



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 04:42 AM EST

PDB ID : 1ON9
Title : Transcarboxylase 12S crystal structure: hexamer assembly and substrate binding to a multienzyme core (with hydrolyzed methylmalonyl-coenzyme a 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 : 2003-02-27
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-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

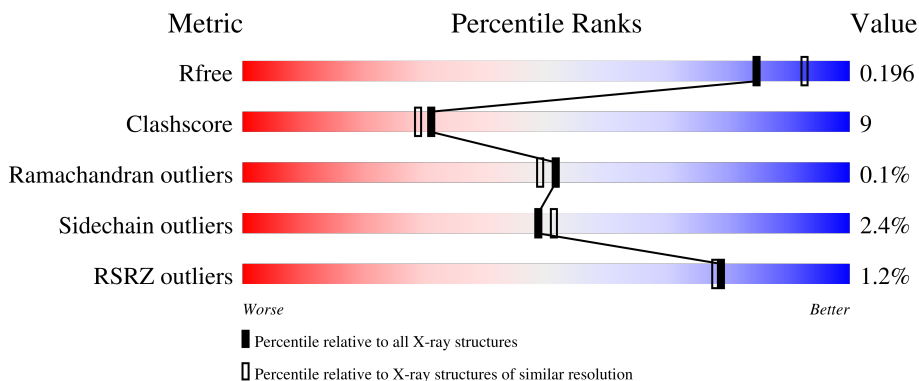
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



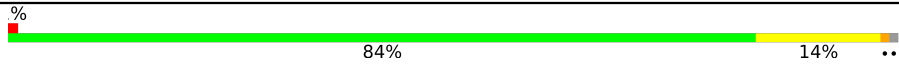

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	523	 81% 16% ..
1	B	523	 84% 14% ..
1	C	523	 83% 15% ..
1	D	523	 78% 17% ..

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Mol	Chain	Length	Quality of chain
1	E	523	
1	F	523	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26869 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.

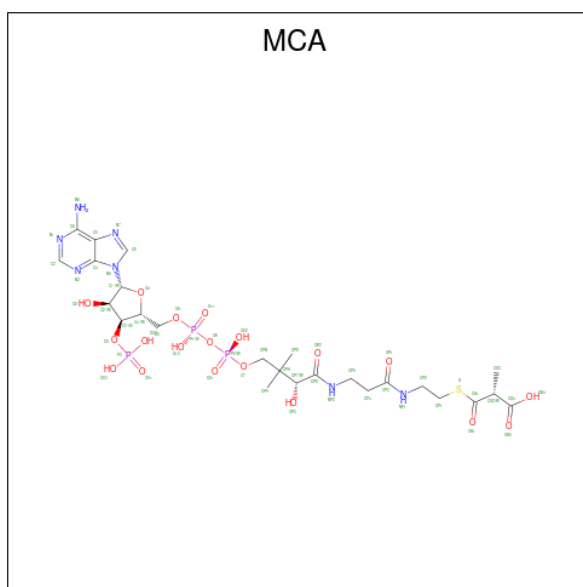
- Molecule 1 is a protein called Methylmalonyl-CoA carboxyltransferase 12S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	3900	2448	679	754	19	0	0	0
1	B	516	3900	2448	679	754	19	0	0	0
1	C	514	3878	2433	674	752	19	0	0	0
1	D	504	3805	2394	660	732	19	0	0	0
1	E	519	3925	2464	684	758	19	0	0	0
1	F	516	3900	2448	679	754	19	0	0	0

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

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

- Molecule 3 is METHYLMALONYL-COENZYME A (three-letter code: MCA) (formula: C₂₅H₄₀N₇O₁₉P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
3	B	1	26	10	5	9	2	0	0
3	C	1	26	10	5	9	2	0	0
3	D	1	31	10	5	13	3	0	0
3	E	1	23	10	5	7	1	0	0
3	F	1	27	10	5	10	2	0	0

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	C O	0	0
			8	6 2		

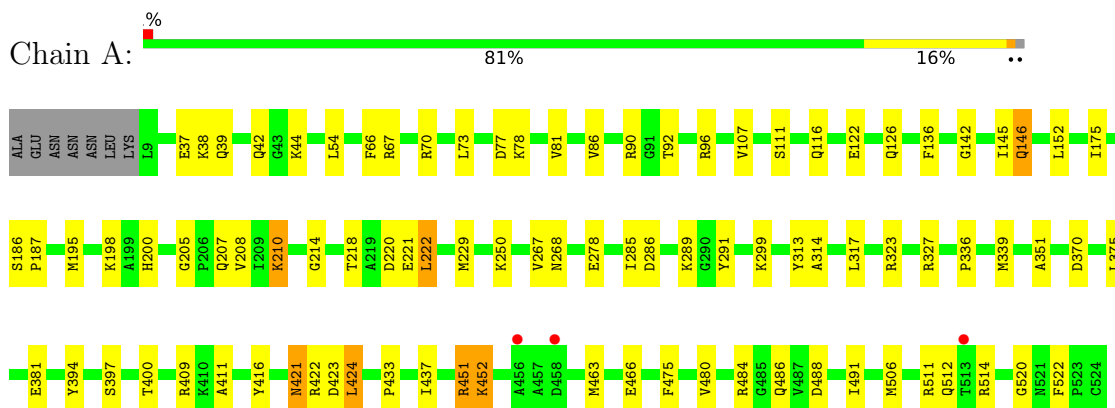
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	558	Total	O	0	0
			558	558		
5	B	616	Total	O	0	0
			616	616		
5	C	557	Total	O	0	0
			557	557		
5	D	492	Total	O	0	0
			492	492		
5	E	610	Total	O	0	0
			610	610		
5	F	557	Total	O	0	0
			557	557		

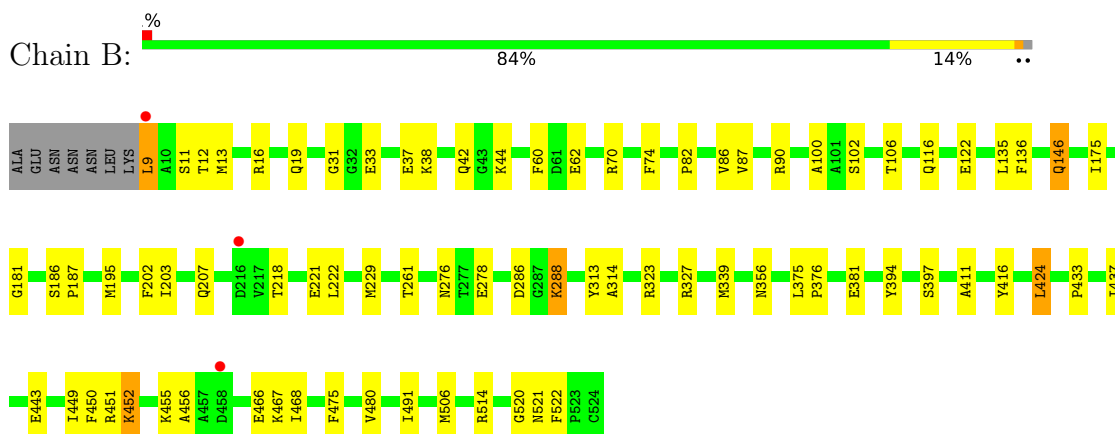
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

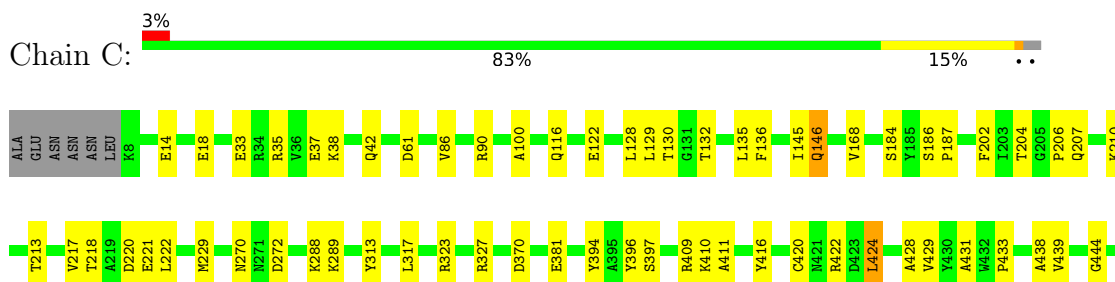
- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

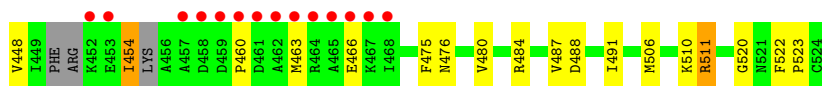


- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

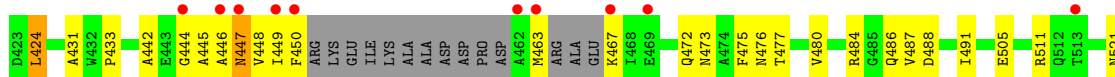
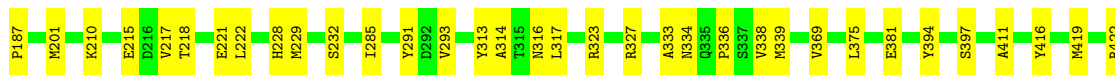
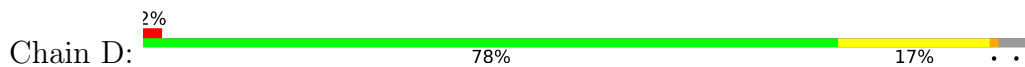


- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

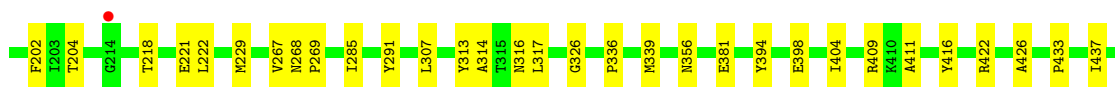
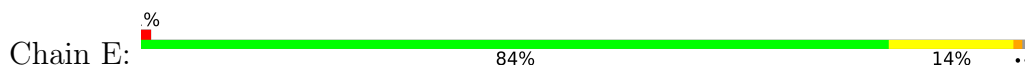




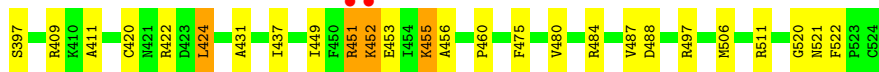
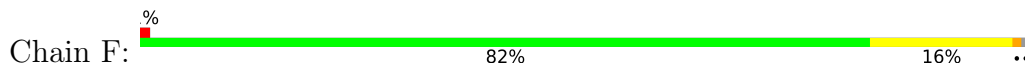
- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit



- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit



- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.81Å 200.02Å 145.90Å 90.00° 102.97° 90.00°	Depositor
Resolution (Å)	29.55 – 2.00 29.54 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.55-2.00) 91.2 (29.54-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.88Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.198 0.150 , 0.196	Depositor DCC
R_{free} test set	10242 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26869	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MCA, CD, MPD

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	0.40	0/3972	0.68	0/5378
1	B	0.42	0/3972	0.69	0/5378
1	C	0.40	0/3947	0.67	1/5342 (0.0%)
1	D	0.38	0/3874	0.66	0/5243
1	E	0.42	0/3997	0.69	0/5411
1	F	0.41	0/3972	0.68	0/5378
All	All	0.40	0/23734	0.68	1/32130 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	ASN	N-CA-C	-5.12	97.19	111.00

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	3900	0	3850	83	0
1	B	3900	0	3850	87	0
1	C	3878	0	3826	72	0
1	D	3805	0	3763	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3925	0	3880	68	0
1	F	3900	0	3850	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	11	0	0
3	B	26	0	11	0	0
3	C	26	0	11	1	0
3	D	31	0	11	1	0
3	E	23	0	11	1	0
3	F	27	0	11	2	0
4	F	8	0	14	0	0
5	A	558	0	0	9	0
5	B	616	0	0	8	0
5	C	557	0	0	10	0
5	D	492	0	0	12	0
5	E	610	0	0	5	0
5	F	557	0	0	10	0
All	All	26869	0	23099	424	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 (424) 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:F:452:LYS:HD2	1:F:453:GLU:N	1.77	1.00
1:B:146:GLN:H	1:B:146:GLN:HE21	1.08	0.98
1:D:7:LEU:HD22	1:D:23:GLN:HE21	1.30	0.97
1:E:422:ARG:HH11	1:E:422:ARG:HG2	1.33	0.93
1:D:477:THR:HG22	1:D:480:VAL:HG23	1.50	0.91
1:A:511:ARG:HH12	1:B:261:THR:HG21	1.36	0.90
1:E:146:GLN:H	1:E:146:GLN:HE21	1.18	0.89
1:B:286:ASP:OD1	1:B:288:LYS:HG2	1.73	0.88
1:C:146:GLN:H	1:C:146:GLN:HE21	1.19	0.88
1:D:13:MET:HB2	1:E:285:ILE:HD11	1.54	0.87
1:F:146:GLN:H	1:F:146:GLN:HE21	1.19	0.86
1:B:146:GLN:H	1:B:146:GLN:NE2	1.72	0.86
1:A:70:ARG:HH11	1:A:70:ARG:HB3	1.40	0.85
1:D:146:GLN:H	1:D:146:GLN:HE21	1.26	0.83
1:F:452:LYS:HD2	1:F:453:GLU:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:THR:OG1	1:B:221:GLU:HG3	1.81	0.81
1:A:145:ILE:HG13	5:D:4397:HOH:O	1.81	0.80
1:C:206:PRO:HD2	1:C:207:GLN:HE22	1.46	0.80
1:A:146:GLN:H	1:A:146:GLN:HE21	1.27	0.79
1:D:218:THR:OG1	1:D:221:GLU:HG3	1.85	0.76
1:E:146:GLN:H	1:E:146:GLN:NE2	1.82	0.76
1:E:16:ARG:NH1	1:F:285:ILE:HD12	2.01	0.76
1:F:451:ARG:NH2	1:F:452:LYS:HG3	2.02	0.75
1:E:78:LYS:HD2	1:E:79:ALA:N	2.03	0.74
1:A:146:GLN:H	1:A:146:GLN:NE2	1.85	0.74
1:A:451:ARG:NH1	1:A:451:ARG:HB2	2.03	0.73
1:F:186:SER:HB3	1:F:187:PRO:HD3	1.69	0.73
1:A:70:ARG:HB3	1:A:70:ARG:NH1	2.02	0.73
1:F:9:LEU:HD23	1:F:19:GLN:HE22	1.52	0.73
1:A:210:LYS:HE2	1:A:214:GLY:HA2	1.71	0.73
1:C:454:ILE:HA	1:C:463:MET:HG2	1.70	0.73
1:F:146:GLN:H	1:F:146:GLN:NE2	1.87	0.72
1:F:247:LEU:HD23	5:F:6486:HOH:O	1.89	0.72
1:D:463:MET:HG3	1:D:467:LYS:HG2	1.70	0.72
1:B:146:GLN:HE21	1:B:146:GLN:N	1.87	0.72
1:C:61:ASP:HB2	5:C:7491:HOH:O	1.89	0.72
1:C:422:ARG:HH11	1:C:422:ARG:HG2	1.52	0.72
1:D:186:SER:HB3	1:D:187:PRO:HD3	1.72	0.72
1:D:7:LEU:HD22	1:D:23:GLN:NE2	2.05	0.71
1:B:452:LYS:H	1:B:452:LYS:HZ2	1.36	0.71
1:E:316:ASN:HB3	1:E:339:MET:HE3	1.71	0.71
1:D:122:GLU:HG3	5:D:4413:HOH:O	1.91	0.71
1:C:454:ILE:HD13	1:C:454:ILE:H	1.56	0.71
1:A:186:SER:HB3	1:A:187:PRO:HD3	1.73	0.70
1:B:506:MET:HE3	5:B:7479:HOH:O	1.92	0.70
1:E:422:ARG:HG2	1:E:422:ARG:NH1	2.07	0.70
1:B:186:SER:HB3	1:B:187:PRO:HD3	1.73	0.69
1:D:477:THR:CG2	1:D:480:VAL:HG23	2.22	0.69
1:D:12:THR:HG23	1:D:15:GLY:H	1.57	0.69
1:D:442:ALA:HB2	1:D:472:GLN:HE21	1.58	0.69
1:D:7:LEU:CD2	1:D:23:GLN:HE21	2.05	0.69
1:C:146:GLN:H	1:C:146:GLN:NE2	1.92	0.68
1:D:35:ARG:HH12	3:D:4004:MCA:P3	2.15	0.68
1:A:207:GLN:HE21	1:A:208:VAL:HG23	1.58	0.68
1:E:70:ARG:HD2	5:F:6349:HOH:O	1.92	0.68
1:E:186:SER:HB3	1:E:187:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ARG:HH12	3:F:4006:MCA:P3	2.18	0.67
1:C:207:GLN:CD	1:C:207:GLN:H	1.97	0.67
1:C:206:PRO:HD2	1:C:207:GLN:NE2	2.10	0.66
1:D:146:GLN:H	1:D:146:GLN:NE2	1.91	0.66
1:C:145:ILE:HG22	1:F:449:ILE:HD11	1.78	0.66
1:C:272:ASP:OD2	5:C:7501:HOH:O	2.14	0.65
1:B:506:MET:HE1	1:C:132:THR:HG21	1.79	0.65
1:F:394:TYR:OH	1:F:520:GLY:HA3	1.97	0.65
1:F:9:LEU:HD23	1:F:19:GLN:NE2	2.13	0.64
1:D:475:PHE:HA	1:D:480:VAL:HG11	1.78	0.64
1:A:422:ARG:NH2	1:A:488:ASP:OD1	2.28	0.64
1:C:122:GLU:HG3	5:C:7472:HOH:O	1.97	0.64
1:F:339:MET:HE2	1:F:375:LEU:HD22	1.79	0.64
1:D:38:LYS:O	1:D:42:GLN:HG3	1.98	0.63
1:F:397:SER:OG	1:F:424:LEU:HD13	1.98	0.63
1:B:33:GLU:O	1:B:37:GLU:HG3	1.98	0.63
1:A:486:GLN:HG2	5:A:7460:HOH:O	1.97	0.63
1:E:218:THR:OG1	1:E:221:GLU:HG3	1.98	0.63
1:B:339:MET:CE	1:B:375:LEU:HD22	2.29	0.63
1:A:90:ARG:CD	1:C:506:MET:HG2	2.29	0.62
1:B:452:LYS:N	1:B:452:LYS:HD3	2.14	0.62
1:B:506:MET:HE1	1:C:132:THR:CG2	2.29	0.62
1:F:497:ARG:HD3	5:F:6205:HOH:O	1.98	0.62
1:C:411:ALA:HB1	1:C:416:TYR:CD2	2.35	0.62
1:A:90:ARG:HD2	1:C:506:MET:HG2	1.81	0.62
1:F:9:LEU:HA	1:F:19:GLN:HE22	1.63	0.62
1:F:21:ALA:O	1:F:25:GLN:HG2	1.99	0.62
1:F:455:LYS:HE2	1:F:456:ALA:HB2	1.82	0.61
1:E:78:LYS:HD2	1:E:78:LYS:C	2.20	0.61
1:C:222:LEU:HD11	1:F:381:GLU:HG3	1.83	0.61
1:E:445:ALA:O	1:E:449:ILE:HG12	2.01	0.60
1:B:288:LYS:NZ	1:B:288:LYS:HB3	2.17	0.60
1:D:394:TYR:CD2	1:D:522:PHE:HD2	2.19	0.60
1:A:451:ARG:HB2	1:A:451:ARG:HH11	1.66	0.60
1:E:34:ARG:HB3	1:E:34:ARG:HH11	1.67	0.60
1:B:455:LYS:HD3	1:B:455:LYS:C	2.23	0.60
1:C:289:LYS:HA	1:C:289:LYS:HE3	1.84	0.60
1:D:477:THR:HG22	1:D:480:VAL:CG2	2.28	0.59
1:A:205:GLY:HA3	1:A:207:GLN:HE22	1.67	0.59
1:B:411:ALA:HB1	1:B:416:TYR:CD2	2.38	0.59
1:C:218:THR:OG1	1:C:221:GLU:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:SER:OG	1:B:424:LEU:HD13	2.02	0.59
1:F:218:THR:OG1	1:F:221:GLU:HG3	2.03	0.58
1:F:339:MET:CE	1:F:375:LEU:HD22	2.33	0.58
1:C:90:ARG:HD3	5:C:7077:HOH:O	2.03	0.58
1:A:452:LYS:HD2	1:A:452:LYS:N	2.17	0.58
1:E:90:ARG:HG2	1:F:506:MET:HG2	1.85	0.58
1:C:33:GLU:O	1:C:37:GLU:HG3	2.03	0.58
1:F:455:LYS:HG3	1:F:456:ALA:N	2.19	0.58
1:D:397:SER:OG	1:D:424:LEU:HD13	2.04	0.58
1:F:38:LYS:O	1:F:42:GLN:HG3	2.04	0.58
1:A:229:MET:O	1:A:313:TYR:HB2	2.04	0.58
1:A:210:LYS:HE2	1:A:210:LYS:O	2.03	0.57
1:C:186:SER:HB3	1:C:187:PRO:HD3	1.86	0.57
1:B:455:LYS:HD3	1:B:456:ALA:N	2.19	0.57
1:C:454:ILE:HA	1:C:463:MET:CG	2.35	0.57
1:B:9:LEU:HD23	1:B:9:LEU:N	2.20	0.57
1:B:82:PRO:HG3	5:B:7608:HOH:O	2.05	0.57
1:A:286:ASP:HB3	1:A:289:LYS:HD3	1.87	0.57
1:B:175:ILE:HB	1:B:195:MET:HG3	1.87	0.57
1:B:506:MET:HE2	1:C:130:THR:CB	2.35	0.57
5:A:7469:HOH:O	1:D:217:VAL:HB	2.04	0.57
1:B:9:LEU:HD12	1:B:16:ARG:NE	2.20	0.56
1:C:394:TYR:OH	1:C:520:GLY:HA3	2.05	0.56
1:D:422:ARG:NH2	1:D:488:ASP:OD1	2.38	0.56
1:F:411:ALA:HB3	1:F:437:ILE:HA	1.87	0.56
1:F:451:ARG:CZ	1:F:452:LYS:HG3	2.35	0.56
1:A:90:ARG:HD3	5:A:7018:HOH:O	2.04	0.56
1:A:218:THR:OG1	1:A:221:GLU:HG3	2.04	0.56
1:A:198:LYS:HE2	5:A:7549:HOH:O	2.05	0.56
1:A:285:ILE:HD12	1:B:11:SER:O	2.05	0.56
1:A:506:MET:HG2	1:B:90:ARG:CD	2.35	0.56
1:D:444:GLY:O	1:D:448:VAL:HG23	2.06	0.56
1:E:229:MET:O	1:E:313:TYR:HB2	2.05	0.56
1:C:381:GLU:HG3	1:F:222:LEU:HD11	1.87	0.56
1:C:410:LYS:HE3	5:C:7374:HOH:O	2.04	0.56
1:A:210:LYS:HE3	5:A:7537:HOH:O	2.05	0.55
1:A:339:MET:HE3	1:A:375:LEU:HD13	1.87	0.55
1:E:146:GLN:HE21	1:E:146:GLN:N	1.97	0.55
1:D:12:THR:HG23	1:D:15:GLY:N	2.20	0.55
1:A:394:TYR:CD2	1:A:522:PHE:HD2	2.25	0.55
1:E:422:ARG:NH2	1:E:488:ASP:OD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:MET:O	1:A:466:GLU:HB3	2.06	0.55
1:C:454:ILE:H	1:C:454:ILE:CD1	2.19	0.55
1:B:276:ASN:OD1	1:B:278:GLU:HB2	2.06	0.55
1:C:35:ARG:HH12	3:C:4003:MCA:P3	2.29	0.55
1:F:146:GLN:HE21	1:F:146:GLN:N	1.98	0.55
1:D:476:ASN:N	1:D:476:ASN:HD22	2.05	0.55
1:A:146:GLN:HE21	1:A:146:GLN:N	2.02	0.54
1:D:228:HIS:HA	1:D:232:SER:HB2	1.90	0.54
1:C:397:SER:OG	1:C:424:LEU:HD13	2.07	0.54
1:D:477:THR:HG23	1:D:480:VAL:H	1.73	0.54
1:F:31:GLY:O	1:F:35:ARG:HG3	2.07	0.54
1:E:433:PRO:HD3	1:E:491:ILE:O	2.08	0.54
1:A:285:ILE:HG23	1:B:16:ARG:NH1	2.22	0.54
1:D:210:LYS:HA	1:D:215:GLU:O	2.07	0.54
1:A:484:ARG:NH2	1:B:70:ARG:NH1	2.55	0.54
1:E:394:TYR:CD2	1:E:522:PHE:HD2	2.25	0.54
1:A:433:PRO:HD3	1:A:491:ILE:O	2.08	0.54
1:D:334:ASN:O	1:D:336:PRO:HD3	2.09	0.54
1:E:404:ILE:HD12	1:E:503:ALA:HB1	1.90	0.54
1:E:514:ARG:HD3	5:E:4547:HOH:O	2.08	0.53
1:D:31:GLY:O	1:D:35:ARG:HD2	2.07	0.53
1:E:411:ALA:HB1	1:E:416:TYR:CD2	2.43	0.53
1:B:475:PHE:HA	1:B:480:VAL:HG11	1.89	0.53
1:D:9:LEU:HD21	1:E:433:PRO:O	2.08	0.53
1:E:34:ARG:HB3	1:E:34:ARG:NH1	2.23	0.53
1:F:35:ARG:HG2	5:F:6445:HOH:O	2.07	0.53
1:A:475:PHE:HA	1:A:480:VAL:HG11	1.89	0.53
1:B:86:VAL:HB	1:B:116:GLN:HG3	1.91	0.53
1:E:422:ARG:HD3	1:E:426:ALA:O	2.07	0.53
1:E:38:LYS:NZ	3:E:4005:MCA:H5'1	2.23	0.53
1:C:422:ARG:HH11	1:C:422:ARG:CG	2.22	0.53
1:E:75:GLY:O	1:E:78:LYS:HE3	2.08	0.53
1:B:514:ARG:NH2	5:B:7547:HOH:O	2.41	0.52
1:B:506:MET:HE2	1:C:130:THR:HB	1.90	0.52
1:A:394:TYR:OH	1:A:520:GLY:HA3	2.09	0.52
1:A:411:ALA:HB3	1:A:437:ILE:HA	1.91	0.52
1:B:433:PRO:HD3	1:B:491:ILE:O	2.10	0.52
1:A:522:PHE:HD1	1:D:522:PHE:CD1	2.26	0.52
1:B:87:VAL:HB	5:B:7559:HOH:O	2.07	0.52
1:B:9:LEU:HA	1:B:19:GLN:HE22	1.75	0.52
1:A:285:ILE:HD11	1:B:13:MET:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:GLU:HG2	5:E:4174:HOH:O	2.08	0.52
1:A:397:SER:OG	1:A:424:LEU:HD13	2.09	0.52
1:C:323:ARG:HA	1:C:327:ARG:O	2.09	0.52
1:A:86:VAL:HB	1:A:116:GLN:HG3	1.91	0.51
1:B:394:TYR:OH	1:B:520:GLY:HA3	2.09	0.51
1:A:506:MET:HG2	1:B:90:ARG:HD2	1.92	0.51
1:D:444:GLY:HA2	1:D:447:ASN:HB3	1.92	0.51
1:B:222:LEU:HD11	1:E:381:GLU:HG3	1.93	0.51
1:F:291:TYR:CZ	1:F:336:PRO:HG2	2.45	0.51
1:A:291:TYR:CZ	1:A:336:PRO:HG2	2.46	0.51
1:E:122:GLU:O	1:E:126:GLN:HG2	2.10	0.51
1:F:451:ARG:HA	5:F:6475:HOH:O	2.09	0.51
1:B:506:MET:HG2	1:C:90:ARG:CD	2.40	0.51
5:B:7492:HOH:O	1:E:521:ASN:HB3	2.09	0.51
1:B:229:MET:O	1:B:313:TYR:HB2	2.11	0.51
1:D:14:GLU:HA	1:D:14:GLU:OE2	2.11	0.51
1:F:394:TYR:CD2	1:F:522:PHE:HD2	2.29	0.51
1:A:522:PHE:HD1	1:D:522:PHE:HD1	1.56	0.51
1:A:285:ILE:HG23	1:B:16:ARG:HH12	1.77	0.50
1:E:38:LYS:O	1:E:42:GLN:HG3	2.11	0.50
1:D:431:ALA:HB2	1:D:487:VAL:HG11	1.93	0.50
1:E:394:TYR:OH	1:E:520:GLY:HA3	2.11	0.50
1:A:38:LYS:O	1:A:42:GLN:HG3	2.11	0.50
1:C:204:THR:HG21	1:F:376:PRO:HB3	1.93	0.50
1:D:7:LEU:HD22	5:D:4166:HOH:O	2.10	0.50
1:C:14:GLU:O	1:C:18:GLU:HG3	2.11	0.50
1:C:454:ILE:HD13	1:C:454:ILE:N	2.25	0.50
1:D:12:THR:HG23	1:D:15:GLY:HA3	1.93	0.50
1:D:90:ARG:NE	1:E:506:MET:HG2	2.26	0.50
1:D:433:PRO:HD3	1:D:491:ILE:O	2.11	0.50
1:E:422:ARG:NH1	1:E:422:ARG:CG	2.70	0.50
1:B:506:MET:O	1:B:506:MET:CE	2.60	0.50
1:B:452:LYS:HZ3	1:B:452:LYS:HB2	1.76	0.49
1:C:86:VAL:HB	1:C:116:GLN:HG3	1.94	0.49
1:D:60:PHE:CE2	1:D:62:GLU:HB2	2.47	0.49
1:A:278:GLU:HB3	1:A:299:LYS:HE2	1.93	0.49
1:C:370:ASP:CG	1:C:409:ARG:HB3	2.31	0.49
1:F:229:MET:O	1:F:313:TYR:HB2	2.12	0.49
5:A:7426:HOH:O	1:D:521:ASN:HB2	2.12	0.49
1:B:506:MET:HG2	1:C:90:ARG:HD2	1.94	0.49
1:A:323:ARG:HA	1:A:327:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:TYR:CE2	1:E:336:PRO:HG2	2.48	0.49
1:F:19:GLN:O	1:F:23:GLN:HG2	2.12	0.49
1:A:145:ILE:HG22	1:D:449:ILE:HD11	1.95	0.49
1:B:506:MET:CE	1:C:130:THR:HB	2.42	0.49
1:E:45:GLN:NE2	1:E:53:ASN:HD22	2.09	0.49
1:E:475:PHE:HA	1:E:480:VAL:HG11	1.94	0.49
1:D:45:GLN:NE2	1:D:53:ASN:HD22	2.10	0.49
1:D:90:ARG:HD3	1:D:91:GLY:N	2.28	0.49
1:F:455:LYS:HG3	1:F:456:ALA:H	1.77	0.49
1:D:21:ALA:O	1:D:25:GLN:HG3	2.13	0.49
1:B:381:GLU:HG3	1:E:222:LEU:HD11	1.95	0.48
1:C:206:PRO:HB3	1:C:217:VAL:O	2.13	0.48
1:C:146:GLN:HE21	1:C:146:GLN:N	2.00	0.48
1:D:201:MET:O	1:D:228:HIS:NE2	2.39	0.48
1:D:486:GLN:HG2	5:D:4344:HOH:O	2.13	0.48
1:F:484:ARG:HD2	5:F:6349:HOH:O	2.12	0.48
1:A:39:GLN:NE2	1:A:44:LYS:HE2	2.28	0.48
1:C:433:PRO:HD3	1:C:491:ILE:O	2.14	0.48
1:C:229:MET:O	1:C:313:TYR:HB2	2.14	0.48
1:C:422:ARG:HD3	5:C:7252:HOH:O	2.14	0.48
1:F:422:ARG:NH2	1:F:488:ASP:OD1	2.40	0.48
1:D:122:GLU:O	1:D:126:GLN:HG2	2.14	0.47
1:D:323:ARG:HA	1:D:327:ARG:O	2.14	0.47
1:D:81:VAL:HG13	1:D:107:VAL:CG1	2.44	0.47
1:D:90:ARG:CD	1:E:506:MET:HG2	2.44	0.47
1:B:376:PRO:HB3	1:E:204:THR:HG21	1.96	0.47
1:C:429:VAL:HG12	1:C:487:VAL:HG12	1.96	0.47
1:E:411:ALA:HB3	1:E:437:ILE:HA	1.97	0.47
1:B:506:MET:HE3	1:B:506:MET:O	2.14	0.47
1:B:339:MET:HE1	1:B:375:LEU:HD22	1.96	0.47
1:B:356:ASN:ND2	5:B:7115:HOH:O	2.45	0.47
1:C:38:LYS:O	1:C:42:GLN:HG3	2.15	0.47
1:A:54:LEU:O	1:A:250:LYS:HE2	2.14	0.47
1:B:323:ARG:HA	1:B:327:ARG:O	2.15	0.47
1:D:445:ALA:O	1:D:449:ILE:HG13	2.15	0.47
1:F:35:ARG:CB	1:F:106:THR:HB	2.45	0.47
1:F:90:ARG:NH1	5:F:6483:HOH:O	2.48	0.47
1:E:24:ARG:O	1:E:28:GLU:HG3	2.15	0.47
1:C:438:ALA:HB2	1:C:476:ASN:CG	2.35	0.46
1:D:146:GLN:HE21	1:D:146:GLN:N	2.04	0.46
1:E:14:GLU:OE2	1:E:14:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:HE	1:C:484:ARG:NE	2.14	0.46
1:B:443:GLU:HA	1:B:468:ILE:HG12	1.98	0.46
1:A:38:LYS:NZ	1:A:38:LYS:HB3	2.31	0.46
1:A:299:LYS:NZ	5:A:7490:HOH:O	2.38	0.46
1:A:370:ASP:CG	1:A:409:ARG:HB3	2.35	0.46
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.81	0.46
1:B:452:LYS:H	1:B:452:LYS:HD3	1.78	0.46
1:C:220:ASP:HB2	5:C:7476:HOH:O	2.16	0.46
1:E:198:LYS:HD2	5:E:4226:HOH:O	2.15	0.46
1:F:370:ASP:CG	1:F:409:ARG:HB3	2.36	0.46
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.81	0.46
1:D:12:THR:HG23	1:D:15:GLY:CA	2.46	0.46
1:D:339:MET:HE1	5:D:4022:HOH:O	2.16	0.46
1:A:207:GLN:CD	1:A:207:GLN:H	2.19	0.46
1:B:74:PHE:CD1	1:E:450:PHE:HZ	2.34	0.45
1:D:316:ASN:HB3	1:D:339:MET:HE3	1.99	0.45
1:D:339:MET:HE2	5:D:4124:HOH:O	2.16	0.45
1:F:455:LYS:CG	1:F:456:ALA:N	2.79	0.45
1:C:510:LYS:O	1:C:511:ARG:HD3	2.15	0.45
1:D:444:GLY:CA	1:D:447:ASN:HB3	2.46	0.45
5:D:4317:HOH:O	1:E:506:MET:HE1	2.17	0.45
1:A:285:ILE:HD11	1:B:12:THR:C	2.36	0.45
1:C:422:ARG:HG2	1:C:422:ARG:NH1	2.28	0.45
1:C:428:ALA:HA	1:C:488:ASP:OD2	2.17	0.45
1:E:291:TYR:CZ	1:E:336:PRO:HG2	2.51	0.45
1:F:200:HIS:HB2	5:F:6202:HOH:O	2.16	0.45
1:C:444:GLY:O	1:C:448:VAL:HG23	2.16	0.45
1:E:6:ASN:OD1	1:E:6:ASN:N	2.50	0.45
1:A:317:LEU:CD2	1:A:351:ALA:HB2	2.47	0.45
1:E:451:ARG:HD2	1:E:452:LYS:HE3	1.97	0.45
1:C:394:TYR:CD2	1:C:522:PHE:HD2	2.35	0.45
1:B:452:LYS:H	1:B:452:LYS:NZ	2.10	0.45
1:D:442:ALA:HB2	1:D:472:GLN:NE2	2.27	0.45
1:F:452:LYS:NZ	1:F:453:GLU:HB2	2.32	0.45
1:F:511:ARG:HH11	1:F:511:ARG:HG3	1.81	0.45
1:B:207:GLN:HA	1:B:207:GLN:NE2	2.32	0.45
1:C:100:ALA:HA	1:C:135:LEU:O	2.17	0.45
1:A:205:GLY:CA	1:A:207:GLN:HE22	2.28	0.44
1:E:86:VAL:HB	1:E:116:GLN:HG3	1.99	0.44
1:F:291:TYR:CE2	1:F:336:PRO:HG2	2.52	0.44
1:F:323:ARG:HA	1:F:327:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:O	1:B:42:GLN:HG3	2.18	0.44
1:C:439:VAL:HA	1:F:152:LEU:HG	1.99	0.44
1:D:446:ALA:O	1:D:450:PHE:HD1	1.99	0.44
1:F:313:TYR:O	1:F:314:ALA:C	2.54	0.44
1:B:181:GLY:HA2	1:B:203:ILE:O	2.16	0.44
1:D:476:ASN:N	1:D:476:ASN:ND2	2.65	0.44
1:A:67:ARG:NH2	5:A:7157:HOH:O	2.49	0.44
1:B:522:PHE:HD1	1:E:522:PHE:CD1	2.36	0.44
1:C:431:ALA:HB2	1:C:487:VAL:HG11	2.00	0.44
1:E:16:ARG:HH11	1:F:285:ILE:HD12	1.81	0.44
1:C:184:SER:O	1:C:187:PRO:HD2	2.18	0.44
1:D:313:TYR:O	1:D:314:ALA:C	2.55	0.44
1:F:83:ALA:HB1	1:F:119:LYS:NZ	2.33	0.44
1:B:102:SER:HB3	5:B:7559:HOH:O	2.17	0.44
1:D:215:GLU:OE1	1:D:215:GLU:HA	2.18	0.44
1:F:22:GLU:O	1:F:26:VAL:HG23	2.17	0.44
1:B:394:TYR:CD2	1:B:522:PHE:HD2	2.36	0.44
1:C:14:GLU:CD	1:C:14:GLU:H	2.21	0.43
1:D:22:GLU:HG3	5:D:4445:HOH:O	2.18	0.43
1:D:94:LEU:HB3	5:D:4226:HOH:O	2.18	0.43
1:B:42:GLN:HB2	1:B:44:LYS:HE2	2.00	0.43
1:A:222:LEU:HD21	1:D:381:GLU:HG3	2.01	0.43
1:F:81:VAL:HG13	1:F:107:VAL:CG1	2.48	0.43
1:A:267:VAL:O	1:A:268:ASN:C	2.57	0.43
1:A:317:LEU:HD22	1:A:351:ALA:HB2	2.00	0.43
1:D:484:ARG:HG3	1:D:484:ARG:HH11	1.84	0.43
1:F:60:PHE:CE2	1:F:62:GLU:HB2	2.53	0.43
1:B:411:ALA:HB3	1:B:437:ILE:HA	2.00	0.43
1:C:128:LEU:CD1	1:C:168:VAL:HG11	2.49	0.43
1:F:451:ARG:HB3	5:F:6474:HOH:O	2.19	0.43
1:A:92:THR:HA	1:A:96:ARG:O	2.19	0.43
1:B:467:LYS:HD3	1:B:467:LYS:HA	1.79	0.43
1:F:451:ARG:N	5:F:6474:HOH:O	2.52	0.43
1:A:86:VAL:HB	1:A:116:GLN:CG	2.49	0.43
1:F:396:TYR:CG	1:F:420:CYS:HB2	2.53	0.43
1:F:431:ALA:HB2	1:F:487:VAL:HG11	2.01	0.43
1:A:122:GLU:O	1:A:126:GLN:HG2	2.19	0.43
1:A:313:TYR:O	1:A:314:ALA:C	2.58	0.43
1:C:210:LYS:O	1:C:213:THR:O	2.36	0.43
1:C:475:PHE:HA	1:C:480:VAL:HG11	2.01	0.43
1:F:92:THR:HA	1:F:96:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:GLU:O	1:F:126:GLN:HG2	2.19	0.43
1:F:175:ILE:HB	1:F:195:MET:HG3	2.01	0.43
1:B:452:LYS:HB2	1:B:452:LYS:NZ	2.34	0.42
1:B:521:ASN:HA	1:E:356:ASN:HD21	1.83	0.42
1:D:31:GLY:HA3	1:D:106:THR:O	2.19	0.42
1:E:269:PRO:HB3	1:E:326:GLY:HA3	2.00	0.42
1:A:421:ASN:HB2	5:A:7083:HOH:O	2.19	0.42
1:A:421:ASN:HD21	1:A:423:ASP:HB2	1.84	0.42
1:E:103:GLN:HG3	1:E:136:PHE:HE2	1.84	0.42
1:E:497:ARG:HD3	5:E:4182:HOH:O	2.19	0.42
1:A:77:ASP:OD1	1:A:78:LYS:N	2.52	0.42
1:E:33:GLU:O	1:E:37:GLU:HG3	2.19	0.42
1:E:100:ALA:HA	1:E:135:LEU:O	2.19	0.42
1:E:450:PHE:CE2	1:E:467:LYS:HD2	2.53	0.42
1:F:302:ASP:HB3	1:F:303:TRP:CD1	2.54	0.42
1:A:200:HIS:CD2	1:A:220:ASP:HA	2.55	0.42
1:B:31:GLY:HA3	1:B:106:THR:O	2.19	0.42
1:A:81:VAL:HG13	1:A:107:VAL:CG1	2.50	0.42
1:B:452:LYS:N	1:B:452:LYS:CD	2.82	0.42
1:D:293:VAL:HG21	1:D:333:ALA:HB1	2.01	0.42
1:B:60:PHE:CE2	1:B:62:GLU:HB2	2.53	0.42
1:B:449:ILE:HG13	1:B:450:PHE:CD1	2.55	0.42
1:A:73:LEU:HD12	1:D:475:PHE:CZ	2.55	0.42
1:A:152:LEU:HD21	1:D:416:TYR:HD1	1.85	0.42
1:C:460:PRO:HG3	5:C:7320:HOH:O	2.20	0.42
1:B:9:LEU:HD12	1:B:16:ARG:HE	1.85	0.41
1:B:100:ALA:HA	1:B:135:LEU:O	2.20	0.41
1:D:316:ASN:HA	1:D:338:VAL:HB	2.02	0.41
1:F:149:ILE:HA	1:F:152:LEU:HB2	2.02	0.41
1:F:397:SER:HG	1:F:424:LEU:HD13	1.85	0.41
1:A:411:ALA:HB1	1:A:416:TYR:CD2	2.54	0.41
1:D:25:GLN:HG3	5:D:4209:HOH:O	2.20	0.41
1:F:128:LEU:CD2	1:F:164:LYS:HE2	2.50	0.41
1:A:175:ILE:HB	1:A:195:MET:HG3	2.02	0.41
1:A:291:TYR:CE1	1:A:336:PRO:HG2	2.55	0.41
1:D:291:TYR:CZ	1:D:336:PRO:HG2	2.56	0.41
1:E:45:GLN:HE22	1:E:53:ASN:HD22	1.68	0.41
1:A:506:MET:HG2	1:B:90:ARG:HD3	2.01	0.41
1:B:411:ALA:HB1	1:B:416:TYR:CG	2.55	0.41
1:A:522:PHE:CD1	1:D:522:PHE:HD1	2.37	0.41
1:D:35:ARG:HH11	1:D:35:ARG:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:ILE:HG13	1:E:450:PHE:CD1	2.56	0.41
1:B:70:ARG:NH1	1:B:70:ARG:HB2	2.35	0.41
1:B:207:GLN:NE2	1:B:207:GLN:CA	2.83	0.41
1:D:473:ASN:N	1:D:473:ASN:HD22	2.19	0.41
1:F:475:PHE:HA	1:F:480:VAL:HG11	2.02	0.41
1:C:522:PHE:HA	1:C:523:PRO:HD3	1.98	0.41
1:F:81:VAL:HG12	1:F:84:ASP:HA	2.03	0.41
1:F:451:ARG:H	1:F:451:ARG:NE	2.18	0.41
1:C:289:LYS:HA	1:C:289:LYS:CE	2.50	0.41
1:A:66:PHE:HB3	5:C:7133:HOH:O	2.21	0.41
1:A:81:VAL:HG13	1:A:107:VAL:HG12	2.03	0.41
5:C:7459:HOH:O	1:F:521:ASN:HB3	2.21	0.41
1:D:94:LEU:HD11	5:D:4193:HOH:O	2.19	0.41
1:D:186:SER:CB	1:D:187:PRO:HD3	2.48	0.41
1:D:229:MET:O	1:D:313:TYR:HB2	2.20	0.41
1:D:411:ALA:HB1	1:D:416:TYR:CD2	2.55	0.41
1:D:511:ARG:NH1	5:D:4210:HOH:O	2.54	0.41
1:E:11:SER:HA	5:E:4431:HOH:O	2.21	0.41
1:B:521:ASN:HA	1:E:356:ASN:ND2	2.36	0.41
1:C:184:SER:C	1:C:187:PRO:HD2	2.41	0.41
1:E:267:VAL:O	1:E:268:ASN:C	2.59	0.41
1:A:400:THR:HG22	1:A:512:GLN:HE21	1.86	0.40
1:D:28:GLU:HG2	1:D:48:ARG:CZ	2.50	0.40
1:F:105:PHE:CZ	3:F:4006:MCA:H5'2	2.56	0.40
1:F:267:VAL:O	1:F:268:ASN:C	2.59	0.40
1:C:288:LYS:HB2	1:C:288:LYS:NZ	2.36	0.40
1:D:369:VAL:HG22	1:D:419:MET:HB3	2.03	0.40
1:A:381:GLU:HG3	1:D:222:LEU:HD11	2.03	0.40
1:B:9:LEU:N	1:B:9:LEU:CD2	2.84	0.40
1:B:339:MET:HE3	1:B:375:LEU:HD22	2.02	0.40
1:C:422:ARG:CG	1:C:422:ARG:NH1	2.81	0.40
1:F:200:HIS:CD2	1:F:220:ASP:HA	2.57	0.40
1:B:122:GLU:HG3	5:B:7545:HOH:O	2.20	0.40
1:B:522:PHE:HD1	1:E:522:PHE:HD1	1.70	0.40
1:C:396:TYR:CD2	1:C:420:CYS:HB2	2.56	0.40
1:E:313:TYR:O	1:E:314:ALA:C	2.60	0.40
1:A:111:SER:HA	1:A:142:GLY:O	2.21	0.40
1:B:313:TYR:O	1:B:314:ALA:C	2.60	0.40
1:D:285:ILE:HD13	1:D:285:ILE:HA	1.98	0.40
1:F:35:ARG:HB2	1:F:106:THR:HB	2.02	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	514/523 (98%)	497 (97%)	17 (3%)	0	100	100
1	B	514/523 (98%)	500 (97%)	14 (3%)	0	100	100
1	C	508/523 (97%)	485 (96%)	23 (4%)	0	100	100
1	D	498/523 (95%)	480 (96%)	18 (4%)	0	100	100
1	E	517/523 (99%)	498 (96%)	18 (4%)	1 (0%)	47	44
1	F	514/523 (98%)	496 (96%)	17 (3%)	1 (0%)	47	44
All	All	3065/3138 (98%)	2956 (96%)	107 (4%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	10	ALA
1	E	409	ARG

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	405/411 (98%)	395 (98%)	10 (2%)	47	49
1	B	405/411 (98%)	397 (98%)	8 (2%)	55	58
1	C	403/411 (98%)	394 (98%)	9 (2%)	52	55
1	D	396/411 (96%)	386 (98%)	10 (2%)	47	49
1	E	408/411 (99%)	399 (98%)	9 (2%)	52	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	405/411 (98%)	394 (97%)	11 (3%)	44	46
All	All	2422/2466 (98%)	2365 (98%)	57 (2%)	49	51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	136	PHE
1	A	146	GLN
1	A	210	LYS
1	A	222	LEU
1	A	421	ASN
1	A	424	LEU
1	A	451	ARG
1	A	452	LYS
1	A	514	ARG
1	B	9	LEU
1	B	136	PHE
1	B	146	GLN
1	B	202	PHE
1	B	288	LYS
1	B	424	LEU
1	B	452	LYS
1	B	466	GLU
1	C	129	LEU
1	C	136	PHE
1	C	146	GLN
1	C	202	PHE
1	C	317	LEU
1	C	424	LEU
1	C	454	ILE
1	C	466	GLU
1	C	511	ARG
1	D	9	LEU
1	D	12	THR
1	D	34	ARG
1	D	136	PHE
1	D	146	GLN
1	D	317	LEU
1	D	375	LEU
1	D	424	LEU
1	D	447	ASN

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Mol	Chain	Res	Type
1	D	505	GLU
1	E	6	ASN
1	E	78	LYS
1	E	90	ARG
1	E	136	PHE
1	E	146	GLN
1	E	152	LEU
1	E	202	PHE
1	E	307	LEU
1	E	317	LEU
1	F	122	GLU
1	F	136	PHE
1	F	146	GLN
1	F	152	LEU
1	F	202	PHE
1	F	356	ASN
1	F	424	LEU
1	F	451	ARG
1	F	452	LYS
1	F	455	LYS
1	F	460	PRO

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	25	GLN
1	A	146	GLN
1	A	207	GLN
1	A	234	ASN
1	A	271	ASN
1	A	356	ASN
1	A	379	GLN
1	A	421	ASN
1	A	486	GLN
1	A	512	GLN
1	A	521	ASN
1	B	19	GLN
1	B	23	GLN
1	B	45	GLN
1	B	146	GLN
1	B	207	GLN

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	356	ASN
1	B	379	GLN
1	C	53	ASN
1	C	146	GLN
1	C	207	GLN
1	C	234	ASN
1	C	271	ASN
1	C	379	GLN
1	D	23	GLN
1	D	25	GLN
1	D	45	GLN
1	D	146	GLN
1	D	162	ASN
1	D	207	GLN
1	D	234	ASN
1	D	271	ASN
1	D	447	ASN
1	D	472	GLN
1	D	473	ASN
1	D	476	ASN
1	D	512	GLN
1	E	45	GLN
1	E	146	GLN
1	E	234	ASN
1	E	268	ASN
1	F	146	GLN
1	F	162	ASN
1	F	234	ASN
1	F	271	ASN
1	F	379	GLN
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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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
3	MCA	C	4003	-	23,28,57	3.18	6 (26%)	23,42,85	1.82	5 (21%)
3	MCA	A	4001	-	26,29,57	2.76	10 (38%)	31,45,85	2.89	9 (29%)
4	MPD	F	6006	-	7,7,7	0.60	0	9,10,10	0.50	0
3	MCA	E	4005	-	22,25,57	1.99	5 (22%)	24,38,85	1.82	4 (16%)
3	MCA	D	4004	-	28,33,57	2.57	11 (39%)	35,52,85	3.52	13 (37%)
3	MCA	F	4006	-	26,29,57	2.73	10 (38%)	31,45,85	2.87	9 (29%)
3	MCA	B	4002	-	22,28,57	2.70	5 (22%)	24,42,85	1.80	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MCA	C	4003	-	-	2/8/30/75	0/3/3/3
3	MCA	A	4001	-	-	2/11/31/75	0/3/3/3
4	MPD	F	6006	-	-	0/5/5/5	-
3	MCA	E	4005	-	-	4/7/27/75	0/3/3/3
3	MCA	D	4004	-	-	8/17/37/75	0/3/3/3
3	MCA	F	4006	-	-	2/11/31/75	0/3/3/3
3	MCA	B	4002	-	-	4/8/30/75	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4002	MCA	O5'-C5'	-10.17	1.19	1.44
3	C	4003	MCA	O5'-C5'	-9.86	1.19	1.44
3	C	4003	MCA	P1-O5'	-8.87	1.37	1.62
3	A	4001	MCA	P1-O5'	-6.89	1.38	1.60
3	F	4006	MCA	P1-O5'	-6.75	1.38	1.60
3	A	4001	MCA	O5'-C5'	-6.54	1.19	1.44
3	F	4006	MCA	O5'-C5'	-6.46	1.19	1.44
3	D	4004	MCA	O5'-C5'	-6.29	1.20	1.44
3	A	4001	MCA	P1-O12	-5.48	1.33	1.54
3	E	4005	MCA	O5'-C5'	-5.40	1.19	1.42
3	F	4006	MCA	P1-O12	-5.39	1.34	1.54
3	D	4004	MCA	P1-O5'	-4.95	1.39	1.59
3	D	4004	MCA	P1-O12	-4.52	1.34	1.55
3	E	4005	MCA	P3-O3'	4.31	1.67	1.59
3	B	4002	MCA	P3-O3'	4.19	1.67	1.59
3	A	4001	MCA	P1-O11	-4.13	1.37	1.50
3	F	4006	MCA	P1-O11	-4.10	1.37	1.50
3	C	4003	MCA	P3-O3'	4.07	1.67	1.59
3	A	4001	MCA	P3-O3'	3.89	1.66	1.59
3	D	4004	MCA	P1-O11	-3.84	1.37	1.50
3	D	4004	MCA	P2-O22	-3.68	1.40	1.54
3	D	4004	MCA	C2-N3	3.64	1.38	1.32
3	D	4004	MCA	P3-O3'	3.60	1.66	1.59
3	D	4004	MCA	P2-O21	-3.58	1.39	1.50
3	A	4001	MCA	C2-N3	3.54	1.37	1.32
3	C	4003	MCA	C2-N3	3.52	1.37	1.32
3	F	4006	MCA	C2-N3	3.49	1.37	1.32
3	B	4002	MCA	C2-N3	3.48	1.37	1.32
3	D	4004	MCA	C4-N3	3.35	1.40	1.35
3	E	4005	MCA	C2-N3	3.28	1.37	1.32
3	F	4006	MCA	P3-O3'	3.26	1.65	1.59
3	F	4006	MCA	C4-N3	3.23	1.40	1.35
3	E	4005	MCA	C4-N3	3.23	1.40	1.35
3	C	4003	MCA	C4-N3	3.13	1.40	1.35
3	B	4002	MCA	C4-N3	3.10	1.39	1.35
3	A	4001	MCA	C4-N3	2.88	1.39	1.35
3	F	4006	MCA	P1-O6	2.72	1.65	1.54
3	A	4001	MCA	P1-O6	2.69	1.65	1.54
3	F	4006	MCA	C2-N1	2.25	1.38	1.33
3	B	4002	MCA	C2-N1	2.06	1.37	1.33
3	C	4003	MCA	C2-N1	2.05	1.37	1.33
3	A	4001	MCA	C2-N1	2.05	1.37	1.33
3	E	4005	MCA	C2-N1	2.05	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4006	MCA	C8-N7	-2.04	1.31	1.34
3	D	4004	MCA	P2-O7	2.04	1.62	1.54
3	A	4001	MCA	C8-N7	-2.01	1.31	1.34
3	D	4004	MCA	C2-N1	2.00	1.37	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4004	MCA	P1-O6-P2	12.71	176.44	132.83
3	F	4006	MCA	P1-O5'-C5'	11.24	149.27	118.30
3	A	4001	MCA	P1-O5'-C5'	11.14	148.97	118.30
3	D	4004	MCA	O33-P3-O31	-7.20	82.48	110.68
3	D	4004	MCA	O33-P3-O32	-6.65	82.23	107.64
3	E	4005	MCA	O3'-P3-O31	-5.65	87.58	109.39
3	C	4003	MCA	O3'-P3-O31	-5.58	87.87	109.39
3	F	4006	MCA	O3'-P3-O31	-5.57	87.89	109.39
3	A	4001	MCA	O3'-P3-O31	-5.57	87.90	109.39
3	D	4004	MCA	O32-P3-O31	5.57	132.48	110.68
3	B	4002	MCA	O3'-P3-O31	-5.55	87.96	109.39
3	A	4001	MCA	O12-P1-O5'	-5.39	92.38	106.73
3	F	4006	MCA	O12-P1-O5'	-5.20	92.91	106.73
3	D	4004	MCA	P1-O5'-C5'	4.70	149.27	121.68
3	D	4004	MCA	O22-P2-O6	4.67	120.29	104.64
3	D	4004	MCA	O6-P2-O21	-4.50	86.22	111.19
3	D	4004	MCA	O22-P2-O21	4.14	126.88	110.68
3	F	4006	MCA	O5'-P1-O11	3.52	116.36	106.47
3	A	4001	MCA	O5'-P1-O11	3.50	116.29	106.47
3	D	4004	MCA	O32-P3-O3'	3.41	121.28	105.99
3	A	4001	MCA	O33-P3-O3'	3.38	121.12	105.99
3	E	4005	MCA	O33-P3-O3'	3.32	120.88	105.99
3	C	4003	MCA	O33-P3-O3'	3.30	120.79	105.99
3	B	4002	MCA	O33-P3-O3'	3.27	120.64	105.99
3	F	4006	MCA	O33-P3-O3'	3.19	120.28	105.99
3	D	4004	MCA	O12-P1-O5'	-3.14	93.14	107.75
3	E	4005	MCA	C5-C6-N6	2.85	124.69	120.35
3	B	4002	MCA	C5-C6-N6	2.81	124.63	120.35
3	C	4003	MCA	C5-C6-N6	2.81	124.63	120.35
3	A	4001	MCA	C5-C6-N6	2.72	124.48	120.35
3	D	4004	MCA	C5-C6-N6	2.65	124.38	120.35
3	F	4006	MCA	C5-C6-N6	2.65	124.38	120.35
3	F	4006	MCA	C1'-N9-C4	-2.46	122.33	126.64
3	B	4002	MCA	C1'-N9-C4	-2.35	122.52	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4004	MCA	C1'-N9-C4	-2.29	122.61	126.64
3	A	4001	MCA	O6-P1-O12	2.28	116.33	107.64
3	C	4003	MCA	C1'-N9-C4	-2.27	122.65	126.64
3	F	4006	MCA	O6-P1-O12	2.19	116.01	107.64
3	A	4001	MCA	C1'-N9-C4	-2.19	122.79	126.64
3	E	4005	MCA	C1'-N9-C4	-2.18	122.82	126.64
3	F	4006	MCA	O2'-C2'-C3'	2.16	117.29	111.17
3	D	4004	MCA	O2'-C2'-C3'	2.11	117.16	111.17
3	C	4003	MCA	O2'-C2'-C3'	2.05	117.00	111.17
3	A	4001	MCA	O12-P1-O11	2.03	118.62	110.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

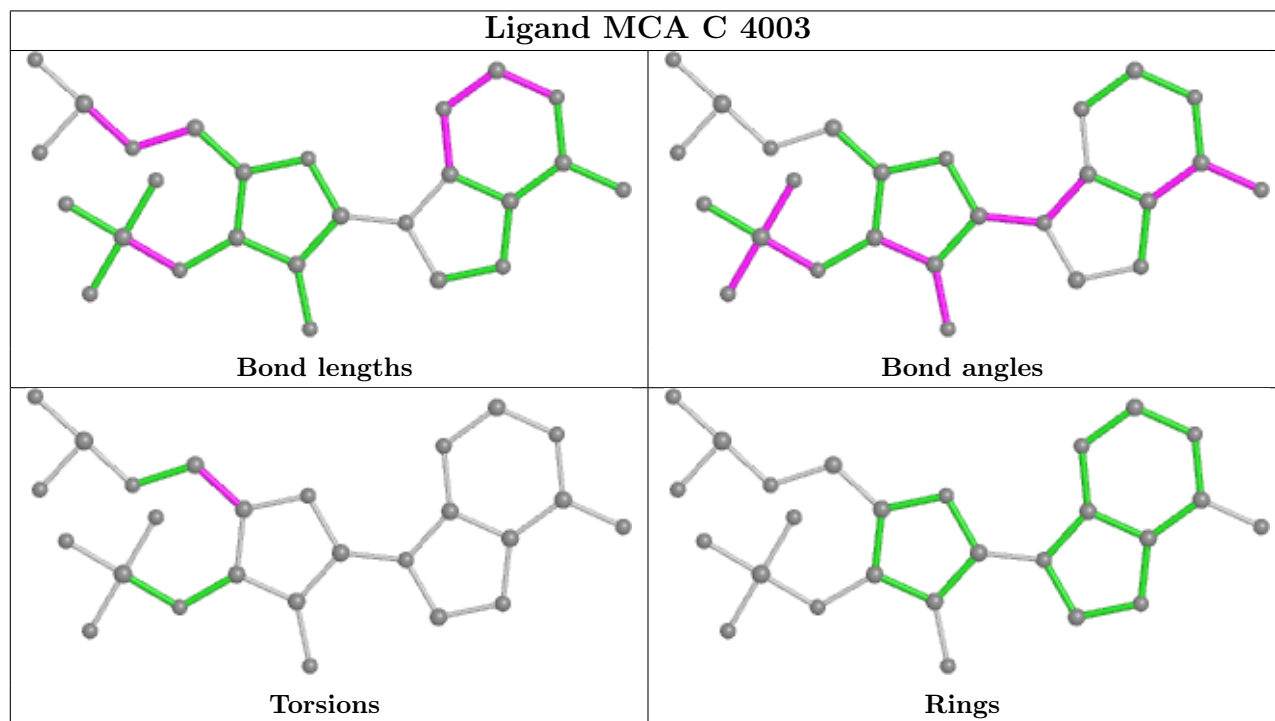
Mol	Chain	Res	Type	Atoms
3	E	4005	MCA	C3'-C4'-C5'-O5'
3	E	4005	MCA	O4'-C4'-C5'-O5'
3	A	4001	MCA	C3'-C4'-C5'-O5'
3	B	4002	MCA	C3'-C4'-C5'-O5'
3	B	4002	MCA	O4'-C4'-C5'-O5'
3	C	4003	MCA	C3'-C4'-C5'-O5'
3	D	4004	MCA	C3'-C4'-C5'-O5'
3	F	4006	MCA	C3'-C4'-C5'-O5'
3	B	4002	MCA	C4'-C3'-O3'-P3
3	D	4004	MCA	C4'-C3'-O3'-P3
3	E	4005	MCA	C4'-C3'-O3'-P3
3	A	4001	MCA	O4'-C4'-C5'-O5'
3	C	4003	MCA	O4'-C4'-C5'-O5'
3	D	4004	MCA	O4'-C4'-C5'-O5'
3	F	4006	MCA	O4'-C4'-C5'-O5'
3	B	4002	MCA	C2'-C3'-O3'-P3
3	E	4005	MCA	C2'-C3'-O3'-P3
3	D	4004	MCA	P1-O6-P2-O21
3	D	4004	MCA	P2-O6-P1-O12
3	D	4004	MCA	C5'-O5'-P1-O6
3	D	4004	MCA	P2-O6-P1-O11
3	D	4004	MCA	C2'-C3'-O3'-P3

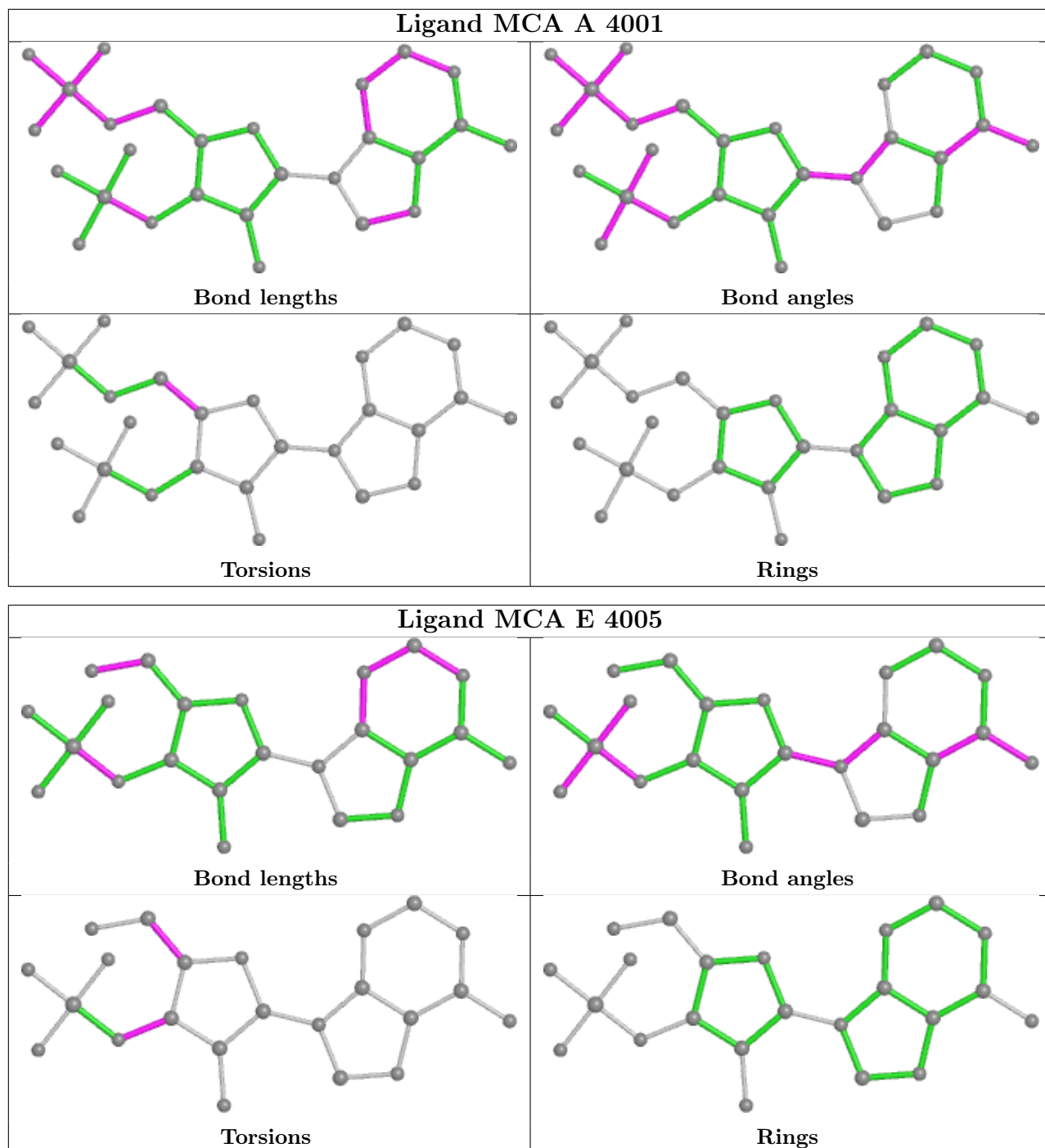
There are no ring outliers.

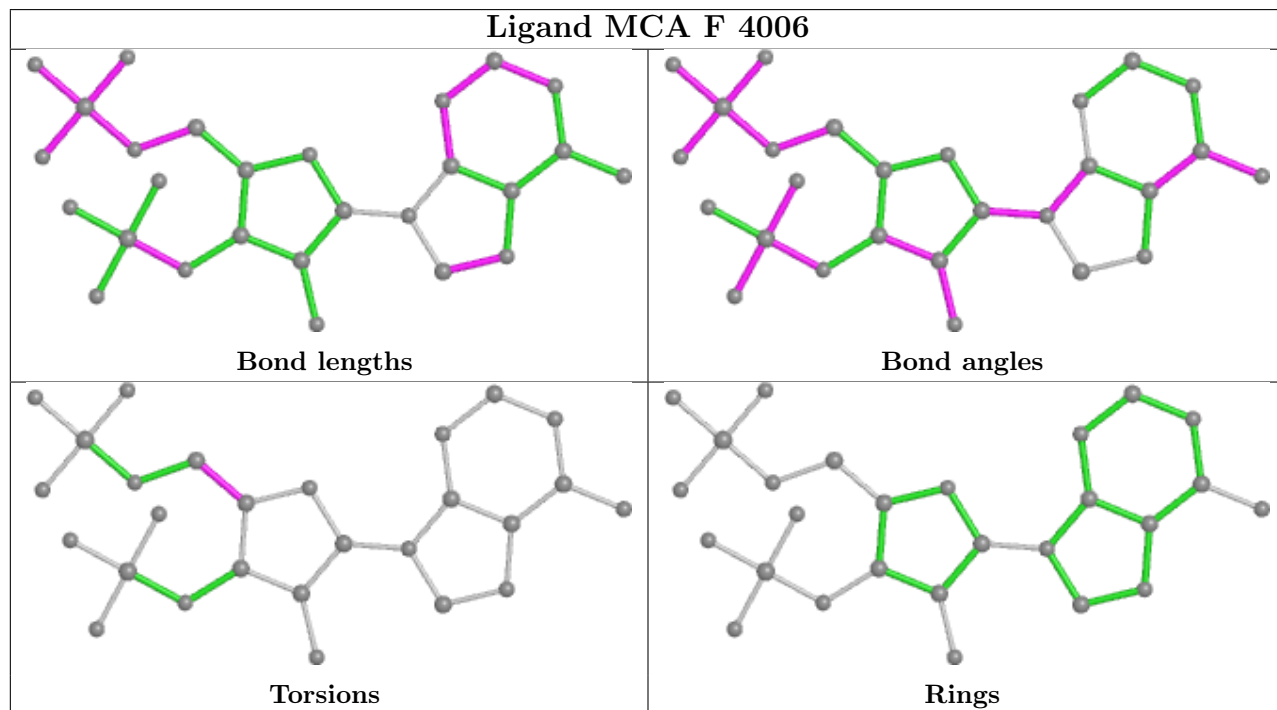
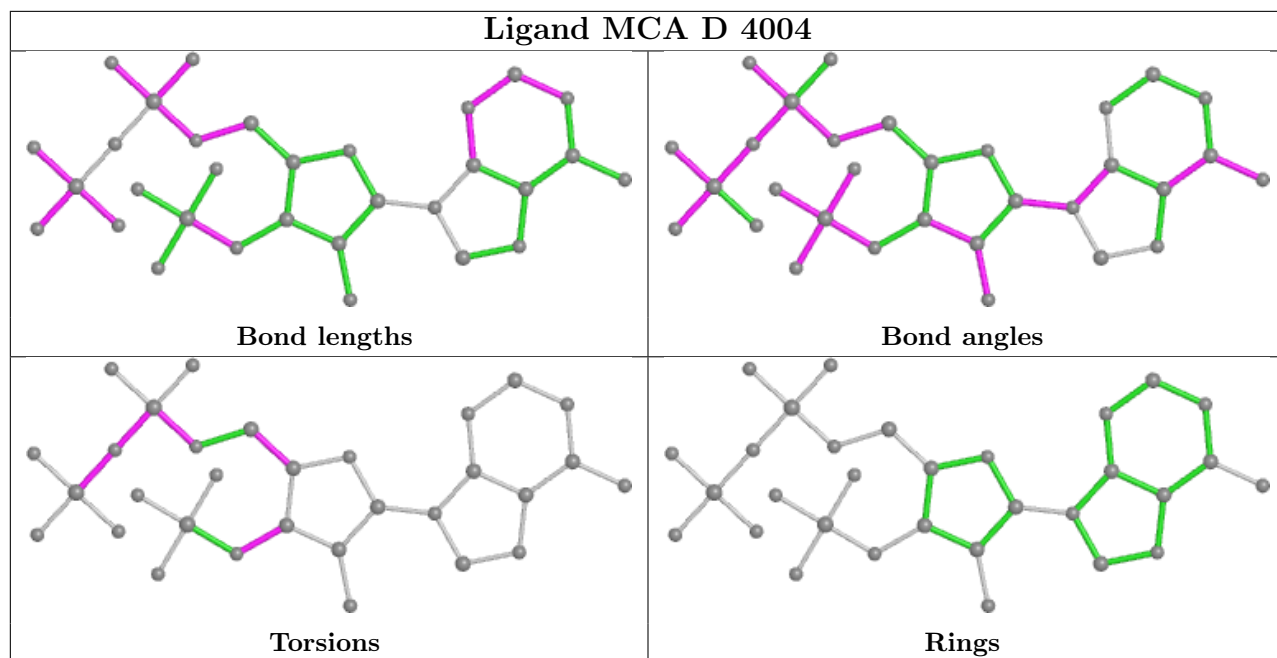
4 monomers are involved in 5 short contacts:

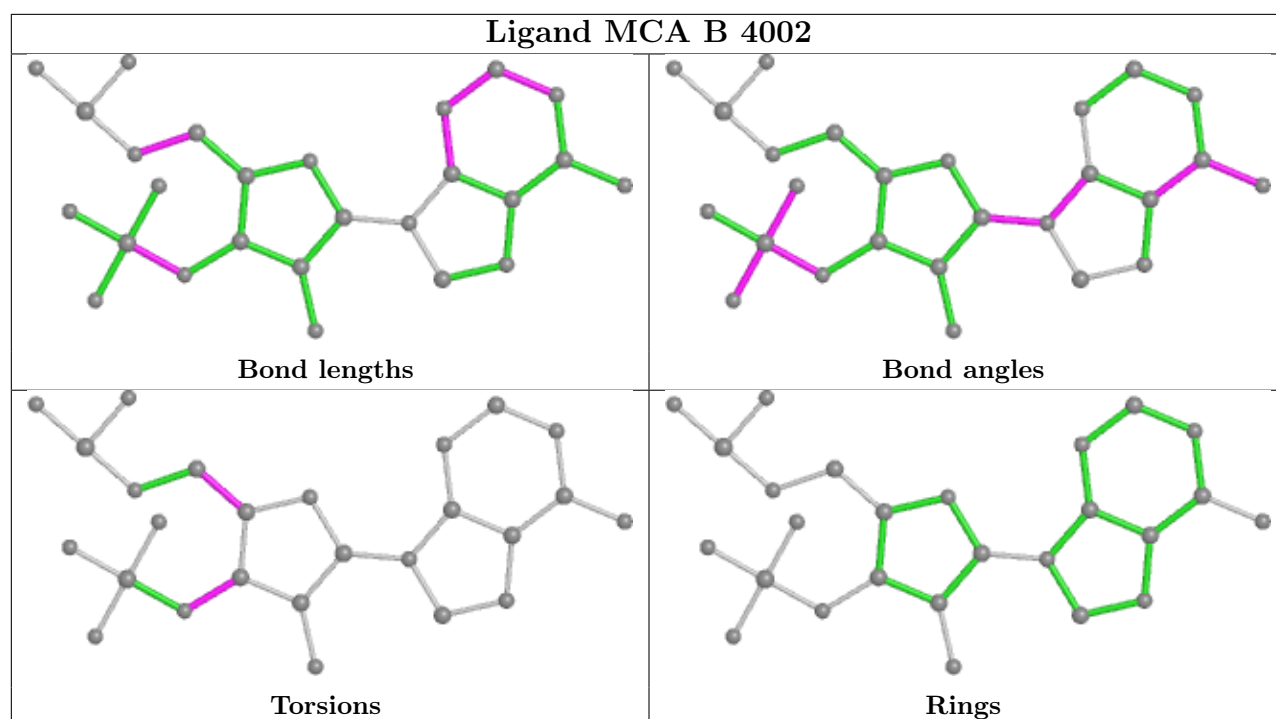
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4003	MCA	1	0
3	E	4005	MCA	1	0
3	D	4004	MCA	1	0
3	F	4006	MCA	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	516/523 (98%)	-0.61	3 (0%) 89 88	8, 16, 41, 62	0
1	B	516/523 (98%)	-0.72	3 (0%) 89 88	6, 14, 34, 69	0
1	C	514/523 (98%)	-0.56	14 (2%) 54 53	8, 15, 48, 96	0
1	D	504/523 (96%)	-0.48	11 (2%) 62 60	8, 19, 45, 105	0
1	E	519/523 (99%)	-0.75	3 (0%) 89 88	7, 14, 33, 51	0
1	F	516/523 (98%)	-0.65	4 (0%) 86 85	8, 16, 37, 69	0
All	All	3085/3138 (98%)	-0.63	38 (1%) 79 78	6, 16, 39, 105	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	462	ALA	8.6
1	D	463	MET	7.3
1	C	464	ARG	5.0
1	C	459	ASP	4.8
1	C	462	ALA	4.6
1	D	450	PHE	4.3
1	C	458	ASP	4.3
1	C	463	MET	4.2
1	C	460	PRO	4.0
1	D	446	ALA	3.8
1	C	465	ALA	3.4
1	D	469	GLU	3.4
1	A	513	THR	3.3
1	C	466	GLU	3.3
1	F	9	LEU	3.1
1	C	453	GLU	3.0
1	C	457	ALA	3.0
1	A	458	ASP	3.0
1	D	447	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	467	LYS	2.8
1	D	444	GLY	2.7
1	D	449	ILE	2.6
1	C	452	LYS	2.6
1	B	9	LEU	2.6
1	D	467	LYS	2.5
1	F	214	GLY	2.5
1	F	451	ARG	2.4
1	F	452	LYS	2.4
1	B	216	ASP	2.4
1	E	214	GLY	2.3
1	E	456	ALA	2.3
1	C	461	ASP	2.3
1	D	7	LEU	2.2
1	A	456	ALA	2.2
1	D	513	THR	2.2
1	C	468	ILE	2.1
1	B	458	ASP	2.1
1	E	455	LYS	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.

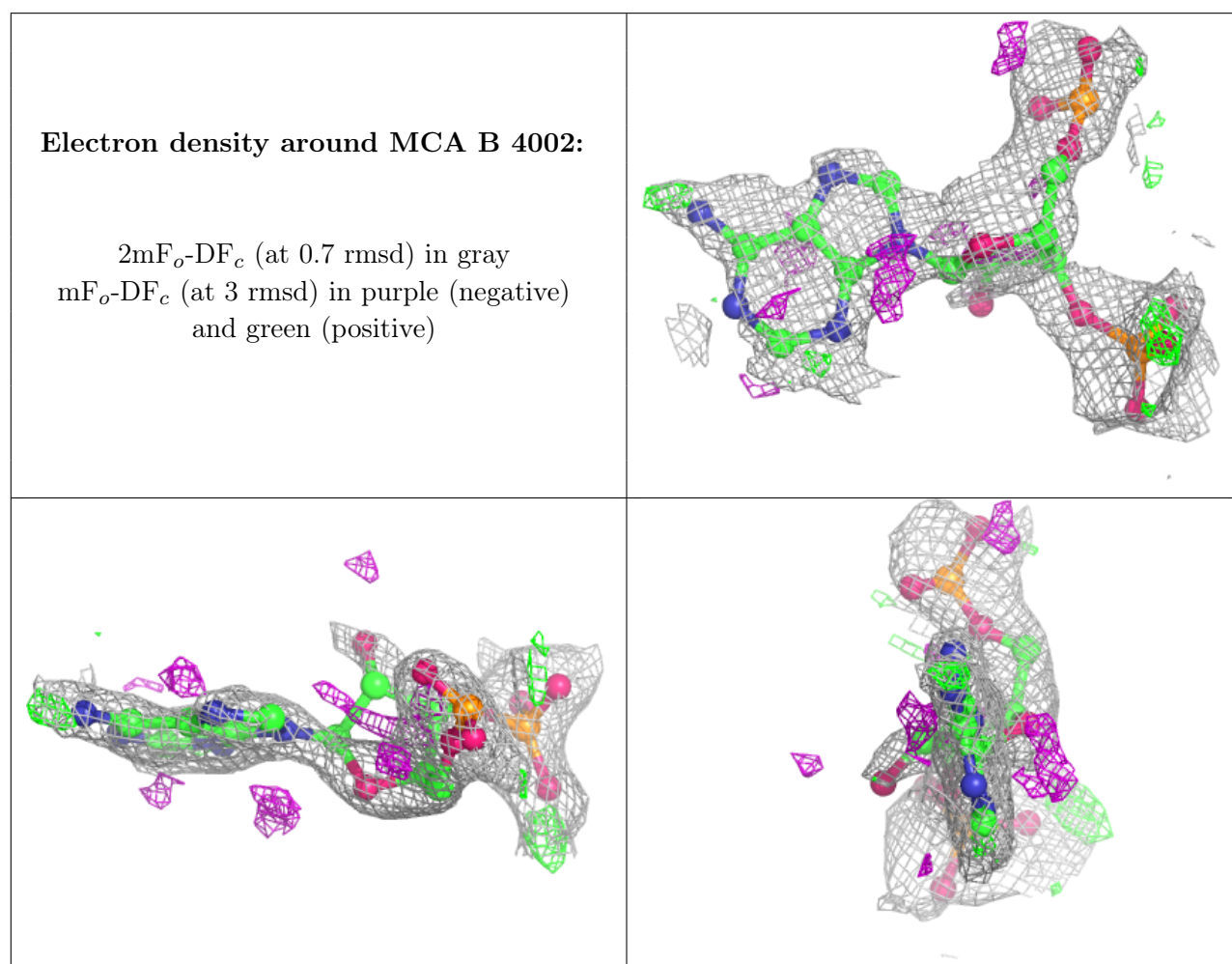
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MCA	B	4002	26/55	0.65	0.24	82,89,92,93	0
3	MCA	C	4003	26/55	0.65	0.23	62,81,94,95	0
3	MCA	D	4004	31/55	0.65	0.22	68,89,110,110	0
3	MCA	E	4005	23/55	0.71	0.20	53,65,76,76	0

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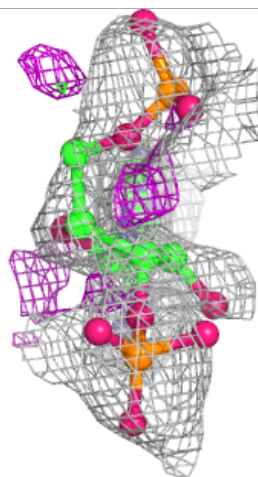
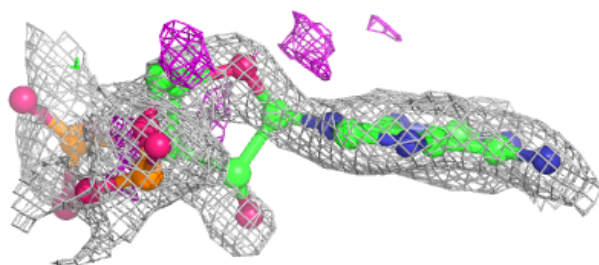
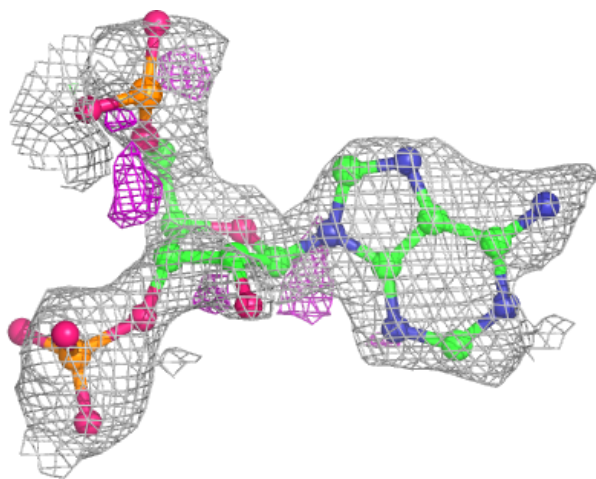
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MCA	F	4006	27/55	0.72	0.18	41,64,82,82	0
3	MCA	A	4001	27/55	0.73	0.22	62,76,85,87	0
4	MPD	F	6006	8/8	0.92	0.10	20,24,28,35	0
2	CD	B	7002	1/1	1.00	0.04	11,11,11,11	0
2	CD	C	7003	1/1	1.00	0.04	14,14,14,14	0
2	CD	A	7001	1/1	1.00	0.04	16,16,16,16	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.



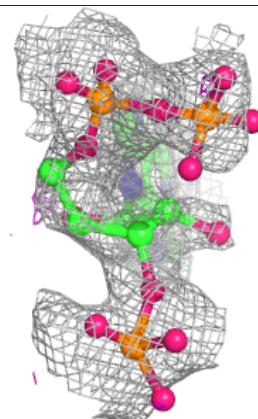
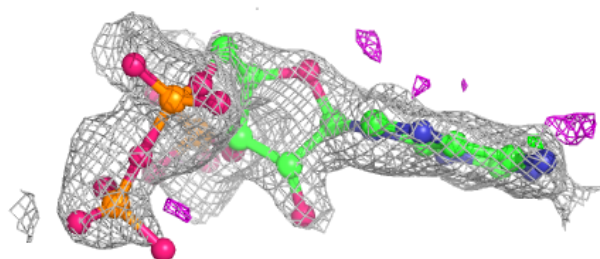
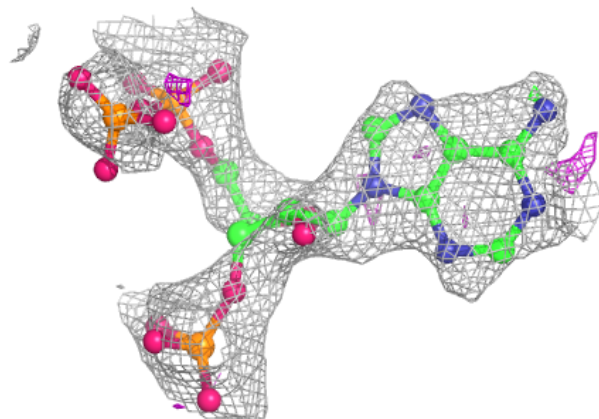
Electron density around MCA C 4003:

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

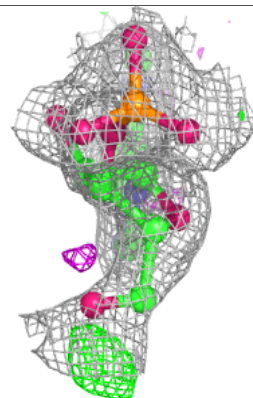
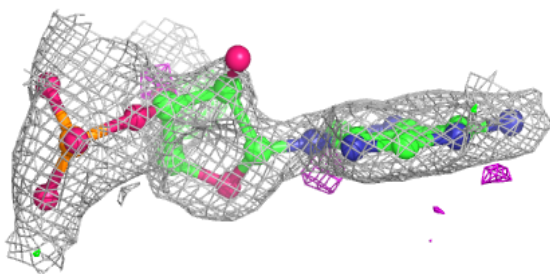
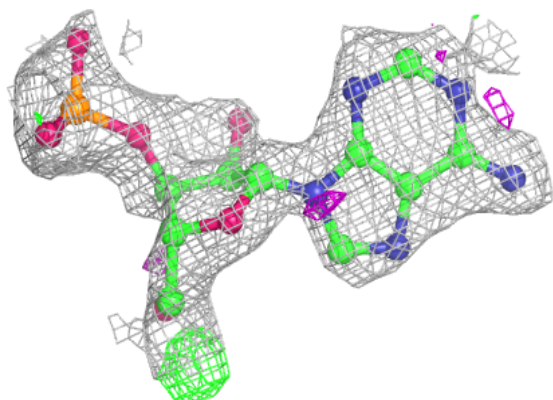


Electron density around MCA D 4004:

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

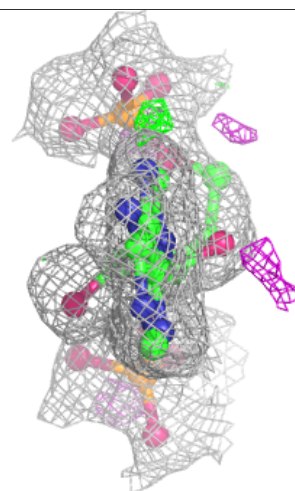
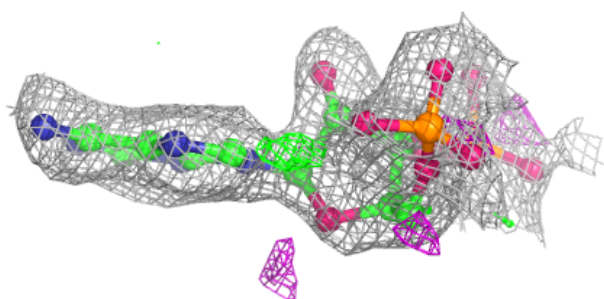
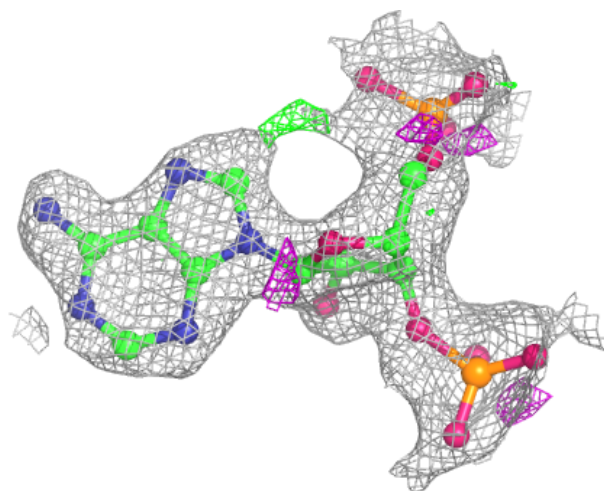
**Electron density around MCA E 4005:**

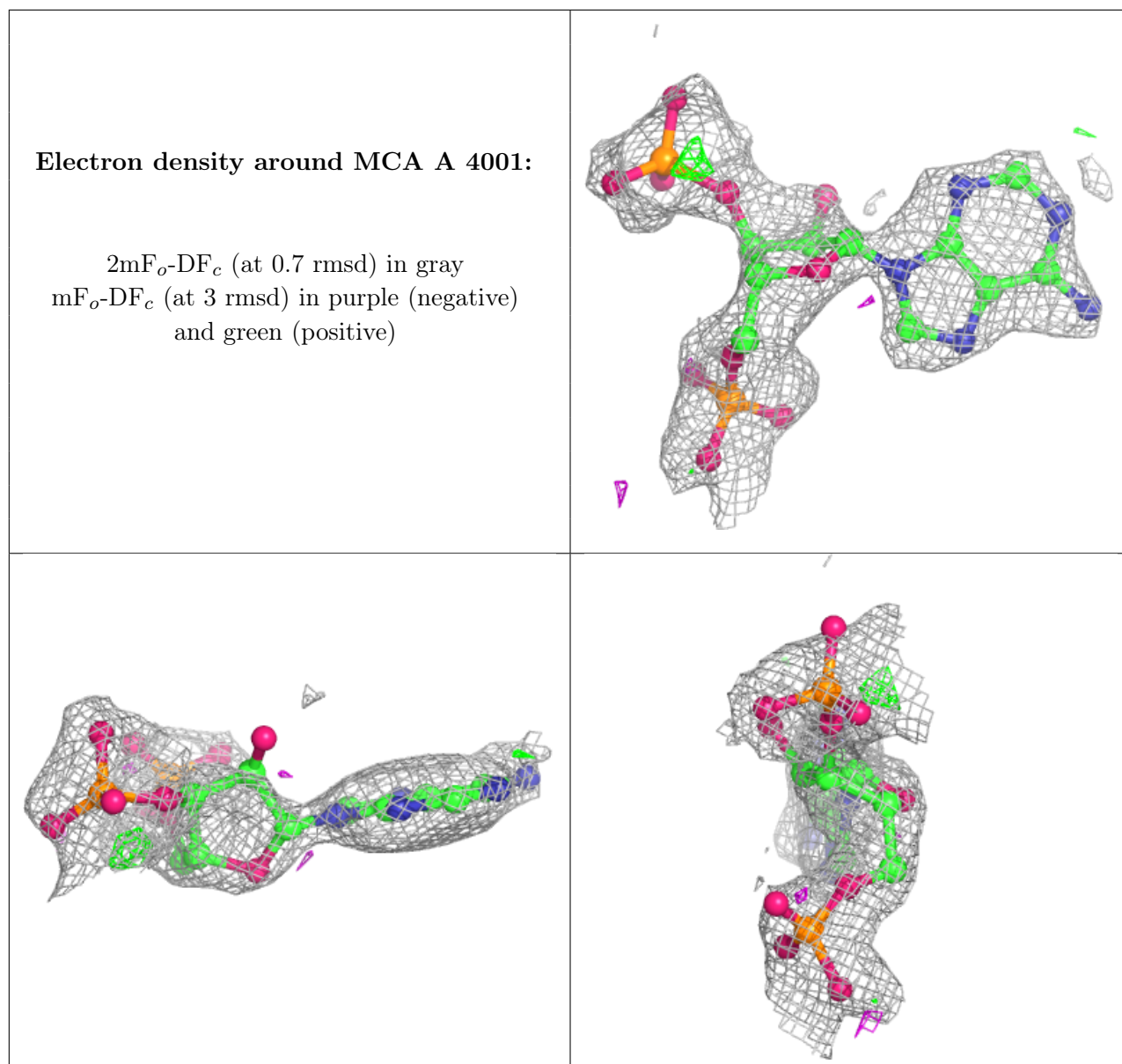
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.