



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:36 PM UTC

PDB ID : 5B0K / pdb_00005b0k
Title : Structure of MoeN5-Sso7d fusion protein in complex with beta-decyl maltoside
Authors : Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2015-10-30
Resolution : 2.75 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

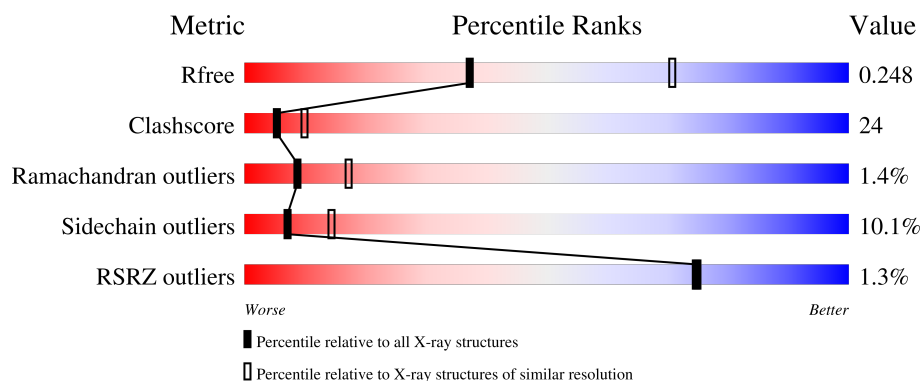
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	343	2% 43% 27% 6% 23%
1	B	343	53% 35% 8% .
1	C	343	41% 29% 6% . 24%
1	D	343	2% 51% 38% 6% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9969 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2013	1243	374	385	11			
1	B	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	C	262	Total	C	N	O	S	0	0	0
			1998	1234	372	381	11			
1	D	331	Total	C	N	O	S	0	0	0
			2525	1567	462	482	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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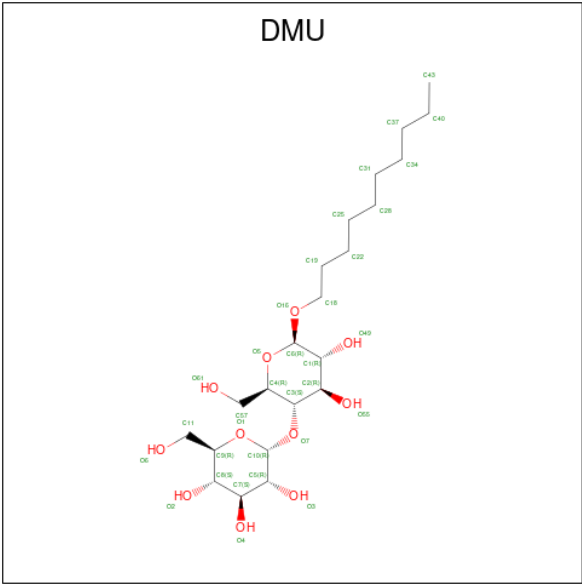
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			33	22	11		
2	A	1	Total	C	O	0	0
			33	22	11		
2	B	1	Total	C	O	0	0
			33	22	11		
2	B	1	Total	C	O	0	0
			33	22	11		

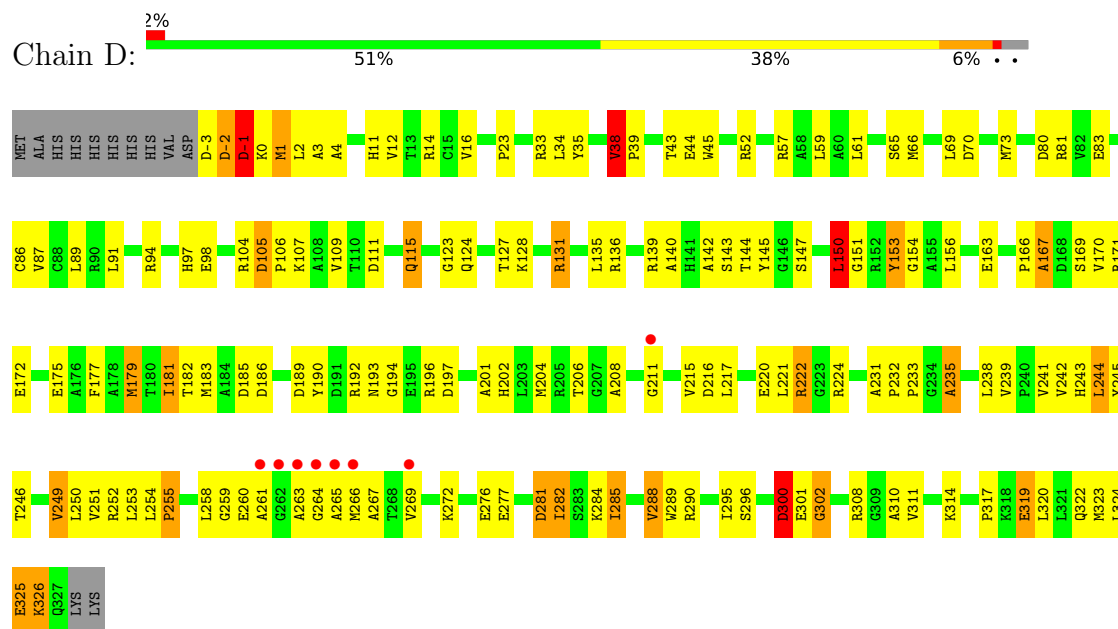
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			33	22	11		
2	D	1	Total	C	O	0	0
			33	22	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	204	Total	O	0	0
			204	204		
3	C	147	Total	O	0	0
			147	147		
3	D	177	Total	O	0	0
			177	177		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.45Å 219.65Å 104.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 25.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.9 (25.00-2.75) 93.7 (25.00-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.182 , 0.248 0.183 , 0.248	Depositor DCC
R_{free} test set	1982 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9969	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: DMU

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	1.21	5/2045 (0.2%)	1.35	15/2780 (0.5%)
1	B	1.13	4/2572 (0.2%)	1.34	22/3478 (0.6%)
1	C	1.19	2/2030 (0.1%)	1.39	27/2759 (1.0%)
1	D	1.09	3/2564 (0.1%)	1.40	26/3467 (0.7%)
All	All	1.15	14/9211 (0.2%)	1.37	90/12484 (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	D	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	ILE	CA-CB	7.55	1.65	1.54
1	D	241	VAL	CA-CB	6.59	1.61	1.54
1	A	182	THR	CA-CB	-5.90	1.44	1.53
1	B	235	ALA	CA-CB	5.81	1.59	1.53
1	B	53	ALA	CA-CB	-5.54	1.44	1.53
1	A	251	VAL	CA-CB	5.54	1.61	1.54
1	A	246	THR	CA-CB	5.22	1.61	1.53
1	D	124	GLN	C-O	-5.22	1.18	1.24
1	B	66	MET	SD-CE	5.21	1.92	1.79
1	C	188	THR	CA-CB	-5.19	1.47	1.53
1	A	192	ARG	CA-C	5.17	1.58	1.52
1	B	66	MET	CG-SD	5.16	1.93	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	THR	CA-CB	5.11	1.62	1.53
1	D	38	VAL	CA-CB	5.04	1.60	1.54

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-2	ASP	N-CA-C	-15.55	94.99	112.72
1	D	-1	ASP	N-CA-C	-11.36	97.58	112.68
1	B	-2	ASP	N-CA-C	-10.14	100.32	112.89
1	A	195	GLU	N-CA-C	-9.62	96.63	110.59
1	D	105	ASP	CA-C-N	-9.20	110.33	121.00
1	D	105	ASP	C-N-CA	-9.20	110.33	121.00
1	B	195	GLU	N-CA-C	-9.08	98.06	110.68
1	C	154	GLY	N-CA-C	-8.92	102.16	112.50
1	A	232	PRO	N-CA-C	8.88	121.54	110.70
1	D	208	ALA	N-CA-C	-8.86	102.48	113.38
1	D	253	LEU	N-CA-C	8.85	121.81	111.02
1	B	253	LEU	N-CA-C	8.69	120.75	111.28
1	D	260	GLU	N-CA-C	-8.67	102.61	113.02
1	D	250	LEU	N-CA-C	7.94	121.91	111.75
1	A	58	ALA	N-CA-C	-7.71	102.96	111.36
1	A	251	VAL	N-CA-C	7.69	117.76	110.53
1	B	251	VAL	N-CA-C	7.65	119.33	111.00
1	A	164	GLY	N-CA-C	-7.54	103.47	115.08
1	C	235	ALA	CA-C-N	7.20	127.82	119.47
1	C	235	ALA	C-N-CA	7.20	127.82	119.47
1	A	104	ARG	N-CA-C	-6.96	103.38	110.97
1	C	172	GLU	N-CA-C	-6.80	103.94	111.36
1	C	231	ALA	CA-C-N	6.66	127.24	120.38
1	C	231	ALA	C-N-CA	6.66	127.24	120.38
1	D	265	ALA	N-CA-C	-6.60	105.09	113.01
1	D	147	SER	N-CA-C	6.54	119.00	111.02
1	B	326	LYS	N-CA-C	-6.50	105.23	113.43
1	D	177	PHE	N-CA-C	-6.47	104.32	111.82
1	C	47	THR	N-CA-C	6.42	121.37	112.45
1	D	222	ARG	N-CA-C	-6.41	104.37	111.36
1	C	208	ALA	N-CA-C	-6.33	105.38	113.23
1	C	197	ASP	N-CA-C	6.31	119.63	110.42
1	D	151	GLY	N-CA-C	-6.29	105.15	112.83
1	B	-3	ASP	N-CA-C	-6.21	105.53	113.23
1	D	115	GLN	N-CA-C	6.20	121.60	111.37
1	A	14	ARG	N-CA-C	-6.16	104.56	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ILE	N-CA-C	-6.12	104.38	110.62
1	A	253	LEU	N-CA-C	6.11	118.86	111.40
1	C	239	VAL	CA-C-N	-6.11	112.56	119.28
1	C	239	VAL	C-N-CA	-6.11	112.56	119.28
1	C	257	HIS	N-CA-C	6.09	120.41	112.92
1	D	300	ASP	N-CA-C	6.08	119.72	109.76
1	D	235	ALA	N-CA-C	-6.00	98.54	108.75
1	A	193	ASN	N-CA-C	5.97	123.53	110.80
1	B	210	ALA	N-CA-C	5.93	118.38	108.96
1	B	183	MET	N-CA-C	-5.87	104.79	111.07
1	D	154	GLY	N-CA-C	-5.84	105.73	112.50
1	B	297	PHE	N-CA-C	5.83	117.00	108.14
1	D	163	GLU	N-CA-C	5.83	119.14	110.52
1	B	103	ALA	N-CA-C	5.77	118.20	110.35
1	D	326	LYS	N-CA-C	-5.72	106.34	113.55
1	C	135	LEU	N-CA-C	5.71	117.50	111.28
1	B	109	VAL	N-CA-C	5.70	116.48	110.72
1	D	23	PRO	N-CA-C	-5.66	105.61	113.81
1	B	26	VAL	N-CA-C	-5.65	105.00	110.42
1	B	273	TYR	N-CA-C	5.62	117.85	109.25
1	C	160	CYS	N-CA-C	-5.62	105.78	113.30
1	D	33	ARG	N-CA-C	5.61	117.84	111.11
1	A	210	ALA	N-CA-C	5.57	119.18	110.32
1	B	170	VAL	N-CA-C	-5.50	105.01	110.62
1	B	108	ALA	N-CA-C	5.48	117.69	111.11
1	A	172	GLU	N-CA-C	-5.39	104.80	111.33
1	B	215	VAL	N-CA-C	-5.39	105.28	110.72
1	A	51	ARG	N-CA-C	-5.36	105.35	111.14
1	D	3	ALA	N-CA-C	-5.36	105.33	111.07
1	B	154	GLY	N-CA-C	-5.36	106.01	112.49
1	C	3	ALA	N-CA-C	-5.36	105.48	112.23
1	D	107	LYS	N-CA-C	-5.34	105.41	112.94
1	B	258	LEU	N-CA-C	-5.34	104.36	112.04
1	C	79	LEU	N-CA-C	-5.31	101.29	109.52
1	C	48	ASP	CA-C-N	5.30	124.75	119.24
1	C	48	ASP	C-N-CA	5.30	124.75	119.24
1	B	163	GLU	N-CA-C	5.29	118.36	110.52
1	C	186	ASP	N-CA-C	5.28	117.04	111.28
1	C	194	GLY	N-CA-C	-5.25	104.31	113.76
1	B	308	ARG	N-CA-C	5.25	117.37	109.23
1	C	170	VAL	N-CA-C	-5.25	104.63	110.62
1	D	190	TYR	N-CA-C	-5.21	105.78	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLY	O-C-N	5.19	124.76	121.85
1	A	167	ALA	N-CA-C	5.16	121.80	110.80
1	C	218	LEU	N-CA-C	5.14	116.56	111.07
1	A	94	ARG	N-CA-C	-5.12	105.78	111.36
1	A	154	GLY	N-CA-C	-5.12	106.59	112.73
1	D	150	LEU	N-CA-C	5.09	117.73	111.82
1	C	86	CYS	N-CA-C	5.08	116.82	111.28
1	B	231	ALA	CA-C-N	-5.05	115.17	120.38
1	B	231	ALA	C-N-CA	-5.05	115.17	120.38
1	C	23	PRO	N-CA-C	-5.04	106.52	113.53
1	C	26	VAL	N-CA-C	5.04	116.36	110.62
1	D	69	LEU	N-CA-C	-5.03	105.99	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Sidechain
1	D	153	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	2013	0	1996	90	0
1	B	2533	0	2532	135	0
1	C	1998	0	1983	106	0
1	D	2525	0	2528	125	0
2	A	66	0	84	11	0
2	B	66	0	84	9	0
2	C	33	0	42	8	0
2	D	33	0	42	3	0
3	A	174	0	0	9	0
3	B	204	0	0	3	0
3	C	147	0	0	2	0
3	D	177	0	0	4	0
All	All	9969	0	9291	448	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 24.

All (448) 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:B:196:ARG:HD3	1:B:197:ASP:H	1.21	1.02
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.09	0.96
1:C:199:ASN:O	1:C:203:LEU:HD12	1.65	0.94
1:C:81:ARG:HD3	1:D:81:ARG:NH2	1.86	0.91
2:A:501:DMU:H33	1:C:78:GLY:HA2	1.53	0.90
1:D:263:ALA:HB1	1:D:266:MET:HG3	1.53	0.89
1:C:1:MET:HE2	3:C:555:HOH:O	1.73	0.89
1:D:263:ALA:HB3	1:D:267:ALA:HB2	1.53	0.88
1:A:190:TYR:HB3	2:A:501:DMU:H40	1.57	0.87
1:B:322:GLN:O	1:B:326:LYS:HG2	1.75	0.87
1:B:33:ARG:CG	1:B:33:ARG:HH21	1.88	0.87
1:B:258:LEU:HD13	1:B:262:GLY:HA2	1.55	0.87
1:A:132:ALA:HB1	1:A:137:GLU:HB2	1.54	0.86
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.57	0.86
1:A:196:ARG:HG3	1:A:197:ASP:H	1.40	0.86
1:C:5:GLU:OE2	1:C:33:ARG:HG2	1.74	0.86
1:D:222:ARG:NH1	1:D:243:HIS:HD2	1.73	0.85
1:B:33:ARG:HH21	1:B:33:ARG:HG2	1.41	0.85
1:A:190:TYR:CE2	2:A:501:DMU:H4	2.12	0.84
1:B:179:MET:HG2	1:B:221:LEU:HD11	1.58	0.84
1:A:172:GLU:HG2	3:A:654:HOH:O	1.77	0.84
1:C:219:GLU:CD	1:C:222:ARG:HE	1.87	0.82
1:D:104:ARG:HG3	1:D:105:ASP:H	1.45	0.82
1:D:38:VAL:HG11	1:D:150:LEU:HD21	1.61	0.81
1:D:94:ARG:HD2	1:D:98:GLU:OE2	1.81	0.81
1:D:131:ARG:NH2	3:D:501:HOH:O	2.10	0.80
1:A:202:HIS:O	1:A:206:THR:HG23	1.81	0.80
1:A:203:LEU:HB3	1:A:209:VAL:HG23	1.64	0.80
1:A:190:TYR:CB	2:A:501:DMU:H40	2.12	0.79
1:D:222:ARG:HH11	1:D:243:HIS:CD2	1.97	0.79
1:C:124:GLN:HE22	1:C:145:TYR:HB3	1.47	0.79
1:C:166:PRO:HD3	1:C:233:PRO:HD2	1.64	0.78
1:B:196:ARG:HD3	1:B:197:ASP:N	1.95	0.78
1:C:124:GLN:NE2	1:C:145:TYR:HB3	1.99	0.78
1:D:264:GLY:H	1:D:266:MET:HG2	1.46	0.78
1:A:185:ASP:HB2	2:A:501:DMU:H8	1.66	0.78
1:A:188:THR:HB	1:A:190:TYR:HE1	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD23	1:B:174:ALA:O	1.87	0.74
1:C:104:ARG:HH11	1:C:162:GLY:HA2	1.51	0.74
1:D:59:LEU:HD22	1:D:153:TYR:HD1	1.51	0.74
1:B:295:ILE:CD1	1:B:324:LEU:HD11	2.18	0.74
1:A:203:LEU:HB3	1:A:209:VAL:CG2	2.18	0.73
1:B:192:ARG:HD2	2:B:501:DMU:H40	1.69	0.73
1:D:179:MET:HG2	1:D:221:LEU:HD11	1.70	0.72
1:B:34:LEU:HD21	1:B:181:ILE:HD13	1.72	0.72
1:B:-4:ASP:HA	1:B:-1:ASP:OD2	1.91	0.71
1:B:285:ILE:HG21	1:B:323:MET:SD	2.31	0.70
1:C:222:ARG:NH1	1:C:243:HIS:HD2	1.89	0.70
1:D:259:GLY:HA2	1:D:322:GLN:NE2	2.06	0.70
1:B:131:ARG:CA	1:B:131:ARG:HH11	2.05	0.70
1:B:319:GLU:HA	1:B:322:GLN:HE21	1.56	0.70
1:C:107:LYS:O	1:C:107:LYS:HD3	1.92	0.70
1:D:-3:ASP:C	1:D:-1:ASP:H	1.97	0.70
1:A:72:LEU:HD13	1:A:84:LEU:HB3	1.74	0.70
1:A:192:ARG:NH2	1:A:195:GLU:HB2	2.06	0.70
1:D:267:ALA:HB1	1:D:282:ILE:HG13	1.73	0.69
1:C:219:GLU:OE1	1:C:222:ARG:NE	2.25	0.69
1:D:111:ASP:O	1:D:115:GLN:HB2	1.92	0.69
1:C:232:PRO:HA	1:C:234:GLY:N	2.09	0.68
1:D:288:VAL:HG23	1:D:324:LEU:HD13	1.74	0.68
1:C:9:ARG:HD2	3:C:533:HOH:O	1.93	0.67
1:C:191:ASP:OD2	1:C:256:ARG:NH1	2.27	0.67
1:B:295:ILE:HD12	1:B:324:LEU:HD11	1.77	0.67
1:A:188:THR:HB	1:A:190:TYR:CE1	2.30	0.67
1:D:45:TRP:CE3	1:D:170:VAL:HG22	2.29	0.67
1:D:259:GLY:HA2	1:D:322:GLN:CD	2.19	0.67
1:B:131:ARG:HH11	1:B:131:ARG:HA	1.60	0.66
1:C:183:MET:HE1	1:C:218:LEU:HG	1.77	0.66
1:A:163:GLU:HA	3:A:652:HOH:O	1.95	0.66
1:B:61:LEU:HD22	1:B:91:LEU:HD22	1.78	0.66
1:B:201:ALA:O	1:B:205:ARG:HG3	1.94	0.66
1:B:124:GLN:HE22	1:B:145:TYR:HB3	1.62	0.65
1:A:10:ASP:CG	1:C:192:ARG:HD2	2.21	0.65
1:B:258:LEU:HD13	1:B:262:GLY:CA	2.27	0.65
1:C:1:MET:O	1:C:4:ALA:HB3	1.96	0.65
1:A:33:ARG:HG2	3:A:611:HOH:O	1.97	0.65
1:D:269:VAL:HG21	1:D:320:LEU:HD22	1.79	0.65
1:A:205:ARG:CZ	1:D:131:ARG:HD3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:HA	1:B:73:MET:HE3	1.79	0.65
1:D:59:LEU:HD22	1:D:153:TYR:CD1	2.33	0.65
1:D:136:ARG:HH11	1:D:136:ARG:HB2	1.61	0.64
1:B:33:ARG:CG	1:B:33:ARG:NH2	2.52	0.64
1:C:38:VAL:HG12	1:C:39:PRO:HD3	1.77	0.64
1:D:238:LEU:O	1:D:242:VAL:HG23	1.98	0.64
1:A:196:ARG:HG3	1:A:197:ASP:N	2.12	0.64
1:B:192:ARG:CD	2:B:501:DMU:H40	2.28	0.63
1:B:196:ARG:CD	1:B:197:ASP:H	2.04	0.63
1:C:1:MET:SD	1:C:2:LEU:HD23	2.38	0.63
1:D:-3:ASP:H3	1:D:-1:ASP:HB2	1.64	0.63
1:D:290:ARG:HB2	1:D:324:LEU:HD21	1.81	0.63
1:B:124:GLN:HE21	1:B:124:GLN:HA	1.63	0.63
1:B:203:LEU:HD22	1:B:209:VAL:HG23	1.81	0.63
1:D:57:ARG:HD3	3:D:537:HOH:O	1.98	0.63
1:A:195:GLU:HG2	1:A:196:ARG:N	2.13	0.63
1:B:1:MET:HE2	1:B:2:LEU:HA	1.80	0.63
1:D:142:ALA:HA	1:D:145:TYR:CE2	2.33	0.63
1:B:150:LEU:HD23	1:B:178:ALA:HB2	1.80	0.62
1:A:145:TYR:CE1	2:A:502:DMU:H4	2.34	0.62
1:D:-2:ASP:O	1:D:2:LEU:HG	1.99	0.62
1:A:127:THR:HA	1:A:141:HIS:CE1	2.34	0.62
1:B:150:LEU:CD2	1:B:178:ALA:HB2	2.29	0.62
1:B:266:MET:HE2	1:B:267:ALA:HB3	1.82	0.62
1:D:183:MET:HE3	1:D:217:LEU:HD23	1.80	0.62
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.65	0.62
1:B:318:LYS:O	1:B:322:GLN:HG3	1.99	0.62
1:A:187:LEU:HD21	1:A:204:MET:CE	2.30	0.62
1:D:59:LEU:CD2	1:D:153:TYR:HD1	2.12	0.61
1:D:45:TRP:CE2	1:D:235:ALA:HB2	2.36	0.61
1:D:281:ASP:O	1:D:284:LYS:HB2	2.01	0.61
1:C:195:GLU:O	1:C:196:ARG:NH2	2.32	0.61
1:B:196:ARG:CZ	1:B:197:ASP:HB3	2.31	0.61
1:D:-3:ASP:H3	1:D:-1:ASP:CB	2.13	0.61
1:A:107:LYS:O	1:A:107:LYS:HD3	2.01	0.60
1:B:90:ARG:HD3	1:B:90:ARG:C	2.26	0.60
1:C:203:LEU:HD12	1:C:203:LEU:H	1.65	0.60
1:D:222:ARG:NH1	1:D:243:HIS:CD2	2.62	0.60
2:B:501:DMU:H30	3:B:667:HOH:O	2.01	0.60
1:B:269:VAL:O	1:B:279:GLU:HA	2.01	0.60
1:A:236:PRO:O	1:A:239:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG12	1:B:39:PRO:HD3	1.84	0.60
1:A:142:ALA:HA	1:A:145:TYR:CE2	2.37	0.60
1:D:80:ASP:HB3	1:D:83:GLU:HG2	1.84	0.59
1:D:136:ARG:NH1	1:D:136:ARG:CB	2.65	0.59
1:C:222:ARG:HH11	1:C:243:HIS:HD2	1.50	0.59
1:D:104:ARG:CG	1:D:105:ASP:H	2.12	0.59
1:B:179:MET:HG2	1:B:221:LEU:CD1	2.31	0.59
1:C:104:ARG:NH1	1:C:162:GLY:HA2	2.18	0.59
1:D:263:ALA:CB	1:D:267:ALA:HB2	2.29	0.59
1:C:139:ARG:HG2	1:C:179:MET:HE1	1.84	0.59
1:C:211:GLY:O	1:C:215:VAL:HG23	2.02	0.59
1:C:196:ARG:O	1:C:199:ASN:HB3	2.03	0.59
1:C:142:ALA:HA	1:C:145:TYR:CE2	2.38	0.58
1:B:272:LYS:HE2	1:B:275:GLY:O	2.03	0.58
1:C:107:LYS:NZ	1:D:97:HIS:ND1	2.50	0.58
1:A:72:LEU:CD1	1:A:84:LEU:HB3	2.34	0.58
1:B:273:TYR:CE2	1:B:274:LYS:HD2	2.38	0.58
1:D:104:ARG:HG3	1:D:105:ASP:N	2.16	0.58
1:D:263:ALA:HB3	1:D:267:ALA:CB	2.31	0.58
1:A:43:THR:HA	3:A:604:HOH:O	2.04	0.58
1:A:124:GLN:NE2	2:A:502:DMU:H17	2.19	0.58
1:B:262:GLY:HA3	3:B:641:HOH:O	2.02	0.58
1:B:186:ASP:O	1:B:198:GLY:HA3	2.04	0.58
1:A:1:MET:HA	1:A:40:HIS:CD2	2.39	0.57
1:A:19:THR:CG2	1:A:87:VAL:HG22	2.34	0.57
1:D:45:TRP:CZ3	1:D:170:VAL:HG22	2.39	0.57
1:D:244:LEU:HD23	1:D:245:TYR:CD2	2.39	0.57
1:A:124:GLN:HE21	2:A:502:DMU:H17	1.69	0.57
1:C:232:PRO:HA	1:C:234:GLY:H	1.68	0.57
1:B:269:VAL:HG23	1:B:282:ILE:CD1	2.34	0.57
1:B:266:MET:HG2	1:B:281:ASP:OD2	2.04	0.57
1:A:38:VAL:CG1	1:A:39:PRO:HD3	2.33	0.57
1:A:195:GLU:HG2	1:A:196:ARG:H	1.68	0.57
1:D:211:GLY:O	1:D:215:VAL:HG23	2.05	0.57
1:B:231:ALA:O	1:B:234:GLY:N	2.29	0.57
1:C:99:LEU:HD13	1:C:156:LEU:HD22	1.87	0.56
1:A:104:ARG:HG2	3:A:722:HOH:O	2.05	0.56
1:A:187:LEU:HD21	1:A:204:MET:HE2	1.86	0.56
1:B:267:ALA:CB	1:B:282:ILE:HG12	2.35	0.56
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.88	0.56
1:D:35:TYR:OH	2:D:401:DMU:H8	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:SD	1:B:37:ARG:HD2	2.45	0.56
1:C:139:ARG:NH1	1:C:224:ARG:HH11	2.03	0.56
1:B:43:THR:HB	1:B:52:ARG:HG3	1.88	0.55
1:C:139:ARG:CG	1:C:179:MET:HE1	2.35	0.55
1:C:222:ARG:HH11	1:C:243:HIS:CD2	2.24	0.55
1:A:230:ALA:HB2	3:A:629:HOH:O	2.07	0.55
1:D:179:MET:HG2	1:D:221:LEU:CD1	2.37	0.55
1:D:70:ASP:HA	1:D:73:MET:HE3	1.88	0.55
1:C:81:ARG:HD3	1:D:81:ARG:HH22	1.66	0.55
1:D:94:ARG:HD3	1:D:98:GLU:HG3	1.87	0.55
1:D:263:ALA:HB1	1:D:266:MET:CG	2.31	0.55
1:A:179:MET:HG2	1:A:221:LEU:HD11	1.89	0.55
1:B:258:LEU:CD1	1:B:262:GLY:HA2	2.33	0.55
1:A:128:LYS:HD3	2:A:502:DMU:O6	2.07	0.55
1:D:136:ARG:HH11	1:D:136:ARG:CB	2.19	0.55
1:B:61:LEU:CD2	1:B:91:LEU:HD22	2.37	0.55
1:D:45:TRP:NE1	1:D:235:ALA:HB2	2.21	0.55
1:D:183:MET:CE	1:D:217:LEU:HD23	2.37	0.55
1:B:267:ALA:C	1:B:282:ILE:HG12	2.32	0.55
1:D:289:TRP:CE2	1:D:296:SER:HB3	2.41	0.55
1:B:147:SER:O	1:B:175:GLU:HG2	2.07	0.54
1:A:9:ARG:HB2	1:A:36:LEU:HD13	1.90	0.54
1:A:12:VAL:HG22	1:A:61:LEU:HD23	1.90	0.54
1:D:220:GLU:O	1:D:224:ARG:HG3	2.07	0.54
1:B:1:MET:CE	1:B:37:ARG:HD3	2.37	0.54
1:B:192:ARG:HG2	1:B:193:ASN:H	1.73	0.54
1:D:136:ARG:NH1	1:D:136:ARG:HB3	2.23	0.54
1:A:190:TYR:HB2	2:A:501:DMU:H40	1.89	0.54
1:C:236:PRO:O	1:C:239:VAL:HG23	2.07	0.54
1:C:81:ARG:HD3	1:D:81:ARG:CZ	2.37	0.53
1:A:25:LEU:HD22	1:A:83:GLU:HB3	1.91	0.53
1:B:289:TRP:CE2	1:B:296:SER:HB3	2.44	0.53
1:C:199:ASN:O	1:C:203:LEU:CD1	2.47	0.53
1:A:81:ARG:HE	1:B:75:ASP:HB2	1.73	0.53
1:B:272:LYS:HA	1:B:276:GLU:O	2.09	0.53
1:C:68:LEU:HD22	1:C:84:LEU:CD2	2.39	0.53
1:D:128:LYS:HE2	2:D:401:DMU:O61	2.09	0.53
1:C:197:ASP:N	1:C:197:ASP:OD1	2.41	0.53
2:C:401:DMU:H29	2:C:401:DMU:H35	1.89	0.53
1:A:192:ARG:O	1:A:195:GLU:HB3	2.09	0.53
1:C:139:ARG:HH11	1:C:224:ARG:HH11	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:HG21	1:D:323:MET:SD	2.49	0.53
1:A:11:HIS:CE1	1:A:57:ARG:NH1	2.76	0.52
1:C:139:ARG:HG3	1:C:179:MET:CE	2.39	0.52
1:D:245:TYR:O	1:D:249:VAL:HG23	2.10	0.52
1:D:308:ARG:HG2	1:D:308:ARG:HH11	1.74	0.52
1:A:229:VAL:HG11	1:A:238:LEU:HB2	1.91	0.52
1:B:295:ILE:O	1:B:310:ALA:HA	2.09	0.52
1:C:205:ARG:HG2	1:C:205:ARG:HH11	1.75	0.52
1:B:254:LEU:HD13	1:B:258:LEU:HD11	1.91	0.52
1:D:295:ILE:O	1:D:310:ALA:HA	2.09	0.52
1:B:282:ILE:HD13	1:B:282:ILE:N	2.24	0.52
1:C:147:SER:HB3	1:C:175:GLU:HG2	1.92	0.52
1:A:46:THR:OG1	3:A:601:HOH:O	2.19	0.52
1:C:55:VAL:HG22	1:C:102:LEU:HD13	1.92	0.52
1:B:114:GLU:O	1:B:115:GLN:C	2.52	0.52
1:B:131:ARG:HH11	1:B:131:ARG:N	2.08	0.52
1:B:1:MET:HE3	1:B:37:ARG:HD3	1.92	0.51
1:B:270:LYS:HZ3	1:B:279:GLU:CD	2.17	0.51
1:C:139:ARG:HG3	1:C:179:MET:HE3	1.91	0.51
1:D:12:VAL:O	1:D:16:VAL:HG23	2.10	0.51
1:D:295:ILE:HD12	1:D:324:LEU:HD22	1.91	0.51
1:A:70:ASP:HA	1:A:73:MET:HE3	1.92	0.51
1:C:90:ARG:HD3	1:C:90:ARG:C	2.35	0.51
1:A:107:LYS:HD3	1:A:107:LYS:C	2.36	0.51
1:C:73:MET:CE	2:C:401:DMU:H25	2.41	0.51
1:B:210:ALA:O	1:B:211:GLY:C	2.53	0.51
1:A:45:TRP:CE3	1:A:170:VAL:HG22	2.45	0.51
1:B:270:LYS:NZ	1:B:279:GLU:OE1	2.43	0.51
1:C:-3:ASP:HB2	1:C:2:LEU:HD11	1.93	0.51
1:B:288:VAL:HG11	1:B:320:LEU:HD11	1.93	0.51
1:D:166:PRO:HD3	1:D:233:PRO:HD2	1.93	0.51
1:B:90:ARG:HD3	1:B:90:ARG:O	2.11	0.50
1:D:65:SER:HB2	1:D:91:LEU:HB2	1.94	0.50
1:B:33:ARG:NH2	1:B:33:ARG:HG3	2.27	0.50
1:C:187:LEU:HD21	1:C:204:MET:CE	2.42	0.50
1:D:140:ALA:O	1:D:143:SER:HB3	2.11	0.50
1:C:139:ARG:HH11	1:C:224:ARG:NH1	2.08	0.50
1:C:183:MET:CE	1:C:218:LEU:HG	2.42	0.50
1:D:322:GLN:HA	1:D:322:GLN:OE1	2.11	0.50
1:C:80:ASP:HB3	1:C:83:GLU:HG2	1.94	0.50
1:C:124:GLN:HG3	2:C:401:DMU:C37	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:GLY:H	1:D:266:MET:CG	2.21	0.50
1:D:285:ILE:HG22	1:D:285:ILE:O	2.11	0.49
1:B:196:ARG:CD	1:B:197:ASP:N	2.71	0.49
1:C:72:LEU:HD12	1:D:81:ARG:NH2	2.26	0.49
1:A:77:THR:OG1	1:A:79:LEU:HD12	2.12	0.49
1:D:189:ASP:OD1	1:D:192:ARG:NH2	2.40	0.49
1:B:188:THR:HG21	1:B:190:TYR:CE1	2.47	0.49
1:B:285:ILE:O	1:B:285:ILE:HG22	2.12	0.49
1:D:131:ARG:HH11	1:D:131:ARG:HB2	1.78	0.49
1:A:16:VAL:HG12	1:A:26:VAL:HG22	1.93	0.49
1:A:158:ALA:HA	1:A:165:GLN:HG2	1.93	0.49
1:C:73:MET:HE1	2:C:401:DMU:H25	1.94	0.49
1:A:81:ARG:HG2	1:A:81:ARG:NH1	2.26	0.49
1:D:201:ALA:HA	1:D:204:MET:HE3	1.94	0.49
2:D:401:DMU:C9	2:D:401:DMU:H29	2.42	0.49
1:B:288:VAL:HG13	1:B:327:GLN:NE2	2.26	0.49
1:A:132:ALA:CB	1:A:137:GLU:HB2	2.36	0.49
1:A:226:LEU:HD22	1:A:239:VAL:HG13	1.95	0.49
1:C:76:ASP:N	1:C:76:ASP:OD1	2.43	0.49
1:A:106:PRO:HB2	1:B:106:PRO:HB2	1.94	0.48
1:B:202:HIS:O	1:B:203:LEU:C	2.55	0.48
1:C:129:ARG:NH2	1:D:80:ASP:OD2	2.43	0.48
1:C:39:PRO:HG3	1:C:63:ILE:HD12	1.95	0.48
1:D:123:GLY:O	1:D:127:THR:HG23	2.13	0.48
1:D:136:ARG:HB3	1:D:136:ARG:CZ	2.44	0.48
1:B:19:THR:O	1:B:19:THR:HG23	2.13	0.48
1:A:112:ILE:HD13	1:A:155:ALA:HB1	1.95	0.48
1:B:127:THR:HA	1:B:141:HIS:CD2	2.48	0.48
1:C:219:GLU:OE1	1:C:219:GLU:HA	2.12	0.48
1:B:266:MET:CE	1:B:267:ALA:N	2.77	0.48
1:D:171:ARG:O	1:D:175:GLU:HG3	2.12	0.48
1:B:185:ASP:HB2	2:B:501:DMU:H11	1.96	0.48
1:B:11:HIS:CG	1:B:57:ARG:HD2	2.49	0.48
2:C:401:DMU:H29	2:C:401:DMU:C9	2.43	0.48
1:A:10:ASP:OD1	1:C:192:ARG:HD2	2.14	0.47
1:B:105:ASP:OD1	1:B:106:PRO:HD2	2.15	0.47
1:C:10:ASP:CG	1:C:14:ARG:HH22	2.22	0.47
1:D:142:ALA:HB1	1:D:182:THR:HG21	1.95	0.47
1:C:205:ARG:HG2	1:C:205:ARG:NH1	2.29	0.47
1:D:105:ASP:OD2	1:D:106:PRO:HD2	2.14	0.47
1:A:78:GLY:N	3:A:606:HOH:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HB2	1:B:255:PRO:HD3	1.96	0.47
1:B:124:GLN:NE2	1:B:145:TYR:HB3	2.28	0.47
1:B:131:ARG:HD2	1:B:199:ASN:ND2	2.30	0.47
1:B:244:LEU:HD12	3:B:645:HOH:O	2.14	0.47
1:D:61:LEU:CD1	1:D:94:ARG:HG3	2.45	0.47
1:D:254:LEU:HD12	1:D:254:LEU:HA	1.67	0.47
1:C:45:TRP:CE2	1:C:235:ALA:HB2	2.50	0.47
1:A:90:ARG:C	1:A:90:ARG:HD3	2.40	0.47
1:C:124:GLN:HG3	2:C:401:DMU:H20	1.97	0.47
1:B:229:VAL:HG13	1:B:235:ALA:O	2.15	0.46
1:D:202:HIS:O	1:D:206:THR:HG23	2.15	0.46
1:D:239:VAL:HG21	3:D:612:HOH:O	2.14	0.46
1:C:11:HIS:CD2	1:C:57:ARG:HD2	2.50	0.46
1:D:185:ASP:O	1:D:186:ASP:C	2.58	0.46
1:D:301:GLU:O	1:D:302:GLY:C	2.57	0.46
1:C:130:SER:HB2	1:C:141:HIS:CE1	2.51	0.46
1:D:-3:ASP:H3	1:D:-1:ASP:H	1.63	0.46
1:C:54:ALA:HA	1:C:57:ARG:HE	1.80	0.46
1:A:45:TRP:CD2	1:A:170:VAL:HG22	2.50	0.46
1:B:297:PHE:CD1	1:B:297:PHE:C	2.94	0.46
1:B:1:MET:CE	1:B:5:GLU:OE1	2.64	0.46
1:A:108:ALA:O	1:A:112:ILE:HG13	2.16	0.46
1:D:-3:ASP:C	1:D:-1:ASP:N	2.66	0.46
1:B:210:ALA:O	1:B:213:ASP:N	2.49	0.46
1:B:293:LYS:HG2	1:B:313:GLU:OE2	2.16	0.46
1:C:232:PRO:HA	1:C:233:PRO:C	2.40	0.46
1:A:192:ARG:HH21	1:A:195:GLU:HB2	1.78	0.45
1:B:324:LEU:C	1:B:326:LYS:H	2.22	0.45
1:A:179:MET:O	1:A:183:MET:HG3	2.16	0.45
1:C:19:THR:O	1:C:19:THR:HG22	2.15	0.45
1:C:231:ALA:HA	1:C:232:PRO:HD3	1.71	0.45
1:D:284:LYS:HD2	1:D:300:ASP:HB3	1.98	0.45
1:D:289:TRP:HA	1:D:324:LEU:HD11	1.98	0.45
1:A:89:LEU:O	1:A:93:LEU:HG	2.16	0.45
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.73	0.45
1:D:325:GLU:OE2	1:D:325:GLU:O	2.35	0.45
1:B:212:GLN:HB2	1:B:263:ALA:O	2.16	0.45
1:B:255:PRO:C	1:B:257:HIS:N	2.74	0.45
1:D:216:ASP:O	1:D:217:LEU:C	2.57	0.45
1:C:34:LEU:CD2	1:C:181:ILE:HG21	2.47	0.45
1:A:205:ARG:NH1	1:D:131:ARG:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:O	1:B:112:ILE:HG13	2.17	0.45
1:B:270:LYS:HA	1:B:278:LYS:O	2.17	0.45
2:B:501:DMU:H26	2:B:501:DMU:H18	1.78	0.45
1:C:139:ARG:CG	1:C:179:MET:CE	2.95	0.45
1:A:198:GLY:O	1:A:201:ALA:HB3	2.16	0.45
1:B:38:VAL:CG1	1:B:39:PRO:HD3	2.47	0.45
1:B:219:GLU:OE1	1:B:219:GLU:HA	2.16	0.45
1:B:268:THR:HG22	1:B:281:ASP:HA	1.99	0.45
1:C:139:ARG:O	1:C:143:SER:HB2	2.17	0.45
1:C:190:TYR:O	1:C:194:GLY:HA2	2.17	0.45
1:D:-3:ASP:N	1:D:0:LYS:H	2.14	0.45
1:D:1:MET:O	1:D:4:ALA:HB3	2.16	0.45
1:A:138:TRP:CH2	1:A:183:MET:HG2	2.51	0.44
1:B:145:TYR:CE1	2:B:502:DMU:H4	2.52	0.44
1:C:165:GLN:HE21	1:C:165:GLN:HB3	1.41	0.44
1:D:109:VAL:HG22	1:D:156:LEU:HD22	1.99	0.44
1:D:254:LEU:HG	1:D:258:LEU:HD13	2.00	0.44
1:D:269:VAL:HG22	1:D:317:PRO:HG3	1.99	0.44
1:C:166:PRO:HD3	1:C:233:PRO:CD	2.42	0.44
1:A:136:ARG:CZ	1:A:136:ARG:HB3	2.48	0.44
1:A:205:ARG:NH1	1:D:131:ARG:CD	2.80	0.44
1:A:233:PRO:O	1:A:234:GLY:O	2.36	0.44
1:B:55:VAL:HG23	1:B:102:LEU:HD13	1.99	0.44
1:D:11:HIS:CD2	1:D:57:ARG:HB2	2.53	0.44
1:A:76:ASP:OD1	1:A:76:ASP:C	2.61	0.43
2:A:501:DMU:C7	1:C:78:GLY:HA2	2.35	0.43
1:B:34:LEU:HD21	1:B:181:ILE:CD1	2.45	0.43
1:B:255:PRO:O	1:B:257:HIS:N	2.50	0.43
1:B:288:VAL:HG13	1:B:327:GLN:HE22	1.82	0.43
1:B:319:GLU:CD	1:B:319:GLU:H	2.26	0.43
1:C:143:SER:O	1:C:147:SER:HB2	2.16	0.43
1:C:200:LEU:O	1:C:200:LEU:HD12	2.19	0.43
1:D:104:ARG:CG	1:D:105:ASP:N	2.76	0.43
1:B:194:GLY:C	1:B:196:ARG:H	2.26	0.43
1:B:285:ILE:CG2	1:B:323:MET:SD	3.04	0.43
1:B:38:VAL:N	1:B:39:PRO:CD	2.82	0.43
1:C:90:ARG:NH1	1:C:90:ARG:HG2	2.33	0.43
1:C:179:MET:HB3	1:C:221:LEU:HD22	2.00	0.43
1:D:314:LYS:HD2	3:D:599:HOH:O	2.17	0.43
1:A:226:LEU:CD2	1:A:239:VAL:HG13	2.48	0.43
1:B:65:SER:HB2	1:B:91:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLN:O	1:B:326:LYS:CG	2.56	0.43
1:D:11:HIS:HD2	1:D:57:ARG:HB2	1.83	0.43
1:A:11:HIS:ND1	1:A:57:ARG:NH1	2.66	0.43
1:C:255:PRO:O	1:C:256:ARG:C	2.62	0.43
1:B:286:LYS:HE3	1:B:299:TYR:O	2.19	0.43
1:C:141:HIS:O	1:C:145:TYR:CD2	2.72	0.43
1:D:39:PRO:O	1:D:43:THR:HG23	2.17	0.43
1:A:131:ARG:HA	1:A:131:ARG:HD3	1.52	0.43
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.81	0.43
1:D:231:ALA:HA	1:D:232:PRO:HD3	1.85	0.43
1:D:44:GLU:OE2	1:D:52:ARG:NH2	2.51	0.43
2:B:502:DMU:H29	2:B:502:DMU:C9	2.49	0.43
1:C:90:ARG:HG2	1:C:90:ARG:HH11	1.84	0.43
1:D:16:VAL:HG13	1:D:87:VAL:HG11	2.01	0.42
1:C:35:TYR:OH	2:C:401:DMU:H8	2.18	0.42
1:B:-4:ASP:O	1:B:-1:ASP:HB2	2.19	0.42
1:B:1:MET:HE3	1:B:5:GLU:OE1	2.18	0.42
1:B:166:PRO:O	1:B:166:PRO:HG2	2.19	0.42
1:B:255:PRO:O	1:B:256:ARG:C	2.61	0.42
1:B:266:MET:HE2	1:B:267:ALA:N	2.34	0.42
1:C:163:GLU:O	1:C:163:GLU:HG2	2.20	0.42
2:C:401:DMU:H22	1:D:89:LEU:HD22	2.00	0.42
1:D:267:ALA:HB1	1:D:319:GLU:OE1	2.19	0.42
1:D:272:LYS:HA	1:D:276:GLU:O	2.20	0.42
1:B:172:GLU:HG3	1:B:228:ALA:HB2	2.00	0.42
1:C:199:ASN:O	1:C:202:HIS:HB3	2.19	0.42
1:D:66:MET:HE2	1:D:66:MET:HA	2.02	0.42
1:B:288:VAL:HG11	1:B:320:LEU:CD1	2.50	0.42
1:C:222:ARG:NH1	1:C:243:HIS:CD2	2.77	0.42
1:D:135:LEU:HA	1:D:135:LEU:HD12	1.65	0.42
1:B:179:MET:O	1:B:180:THR:C	2.62	0.42
1:C:62:ASP:O	1:C:63:ILE:C	2.61	0.42
1:C:252:ARG:NH1	1:C:253:LEU:HD21	2.35	0.42
1:D:14:ARG:HE	1:D:14:ARG:HB2	1.47	0.42
1:D:194:GLY:HA2	1:D:196:ARG:HH12	1.83	0.42
1:A:22:SER:HB2	1:A:23:PRO:CD	2.50	0.42
1:C:29:THR:HG22	1:C:30:ALA:N	2.35	0.42
1:C:51:ARG:HH21	1:C:51:ARG:HD3	1.67	0.42
1:C:165:GLN:O	1:C:167:ALA:N	2.52	0.42
1:C:179:MET:HG2	1:C:221:LEU:HD21	2.01	0.42
1:D:282:ILE:O	1:D:282:ILE:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:HD3	1:B:162:GLY:N	2.34	0.42
1:B:168:ASP:OD2	1:B:168:ASP:N	2.33	0.42
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.85	0.42
1:A:241:VAL:O	1:A:242:VAL:C	2.62	0.42
1:B:282:ILE:HG22	1:B:282:ILE:O	2.20	0.42
1:C:187:LEU:HD22	1:C:201:ALA:HB2	2.02	0.42
1:B:-4:ASP:HA	1:B:-1:ASP:HB2	2.02	0.41
1:B:321:LEU:O	1:B:324:LEU:HB2	2.20	0.41
1:C:45:TRP:CE3	1:C:170:VAL:HG22	2.54	0.41
1:D:34:LEU:HD21	1:D:181:ILE:HG21	2.01	0.41
1:C:192:ARG:HE	1:C:192:ARG:HB3	1.61	0.41
1:A:44:GLU:HG2	1:A:238:LEU:HG	2.02	0.41
1:B:266:MET:HE3	1:B:267:ALA:H	1.85	0.41
1:D:246:THR:O	1:D:246:THR:HG22	2.19	0.41
1:D:252:ARG:O	1:D:255:PRO:HD2	2.19	0.41
1:B:150:LEU:O	1:B:153:TYR:N	2.51	0.41
1:C:51:ARG:HD3	1:C:161:GLY:O	2.19	0.41
1:D:45:TRP:CD2	1:D:170:VAL:HG22	2.55	0.41
1:A:-5:VAL:HB	1:A:-4:ASP:H	1.66	0.41
1:D:94:ARG:HD2	1:D:98:GLU:CD	2.44	0.41
1:C:73:MET:HE1	1:D:86:CYS:SG	2.60	0.41
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.92	0.41
1:B:221:LEU:HA	1:B:221:LEU:HD23	1.89	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.88	0.41
1:A:80:ASP:OD2	1:A:83:GLU:HG3	2.20	0.41
1:A:116:ASP:N	1:A:116:ASP:OD1	2.54	0.41
1:A:200:LEU:O	1:A:204:MET:HG3	2.21	0.41
1:B:192:ARG:NE	2:B:501:DMU:H40	2.36	0.41
1:C:230:ALA:O	1:C:231:ALA:C	2.63	0.41
1:D:166:PRO:O	1:D:167:ALA:C	2.63	0.41
1:C:44:GLU:HG2	1:C:238:LEU:HG	2.03	0.41
1:C:254:LEU:N	1:C:255:PRO:CD	2.84	0.41
1:B:173:PHE:O	1:B:174:ALA:C	2.64	0.40
1:A:187:LEU:CD2	1:A:204:MET:CE	2.98	0.40
1:B:192:ARG:HD2	2:B:501:DMU:C11	2.44	0.40
1:C:186:ASP:OD1	1:C:199:ASN:HA	2.21	0.40
1:B:1:MET:SD	1:B:37:ARG:CD	3.09	0.40
1:D:322:GLN:O	1:D:326:LYS:HG3	2.21	0.40
1:A:78:GLY:HA2	3:A:606:HOH:O	2.21	0.40
1:B:24:ASP:O	1:B:27:ALA:HB3	2.22	0.40
1:B:239:VAL:N	1:B:240:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ARG:HA	1:B:131:ARG:HD3	1.90	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	262/343 (76%)	249 (95%)	8 (3%)	5 (2%)	6	12
1	B	330/343 (96%)	295 (89%)	28 (8%)	7 (2%)	5	11
1	C	260/343 (76%)	245 (94%)	14 (5%)	1 (0%)	30	50
1	D	329/343 (96%)	308 (94%)	17 (5%)	4 (1%)	10	20
All	All	1181/1372 (86%)	1097 (93%)	67 (6%)	17 (1%)	9	17

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	GLY
1	B	193	ASN
1	B	234	GLY
1	B	302	GLY
1	D	167	ALA
1	A	115	GLN
1	C	234	GLY
1	D	261	ALA
1	D	302	GLY
1	B	33	ARG
1	B	115	GLN
1	B	143	SER
1	B	305	LYS
1	A	167	ALA

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Mol	Chain	Res	Type
1	A	193	ASN
1	A	199	ASN
1	D	249	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/270 (77%)	184 (88%)	24 (12%)	5	10
1	B	260/270 (96%)	235 (90%)	25 (10%)	8	15
1	C	206/270 (76%)	186 (90%)	20 (10%)	8	15
1	D	259/270 (96%)	234 (90%)	25 (10%)	8	15
All	All	933/1080 (86%)	839 (90%)	94 (10%)	7	14

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	5	GLU
1	A	18	GLN
1	A	23	PRO
1	A	47	THR
1	A	81	ARG
1	A	94	ARG
1	A	107	LYS
1	A	115	GLN
1	A	129	ARG
1	A	131	ARG
1	A	137	GLU
1	A	139	ARG
1	A	141	HIS
1	A	165	GLN
1	A	181	ILE
1	A	182	THR
1	A	188	THR

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Mol	Chain	Res	Type
1	A	189	ASP
1	A	190	TYR
1	A	191	ASP
1	A	195	GLU
1	A	197	ASP
1	A	255	PRO
1	B	-2	ASP
1	B	1	MET
1	B	14	ARG
1	B	18	GLN
1	B	19	THR
1	B	33	ARG
1	B	124	GLN
1	B	131	ARG
1	B	168	ASP
1	B	179	MET
1	B	186	ASP
1	B	188	THR
1	B	191	ASP
1	B	196	ARG
1	B	199	ASN
1	B	233	PRO
1	B	266	MET
1	B	281	ASP
1	B	284	LYS
1	B	285	ILE
1	B	288	VAL
1	B	293	LYS
1	B	296	SER
1	B	311	VAL
1	B	325	GLU
1	C	23	PRO
1	C	29	THR
1	C	38	VAL
1	C	47	THR
1	C	52	ARG
1	C	65	SER
1	C	72	LEU
1	C	94	ARG
1	C	107	LYS
1	C	144	THR
1	C	165	GLN

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Mol	Chain	Res	Type
1	C	179	MET
1	C	186	ASP
1	C	197	ASP
1	C	200	LEU
1	C	212	GLN
1	C	219	GLU
1	C	224	ARG
1	C	246	THR
1	C	251	VAL
1	D	-1	ASP
1	D	1	MET
1	D	38	VAL
1	D	131	ARG
1	D	139	ARG
1	D	144	THR
1	D	150	LEU
1	D	169	SER
1	D	172	GLU
1	D	179	MET
1	D	181	ILE
1	D	193	ASN
1	D	197	ASP
1	D	244	LEU
1	D	251	VAL
1	D	255	PRO
1	D	277	GLU
1	D	281	ASP
1	D	282	ILE
1	D	285	ILE
1	D	288	VAL
1	D	300	ASP
1	D	311	VAL
1	D	319	GLU
1	D	325	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	115	GLN
1	A	199	ASN
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	124	GLN
1	B	199	ASN
1	B	212	GLN
1	B	322	GLN
1	C	124	GLN
1	C	165	GLN
1	C	243	HIS
1	D	11	HIS
1	D	165	GLN
1	D	243	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
2	DMU	B	502	-	34,34,34	0.91	1 (2%)	45,45,45	0.84	0
2	DMU	D	401	-	34,34,34	0.79	1 (2%)	45,45,45	0.75	2 (4%)
2	DMU	A	502	-	34,34,34	0.82	1 (2%)	45,45,45	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMU	B	501	-	34,34,34	1.01	1 (2%)	45,45,45	0.84	1 (2%)
2	DMU	A	501	-	34,34,34	0.91	1 (2%)	45,45,45	0.65	0
2	DMU	C	401	-	34,34,34	0.78	1 (2%)	45,45,45	0.80	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
2	DMU	B	502	-	-	10/19/59/59	0/2/2/2
2	DMU	D	401	-	-	6/19/59/59	0/2/2/2
2	DMU	A	502	-	-	6/19/59/59	0/2/2/2
2	DMU	B	501	-	-	10/19/59/59	0/2/2/2
2	DMU	A	501	-	-	9/19/59/59	0/2/2/2
2	DMU	C	401	-	-	9/19/59/59	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	DMU	O16-C18	3.87	1.53	1.43
2	A	501	DMU	O16-C18	3.74	1.53	1.43
2	D	401	DMU	O16-C18	3.64	1.52	1.43
2	B	501	DMU	O16-C18	3.36	1.52	1.43
2	A	502	DMU	O16-C18	3.36	1.52	1.43
2	C	401	DMU	O16-C18	3.06	1.51	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	DMU	C18-O16-C6	-3.37	107.93	113.68
2	D	401	DMU	C18-O16-C6	-2.41	109.56	113.68
2	B	501	DMU	O7-C10-O1	-2.02	105.39	110.69
2	D	401	DMU	C57-C4-C3	-2.01	107.74	113.38

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	DMU	O6-C11-C9-C8
2	C	401	DMU	O6-C11-C9-C8
2	A	502	DMU	O6-C11-C9-O1
2	B	502	DMU	O6-C11-C9-O1
2	C	401	DMU	O5-C4-C57-O61
2	B	501	DMU	O5-C6-O16-C18
2	A	502	DMU	O5-C4-C57-O61
2	A	501	DMU	O16-C18-C19-C22
2	D	401	DMU	O5-C4-C57-O61
2	C	401	DMU	O6-C11-C9-O1
2	D	401	DMU	O6-C11-C9-O1
2	A	502	DMU	C3-C4-C57-O61
2	C	401	DMU	C3-C4-C57-O61
2	B	501	DMU	C1-C6-O16-C18
2	B	502	DMU	O6-C11-C9-C8
2	D	401	DMU	C3-C4-C57-O61
2	B	501	DMU	O5-C4-C57-O61
2	A	502	DMU	O6-C11-C9-C8
2	B	502	DMU	O5-C4-C57-O61
2	B	502	DMU	C19-C22-C25-C28
2	B	502	DMU	C3-C4-C57-O61
2	A	501	DMU	C3-C4-C57-O61
2	B	502	DMU	O16-C18-C19-C22
2	A	501	DMU	O5-C4-C57-O61
2	A	501	DMU	C28-C31-C34-C37
2	B	501	DMU	C25-C28-C31-C34
2	C	401	DMU	C31-C34-C37-C40
2	D	401	DMU	C25-C28-C31-C34
2	A	502	DMU	C18-C19-C22-C25
2	B	502	DMU	C25-C28-C31-C34
2	B	501	DMU	C31-C34-C37-C40
2	A	501	DMU	O1-C10-O7-C3
2	B	501	DMU	C28-C31-C34-C37
2	C	401	DMU	C18-C19-C22-C25
2	A	501	DMU	O6-C11-C9-O1
2	C	401	DMU	C28-C31-C34-C37
2	B	501	DMU	C19-C22-C25-C28
2	B	501	DMU	C22-C25-C28-C31
2	C	401	DMU	C19-C22-C25-C28
2	C	401	DMU	C25-C28-C31-C34
2	B	501	DMU	C3-C4-C57-O61
2	B	501	DMU	C34-C37-C40-C43
2	B	502	DMU	C19-C18-O16-C6

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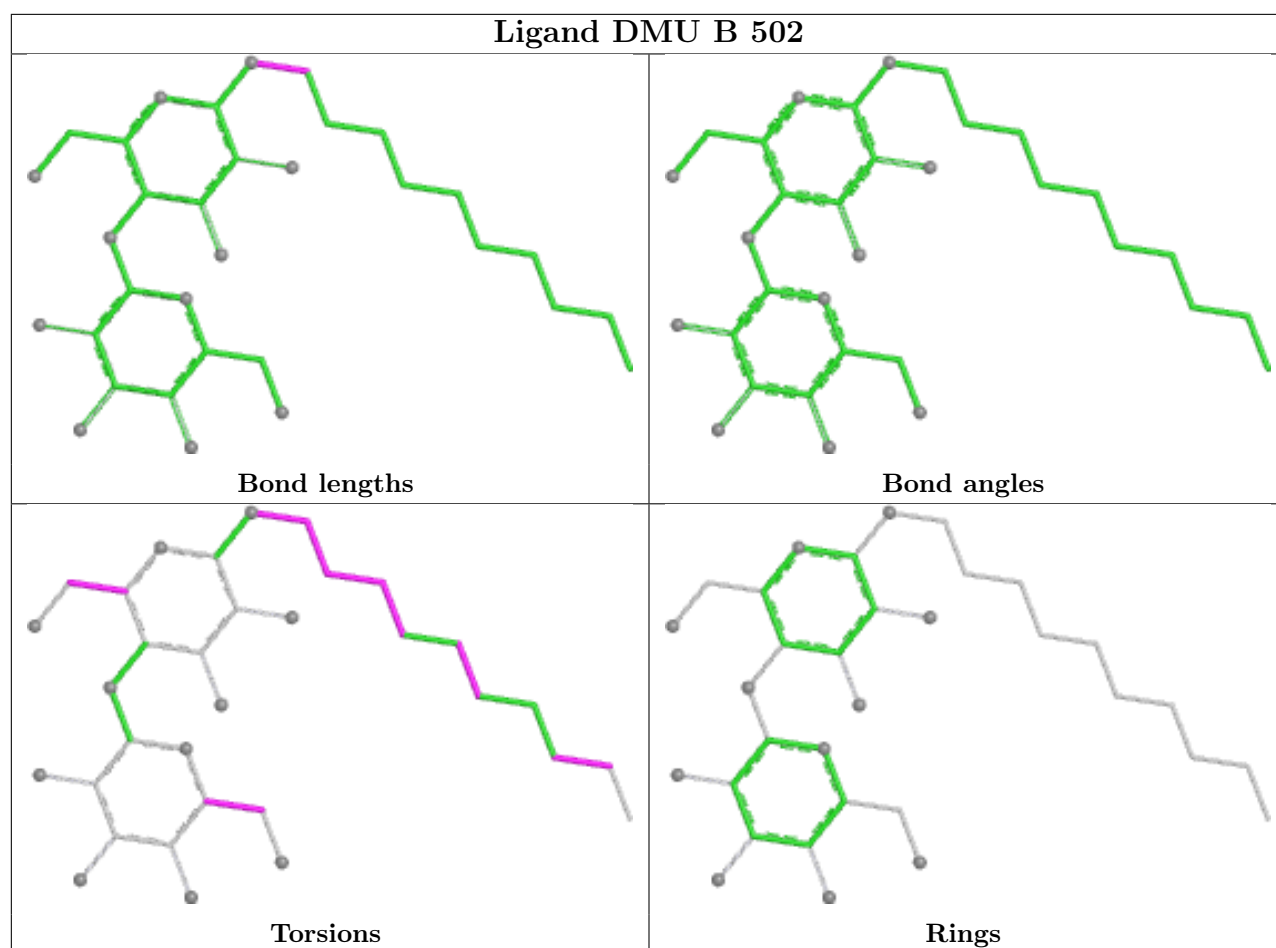
Mol	Chain	Res	Type	Atoms
2	A	501	DMU	C31-C34-C37-C40
2	A	501	DMU	C5-C10-O7-C3
2	B	502	DMU	C34-C37-C40-C43
2	D	401	DMU	C18-C19-C22-C25
2	B	502	DMU	C18-C19-C22-C25
2	A	501	DMU	C18-C19-C22-C25
2	A	502	DMU	C25-C28-C31-C34

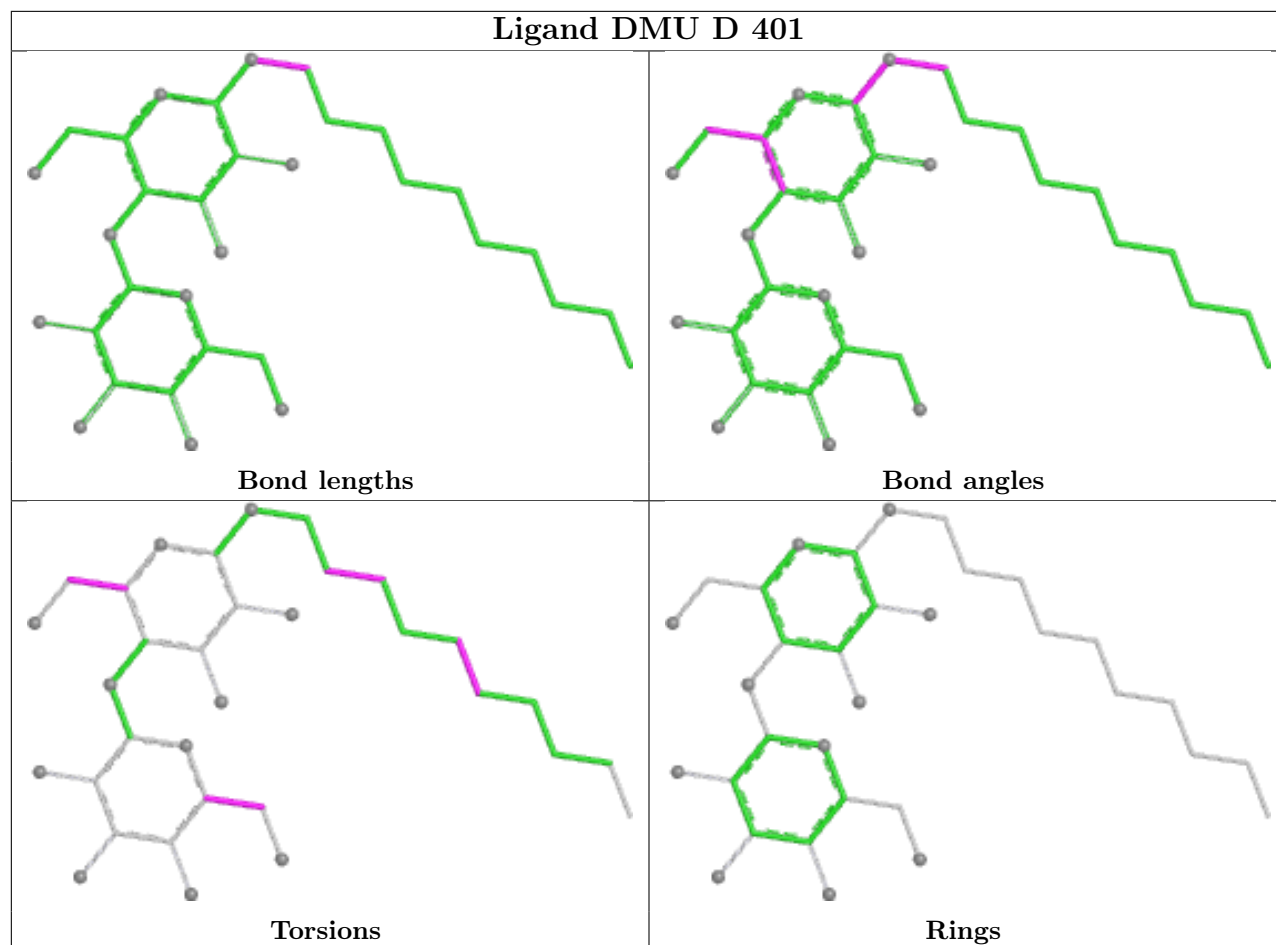
There are no ring outliers.

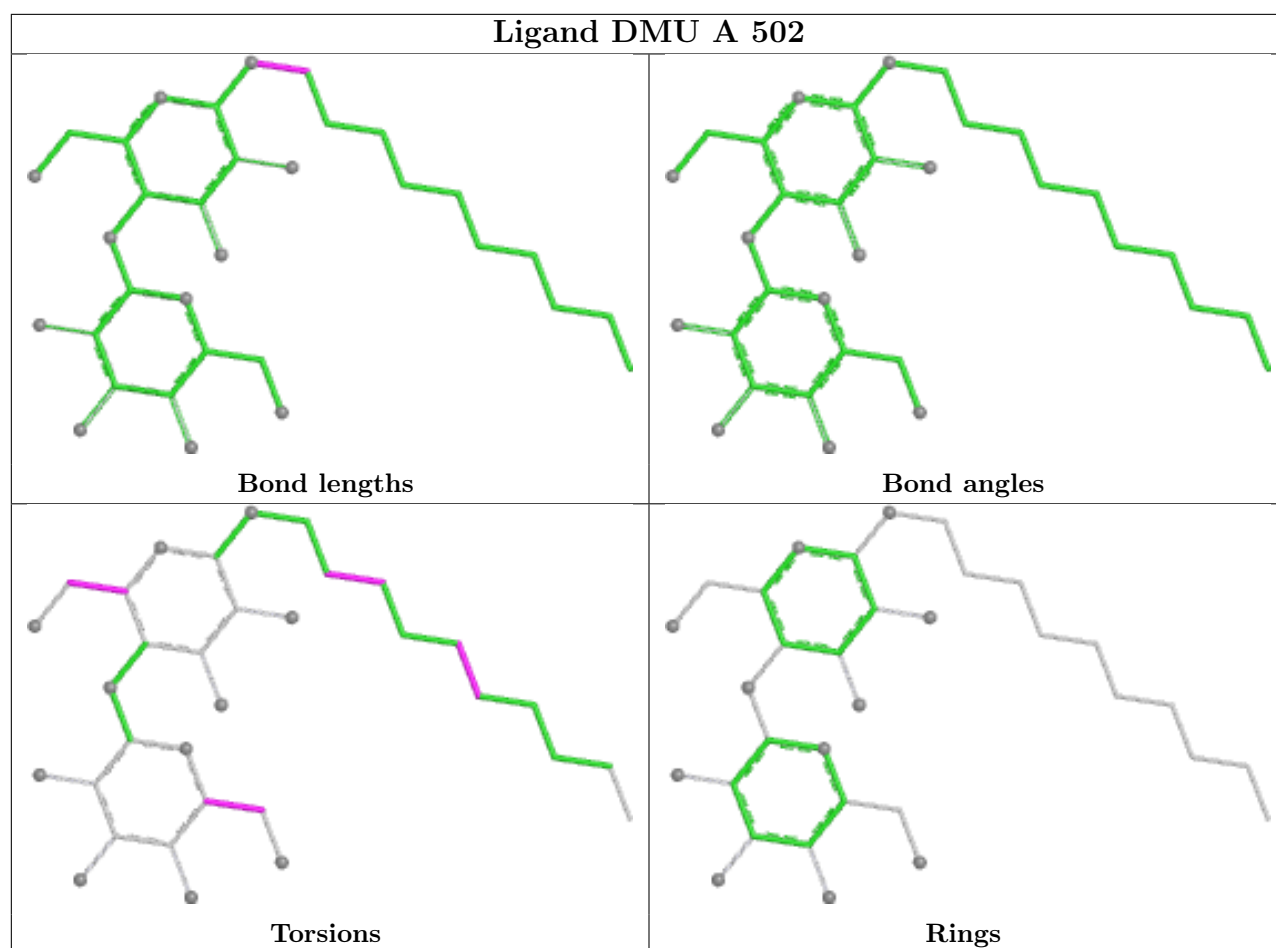
6 monomers are involved in 31 short contacts:

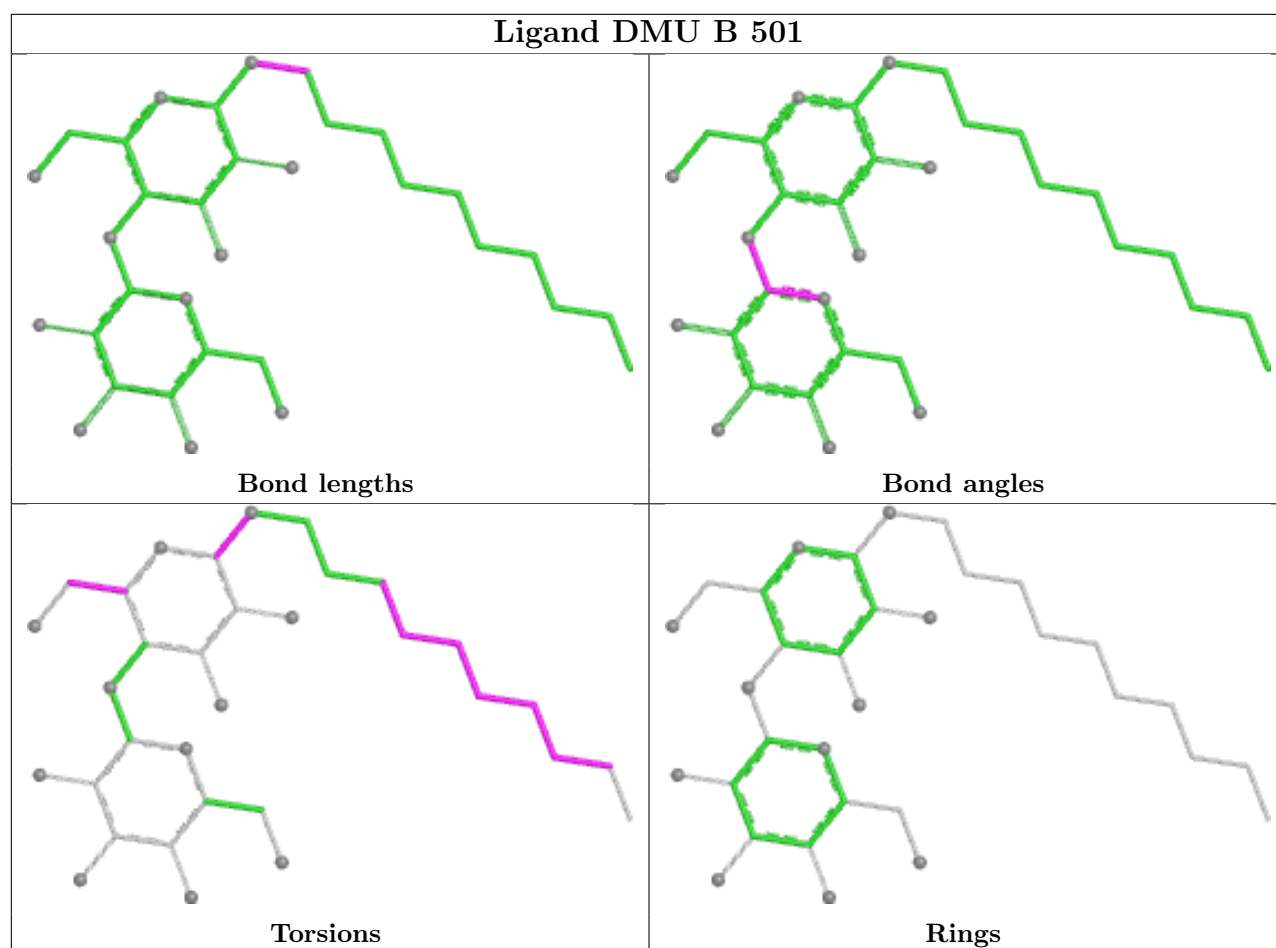
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	DMU	2	0
2	D	401	DMU	3	0
2	A	502	DMU	4	0
2	B	501	DMU	7	0
2	A	501	DMU	7	0
2	C	401	DMU	8	0

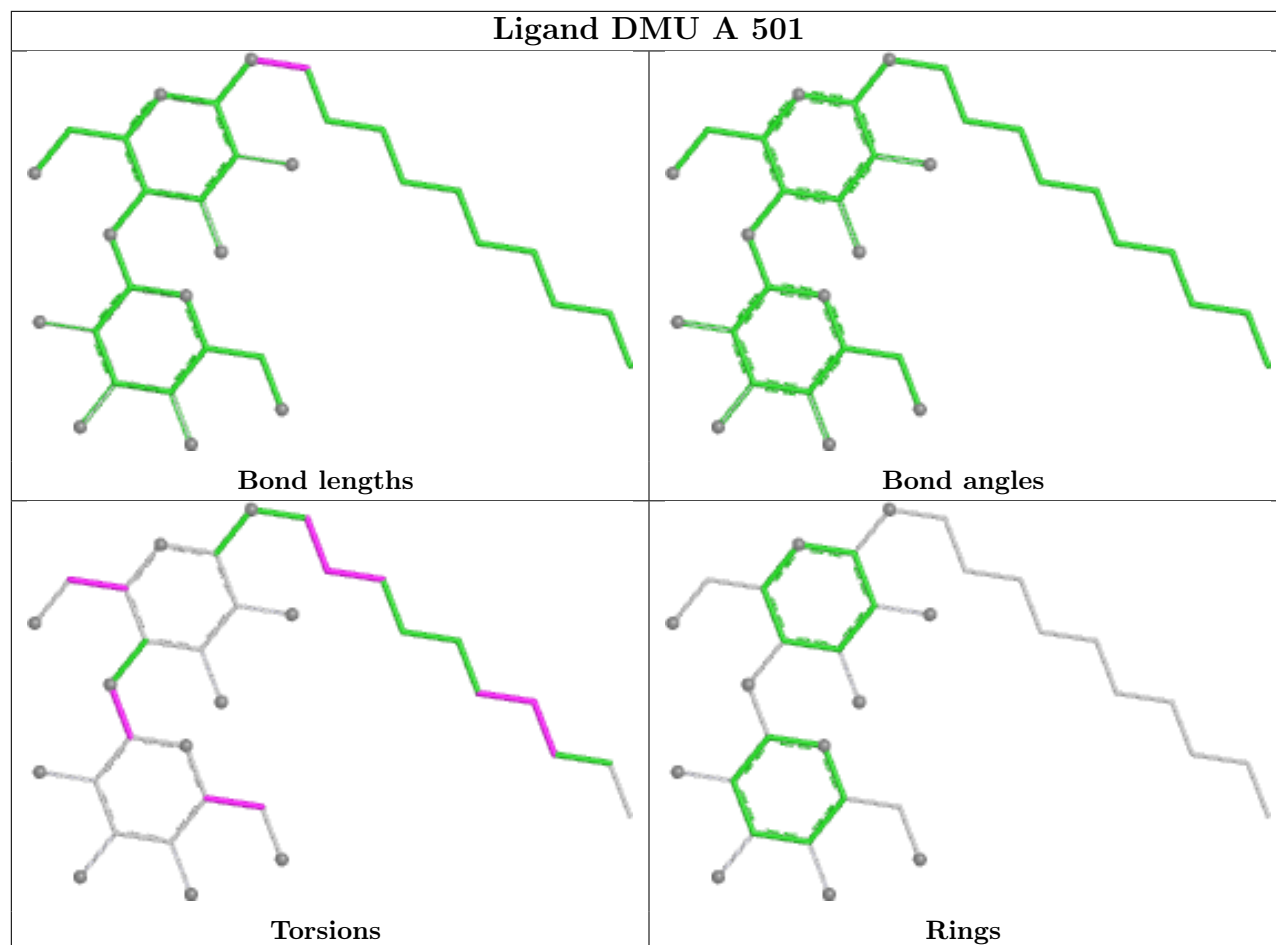
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

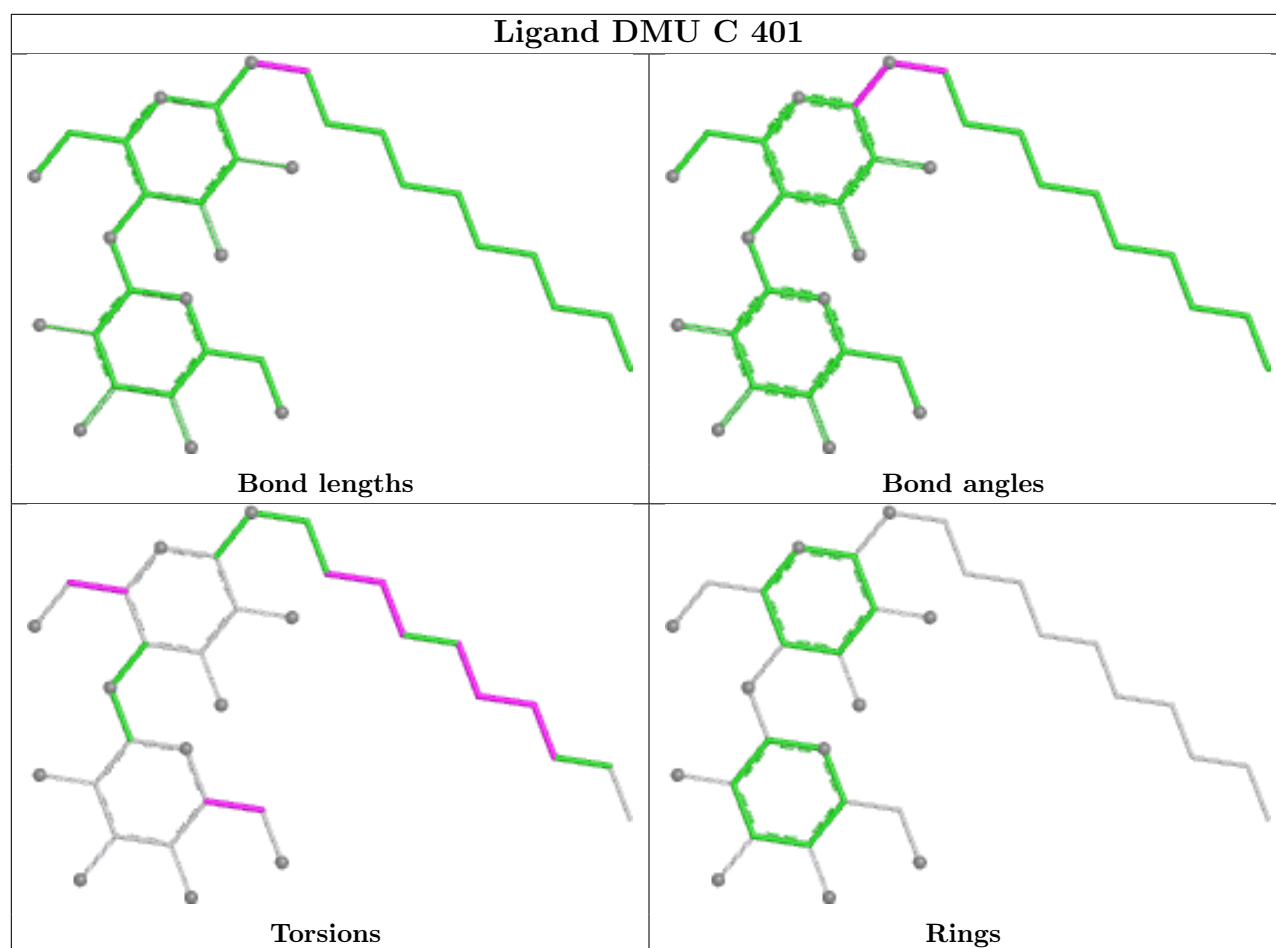












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	264/343 (76%)	-0.55	5 (1%) 66 64	13, 31, 60, 102	0
1	B	332/343 (96%)	-0.37	3 (0%) 81 81	17, 37, 82, 117	0
1	C	262/343 (76%)	-0.56	0 100 100	15, 34, 58, 74	0
1	D	331/343 (96%)	-0.28	8 (2%) 59 57	16, 38, 94, 126	0
All	All	1189/1372 (86%)	-0.43	16 (1%) 75 75	13, 35, 84, 126	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ASN	4.5
1	D	261	ALA	3.2
1	B	194	GLY	3.0
1	B	190	TYR	2.8
1	D	266	MET	2.7
1	D	263	ALA	2.7
1	A	192	ARG	2.6
1	D	264	GLY	2.6
1	D	265	ALA	2.5
1	A	164	GLY	2.5
1	A	193	ASN	2.5
1	D	262	GLY	2.3
1	A	190	TYR	2.2
1	D	269	VAL	2.1
1	D	211	GLY	2.0
1	A	194	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

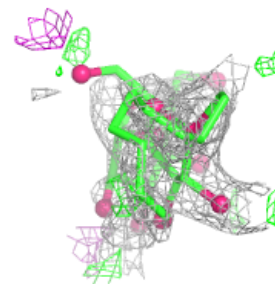
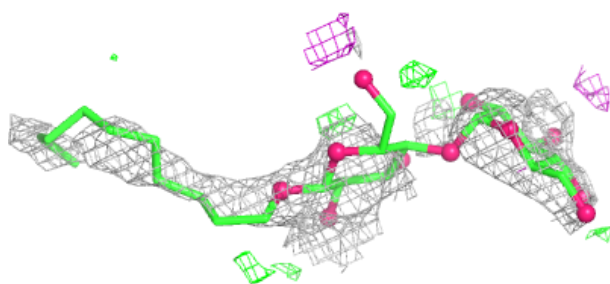
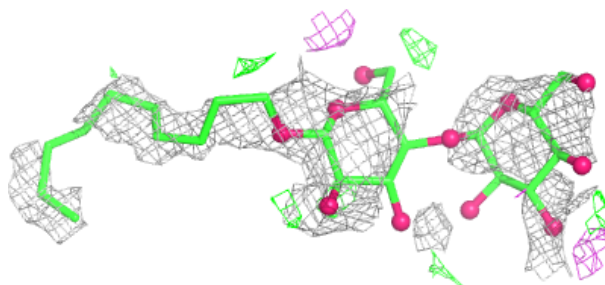
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	DMU	A	501	33/33	0.79	0.21	84,112,120,121	0
2	DMU	B	501	33/33	0.80	0.18	65,88,97,97	0
2	DMU	C	401	33/33	0.87	0.12	41,64,72,72	0
2	DMU	B	502	33/33	0.88	0.13	50,65,72,73	0
2	DMU	D	401	33/33	0.90	0.11	43,63,67,71	0
2	DMU	A	502	33/33	0.91	0.10	41,64,70,71	0

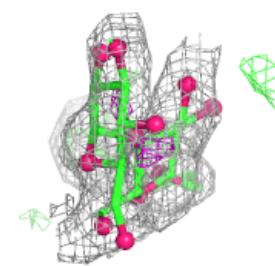
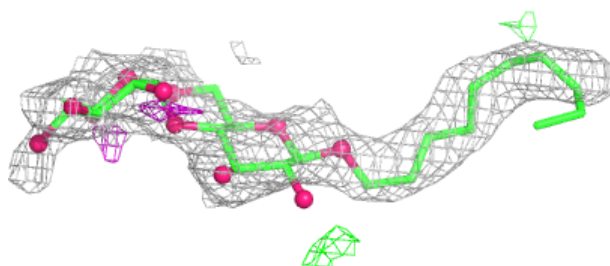
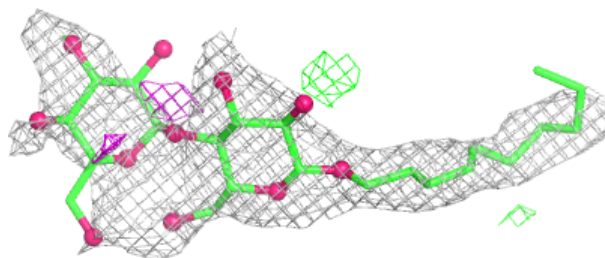
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU A 501:

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

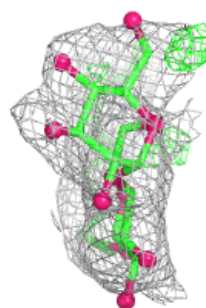
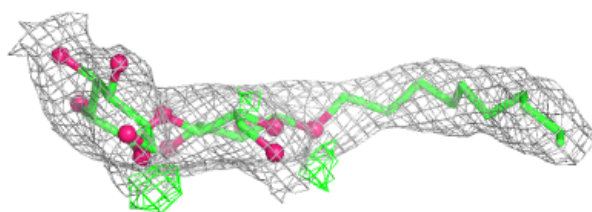
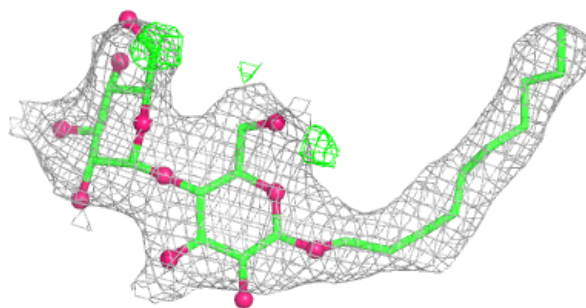
**Electron density around DMU B 501:**

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

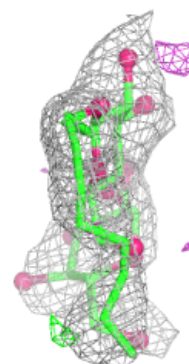
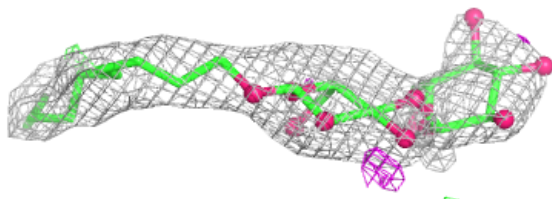
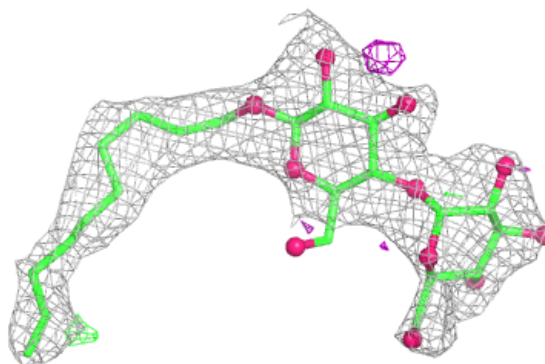


Electron density around DMU C 401:

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

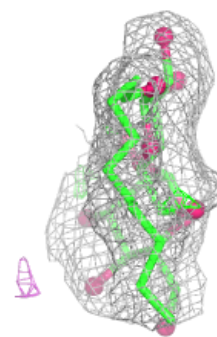
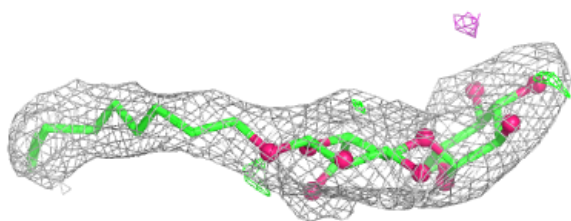
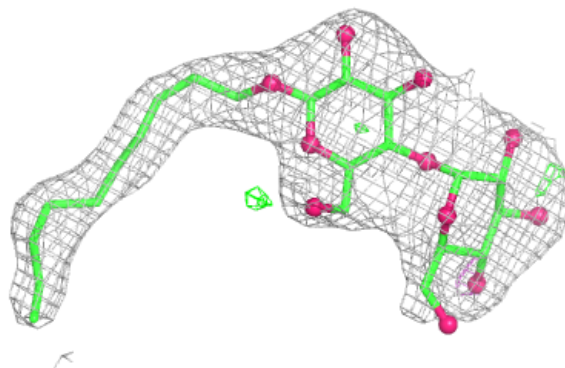
**Electron density around DMU B 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

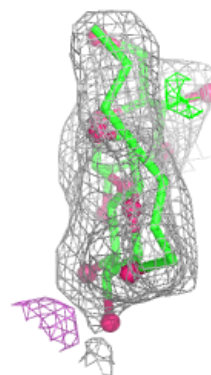
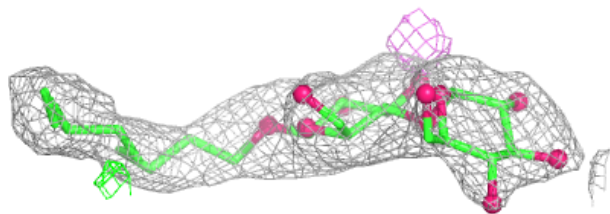
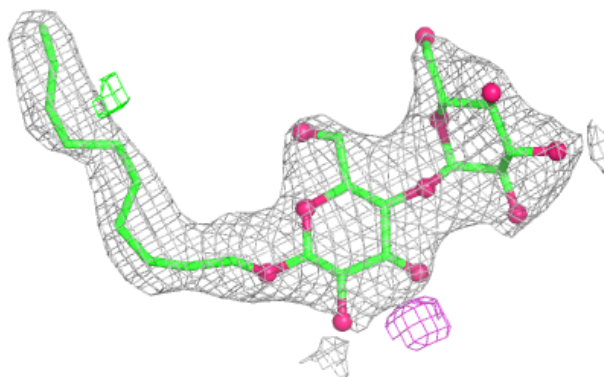


Electron density around DMU D 401:

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

**Electron density around DMU A 502:**

$2mF_o-DF_c$ (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.