Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 02:32 AM EST

PDB ID	:	1ON3
Title	:	Transcarboxylase 12S crystal structure: hexamer assembly and substrate binding to a multienzyme core (with methylmalonyl-coenzyme a and methylmalonic acid bound)
Authors	:	Hall, P.R.; Wang, Y.-F.; Rivera-Hainaj, R.E.; Zheng, X.; Pustai-Carey, M.; Carey, P.R.; Yee, V.C.
Deposited on	:	2003-02-26
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

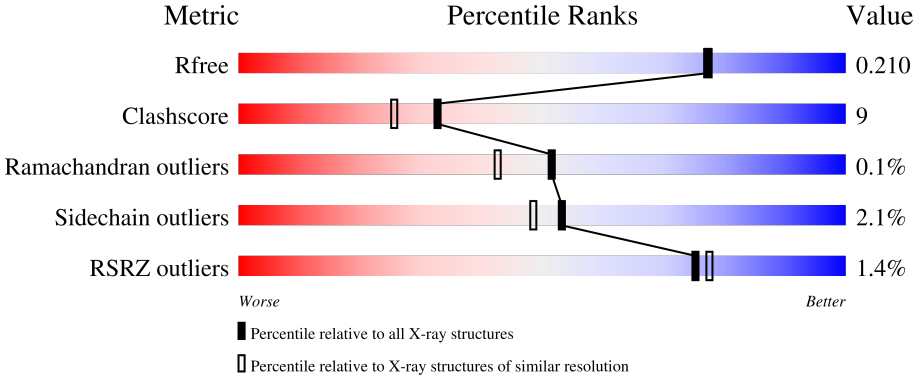
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	523	.% 85% 13% ••
1	B	523	2% 85% 13% ••
1	C	523	2% 81% 16% ••
1	D	523	2% 75% 22% ••
1	E	523	.% 87% 11% ••

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Mol	Chain	Length	Quality of chain
1	F	523	85% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MCA	A	4001	X	-	-	-
3	MCA	B	4002	X	-	-	-
3	MCA	C	4003	X	-	-	-
3	MCA	D	4004	X	-	-	-
3	MCA	E	4005	X	-	-	-
3	MCA	F	4006	X	-	-	-
4	DXX	A	5001	-	X	-	-
4	DXX	B	5002	-	X	-	-
4	DXX	C	5003	-	X	-	-
4	DXX	D	5004	-	X	-	-
4	DXX	E	5005	-	X	-	-
4	DXX	F	5006	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27244 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.

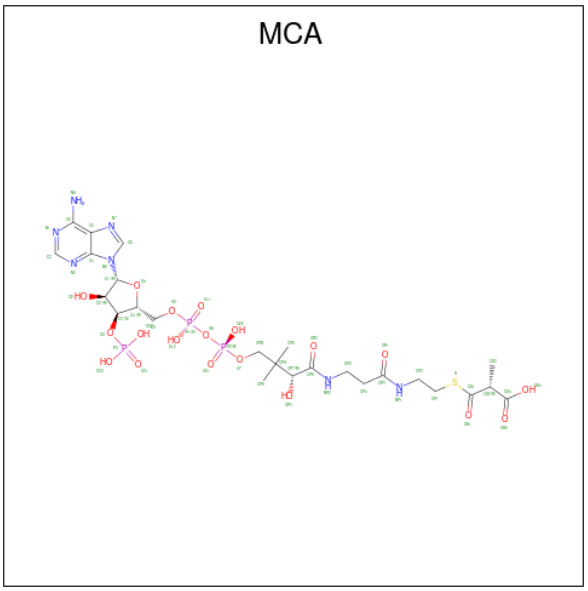
- Molecule 1 is a protein called Methylmalonyl-CoA carboxyltransferase 12S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	517	3929	2466	687	757	19	0	4	0
1	B	516	3929	2466	686	758	19	0	6	0
1	C	510	3859	2423	672	745	19	0	1	0
1	D	513	3893	2446	678	750	19	0	3	0
1	E	520	3959	2483	690	767	19	0	6	0
1	F	517	3913	2456	681	757	19	0	2	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

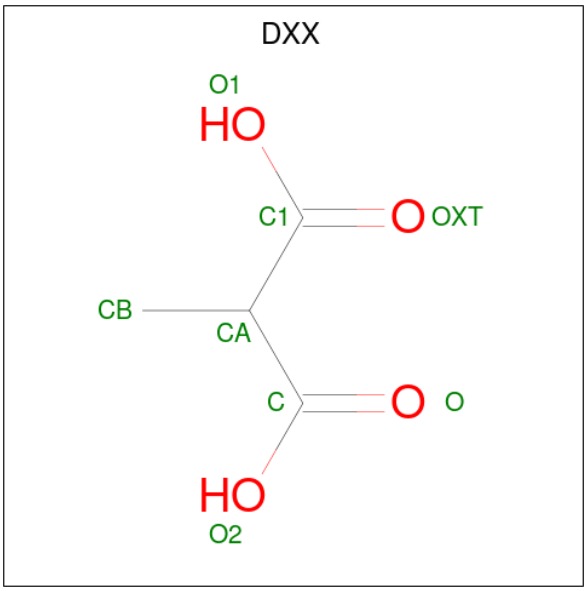
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is METHYLMALONYL-COENZYME A (three-letter code: MCA) (formula: $C_{25}H_{40}N_7O_{19}P_3S$).



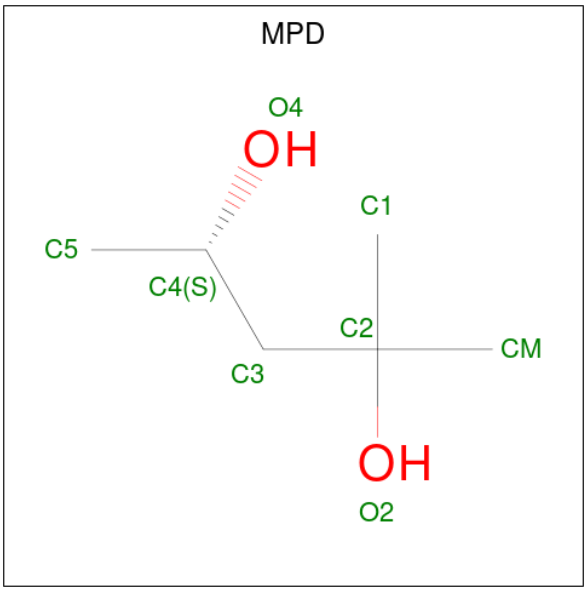
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	55	25	7	19	3	1	0	0
3	B	1	55	25	7	19	3	1	0	0
3	C	1	55	25	7	19	3	1	0	0
3	D	1	55	25	7	19	3	1	0	0
3	E	1	55	25	7	19	3	1	0	0
3	F	1	55	25	7	19	3	1	0	0

- Molecule 4 is METHYLMALONIC ACID (three-letter code: DXX) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
4	B	1	7	4	3	0	0
4	C	1	7	4	3	0	0
4	D	1	7	4	3	0	0
4	E	1	7	4	3	0	0
4	F	1	7	4	3	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	8	6	2	0	0
5	B	1	8	6	2	0	0
5	F	1	8	6	2	0	0

- Molecule 6 is water.

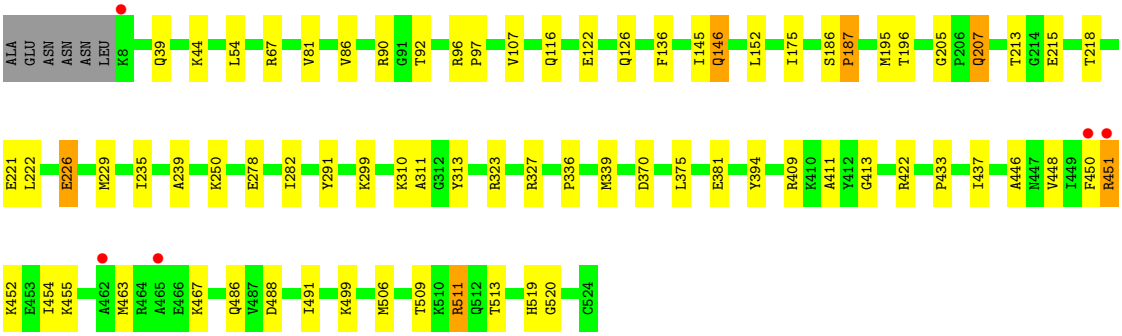
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	553	553	553	0	0
6	B	555	555	555	0	0
6	C	590	590	590	0	0
6	D	509	509	509	0	0
6	E	606	606	606	0	0
6	F	550	550	550	0	0

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.

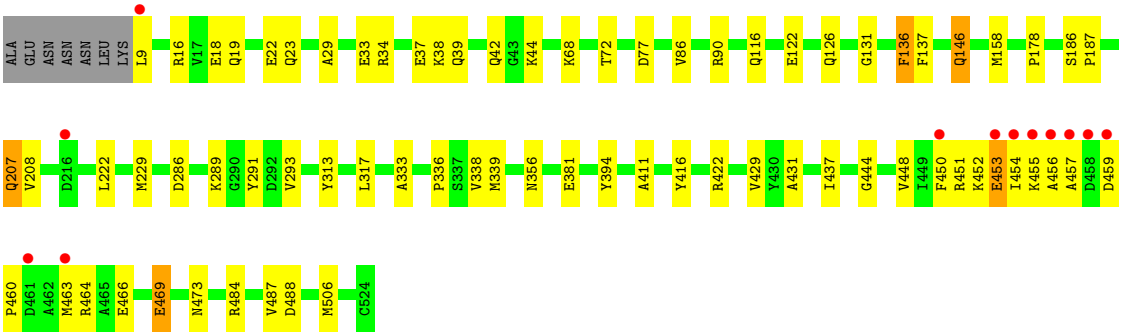
• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

Chain A:



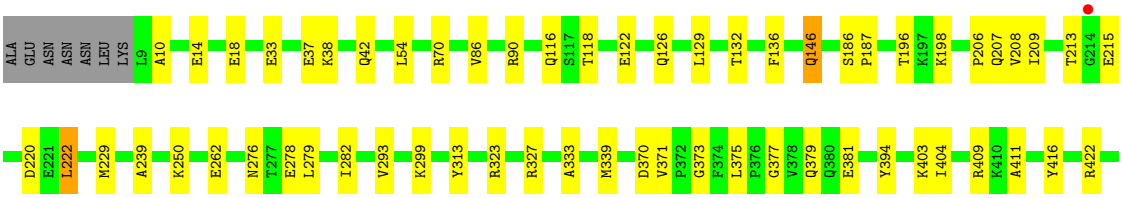
• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

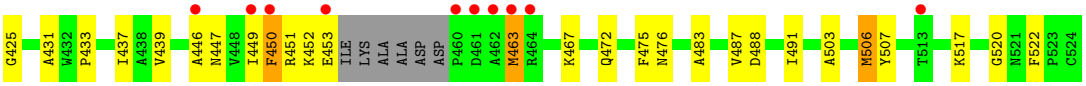
Chain B:



• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

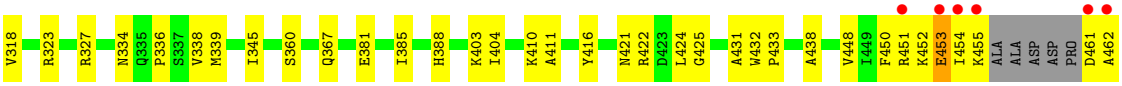
Chain C:

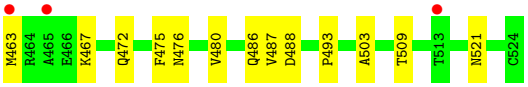




• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

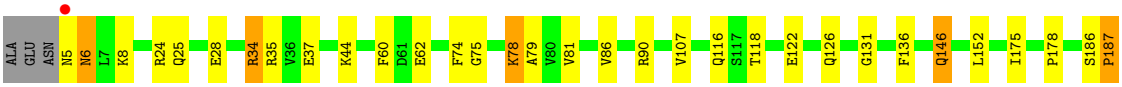
Chain D:

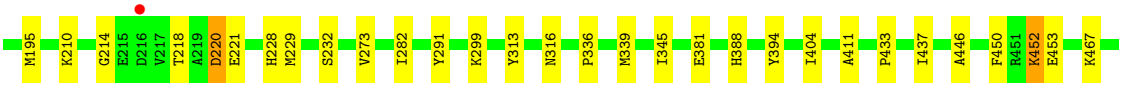




• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

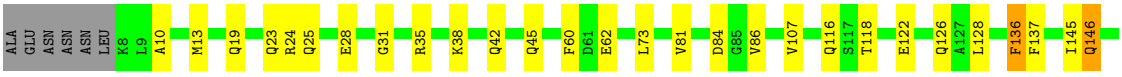
Chain E:

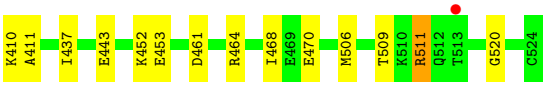




• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.81Å 200.71Å 146.35Å 90.00° 102.43° 90.00°	Depositor
Resolution (Å)	19.97 – 1.90 29.64 – 1.89	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.97-1.90) 90.4 (29.64-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.168 , 0.213 0.166 , 0.210	Depositor DCC
R_{free} test set	10568 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27244	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: MCA, MPD, CD, DXX

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	0.39	0/4019	0.65	0/5438
1	B	0.40	0/4025	0.66	0/5448
1	C	0.40	0/3934	0.66	0/5324
1	D	0.36	0/3975	0.63	0/5377
1	E	0.39	0/4055	0.66	0/5488
1	F	0.39	0/3993	0.66	0/5405
All	All	0.39	0/24001	0.65	0/32480

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3929	0	3885	70	0
1	B	3929	0	3880	77	0
1	C	3859	0	3809	77	0
1	D	3893	0	3854	108	0
1	E	3959	0	3905	63	0
1	F	3913	0	3865	65	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	55	0	33	1	0
3	B	55	0	33	1	0
3	C	55	0	33	1	0
3	D	55	0	33	0	0
3	E	55	0	33	3	0
3	F	55	0	33	1	0
4	A	7	0	3	0	0
4	B	7	0	3	1	0
4	C	7	0	3	0	0
4	D	7	0	3	0	0
4	E	7	0	3	0	0
4	F	7	0	3	0	0
5	A	8	0	14	1	0
5	B	8	0	14	0	0
5	F	8	0	14	0	0
6	A	553	0	0	9	0
6	B	555	0	0	9	0
6	C	590	0	0	7	0
6	D	509	0	0	20	0
6	E	606	0	0	12	0
6	F	550	0	0	9	0
All	All	27244	0	23456	412	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 9.

All (412) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HD2	1:E:506:MET:HG3	1.23	1.12
1:E:452:LYS:HD2	1:E:453:GLU:H	1.03	1.06
1:E:452:LYS:HD2	1:E:453:GLU:N	1.69	1.06
1:D:244:ALA:HB3	6:D:5492:HOH:O	1.57	1.05
1:A:511:ARG:HH12	1:B:131:GLY:HA3	1.29	0.95
1:C:213:THR:HG23	1:C:215:GLU:H	1.34	0.92
1:F:146:GLN:H	1:F:146:GLN:HE21	1.16	0.91
1:C:146:GLN:H	1:C:146:GLN:HE21	1.13	0.90
1:B:146:GLN:H	1:B:146:GLN:HE21	1.18	0.86
1:E:146:GLN:H	1:E:146:GLN:HE21	1.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:ASN:HD22	1:D:486[A]:GLN:HE22	1.21	0.84
1:F:206:PRO:HD2	1:F:207:GLN:HE22	1.43	0.83
1:A:90:ARG:HD2	1:C:506:MET:HG3	1.61	0.82
1:B:146:GLN:HE22	3:B:4002:MCA:H2	1.45	0.81
1:C:146:GLN:HE22	3:C:4003:MCA:H2	1.44	0.80
1:B:146:GLN:H	1:B:146:GLN:NE2	1.79	0.79
1:F:146:GLN:HE22	3:F:4006:MCA:H2	1.48	0.79
1:C:186:SER:HB3	1:C:187:PRO:HD3	1.64	0.79
1:D:286:ASP:HB3	1:D:289:LYS:HE2	1.65	0.79
1:C:222:LEU:HD21	1:F:381:GLU:HG3	1.65	0.78
1:F:207:GLN:CD	1:F:207:GLN:H	1.87	0.78
1:E:118:THR:O	1:E:122[B]:GLU:HG3	1.85	0.77
1:D:388:HIS:HB2	6:D:5485:HOH:O	1.85	0.76
1:A:90:ARG:CD	1:C:506:MET:HG3	2.16	0.76
1:F:118:THR:O	1:F:122:GLU:HG3	1.84	0.76
1:B:506:MET:HE3	6:B:7291:HOH:O	1.86	0.76
1:D:433:PRO:HB2	1:F:13:MET:HE1	1.68	0.75
1:A:511:ARG:HH12	1:B:131:GLY:CA	1.98	0.75
1:A:186:SER:HB3	1:A:187:PRO:HD3	1.69	0.74
1:F:146:GLN:H	1:F:146:GLN:NE2	1.85	0.74
1:D:280:ARG:HG2	1:D:493:PRO:HG2	1.70	0.74
1:B:186:SER:HB3	1:B:187:PRO:HD3	1.69	0.73
1:A:146:GLN:H	1:A:146:GLN:HE21	1.36	0.73
1:D:12:THR:HG23	1:D:15:GLY:H	1.52	0.73
1:C:146:GLN:H	1:C:146:GLN:NE2	1.86	0.72
1:D:122:GLU:HG3	6:D:5419:HOH:O	1.89	0.72
1:C:209:ILE:O	1:C:213:THR:HG22	1.89	0.72
1:A:207:GLN:CD	1:A:207:GLN:H	1.92	0.71
1:B:381:GLU:HG3	6:E:5610:HOH:O	1.88	0.71
1:B:459:ASP:N	1:B:460:PRO:HD3	2.05	0.71
1:D:186:SER:HB3	1:D:187:PRO:HD3	1.72	0.71
1:B:158:MET:HE1	6:B:7287:HOH:O	1.88	0.71
1:F:299:LYS:HE2	6:F:6486:HOH:O	1.90	0.71
1:F:228:HIS:HA	1:F:232[B]:SER:OG	1.92	0.70
1:E:78:LYS:HD2	1:E:79:ALA:N	2.07	0.69
1:E:146:GLN:HE22	3:E:4005:MCA:H2	1.56	0.69
1:E:5:ASN:HD21	1:F:470:GLU:HA	1.56	0.69
1:A:90:ARG:HD2	1:C:506:MET:CG	2.22	0.68
1:A:226:GLU:HG2	6:A:7385:HOH:O	1.92	0.68
1:D:385:ILE:HA	6:D:5485:HOH:O	1.93	0.68
1:E:78:LYS:HD2	1:E:78:LYS:C	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:THR:OG1	1:D:221:GLU:HG3	1.94	0.68
1:E:75:GLY:O	1:E:78:LYS:HE3	1.91	0.68
1:D:421:ASN:ND2	1:D:486[A]:GLN:HE22	1.91	0.68
1:E:186:SER:HB3	1:E:187:PRO:HD3	1.74	0.67
1:A:122:GLU:O	1:A:126[B]:GLN:HG2	1.95	0.67
1:A:207:GLN:H	1:A:207:GLN:NE2	1.91	0.66
1:D:90:ARG:CD	1:E:506:MET:HG3	2.14	0.66
1:B:222:LEU:HD11	1:E:381:GLU:HG3	1.76	0.66
1:F:206:PRO:HD2	1:F:207:GLN:NE2	2.09	0.66
1:E:5:ASN:ND2	1:F:470:GLU:HA	2.10	0.66
1:A:97:PRO:HB3	1:C:506:MET:CE	2.25	0.66
1:F:453:GLU:HG3	6:F:6067:HOH:O	1.96	0.65
1:A:218:THR:OG1	1:A:221:GLU:HG3	1.96	0.65
1:D:450:PHE:CE2	1:D:467:LYS:HE2	2.32	0.65
1:B:207:GLN:H	1:B:207:GLN:CD	1.97	0.65
1:D:385:ILE:HD12	6:D:5485:HOH:O	1.96	0.65
1:E:228:HIS:HA	1:E:232[A]:SER:OG	1.97	0.65
1:A:450:PHE:CD1	1:A:467:LYS:HB3	2.32	0.65
1:E:37:GLU:HG3	6:E:5566:HOH:O	1.95	0.65
1:D:239:ALA:HB1	6:D:5492:HOH:O	1.96	0.64
1:A:226:GLU:CD	1:A:226:GLU:H	2.01	0.64
1:B:208:VAL:HG21	4:B:5002:DXX:HB1	1.79	0.64
1:A:86:VAL:HB	1:A:116:GLN:HG3	1.80	0.63
1:D:345:ILE:HA	6:D:5485:HOH:O	1.99	0.63
1:C:207:GLN:CD	1:C:207:GLN:H	2.01	0.63
1:A:452:LYS:O	1:A:455:LYS:HG2	1.98	0.63
1:D:452:LYS:HB2	1:D:452:LYS:NZ	2.13	0.63
1:D:433:PRO:HB2	1:F:13:MET:CE	2.29	0.63
1:C:449:ILE:HD11	1:F:145:ILE:HG22	1.80	0.63
1:B:122[A]:GLU:HG3	6:B:7398:HOH:O	1.98	0.63
1:B:122[B]:GLU:HG3	6:B:7398:HOH:O	1.98	0.63
1:C:506:MET:CE	6:C:7040:HOH:O	2.46	0.63
1:D:472:GLN:NE2	1:D:476:ASN:HB2	2.14	0.63
1:A:486[B]:GLN:NE2	6:A:7067:HOH:O	2.32	0.62
1:C:411:ALA:HB1	1:C:416:TYR:CD2	2.34	0.62
1:B:146:GLN:HE21	1:B:146:GLN:N	1.95	0.62
1:C:146:GLN:HE21	1:C:146:GLN:N	1.92	0.62
1:D:77:ASP:CG	1:D:78:LYS:HD3	2.19	0.62
1:D:143:ALA:HB1	1:D:151:SER:OG	2.00	0.62
1:D:345:ILE:HG12	6:D:5485:HOH:O	2.00	0.62
1:E:24:ARG:O	1:E:28:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLU:HB3	1:A:299:LYS:NZ	2.15	0.61
1:B:455:LYS:HE3	1:B:456:ALA:HB2	1.82	0.61
1:C:118:THR:HA	6:C:7392:HOH:O	1.99	0.61
1:A:146:GLN:HE22	3:A:4001:MCA:H2	1.65	0.61
1:B:450:PHE:HZ	1:E:74:PHE:CD1	2.19	0.61
1:E:34:ARG:HA	1:E:34:ARG:HH11	1.65	0.61
1:D:452:LYS:O	1:D:455:LYS:HE3	2.00	0.61
1:C:472:GLN:OE1	1:C:476:ASN:HB2	2.00	0.61
1:E:282:ILE:HD11	1:E:299:LYS:HD2	1.83	0.61
1:B:454:ILE:HA	1:B:463:MET:HG2	1.83	0.60
1:D:451:ARG:HD3	6:D:5273:HOH:O	2.02	0.60
1:F:158:MET:HE3	6:F:6322:HOH:O	2.02	0.60
1:E:5:ASN:HD21	1:F:470:GLU:CA	2.14	0.59
1:D:338:VAL:HG12	1:D:339:MET:HG3	1.85	0.59
1:B:19:GLN:O	1:B:23:GLN:HG2	2.03	0.59
1:D:90:ARG:HD2	1:E:506:MET:CG	2.15	0.59
1:F:509:THR:O	1:F:511:ARG:HD3	2.03	0.59
1:A:97:PRO:CB	1:C:506:MET:HE1	2.33	0.58
1:D:12:THR:O	1:D:16:ARG:HG3	2.02	0.58
1:F:146:GLN:HE21	1:F:146:GLN:N	1.95	0.58
1:A:222:LEU:HD11	1:D:381:GLU:HG3	1.85	0.58
1:A:278:GLU:HB3	1:A:299:LYS:HZ3	1.69	0.58
1:B:286:ASP:HB3	1:B:289:LYS:HE2	1.84	0.58
1:C:506:MET:HE2	6:C:7040:HOH:O	2.02	0.58
1:A:97:PRO:HB3	1:C:506:MET:HE1	1.86	0.58
1:C:118:THR:O	1:C:122:GLU:HG3	2.04	0.58
1:C:431:ALA:HB2	1:C:487:VAL:HG11	1.86	0.58
1:D:422:ARG:NH2	1:D:488:ASP:OD1	2.37	0.57
1:C:422:ARG:NH2	1:C:488:ASP:OD1	2.35	0.57
1:A:381:GLU:HG3	1:D:222:LEU:HD11	1.85	0.57
1:A:451:ARG:HD3	1:A:451:ARG:C	2.25	0.57
1:F:186:SER:HB3	1:F:187:PRO:HD3	1.85	0.57
1:F:19:GLN:O	1:F:23:GLN:HG2	2.04	0.57
5:A:6001:MPD:H31	6:A:7122:HOH:O	2.05	0.57
1:C:198:LYS:HE2	6:C:7406:HOH:O	2.04	0.57
1:A:146:GLN:H	1:A:146:GLN:NE2	2.02	0.57
1:B:86:VAL:HB	1:B:116:GLN:HG3	1.86	0.56
1:A:229:MET:O	1:A:313:TYR:HB2	2.05	0.56
1:C:90:ARG:HD3	6:C:7322:HOH:O	2.04	0.56
1:D:454:ILE:HG12	1:D:463:MET:HG3	1.86	0.56
1:A:39:GLN:NE2	1:A:44[A]:LYS:HE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ALA:HB3	6:A:7272:HOH:O	2.05	0.56
1:B:422:ARG:NH2	1:B:488:ASP:OD1	2.27	0.56
1:D:453:GLU:CD	1:D:453:GLU:H	2.06	0.56
1:E:506:MET:HE1	6:E:5041:HOH:O	2.06	0.56
1:B:33:GLU:OE2	1:B:37:GLU:HG3	2.06	0.56
1:A:145:ILE:HD12	1:D:448:VAL:HG11	1.87	0.56
1:D:286:ASP:HB3	1:D:289:LYS:CE	2.36	0.56
1:B:464:ARG:HG3	1:B:464:ARG:HH11	1.71	0.56
1:D:286:ASP:CB	1:D:289:LYS:HE2	2.36	0.56
1:B:38:LYS:O	1:B:42:GLN:HG3	2.06	0.55
1:D:97:PRO:HB3	1:E:506:MET:HE3	1.87	0.55
1:F:38:LYS:O	1:F:42:GLN:HG3	2.06	0.55
1:E:218:THR:OG1	1:E:221:GLU:HG3	2.06	0.55
1:B:411:ALA:HB1	1:B:416:TYR:CD2	2.41	0.55
1:B:506:MET:HE2	1:B:506:MET:O	2.06	0.55
1:A:509:THR:O	1:A:511:ARG:HD3	2.07	0.55
1:B:207:GLN:H	1:B:207:GLN:NE2	2.05	0.55
1:E:453:GLU:OE1	1:E:467:LYS:HE3	2.06	0.55
1:D:217:VAL:HG12	6:D:5367:HOH:O	2.05	0.55
1:A:97:PRO:HB3	1:C:506:MET:HE3	1.88	0.55
1:F:218:THR:OG1	1:F:221:GLU:HG3	2.06	0.55
1:F:394:TYR:OH	1:F:520:GLY:HA3	2.06	0.55
1:B:291:TYR:CE2	1:B:336:PRO:HG3	2.42	0.55
1:E:35[B]:ARG:NH1	6:E:5574:HOH:O	2.40	0.55
1:A:506:MET:HG2	1:B:90[B]:ARG:HD2	1.87	0.55
1:B:86:VAL:CG1	1:B:116:GLN:HG3	2.37	0.55
1:E:35[B]:ARG:NH1	6:E:5406:HOH:O	2.40	0.54
1:D:410:LYS:HE2	6:D:5249:HOH:O	2.08	0.54
1:F:81:VAL:HG13	1:F:107:VAL:CG1	2.36	0.54
1:C:282:ILE:HD11	1:C:299:LYS:HD2	1.87	0.54
1:B:444:GLY:O	1:B:448:VAL:HG23	2.07	0.54
1:C:381:GLU:HG3	1:F:222:LEU:HD11	1.90	0.54
1:E:8:LYS:HE3	6:E:5543:HOH:O	2.08	0.54
1:B:506:MET:HE1	1:C:132:THR:HG21	1.90	0.54
1:C:213:THR:HG21	1:C:215:GLU:OE2	2.07	0.54
1:A:175:ILE:HB	1:A:195:MET:HG2	1.89	0.54
1:B:18:GLU:O	1:B:22:GLU:HG3	2.08	0.54
1:C:14:GLU:O	1:C:18:GLU:HG3	2.07	0.54
1:C:86:VAL:HB	1:C:116:GLN:HG3	1.89	0.54
1:D:461:ASP:C	1:D:463:MET:H	2.10	0.54
1:B:460:PRO:HA	1:B:463:MET:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:GLU:HG3	1:D:37:GLU:OE2	2.07	0.54
1:E:6:ASN:HB2	6:E:5363:HOH:O	2.08	0.54
1:D:175:ILE:HB	1:D:195:MET:HG2	1.90	0.53
1:C:33:GLU:O	1:C:37:GLU:HG3	2.09	0.53
1:D:60:PHE:CE2	1:D:62:GLU:HB2	2.44	0.53
1:A:411:ALA:HB3	1:A:437:ILE:HA	1.91	0.53
1:B:469:GLU:HG3	1:B:473:ASN:HD21	1.74	0.53
1:A:207:GLN:NE2	1:A:207:GLN:N	2.57	0.53
1:D:7:LEU:N	1:D:7:LEU:HD13	2.24	0.52
6:D:5271:HOH:O	1:E:506:MET:HG2	2.10	0.52
1:A:506:MET:HG2	1:B:90[B]:ARG:CD	2.39	0.52
1:D:33:GLU:O	1:D:37:GLU:HG3	2.08	0.52
1:C:433:PRO:HD3	1:C:491:ILE:O	2.09	0.52
1:E:146:GLN:H	1:E:146:GLN:NE2	2.00	0.52
1:B:469:GLU:HG3	1:B:473:ASN:ND2	2.24	0.52
1:D:32:GLY:O	1:D:36:VAL:HG23	2.10	0.52
1:E:220:ASP:HB3	6:E:5497:HOH:O	2.08	0.52
1:E:316:ASN:HB3	1:E:339:MET:HE3	1.91	0.52
1:D:433:PRO:CG	1:F:13:MET:HE2	2.40	0.51
1:E:178:PRO:HG3	6:E:5458:HOH:O	2.10	0.51
1:B:459:ASP:N	1:B:460:PRO:CD	2.71	0.51
1:B:452:LYS:HG2	6:B:7387:HOH:O	2.08	0.51
1:A:339:MET:CE	1:A:375:LEU:HD22	2.41	0.51
1:E:131:GLY:HA3	1:F:511:ARG:HH12	1.76	0.51
1:C:404:ILE:HD13	1:C:503:ALA:HB3	1.93	0.51
1:B:207:GLN:HG2	1:B:208:VAL:H	1.76	0.51
1:C:206:PRO:HB2	1:C:207:GLN:NE2	2.26	0.50
1:A:339:MET:HE3	1:A:375:LEU:HD22	1.93	0.50
1:C:198:LYS:HD2	1:C:198:LYS:N	2.26	0.50
1:B:454:ILE:HG12	1:B:463:MET:HG3	1.93	0.50
1:B:506:MET:HE1	1:C:132:THR:CG2	2.42	0.50
1:C:394:TYR:CD2	1:C:522:PHE:HD2	2.29	0.50
1:A:463:MET:O	1:A:467:LYS:HG2	2.11	0.50
1:D:81:VAL:HG13	1:D:107:VAL:CG1	2.42	0.50
1:E:506:MET:O	1:E:506:MET:SD	2.70	0.50
1:C:229:MET:O	1:C:313:TYR:HB2	2.12	0.49
1:E:452:LYS:CD	1:E:453:GLU:N	2.60	0.49
1:B:451:ARG:HG3	1:B:452:LYS:H	1.76	0.49
1:D:34:ARG:HD3	1:D:34:ARG:C	2.33	0.49
1:E:394:TYR:OH	1:E:520:GLY:HA3	2.12	0.49
1:E:446:ALA:HA	1:E:450:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:VAL:HB	1:F:116:GLN:HG3	1.94	0.49
1:D:308:GLU:OE2	1:D:318:VAL:HG13	2.11	0.49
1:D:240:GLU:N	6:D:5492:HOH:O	2.45	0.49
1:C:451:ARG:HG3	1:C:452:LYS:HG3	1.95	0.49
1:C:447:ASN:HD22	1:C:447:ASN:N	2.09	0.48
1:F:443:GLU:HA	1:F:468:ILE:HG12	1.94	0.48
1:E:175:ILE:HB	1:E:195:MET:HG3	1.94	0.48
1:A:394:TYR:OH	1:A:520:GLY:HA3	2.12	0.48
1:C:379:GLN:HA	1:C:379:GLN:NE2	2.29	0.48
1:E:44:LYS:NZ	6:E:5413:HOH:O	2.45	0.48
1:C:122:GLU:O	1:C:126:GLN:HG2	2.13	0.48
1:D:97:PRO:CB	1:E:506:MET:HE3	2.44	0.48
1:D:323:ARG:HA	1:D:327:ARG:O	2.13	0.48
1:C:371:VAL:HG22	1:C:373:GLY:H	1.78	0.48
1:C:439:VAL:HA	1:F:152:LEU:HG	1.96	0.48
1:C:208:VAL:HG23	6:C:7333:HOH:O	2.13	0.48
1:C:463:MET:HA	1:C:463:MET:CE	2.43	0.48
1:E:90:ARG:HG3	1:F:506:MET:HE3	1.95	0.48
1:B:454:ILE:O	1:B:460:PRO:HG3	2.13	0.48
1:A:282:ILE:HD11	1:A:299:LYS:HD2	1.96	0.48
1:F:122:GLU:O	1:F:126:GLN:HG2	2.14	0.48
1:F:291:TYR:CZ	1:F:336:PRO:HG2	2.49	0.48
1:D:295:ASP:O	1:D:299:LYS:HE2	2.13	0.47
1:D:411:ALA:HB1	1:D:416:TYR:CD2	2.49	0.47
1:A:370:ASP:CG	1:A:409:ARG:HB3	2.35	0.47
1:D:433:PRO:HG2	1:F:13:MET:HE2	1.96	0.47
1:B:506:MET:O	1:B:506:MET:CE	2.62	0.47
1:F:229:MET:O	1:F:313:TYR:HB2	2.14	0.47
1:E:446:ALA:HA	1:E:450:PHE:HD1	1.80	0.47
1:F:24:ARG:O	1:F:28:GLU:HG3	2.15	0.47
1:F:250:LYS:HE2	6:F:6472:HOH:O	2.15	0.47
1:A:422:ARG:NH2	1:A:488:ASP:OD1	2.35	0.47
1:B:286:ASP:CB	1:B:289:LYS:HE2	2.45	0.47
1:D:454:ILE:HG12	1:D:463:MET:CG	2.45	0.47
1:A:126[A]:GLN:NE2	1:C:507:TYR:OH	2.48	0.47
1:C:446:ALA:HA	1:C:450:PHE:CD1	2.50	0.47
1:D:201:MET:O	1:D:228:HIS:NE2	2.41	0.46
1:D:450:PHE:CD2	1:D:467:LYS:HE2	2.49	0.46
1:D:334:ASN:O	1:D:336:PRO:HD3	2.15	0.46
1:D:432:TRP:CD2	1:D:493:PRO:HB3	2.51	0.46
1:B:484:ARG:HD2	1:C:70:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:LYS:HA	1:D:455:LYS:HE3	1.97	0.46
1:B:455:LYS:HE2	1:B:455:LYS:HB3	1.81	0.46
1:C:38:LYS:O	1:C:42:GLN:HG3	2.14	0.46
1:D:461:ASP:O	1:D:462:ALA:HB3	2.16	0.46
1:D:475:PHE:HA	1:D:480:VAL:HG11	1.98	0.46
1:D:509:THR:HB	6:D:5487:HOH:O	2.14	0.46
1:B:29:ALA:HB1	6:B:7347:HOH:O	2.16	0.46
1:C:506:MET:CE	1:C:506:MET:HA	2.45	0.46
1:E:210:LYS:HD2	1:E:214:GLY:C	2.35	0.46
1:B:229:MET:O	1:B:313:TYR:HB2	2.16	0.46
1:E:345:ILE:HG23	1:E:388:HIS:CG	2.51	0.46
1:F:42:GLN:O	1:F:198:LYS:HE2	2.15	0.46
1:A:67:ARG:HD2	1:C:483:ALA:O	2.16	0.46
1:C:279:LEU:HD21	1:C:299:LYS:HB2	1.98	0.46
1:E:291:TYR:CE2	1:E:336:PRO:HG2	2.51	0.46
1:B:39:GLN:NE2	1:B:44:LYS:HE2	2.31	0.45
1:D:345:ILE:HG21	6:D:5491:HOH:O	2.16	0.45
1:F:372:PRO:HB3	1:F:410:LYS:HD3	1.98	0.45
1:C:323:ARG:HA	1:C:327:ARG:O	2.16	0.45
1:F:207:GLN:NE2	6:F:6191:HOH:O	2.49	0.45
1:C:506:MET:HE1	6:C:7040:HOH:O	2.13	0.45
1:D:9:LEU:HD13	1:D:16:ARG:NH1	2.32	0.45
1:E:5:ASN:HB3	6:E:5543:HOH:O	2.16	0.45
1:E:34:ARG:HH11	1:E:34:ARG:CA	2.29	0.45
1:B:411:ALA:HB3	1:B:437:ILE:HA	1.98	0.45
1:A:413:GLY:HA2	1:D:152:LEU:HD13	1.97	0.45
1:A:446:ALA:C	1:A:448:VAL:H	2.20	0.45
1:D:77:ASP:OD2	1:D:78:LYS:HD3	2.17	0.45
1:C:394:TYR:OH	1:C:520:GLY:HA3	2.16	0.45
1:A:122:GLU:O	1:A:126[A]:GLN:HG3	2.16	0.45
1:B:457:ALA:C	1:B:459:ASP:H	2.20	0.45
1:E:81:VAL:HG13	1:E:107:VAL:CG1	2.47	0.45
1:E:229:MET:O	1:E:313:TYR:HB2	2.17	0.45
1:D:404:ILE:HD12	1:D:503:ALA:HB1	1.99	0.45
1:D:136:PHE:HD2	1:D:137:PHE:N	2.15	0.44
1:F:370:ASP:CG	1:F:409:ARG:HB3	2.37	0.44
1:B:506:MET:HG2	1:C:90:ARG:HD2	1.98	0.44
1:A:81:VAL:HG13	1:A:107:VAL:CG1	2.48	0.44
1:C:377:GLY:HA3	6:F:6338:HOH:O	2.17	0.44
1:B:452:LYS:O	1:B:455:LYS:HE2	2.17	0.44
1:D:44:LYS:NZ	6:D:5499:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:VAL:HG12	1:F:84:ASP:HA	1.99	0.44
1:D:178:PRO:HG3	6:D:5343:HOH:O	2.18	0.44
1:D:452:LYS:HB2	1:D:452:LYS:HZ2	1.80	0.44
1:D:452:LYS:O	1:D:454:ILE:N	2.49	0.44
1:A:235:ILE:O	1:A:310:LYS:HG2	2.17	0.44
1:B:450:PHE:HA	1:B:453:GLU:HG2	2.00	0.44
1:C:207:GLN:CD	1:C:207:GLN:N	2.69	0.44
1:F:287:GLY:HA3	6:F:6514:HOH:O	2.18	0.44
1:A:454:ILE:HA	1:A:463:MET:HG2	1.98	0.44
1:B:431:ALA:HB2	1:B:487:VAL:HG11	1.99	0.44
1:D:138:TYR:CE2	1:D:173:ALA:HB1	2.52	0.44
1:A:513:THR:HA	6:A:7462:HOH:O	2.17	0.44
1:B:136:PHE:HD2	1:B:137:PHE:N	2.15	0.44
1:C:447:ASN:N	1:C:447:ASN:ND2	2.65	0.44
1:C:450:PHE:CE2	1:C:467:LYS:HD2	2.53	0.44
1:A:54:LEU:O	1:A:250:LYS:HE2	2.18	0.44
1:D:422:ARG:O	1:D:422:ARG:HG3	2.17	0.44
1:C:411:ALA:HB3	1:C:437:ILE:HA	1.99	0.43
1:E:60:PHE:CE2	1:E:62:GLU:HB2	2.53	0.43
1:B:454:ILE:HG22	1:B:460:PRO:HB3	2.00	0.43
1:F:411:ALA:HB3	1:F:437:ILE:HA	2.00	0.43
1:C:339:MET:CE	1:C:375:LEU:HD22	2.48	0.43
1:C:370:ASP:CG	1:C:409:ARG:HB3	2.37	0.43
1:A:511:ARG:NH1	1:B:131:GLY:HA3	2.13	0.43
1:B:338:VAL:HG12	1:B:339:MET:HE3	2.01	0.43
1:D:174:ILE:HD11	1:D:249:ALA:HB2	2.01	0.43
1:D:433:PRO:HD3	1:D:493:PRO:HD3	1.99	0.43
1:D:467:LYS:HE3	1:D:467:LYS:HA	1.99	0.43
1:F:228:HIS:HA	1:F:232[B]:SER:HG	1.82	0.43
1:A:186:SER:HB3	1:A:187:PRO:CD	2.43	0.43
1:A:433:PRO:HD3	1:A:491:ILE:O	2.19	0.43
1:B:72:THR:HB	1:B:77:ASP:HB3	2.01	0.43
1:C:293:VAL:HG21	1:C:333:ALA:HB1	1.99	0.43
1:A:92:THR:HA	1:A:96:ARG:O	2.19	0.43
1:B:68:LYS:HE3	6:B:7024:HOH:O	2.19	0.43
1:B:86:VAL:CB	1:B:116:GLN:HG3	2.49	0.43
1:D:38:LYS:O	1:D:42:GLN:HG3	2.18	0.43
1:A:205:GLY:HA3	1:A:207:GLN:HE22	1.84	0.43
1:D:433:PRO:CD	1:D:493:PRO:HD3	2.49	0.43
1:E:411:ALA:HB3	1:E:437:ILE:HA	2.01	0.43
1:E:433:PRO:HD3	1:E:491:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:TYR:CZ	1:A:336:PRO:HG2	2.54	0.43
1:D:94:LEU:HB3	6:D:5365:HOH:O	2.19	0.43
1:D:461:ASP:C	1:D:463:MET:N	2.71	0.43
1:F:13:MET:CE	1:F:13:MET:HA	2.49	0.43
1:E:273:VAL:HG22	6:E:5510:HOH:O	2.18	0.42
1:F:31:GLY:O	1:F:35:ARG:HG3	2.19	0.42
1:F:158:MET:HE3	1:F:186:SER:HB2	2.01	0.42
1:B:506:MET:HG2	1:C:90:ARG:CD	2.49	0.42
1:C:276:ASN:OD1	1:C:278:GLU:HB2	2.19	0.42
1:D:403:LYS:HE3	1:D:425:GLY:O	2.18	0.42
1:D:438:ALA:HB2	1:D:476:ASN:ND2	2.35	0.42
1:F:10:ALA:HB1	6:F:6463:HOH:O	2.18	0.42
1:A:323:ARG:HA	1:A:327:ARG:O	2.19	0.42
1:D:452:LYS:C	1:D:454:ILE:H	2.23	0.42
1:D:229:MET:O	1:D:313:TYR:HB2	2.18	0.42
1:D:138:TYR:HE2	1:D:173:ALA:HB1	1.85	0.42
1:D:476:ASN:OD1	1:D:476:ASN:N	2.52	0.42
1:B:356[B]:ASN:ND2	6:B:7043:HOH:O	2.52	0.42
1:D:313:TYR:O	1:D:314:ALA:C	2.56	0.42
1:B:291:TYR:CZ	1:B:336:PRO:HG3	2.54	0.42
1:D:280:ARG:CG	1:D:493:PRO:HG2	2.46	0.42
1:F:45:GLN:NE2	1:F:246:GLU:OE1	2.53	0.42
1:D:92:THR:HA	1:D:96:ARG:O	2.20	0.42
6:A:7049:HOH:O	1:D:521:ASN:HB2	2.18	0.42
1:C:517:LYS:HE2	1:F:168:VAL:CG2	2.49	0.42
1:D:210:LYS:HA	1:D:215:GLU:O	2.20	0.42
1:D:241:ASP:N	6:D:5492:HOH:O	2.27	0.42
1:A:213:THR:OG1	1:A:215:GLU:HG3	2.20	0.41
1:B:9:LEU:HD13	1:B:16:ARG:NH1	2.35	0.41
1:B:34:ARG:HG2	1:B:34:ARG:HH11	1.84	0.41
1:F:128:LEU:CD2	1:F:164:LYS:HE2	2.50	0.41
1:E:146:GLN:NE2	3:E:4005:MCA:H2	2.28	0.41
1:A:452:LYS:HA	1:A:455:LYS:HE2	2.02	0.41
1:D:292:ASP:OD1	1:D:294:ARG:HB2	2.20	0.41
1:D:431:ALA:HB2	1:D:487:VAL:HG11	2.02	0.41
1:E:86:VAL:HB	1:E:116:GLN:HG3	2.02	0.41
1:A:499:LYS:HA	1:A:499:LYS:HD3	1.90	0.41
1:B:178:PRO:HG3	6:B:7357:HOH:O	2.20	0.41
1:D:54:LEU:O	1:D:250:LYS:HE2	2.21	0.41
1:B:394:TYR:C	1:B:394:TYR:CD2	2.92	0.41
1:D:452:LYS:O	1:D:455:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35[A]:ARG:NH2	3:E:4005:MCA:O33	2.53	0.41
1:F:452:LYS:HG2	6:F:6359:HOH:O	2.21	0.41
1:B:454:ILE:HA	1:B:463:MET:CG	2.50	0.41
1:C:196:THR:HA	1:C:239:ALA:O	2.20	0.41
1:C:475:PHE:CZ	1:F:73:LEU:HD12	2.55	0.41
1:E:5:ASN:ND2	1:F:470:GLU:O	2.54	0.41
1:E:404:ILE:HD12	1:E:503:ALA:HB1	2.02	0.41
1:A:311:ALA:N	6:A:7272:HOH:O	2.53	0.41
1:C:54:LEU:O	1:C:250:LYS:HE2	2.20	0.41
1:C:222:LEU:HD21	1:F:381:GLU:CG	2.45	0.41
1:F:136:PHE:HD2	1:F:137:PHE:N	2.18	0.41
1:F:323:ARG:HA	1:F:327:ARG:O	2.21	0.41
1:F:461:ASP:HA	1:F:464:ARG:NH1	2.36	0.41
1:D:302:ASP:HB3	1:D:303:TRP:CD1	2.56	0.41
1:B:429:VAL:HG12	1:B:487:VAL:HG12	2.02	0.41
1:C:452:LYS:O	1:C:453:GLU:HB3	2.21	0.41
1:D:35:ARG:HH11	1:D:35:ARG:HG2	1.86	0.41
1:D:236:HIS:HB3	1:D:309:VAL:HG13	2.03	0.41
1:D:433:PRO:HD2	1:F:13:MET:HE2	2.02	0.41
1:F:60:PHE:CE2	1:F:62:GLU:HB2	2.56	0.41
1:C:403:LYS:HE3	1:C:425:GLY:O	2.20	0.41
1:E:34:ARG:HB2	1:E:34:ARG:NH1	2.35	0.41
1:A:229:MET:CE	6:A:7272:HOH:O	2.68	0.40
1:A:519:HIS:CE1	1:D:360[B]:SER:OG	2.73	0.40
1:A:196:THR:HA	1:A:239:ALA:O	2.21	0.40
1:B:293:VAL:HG21	1:B:333:ALA:HB1	2.03	0.40
1:D:200:HIS:HB2	6:D:5311:HOH:O	2.21	0.40
1:D:244:ALA:O	1:D:248:ILE:HG13	2.21	0.40
1:F:13:MET:HE3	1:F:13:MET:O	2.22	0.40
1:A:499:LYS:HD3	6:A:7424:HOH:O	2.21	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	519/523 (99%)	499 (96%)	20 (4%)	0	100	100
1	B	520/523 (99%)	494 (95%)	26 (5%)	0	100	100
1	C	507/523 (97%)	486 (96%)	20 (4%)	1 (0%)	47	38
1	D	512/523 (98%)	485 (95%)	26 (5%)	1 (0%)	47	38
1	E	524/523 (100%)	506 (97%)	18 (3%)	0	100	100
1	F	517/523 (99%)	497 (96%)	20 (4%)	0	100	100
All	All	3099/3138 (99%)	2967 (96%)	130 (4%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	10	ALA
1	D	453	GLU

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	410/411 (100%)	402 (98%)	8 (2%)	55	51
1	B	411/411 (100%)	404 (98%)	7 (2%)	60	57
1	C	402/411 (98%)	393 (98%)	9 (2%)	52	47
1	D	407/411 (99%)	401 (98%)	6 (2%)	65	62
1	E	415/411 (101%)	404 (97%)	11 (3%)	44	38
1	F	408/411 (99%)	399 (98%)	9 (2%)	52	47
All	All	2453/2466 (100%)	2403 (98%)	50 (2%)	53	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	PHE
1	A	146	GLN
1	A	152	LEU
1	A	187	PRO
1	A	207	GLN
1	A	226	GLU
1	A	451	ARG
1	A	511	ARG
1	B	136	PHE
1	B	146	GLN
1	B	207	GLN
1	B	317	LEU
1	B	453	GLU
1	B	466	GLU
1	B	469	GLU
1	C	129	LEU
1	C	136	PHE
1	C	146	GLN
1	C	220	ASP
1	C	222	LEU
1	C	262	GLU
1	C	450	PHE
1	C	463	MET
1	C	506	MET
1	D	7	LEU
1	D	34	ARG
1	D	136	PHE
1	D	299	LYS
1	D	367	GLN
1	D	424	LEU
1	E	6	ASN
1	E	25	GLN
1	E	34	ARG
1	E	78	LYS
1	E	136	PHE
1	E	146	GLN
1	E	152	LEU
1	E	187	PRO
1	E	220	ASP
1	E	452	LYS
1	E	506	MET
1	F	25	GLN
1	F	136	PHE

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Mol	Chain	Res	Type
1	F	146	GLN
1	F	152	LEU
1	F	195	MET
1	F	220	ASP
1	F	268	ASN
1	F	307	LEU
1	F	511	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	42	GLN
1	A	45	GLN
1	A	53	ASN
1	A	146	GLN
1	A	207	GLN
1	A	271	ASN
1	A	356	ASN
1	A	447	ASN
1	A	512	GLN
1	B	25	GLN
1	B	146	GLN
1	B	207	GLN
1	B	234	ASN
1	B	268	ASN
1	B	379	GLN
1	B	473	ASN
1	C	45	GLN
1	C	53	ASN
1	C	146	GLN
1	C	207	GLN
1	C	234	ASN
1	C	268	ASN
1	C	271	ASN
1	C	379	GLN
1	C	447	ASN
1	C	473	ASN
1	D	23	GLN
1	D	45	GLN
1	D	53	ASN
1	D	234	ASN

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Mol	Chain	Res	Type
1	D	271	ASN
1	E	5	ASN
1	E	25	GLN
1	E	45	GLN
1	E	53	ASN
1	E	146	GLN
1	E	234	ASN
1	E	268	ASN
1	F	25	GLN
1	F	45	GLN
1	F	53	ASN
1	F	146	GLN
1	F	162	ASN
1	F	207	GLN
1	F	234	ASN
1	F	268	ASN
1	F	271	ASN
1	F	512	GLN

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)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DXX	C	5003	-	5,6,7	2.37	3 (60%)	4,7,9	3.34	3 (75%)
3	MCA	E	4005	-	49,57,57	4.17	25 (51%)	61,85,85	4.81	22 (36%)
3	MCA	F	4006	-	49,57,57	4.15	25 (51%)	61,85,85	4.80	23 (37%)
5	MPD	A	6001	-	7,7,7	0.47	0	9,10,10	0.51	0
5	MPD	F	6006	-	7,7,7	0.57	0	9,10,10	0.53	0
5	MPD	B	6002	-	7,7,7	0.53	0	9,10,10	0.44	0
4	DXX	D	5004	-	5,6,7	2.57	3 (60%)	4,7,9	3.33	3 (75%)
4	DXX	E	5005	-	5,6,7	2.51	3 (60%)	4,7,9	3.21	3 (75%)
4	DXX	A	5001	-	5,6,7	2.40	4 (80%)	4,7,9	3.38	3 (75%)
3	MCA	A	4001	-	49,57,57	4.14	25 (51%)	61,85,85	4.80	25 (40%)
3	MCA	C	4003	-	49,57,57	4.14	26 (53%)	61,85,85	4.84	22 (36%)
4	DXX	F	5006	-	5,6,7	2.30	3 (60%)	4,7,9	3.37	3 (75%)
4	DXX	B	5002	-	5,6,7	2.40	3 (60%)	4,7,9	3.33	3 (75%)
3	MCA	D	4004	-	49,57,57	4.16	22 (44%)	61,85,85	4.81	24 (39%)
3	MCA	B	4002	-	49,57,57	4.17	24 (48%)	61,85,85	4.83	25 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DXX	C	5003	-	-	2/6/6/8	-
3	MCA	E	4005	-	1/1/14/16	18/55/75/75	0/3/3/3
3	MCA	F	4006	-	1/1/14/16	12/55/75/75	0/3/3/3
5	MPD	A	6001	-	-	0/5/5/5	-
5	MPD	F	6006	-	-	0/5/5/5	-
5	MPD	B	6002	-	-	3/5/5/5	-
4	DXX	D	5004	-	-	3/6/6/8	-
4	DXX	E	5005	-	-	2/6/6/8	-
4	DXX	A	5001	-	-	1/6/6/8	-
3	MCA	A	4001	-	1/1/14/16	14/55/75/75	0/3/3/3
3	MCA	C	4003	-	1/1/14/16	17/55/75/75	0/3/3/3
4	DXX	F	5006	-	-	4/6/6/8	-
4	DXX	B	5002	-	-	2/6/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MCA	D	4004	-	1/1/14/16	11/55/75/75	0/3/3/3
3	MCA	B	4002	-	1/1/14/16	18/55/75/75	0/3/3/3

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4005	MCA	CS2-CS1	-16.00	1.40	1.53
3	C	4003	MCA	CS2-CS1	-15.81	1.40	1.53
3	A	4001	MCA	CS2-CS1	-15.62	1.41	1.53
3	F	4006	MCA	CS2-CS1	-15.50	1.41	1.53
3	B	4002	MCA	CS2-CS1	-15.48	1.41	1.53
3	D	4004	MCA	CS2-CS1	-15.27	1.41	1.53
3	D	4004	MCA	OP3-CP7	-10.33	1.23	1.42
3	F	4006	MCA	OP3-CP7	-10.07	1.23	1.42
3	A	4001	MCA	OP3-CP7	-10.06	1.23	1.42
3	B	4002	MCA	OP3-CP7	-9.90	1.24	1.42
3	C	4003	MCA	OP3-CP7	-9.76	1.24	1.42
3	E	4005	MCA	OP3-CP7	-9.60	1.24	1.42
3	B	4002	MCA	CP6-NP2	7.22	1.49	1.33
3	D	4004	MCA	CP6-NP2	7.20	1.49	1.33
3	E	4005	MCA	O7-CPB	-7.19	1.20	1.43
3	A	4001	MCA	O7-CPB	-7.18	1.20	1.43
3	D	4004	MCA	O7-CPB	-7.12	1.20	1.43
3	C	4003	MCA	O7-CPB	-7.11	1.20	1.43
3	F	4006	MCA	O7-CPB	-7.11	1.20	1.43
3	C	4003	MCA	CP6-NP2	7.11	1.49	1.33
3	F	4006	MCA	CP6-NP2	7.05	1.49	1.33
3	B	4002	MCA	O7-CPB	-7.01	1.21	1.43
3	D	4004	MCA	CP1-S	-6.78	1.53	1.81
3	E	4005	MCA	CP1-S	-6.77	1.53	1.81
3	B	4002	MCA	CP1-S	-6.71	1.53	1.81
3	E	4005	MCA	CS3-CS2	-6.70	1.32	1.53
3	E	4005	MCA	CP6-NP2	6.69	1.48	1.33
3	F	4006	MCA	CP1-S	-6.62	1.54	1.81
3	A	4001	MCA	CP3-NP1	6.58	1.48	1.33
3	A	4001	MCA	CS3-CS2	-6.57	1.33	1.53
3	A	4001	MCA	CP6-NP2	6.56	1.47	1.33
3	C	4003	MCA	CP1-S	-6.56	1.54	1.81
3	B	4002	MCA	CP3-NP1	6.55	1.48	1.33
3	B	4002	MCA	CS3-CS2	-6.53	1.33	1.53
3	A	4001	MCA	CP1-S	-6.52	1.54	1.81
3	D	4004	MCA	CS3-CS2	-6.51	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4004	MCA	CP3-NP1	6.50	1.48	1.33
3	F	4006	MCA	CP3-NP1	6.48	1.48	1.33
3	F	4006	MCA	CS3-CS2	-6.48	1.33	1.53
3	C	4003	MCA	CP3-NP1	6.37	1.47	1.33
3	E	4005	MCA	OP1-CP3	6.36	1.36	1.23
3	B	4002	MCA	O5'-C5'	-6.34	1.20	1.44
3	C	4003	MCA	O5'-C5'	-6.32	1.20	1.44
3	D	4004	MCA	O5'-C5'	-6.27	1.20	1.44
3	F	4006	MCA	O5'-C5'	-6.21	1.20	1.44
3	A	4001	MCA	O5'-C5'	-6.20	1.20	1.44
3	E	4005	MCA	O5'-C5'	-6.16	1.21	1.44
3	B	4002	MCA	OP1-CP3	6.14	1.35	1.23
3	A	4001	MCA	OP1-CP3	6.12	1.35	1.23
3	C	4003	MCA	CS3-CS2	-6.12	1.34	1.53
3	E	4005	MCA	CP3-NP1	6.10	1.47	1.33
3	F	4006	MCA	OP1-CP3	6.07	1.35	1.23
3	D	4004	MCA	OP1-CP3	5.92	1.35	1.23
3	C	4003	MCA	OP1-CP3	5.92	1.35	1.23
3	D	4004	MCA	P1-O5'	-5.05	1.38	1.59
3	F	4006	MCA	P1-O5'	-4.99	1.39	1.59
3	C	4003	MCA	P1-O5'	-4.97	1.39	1.59
3	E	4005	MCA	P1-O5'	-4.96	1.39	1.59
3	B	4002	MCA	P1-O5'	-4.91	1.39	1.59
3	A	4001	MCA	P1-O5'	-4.89	1.39	1.59
3	B	4002	MCA	P1-O12	-4.54	1.34	1.55
3	E	4005	MCA	P1-O12	-4.53	1.34	1.55
3	F	4006	MCA	OS1-CS1	4.52	1.27	1.20
3	D	4004	MCA	P1-O12	-4.47	1.34	1.55
3	C	4003	MCA	P1-O12	-4.47	1.34	1.55
3	A	4001	MCA	P1-O12	-4.47	1.34	1.55
3	F	4006	MCA	P1-O12	-4.42	1.34	1.55
3	B	4002	MCA	P3-O3'	4.19	1.67	1.59
3	B	4002	MCA	OS1-CS1	4.17	1.26	1.20
3	A	4001	MCA	OS1-CS1	4.13	1.26	1.20
3	D	4004	MCA	OS1-CS1	4.11	1.26	1.20
3	E	4005	MCA	OS1-CS1	4.09	1.26	1.20
3	C	4003	MCA	OS1-CS1	4.04	1.26	1.20
3	D	4004	MCA	P3-O3'	3.94	1.66	1.59
3	D	4004	MCA	P1-O11	-3.93	1.37	1.50
3	F	4006	MCA	P3-O3'	3.92	1.66	1.59
3	C	4003	MCA	P1-O11	-3.91	1.37	1.50
4	E	5005	DXX	CB-CA	-3.86	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4002	MCA	P1-O11	-3.86	1.37	1.50
3	E	4005	MCA	C2-N3	3.85	1.38	1.32
3	E	4005	MCA	P1-O11	-3.83	1.37	1.50
3	F	4006	MCA	P1-O11	-3.80	1.37	1.50
3	B	4002	MCA	C2-N3	3.75	1.38	1.32
4	D	5004	DXX	CB-CA	-3.73	1.40	1.52
3	A	4001	MCA	P1-O11	-3.70	1.37	1.50
3	D	4004	MCA	C2-N3	3.69	1.38	1.32
3	F	4006	MCA	C2-N3	3.65	1.38	1.32
3	F	4006	MCA	CS1-S	-3.62	1.63	1.75
3	C	4003	MCA	C4-N3	3.56	1.40	1.35
3	A	4001	MCA	C2-N3	3.55	1.37	1.32
3	A	4001	MCA	P3-O3'	3.55	1.66	1.59
4	A	5001	DXX	CB-CA	-3.55	1.41	1.52
4	B	5002	DXX	CB-CA	-3.54	1.41	1.52
3	C	4003	MCA	C2-N3	3.53	1.37	1.32
4	C	5003	DXX	CB-CA	-3.53	1.41	1.52
3	B	4002	MCA	CS1-S	-3.53	1.63	1.75
3	C	4003	MCA	P3-O3'	3.51	1.65	1.59
3	A	4001	MCA	CS1-S	-3.45	1.63	1.75
3	D	4004	MCA	P2-O21	-3.44	1.38	1.50
3	A	4001	MCA	P2-O21	-3.40	1.38	1.50
4	F	5006	DXX	CB-CA	-3.36	1.41	1.52
3	D	4004	MCA	CS1-S	-3.36	1.63	1.75
3	E	4005	MCA	P2-O21	-3.35	1.39	1.50
3	B	4002	MCA	P2-O21	-3.31	1.39	1.50
3	E	4005	MCA	CS1-S	-3.30	1.64	1.75
3	F	4006	MCA	P2-O21	-3.28	1.39	1.50
3	B	4002	MCA	P2-O22	-3.27	1.40	1.55
3	C	4003	MCA	P2-O21	-3.19	1.39	1.50
3	D	4004	MCA	P2-O22	-3.19	1.40	1.55
3	E	4005	MCA	C4-N3	3.14	1.40	1.35
3	A	4001	MCA	P2-O22	-3.12	1.40	1.55
3	F	4006	MCA	P2-O22	-3.12	1.40	1.55
3	C	4003	MCA	P2-O22	-3.10	1.40	1.55
3	E	4005	MCA	P3-O3'	3.09	1.65	1.59
3	E	4005	MCA	P2-O22	-3.00	1.41	1.55
3	C	4003	MCA	CS1-S	-2.99	1.65	1.75
3	E	4005	MCA	CP4-CP3	-2.98	1.45	1.51
3	D	4004	MCA	CP4-CP3	-2.95	1.45	1.51
4	D	5004	DXX	CA-C	-2.94	1.43	1.51
3	C	4003	MCA	OP2-CP6	2.93	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4001	MCA	C4-N3	2.92	1.39	1.35
3	B	4002	MCA	CP4-CP3	-2.89	1.45	1.51
3	B	4002	MCA	C4-N3	2.88	1.39	1.35
3	D	4004	MCA	C4-N3	2.83	1.39	1.35
3	C	4003	MCA	CP4-CP3	-2.80	1.46	1.51
3	E	4005	MCA	OP2-CP6	2.80	1.29	1.23
3	D	4004	MCA	OP2-CP6	2.79	1.28	1.23
3	D	4004	MCA	CP5-CP4	-2.75	1.42	1.51
3	A	4001	MCA	OP2-CP6	2.73	1.28	1.23
3	F	4006	MCA	CP4-CP3	-2.71	1.46	1.51
3	F	4006	MCA	CP5-CP4	-2.70	1.42	1.51
3	B	4002	MCA	CP5-CP4	-2.66	1.43	1.51
3	C	4003	MCA	CP5-CP4	-2.65	1.43	1.51
3	A	4001	MCA	CP4-CP3	-2.64	1.46	1.51
4	E	5005	DXX	CA-C	-2.63	1.44	1.51
3	F	4006	MCA	C4-N3	2.62	1.39	1.35
4	A	5001	DXX	O1-C1	-2.61	1.31	1.42
3	F	4006	MCA	OP2-CP6	2.53	1.28	1.23
3	A	4001	MCA	CP5-CP4	-2.51	1.43	1.51
3	E	4005	MCA	CP5-CP4	-2.50	1.43	1.51
3	B	4002	MCA	OP2-CP6	2.46	1.28	1.23
3	B	4002	MCA	OS4-CS4	-2.45	1.22	1.30
4	B	5002	DXX	CA-C	-2.44	1.44	1.51
4	D	5004	DXX	O1-C1	-2.41	1.32	1.42
4	E	5005	DXX	O1-C1	-2.39	1.32	1.42
4	F	5006	DXX	O1-C1	-2.38	1.32	1.42
4	B	5002	DXX	O1-C1	-2.38	1.32	1.42
4	C	5003	DXX	CA-C	-2.38	1.44	1.51
4	F	5006	DXX	CA-C	-2.35	1.44	1.51
4	C	5003	DXX	O1-C1	-2.35	1.32	1.42
3	C	4003	MCA	C2-N1	2.33	1.38	1.33
3	C	4003	MCA	C8-N7	-2.26	1.30	1.34
3	B	4002	MCA	C5'-C4'	2.25	1.58	1.51
3	E	4005	MCA	C5'-C4'	2.23	1.58	1.51
3	F	4006	MCA	C8-N7	-2.21	1.30	1.34
3	E	4005	MCA	C2-N1	2.21	1.38	1.33
3	A	4001	MCA	C5'-C4'	2.20	1.58	1.51
3	C	4003	MCA	C5'-C4'	2.15	1.58	1.51
3	F	4006	MCA	C5'-C4'	2.12	1.58	1.51
3	F	4006	MCA	C2-N1	2.12	1.37	1.33
3	E	4005	MCA	OS4-CS4	-2.10	1.23	1.30
4	A	5001	DXX	CA-C	-2.10	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4003	MCA	OS4-CS4	-2.10	1.23	1.30
3	A	4001	MCA	C8-N7	-2.09	1.31	1.34
3	A	4001	MCA	OS4-CS4	-2.08	1.23	1.30
4	A	5001	DXX	O2-C	-2.05	1.23	1.30

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	4005	MCA	CP4-CP5-NP2	16.16	144.52	111.90
3	D	4004	MCA	CP4-CP5-NP2	16.04	144.28	111.90
3	C	4003	MCA	CP4-CP5-NP2	15.88	143.96	111.90
3	A	4001	MCA	CP4-CP5-NP2	15.81	143.81	111.90
3	F	4006	MCA	CP4-CP5-NP2	15.77	143.74	111.90
3	B	4002	MCA	CP4-CP5-NP2	15.77	143.72	111.90
3	C	4003	MCA	OS1-CS1-CS2	-14.44	100.91	124.12
3	E	4005	MCA	OS1-CS1-CS2	-14.02	101.58	124.12
3	B	4002	MCA	OS1-CS1-CS2	-13.81	101.91	124.12
3	A	4001	MCA	OS1-CS1-CS2	-13.75	102.02	124.12
3	D	4004	MCA	OS1-CS1-CS2	-13.56	102.32	124.12
3	F	4006	MCA	OS1-CS1-CS2	-12.97	103.26	124.12
3	D	4004	MCA	P2-O6-P1	12.48	175.66	132.83
3	C	4003	MCA	CP4-CP3-NP1	12.39	137.28	116.42
3	B	4002	MCA	P2-O6-P1	12.20	174.69	132.83
3	F	4006	MCA	CP4-CP3-NP1	12.16	136.89	116.42
3	E	4005	MCA	CP4-CP3-NP1	12.13	136.85	116.42
3	D	4004	MCA	CP4-CP3-NP1	12.07	136.74	116.42
3	B	4002	MCA	CP4-CP3-NP1	12.00	136.63	116.42
3	A	4001	MCA	CP4-CP3-NP1	11.98	136.59	116.42
3	F	4006	MCA	P2-O6-P1	11.94	173.81	132.83
3	C	4003	MCA	P2-O6-P1	11.88	173.59	132.83
3	A	4001	MCA	P2-O6-P1	11.68	172.90	132.83
3	E	4005	MCA	P2-O6-P1	11.66	172.83	132.83
3	B	4002	MCA	O7-CPB-CPA	11.38	128.84	110.55
3	F	4006	MCA	O7-CPB-CPA	11.13	128.45	110.55
3	A	4001	MCA	O7-CPB-CPA	10.76	127.85	110.55
3	D	4004	MCA	O7-CPB-CPA	10.67	127.70	110.55
3	E	4005	MCA	O7-CPB-CPA	10.54	127.50	110.55
3	C	4003	MCA	O7-CPB-CPA	10.27	127.05	110.55
3	D	4004	MCA	OS1-CS1-S	9.37	136.41	123.80
3	C	4003	MCA	CP5-CP4-CP3	9.22	127.71	112.36
3	D	4004	MCA	OP1-CP3-CP4	-8.96	105.64	122.02
3	B	4002	MCA	OP1-CP3-CP4	-8.93	105.68	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4006	MCA	OS1-CS1-S	8.92	135.81	123.80
3	A	4001	MCA	CP5-CP4-CP3	8.91	127.19	112.36
3	F	4006	MCA	OP1-CP3-CP4	-8.90	105.74	122.02
3	A	4001	MCA	OP1-CP3-CP4	-8.89	105.75	122.02
3	B	4002	MCA	CP5-CP4-CP3	8.86	127.11	112.36
3	C	4003	MCA	OP1-CP3-CP4	-8.79	105.94	122.02
3	F	4006	MCA	CP5-CP4-CP3	8.79	126.99	112.36
3	E	4005	MCA	OP1-CP3-CP4	-8.75	106.01	122.02
3	A	4001	MCA	OS1-CS1-S	8.66	135.45	123.80
3	B	4002	MCA	OS1-CS1-S	8.64	135.43	123.80
3	E	4005	MCA	CP5-CP4-CP3	8.42	126.38	112.36
3	D	4004	MCA	CP5-CP4-CP3	8.36	126.28	112.36
3	E	4005	MCA	OS1-CS1-S	8.30	134.98	123.80
3	C	4003	MCA	OS1-CS1-S	8.20	134.84	123.80
3	C	4003	MCA	CP1-S-CS1	-7.42	79.41	101.75
3	E	4005	MCA	CP1-S-CS1	-7.22	80.04	101.75
3	F	4006	MCA	CP1-S-CS1	-7.14	80.26	101.75
3	B	4002	MCA	CP1-S-CS1	-7.04	80.58	101.75
3	D	4004	MCA	CP1-S-CS1	-6.95	80.84	101.75
3	A	4001	MCA	CP1-S-CS1	-6.87	81.07	101.75
3	A	4001	MCA	CP9-CPA-CP7	6.69	120.42	108.82
3	B	4002	MCA	CP9-CPA-CP7	6.68	120.41	108.82
3	E	4005	MCA	CP9-CPA-CP7	6.60	120.26	108.82
3	C	4003	MCA	CP9-CPA-CP7	6.51	120.11	108.82
3	D	4004	MCA	CP9-CPA-CP7	6.47	120.04	108.82
3	F	4006	MCA	CP9-CPA-CP7	6.41	119.93	108.82
3	C	4003	MCA	CP2-NP1-CP3	-6.26	111.22	122.84
3	E	4005	MCA	CP2-NP1-CP3	-6.12	111.47	122.84
3	F	4006	MCA	O3'-P3-O31	-5.65	87.57	109.39
3	C	4003	MCA	O3'-P3-O31	-5.65	87.59	109.39
3	D	4004	MCA	O3'-P3-O31	-5.60	87.79	109.39
3	A	4001	MCA	O3'-P3-O31	-5.54	88.01	109.39
4	A	5001	DXX	CB-CA-C	5.49	123.81	108.94
3	B	4002	MCA	O3'-P3-O31	-5.49	88.19	109.39
3	E	4005	MCA	O3'-P3-O31	-5.48	88.23	109.39
3	F	4006	MCA	CP2-NP1-CP3	-5.42	112.77	122.84
3	A	4001	MCA	CP5-NP2-CP6	-5.39	112.98	122.59
3	A	4001	MCA	P1-O5'-C5'	5.36	153.13	121.68
4	B	5002	DXX	CB-CA-C	5.31	123.31	108.94
3	E	4005	MCA	P1-O5'-C5'	5.29	152.73	121.68
3	F	4006	MCA	P1-O5'-C5'	5.29	152.71	121.68
4	F	5006	DXX	CB-CA-C	5.27	123.20	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	4002	MCA	CP2-NP1-CP3	-5.26	113.06	122.84
4	C	5003	DXX	CB-CA-C	5.24	123.14	108.94
3	C	4003	MCA	P1-O5'-C5'	5.24	152.42	121.68
3	D	4004	MCA	CP2-NP1-CP3	-5.23	113.13	122.84
3	B	4002	MCA	P1-O5'-C5'	5.21	152.22	121.68
3	F	4006	MCA	CP5-NP2-CP6	-5.18	113.34	122.59
4	D	5004	DXX	CB-CA-C	5.16	122.92	108.94
3	A	4001	MCA	CP2-NP1-CP3	-5.15	113.28	122.84
3	D	4004	MCA	P1-O5'-C5'	5.13	151.77	121.68
3	B	4002	MCA	CP5-NP2-CP6	-4.92	113.81	122.59
4	E	5005	DXX	CB-CA-C	4.90	122.22	108.94
3	E	4005	MCA	CP5-NP2-CP6	-4.84	113.95	122.59
3	C	4003	MCA	CP5-NP2-CP6	-4.76	114.09	122.59
3	D	4004	MCA	CP5-NP2-CP6	-4.55	114.48	122.59
3	A	4001	MCA	CS2-CS1-S	-3.76	107.74	111.81
3	D	4004	MCA	CP1-CP2-NP1	-3.40	105.26	112.42
3	C	4003	MCA	OP1-CP3-NP1	-3.30	116.78	123.01
3	F	4006	MCA	CS2-CS1-S	-3.27	108.27	111.81
3	A	4001	MCA	O33-P3-O3'	3.26	120.60	105.99
3	F	4006	MCA	O33-P3-O3'	3.24	120.53	105.99
3	B	4002	MCA	O33-P3-O3'	3.24	120.50	105.99
3	B	4002	MCA	CP1-CP2-NP1	-3.23	105.63	112.42
4	D	5004	DXX	O-C-CA	-3.22	111.47	122.02
3	D	4004	MCA	O33-P3-O3'	3.21	120.37	105.99
4	E	5005	DXX	O-C-CA	-3.17	111.63	122.02
3	E	4005	MCA	O12-P1-O5'	-3.15	93.14	107.75
4	F	5006	DXX	O-C-CA	-3.14	111.71	122.02
3	C	4003	MCA	O33-P3-O3'	3.14	120.05	105.99
3	E	4005	MCA	OP1-CP3-NP1	-3.12	117.13	123.01
3	B	4002	MCA	CS2-CS1-S	-3.11	108.44	111.81
3	F	4006	MCA	O12-P1-O5'	-3.10	93.37	107.75
4	C	5003	DXX	O-C-CA	-3.09	111.88	122.02
3	E	4005	MCA	CP9-CPA-CPB	3.09	113.27	108.23
3	E	4005	MCA	O22-P2-O21	3.08	127.48	112.24
3	A	4001	MCA	O12-P1-O5'	-3.08	93.46	107.75
3	E	4005	MCA	O33-P3-O3'	3.07	119.75	105.99
3	B	4002	MCA	O12-P1-O5'	-3.03	93.67	107.75
3	C	4003	MCA	O12-P1-O5'	-3.03	93.69	107.75
4	B	5002	DXX	O-C-CA	-3.02	112.10	122.02
3	F	4006	MCA	O22-P2-O21	3.02	127.19	112.24
3	C	4003	MCA	O22-P2-O21	3.02	127.15	112.24
3	D	4004	MCA	O12-P1-O5'	-3.01	93.76	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4006	MCA	CP9-CPA-CPB	2.99	113.11	108.23
3	F	4006	MCA	OP1-CP3-NP1	-2.99	117.37	123.01
3	A	4001	MCA	O22-P2-O21	2.99	127.01	112.24
3	A	4001	MCA	CP1-CP2-NP1	-2.98	106.16	112.42
3	D	4004	MCA	O22-P2-O21	2.97	126.90	112.24
3	B	4002	MCA	O22-P2-O21	2.96	126.89	112.24
3	F	4006	MCA	CP1-CP2-NP1	-2.95	106.23	112.42
3	E	4005	MCA	CS2-CS1-S	-2.90	108.67	111.81
4	A	5001	DXX	O-C-CA	-2.88	112.57	122.02
3	D	4004	MCA	OP1-CP3-NP1	-2.86	117.61	123.01
3	B	4002	MCA	CP9-CPA-CPB	2.86	112.90	108.23
3	A	4001	MCA	OP1-CP3-NP1	-2.84	117.65	123.01
3	A	4001	MCA	CP9-CPA-CPB	2.83	112.85	108.23
3	B	4002	MCA	OP1-CP3-NP1	-2.82	117.69	123.01
3	E	4005	MCA	CP1-CP2-NP1	-2.79	106.54	112.42
4	F	5006	DXX	O2-C-CA	2.76	124.77	115.28
3	D	4004	MCA	CS2-CS1-S	-2.76	108.82	111.81
3	D	4004	MCA	C5-C6-N6	2.75	124.53	120.35
4	C	5003	DXX	O2-C-CA	2.73	124.66	115.28
3	F	4006	MCA	C5-C6-N6	2.70	124.46	120.35
3	C	4003	MCA	CP9-CPA-CPB	2.70	112.64	108.23
4	D	5004	DXX	O2-C-CA	2.70	124.55	115.28
4	E	5005	DXX	O2-C-CA	2.67	124.47	115.28
3	D	4004	MCA	CP9-CPA-CPB	2.66	112.57	108.23
3	B	4002	MCA	C5-C6-N6	2.65	124.38	120.35
4	A	5001	DXX	O2-C-CA	2.64	124.35	115.28
4	B	5002	DXX	O2-C-CA	2.63	124.32	115.28
3	C	4003	MCA	CP1-CP2-NP1	-2.54	107.09	112.42
3	C	4003	MCA	CS2-CS1-S	-2.50	109.10	111.81
3	A	4001	MCA	C5-C6-N6	2.47	124.11	120.35
3	E	4005	MCA	C5-C6-N6	2.46	124.09	120.35
3	F	4006	MCA	O2'-C2'-C3'	2.42	118.03	111.17
3	C	4003	MCA	C5-C6-N6	2.34	123.91	120.35
3	B	4002	MCA	O2'-C2'-C3'	2.25	117.56	111.17
3	D	4004	MCA	OP3-CP7-CPA	2.11	115.22	110.25
3	B	4002	MCA	C1'-N9-C4	-2.09	122.97	126.64
3	A	4001	MCA	CP7-CP6-NP2	2.03	120.61	116.58
3	A	4001	MCA	CP8-CPA-CP7	2.01	112.31	108.82
3	A	4001	MCA	C1'-N9-C4	-2.01	123.11	126.64
3	D	4004	MCA	C1'-N9-C4	-2.01	123.11	126.64
3	B	4002	MCA	CP7-CP6-NP2	2.01	120.57	116.58

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	4001	MCA	CS2
3	B	4002	MCA	CS2
3	C	4003	MCA	CS2
3	D	4004	MCA	CS2
3	E	4005	MCA	CS2
3	F	4006	MCA	CS2

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4001	MCA	P1-O6-P2-O7
3	A	4001	MCA	CP7-CP6-NP2-CP5
3	A	4001	MCA	CP3-CP4-CP5-NP2
3	A	4001	MCA	CS2-CS1-S-CP1
3	B	4002	MCA	CP7-CP6-NP2-CP5
3	B	4002	MCA	CP3-CP4-CP5-NP2
3	B	4002	MCA	CS2-CS1-S-CP1
3	B	4002	MCA	S-CS1-CS2-CS4
3	C	4003	MCA	CP7-CP6-NP2-CP5
3	C	4003	MCA	CS2-CS1-S-CP1
3	C	4003	MCA	CS1-CS2-CS4-OS4
3	D	4004	MCA	O4'-C4'-C5'-O5'
3	D	4004	MCA	CS2-CS1-S-CP1
3	E	4005	MCA	CP7-CP6-NP2-CP5
3	E	4005	MCA	CS2-CS1-S-CP1
3	E	4005	MCA	CS1-CS2-CS4-OS4
3	F	4006	MCA	CP7-CP6-NP2-CP5
3	F	4006	MCA	CP3-CP4-CP5-NP2
3	F	4006	MCA	CS2-CS1-S-CP1
4	A	5001	DXX	O1-C1-CA-CB
4	B	5002	DXX	O1-C1-CA-CB
4	D	5004	DXX	O1-C1-CA-CB
4	E	5005	DXX	O1-C1-CA-CB
4	F	5006	DXX	O1-C1-CA-CB
3	A	4001	MCA	CP4-CP5-NP2-CP6
3	B	4002	MCA	CP4-CP5-NP2-CP6
3	C	4003	MCA	CP4-CP5-NP2-CP6
3	E	4005	MCA	CP4-CP5-NP2-CP6
3	F	4006	MCA	CP4-CP5-NP2-CP6
3	B	4002	MCA	OP2-CP6-NP2-CP5
3	C	4003	MCA	OP2-CP6-NP2-CP5
3	F	4006	MCA	OP2-CP6-NP2-CP5
3	A	4001	MCA	OP2-CP6-NP2-CP5

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Mol	Chain	Res	Type	Atoms
3	A	4001	MCA	C3'-C4'-C5'-O5'
3	B	4002	MCA	C3'-C4'-C5'-O5'
3	C	4003	MCA	C3'-C4'-C5'-O5'
3	D	4004	MCA	C3'-C4'-C5'-O5'
3	E	4005	MCA	C3'-C4'-C5'-O5'
3	F	4006	MCA	C3'-C4'-C5'-O5'
3	A	4001	MCA	O4'-C4'-C5'-O5'
3	B	4002	MCA	O4'-C4'-C5'-O5'
3	C	4003	MCA	O4'-C4'-C5'-O5'
3	E	4005	MCA	O4'-C4'-C5'-O5'
3	F	4006	MCA	O4'-C4'-C5'-O5'
3	D	4004	MCA	CP4-CP5-NP2-CP6
3	E	4005	MCA	C4'-C3'-O3'-P3
3	D	4004	MCA	OS1-CS1-CS2-CS3
3	E	4005	MCA	OP2-CP6-NP2-CP5
3	E	4005	MCA	C2'-C3'-O3'-P3
3	B	4002	MCA	NP2-CP6-CP7-CPA
4	F	5006	DXX	O-C-CA-CB
4	F	5006	DXX	O2-C-CA-CB
3	B	4002	MCA	P1-O6-P2-O7
3	C	4003	MCA	P1-O6-P2-O7
3	E	4005	MCA	P1-O6-P2-O7
3	F	4006	MCA	P1-O6-P2-O7
4	D	5004	DXX	O-C-CA-C1
4	D	5004	DXX	O2-C-CA-C1
5	B	6002	MPD	O2-C2-C3-C4
3	C	4003	MCA	CP3-CP4-CP5-NP2
3	E	4005	MCA	CS1-CS2-CS4-OS5
3	B	4002	MCA	P2-O6-P1-O11
3	D	4004	MCA	P2-O6-P1-O11
3	B	4002	MCA	CPB-O7-P2-O21
3	B	4002	MCA	OS1-CS1-CS2-CS3
3	C	4003	MCA	OS1-CS1-CS2-CS3
3	E	4005	MCA	OS1-CS1-CS2-CS3
3	A	4001	MCA	C4'-C3'-O3'-P3
3	C	4003	MCA	CP1-CP2-NP1-CP3
5	B	6002	MPD	C1-C2-C3-C4
5	B	6002	MPD	CM-C2-C3-C4
3	C	4003	MCA	C4'-C3'-O3'-P3
3	C	4003	MCA	P2-O6-P1-O11
3	D	4004	MCA	CP3-CP4-CP5-NP2
3	A	4001	MCA	OS1-CS1-CS2-CS3

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Mol	Chain	Res	Type	Atoms
3	F	4006	MCA	OS1-CS1-CS2-CS3
3	B	4002	MCA	C4'-C3'-O3'-P3
3	D	4004	MCA	C4'-C3'-O3'-P3
3	B	4002	MCA	CP9-CPA-CPB-O7
3	E	4005	MCA	CP9-CPA-CPB-O7
3	C	4003	MCA	NP2-CP6-CP7-CPA
3	D	4004	MCA	NP2-CP6-CP7-CPA
4	C	5003	DXX	O1-C1-CA-CB
3	A	4001	MCA	CP2-CP1-S-CS1
3	B	4002	MCA	CP2-CP1-S-CS1
3	C	4003	MCA	CP2-CP1-S-CS1
3	D	4004	MCA	CP2-CP1-S-CS1
3	E	4005	MCA	CP2-CP1-S-CS1
3	F	4006	MCA	CP2-CP1-S-CS1
3	A	4001	MCA	P2-O6-P1-O11
3	E	4005	MCA	P2-O6-P1-O11
4	E	5005	DXX	O2-C-CA-CB
3	B	4002	MCA	CP8-CPA-CPB-O7
3	E	4005	MCA	S-CS1-CS2-CS4
3	C	4003	MCA	CS1-CS2-CS4-OS5
3	E	4005	MCA	P2-O6-P1-O12
3	A	4001	MCA	CPB-O7-P2-O21
3	E	4005	MCA	CPB-O7-P2-O21
3	F	4006	MCA	CPB-O7-P2-O21
4	B	5002	DXX	O1-C1-CA-C
4	C	5003	DXX	O1-C1-CA-C
4	F	5006	DXX	O1-C1-CA-C
3	A	4001	MCA	OP2-CP6-CP7-CPA
3	B	4002	MCA	OP2-CP6-CP7-CPA
3	C	4003	MCA	OP2-CP6-CP7-CPA
3	D	4004	MCA	OP2-CP6-CP7-CPA
3	F	4006	MCA	OP2-CP6-CP7-CPA

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4005	MCA	3	0
3	F	4006	MCA	1	0
5	A	6001	MPD	1	0
3	A	4001	MCA	1	0
3	C	4003	MCA	1	0

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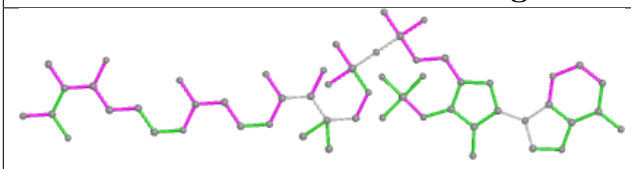
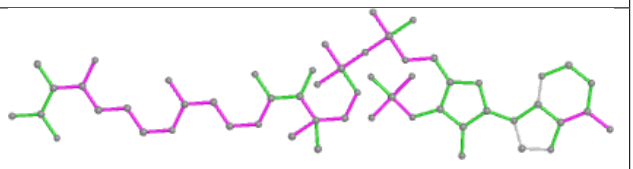
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	DXX	1	0
3	B	4002	MCA	1	0

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

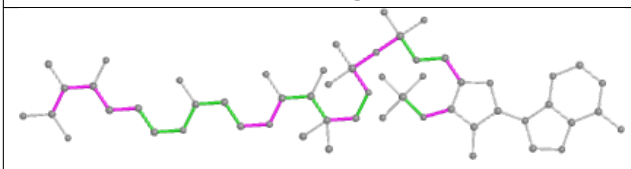
Ligand MCA E 4005



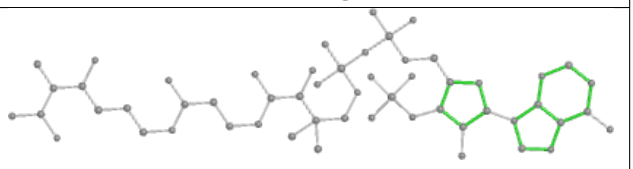
Bond lengths



Bond angles

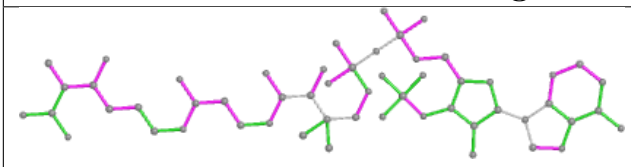


Torsions

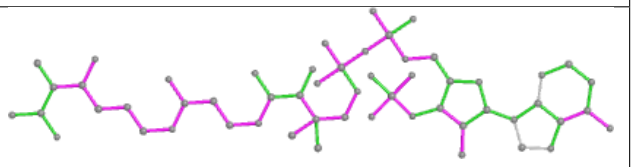


Rings

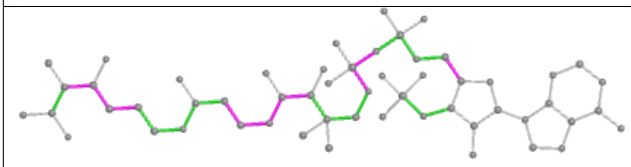
Ligand MCA F 4006



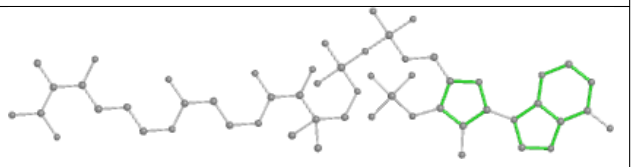
Bond lengths



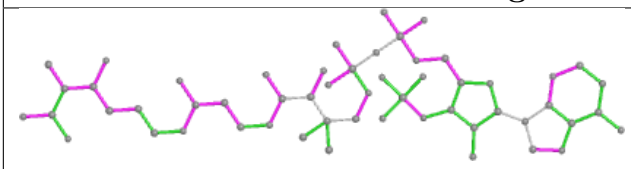
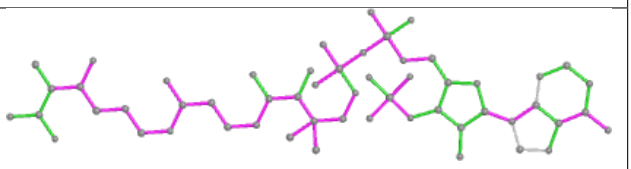
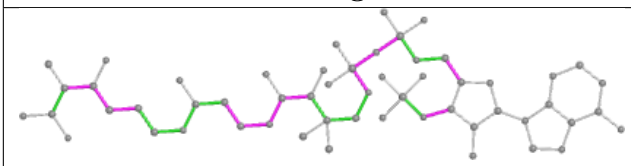
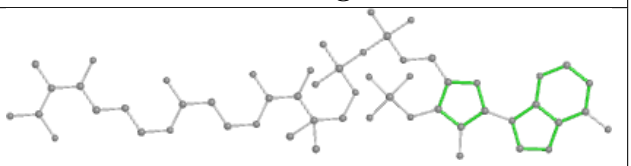
Bond angles

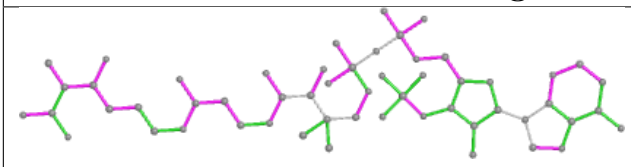
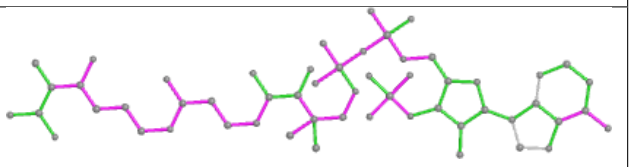
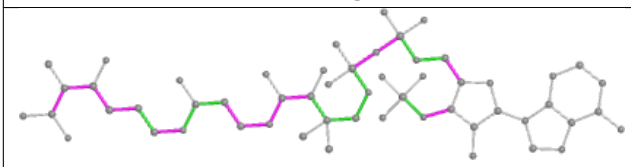
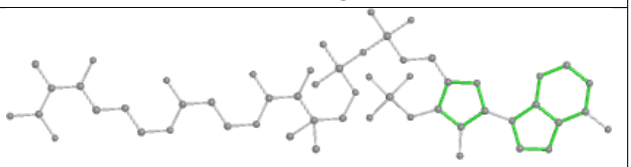


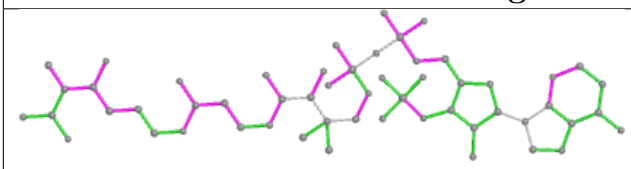
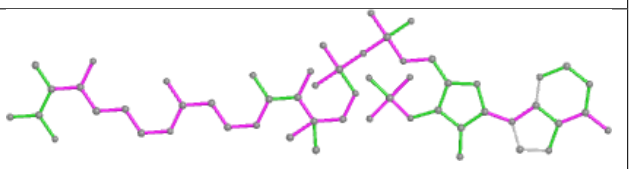
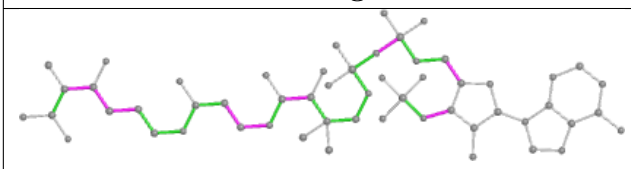
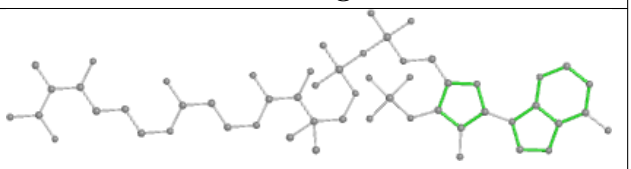
Torsions

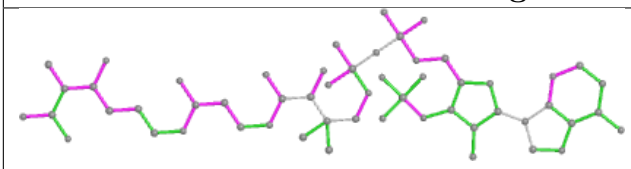
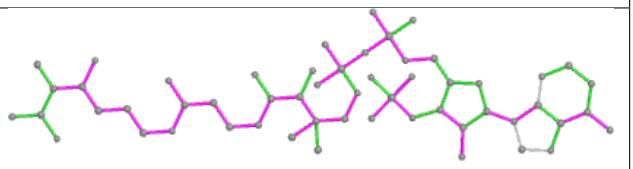
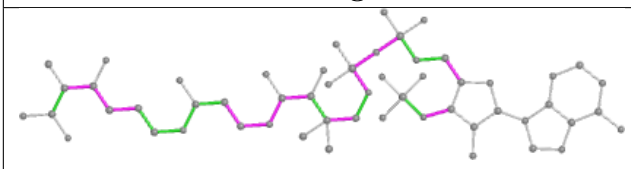
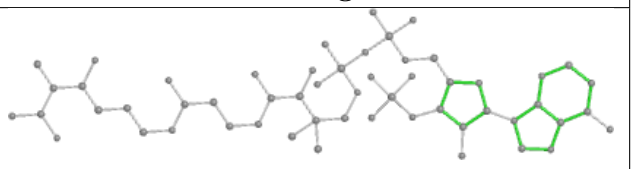


Rings

Ligand MCA A 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MCA C 4003	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MCA D 4004	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MCA B 4002	
 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	517/523 (98%)	-0.41	5 (0%)	82	84	10, 19, 43, 68	0
1	B	516/523 (98%)	-0.40	12 (2%)	60	63	8, 17, 46, 86	0
1	C	510/523 (97%)	-0.41	11 (2%)	62	64	10, 17, 45, 83	0
1	D	513/523 (98%)	-0.17	12 (2%)	60	63	13, 23, 47, 78	0
1	E	520/523 (99%)	-0.56	3 (0%)	89	90	8, 16, 35, 67	0
1	F	517/523 (98%)	-0.45	1 (0%)	95	95	9, 19, 36, 67	0
All	All	3093/3138 (98%)	-0.40	44 (1%)	75	77	8, 19, 42, 86	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	ASP	8.9
1	B	454	ILE	7.5
1	D	461	ASP	4.6
1	D	454	ILE	4.2
1	C	460	PRO	3.9
1	C	513	THR	3.8
1	D	7	LEU	3.8
1	C	462	ALA	3.7
1	B	459	ASP	3.5
1	D	513	THR	3.5
1	D	451	ARG	3.3
1	E	5	ASN	3.3
1	B	450	PHE	2.9
1	C	463	MET	2.9
1	B	463	MET	2.9
1	D	455	LYS	2.9
1	B	461	ASP	2.8
1	A	450	PHE	2.8
1	D	465	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	446	ALA	2.7
1	B	457	ALA	2.7
1	B	456	ALA	2.6
1	C	450	PHE	2.6
1	A	8	LYS	2.6
1	C	214	GLY	2.6
1	D	462	ALA	2.5
1	B	9	LEU	2.5
1	C	461	ASP	2.5
1	F	513	THR	2.5
1	C	464	ARG	2.4
1	A	465	ALA	2.3
1	A	451	ARG	2.3
1	C	453	GLU	2.3
1	B	216	ASP	2.3
1	D	34	ARG	2.2
1	E	216	ASP	2.2
1	D	463	MET	2.2
1	B	455	LYS	2.2
1	E	513	THR	2.1
1	D	9	LEU	2.1
1	D	453	GLU	2.1
1	A	462	ALA	2.1
1	C	449	ILE	2.1
1	B	453	GLU	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)

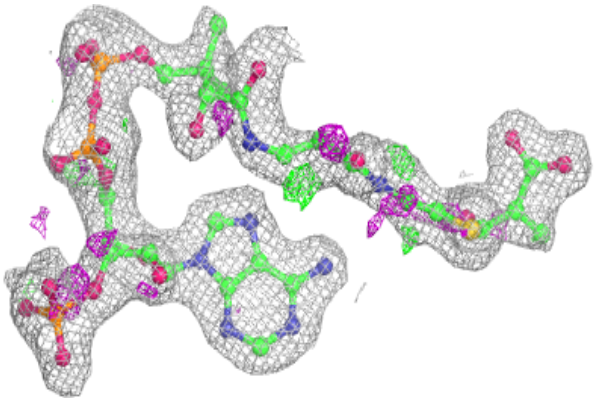
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

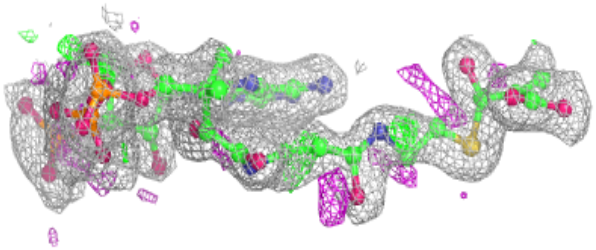
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DXX	B	5002	7/8	0.76	0.22	55,58,58,60	0
4	DXX	C	5003	7/8	0.84	0.12	32,44,45,51	0
4	DXX	D	5004	7/8	0.84	0.15	40,49,49,51	0
4	DXX	A	5001	7/8	0.89	0.17	27,38,44,44	0
5	MPD	B	6002	8/8	0.89	0.15	32,36,39,40	0
4	DXX	E	5005	7/8	0.90	0.12	29,43,46,46	0
5	MPD	A	6001	8/8	0.90	0.17	29,39,48,50	0
3	MCA	B	4002	55/55	0.90	0.12	19,41,59,64	0
4	DXX	F	5006	7/8	0.91	0.11	29,42,46,48	0
3	MCA	D	4004	55/55	0.92	0.11	26,42,57,60	0
3	MCA	F	4006	55/55	0.92	0.10	23,35,51,55	0
3	MCA	A	4001	55/55	0.93	0.10	21,38,50,54	0
3	MCA	C	4003	55/55	0.93	0.10	14,29,46,51	0
5	MPD	F	6006	8/8	0.93	0.11	27,31,40,47	0
3	MCA	E	4005	55/55	0.94	0.09	15,29,41,44	0
2	CD	C	7003	1/1	0.99	0.04	16,16,16,16	0
2	CD	A	7001	1/1	0.99	0.04	20,20,20,20	0
2	CD	B	7002	1/1	1.00	0.03	13,13,13,13	0

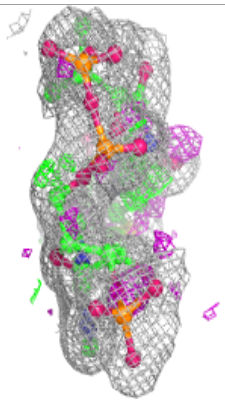
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MCA B 4002:

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

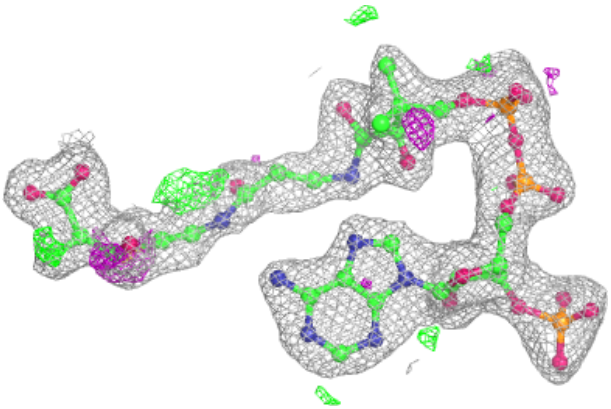


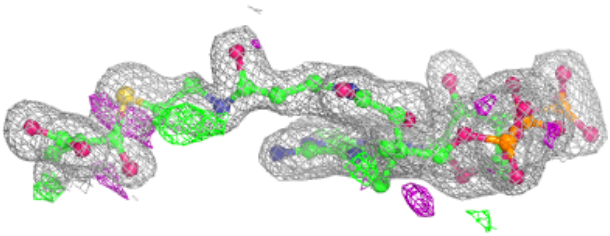




Electron density around MCA D 4004:

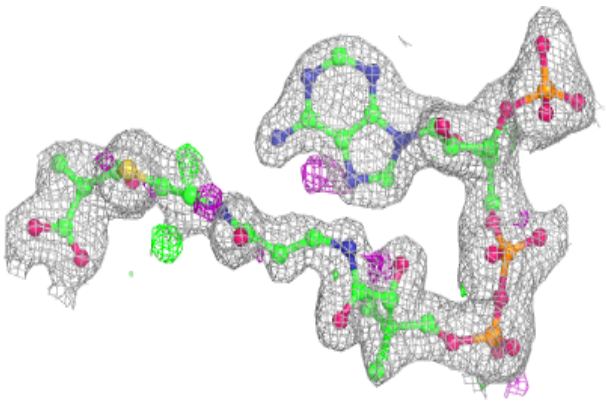
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

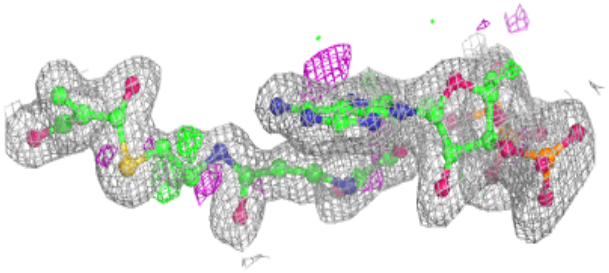


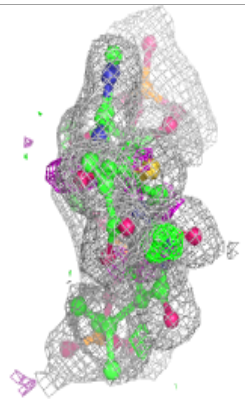


Electron density around MCA F 4006:

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

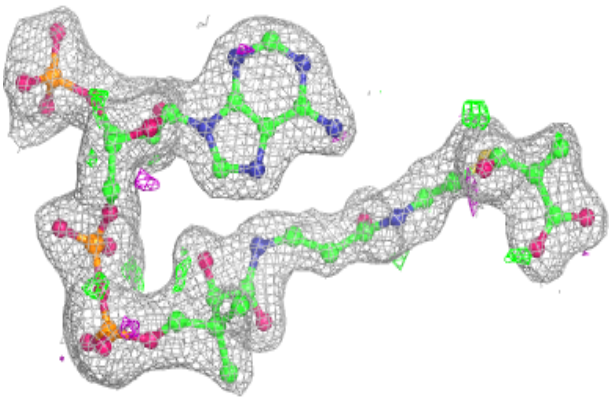


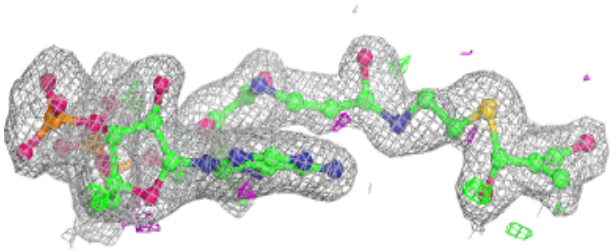


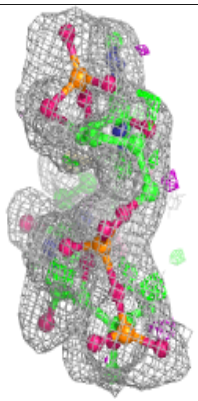


Electron density around MCA A 4001:

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

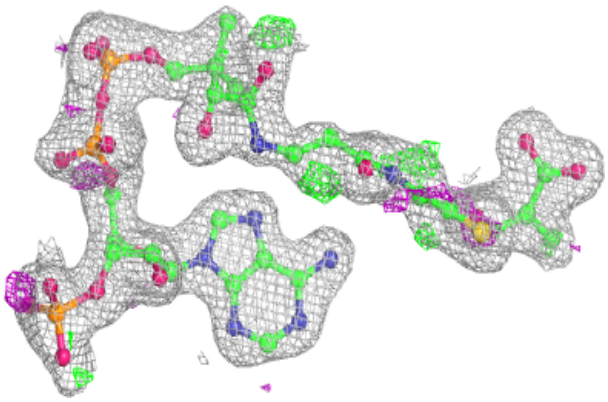


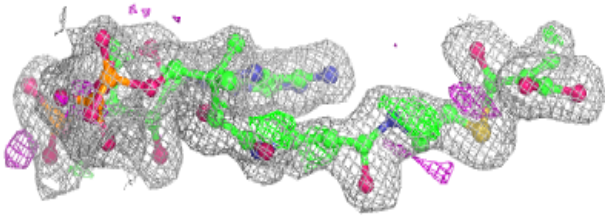


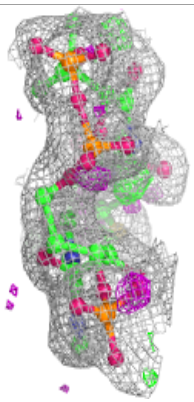


Electron density around MCA C 4003:

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

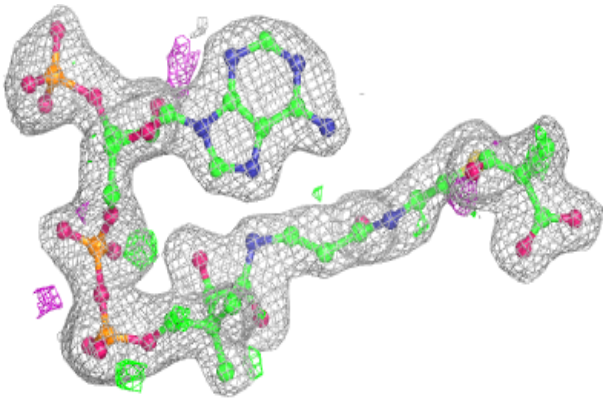


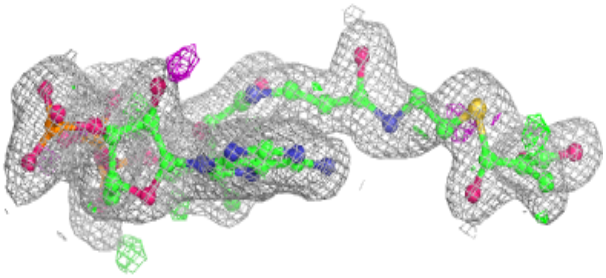




Electron density around MCA E 4005:

$2mF_o$-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.