Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 01:17 PM JST

PDB ID	:	5B0K
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 (i) 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 (i)) were used in the production of this report:

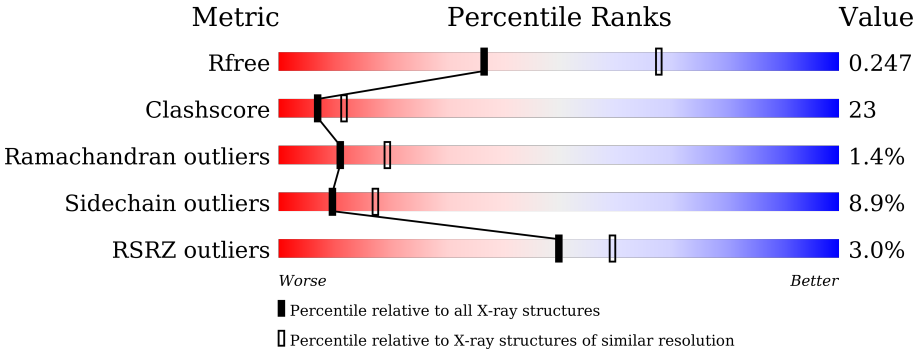
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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%, 47%, 25%, •, 23%
1	B	343	3%, 58%, 32%, 6%, •
1	C	343	%, 45%, 27%, •, 24%
1	D	343	5%, 57%, 34%, •, •, •

2 Entry composition (i)

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

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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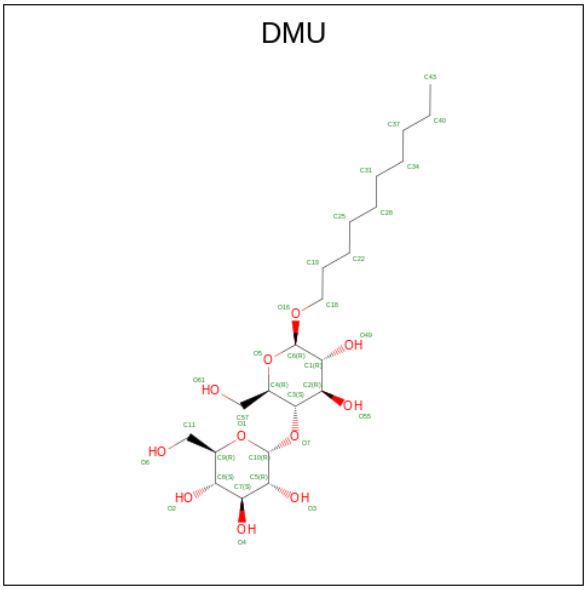
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
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 (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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

- Molecule 3 is water.

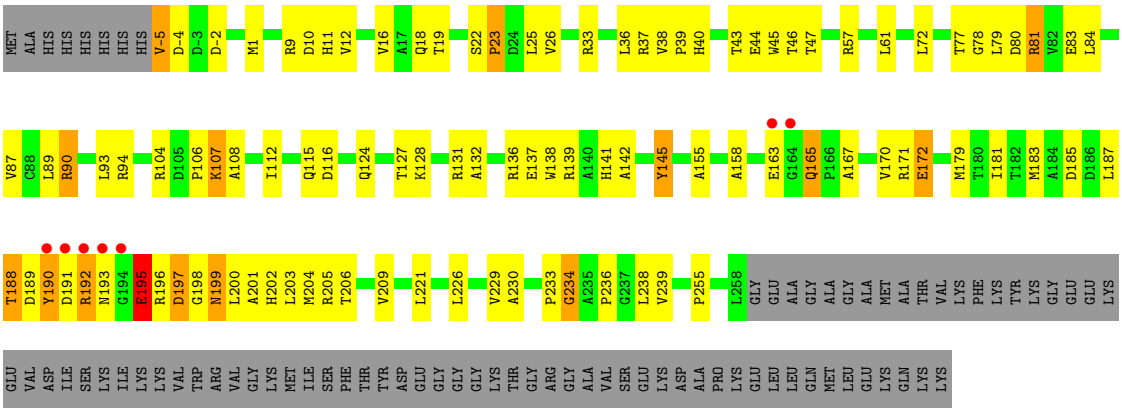
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	174	174	174	0	0
			Total	O		
3	B	204	204	204	0	0
			Total	O		
3	C	147	147	147	0	0
			Total	O		
3	D	177	177	177	0	0

3 Residue-property plots (i)

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.

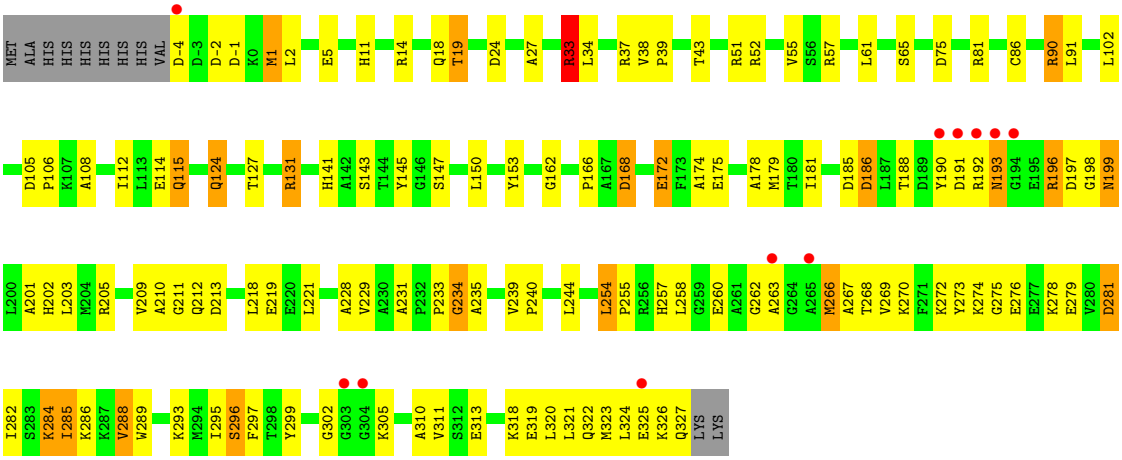
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain A:



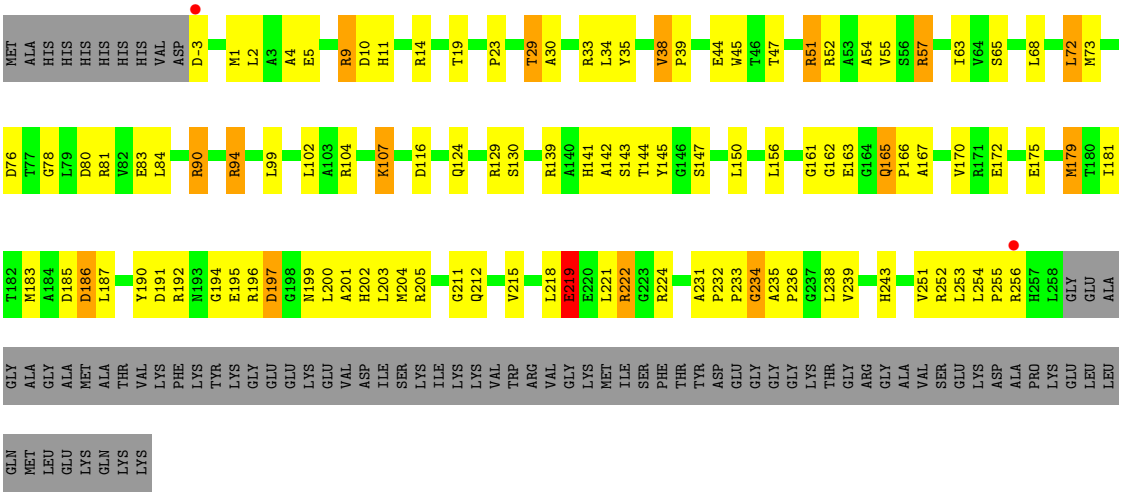
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain B:



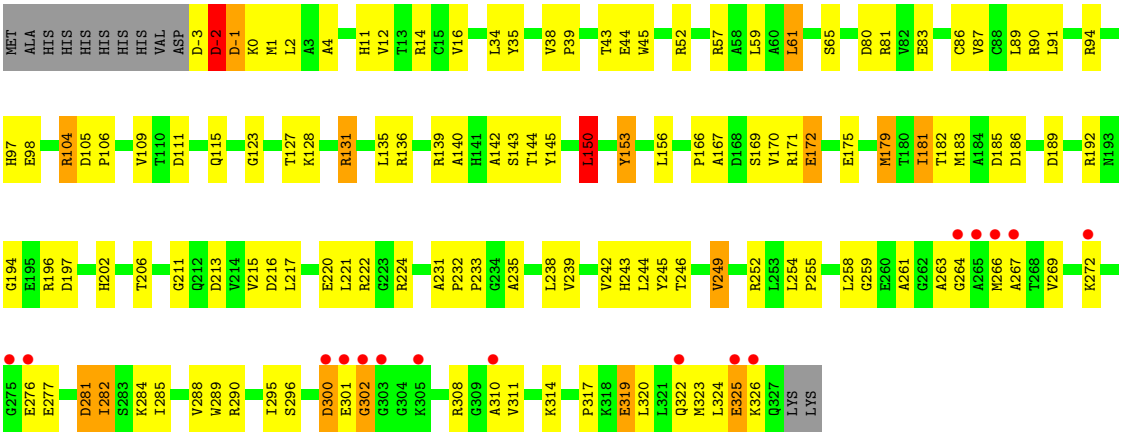
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

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 24.43 – 2.72	Depositor EDS
% Data completeness (in resolution range)	93.9 (25.00-2.75) 92.9 (24.43-2.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.182 , 0.248 0.178 , 0.247	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 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.91	1/2045 (0.0%)	1.03	4/2780 (0.1%)
1	B	0.89	3/2572 (0.1%)	0.98	3/3478 (0.1%)
1	C	0.93	2/2030 (0.1%)	1.02	7/2759 (0.3%)
1	D	0.85	1/2564 (0.0%)	0.99	4/3467 (0.1%)
All	All	0.89	7/9211 (0.1%)	1.00	18/12484 (0.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	GLU	CG-CD	6.52	1.61	1.51
1	C	172	GLU	CG-CD	6.36	1.61	1.51
1	C	219	GLU	CG-CD	5.58	1.60	1.51
1	B	172	GLU	CG-CD	5.58	1.60	1.51
1	A	172	GLU	CG-CD	5.50	1.60	1.51
1	B	86	CYS	CB-SG	-5.22	1.73	1.81
1	B	260	GLU	CB-CG	5.05	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	94	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	94	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	37	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	C	9	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	D	-2	ASP	N-CA-C	-5.93	94.99	111.00
1	D	150	LEU	CA-CB-CG	-5.87	101.81	115.30
1	C	57	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	222	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	254	LEU	CA-CB-CG	5.48	127.90	115.30
1	D	213	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	A	37	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	C	116	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	195	GLU	N-CA-C	-5.32	96.63	111.00
1	A	171	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	81	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	D	61	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	86	CYS	CA-CB-SG	-5.03	104.95	114.00
1	C	51	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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 (i)

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	88	0
1	B	2533	0	2532	127	0
1	C	1998	0	1983	102	0
1	D	2525	0	2528	117	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	426	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 23.

All (426) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:219:GLU:CD	1:C:222:ARG:HE	1.87	0.78
1:A:188:THR:HB	1:A:190:TYR:HE1	1.51	0.76
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:D:-3:ASP:H2	1:D:0:LYS:H	1.36	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:C:139:ARG:HG3	1:C:179:MET:HE3	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: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:B:131:ARG:HH11	1:B:131:ARG:HA	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1:MET:HE2	1:B:2:LEU:HA	1.78	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:D:-3:ASP:C	1:D:-1:ASP:H	1.97	0.63
1:C:1:MET:SD	1:C:2:LEU:HD23	2.38	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: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:D:259:GLY:HA2	1:D:322:GLN:CD	2.19	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: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:B:266:MET:HE2	1:B:267:ALA:HB3	1.82	0.61
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:A:107:LYS:O	1:A:107:LYS:HD3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:10:ASP:CG	1:C:192:ARG:HD2	2.21	0.60
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:TYR:OH	2:D:401:DMU:H8	2.06	0.56
1:B:90:ARG:HD3	1:B:90:ARG:C	2.26	0.56
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: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: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: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
1:D:183:MET:HE3	1:D:217:LEU:HD23	1.90	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: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:C:139:ARG:HG3	1:C:179:MET:CE	2.39	0.52
1:B:131:ARG:HH11	1:B:131:ARG:N	2.08	0.52
1:D:12:VAL:O	1:D:16:VAL:HG23	2.10	0.51
1:C:73:MET:HE1	2:C:401:DMU:H25	1.92	0.51
1:D:295:ILE:HD12	1:D:324:LEU:HD22	1.91	0.51
1:C:73:MET:CE	2:C:401:DMU:H25	2.41	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
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:B:267:ALA:C	1:B:282:ILE:HG12	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:81:ARG:HG2	1:A:81:ARG:NH1	2.26	0.49
1:B:270:LYS:HZ3	1:B:279:GLU:CD	2.15	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: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: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
1:B:254:LEU:HB2	1:B:255:PRO:HD3	1.96	0.47
1:D:104:ARG:CG	1:D:105:ASP:N	2.76	0.47
1:B:114:GLU:O	1:B:115:GLN:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD21	1:A:204:MET:HE3	1.96	0.47
1:A:107:LYS:HD3	1:A:107:LYS:C	2.36	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:C:90:ARG:HD3	1:C:90:ARG:C	2.35	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:B:210:ALA:O	1:B:211:GLY:C	2.53	0.46
1:C:130:SER:HB2	1:C:141:HIS:CE1	2.51	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: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: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:A:192:ARG:HH21	1:A:195:GLU:HB2	1.78	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:B:266:MET:HE2	1:B:267:ALA:N	2.31	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:202:HIS:O	1:B:203:LEU:C	2.55	0.44
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: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:B:1:MET:HE3	1:B:37:ARG:HD3	2.00	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
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:139:ARG:HG2	1:C:179:MET:HE1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-4:ASP:O	1:B:-1:ASP:HB2	2.19	0.42
1:B:166:PRO:O	1:B:166:PRO:HG2	2.19	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:187:LEU:HD21	1:C:204:MET:HE1	2.02	0.42
1:C:199:ASN:O	1:C:202:HIS:HB3	2.19	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:D:301:GLU:O	1:D:302:GLY:C	2.57	0.42
1:C:1:MET:HE2	3:C:555:HOH:O	2.19	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
1:A:90:ARG:C	1:A:90:ARG:HD3	2.40	0.42
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: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:D:185:ASP:O	1:D:186:ASP:C	2.58	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:297:PHE:CD1	1:B:297:PHE:C	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:73:MET:HE2	1:D:86:CYS:SG	2.61	0.41
1:D:-3:ASP:H2	1:D:-1:ASP:CB	2.34	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:C:10:ASP:CG	1:C:14:ARG:HH22	2.22	0.41
1:C:232:PRO:HA	1:C:233:PRO:C	2.40	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:B:255:PRO:C	1:B:257:HIS:N	2.74	0.41
1:B:324:LEU:C	1:B:326:LYS:H	2.22	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:A:187:LEU:HD21	1:A:204:MET:HE2	2.01	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
1:B:131:ARG:HA	1:B:131:ARG:HD3	1.90	0.40
1:D:216:ASP:O	1:D:217:LEU:C	2.57	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%)	8 14
1	B	330/343 (96%)	295 (89%)	28 (8%)	7 (2%)	7 12
1	C	260/343 (76%)	245 (94%)	14 (5%)	1 (0%)	34 53
1	D	329/343 (96%)	308 (94%)	17 (5%)	4 (1%)	13 23
All	All	1181/1372 (86%)	1097 (93%)	67 (6%)	17 (1%)	11 19

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
1	A	193	ASN
1	A	199	ASN
1	D	249	VAL

5.3.2 Protein sidechains (i)

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%)	187 (90%)	21 (10%)	7 12
1	B	260/270 (96%)	237 (91%)	23 (9%)	10 17
1	C	206/270 (76%)	187 (91%)	19 (9%)	9 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	259/270 (96%)	239 (92%)	20 (8%)	13 22
All	All	933/1080 (86%)	850 (91%)	83 (9%)	9 17

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	-2	ASP
1	A	18	GLN
1	A	23	PRO
1	A	47	THR
1	A	81	ARG
1	A	90	ARG
1	A	94	ARG
1	A	107	LYS
1	A	139	ARG
1	A	165	GLN
1	A	181	ILE
1	A	188	THR
1	A	189	ASP
1	A	190	TYR
1	A	191	ASP
1	A	192	ARG
1	A	195	GLU
1	A	197	ASP
1	A	199	ASN
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	90	ARG
1	B	124	GLN
1	B	131	ARG
1	B	168	ASP
1	B	186	ASP
1	B	191	ASP
1	B	196	ARG
1	B	199	ASN
1	B	233	PRO

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Mol	Chain	Res	Type
1	B	266	MET
1	B	281	ASP
1	B	284	LYS
1	B	285	ILE
1	B	288	VAL
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	90	ARG
1	C	94	ARG
1	C	107	LYS
1	C	144	THR
1	C	165	GLN
1	C	179	MET
1	C	185	ASP
1	C	186	ASP
1	C	197	ASP
1	C	212	GLN
1	C	219	GLU
1	C	251	VAL
1	D	-2	ASP
1	D	-1	ASP
1	D	90	ARG
1	D	104	ARG
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	197	ASP
1	D	277	GLU
1	D	281	ASP

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Mol	Chain	Res	Type
1	D	282	ILE
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	199	ASN
1	B	18	GLN
1	B	124	GLN
1	B	199	ASN
1	B	322	GLN
1	C	124	GLN
1	C	141	HIS
1	C	165	GLN
1	C	243	HIS
1	D	11	HIS
1	D	165	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	501	-	34,34,34	0.90	1 (2%)	45,45,45	0.64	0
2	DMU	C	401	-	34,34,34	0.76	1 (2%)	45,45,45	0.81	1 (2%)
2	DMU	D	401	-	34,34,34	0.79	1 (2%)	45,45,45	0.75	1 (2%)
2	DMU	B	501	-	34,34,34	1.01	1 (2%)	45,45,45	0.83	1 (2%)
2	DMU	A	502	-	34,34,34	0.81	1 (2%)	45,45,45	0.66	0
2	DMU	B	502	-	34,34,34	0.90	1 (2%)	45,45,45	0.84	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	DMU	A	501	-	-	9/19/59/59	0/2/2/2
2	DMU	C	401	-	-	9/19/59/59	0/2/2/2
2	DMU	D	401	-	-	6/19/59/59	0/2/2/2
2	DMU	B	501	-	-	10/19/59/59	0/2/2/2
2	DMU	A	502	-	-	6/19/59/59	0/2/2/2
2	DMU	B	502	-	-	10/19/59/59	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	3.79	1.53	1.43
2	A	501	DMU	O16-C18	3.67	1.53	1.43
2	D	401	DMU	O16-C18	3.57	1.52	1.43
2	B	501	DMU	O16-C18	3.29	1.52	1.43
2	A	502	DMU	O16-C18	3.29	1.52	1.43
2	C	401	DMU	O16-C18	3.00	1.51	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	DMU	C18-O16-C6	-3.56	107.93	113.84
2	D	401	DMU	C18-O16-C6	-2.58	109.56	113.84
2	B	501	DMU	C18-O16-C6	-2.02	110.50	113.84

There are no chirality outliers.

All (50) torsion outliers are listed below:

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

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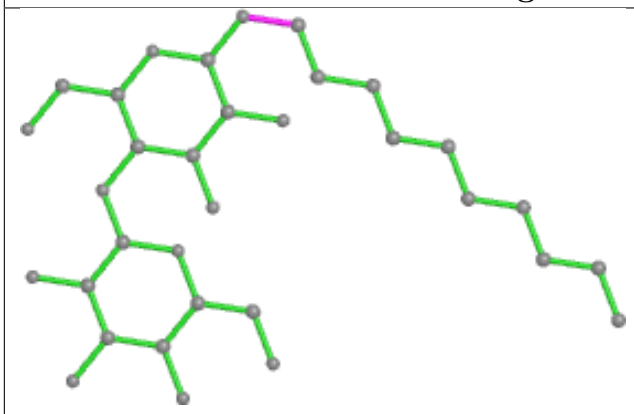
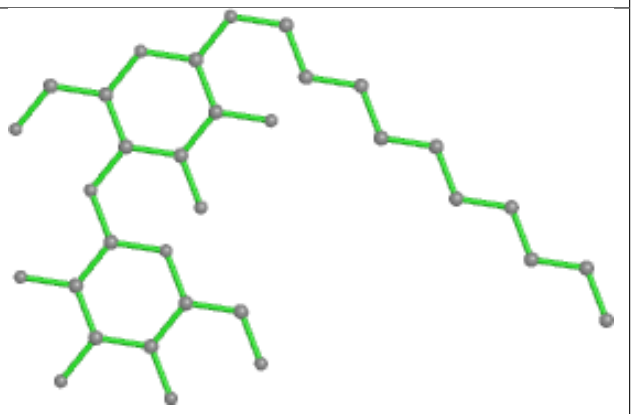
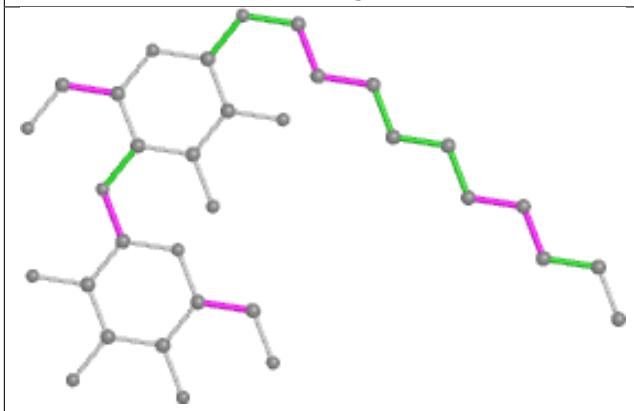
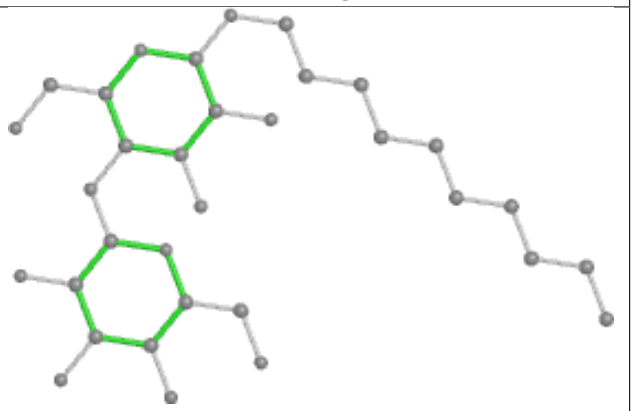
Mol	Chain	Res	Type	Atoms
2	A	502	DMU	C18-C19-C22-C25
2	B	501	DMU	C28-C31-C34-C37
2	C	401	DMU	C19-C22-C25-C28
2	C	401	DMU	C25-C28-C31-C34
2	C	401	DMU	C18-C19-C22-C25
2	A	501	DMU	O6-C11-C9-O1
2	B	501	DMU	C3-C4-C57-O61
2	A	501	DMU	C5-C10-O7-C3
2	B	501	DMU	C34-C37-C40-C43
2	A	501	DMU	C31-C34-C37-C40
2	B	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.

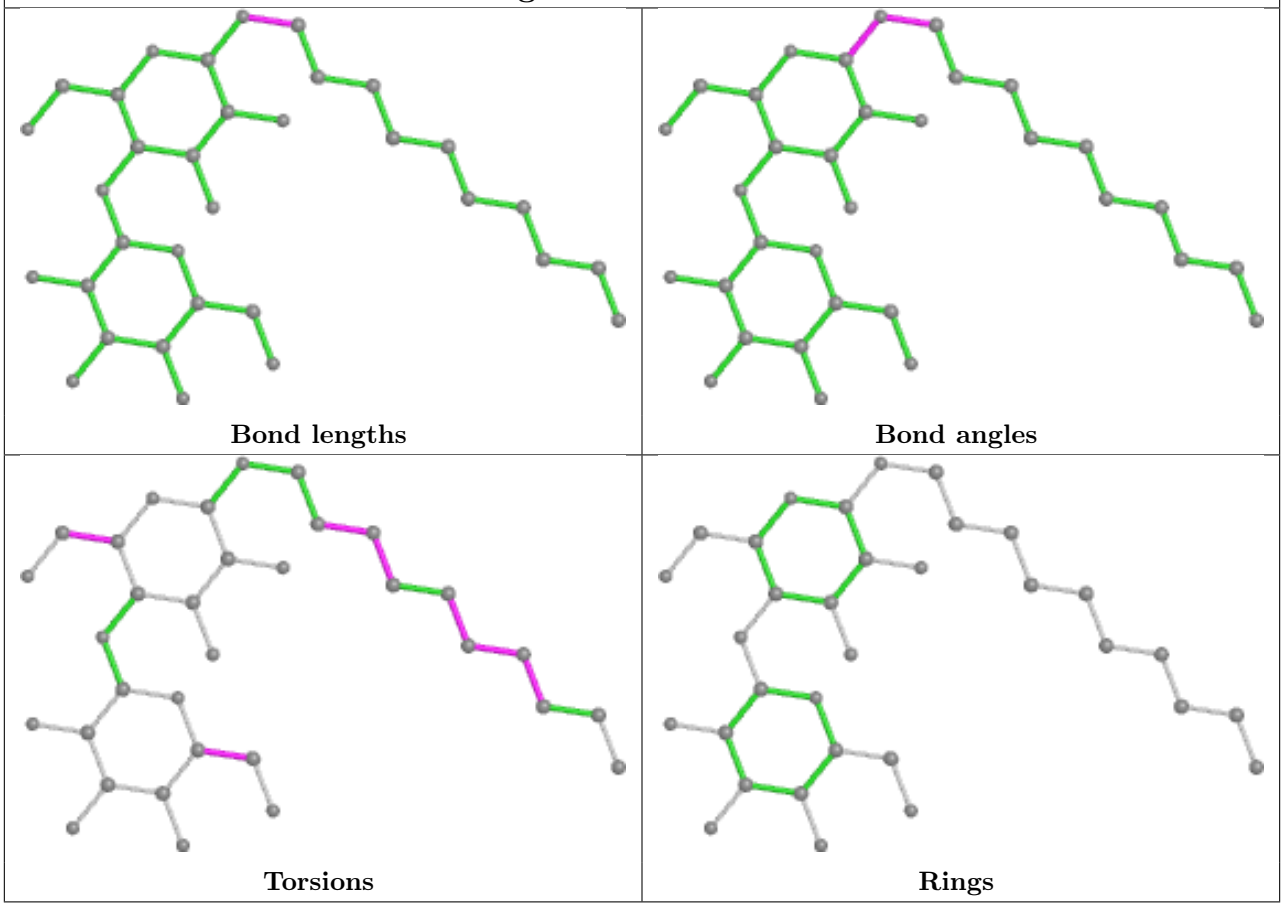
6 monomers are involved in 31 short contacts:

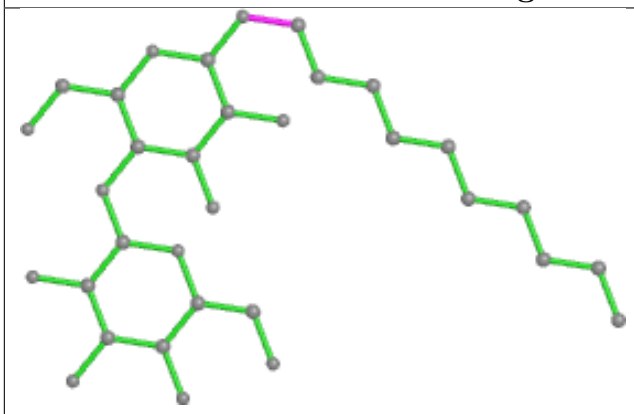
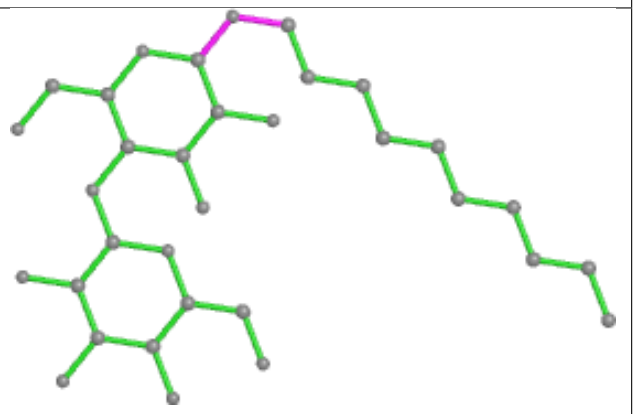
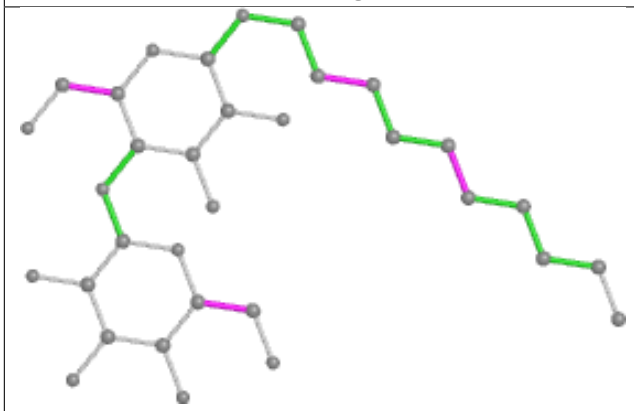
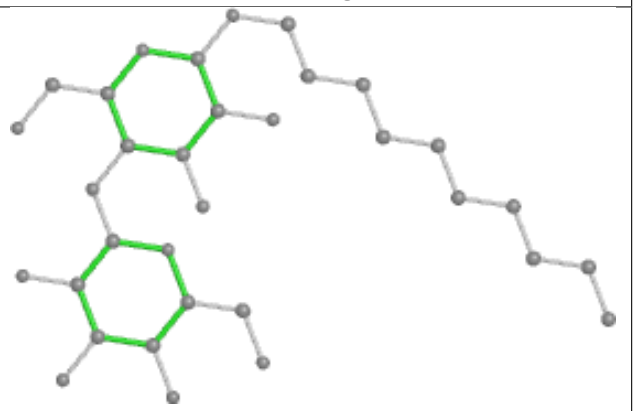
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	DMU	7	0
2	C	401	DMU	8	0
2	D	401	DMU	3	0
2	B	501	DMU	7	0
2	A	502	DMU	4	0
2	B	502	DMU	2	0

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

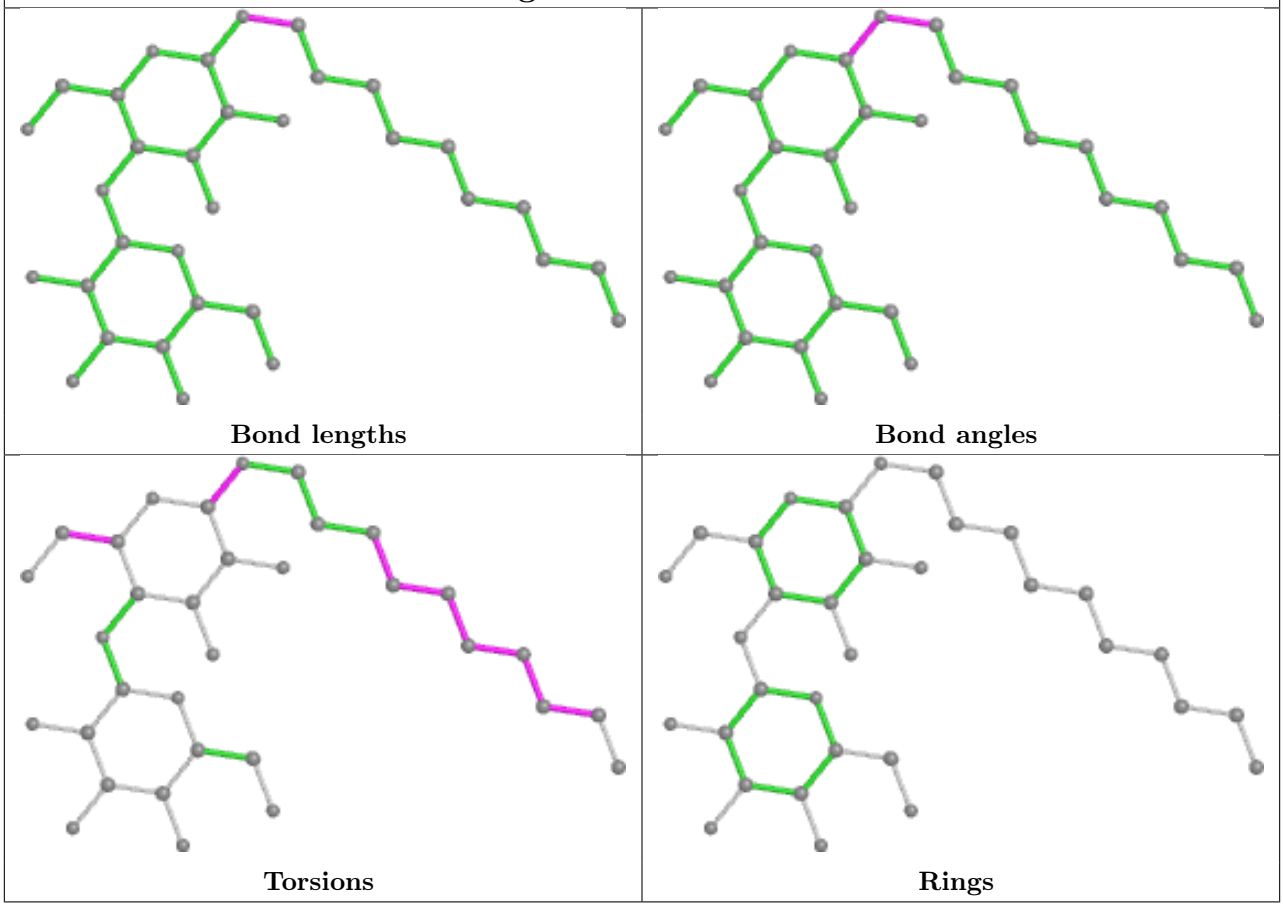
Ligand DMU A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DMU C 401

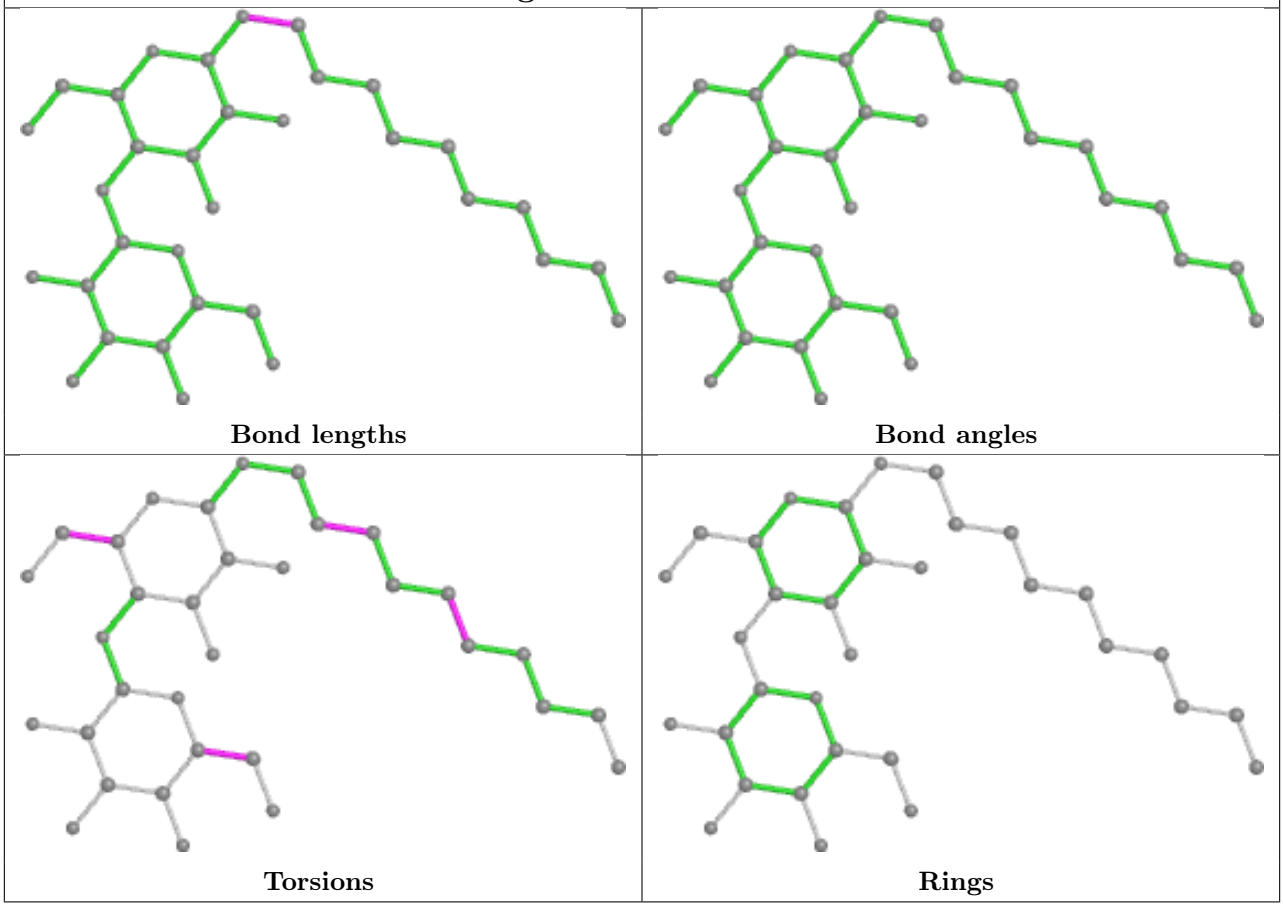


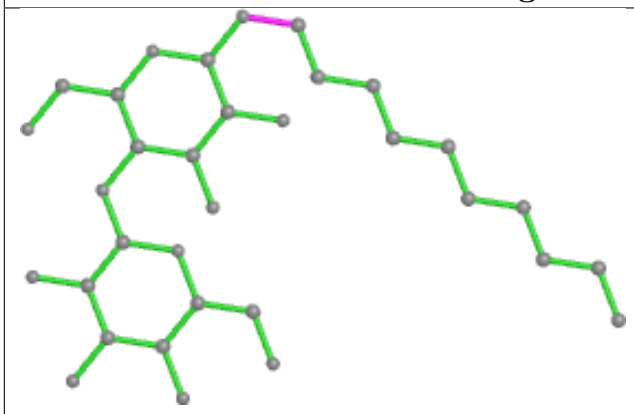
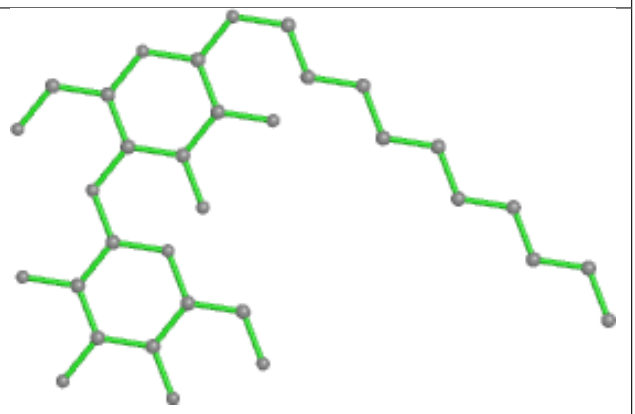
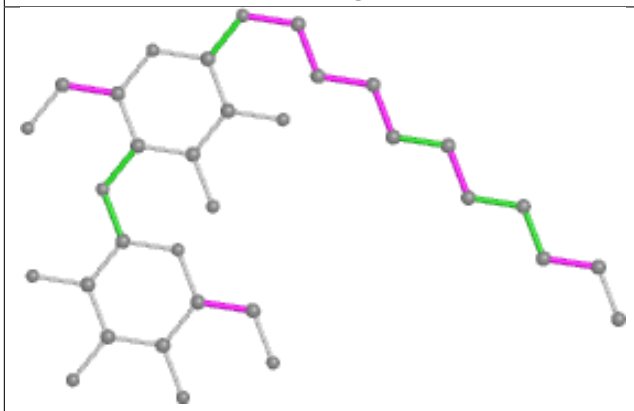
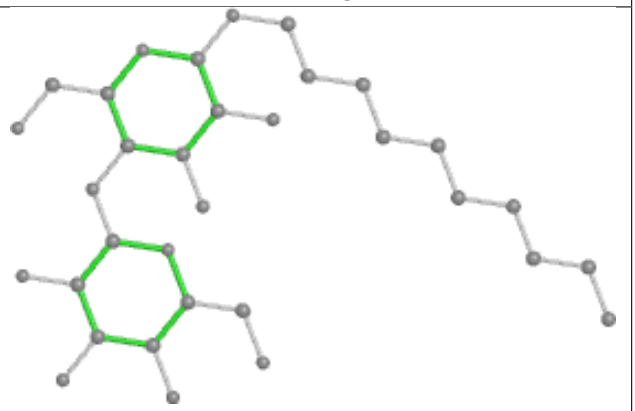
Ligand DMU D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DMU B 501



Ligand DMU A 502



Ligand DMU B 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

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%)	-0.48	7 (2%)	54	63	13, 31, 60, 102	0
1	B	332/343 (96%)	-0.21	11 (3%)	46	54	17, 37, 82, 117	0
1	C	262/343 (76%)	-0.55	2 (0%)	86	90	15, 34, 58, 74	0
1	D	331/343 (96%)	-0.20	16 (4%)	30	36	16, 38, 94, 126	0
All	All	1189/1372 (86%)	-0.34	36 (3%)	50	59	13, 35, 84, 126	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ASN	9.4
1	D	266	MET	8.5
1	B	192	ARG	5.2
1	D	267	ALA	5.1
1	A	193	ASN	4.9
1	D	265	ALA	4.8
1	B	194	GLY	4.7
1	A	192	ARG	4.5
1	B	191	ASP	3.7
1	B	304	GLY	3.5
1	D	275	GLY	3.5
1	A	194	GLY	3.2
1	D	272	LYS	3.2
1	B	-4	ASP	3.1
1	C	-3	ASP	3.0
1	D	301	GLU	3.0
1	B	303	GLY	3.0
1	D	276	GLU	3.0
1	A	191	ASP	2.9
1	A	164	GLY	2.9
1	D	264	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	265	ALA	2.9
1	D	305	LYS	2.8
1	D	300	ASP	2.7
1	B	190	TYR	2.5
1	D	303	GLY	2.5
1	B	263	ALA	2.5
1	B	325	GLU	2.4
1	D	325	GLU	2.4
1	A	163	GLU	2.3
1	D	302	GLY	2.3
1	D	322	GLN	2.2
1	D	326	LYS	2.2
1	A	190	TYR	2.2
1	C	256	ARG	2.2
1	D	310	ALA	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 monosaccharides 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.

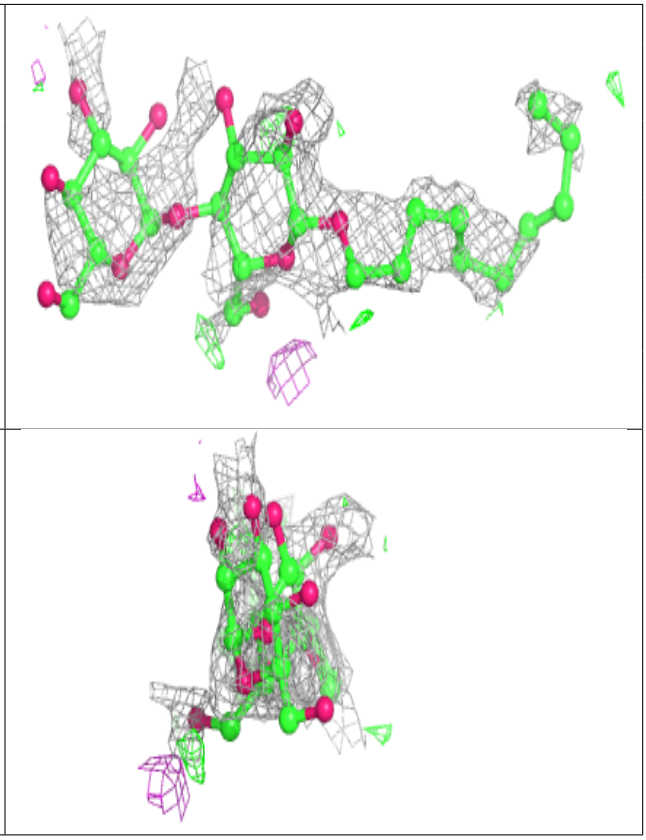
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DMU	A	501	33/33	0.67	0.38	84,112,120,121	0
2	DMU	B	501	33/33	0.69	0.33	65,88,97,97	0
2	DMU	B	502	33/33	0.86	0.22	50,65,72,73	0
2	DMU	A	502	33/33	0.89	0.21	41,64,70,71	0
2	DMU	C	401	33/33	0.90	0.20	41,64,72,72	0
2	DMU	D	401	33/33	0.92	0.18	43,63,67,71	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.

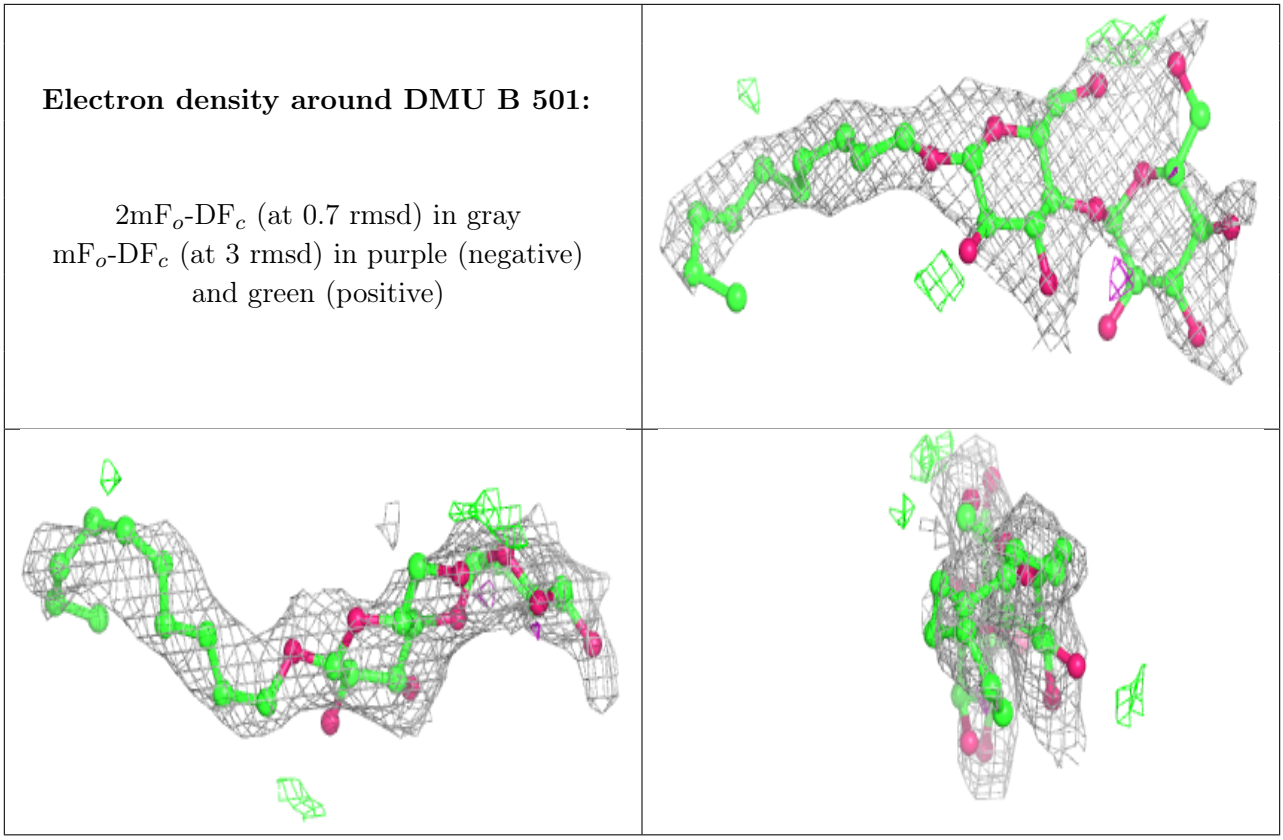
Electron density around DMU A 501:

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



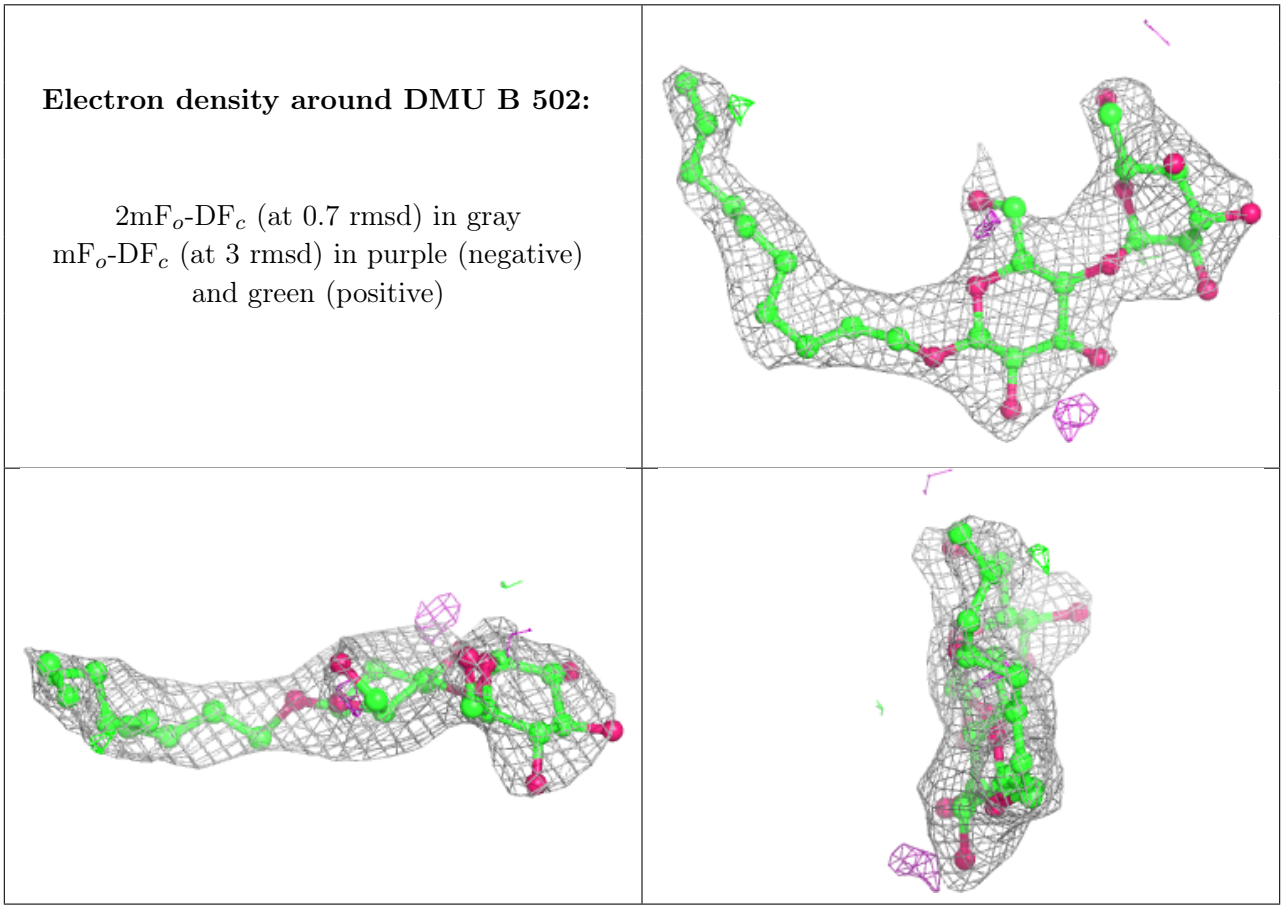
Electron density around DMU B 501:

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



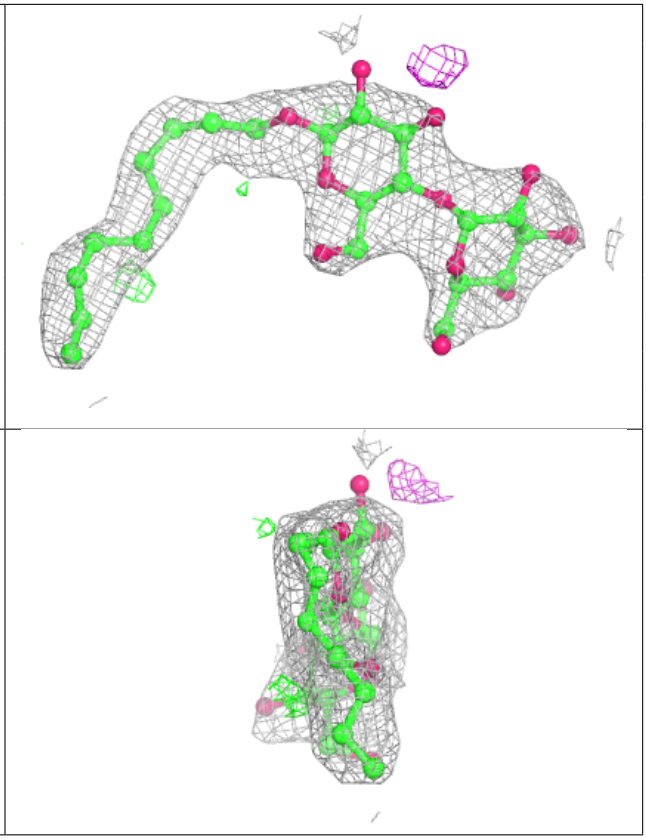
Electron density around DMU B 502:

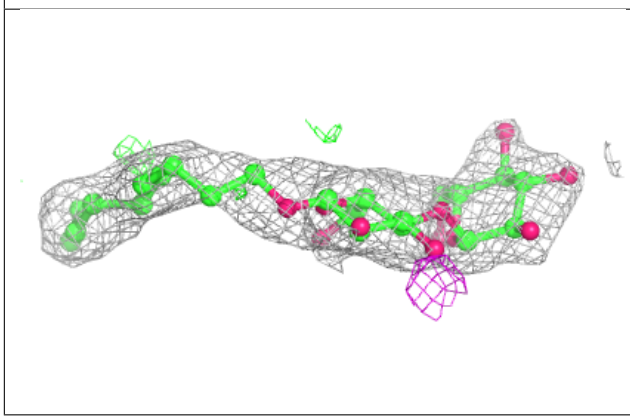
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DMU A 502:

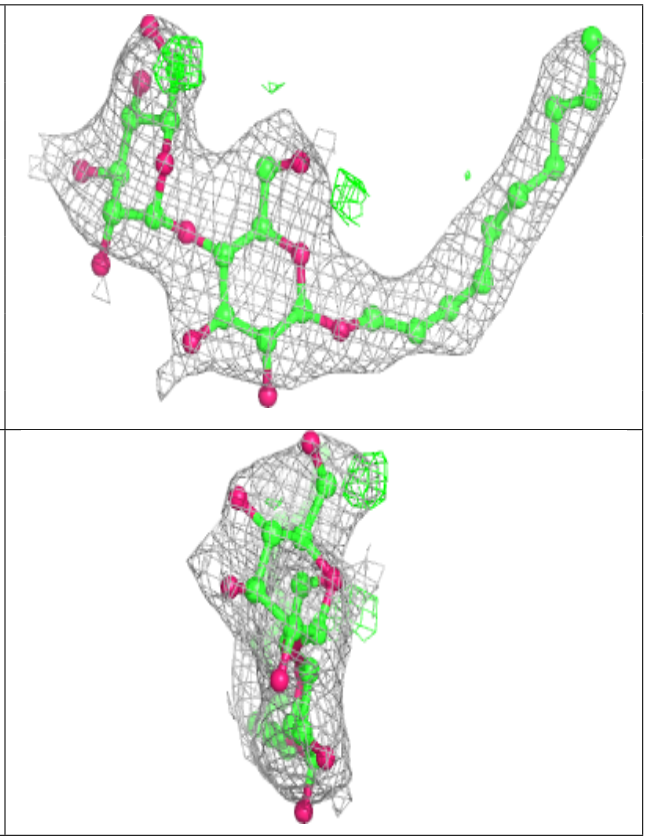
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

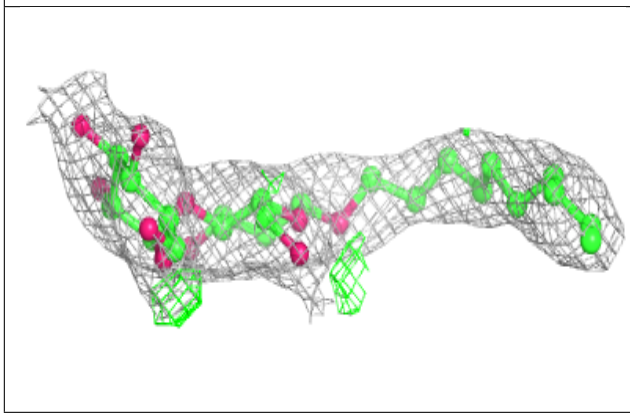




Electron density around DMU C 401:

$2mF_o$-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 D 401:

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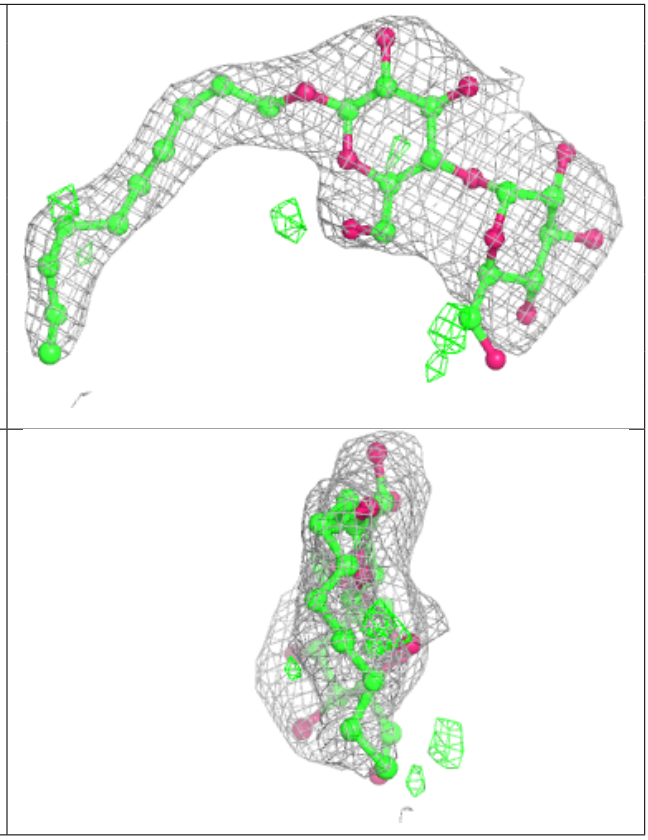
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.