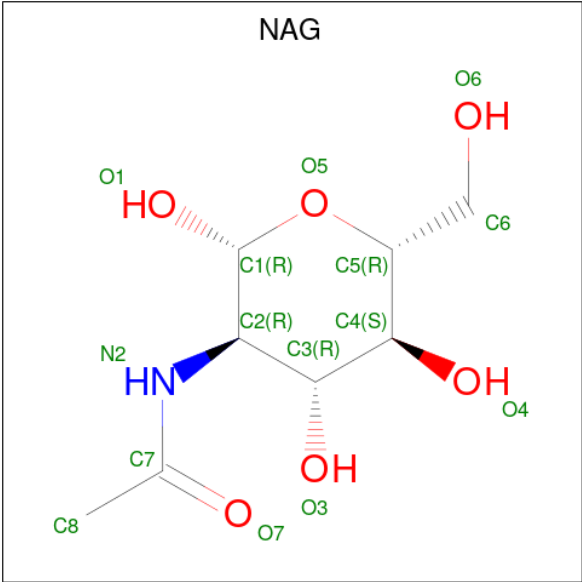
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	547	4% 54% 36% 8% ..
1	B	547	% 61% 31% 6% ..
1	C	547	2% 58% 34% 6% ..
1	D	547	3% 56% 33% 9% ..
2	E	3	67% 33%

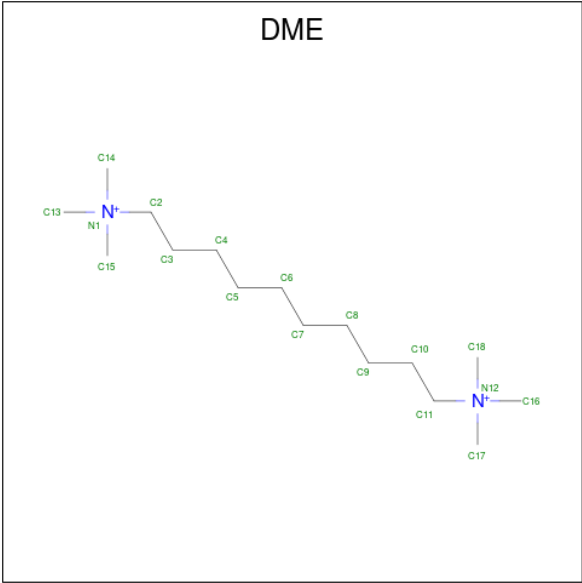
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DME	B	996	-	-	X	-
4	DME	C	997	-	-	X	-
5	GOL	C	951	-	-	X	-
6	PO4	B	548	-	X	-	-
6	PO4	C	548	-	X	-	-
6	PO4	C	998	-	X	-	-



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is DECAMETHONIUM ION (CCD ID: DME) (formula: $C_{16}H_{38}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			18	16	2		
4	B	1	Total	C	N	0	0
			18	16	2		
4	C	1	Total	C	N	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	N	0	0
			18	16	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		

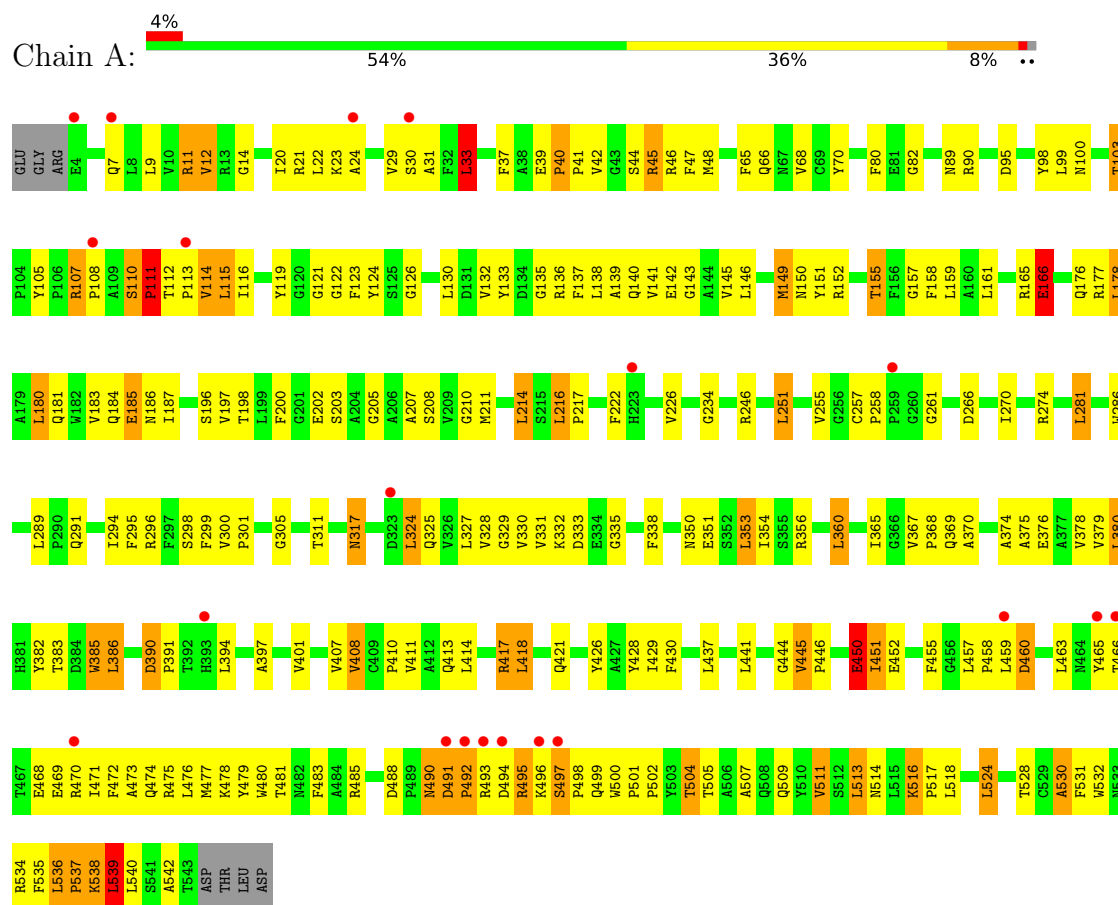
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total	O	0	0
			27	27		
7	B	49	Total	O	0	0
			49	49		
7	C	59	Total	O	0	0
			59	59		
7	D	52	Total	O	0	0
			52	52		

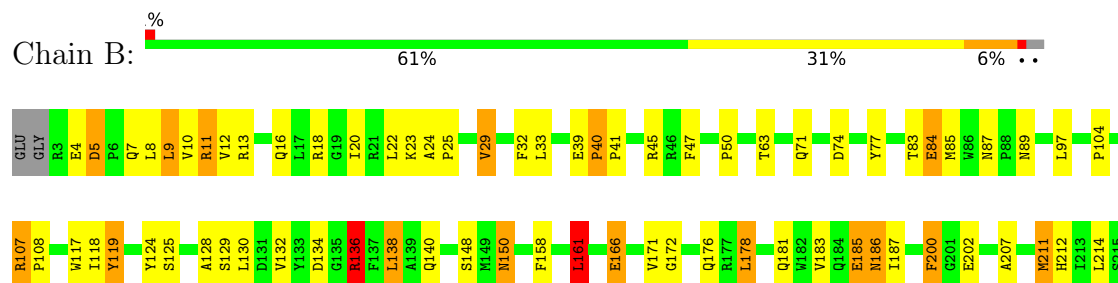
3 Residue-property plots

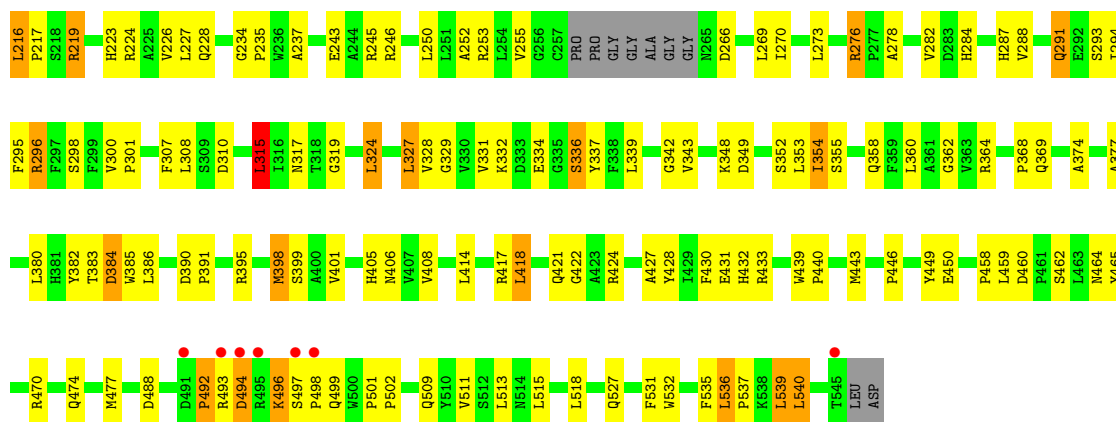
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ACETYLCHOLINESTERASE

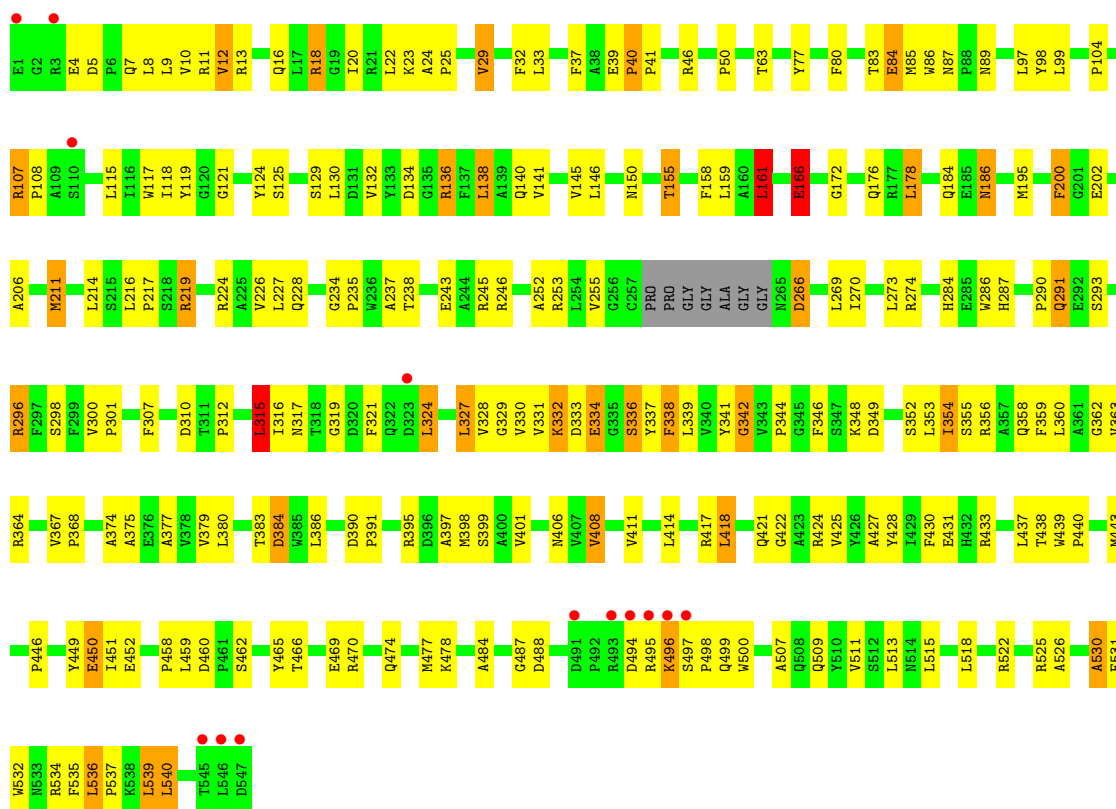


• Molecule 1: ACETYLCHOLINESTERASE

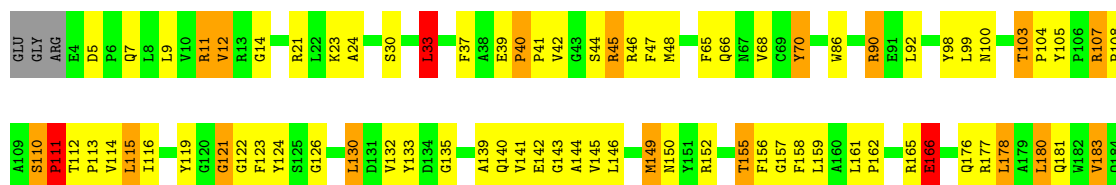


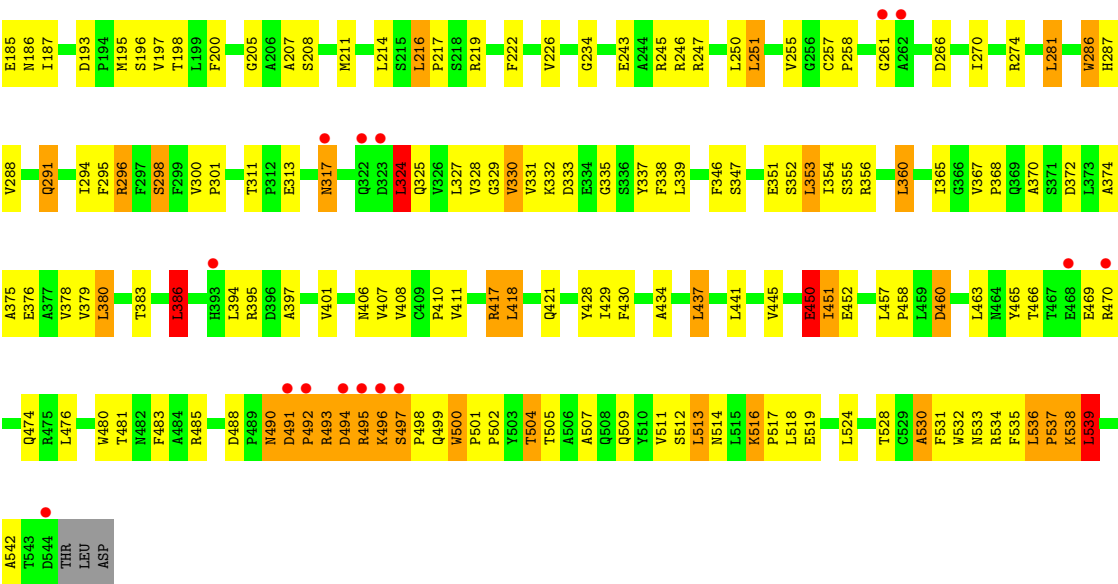


● Molecule 1: ACETYLCHOLINESTERASE



● Molecule 1: ACETYLCHOLINESTERASE





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	136.55Å 173.13Å 224.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.90) 91.0 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.200 , 0.248 0.202 , 0.244	Depositor DCC
R_{free} test set	2378 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.1	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	17084	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DME, NAG, FUL, GOL, PO4

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	0.62	0/4313	1.20	37/5898 (0.6%)
1	B	0.67	1/4292 (0.0%)	1.20	40/5868 (0.7%)
1	C	0.69	1/4309 (0.0%)	1.22	44/5892 (0.7%)
1	D	0.62	0/4318	1.20	33/5905 (0.6%)
All	All	0.65	2/17232 (0.0%)	1.20	154/23563 (0.7%)

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
1	C	0	1
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	195	MET	SD-CE	7.10	1.97	1.79
1	B	398	MET	SD-CE	-5.68	1.65	1.79

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	ASP	CA-C-N	11.28	133.93	119.84
1	A	491	ASP	C-N-CA	11.28	133.93	119.84
1	B	186	ASN	N-CA-C	10.37	125.04	112.38
1	D	491	ASP	CA-C-N	10.31	132.73	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	491	ASP	C-N-CA	10.31	132.73	119.84
1	D	354	ILE	N-CA-C	9.27	120.16	110.05
1	A	354	ILE	N-CA-C	9.02	119.88	110.05
1	D	335	GLY	N-CA-C	8.98	124.37	114.40
1	C	186	ASN	N-CA-C	8.52	123.24	113.01
1	C	495	ARG	N-CA-C	-8.46	101.69	113.20
1	D	408	VAL	N-CA-C	8.45	119.02	110.23
1	B	298	SER	N-CA-C	7.92	119.61	110.97
1	D	39	GLU	CA-C-N	7.68	128.30	120.38
1	D	39	GLU	C-N-CA	7.68	128.30	120.38
1	C	298	SER	N-CA-C	7.64	119.30	110.97
1	A	126	GLY	N-CA-C	7.59	119.16	111.95
1	A	335	GLY	N-CA-C	7.58	122.81	114.40
1	A	408	VAL	N-CA-C	7.37	117.89	110.23
1	C	408	VAL	N-CA-C	7.32	118.04	110.36
1	C	450	GLU	N-CA-C	-7.30	104.98	114.04
1	D	460	ASP	CA-C-N	7.24	126.74	118.85
1	D	460	ASP	C-N-CA	7.24	126.74	118.85
1	C	161	LEU	N-CA-C	-7.20	96.27	108.94
1	C	40	PRO	CA-C-N	7.15	128.77	119.84
1	C	40	PRO	C-N-CA	7.15	128.77	119.84
1	B	450	GLU	N-CA-C	-7.04	105.31	114.04
1	C	307	PHE	N-CA-C	-6.94	103.65	111.07
1	B	237	ALA	N-CA-C	6.89	119.63	111.71
1	B	161	LEU	N-CA-C	-6.88	96.84	108.94
1	A	166	GLU	N-CA-C	6.82	121.30	112.92
1	A	324	LEU	N-CA-C	6.74	120.00	110.23
1	D	166	GLU	N-CA-C	6.62	121.06	112.92
1	B	408	VAL	N-CA-C	6.61	117.30	110.36
1	B	422	GLY	N-CA-C	6.55	122.76	114.25
1	A	460	ASP	CA-C-N	6.44	125.87	118.85
1	A	460	ASP	C-N-CA	6.44	125.87	118.85
1	A	40	PRO	CA-C-N	6.43	127.88	119.84
1	A	40	PRO	C-N-CA	6.43	127.88	119.84
1	B	332	LYS	N-CA-C	6.43	119.98	111.75
1	B	40	PRO	CA-C-N	6.42	127.87	119.84
1	B	40	PRO	C-N-CA	6.42	127.87	119.84
1	C	5	ASP	CA-C-N	6.42	125.99	119.19
1	C	5	ASP	C-N-CA	6.42	125.99	119.19
1	A	530	ALA	N-CA-C	-6.40	104.16	112.23
1	D	324	LEU	N-CA-C	6.38	119.48	110.23
1	B	307	PHE	N-CA-C	-6.38	104.33	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	488	ASP	CA-C-N	6.37	126.50	119.87
1	B	488	ASP	C-N-CA	6.37	126.50	119.87
1	C	158	PHE	N-CA-C	6.27	123.49	114.39
1	D	493	ARG	N-CA-C	-6.27	103.54	112.13
1	C	526	ALA	N-CA-C	6.24	118.63	111.02
1	D	509	GLN	N-CA-C	6.24	119.41	109.24
1	C	141	VAL	N-CA-C	6.21	117.00	110.72
1	A	298	SER	N-CA-C	6.21	117.85	111.14
1	B	39	GLU	CA-C-N	6.20	126.77	120.38
1	B	39	GLU	C-N-CA	6.20	126.77	120.38
1	D	500	TRP	CA-C-N	6.20	126.76	120.38
1	D	500	TRP	C-N-CA	6.20	126.76	120.38
1	C	338	PHE	N-CA-C	6.19	119.00	111.82
1	A	509	GLN	N-CA-C	6.19	119.33	109.24
1	D	126	GLY	N-CA-C	6.18	117.82	111.95
1	B	5	ASP	N-CA-C	-6.13	100.72	109.24
1	C	237	ALA	N-CA-C	6.09	119.81	112.38
1	D	539	LEU	N-CA-C	-6.08	104.73	111.36
1	A	39	GLU	CA-C-N	6.06	126.63	120.38
1	A	39	GLU	C-N-CA	6.06	126.63	120.38
1	C	315	LEU	N-CA-C	6.04	117.87	111.28
1	D	298	SER	N-CA-C	6.04	117.67	111.14
1	B	136	ARG	N-CA-C	6.04	118.63	111.33
1	C	332	LYS	N-CA-C	6.03	119.47	111.75
1	A	445	VAL	CA-C-N	5.99	125.96	120.21
1	A	445	VAL	C-N-CA	5.99	125.96	120.21
1	D	33	LEU	N-CA-C	5.99	119.66	110.20
1	A	450	GLU	N-CA-C	-5.94	106.57	113.88
1	B	431	GLU	N-CA-C	5.92	121.24	113.30
1	C	530	ALA	N-CA-C	-5.91	104.92	111.36
1	C	390	ASP	CA-C-N	5.90	125.77	119.28
1	C	390	ASP	C-N-CA	5.90	125.77	119.28
1	C	349	ASP	N-CA-C	5.87	118.91	111.69
1	A	33	LEU	N-CA-C	5.82	119.02	109.76
1	B	150	ASN	N-CA-C	-5.81	100.82	110.17
1	B	315	LEU	N-CA-C	5.76	118.30	111.33
1	C	166	GLU	N-CA-C	5.73	119.89	113.01
1	D	40	PRO	CA-C-N	5.72	126.99	119.84
1	D	40	PRO	C-N-CA	5.72	126.99	119.84
1	C	384	ASP	N-CA-C	-5.71	98.44	108.20
1	D	542	ALA	N-CA-C	-5.69	106.26	113.43
1	B	390	ASP	CA-C-N	5.65	125.49	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	ASP	C-N-CA	5.65	125.49	119.28
1	B	349	ASP	N-CA-C	5.63	118.62	111.69
1	B	234	GLY	CA-C-N	5.63	125.24	119.56
1	B	234	GLY	C-N-CA	5.63	125.24	119.56
1	D	530	ALA	N-CA-C	-5.62	105.30	111.82
1	C	488	ASP	CA-C-N	5.62	125.72	119.87
1	C	488	ASP	C-N-CA	5.62	125.72	119.87
1	C	145	VAL	N-CA-C	-5.62	99.06	107.37
1	C	235	PRO	N-CA-C	5.61	120.92	113.57
1	B	130	LEU	N-CA-C	5.54	118.04	110.24
1	C	431	GLU	N-CA-C	5.52	120.72	112.94
1	A	305	GLY	N-CA-C	-5.50	107.18	115.32
1	D	130	LEU	N-CA-C	5.50	117.83	110.35
1	C	334	GLU	N-CA-C	5.47	118.00	111.71
1	B	384	ASP	N-CA-C	-5.46	98.86	108.20
1	A	130	LEU	N-CA-C	5.45	117.76	110.35
1	C	367	VAL	CA-C-N	5.42	125.24	119.28
1	C	367	VAL	C-N-CA	5.42	125.24	119.28
1	D	141	VAL	N-CA-C	5.41	115.67	110.74
1	B	119	TYR	N-CA-C	5.41	117.67	110.53
1	A	110	SER	CA-C-N	5.38	126.56	119.84
1	A	110	SER	C-N-CA	5.38	126.56	119.84
1	A	386	LEU	N-CA-C	-5.38	105.85	112.90
1	B	464	ASN	N-CA-C	5.35	120.48	113.20
1	D	533	ASN	N-CA-C	5.35	118.03	111.82
1	D	490	ASN	N-CA-C	5.33	118.62	110.20
1	D	158	PHE	N-CA-C	5.33	122.12	114.39
1	C	293	SER	N-CA-C	5.32	116.08	108.74
1	B	158	PHE	N-CA-C	5.32	122.33	114.09
1	B	235	PRO	N-CA-C	5.29	120.47	113.86
1	A	158	PHE	N-CA-C	5.27	122.22	113.89
1	C	130	LEU	N-CA-C	5.27	117.87	110.23
1	C	234	GLY	CA-C-N	5.26	124.77	119.19
1	C	234	GLY	C-N-CA	5.26	124.77	119.19
1	C	425	VAL	N-CA-C	5.22	116.10	108.53
1	B	125	SER	N-CA-C	5.22	116.22	108.60
1	B	343	VAL	CA-C-N	5.22	125.47	119.83
1	B	343	VAL	C-N-CA	5.22	125.47	119.83
1	A	511	VAL	N-CA-C	5.20	116.86	108.85
1	B	107	ARG	CA-C-N	5.20	125.20	119.90
1	B	107	ARG	C-N-CA	5.20	125.20	119.90
1	A	286	TRP	N-CA-C	5.19	119.48	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	450	GLU	N-CA-C	-5.19	107.50	113.88
1	B	334	GLU	N-CA-C	5.18	117.67	111.71
1	A	114	VAL	N-CA-C	5.18	115.77	108.36
1	A	390	ASP	CA-C-N	5.18	125.22	119.32
1	A	390	ASP	C-N-CA	5.18	125.22	119.32
1	B	207	ALA	N-CA-C	-5.16	105.55	111.07
1	A	542	ALA	N-CA-C	-5.14	106.95	113.43
1	B	74	ASP	N-CA-C	5.14	116.86	108.63
1	C	39	GLU	CA-C-N	5.14	125.68	120.38
1	C	39	GLU	C-N-CA	5.14	125.68	120.38
1	D	286	TRP	N-CA-C	5.13	119.54	113.28
1	D	110	SER	CA-C-N	5.11	126.23	119.84
1	D	110	SER	C-N-CA	5.11	126.23	119.84
1	C	422	GLY	N-CA-C	5.10	120.88	114.25
1	A	385	TRP	N-CA-C	5.09	118.97	112.87
1	A	539	LEU	N-CA-C	-5.04	105.86	111.36
1	B	71	GLN	N-CA-C	5.04	115.18	108.38
1	C	107	ARG	CA-C-N	5.04	125.04	119.90
1	C	107	ARG	C-N-CA	5.04	125.04	119.90
1	A	382	TYR	N-CA-C	5.03	119.42	113.28
1	C	266	ASP	N-CA-C	5.02	117.40	111.33
1	C	125	SER	N-CA-C	5.01	115.14	108.38
1	A	490	ASN	N-CA-C	5.01	118.11	110.20
1	D	386	LEU	N-CA-C	-5.01	105.92	112.23

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	TYR	Sidechain
1	C	98	TYR	Sidechain
1	D	70	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	4187	0	4068	166	0
1	B	4169	0	4048	140	0
1	C	4186	0	4053	162	0
1	D	4192	0	4070	179	0
2	E	38	0	34	2	0
3	A	14	0	13	1	0
4	A	18	0	38	1	0
4	B	18	0	38	13	0
4	C	18	0	38	19	0
4	D	18	0	38	7	0
5	A	6	0	8	2	0
5	B	6	0	8	1	0
5	C	6	0	8	7	0
5	D	6	0	8	1	0
6	B	5	0	0	0	0
6	C	10	0	0	0	0
7	A	27	0	0	2	0
7	B	49	0	0	1	0
7	C	59	0	0	1	0
7	D	52	0	0	4	0
All	All	17084	0	16470	652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (652) 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:D:428:TYR:HB2	1:D:513:LEU:HD23	1.33	1.10
1:A:261:GLY:HA3	4:C:997:DME:H152	1.29	1.09
1:B:219:ARG:HG3	1:B:219:ARG:HH11	1.23	0.99
1:A:428:TYR:HB2	1:A:513:LEU:HD23	1.44	0.98
1:B:84:GLU:HA	1:B:87:ASN:HD22	1.31	0.96
1:A:261:GLY:HA3	4:C:997:DME:C15	1.95	0.95
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.31	0.95
1:D:429:ILE:HD11	1:D:524:LEU:HD21	1.45	0.95
1:C:84:GLU:HA	1:C:87:ASN:HD22	1.34	0.93
1:A:429:ILE:HD11	1:A:524:LEU:HD21	1.53	0.91
1:C:219:ARG:HH11	1:C:219:ARG:HG2	1.37	0.89
1:B:498:PRO:HB2	1:B:518:LEU:HB2	1.55	0.88
1:D:329:GLY:HA3	1:D:428:TYR:CZ	2.08	0.88
1:D:329:GLY:HA3	1:D:428:TYR:CE2	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ARG:HH11	1:D:11:ARG:HB2	1.41	0.85
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.40	0.85
1:C:341:TYR:CD2	4:C:997:DME:H22	2.11	0.84
1:D:107:ARG:HG3	1:D:107:ARG:HH11	1.42	0.84
1:B:219:ARG:HG3	1:B:219:ARG:NH1	1.91	0.83
1:B:319:GLY:H	1:B:421:GLN:HE22	1.25	0.83
1:D:534:ARG:HG3	1:D:534:ARG:HH11	1.44	0.83
1:A:30:SER:HB2	1:A:103:THR:HG22	1.60	0.81
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.43	0.80
1:B:161:LEU:HD22	1:B:270:ILE:HD11	1.62	0.80
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.16	0.80
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.62	0.80
1:C:286:TRP:CH2	4:C:997:DME:C15	2.65	0.80
1:C:286:TRP:CH2	4:C:997:DME:H151	2.16	0.79
1:C:498:PRO:HB2	1:C:518:LEU:HB2	1.63	0.79
1:A:226:VAL:HG11	1:A:480:TRP:HE1	1.48	0.79
1:B:41:PRO:HD3	1:B:97:LEU:HD12	1.66	0.78
1:C:286:TRP:CZ2	4:C:997:DME:H151	2.18	0.78
1:D:266:ASP:O	1:D:270:ILE:HG12	1.85	0.77
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.49	0.77
1:B:124:TYR:OH	4:B:996:DME:H82	1.84	0.77
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.68	0.76
1:B:136:ARG:HH11	1:B:136:ARG:HG2	1.50	0.75
1:C:161:LEU:HD22	1:C:270:ILE:HD11	1.68	0.74
7:A:1009:HOH:O	1:B:527:GLN:HG3	1.88	0.74
1:C:219:ARG:HG2	1:C:219:ARG:NH1	2.02	0.73
1:B:291:GLN:HE21	1:B:368:PRO:HB2	1.53	0.73
1:B:319:GLY:H	1:B:421:GLN:NE2	1.86	0.72
1:D:528:THR:O	1:D:531:PHE:HB3	1.88	0.72
1:C:329:GLY:HA3	1:C:428:TYR:CE2	2.25	0.72
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.25	0.71
1:C:104:PRO:HD2	1:C:108:PRO:HD3	1.71	0.71
1:C:7:GLN:NE2	1:C:107:ARG:H	1.88	0.71
1:D:45:ARG:HG3	1:D:45:ARG:NH1	1.98	0.71
1:D:367:VAL:HG12	1:D:370:ALA:HB2	1.73	0.71
1:D:460:ASP:HB3	1:D:463:LEU:HD12	1.72	0.71
1:D:535:PHE:O	1:D:538:LYS:HG2	1.90	0.70
1:A:528:THR:O	1:A:531:PHE:HB3	1.92	0.70
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.05	0.70
1:D:161:LEU:HD22	1:D:270:ILE:HD11	1.74	0.70
1:D:65:PHE:HB2	1:D:90:ARG:HH11	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:O	1:A:183:VAL:HG12	1.92	0.69
1:C:291:GLN:HE21	1:C:368:PRO:HB2	1.58	0.69
1:C:338:PHE:HE2	4:C:997:DME:H71	1.56	0.69
1:A:535:PHE:O	1:A:538:LYS:HG2	1.92	0.69
1:D:428:TYR:CB	1:D:513:LEU:HD23	2.18	0.69
1:D:30:SER:HB2	1:D:103:THR:HG22	1.73	0.69
1:C:494:ASP:C	1:C:496:LYS:H	2.00	0.67
4:B:996:DME:H153	1:D:261:GLY:HA2	1.76	0.67
1:A:116:ILE:HD11	1:A:183:VAL:HG11	1.75	0.67
1:C:319:GLY:H	1:C:421:GLN:HE22	1.42	0.67
1:A:149:MET:HE2	1:A:176:GLN:HA	1.74	0.67
1:D:337:TYR:HE2	4:D:999:DME:H71	1.60	0.67
1:C:310:ASP:HB3	1:C:315:LEU:HD13	1.77	0.66
1:D:347:SER:HB2	2:E:1:NAG:H62	1.76	0.66
1:D:24:ALA:HB3	1:D:140:GLN:HG3	1.77	0.66
1:D:44:SER:HA	1:D:274:ARG:HD2	1.78	0.66
1:D:250:LEU:HD23	1:D:288:VAL:HG12	1.78	0.66
1:A:261:GLY:CA	4:C:997:DME:H152	2.17	0.66
1:B:494:ASP:C	1:B:496:LYS:H	2.03	0.66
1:D:534:ARG:HG3	1:D:534:ARG:NH1	2.11	0.66
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.76	0.66
1:A:397:ALA:O	1:A:401:VAL:HG23	1.96	0.66
1:C:286:TRP:CH2	4:C:997:DME:H153	2.31	0.65
1:A:266:ASP:O	1:A:270:ILE:HG12	1.97	0.65
1:B:459:LEU:HD23	1:B:470:ARG:HG2	1.79	0.65
1:C:226:VAL:HG13	1:C:327:LEU:HB3	1.79	0.65
1:A:44:SER:HA	1:A:274:ARG:HD2	1.79	0.65
1:A:365:ILE:O	1:A:368:PRO:HD3	1.96	0.65
1:D:245:ARG:HD2	7:D:1000:HOH:O	1.97	0.64
1:C:440:PRO:HG2	1:C:443:MET:HG3	1.78	0.64
1:D:452:GLU:OE2	5:D:952:GOL:O1	2.12	0.64
1:A:294:ILE:HG12	1:A:365:ILE:HG22	1.79	0.64
1:A:460:ASP:HB3	1:A:463:LEU:HD12	1.80	0.64
1:A:497:SER:CB	1:A:498:PRO:HD3	2.27	0.64
1:B:310:ASP:HB3	1:B:315:LEU:HD13	1.79	0.64
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.32	0.64
1:B:252:ALA:HA	1:B:273:LEU:HD21	1.80	0.63
1:C:117:TRP:HB2	1:C:200:PHE:CE1	2.33	0.63
1:B:294:ILE:HA	4:B:996:DME:C3	2.28	0.63
1:A:450:GLU:HG2	1:A:451:ILE:N	2.12	0.63
1:D:417:ARG:HG3	1:D:417:ARG:HH11	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.32	0.63
1:B:136:ARG:HH11	1:B:136:ARG:CG	2.12	0.63
1:A:452:GLU:OE2	5:A:954:GOL:O1	2.17	0.62
1:C:219:ARG:NH2	1:C:324:LEU:HG	2.13	0.62
1:A:114:VAL:HG23	1:A:197:VAL:HA	1.80	0.62
1:B:226:VAL:HG13	1:B:327:LEU:HB3	1.80	0.62
1:B:317:ASN:ND2	1:B:417:ARG:HE	1.97	0.62
1:B:348:LYS:HA	1:B:440:PRO:HG3	1.81	0.62
1:A:11:ARG:HH11	1:A:11:ARG:HB2	1.65	0.62
1:A:207:ALA:O	1:A:211:MET:HG2	1.99	0.62
1:A:534:ARG:HG3	1:A:534:ARG:NH1	2.14	0.62
1:D:497:SER:CB	1:D:498:PRO:HD3	2.30	0.62
1:D:450:GLU:HG2	1:D:451:ILE:N	2.14	0.62
1:B:77:TYR:CD2	1:B:348:LYS:HD3	2.35	0.61
1:D:498:PRO:HB2	1:D:518:LEU:HB2	1.80	0.61
1:D:12:VAL:HG12	1:D:14:GLY:H	1.65	0.61
1:B:446:PRO:HG2	1:B:449:TYR:CD2	2.35	0.61
1:C:329:GLY:HA3	1:C:428:TYR:CZ	2.36	0.61
1:B:352:SER:O	1:B:395:ARG:HG3	2.01	0.60
1:A:155:THR:HG22	1:A:159:LEU:HD12	1.83	0.60
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.36	0.60
1:B:50:PRO:HB2	1:B:178:LEU:HD12	1.83	0.60
1:B:117:TRP:HB2	1:B:200:PHE:CE1	2.37	0.60
4:D:999:DME:H92	4:D:999:DME:H182	1.83	0.60
1:B:317:ASN:HD22	1:B:417:ARG:HH21	1.49	0.60
1:D:470:ARG:O	1:D:474:GLN:HG3	2.01	0.60
1:D:300:VAL:HB	1:D:301:PRO:HD2	1.84	0.60
1:D:356:ARG:HA	1:D:394:LEU:HD13	1.84	0.60
1:A:197:VAL:HB	1:A:222:PHE:HA	1.84	0.59
1:A:37:PHE:HD1	1:A:178:LEU:HD12	1.66	0.59
1:C:224:ARG:HG3	1:C:224:ARG:HH11	1.67	0.59
1:C:337:TYR:CE1	4:C:997:DME:H61	2.36	0.59
1:A:113:PRO:HA	1:A:196:SER:OG	2.02	0.59
1:A:532:TRP:O	1:A:537:PRO:HD3	2.02	0.59
1:A:473:ALA:O	1:A:477:MET:HG3	2.02	0.59
1:B:211:MET:HG3	1:B:308:LEU:HD21	1.84	0.59
1:B:293:SER:O	4:B:996:DME:H132	2.01	0.59
1:C:362:GLY:HA3	1:C:398:MET:HE3	1.84	0.59
1:D:113:PRO:HA	1:D:196:SER:OG	2.03	0.59
1:C:20:ILE:HB	1:C:63:THR:HG22	1.83	0.59
1:D:114:VAL:HG11	1:D:187:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:HA3	1:A:146:LEU:HD22	1.83	0.59
1:C:319:GLY:H	1:C:421:GLN:NE2	2.00	0.59
1:C:452:GLU:CD	5:C:951:GOL:H11	2.28	0.59
1:D:287:HIS:HB3	7:D:1034:HOH:O	2.02	0.59
1:C:77:TYR:CD2	1:C:348:LYS:HD3	2.37	0.59
1:D:374:ALA:HA	1:D:539:LEU:HD13	1.85	0.59
1:B:362:GLY:HA3	1:B:398:MET:HE3	1.85	0.59
1:C:266:ASP:O	1:C:270:ILE:HG12	2.02	0.59
1:D:162:PRO:HG2	7:D:1000:HOH:O	2.03	0.59
1:B:470:ARG:O	1:B:474:GLN:HG3	2.03	0.59
1:B:339:LEU:HD11	1:B:399:SER:HA	1.86	0.58
1:C:337:TYR:HE1	4:C:997:DME:H61	1.67	0.58
1:D:45:ARG:HH11	1:D:45:ARG:CG	2.12	0.58
1:D:504:THR:OG1	1:D:507:ALA:HB3	2.03	0.58
1:B:328:VAL:O	1:B:427:ALA:HA	2.03	0.58
1:A:12:VAL:HG12	1:A:14:GLY:H	1.67	0.58
1:A:470:ARG:O	1:A:474:GLN:HG3	2.03	0.58
1:C:353:LEU:HB3	1:C:391:PRO:HB2	1.85	0.58
1:C:332:LYS:HG2	1:C:333:ASP:OD1	2.04	0.58
1:B:498:PRO:CB	1:B:518:LEU:HB2	2.31	0.58
1:C:134:ASP:OD1	1:C:136:ARG:HB3	2.03	0.58
1:A:66:GLN:HG3	1:A:98:TYR:CG	2.38	0.57
1:C:85:MET:HE1	5:C:951:GOL:O1	2.04	0.57
1:C:341:TYR:CD2	4:C:997:DME:C2	2.84	0.57
1:D:197:VAL:HB	1:D:222:PHE:HA	1.86	0.57
1:B:354:ILE:HB	1:B:358:GLN:OE1	2.04	0.57
1:C:216:LEU:HB3	1:C:217:PRO:HD3	1.86	0.57
1:C:338:PHE:CE2	4:C:997:DME:H71	2.38	0.57
1:A:374:ALA:HA	1:A:539:LEU:HD13	1.86	0.57
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.85	0.57
1:B:84:GLU:HA	1:B:87:ASN:ND2	2.11	0.57
1:C:355:SER:OG	1:C:358:GLN:HG3	2.05	0.57
1:A:114:VAL:HG12	1:A:145:VAL:HB	1.87	0.57
1:C:414:LEU:HG	1:C:418:LEU:HD22	1.85	0.57
1:D:114:VAL:HG23	1:D:197:VAL:HA	1.87	0.57
1:C:437:LEU:HA	5:C:951:GOL:H32	1.87	0.57
1:D:365:ILE:O	1:D:368:PRO:HD3	2.05	0.57
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.87	0.57
1:D:226:VAL:HG11	1:D:480:TRP:HE1	1.70	0.57
1:D:155:THR:HG22	1:D:159:LEU:HB2	1.86	0.56
1:C:300:VAL:HB	1:C:301:PRO:CD	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:TRP:O	1:D:537:PRO:HD3	2.05	0.56
1:A:181:GLN:O	1:A:185:GLU:HG2	2.04	0.56
1:B:176:GLN:OE1	1:B:212:HIS:HE1	1.88	0.56
1:B:293:SER:O	4:B:996:DME:C13	2.53	0.56
1:A:375:ALA:O	1:A:379:VAL:HG23	2.06	0.56
1:A:119:TYR:CE1	1:A:151:TYR:CE1	2.94	0.56
1:C:202:GLU:HA	1:C:228:GLN:O	2.06	0.56
1:C:328:VAL:O	1:C:427:ALA:HA	2.06	0.56
1:C:460:ASP:OD1	1:C:462:SER:HB3	2.05	0.56
1:D:114:VAL:HG12	1:D:145:VAL:HB	1.88	0.56
1:C:535:PHE:CE2	1:C:539:LEU:HD12	2.40	0.56
1:A:65:PHE:HE1	1:A:100:ASN:ND2	2.04	0.55
1:A:417:ARG:HH11	1:A:417:ARG:HG3	1.71	0.55
1:C:41:PRO:HD3	1:C:97:LEU:HD12	1.87	0.55
1:A:139:ALA:O	1:A:143:GLY:HA2	2.06	0.55
1:B:266:ASP:O	1:B:270:ILE:HG12	2.06	0.55
1:C:252:ALA:HA	1:C:273:LEU:HD21	1.88	0.55
1:A:498:PRO:HB2	1:A:518:LEU:HB2	1.88	0.55
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.88	0.55
1:B:433:ARG:NH2	1:B:439:TRP:O	2.33	0.55
1:C:498:PRO:CB	1:C:518:LEU:HB2	2.32	0.55
1:D:65:PHE:HB2	1:D:90:ARG:NH1	2.21	0.55
1:B:300:VAL:HB	1:B:301:PRO:CD	2.36	0.55
4:B:996:DME:H41	4:B:996:DME:H142	1.87	0.55
1:A:119:TYR:HE2	1:A:150:ASN:HA	1.72	0.55
1:A:132:VAL:HG23	1:A:133:TYR:CD1	2.42	0.55
1:C:252:ALA:CB	1:C:269:LEU:HD21	2.37	0.55
1:A:516:LYS:HE3	1:A:516:LYS:HA	1.89	0.55
1:B:161:LEU:HD21	1:B:269:LEU:HD13	1.89	0.55
1:C:166:GLU:H	1:C:166:GLU:CD	2.15	0.55
1:D:207:ALA:O	1:D:211:MET:HG2	2.07	0.54
1:C:458:PRO:HA	1:C:465:TYR:CD2	2.43	0.54
1:B:11:ARG:HG3	1:B:16:GLN:HG2	1.89	0.54
1:D:329:GLY:O	1:D:330:VAL:HG23	2.07	0.54
1:D:397:ALA:O	1:D:401:VAL:HG23	2.07	0.54
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.42	0.54
1:D:132:VAL:HG23	1:D:133:TYR:CD1	2.42	0.54
1:C:459:LEU:HD23	1:C:470:ARG:HG2	1.88	0.54
1:D:112:THR:HG23	1:D:113:PRO:HD2	1.90	0.54
1:D:116:ILE:HD11	1:D:183:VAL:HG11	1.90	0.54
1:D:155:THR:HG22	1:D:159:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ASN:ND2	1:C:417:ARG:HE	2.05	0.54
1:D:123:PHE:HB2	1:D:300:VAL:HG12	1.88	0.54
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.43	0.54
1:C:224:ARG:HG3	1:C:224:ARG:NH1	2.22	0.54
1:C:138:LEU:HD13	1:C:477:MET:HE3	1.90	0.54
1:C:84:GLU:HA	1:C:87:ASN:ND2	2.15	0.53
1:D:300:VAL:HB	1:D:301:PRO:CD	2.38	0.53
1:A:112:THR:HG23	1:A:113:PRO:HD2	1.90	0.53
1:A:123:PHE:HB2	1:A:300:VAL:HG12	1.91	0.53
1:C:77:TYR:CE2	1:C:348:LYS:HD3	2.44	0.53
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.18	0.53
1:D:66:GLN:HG3	1:D:98:TYR:CG	2.44	0.53
1:A:45:ARG:HH11	1:A:45:ARG:CG	2.15	0.53
1:A:205:GLY:O	1:A:208:SER:HB2	2.08	0.53
1:C:184:GLN:HA	1:C:184:GLN:HE21	1.73	0.53
1:C:433:ARG:NH2	1:C:439:TRP:O	2.37	0.53
1:A:141:VAL:HG21	1:A:459:LEU:CD2	2.39	0.53
1:D:200:PHE:HB2	1:D:226:VAL:HB	1.91	0.53
1:B:202:GLU:HA	1:B:228:GLN:O	2.09	0.52
1:A:468:GLU:HA	1:A:471:ILE:HD12	1.89	0.52
1:D:119:TYR:HE2	1:D:150:ASN:HA	1.73	0.52
1:A:475:ARG:O	1:A:478:LYS:HB2	2.09	0.52
1:B:8:LEU:O	1:B:18:ARG:HA	2.08	0.52
1:A:152:ARG:O	1:A:157:GLY:HA3	2.10	0.52
1:A:488:ASP:OD1	1:A:490:ASN:HB2	2.10	0.52
1:A:504:THR:OG1	1:A:507:ALA:HB3	2.10	0.52
1:C:341:TYR:CE2	4:C:997:DME:H22	2.45	0.52
1:C:494:ASP:C	1:C:496:LYS:N	2.67	0.52
1:B:414:LEU:HG	1:B:418:LEU:HD22	1.92	0.52
1:C:85:MET:CE	5:C:951:GOL:O1	2.58	0.52
1:A:444:GLY:O	1:A:446:PRO:HD3	2.10	0.52
1:C:348:LYS:HA	1:C:440:PRO:HG3	1.91	0.52
1:D:251:LEU:O	1:D:251:LEU:HG	2.07	0.52
1:A:331:VAL:HB	1:A:445:VAL:HG12	1.91	0.51
1:A:407:VAL:O	1:A:411:VAL:HG23	2.10	0.51
1:C:172:GLY:O	1:C:176:GLN:HG3	2.10	0.51
1:D:115:LEU:HD12	1:D:198:THR:HB	1.92	0.51
1:D:251:LEU:HD21	1:D:281:LEU:HD12	1.92	0.51
1:B:291:GLN:NE2	1:B:368:PRO:HB2	2.22	0.51
4:B:996:DME:C15	1:D:261:GLY:HA2	2.39	0.51
1:C:536:LEU:HD13	1:C:540:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.46	0.51
1:B:252:ALA:CB	1:B:269:LEU:HD21	2.40	0.51
1:C:452:GLU:OE2	5:C:951:GOL:H11	2.09	0.51
1:D:243:GLU:O	1:D:247:ARG:HG3	2.10	0.51
1:B:7:GLN:NE2	1:B:107:ARG:H	2.08	0.51
1:B:20:ILE:HB	1:B:63:THR:HG22	1.93	0.51
1:B:531:PHE:CZ	1:B:536:LEU:HG	2.45	0.51
1:C:227:LEU:HB2	1:C:328:VAL:HG12	1.93	0.51
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.20	0.51
1:C:80:PHE:CE1	1:C:438:THR:HB	2.46	0.51
1:D:48:MET:HE1	1:D:165:ARG:HH21	1.76	0.51
1:D:488:ASP:OD1	1:D:490:ASN:HB2	2.11	0.51
1:D:375:ALA:O	1:D:379:VAL:HG23	2.11	0.51
1:B:460:ASP:OD1	1:B:462:SER:HB3	2.11	0.51
1:D:139:ALA:O	1:D:143:GLY:HA2	2.10	0.51
1:D:356:ARG:HH12	1:D:383:THR:HG23	1.76	0.51
1:D:511:VAL:HB	1:D:518:LEU:HD22	1.92	0.51
1:A:356:ARG:HH12	1:A:383:THR:HG23	1.75	0.51
1:B:536:LEU:HD13	1:B:540:LEU:CD2	2.41	0.51
1:A:89:ASN:O	1:A:90:ARG:HD3	2.11	0.50
1:C:136:ARG:HB3	1:C:136:ARG:HH11	1.75	0.50
1:C:452:GLU:OE1	5:C:951:GOL:H11	2.10	0.50
1:D:110:SER:HB2	1:D:111:PRO:HD2	1.93	0.50
4:D:999:DME:H173	4:D:999:DME:C9	2.41	0.50
1:A:328:VAL:HG12	1:A:329:GLY:N	2.26	0.50
1:D:294:ILE:HG12	1:D:365:ILE:HG22	1.94	0.50
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.94	0.50
1:B:310:ASP:HB3	1:B:315:LEU:CD1	2.40	0.50
1:C:466:THR:OG1	1:C:469:GLU:HG3	2.11	0.50
1:D:205:GLY:O	1:D:208:SER:HB2	2.11	0.50
1:A:7:GLN:CB	1:A:105:TYR:HE1	2.25	0.50
1:A:41:PRO:HA	1:A:45:ARG:HB3	1.93	0.50
1:A:466:THR:OG1	1:A:469:GLU:HG3	2.10	0.50
1:C:89:ASN:OD1	1:C:129:SER:HB2	2.12	0.50
1:D:135:GLY:HA3	1:D:146:LEU:HD22	1.93	0.50
1:A:21:ARG:HH21	1:A:23:LYS:NZ	2.10	0.50
1:B:535:PHE:CE2	1:B:539:LEU:HD12	2.47	0.50
1:A:367:VAL:HG12	1:A:370:ALA:HB2	1.94	0.49
1:A:251:LEU:HD21	1:A:281:LEU:HD12	1.94	0.49
1:C:339:LEU:HD11	1:C:399:SER:HA	1.94	0.49
1:D:166:GLU:HB2	1:D:274:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HD22	1:B:270:ILE:CD1	2.39	0.49
1:C:12:VAL:HG22	1:C:186:ASN:HB3	1.94	0.49
1:C:536:LEU:N	1:C:537:PRO:HD2	2.27	0.49
1:A:407:VAL:O	1:A:410:PRO:HD2	2.12	0.49
1:C:352:SER:O	1:C:395:ARG:HG3	2.13	0.49
1:B:124:TYR:OH	4:B:996:DME:C8	2.57	0.49
1:B:250:LEU:HD23	1:B:288:VAL:HG12	1.95	0.49
1:B:355:SER:OG	1:B:358:GLN:HG3	2.12	0.49
1:D:11:ARG:HH11	1:D:11:ARG:CB	2.20	0.49
1:D:466:THR:OG1	1:D:469:GLU:HG3	2.12	0.49
1:B:216:LEU:HB3	1:B:217:PRO:HD3	1.94	0.49
1:B:331:VAL:HG12	1:B:430:PHE:HB3	1.95	0.49
1:D:327:LEU:HD23	1:D:328:VAL:N	2.27	0.49
1:A:22:LEU:HD13	1:A:31:ALA:HB3	1.95	0.49
1:B:89:ASN:OD1	1:B:129:SER:HB2	2.13	0.49
1:C:219:ARG:HH21	1:C:324:LEU:HG	1.77	0.49
1:A:122:GLY:O	1:A:123:PHE:HB2	2.13	0.49
1:C:32:PHE:N	1:C:32:PHE:CD1	2.80	0.49
1:C:362:GLY:HA3	1:C:398:MET:CE	2.43	0.49
1:A:407:VAL:C	1:A:410:PRO:HD2	2.38	0.49
1:B:293:SER:O	4:B:996:DME:H22	2.13	0.49
1:C:446:PRO:HG2	1:C:449:TYR:CD1	2.47	0.49
1:C:535:PHE:CB	1:D:380:LEU:HD12	2.42	0.49
1:D:33:LEU:HD12	1:D:100:ASN:HB3	1.95	0.49
1:D:313:GLU:HB2	7:D:1046:HOH:O	2.12	0.49
1:A:327:LEU:HD23	1:A:328:VAL:N	2.28	0.48
1:B:255:VAL:HG12	1:B:284:HIS:ND1	2.27	0.48
1:D:352:SER:O	1:D:395:ARG:HG3	2.13	0.48
1:A:42:VAL:O	1:A:45:ARG:HB2	2.13	0.48
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.78	0.48
1:C:80:PHE:O	1:C:84:GLU:HG2	2.13	0.48
1:C:354:ILE:HB	1:C:358:GLN:OE1	2.13	0.48
1:C:470:ARG:O	1:C:474:GLN:HG3	2.13	0.48
1:D:86:TRP:CZ3	4:D:999:DME:H161	2.48	0.48
1:C:37:PHE:CD1	1:C:99:LEU:HD23	2.49	0.48
1:D:530:ALA:O	1:D:534:ARG:HB2	2.13	0.48
1:A:124:TYR:CD1	1:A:124:TYR:C	2.91	0.48
1:B:294:ILE:HA	4:B:996:DME:H31	1.94	0.48
1:D:149:MET:HE2	1:D:176:GLN:HA	1.95	0.48
1:A:493:ARG:O	1:A:495:ARG:N	2.47	0.48
1:C:211:MET:CE	1:C:301:PRO:HG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ALA:O	1:C:379:VAL:HG23	2.13	0.48
4:C:997:DME:C14	4:C:997:DME:H42	2.43	0.48
1:B:440:PRO:HG2	1:B:443:MET:HG3	1.96	0.48
1:B:536:LEU:N	1:B:537:PRO:HD2	2.28	0.48
1:C:219:ARG:HH11	1:C:219:ARG:CG	2.18	0.48
1:D:494:ASP:O	1:D:496:LYS:N	2.40	0.48
1:A:107:ARG:HG3	1:A:107:ARG:NH1	2.20	0.48
1:C:269:LEU:HD23	1:C:269:LEU:O	2.13	0.48
1:D:142:GLU:CB	1:D:481:THR:HG21	2.44	0.48
1:C:184:GLN:HA	1:C:184:GLN:NE2	2.29	0.47
1:C:255:VAL:HG12	1:C:284:HIS:ND1	2.28	0.47
1:A:110:SER:HB2	1:A:111:PRO:HD2	1.96	0.47
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.95	0.47
1:B:47:PHE:O	1:B:171:VAL:HG11	2.14	0.47
1:C:243:GLU:HA	1:C:243:GLU:OE1	2.14	0.47
1:C:374:ALA:O	1:C:377:ALA:HB3	2.13	0.47
1:A:48:MET:HE1	1:A:165:ARG:HH21	1.79	0.47
1:A:329:GLY:HA3	1:A:428:TYR:CD2	2.49	0.47
1:B:172:GLY:O	1:B:176:GLN:HG3	2.15	0.47
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.49	0.47
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.95	0.47
1:A:317:ASN:HB2	1:A:417:ARG:NH1	2.29	0.47
1:D:347:SER:HB2	2:E:1:NAG:C6	2.43	0.47
1:B:362:GLY:HA3	1:B:398:MET:CE	2.43	0.47
1:C:296:ARG:NH2	1:C:406:ASN:OD1	2.47	0.47
1:C:300:VAL:HB	1:C:301:PRO:HD2	1.96	0.47
1:C:331:VAL:HG22	1:C:334:GLU:OE2	2.15	0.47
1:D:37:PHE:HD1	1:D:178:LEU:HD12	1.79	0.47
1:D:328:VAL:CG1	1:D:411:VAL:HG13	2.44	0.47
1:A:142:GLU:CB	1:A:481:THR:HG21	2.44	0.47
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.79	0.47
1:C:8:LEU:O	1:C:18:ARG:HA	2.14	0.47
1:C:511:VAL:HB	1:C:518:LEU:HD22	1.95	0.47
1:D:495:ARG:O	1:D:496:LYS:C	2.58	0.47
1:A:210:GLY:O	1:A:214:LEU:HD22	2.14	0.47
1:D:516:LYS:HE2	1:D:516:LYS:HA	1.96	0.47
1:A:138:LEU:HD11	1:A:455:PHE:HA	1.97	0.47
1:B:166:GLU:CD	1:B:166:GLU:H	2.21	0.47
1:B:211:MET:HE2	1:B:301:PRO:HG2	1.95	0.47
1:B:536:LEU:HD13	1:B:540:LEU:HD23	1.97	0.47
1:C:119:TYR:HE2	1:C:150:ASN:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:GLY:C	1:C:398:MET:HE1	2.40	0.47
1:C:531:PHE:CZ	1:C:536:LEU:HG	2.49	0.47
1:D:418:LEU:HD12	1:D:418:LEU:HA	1.69	0.47
1:B:29:VAL:CG2	1:B:140:GLN:HB2	2.45	0.47
1:C:346:PHE:HA	1:C:352:SER:OG	2.15	0.47
1:D:70:TYR:HB3	1:D:156:PHE:CE2	2.50	0.47
1:D:317:ASN:HB2	1:D:417:ARG:NH1	2.30	0.47
1:D:374:ALA:O	1:D:378:VAL:HG23	2.15	0.47
1:A:331:VAL:HG12	1:A:430:PHE:HB3	1.97	0.46
1:A:374:ALA:O	1:A:378:VAL:HG23	2.15	0.46
1:D:45:ARG:O	1:D:48:MET:HB2	2.14	0.46
1:D:339:LEU:HD13	1:D:346:PHE:CE2	2.50	0.46
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.47	0.46
1:B:494:ASP:C	1:B:496:LYS:N	2.71	0.46
1:C:29:VAL:CG2	1:C:140:GLN:HB2	2.45	0.46
1:A:451:ILE:H	1:A:451:ILE:HG12	1.49	0.46
1:B:128:ALA:HB1	7:B:1021:HOH:O	2.15	0.46
1:C:245:ARG:NH2	1:C:266:ASP:OD2	2.49	0.46
1:D:121:GLY:HA2	4:D:999:DME:H101	1.97	0.46
1:B:432:HIS:CE1	1:B:515:LEU:HD11	2.51	0.46
1:C:138:LEU:HD23	1:C:146:LEU:CD1	2.46	0.46
1:C:161:LEU:HD21	1:C:269:LEU:HD13	1.98	0.46
1:C:331:VAL:HG12	1:C:430:PHE:HB3	1.98	0.46
1:C:85:MET:SD	5:C:951:GOL:O1	2.73	0.46
1:D:181:GLN:O	1:D:185:GLU:HG2	2.15	0.46
1:A:37:PHE:CD1	1:A:178:LEU:HD12	2.48	0.46
1:D:429:ILE:CD1	1:D:524:LEU:HD21	2.33	0.46
1:A:114:VAL:HG11	1:A:187:ILE:HG12	1.98	0.46
1:B:278:ALA:O	1:B:282:VAL:HG23	2.16	0.46
1:B:317:ASN:ND2	1:B:417:ARG:HH21	2.12	0.46
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.34	0.46
1:A:300:VAL:HB	1:A:301:PRO:CD	2.46	0.46
1:C:24:ALA:HB3	1:C:140:GLN:HG3	1.97	0.46
1:C:530:ALA:O	1:C:534:ARG:HB2	2.16	0.46
1:D:329:GLY:HA3	1:D:428:TYR:CD2	2.50	0.46
1:A:115:LEU:HD12	1:A:198:THR:HB	1.98	0.45
1:C:329:GLY:HA3	1:C:428:TYR:CD2	2.50	0.45
1:D:331:VAL:HG12	1:D:430:PHE:HB3	1.98	0.45
1:B:4:GLU:HG2	1:B:9:LEU:HB2	1.97	0.45
1:B:161:LEU:CD2	1:B:270:ILE:HD11	2.39	0.45
1:B:243:GLU:OE1	1:B:243:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PHE:H	4:B:996:DME:H31	1.80	0.45
1:A:33:LEU:CD1	1:A:33:LEU:N	2.79	0.45
1:A:457:LEU:N	1:A:458:PRO:CD	2.80	0.45
1:B:128:ALA:HB1	1:B:148:SER:OG	2.16	0.45
1:B:532:TRP:O	1:B:537:PRO:HD3	2.16	0.45
1:C:161:LEU:HD22	1:C:270:ILE:CD1	2.44	0.45
1:D:329:GLY:HA3	1:D:428:TYR:CE1	2.48	0.45
1:A:408:VAL:O	1:A:411:VAL:HB	2.17	0.45
1:D:21:ARG:HH21	1:D:23:LYS:NZ	2.14	0.45
1:C:50:PRO:HB2	1:C:178:LEU:HD12	1.97	0.45
1:A:530:ALA:O	1:A:534:ARG:HB2	2.17	0.45
1:B:10:VAL:HG22	1:B:107:ARG:NH1	2.32	0.45
1:C:29:VAL:HG21	1:C:140:GLN:HB2	1.99	0.45
1:D:42:VAL:O	1:D:45:ARG:HB2	2.16	0.45
1:A:33:LEU:N	1:A:33:LEU:HD13	2.32	0.45
1:A:136:ARG:HG2	1:A:137:PHE:N	2.32	0.45
1:B:219:ARG:NH2	1:B:324:LEU:HG	2.32	0.45
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.52	0.44
1:A:112:THR:HG21	1:A:143:GLY:O	2.17	0.44
1:A:501:PRO:HA	1:A:502:PRO:HD3	1.92	0.44
1:C:40:PRO:HA	1:C:41:PRO:HD2	1.74	0.44
1:C:515:LEU:HD23	1:C:515:LEU:HA	1.81	0.44
1:B:29:VAL:HG21	1:B:140:GLN:HB2	1.99	0.44
1:C:536:LEU:HD23	1:C:536:LEU:HA	1.79	0.44
1:D:112:THR:HG21	1:D:143:GLY:O	2.17	0.44
1:D:180:LEU:O	1:D:183:VAL:HG12	2.16	0.44
1:C:252:ALA:HB2	1:C:269:LEU:HD21	2.00	0.44
1:A:45:ARG:O	1:A:48:MET:HB2	2.18	0.44
1:B:77:TYR:CE2	1:B:348:LYS:HD3	2.51	0.44
4:C:997:DME:H182	4:C:997:DME:H102	1.62	0.44
1:D:417:ARG:HH11	1:D:417:ARG:CG	2.30	0.44
1:B:459:LEU:HD21	1:B:474:GLN:HG2	1.98	0.44
1:C:380:LEU:HD22	1:D:535:PHE:CB	2.47	0.44
1:A:166:GLU:HB2	1:A:274:ARG:HH12	1.82	0.44
1:A:497:SER:CB	1:A:498:PRO:CD	2.94	0.44
1:B:300:VAL:HB	1:B:301:PRO:HD2	2.00	0.44
1:C:11:ARG:NH1	1:C:11:ARG:HG3	2.32	0.44
1:C:224:ARG:HD3	1:C:487:GLY:HA2	1.99	0.44
1:C:507:ALA:HA	1:C:522:ARG:HH21	1.82	0.44
1:D:356:ARG:HG2	1:D:360:LEU:CD2	2.48	0.44
1:D:512:SER:HB3	1:D:519:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLN:HE22	1:C:107:ARG:H	1.65	0.44
1:B:124:TYR:HH	4:B:996:DME:H82	1.78	0.44
1:D:155:THR:HG22	1:D:159:LEU:CD1	2.48	0.44
1:D:372:ASP:O	1:D:375:ALA:HB3	2.18	0.44
1:B:336:SER:O	1:B:337:TYR:C	2.61	0.44
1:D:104:PRO:HG2	1:D:108:PRO:HD3	2.00	0.44
1:D:152:ARG:O	1:D:157:GLY:HA3	2.18	0.44
1:D:177:ARG:CZ	1:D:217:PRO:HB2	2.48	0.44
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.80	0.43
1:A:491:ASP:HA	1:A:492:PRO:HD2	1.56	0.43
1:C:206:ALA:O	1:C:227:LEU:HD23	2.18	0.43
1:C:363:VAL:N	1:C:398:MET:HE1	2.33	0.43
1:D:41:PRO:HA	1:D:45:ARG:HB3	1.99	0.43
1:D:124:TYR:CD1	1:D:124:TYR:C	2.96	0.43
1:D:291:GLN:HE21	1:D:291:GLN:HB2	1.60	0.43
1:B:4:GLU:HG3	1:B:5:ASP:N	2.34	0.43
1:B:287:HIS:CD2	1:B:287:HIS:N	2.86	0.43
1:D:407:VAL:C	1:D:410:PRO:HD2	2.42	0.43
1:D:524:LEU:HA	1:D:524:LEU:HD23	1.73	0.43
1:A:226:VAL:HG11	1:A:480:TRP:NE1	2.25	0.43
1:B:40:PRO:HA	1:B:41:PRO:HD2	1.80	0.43
1:B:211:MET:CE	1:B:301:PRO:HG2	2.49	0.43
1:B:382:TYR:CD2	1:B:401:VAL:HG22	2.53	0.43
1:D:11:ARG:HB2	1:D:11:ARG:NH1	2.21	0.43
1:C:466:THR:HG23	1:C:469:GLU:OE1	2.18	0.43
1:D:311:THR:HG22	1:D:313:GLU:H	1.82	0.43
1:A:138:LEU:HG	1:A:477:MET:HE3	2.00	0.43
1:A:356:ARG:O	1:A:360:LEU:HD22	2.19	0.43
1:A:426:TYR:HD2	1:A:500:TRP:CD1	2.36	0.43
1:D:112:THR:HG21	1:D:144:ALA:HA	2.00	0.43
1:A:99:LEU:C	1:A:99:LEU:HD12	2.44	0.43
1:C:9:LEU:HD11	1:C:16:GLN:NE2	2.33	0.43
1:D:367:VAL:CG1	1:D:370:ALA:HB2	2.45	0.43
1:B:32:PHE:CD1	1:B:32:PHE:N	2.86	0.43
1:B:183:VAL:HG13	1:B:187:ILE:HB	2.01	0.43
1:D:86:TRP:CE3	4:D:999:DME:H161	2.54	0.43
1:D:518:LEU:HA	1:D:518:LEU:HD23	1.79	0.43
1:A:202:GLU:O	1:A:205:GLY:N	2.52	0.43
1:A:295:PHE:CE2	1:A:338:PHE:CZ	3.07	0.43
1:C:246:ARG:HH11	1:C:246:ARG:HD3	1.61	0.43
1:D:328:VAL:HG11	1:D:411:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:VAL:O	1:D:411:VAL:HG23	2.19	0.43
1:A:356:ARG:HA	1:A:394:LEU:HD13	2.00	0.43
1:A:472:PHE:CE1	1:A:476:LEU:HD11	2.54	0.43
1:B:223:HIS:CD2	1:B:223:HIS:N	2.87	0.43
1:C:321:PHE:CD2	1:C:418:LEU:HD12	2.54	0.43
1:A:12:VAL:HG13	1:A:186:ASN:OD1	2.19	0.43
1:C:336:SER:O	1:C:337:TYR:C	2.62	0.43
1:D:12:VAL:HG13	1:D:186:ASN:OD1	2.19	0.43
1:D:250:LEU:HD23	1:D:288:VAL:HA	2.00	0.43
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.78	0.42
1:C:269:LEU:HD23	1:C:269:LEU:C	2.44	0.42
1:C:532:TRP:O	1:C:537:PRO:HD3	2.18	0.42
1:D:33:LEU:N	1:D:33:LEU:HD13	2.34	0.42
1:D:351:GLU:HB2	1:D:353:LEU:HD22	2.01	0.42
1:D:386:LEU:HD23	1:D:386:LEU:HA	1.94	0.42
1:D:493:ARG:O	1:D:495:ARG:N	2.52	0.42
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.49	0.42
1:C:226:VAL:HA	1:C:327:LEU:O	2.19	0.42
1:C:450:GLU:HG2	1:C:451:ILE:N	2.35	0.42
1:A:40:PRO:HG3	1:A:95:ASP:OD1	2.19	0.42
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.83	0.42
1:B:134:ASP:OD1	1:B:136:ARG:NH1	2.53	0.42
1:C:327:LEU:HD21	1:C:500:TRP:CH2	2.55	0.42
1:D:46:ARG:HB3	1:D:274:ARG:HG2	2.00	0.42
1:D:99:LEU:C	1:D:99:LEU:HD12	2.45	0.42
1:D:193:ASP:OD1	1:D:195:MET:HB2	2.19	0.42
1:D:331:VAL:HB	1:D:445:VAL:HG12	2.01	0.42
1:B:138:LEU:HD13	1:B:477:MET:HG2	2.00	0.42
1:C:121:GLY:CA	4:C:997:DME:H91	2.49	0.42
1:C:211:MET:HE2	1:C:301:PRO:HG2	2.00	0.42
1:C:291:GLN:NE2	1:C:368:PRO:HB2	2.31	0.42
1:C:397:ALA:O	1:C:401:VAL:HG23	2.19	0.42
1:D:46:ARG:HD3	1:D:47:PHE:CZ	2.54	0.42
1:A:476:LEU:HA	1:A:479:TYR:HD2	1.85	0.42
1:B:185:GLU:HB2	1:B:186:ASN:H	1.66	0.42
1:B:224:ARG:HG3	1:B:224:ARG:HH11	1.85	0.42
1:C:312:PRO:O	1:C:316:ILE:HG12	2.20	0.42
1:D:286:TRP:CZ2	4:D:999:DME:H142	2.55	0.42
1:B:383:THR:HG22	1:B:384:ASP:N	2.34	0.42
1:C:80:PHE:HE1	1:C:438:THR:HB	1.84	0.42
1:C:85:MET:HE2	1:C:86:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:NH1	1:D:107:ARG:CG	2.82	0.42
1:D:132:VAL:HA	1:D:457:LEU:HD21	2.02	0.42
1:A:380:LEU:HA	1:A:385:TRP:HZ2	1.84	0.42
1:B:224:ARG:HG3	1:B:224:ARG:NH1	2.35	0.42
1:C:359:PHE:O	1:C:363:VAL:HG23	2.20	0.42
1:C:540:LEU:HD13	1:C:540:LEU:HA	1.78	0.42
1:D:130:LEU:HD23	1:D:130:LEU:HA	1.92	0.42
1:D:296:ARG:NH2	1:D:406:ASN:OD1	2.53	0.42
1:A:46:ARG:HD3	1:A:47:PHE:CZ	2.54	0.42
1:B:138:LEU:HD13	1:B:477:MET:HE3	2.02	0.42
1:B:535:PHE:HE2	1:B:539:LEU:HD12	1.83	0.42
1:D:434:ALA:O	1:D:437:LEU:HB2	2.19	0.42
1:B:374:ALA:O	1:B:377:ALA:HB3	2.20	0.42
1:D:476:LEU:HD21	1:D:513:LEU:HD12	2.02	0.42
1:D:491:ASP:HA	1:D:492:PRO:HD2	1.58	0.42
1:A:524:LEU:HA	1:A:524:LEU:HD23	1.82	0.42
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.87	0.42
1:C:124:TYR:OH	4:C:997:DME:H42	2.19	0.42
1:D:325:GLN:O	1:D:483:PHE:HZ	2.03	0.42
1:D:501:PRO:HA	1:D:502:PRO:HD3	1.90	0.42
1:A:328:VAL:CG1	1:A:411:VAL:HG13	2.50	0.41
1:A:414:LEU:O	1:A:418:LEU:HB2	2.20	0.41
1:B:428:TYR:CD1	1:B:428:TYR:C	2.98	0.41
1:C:10:VAL:HG22	1:C:107:ARG:NH1	2.35	0.41
1:D:250:LEU:CD2	1:D:288:VAL:HG12	2.49	0.41
1:D:324:LEU:HD23	1:D:325:GLN:H	1.85	0.41
1:D:457:LEU:N	1:D:458:PRO:CD	2.83	0.41
1:D:538:LYS:HE3	1:D:538:LYS:HB3	1.94	0.41
1:A:330:VAL:CG1	1:A:331:VAL:N	2.83	0.41
1:C:342:GLY:O	1:C:344:PRO:HD3	2.21	0.41
1:D:48:MET:HE1	1:D:165:ARG:NH2	2.35	0.41
1:D:295:PHE:CE2	1:D:338:PHE:CZ	3.07	0.41
1:A:211:MET:HE3	1:A:301:PRO:HG2	2.01	0.41
1:A:516:LYS:HE3	1:A:516:LYS:CA	2.50	0.41
1:B:243:GLU:OE1	1:B:246:ARG:NH1	2.53	0.41
1:C:155:THR:HG22	1:C:159:LEU:HD12	2.02	0.41
1:D:119:TYR:CE2	1:D:150:ASN:HA	2.53	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.89	0.41
1:A:351:GLU:HB2	1:A:353:LEU:HD22	2.02	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD2	1.80	0.41
1:B:294:ILE:HA	4:B:996:DME:H22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD12	1:B:418:LEU:HA	1.91	0.41
1:A:536:LEU:HB3	1:A:537:PRO:HD3	2.03	0.41
1:B:85:MET:SD	5:B:953:GOL:O1	2.72	0.41
1:C:383:THR:HG22	1:C:384:ASP:N	2.35	0.41
1:A:20:ILE:HG12	1:A:21:ARG:N	2.35	0.41
1:A:350:ASN:ND2	3:A:709:NAG:C7	2.83	0.41
1:B:41:PRO:HA	1:B:45:ARG:HB3	2.03	0.41
1:D:70:TYR:CD1	1:D:92:LEU:HB3	2.55	0.41
1:D:142:GLU:HG3	1:D:481:THR:HG21	2.03	0.41
1:D:211:MET:HE3	1:D:301:PRO:HG2	2.02	0.41
1:D:534:ARG:NH1	1:D:534:ARG:CG	2.80	0.41
1:D:536:LEU:HB3	1:D:537:PRO:HD3	2.02	0.41
1:B:255:VAL:HG21	1:B:276:ARG:HG3	2.02	0.41
1:B:518:LEU:HD23	1:B:518:LEU:HA	1.94	0.41
1:C:287:HIS:CD2	1:C:287:HIS:N	2.89	0.41
1:C:356:ARG:NH2	1:C:383:THR:CG2	2.84	0.41
1:A:48:MET:HE1	1:A:165:ARG:NH2	2.36	0.41
1:A:159:LEU:HA	1:A:299:PHE:CD1	2.56	0.41
1:A:413:GLN:O	1:A:417:ARG:HB2	2.20	0.41
1:A:513:LEU:HD13	1:A:513:LEU:HA	1.87	0.41
1:B:13:ARG:NE	1:B:185:GLU:HB3	2.35	0.41
1:C:243:GLU:OE1	1:C:246:ARG:NH1	2.54	0.41
1:C:290:PRO:C	1:C:291:GLN:HG3	2.46	0.41
1:D:113:PRO:HA	1:D:196:SER:HG	1.86	0.41
1:D:122:GLY:O	1:D:123:PHE:HB2	2.20	0.41
1:A:202:GLU:O	1:A:203:SER:C	2.63	0.41
1:A:257:CYS:HA	1:A:258:PRO:HA	1.80	0.41
1:A:452:GLU:CD	5:A:954:GOL:O1	2.64	0.41
1:B:511:VAL:HB	1:B:518:LEU:HD22	2.02	0.41
1:C:46:ARG:HB3	1:C:274:ARG:HG2	2.02	0.41
1:C:115:LEU:HD21	1:C:484:ALA:HB2	2.02	0.41
1:D:216:LEU:HA	1:D:219:ARG:HG2	2.03	0.41
1:D:257:CYS:HA	1:D:258:PRO:HA	1.73	0.41
1:D:327:LEU:HD23	1:D:327:LEU:C	2.46	0.41
1:D:407:VAL:O	1:D:410:PRO:HD2	2.21	0.41
1:D:428:TYR:CD1	1:D:428:TYR:C	2.99	0.41
1:A:325:GLN:O	1:A:483:PHE:HZ	2.04	0.41
1:A:428:TYR:CD1	1:A:428:TYR:C	2.99	0.41
1:D:500:TRP:HA	1:D:501:PRO:HD2	1.89	0.41
1:A:155:THR:HG22	1:A:159:LEU:CD1	2.51	0.40
1:A:187:ILE:HD12	1:A:187:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:998:DME:H102	4:A:998:DME:H173	1.86	0.40
1:B:41:PRO:CD	1:B:97:LEU:HD12	2.43	0.40
1:D:68:VAL:HG23	1:D:90:ARG:HB2	2.03	0.40
1:A:469:GLU:O	1:A:472:PHE:HB3	2.21	0.40
1:B:380:LEU:HA	1:B:385:TRP:HZ2	1.87	0.40
1:A:107:ARG:HG2	1:A:108:PRO:HD2	2.03	0.40
1:C:290:PRO:HA	7:C:1010:HOH:O	2.20	0.40
1:C:330:VAL:HG21	1:C:408:VAL:HG22	2.04	0.40
1:A:99:LEU:HA	1:A:149:MET:HA	2.03	0.40
1:A:161:LEU:HD22	1:A:270:ILE:HD11	2.04	0.40
1:A:208:SER:O	1:A:211:MET:N	2.55	0.40
1:B:245:ARG:NH2	1:B:266:ASP:OD2	2.55	0.40
1:B:317:ASN:ND2	1:B:417:ARG:NE	2.67	0.40
1:C:80:PHE:CZ	1:C:438:THR:O	2.74	0.40
1:C:535:PHE:C	1:C:537:PRO:HD2	2.47	0.40
4:C:997:DME:H72	4:C:997:DME:H101	1.54	0.40
1:D:193:ASP:C	1:D:195:MET:H	2.27	0.40
1:A:369:GLN:HB3	7:A:1000:HOH:O	2.21	0.40
1:B:181:GLN:O	1:B:185:GLU:HG3	2.22	0.40
1:B:492:PRO:HB2	1:B:493:ARG:H	1.78	0.40
1:B:501:PRO:HA	1:B:502:PRO:HD3	1.78	0.40
1:C:317:ASN:HD22	1:C:417:ARG:HH21	1.70	0.40
1:D:7:GLN:CB	1:D:105:TYR:HE1	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/547 (98%)	482 (90%)	45 (8%)	11 (2%)	6	22
1	B	532/547 (97%)	493 (93%)	33 (6%)	6 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	536/547 (98%)	497 (93%)	36 (7%)	3 (1%)	21	51
1	D	539/547 (98%)	486 (90%)	43 (8%)	10 (2%)	6	23
All	All	2145/2188 (98%)	1958 (91%)	157 (7%)	30 (1%)	9	30

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	PRO
1	A	494	ASP
1	A	497	SER
1	B	496	LYS
1	B	497	SER
1	C	496	LYS
1	D	494	ASP
1	D	495	ARG
1	D	497	SER
1	A	111	PRO
1	A	184	GLN
1	A	495	ARG
1	B	492	PRO
1	B	494	ASP
1	C	497	SER
1	D	111	PRO
1	D	234	GLY
1	D	492	PRO
1	A	234	GLY
1	A	517	PRO
1	B	185	GLU
1	D	517	PRO
1	A	185	GLU
1	A	496	LYS
1	C	342	GLY
1	A	121	GLY
1	D	121	GLY
1	D	496	LYS
1	B	342	GLY
1	D	5	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/447 (98%)	384 (88%)	52 (12%)	5	16
1	B	435/447 (97%)	393 (90%)	42 (10%)	8	25
1	C	435/447 (97%)	389 (89%)	46 (11%)	6	22
1	D	436/447 (98%)	381 (87%)	55 (13%)	4	14
All	All	1742/1788 (97%)	1547 (89%)	195 (11%)	6	19

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	ARG
1	A	12	VAL
1	A	29	VAL
1	A	33	LEU
1	A	45	ARG
1	A	103	THR
1	A	107	ARG
1	A	111	PRO
1	A	115	LEU
1	A	149	MET
1	A	155	THR
1	A	166	GLU
1	A	178	LEU
1	A	180	LEU
1	A	214	LEU
1	A	216	LEU
1	A	246	ARG
1	A	251	LEU
1	A	255	VAL
1	A	281	LEU
1	A	291	GLN
1	A	296	ARG
1	A	311	THR

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Mol	Chain	Res	Type
1	A	317	ASN
1	A	324	LEU
1	A	332	LYS
1	A	333	ASP
1	A	353	LEU
1	A	360	LEU
1	A	376	GLU
1	A	380	LEU
1	A	386	LEU
1	A	417	ARG
1	A	418	LEU
1	A	421	GLN
1	A	437	LEU
1	A	441	LEU
1	A	450	GLU
1	A	451	ILE
1	A	485	ARG
1	A	499	GLN
1	A	504	THR
1	A	505	THR
1	A	513	LEU
1	A	514	ASN
1	A	516	LYS
1	A	524	LEU
1	A	536	LEU
1	A	537	PRO
1	A	538	LYS
1	A	539	LEU
1	B	9	LEU
1	B	11	ARG
1	B	12	VAL
1	B	22	LEU
1	B	23	LYS
1	B	25	PRO
1	B	29	VAL
1	B	33	LEU
1	B	83	THR
1	B	84	GLU
1	B	118	ILE
1	B	132	VAL
1	B	136	ARG
1	B	138	LEU

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Mol	Chain	Res	Type
1	B	161	LEU
1	B	166	GLU
1	B	178	LEU
1	B	200	PHE
1	B	211	MET
1	B	214	LEU
1	B	216	LEU
1	B	219	ARG
1	B	253	ARG
1	B	276	ARG
1	B	291	GLN
1	B	296	ARG
1	B	315	LEU
1	B	324	LEU
1	B	327	LEU
1	B	336	SER
1	B	354	ILE
1	B	360	LEU
1	B	364	ARG
1	B	386	LEU
1	B	418	LEU
1	B	424	ARG
1	B	499	GLN
1	B	509	GLN
1	B	513	LEU
1	B	536	LEU
1	B	539	LEU
1	B	540	LEU
1	C	4	GLU
1	C	12	VAL
1	C	13	ARG
1	C	18	ARG
1	C	22	LEU
1	C	23	LYS
1	C	25	PRO
1	C	29	VAL
1	C	33	LEU
1	C	83	THR
1	C	84	GLU
1	C	118	ILE
1	C	132	VAL
1	C	136	ARG

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Mol	Chain	Res	Type
1	C	138	LEU
1	C	155	THR
1	C	161	LEU
1	C	166	GLU
1	C	178	LEU
1	C	200	PHE
1	C	211	MET
1	C	214	LEU
1	C	219	ARG
1	C	238	THR
1	C	253	ARG
1	C	291	GLN
1	C	296	ARG
1	C	315	LEU
1	C	324	LEU
1	C	327	LEU
1	C	336	SER
1	C	354	ILE
1	C	360	LEU
1	C	364	ARG
1	C	386	LEU
1	C	411	VAL
1	C	418	LEU
1	C	424	ARG
1	C	478	LYS
1	C	499	GLN
1	C	509	GLN
1	C	513	LEU
1	C	525	ARG
1	C	536	LEU
1	C	539	LEU
1	C	540	LEU
1	D	9	LEU
1	D	11	ARG
1	D	12	VAL
1	D	33	LEU
1	D	40	PRO
1	D	45	ARG
1	D	90	ARG
1	D	103	THR
1	D	107	ARG
1	D	111	PRO

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Mol	Chain	Res	Type
1	D	115	LEU
1	D	149	MET
1	D	155	THR
1	D	166	GLU
1	D	178	LEU
1	D	180	LEU
1	D	183	VAL
1	D	214	LEU
1	D	216	LEU
1	D	246	ARG
1	D	251	LEU
1	D	255	VAL
1	D	281	LEU
1	D	291	GLN
1	D	296	ARG
1	D	298	SER
1	D	317	ASN
1	D	324	LEU
1	D	330	VAL
1	D	332	LYS
1	D	333	ASP
1	D	353	LEU
1	D	355	SER
1	D	360	LEU
1	D	376	GLU
1	D	380	LEU
1	D	386	LEU
1	D	417	ARG
1	D	418	LEU
1	D	421	GLN
1	D	437	LEU
1	D	441	LEU
1	D	450	GLU
1	D	451	ILE
1	D	485	ARG
1	D	499	GLN
1	D	504	THR
1	D	505	THR
1	D	513	LEU
1	D	514	ASN
1	D	516	LYS
1	D	536	LEU

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Mol	Chain	Res	Type
1	D	537	PRO
1	D	538	LYS
1	D	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	212	HIS
1	A	228	GLN
1	A	291	GLN
1	A	421	GLN
1	A	482	ASN
1	A	499	GLN
1	A	514	ASN
1	A	527	GLN
1	B	7	GLN
1	B	212	HIS
1	B	223	HIS
1	B	291	GLN
1	B	317	ASN
1	B	393	HIS
1	B	405	HIS
1	B	421	GLN
1	B	509	GLN
1	C	7	GLN
1	C	16	GLN
1	C	184	GLN
1	C	287	HIS
1	C	291	GLN
1	C	317	ASN
1	C	325	GLN
1	C	421	GLN
1	C	474	GLN
1	C	509	GLN
1	C	533	ASN
1	D	16	GLN
1	D	66	GLN
1	D	228	GLN
1	D	291	GLN
1	D	317	ASN
1	D	482	ASN

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Mol	Chain	Res	Type
1	D	499	GLN
1	D	514	ASN
1	D	527	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 ⓘ

3 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	0.74	0	17,19,21	0.65	0
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	0.51	0
2	FUL	E	3	2	10,10,11	0.62	0	14,14,16	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	FUL	E	3	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

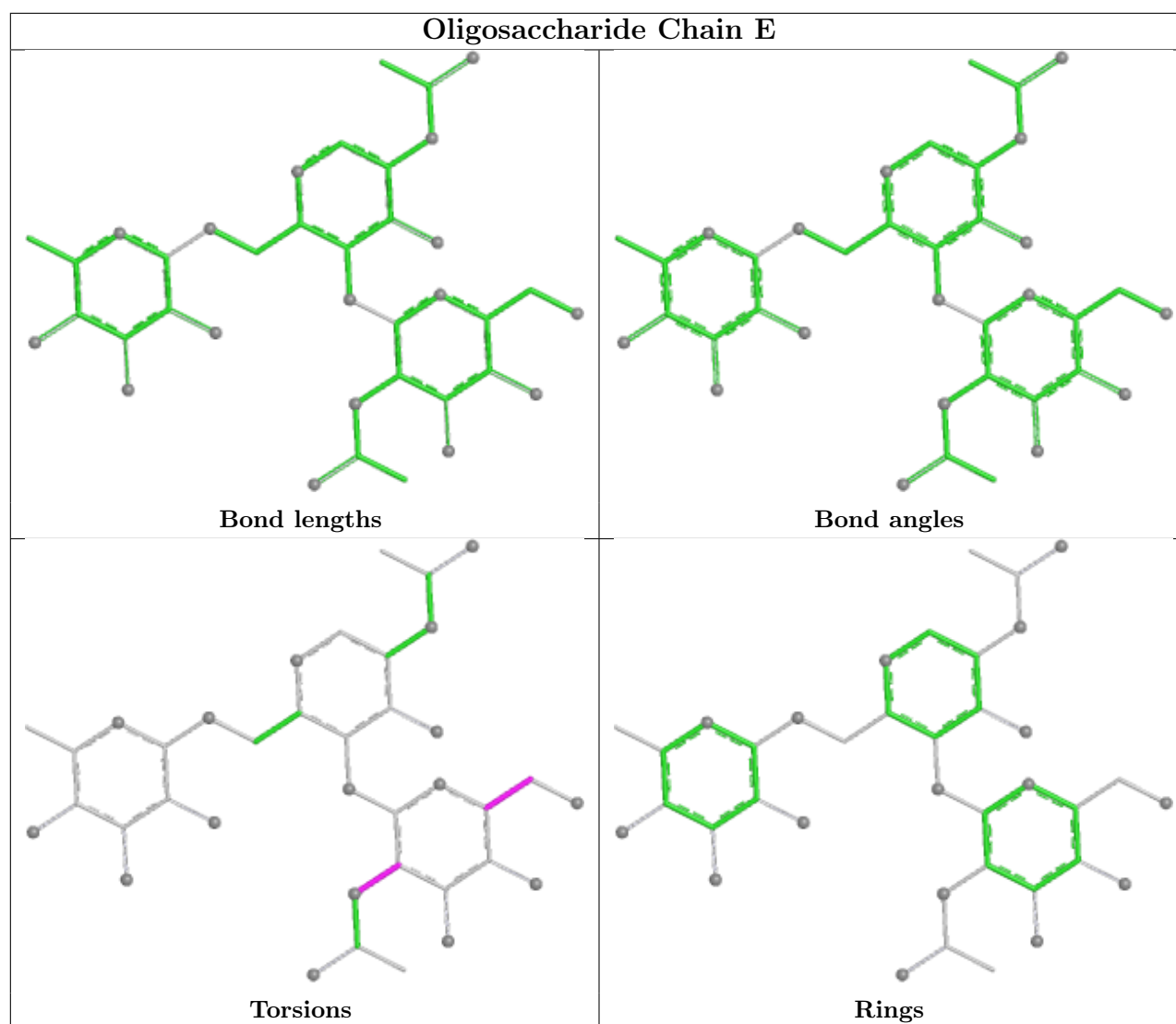
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	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](#)

12 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	$\# Z > 2$
5	GOL	B	953	-	5,5,5	0.87	0	5,5,5	0.59	0
4	DME	B	996	-	17,17,17	0.82	0	22,22,22	0.83	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	D	952	-	5,5,5	0.74	0	5,5,5	0.65	0
3	NAG	A	709	1	14,14,15	0.99	1 (7%)	17,19,21	0.78	0
5	GOL	C	951	-	5,5,5	0.75	0	5,5,5	0.48	0
6	PO4	B	548	-	4,4,4	4.14	4 (100%)	6,6,6	0.62	0
6	PO4	C	548	-	4,4,4	3.86	4 (100%)	6,6,6	1.19	0
4	DME	C	997	-	17,17,17	0.68	0	22,22,22	0.69	0
4	DME	D	999	-	17,17,17	0.64	0	22,22,22	0.82	2 (9%)
5	GOL	A	954	-	5,5,5	0.66	0	5,5,5	0.61	0
4	DME	A	998	-	17,17,17	0.57	0	22,22,22	0.73	0
6	PO4	C	998	-	4,4,4	4.95	4 (100%)	6,6,6	1.16	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	953	-	-	0/4/4/4	-
4	DME	B	996	-	-	8/15/15/15	-
5	GOL	D	952	-	-	0/4/4/4	-
3	NAG	A	709	1	-	2/6/23/26	0/1/1/1
5	GOL	C	951	-	-	2/4/4/4	-
4	DME	C	997	-	-	10/15/15/15	-
4	DME	D	999	-	-	5/15/15/15	-
5	GOL	A	954	-	-	1/4/4/4	-
4	DME	A	998	-	-	3/15/15/15	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	998	PO4	P-O1	7.35	1.67	1.50
6	C	548	PO4	P-O1	5.87	1.64	1.50
6	B	548	PO4	P-O1	5.78	1.64	1.50
6	C	998	PO4	P-O2	4.21	1.66	1.54
6	C	998	PO4	P-O3	3.85	1.65	1.54
6	B	548	PO4	P-O3	3.65	1.65	1.54
6	C	998	PO4	P-O4	3.41	1.64	1.54
6	B	548	PO4	P-O4	3.31	1.64	1.54
6	B	548	PO4	P-O2	3.30	1.64	1.54
6	C	548	PO4	P-O2	3.08	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	548	PO4	P-O4	2.91	1.63	1.54
6	C	548	PO4	P-O3	2.68	1.62	1.54
3	A	709	NAG	C1-C2	2.11	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	999	DME	C11-C10-C9	2.23	120.41	110.81
4	B	996	DME	C2-C3-C4	2.21	120.32	110.81
6	C	998	PO4	O3-P-O2	2.17	114.67	107.91
4	D	999	DME	C2-C3-C4	2.11	119.91	110.81

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	951	GOL	C1-C2-C3-O3
4	D	999	DME	C9-C10-C11-N12
4	B	996	DME	C3-C2-N1-C15
4	B	996	DME	C3-C2-N1-C13
3	A	709	NAG	O5-C5-C6-O6
4	B	996	DME	N1-C2-C3-C4
4	B	996	DME	C3-C2-N1-C14
3	A	709	NAG	C4-C5-C6-O6
4	C	997	DME	N1-C2-C3-C4
5	C	951	GOL	O2-C2-C3-O3
4	D	999	DME	N1-C2-C3-C4
4	A	998	DME	C9-C10-C11-N12
4	C	997	DME	C9-C10-C11-N12
4	D	999	DME	C4-C5-C6-C7
4	C	997	DME	C6-C7-C8-C9
4	C	997	DME	C7-C8-C9-C10
4	D	999	DME	C6-C7-C8-C9
4	C	997	DME	C5-C6-C7-C8
4	B	996	DME	C7-C8-C9-C10
4	C	997	DME	C10-C11-N12-C18
4	C	997	DME	C10-C11-N12-C17
4	C	997	DME	C10-C11-N12-C16
5	A	954	GOL	C1-C2-C3-O3
4	D	999	DME	C7-C8-C9-C10
4	A	998	DME	C7-C8-C9-C10
4	A	998	DME	C5-C6-C7-C8

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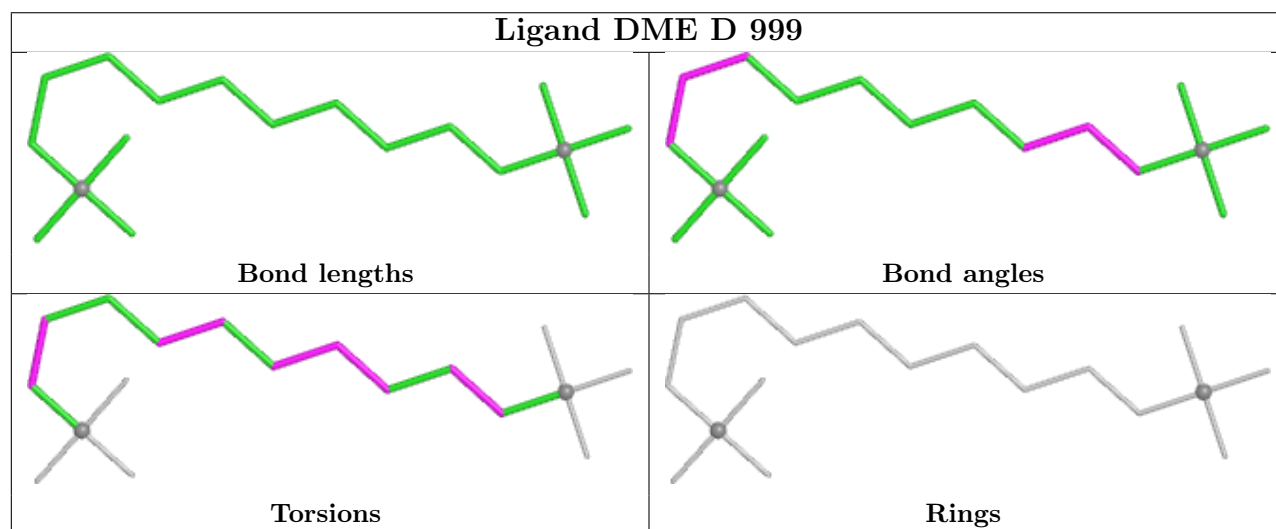
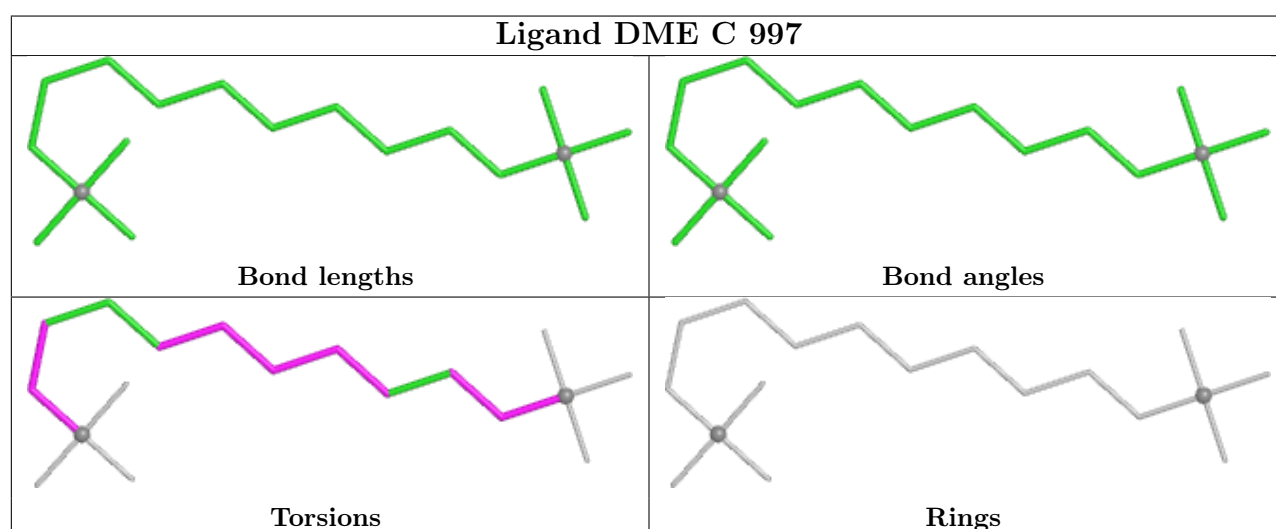
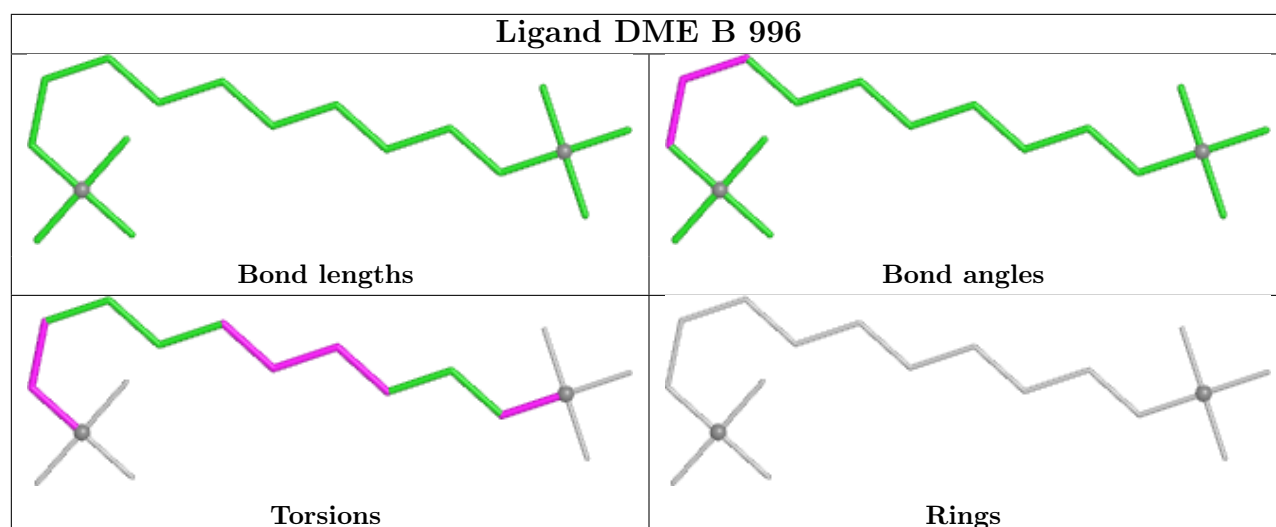
Mol	Chain	Res	Type	Atoms
4	B	996	DME	C5-C6-C7-C8
4	C	997	DME	C4-C5-C6-C7
4	B	996	DME	C10-C11-N12-C17
4	C	997	DME	C3-C2-N1-C14
4	B	996	DME	C6-C7-C8-C9

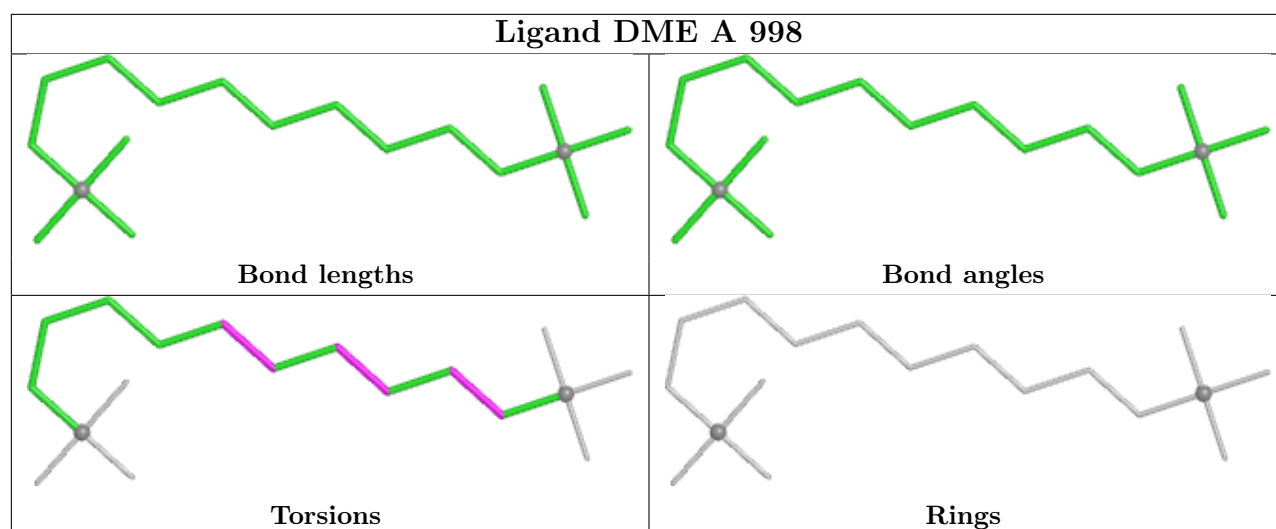
There are no ring outliers.

9 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	953	GOL	1	0
4	B	996	DME	13	0
5	D	952	GOL	1	0
3	A	709	NAG	1	0
5	C	951	GOL	7	0
4	C	997	DME	19	0
4	D	999	DME	7	0
5	A	954	GOL	2	0
4	A	998	DME	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	540/547 (98%)	-0.07	20 (3%) 45 37	20, 50, 79, 80	0
1	B	536/547 (97%)	-0.63	7 (1%) 75 67	13, 35, 61, 80	0
1	C	540/547 (98%)	-0.59	13 (2%) 59 50	11, 34, 64, 80	0
1	D	541/547 (98%)	-0.31	15 (2%) 55 46	16, 44, 79, 80	0
All	All	2157/2188 (98%)	-0.40	55 (2%) 58 48	11, 40, 75, 80	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	ASP	6.2
1	C	546	LEU	5.9
1	A	494	ASP	5.8
1	C	545	THR	5.7
1	D	544	ASP	4.9
1	A	497	SER	4.7
1	B	493	ARG	4.7
1	D	494	ASP	4.6
1	A	493	ARG	4.4
1	D	323	ASP	3.7
1	C	1	GLU	3.7
1	A	491	ASP	3.5
1	D	497	SER	3.4
1	B	497	SER	3.3
1	C	497	SER	3.3
1	A	496	LYS	3.2
1	C	110	SER	3.1
1	B	545	THR	3.1
1	A	4	GLU	2.9
1	D	393	HIS	2.9
1	D	495	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	494	ASP	2.8
1	A	24	ALA	2.7
1	D	317	ASN	2.7
1	D	496	LYS	2.6
1	A	108	PRO	2.6
1	A	223	HIS	2.6
1	D	492	PRO	2.6
1	D	322	GLN	2.6
1	A	470	ARG	2.6
1	C	495	ARG	2.6
1	B	495	ARG	2.5
1	C	493	ARG	2.5
1	A	393	HIS	2.5
1	C	547	ASP	2.5
1	A	323	ASP	2.4
1	D	262	ALA	2.4
1	A	492	PRO	2.4
1	D	491	ASP	2.3
1	C	491	ASP	2.3
1	A	459	LEU	2.3
1	C	3	ARG	2.3
1	A	259	PRO	2.3
1	D	468	GLU	2.2
1	A	113	PRO	2.2
1	C	496	LYS	2.2
1	B	491	ASP	2.2
1	D	261	GLY	2.1
1	A	7	GLN	2.1
1	B	498	PRO	2.1
1	C	323	ASP	2.1
1	A	30	SER	2.1
1	A	466	THR	2.1
1	D	470	ARG	2.1
1	A	465	TYR	2.0

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

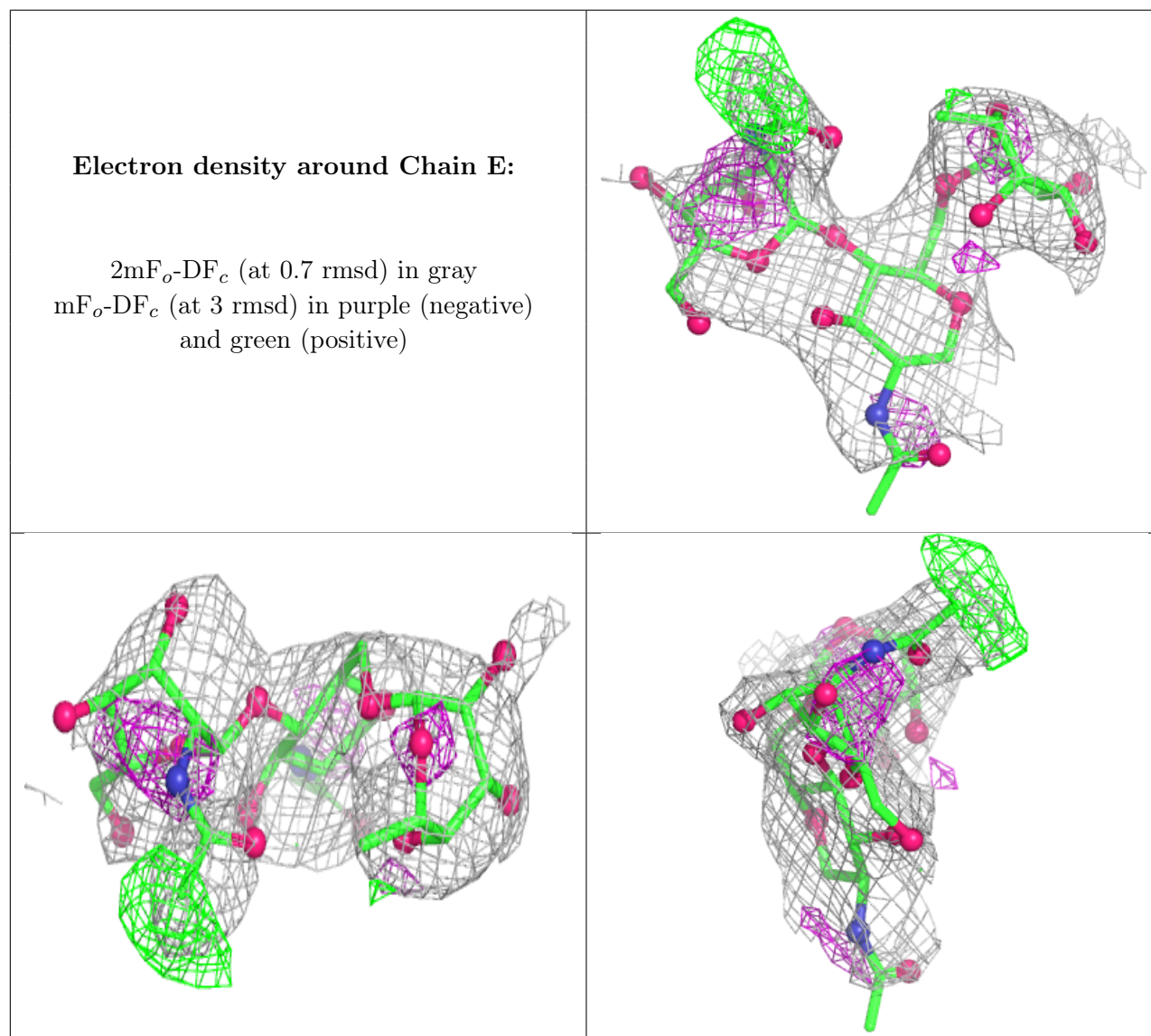
There are no non-standard protein/DNA/RNA residues in this entry.

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
2	NAG	E	2	14/15	0.63	0.20	80,80,80,80	0
2	FUL	E	3	10/11	0.64	0.17	80,80,80,80	0
2	NAG	E	1	14/15	0.83	0.15	80,80,80,80	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.



6.4 Ligands

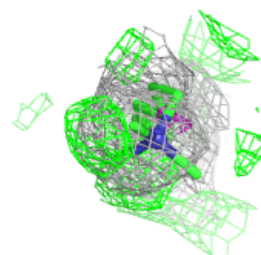
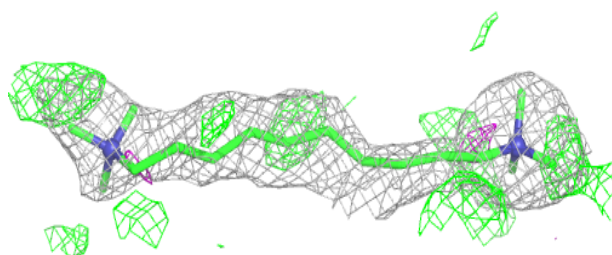
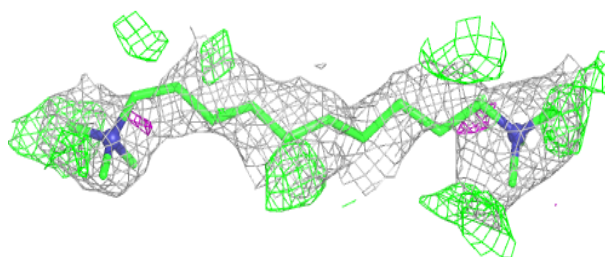
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	709	14/15	0.68	0.18	75,80,80,80	0
4	DME	B	996	18/18	0.76	0.24	44,65,80,80	0
4	DME	C	997	18/18	0.83	0.25	53,77,80,80	0
6	PO4	C	998	5/5	0.83	0.21	80,80,80,80	0
5	GOL	D	952	6/6	0.84	0.16	48,54,55,61	0
4	DME	D	999	18/18	0.85	0.20	40,68,80,80	0
6	PO4	C	548	5/5	0.85	0.19	80,80,80,80	0
5	GOL	A	954	6/6	0.85	0.17	66,74,75,76	0
6	PO4	B	548	5/5	0.86	0.19	80,80,80,80	0
4	DME	A	998	18/18	0.87	0.22	70,79,80,80	0
5	GOL	B	953	6/6	0.93	0.12	33,36,48,53	0
5	GOL	C	951	6/6	0.95	0.07	31,36,38,42	0

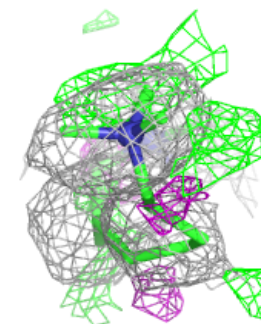
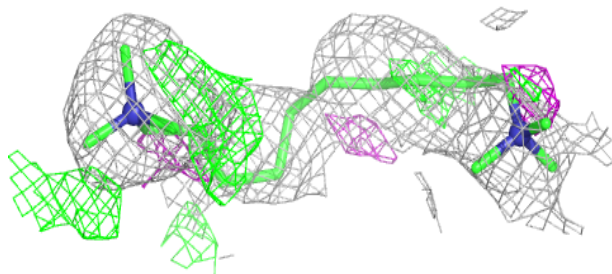
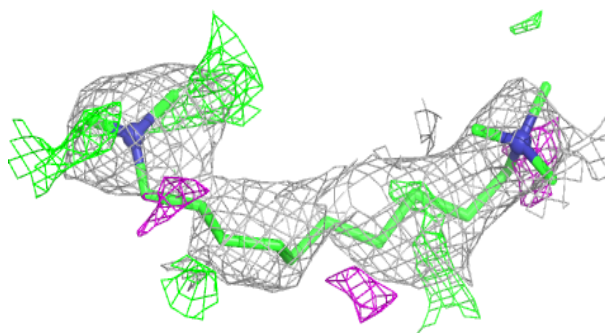
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DME B 996:

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

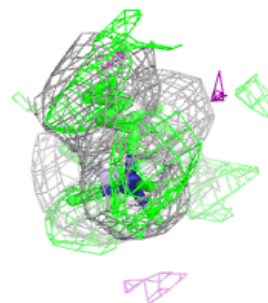
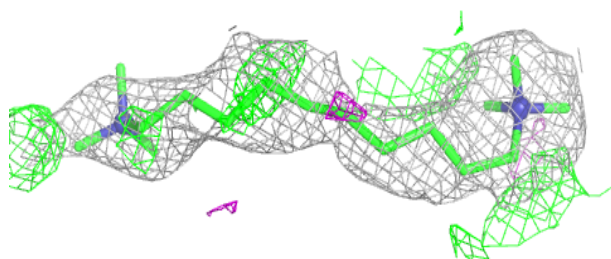
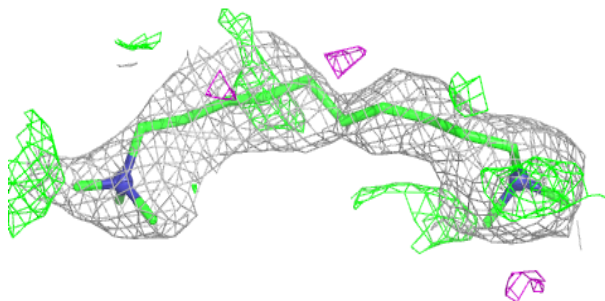
**Electron density around DME C 997:**

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

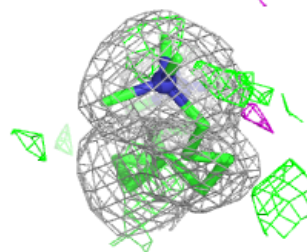
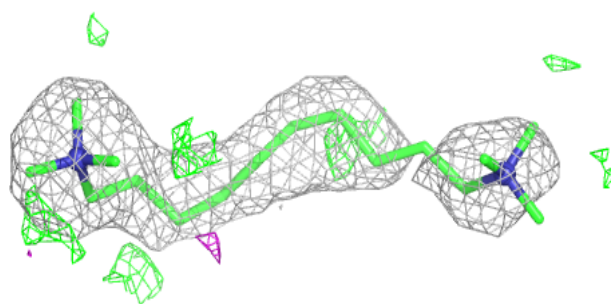
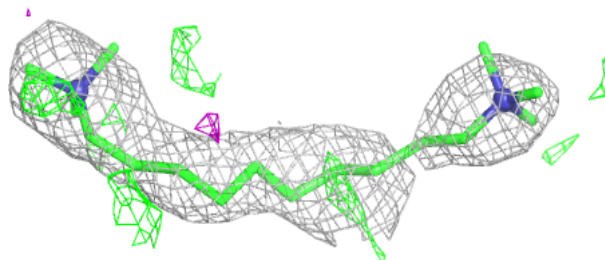


Electron density around DME D 999:

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

**Electron density around DME A 998:**

$2mF_o-DF_c$ (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.