



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:25 PM UTC

PDB ID : 5B0J / pdb_00005b0j
Title : Structure of MoeN5-Sso7d fusion protein in complex with beta-undecyl maltoside
Authors : Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.; Oldfield, E.O.
Deposited on : 2015-10-30
Resolution : 2.50 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

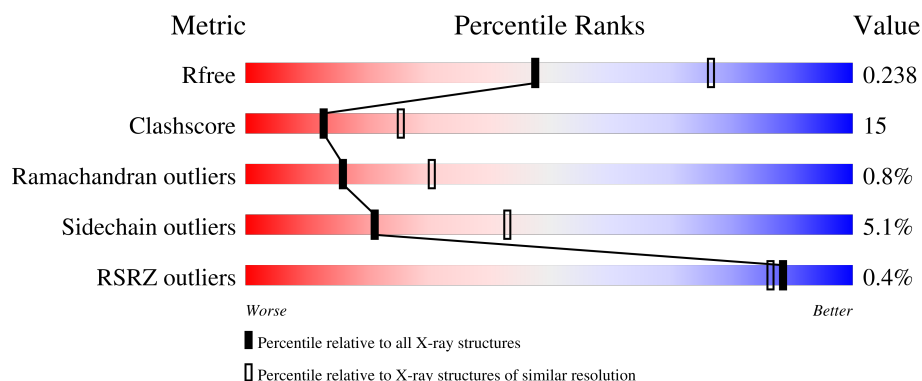
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	B	343	
1	C	343	
1	D	343	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9914 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	269	Total	C	N	O	S	0	0	0
			2056	1268	385	392	11			
1	D	333	Total	C	N	O	S	0	0	0
			2544	1579	466	485	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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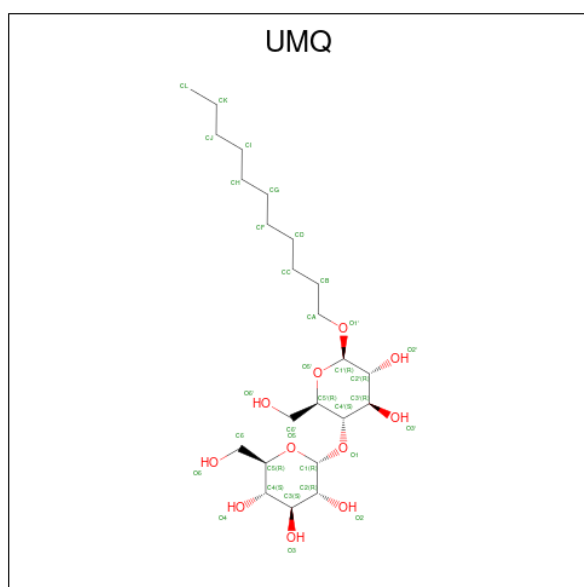
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP 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 UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			34	23	11		
2	D	1	Total	C	O	0	0
			34	23	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		

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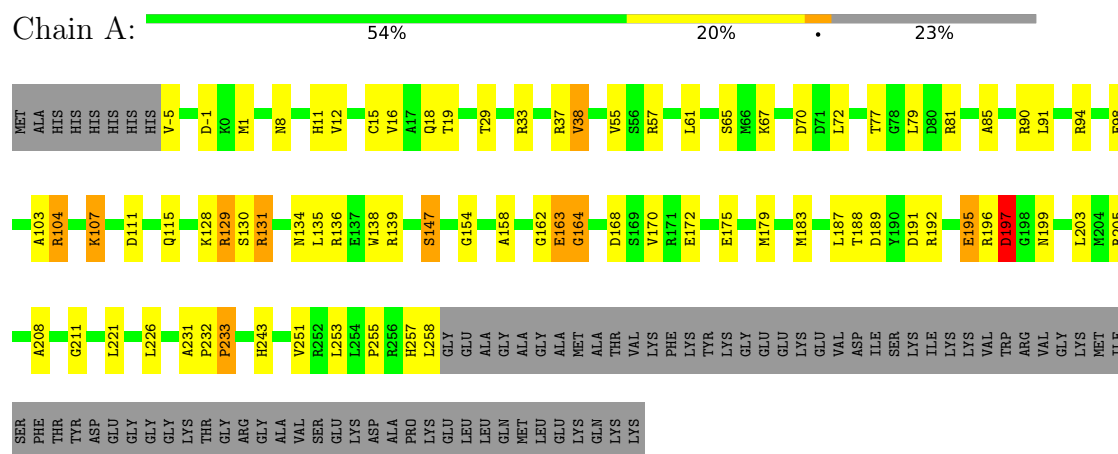
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	191	Total 191	O 191	0	0
3	C	146	Total 146	O 146	0	0
3	D	191	Total 191	O 191	0	0

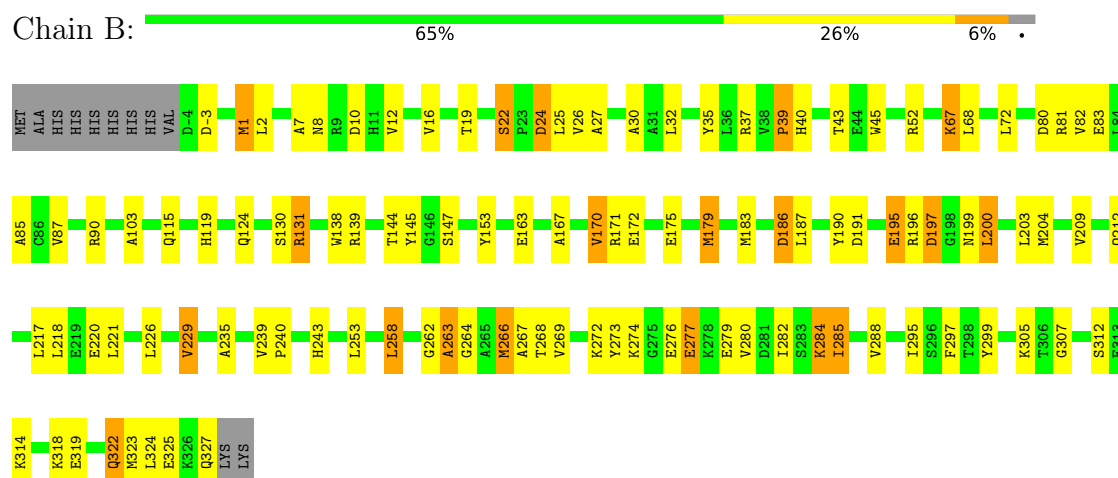
3 Residue-property plots

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.

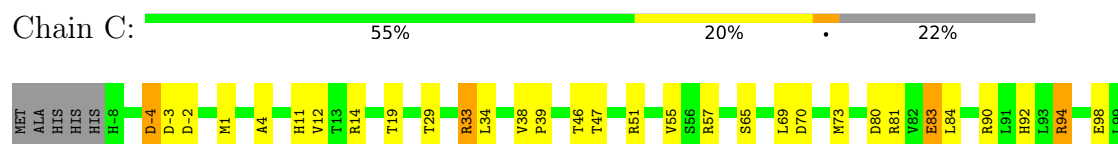
• Molecule 1: MoeN5,DNA-binding protein 7d

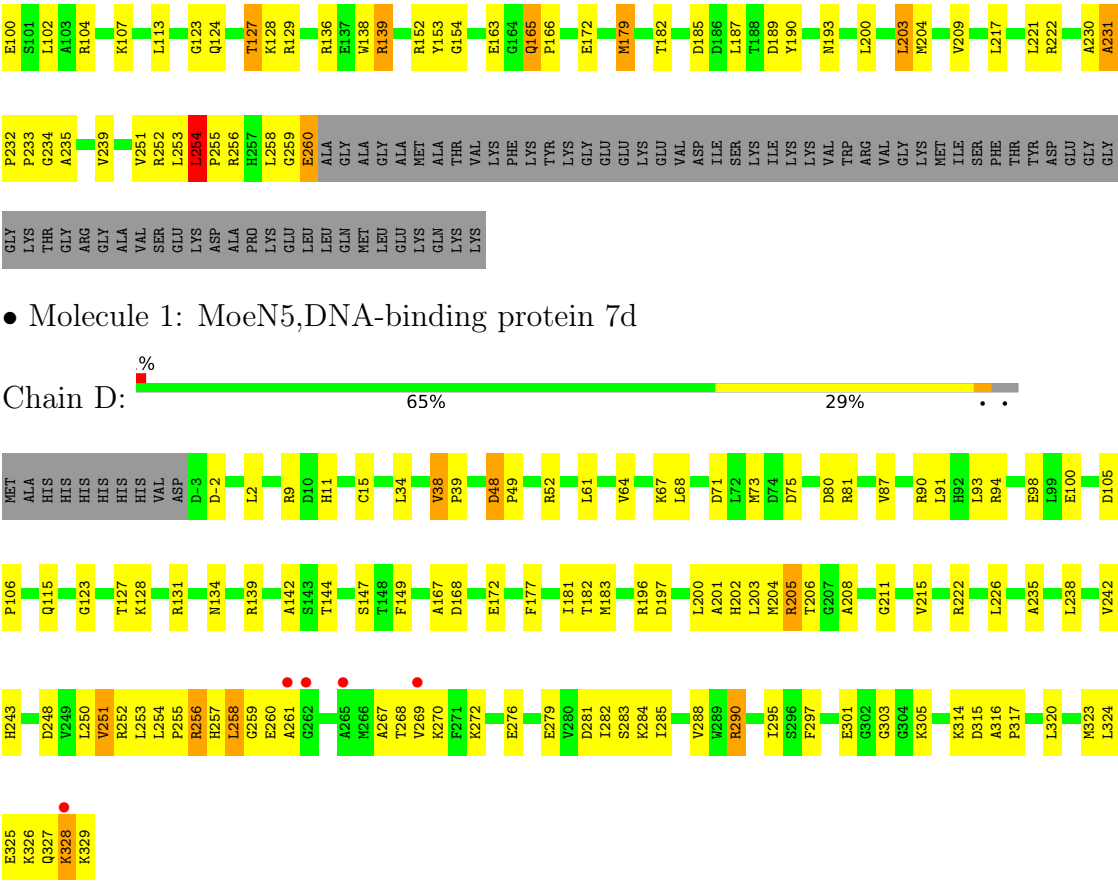


• Molecule 1: MoeN5,DNA-binding protein 7d



• Molecule 1: MoeN5,DNA-binding protein 7d





● Molecule 1: MoeN5,DNA-binding protein 7d

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.78Å 217.79Å 104.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 25.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (25.00-2.50) 96.0 (25.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.238 0.174 , 0.238	Depositor DCC
R_{free} test set	2661 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9914	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: UMQ

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	1.10	1/2045 (0.0%)	1.23	15/2780 (0.5%)
1	B	1.06	1/2572 (0.0%)	1.25	19/3478 (0.5%)
1	C	1.10	1/2091 (0.0%)	1.29	20/2842 (0.7%)
1	D	1.03	0/2583	1.26	14/3489 (0.4%)
All	All	1.07	3/9291 (0.0%)	1.26	68/12589 (0.5%)

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	B	0	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	SD-CE	9.27	2.02	1.79
1	A	55	VAL	CA-CB	-5.28	1.47	1.54
1	C	73	MET	SD-CE	-5.26	1.66	1.79

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-2	ASP	N-CA-C	-13.28	96.42	112.89
1	C	163	GLU	N-CA-C	8.88	123.10	110.23
1	C	104	ARG	N-CA-C	-8.43	102.05	111.07
1	D	326	LYS	N-CA-C	-8.34	103.62	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	GLU	CB-CA-C	-8.08	98.13	110.90
1	B	285	ILE	N-CA-C	7.84	120.14	108.54
1	B	264	GLY	N-CA-C	-7.81	103.93	114.95
1	D	147	SER	N-CA-C	7.40	118.99	111.07
1	B	163	GLU	N-CA-C	7.33	120.83	110.50
1	B	103	ALA	N-CA-C	7.32	120.19	110.53
1	A	104	ARG	N-CA-C	-7.02	103.31	110.97
1	A	253	LEU	N-CA-C	6.99	119.93	111.40
1	B	190	TYR	N-CA-C	-6.92	103.73	111.28
1	C	251	VAL	N-CA-C	6.64	118.61	111.58
1	A	163	GLU	N-CA-C	6.58	124.82	110.80
1	D	208	ALA	N-CA-C	-6.55	105.11	113.23
1	C	47	THR	N-CA-C	6.54	119.73	111.69
1	C	231	ALA	CA-C-N	6.47	127.05	120.38
1	C	231	ALA	C-N-CA	6.47	127.05	120.38
1	B	297	PHE	N-CA-C	6.46	118.03	108.60
1	C	203	LEU	N-CA-C	-6.42	104.38	111.82
1	C	235	ALA	CA-C-N	6.38	126.13	119.05
1	C	235	ALA	C-N-CA	6.38	126.13	119.05
1	B	170	VAL	N-CA-C	-6.34	104.33	110.42
1	A	131	ARG	N-CA-C	6.26	119.07	110.24
1	C	33	ARG	N-CA-C	6.19	118.57	111.02
1	D	235	ALA	N-CA-C	-6.15	98.11	108.94
1	D	257	HIS	N-CA-C	-5.94	106.00	113.72
1	A	103	ALA	N-CA-C	5.91	118.39	110.35
1	B	22	SER	CA-C-N	-5.82	113.77	119.64
1	B	22	SER	C-N-CA	-5.82	113.77	119.64
1	D	48	ASP	CA-C-N	5.80	125.66	119.28
1	D	48	ASP	C-N-CA	5.80	125.66	119.28
1	B	24	ASP	CB-CA-C	-5.80	98.88	110.42
1	B	312	SER	N-CA-C	-5.79	102.33	110.50
1	A	251	VAL	N-CA-C	5.79	117.71	111.58
1	D	11	HIS	N-CA-C	-5.76	105.08	111.36
1	B	258	LEU	N-CA-C	-5.76	104.25	112.13
1	D	52	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	C	-4	ASP	N-CA-C	-5.68	99.53	108.63
1	D	250	LEU	N-CA-C	5.61	117.40	111.28
1	B	220	GLU	N-CA-C	-5.61	105.07	111.07
1	C	138	TRP	N-CA-C	-5.60	105.17	111.28
1	B	130	SER	N-CA-C	5.56	118.30	108.24
1	A	154	GLY	N-CA-C	-5.56	106.05	112.50
1	A	170	VAL	N-CA-C	-5.50	105.01	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	LEU	N-CA-C	-5.49	105.30	111.28
1	A	195	GLU	N-CA-C	5.43	117.59	108.73
1	B	253	LEU	N-CA-C	5.41	118.00	111.40
1	C	193	ASN	CB-CA-C	-5.34	100.70	109.99
1	C	4	ALA	N-CA-C	-5.31	105.39	111.07
1	D	167	ALA	N-CA-C	5.30	122.09	110.80
1	D	256	ARG	N-CA-C	5.30	122.09	110.80
1	B	30	ALA	N-CA-C	-5.30	106.77	113.18
1	B	195	GLU	N-CA-C	5.24	118.09	109.76
1	A	70	ASP	N-CA-C	-5.23	105.48	111.07
1	B	277	GLU	N-CA-C	-5.19	101.23	109.59
1	A	147	SER	N-CA-C	5.18	116.61	111.07
1	D	290	ARG	N-CA-C	5.17	117.91	109.59
1	A	197	ASP	N-CA-C	5.16	117.65	109.96
1	C	254	LEU	N-CA-C	5.16	121.21	109.81
1	C	239	VAL	CA-C-N	-5.09	114.42	119.56
1	C	239	VAL	C-N-CA	-5.09	114.42	119.56
1	B	200	LEU	N-CA-C	5.06	118.23	111.75
1	A	231	ALA	N-CA-C	-5.03	103.14	110.08
1	A	38	VAL	CA-C-N	-5.02	114.44	119.56
1	A	38	VAL	C-N-CA	-5.02	114.44	119.56
1	C	154	GLY	N-CA-C	-5.02	106.68	112.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	153	TYR	Sidechain
1	C	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	58	0
1	B	2533	0	2532	80	0
1	C	2056	0	2026	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2544	0	2554	87	0
2	C	34	0	44	3	0
2	D	34	0	44	5	0
3	A	172	0	0	5	0
3	B	191	0	0	3	0
3	C	146	0	0	4	0
3	D	191	0	0	2	0
All	All	9914	0	9196	278	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 15.

All (278) 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:1:MET:SD	1:B:1:MET:CE	2.02	1.47
1:D:325:GLU:HA	1:D:329:LYS:HB3	1.48	0.96
1:B:10:ASP:HB3	3:B:471:HOH:O	1.68	0.93
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.33	0.91
1:C:69:LEU:HD23	2:C:401:UMQ:HL2	1.53	0.89
1:B:179:MET:HG2	1:B:221:LEU:HD11	1.55	0.87
1:D:268:THR:HG22	1:D:281:ASP:HA	1.58	0.86
1:B:131:ARG:HG3	1:B:197:ASP:HB3	1.60	0.83
1:D:168:ASP:O	1:D:172:GLU:HG3	1.78	0.83
1:D:75:ASP:HB2	1:D:81:ARG:NH1	1.95	0.82
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.26	0.81
1:A:11:HIS:CE1	1:A:57:ARG:HH11	2.00	0.80
1:B:139:ARG:HG3	1:B:179:MET:HE1	1.64	0.80
1:C:81:ARG:HD3	1:D:81:ARG:NH2	1.96	0.80
1:D:281:ASP:HB3	1:D:284:LYS:HZ3	1.48	0.78
1:C:187:LEU:HD21	1:C:204:MET:HE1	1.66	0.77
1:D:325:GLU:CB	1:D:329:LYS:HD3	2.16	0.76
1:C:69:LEU:CD2	2:C:401:UMQ:HL2	2.16	0.76
1:C:203:LEU:HB3	1:C:209:VAL:HG23	1.68	0.76
1:D:281:ASP:HB3	1:D:284:LYS:NZ	2.01	0.76
1:B:1:MET:HG2	1:B:37:ARG:NH2	2.03	0.73
1:C:259:GLY:O	1:C:260:GLU:HB2	1.89	0.73
1:D:48:ASP:OD1	1:D:49:PRO:HD2	1.89	0.72
1:C:139:ARG:HG2	1:C:179:MET:HE1	1.72	0.71
1:A:11:HIS:CE1	1:A:57:ARG:NH1	2.57	0.71
1:A:77:THR:OG1	1:A:79:LEU:HD12	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.58	0.69
1:B:179:MET:HG2	1:B:221:LEU:CD1	2.22	0.69
1:B:1:MET:HG2	1:B:37:ARG:HH21	1.56	0.69
1:D:38:VAL:HG12	1:D:39:PRO:HD3	1.75	0.68
1:B:267:ALA:HB3	1:B:282:ILE:HG13	1.75	0.68
1:D:269:VAL:HG22	1:D:317:PRO:HG3	1.74	0.68
1:B:285:ILE:HG22	1:B:323:MET:HE1	1.75	0.68
1:A:232:PRO:HA	1:A:233:PRO:C	2.18	0.68
1:C:46:THR:HG21	1:C:51:ARG:HG2	1.77	0.67
1:B:22:SER:O	1:B:26:VAL:HG23	1.95	0.66
1:D:272:LYS:HG2	1:D:276:GLU:O	1.95	0.66
1:D:325:GLU:HB3	1:D:329:LYS:HD3	1.78	0.66
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.11	0.65
1:D:254:LEU:HG	1:D:258:LEU:HD13	1.78	0.64
1:C:1:MET:SD	1:C:1:MET:C	2.81	0.64
1:D:270:LYS:HG3	1:D:279:GLU:HG3	1.80	0.64
1:B:273:TYR:CE2	1:B:274:LYS:HD2	2.33	0.63
1:D:269:VAL:HG22	1:D:317:PRO:CG	2.28	0.63
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.81	0.62
1:A:197:ASP:HB2	3:A:441:HOH:O	1.97	0.62
1:B:203:LEU:HB3	1:B:209:VAL:HG23	1.79	0.62
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.82	0.61
1:B:200:LEU:HG	1:B:204:MET:HE2	1.81	0.61
1:D:325:GLU:HB2	1:D:329:LYS:HD3	1.82	0.61
1:B:186:ASP:OD1	1:B:200:LEU:N	2.32	0.61
1:B:267:ALA:HB3	1:B:282:ILE:CG1	2.30	0.61
1:A:94:ARG:HD2	1:A:98:GLU:OE2	2.01	0.60
1:A:164:GLY:N	3:A:403:HOH:O	2.35	0.60
1:D:238:LEU:O	1:D:242:VAL:HG23	2.01	0.60
1:C:127:THR:HG22	3:C:581:HOH:O	2.01	0.60
1:D:90:ARG:NH1	1:D:94:ARG:HB2	2.17	0.60
1:D:295:ILE:HD12	1:D:324:LEU:HD22	1.83	0.60
1:C:124:GLN:HE21	2:C:401:UMQ:HG2	1.66	0.59
1:B:19:THR:HG22	1:B:19:THR:O	2.02	0.59
1:D:329:LYS:OXT	1:D:329:LYS:HG2	2.02	0.59
1:A:61:LEU:HD13	1:A:94:ARG:HG3	1.83	0.59
1:A:107:LYS:O	1:A:107:LYS:HD3	2.03	0.59
1:D:252:ARG:O	1:D:255:PRO:HD2	2.02	0.59
1:B:12:VAL:O	1:B:16:VAL:HG23	2.02	0.58
1:D:269:VAL:HG21	1:D:320:LEU:HD22	1.85	0.58
1:D:149:PHE:CE1	2:D:401:UMQ:HD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:O	1:A:172:GLU:HG3	2.03	0.58
1:B:319:GLU:HA	1:B:322:GLN:NE2	2.19	0.58
1:B:139:ARG:HG3	1:B:179:MET:CE	2.34	0.57
1:D:211:GLY:O	1:D:215:VAL:HG23	2.05	0.57
1:A:11:HIS:CD2	1:A:57:ARG:HD2	2.40	0.57
1:C:187:LEU:HD21	1:C:204:MET:CE	2.33	0.57
1:C:-3:ASP:O	1:C:-2:ASP:C	2.49	0.56
1:D:48:ASP:OD1	1:D:49:PRO:CD	2.53	0.56
1:B:2:LEU:HD23	1:B:37:ARG:HH12	1.69	0.56
1:C:38:VAL:HG12	1:C:39:PRO:HD3	1.87	0.56
1:C:81:ARG:HD3	1:D:81:ARG:CZ	2.35	0.56
1:C:123:GLY:O	1:C:127:THR:HG23	2.06	0.56
1:B:139:ARG:CG	1:B:179:MET:HE1	2.35	0.56
1:C:254:LEU:HD22	1:C:258:LEU:HG	1.88	0.56
1:B:258:LEU:HD13	1:B:262:GLY:HA2	1.88	0.56
1:C:90:ARG:HD3	1:C:90:ARG:C	2.31	0.56
1:A:192:ARG:HD2	1:C:80:ASP:HB2	1.88	0.55
1:C:94:ARG:HD2	1:C:98:GLU:OE2	2.07	0.55
1:D:288:VAL:HG22	1:D:297:PHE:HB3	1.88	0.55
1:D:34:LEU:HD21	1:D:181:ILE:HG21	1.87	0.55
1:D:252:ARG:NH1	1:D:253:LEU:HD21	2.21	0.55
1:B:183:MET:HE1	1:B:218:LEU:HG	1.88	0.55
1:B:266:MET:HE3	1:B:266:MET:HA	1.88	0.55
1:A:33:ARG:HG2	3:A:404:HOH:O	2.06	0.55
1:B:45:TRP:CE3	1:B:170:VAL:HG22	2.41	0.55
1:C:14:ARG:HH21	1:C:14:ARG:HG3	1.72	0.54
1:A:65:SER:HB2	1:A:91:LEU:HB2	1.89	0.54
1:D:123:GLY:O	1:D:127:THR:HG23	2.08	0.54
1:C:11:HIS:CD2	1:C:57:ARG:HD2	2.42	0.54
1:C:259:GLY:O	1:C:260:GLU:CB	2.54	0.54
1:A:192:ARG:HA	3:A:434:HOH:O	2.07	0.54
1:A:163:GLU:HA	1:A:163:GLU:OE1	2.08	0.54
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.72	0.54
1:A:77:THR:CB	1:A:79:LEU:HD12	2.38	0.53
1:B:203:LEU:HB3	1:B:209:VAL:CG2	2.38	0.53
1:B:319:GLU:HA	1:B:322:GLN:HE21	1.73	0.53
1:C:12:VAL:CG1	1:C:29:THR:HG21	2.37	0.53
1:A:33:ARG:HG2	1:A:33:ARG:NH1	2.24	0.53
1:B:32:LEU:HB3	1:B:35:TYR:HD2	1.74	0.52
1:D:259:GLY:C	1:D:260:GLU:HG2	2.34	0.52
1:A:111:ASP:O	1:A:115:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:MET:O	1:B:327:GLN:HB2	2.10	0.52
1:D:94:ARG:HD2	1:D:98:GLU:OE2	2.09	0.52
1:D:105:ASP:OD2	1:D:106:PRO:HD2	2.10	0.52
1:A:203:LEU:HD22	1:A:208:ALA:HB3	1.91	0.52
1:B:131:ARG:NH1	1:B:131:ARG:CG	2.73	0.52
1:A:129:ARG:HG3	1:A:129:ARG:NH1	2.23	0.51
1:A:131:ARG:HG3	1:A:197:ASP:HB3	1.92	0.51
1:A:232:PRO:HA	1:A:233:PRO:O	2.10	0.51
1:B:318:LYS:HB2	1:B:319:GLU:OE2	2.10	0.51
1:D:251:VAL:HG23	1:D:251:VAL:O	2.09	0.51
1:A:147:SER:O	1:A:175:GLU:HG2	2.10	0.51
1:C:33:ARG:HG2	1:C:33:ARG:HH11	1.74	0.51
1:D:290:ARG:HE	1:D:324:LEU:HD21	1.76	0.51
1:D:222:ARG:NH1	1:D:243:HIS:HD2	2.02	0.51
1:A:192:ARG:HG3	3:A:405:HOH:O	2.12	0.50
1:B:269:VAL:O	1:B:279:GLU:HA	2.11	0.50
1:B:272:LYS:HG2	1:B:276:GLU:O	2.11	0.50
1:A:196:ARG:HD2	1:A:196:ARG:N	2.26	0.50
1:B:90:ARG:HD3	1:B:90:ARG:C	2.36	0.50
1:D:323:MET:O	1:D:327:GLN:HB2	2.12	0.50
1:A:138:TRP:CH2	1:A:183:MET:HG2	2.47	0.50
1:B:266:MET:HE2	1:B:267:ALA:N	2.27	0.50
1:D:61:LEU:CD1	1:D:94:ARG:HG3	2.41	0.50
1:D:87:VAL:O	1:D:91:LEU:HG	2.11	0.50
1:B:35:TYR:CE2	1:B:67:LYS:HG3	2.47	0.49
1:B:131:ARG:HH11	1:B:131:ARG:CG	2.10	0.49
1:A:205:ARG:HD3	1:D:131:ARG:HD3	1.94	0.49
1:B:22:SER:HB3	1:B:83:GLU:OE2	2.12	0.49
1:B:295:ILE:CD1	1:B:324:LEU:HD11	2.43	0.49
1:C:12:VAL:HG12	1:C:29:THR:HG21	1.93	0.49
1:D:269:VAL:HG23	1:D:282:ILE:CD1	2.43	0.49
1:A:67:LYS:HD2	1:A:67:LYS:O	2.13	0.49
1:B:267:ALA:HB2	1:B:319:GLU:OE1	2.13	0.49
1:D:281:ASP:CB	1:D:284:LYS:NZ	2.74	0.49
1:B:138:TRP:CH2	1:B:183:MET:HG2	2.48	0.49
1:B:229:VAL:HG13	1:B:235:ALA:O	2.13	0.49
1:C:-4:ASP:CG	1:C:1:MET:HE2	2.38	0.49
1:D:128:LYS:HE2	2:D:401:UMQ:O6'	2.13	0.48
1:D:202:HIS:O	1:D:206:THR:HG22	2.13	0.48
1:D:301:GLU:O	1:D:301:GLU:HG3	2.12	0.48
1:A:1:MET:SD	1:A:37:ARG:HD3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:O	1:A:187:LEU:HG	2.13	0.48
1:B:147:SER:HB3	1:B:175:GLU:HB3	1.95	0.48
1:D:295:ILE:CD1	1:D:324:LEU:HD22	2.43	0.48
1:A:104:ARG:NH1	1:A:158:ALA:O	2.46	0.48
1:D:149:PHE:CZ	2:D:401:UMQ:HD1	2.48	0.48
1:A:195:GLU:C	1:A:196:ARG:HD2	2.38	0.48
1:C:70:ASP:OD2	1:C:128:LYS:NZ	2.47	0.48
1:A:196:ARG:O	1:A:199:ASN:HB3	2.13	0.47
1:B:272:LYS:HA	1:B:276:GLU:O	2.13	0.47
1:C:38:VAL:N	1:C:39:PRO:CD	2.77	0.47
1:C:203:LEU:HB3	1:C:209:VAL:CG2	2.41	0.47
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.79	0.47
1:B:187:LEU:HD21	1:B:204:MET:CE	2.44	0.47
1:D:269:VAL:HG23	1:D:282:ILE:HD11	1.96	0.47
1:A:81:ARG:NH2	1:B:72:LEU:O	2.47	0.47
1:B:179:MET:HE3	1:B:217:LEU:HD11	1.96	0.47
1:C:165:GLN:HE21	1:C:165:GLN:HB3	1.48	0.47
1:A:81:ARG:NH2	1:B:72:LEU:HD12	2.30	0.47
1:D:196:ARG:O	1:D:197:ASP:C	2.57	0.46
1:D:327:GLN:O	1:D:329:LYS:N	2.49	0.46
1:A:104:ARG:HE	1:A:162:GLY:HA2	1.80	0.46
1:B:80:ASP:OD1	1:B:82:VAL:HB	2.16	0.46
1:D:75:ASP:CB	1:D:81:ARG:NH1	2.75	0.46
1:D:115:GLN:NE2	3:D:502:HOH:O	2.37	0.46
1:A:12:VAL:O	1:A:16:VAL:HG23	2.14	0.46
1:A:15:CYS:O	1:A:19:THR:HG22	2.15	0.46
1:D:301:GLU:O	1:D:305:LYS:HB2	2.15	0.46
1:C:55:VAL:HG22	1:C:102:LEU:HD13	1.98	0.46
1:C:259:GLY:O	1:C:260:GLU:CD	2.59	0.46
1:A:195:GLU:N	1:A:196:ARG:NH1	2.64	0.46
1:B:37:ARG:NE	3:B:402:HOH:O	2.34	0.46
1:B:131:ARG:HG3	1:B:197:ASP:CB	2.40	0.46
1:D:134:ASN:OD1	1:D:134:ASN:C	2.59	0.46
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.98	0.46
1:B:226:LEU:HD11	1:B:243:HIS:CE1	2.51	0.46
1:D:75:ASP:OD2	1:D:81:ARG:HD2	2.16	0.46
1:C:230:ALA:O	1:C:231:ALA:C	2.60	0.45
1:A:107:LYS:HD3	1:A:107:LYS:C	2.42	0.45
1:C:189:ASP:O	1:C:190:TYR:C	2.57	0.45
1:D:201:ALA:HA	1:D:204:MET:HE2	1.98	0.45
1:B:195:GLU:C	1:B:196:ARG:HH11	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ARG:HG2	1:C:33:ARG:NH1	2.32	0.45
1:C:100:GLU:OE1	1:D:100:GLU:OE1	2.34	0.45
1:A:61:LEU:CD1	1:A:94:ARG:HG3	2.47	0.45
1:B:43:THR:HA	3:B:432:HOH:O	2.17	0.45
1:B:124:GLN:NE2	1:B:145:TYR:HB3	2.32	0.45
1:D:254:LEU:N	1:D:255:PRO:CD	2.80	0.45
1:D:314:LYS:C	1:D:316:ALA:H	2.24	0.45
1:C:166:PRO:HD3	1:C:233:PRO:HD2	1.99	0.45
1:D:327:GLN:HB3	1:D:328:LYS:H	1.45	0.45
1:B:273:TYR:O	1:B:276:GLU:HB2	2.17	0.44
1:D:281:ASP:OD2	1:D:283:SER:HB3	2.18	0.44
1:D:90:ARG:HD3	1:D:90:ARG:C	2.43	0.44
1:C:254:LEU:N	1:C:255:PRO:CD	2.81	0.44
1:D:205:ARG:NH2	1:D:256:ARG:HH21	2.14	0.44
1:D:267:ALA:O	1:D:282:ILE:HG12	2.17	0.44
2:D:401:UMQ:HB2	2:D:401:UMQ:HF2	1.79	0.44
1:C:136:ARG:NH1	3:C:507:HOH:O	2.50	0.44
1:D:9:ARG:HD2	3:D:553:HOH:O	2.17	0.44
1:D:282:ILE:C	1:D:284:LYS:H	2.26	0.44
1:C:83:GLU:O	1:C:84:LEU:C	2.60	0.44
1:A:179:MET:HG2	1:A:221:LEU:HD11	2.00	0.43
1:C:139:ARG:CG	1:C:179:MET:HE1	2.46	0.43
1:B:171:ARG:O	1:B:175:GLU:HG3	2.18	0.43
1:C:14:ARG:HH21	1:C:14:ARG:CG	2.31	0.43
1:C:172:GLU:HA	1:C:172:GLU:OE1	2.18	0.43
1:D:248:ASP:O	1:D:252:ARG:HB3	2.17	0.43
1:D:183:MET:HE3	1:D:200:LEU:HD21	2.01	0.43
1:D:177:PHE:CE1	1:D:181:ILE:HD11	2.54	0.43
1:C:152:ARG:HB2	3:C:501:HOH:O	2.19	0.43
1:A:90:ARG:NH1	1:A:94:ARG:HB2	2.33	0.43
1:B:68:LEU:HA	1:B:68:LEU:HD23	1.69	0.43
1:C:46:THR:CG2	1:C:51:ARG:HG2	2.45	0.43
1:C:51:ARG:HE	1:C:51:ARG:HB2	1.52	0.43
1:A:72:LEU:HD21	1:A:85:ALA:HB2	2.00	0.43
1:C:182:THR:O	1:C:185:ASP:HB2	2.19	0.43
1:C:200:LEU:HG	1:C:204:MET:HE2	2.01	0.43
1:C:81:ARG:HH21	1:C:81:ARG:HB2	1.83	0.43
1:C:222:ARG:HD2	3:C:537:HOH:O	2.19	0.43
1:C:231:ALA:HA	1:C:232:PRO:HD3	1.70	0.43
1:D:67:LYS:HE3	1:D:71:ASP:OD1	2.19	0.43
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:HA	1:B:280:VAL:O	2.19	0.42
1:A:195:GLU:N	1:A:196:ARG:HH11	2.18	0.42
1:A:188:THR:CG2	1:A:192:ARG:NH1	2.82	0.42
1:A:188:THR:HG21	1:A:192:ARG:NH1	2.35	0.42
1:B:-3:ASP:O	1:B:1:MET:HB2	2.19	0.42
1:B:24:ASP:O	1:B:27:ALA:N	2.51	0.42
1:B:277:GLU:HA	1:B:277:GLU:OE2	2.20	0.42
1:C:65:SER:OG	1:C:92:HIS:HB2	2.19	0.42
1:D:75:ASP:HB2	1:D:81:ARG:HH12	1.77	0.42
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.87	0.42
1:C:81:ARG:CD	1:D:81:ARG:NH2	2.76	0.42
1:B:40:HIS:CE1	1:B:52:ARG:NH2	2.88	0.42
1:B:72:LEU:HD21	1:B:85:ALA:HB2	2.01	0.42
1:D:149:PHE:CD1	2:D:401:UMQ:HD1	2.55	0.42
1:A:255:PRO:C	1:A:257:HIS:N	2.77	0.42
1:B:119:HIS:CE1	1:B:144:THR:HG22	2.55	0.42
1:B:183:MET:CE	1:B:218:LEU:HG	2.50	0.42
1:D:64:VAL:O	1:D:68:LEU:HG	2.19	0.42
1:D:226:LEU:HD23	1:D:226:LEU:HA	1.89	0.42
1:B:212:GLN:HB2	1:B:263:ALA:O	2.20	0.42
1:C:80:ASP:OD2	1:C:80:ASP:C	2.61	0.42
1:B:80:ASP:O	1:B:81:ARG:C	2.60	0.41
1:C:179:MET:HG2	1:C:221:LEU:HD11	2.01	0.41
1:C:258:LEU:HD23	1:C:258:LEU:HA	1.70	0.41
1:D:142:ALA:HB1	1:D:182:THR:HG21	2.01	0.41
1:D:2:LEU:HA	1:D:2:LEU:HD23	1.84	0.41
1:D:252:ARG:HH12	1:D:253:LEU:HD21	1.85	0.41
1:C:129:ARG:HH21	1:D:80:ASP:CG	2.28	0.41
1:D:203:LEU:HA	1:D:206:THR:HG22	2.01	0.41
1:A:134:ASN:O	1:A:135:LEU:C	2.63	0.41
1:D:267:ALA:C	1:D:282:ILE:HG12	2.46	0.41
1:A:-5:VAL:HG13	1:A:-1:ASP:HB2	2.01	0.41
1:A:8:ASN:O	1:A:12:VAL:HG23	2.20	0.41
1:B:16:VAL:HG13	1:B:87:VAL:HG11	2.02	0.41
1:C:-4:ASP:HB3	1:C:1:MET:CE	2.51	0.41
1:C:12:VAL:HG11	1:C:29:THR:CG2	2.51	0.41
1:B:39:PRO:O	1:B:43:THR:HG23	2.20	0.41
1:B:299:TYR:O	1:B:307:GLY:N	2.51	0.41
1:C:113:LEU:HB3	1:D:93:LEU:HD22	2.02	0.41
1:A:211:GLY:HA3	1:A:258:LEU:HD13	2.03	0.40
1:A:226:LEU:HD11	1:A:243:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ALA:O	1:B:8:ASN:C	2.62	0.40
1:B:24:ASP:HB2	1:B:25:LEU:H	1.71	0.40
1:C:252:ARG:NH1	1:C:253:LEU:HD21	2.35	0.40
1:A:134:ASN:OD1	1:A:136:ARG:HB3	2.22	0.40
1:D:255:PRO:O	1:D:258:LEU:HB2	2.21	0.40
1:B:322:GLN:HE21	1:B:322:GLN:HB2	1.58	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%)	252 (96%)	8 (3%)	2 (1%)	16	31
1	B	330/343 (96%)	307 (93%)	20 (6%)	3 (1%)	14	27
1	C	267/343 (78%)	259 (97%)	7 (3%)	1 (0%)	30	49
1	D	331/343 (96%)	303 (92%)	24 (7%)	4 (1%)	10	20
All	All	1190/1372 (87%)	1121 (94%)	59 (5%)	10 (1%)	16	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	261	ALA
1	B	263	ALA
1	D	303	GLY
1	D	328	LYS
1	B	305	LYS
1	A	233	PRO
1	D	315	ASP
1	A	164	GLY
1	C	234	GLY

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Mol	Chain	Res	Type
1	B	167	ALA

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%)	197 (95%)	11 (5%)	20	42
1	B	260/270 (96%)	243 (94%)	17 (6%)	15	32
1	C	212/270 (78%)	201 (95%)	11 (5%)	21	42
1	D	261/270 (97%)	252 (97%)	9 (3%)	32	60
All	All	941/1080 (87%)	893 (95%)	48 (5%)	21	43

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	29	THR
1	A	38	VAL
1	A	107	LYS
1	A	128	LYS
1	A	129	ARG
1	A	130	SER
1	A	139	ARG
1	A	189	ASP
1	A	191	ASP
1	A	197	ASP
1	B	39	PRO
1	B	67	LYS
1	B	115	GLN
1	B	131	ARG
1	B	172	GLU
1	B	179	MET
1	B	186	ASP
1	B	191	ASP
1	B	197	ASP

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Mol	Chain	Res	Type
1	B	199	ASN
1	B	229	VAL
1	B	266	MET
1	B	284	LYS
1	B	288	VAL
1	B	314	LYS
1	B	322	GLN
1	B	325	GLU
1	C	19	THR
1	C	34	LEU
1	C	94	ARG
1	C	107	LYS
1	C	127	THR
1	C	139	ARG
1	C	165	GLN
1	C	179	MET
1	C	254	LEU
1	C	256	ARG
1	C	260	GLU
1	D	15	CYS
1	D	38	VAL
1	D	73	MET
1	D	139	ARG
1	D	144	THR
1	D	205	ARG
1	D	251	VAL
1	D	258	LEU
1	D	285	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	18	GLN
1	A	115	GLN
1	B	8	ASN
1	B	11	HIS
1	B	18	GLN
1	B	40	HIS
1	B	124	GLN
1	B	202	HIS
1	B	322	GLN

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Mol	Chain	Res	Type
1	C	165	GLN
1	D	199	ASN
1	D	243	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	UMQ	D	401	-	35,35,35	0.97	1 (2%)	46,46,46	0.81	1 (2%)
2	UMQ	C	401	-	35,35,35	0.82	2 (5%)	46,46,46	0.88	2 (4%)

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	UMQ	D	401	-	-	9/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMQ	C	401	-	-	7/20/60/60	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	UMQ	O1'-CA	4.32	1.54	1.43
2	C	401	UMQ	O1'-CA	3.13	1.51	1.43
2	C	401	UMQ	O5-C1	2.02	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	UMQ	CA-O1'-C1'	-2.81	108.89	113.68
2	C	401	UMQ	C3-C4-C5	-2.61	105.51	110.23
2	C	401	UMQ	CA-O1'-C1'	-2.19	109.94	113.68

There are no chirality outliers.

All (16) torsion outliers are listed below:

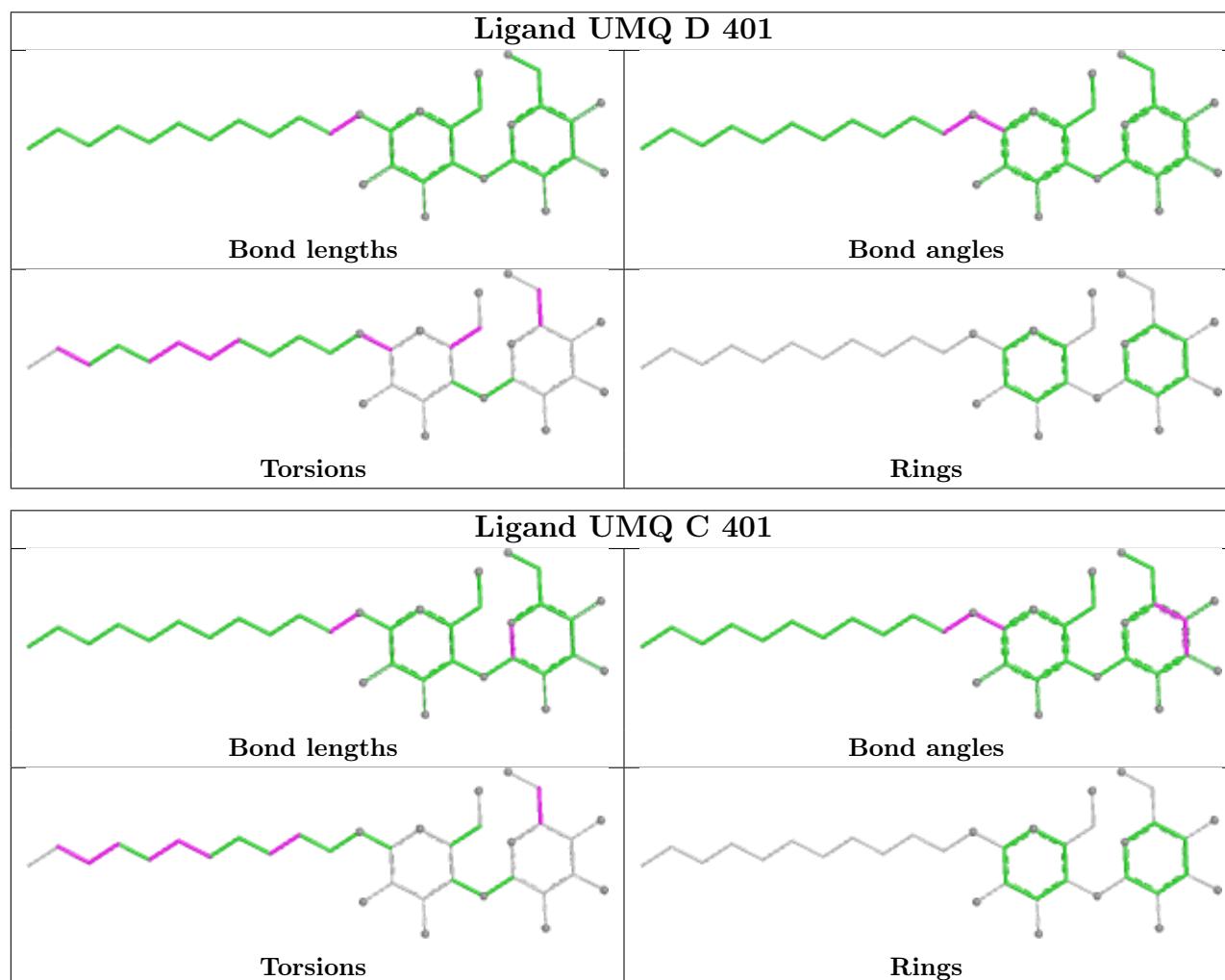
Mol	Chain	Res	Type	Atoms
2	D	401	UMQ	O5'-C5'-C6'-O6'
2	D	401	UMQ	CF-CG-CH-CI
2	D	401	UMQ	C4'-C5'-C6'-O6'
2	C	401	UMQ	C4-C5-C6-O6
2	C	401	UMQ	CA-CB-CC-CD
2	C	401	UMQ	CD-CF-CG-CH
2	D	401	UMQ	CC-CD-CF-CG
2	D	401	UMQ	CD-CF-CG-CH
2	D	401	UMQ	CI-CJ-CK-CL
2	D	401	UMQ	C2'-C1'-O1'-CA
2	D	401	UMQ	O5'-C1'-O1'-CA
2	C	401	UMQ	O5-C5-C6-O6
2	C	401	UMQ	CH-CI-CJ-CK
2	D	401	UMQ	C4-C5-C6-O6
2	C	401	UMQ	CF-CG-CH-CI
2	C	401	UMQ	CI-CJ-CK-CL

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	UMQ	5	0
2	C	401	UMQ	3	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.61	0	100 100	22, 38, 69, 105	0
1	B	332/343 (96%)	-0.50	0	100 100	24, 43, 86, 100	0
1	C	269/343 (78%)	-0.64	0	100 100	21, 38, 63, 101	0
1	D	333/343 (97%)	-0.41	5 (1%)	72 68	22, 41, 110, 133	0
All	All	1198/1372 (87%)	-0.53	5 (0%)	88 86	21, 40, 93, 133	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	ALA	2.9
1	D	269	VAL	2.9
1	D	262	GLY	2.6
1	D	265	ALA	2.6
1	D	328	LYS	2.5

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.

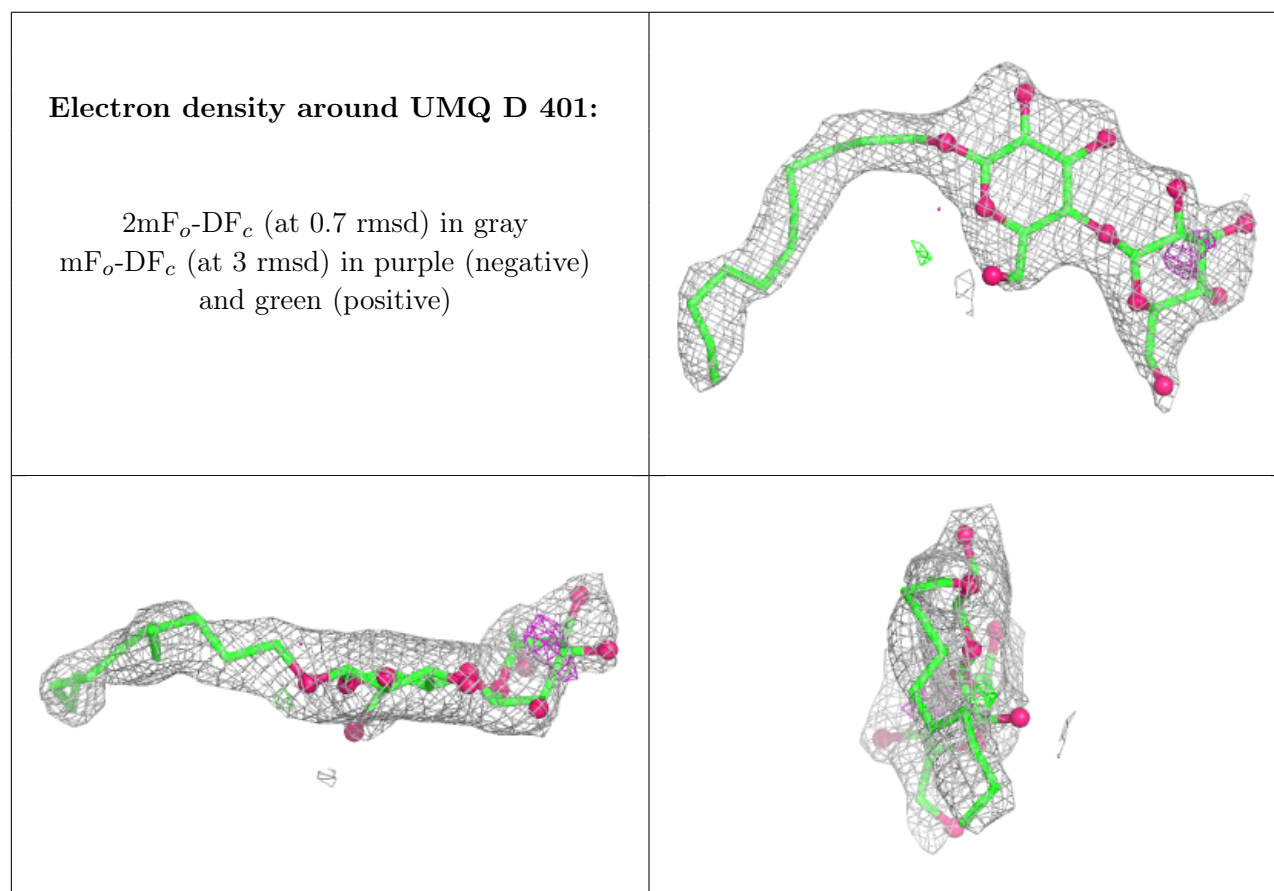
6.4 Ligands [i](#)

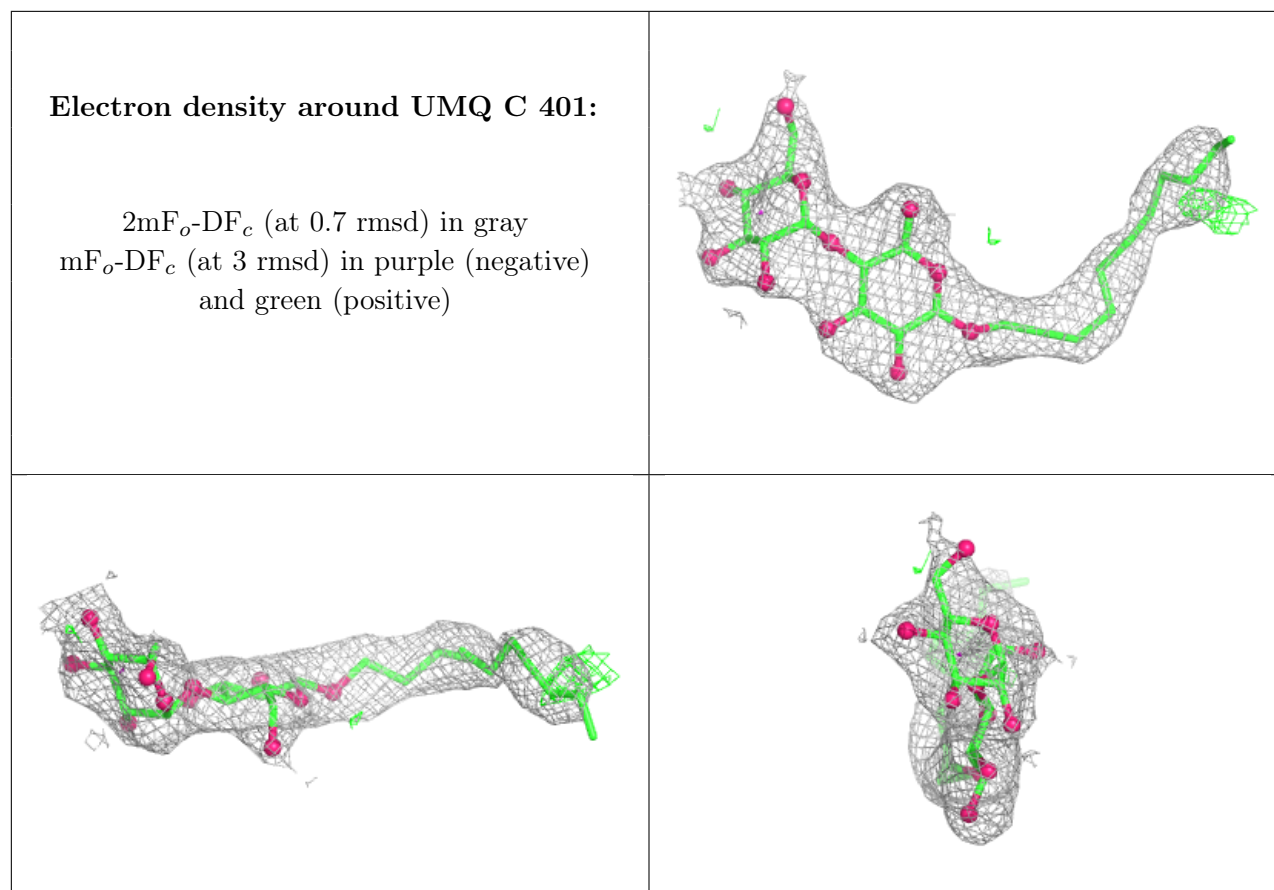
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	UMQ	D	401	34/34	0.91	0.12	56,75,78,81	0
2	UMQ	C	401	34/34	0.92	0.11	56,64,73,75	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.