Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 02:06 AM EDT

PDB ID	:	4JAE
Title	:	STRUCTURAL DETERMINATION OF THE A50T:S279G:S280K:V281K:K282E:H283N VARIANT OF CITRATE SYNTHASE FROM E. COLI complexed WITH S-CARBOXYMETHYL-COA
Authors	:	Maurus, R.; Brayer, G.D.
Deposited on	:	2013-02-18
Resolution	:	2.70 Å(reported)

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

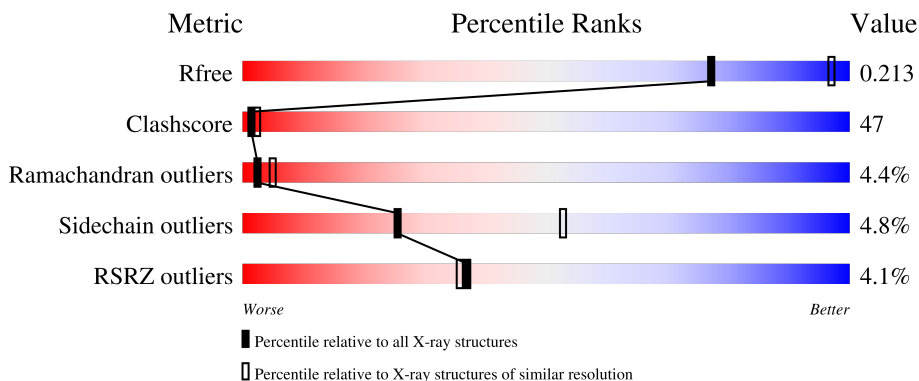|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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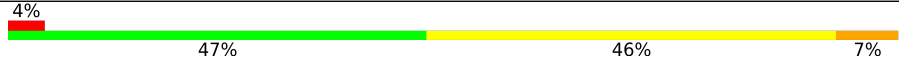*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	Percentile Ranks	Value
Rfree		0.213
Clashscore		47
Ramachandran outliers		4.4%
Sidechain outliers		4.8%
RSRZ outliers		4.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	426	4% · 48% 45% 7%
1	B	426	4% · 47% 46% 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7081 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total 3365	C 2132	N 578	O 630	S 25	0	0	0
1	B	426	Total 3365	C 2132	N 578	O 630	S 25	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ASP	ASN	SEE REMARK 999	UNP P0ABH7
A	50	THR	ALA	engineered mutation	UNP P0ABH7
A	279	GLY	SER	engineered mutation	UNP P0ABH7
A	280	LYS	SER	engineered mutation	UNP P0ABH7
A	281	LYS	VAL	engineered mutation	UNP P0ABH7
A	282	GLU	LYS	engineered mutation	UNP P0ABH7
A	283	ASN	HIS	engineered mutation	UNP P0ABH7
B	1010	ASP	ASN	SEE REMARK 999	UNP P0ABH7
B	1050	THR	ALA	engineered mutation	UNP P0ABH7
B	1279	GLY	SER	engineered mutation	UNP P0ABH7
B	1280	LYS	SER	engineered mutation	UNP P0ABH7
B	1281	LYS	VAL	engineered mutation	UNP P0ABH7
B	1282	GLU	LYS	engineered mutation	UNP P0ABH7
B	1283	ASN	HIS	engineered mutation	UNP P0ABH7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is CARBOXYMETHYL COENZYME *A (three-letter code: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$).
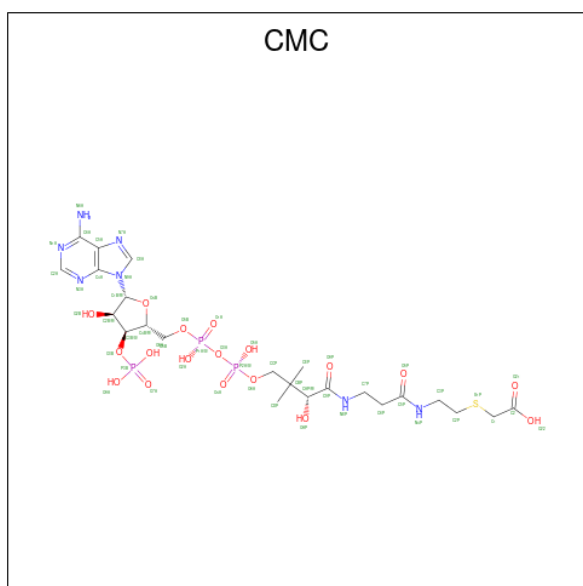
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 52	C 23	N 7	O 18	P 3	S 1	0	0
3	B	1	Total 52	C 23	N 7	O 18	P 3	S 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total 104	O 104	0	0
4	B	123	Total 123	O 123	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Citrate synthase

Chain A:

- Molecule 1: Citrate synthase

Chain B:
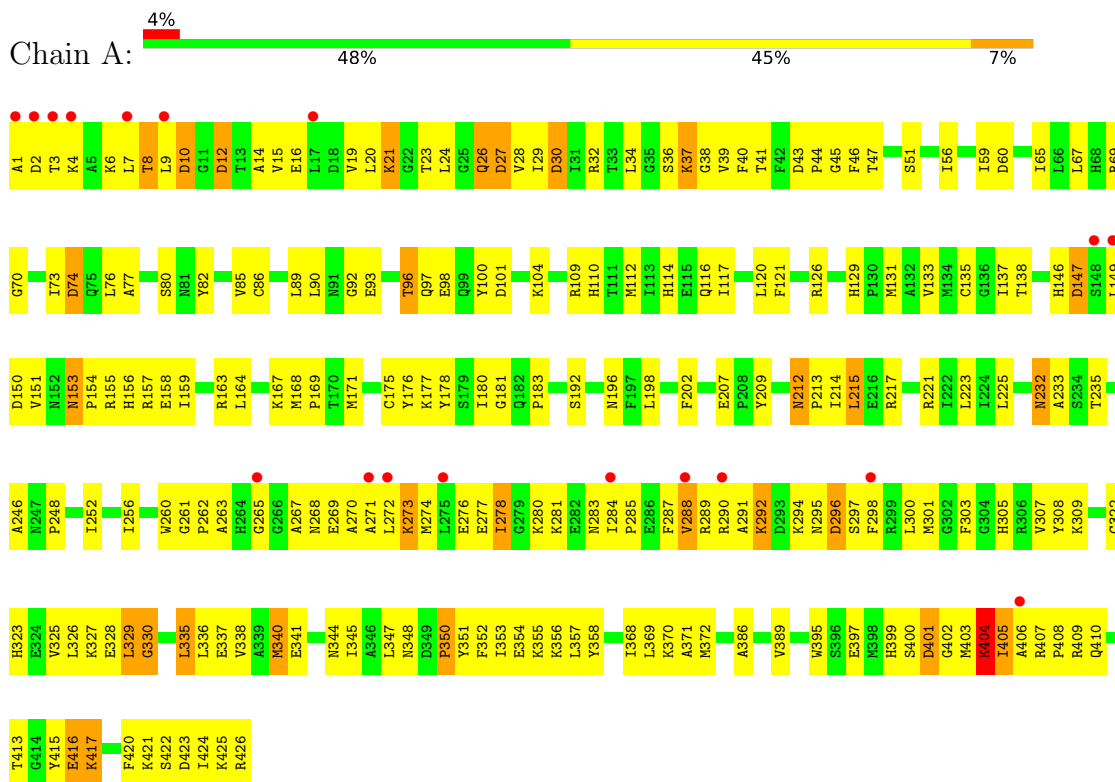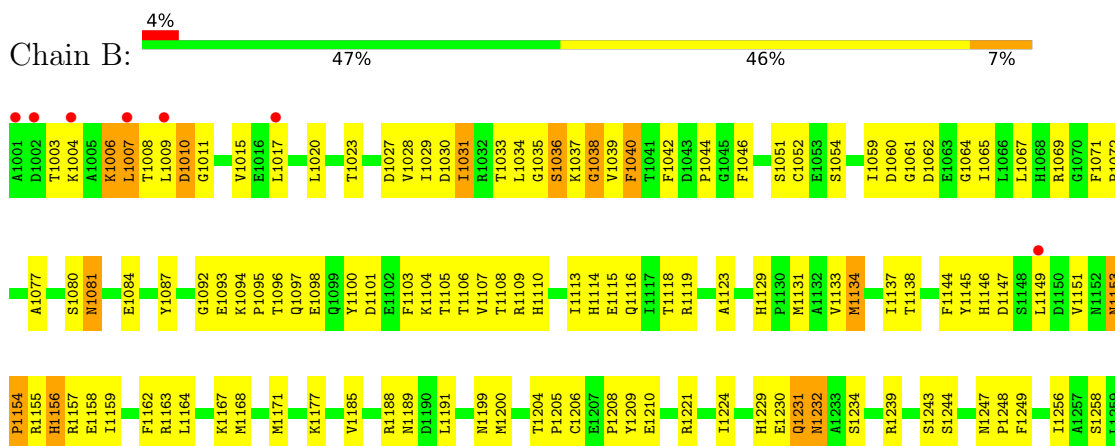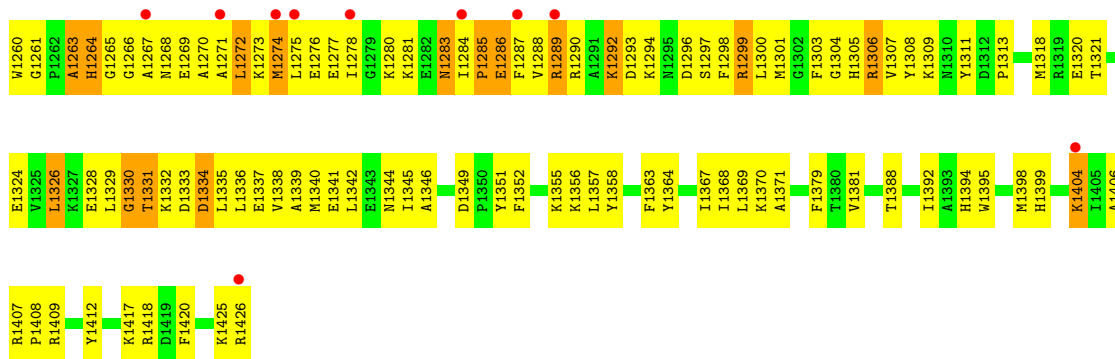
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	164.49Å 164.49Å 157.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 41.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.70) 98.2 (41.12-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.216 0.176 , 0.213	Depositor DCC
R_{free} test set	2093 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7081	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CMC, SO4

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	0.41	0/3441	0.67	1/4649 (0.0%)
1	B	0.42	0/3441	0.67	1/4649 (0.0%)
All	All	0.42	0/6882	0.67	2/9298 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1010	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	10	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3365	0	3315	339	0
1	B	3365	0	3312	349	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	52	0	33	16	0
3	B	52	0	33	16	0
4	A	104	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	123	0	0	9	0
All	All	7081	0	6693	636	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 47.

All (636) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1283:ASN:O	1:B:1288:VAL:HG21	1.18	1.27
1:A:352:PHE:HA	1:A:357:LEU:HD23	1.31	1.10
1:A:404:LYS:H	1:A:404:LYS:HD3	1.20	1.05
1:B:1289:ARG:HA	1:B:1292:LYS:HB3	1.36	1.04
1:A:284:ILE:HG12	1:A:289:ARG:HH11	1.18	1.02
1:A:425:LYS:H	1:B:1097:GLN:HE22	1.06	1.01
1:A:289:ARG:HH12	1:A:290:ARG:HG2	1.23	0.99
1:A:21:LYS:HE2	1:A:21:LYS:H	1.23	0.99
1:A:46:PHE:CD1	1:B:1408:PRO:HG3	1.98	0.98
1:B:1283:ASN:O	1:B:1288:VAL:CG2	2.12	0.98
1:A:298:PHE:HA	1:A:301:MET:HE2	1.46	0.97
1:B:1109:ARG:O	3:B:2003:CMC:H2B	1.65	0.97
1:A:232:ASN:HB2	1:B:1407:ARG:HH21	1.29	0.96
1:B:1425:LYS:HE2	1:B:1425:LYS:HA	1.45	0.96
1:B:1278:ILE:HG23	1:B:1280:LYS:HE2	1.47	0.95
1:B:1145:TYR:HB3	1:B:1163:ARG:NH2	1.80	0.95
1:B:1230:GLU:HG2	1:B:1231:GLN:H	1.30	0.94
1:A:215:LEU:HD11	1:A:329:LEU:HD21	1.52	0.92
1:A:151:VAL:HB	1:A:399:HIS:NE2	1.85	0.91
1:A:1:ALA:HA	1:A:4:LYS:HD2	1.51	0.91
1:B:1267:ALA:HA	1:B:1270:ALA:HB3	1.53	0.91
1:A:298:PHE:HB3	1:A:303:PHE:HB2	1.53	0.89
1:B:1275:LEU:HD21	1:B:1301:MET:SD	2.13	0.89
1:A:289:ARG:NH1	1:A:290:ARG:HG2	1.88	0.89
1:B:1163:ARG:HH11	3:B:2003:CMC:H133	1.37	0.89
1:A:408:PRO:HB2	1:B:1051:SER:HB3	1.55	0.87
1:B:1145:TYR:HB3	1:B:1163:ARG:HH21	1.38	0.87
1:B:1154:PRO:HG3	1:B:1157:ARG:HH11	1.40	0.87
1:A:4:LYS:HG2	1:A:27:ASP:OD2	1.74	0.86
1:A:425:LYS:N	1:B:1097:GLN:HE22	1.73	0.86
1:A:45:GLY:H	1:B:1404:LYS:HE2	1.40	0.85
1:A:262:PRO:HB2	1:A:300:LEU:HD11	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG12	1:A:289:ARG:NH1	1.92	0.85
1:B:1351:TYR:O	1:B:1355:LYS:HD3	1.76	0.85
1:B:1337:GLU:OE1	1:B:1337:GLU:HA	1.76	0.84
1:B:1204:THR:HG22	1:B:1206:CYS:H	1.42	0.84
1:A:153:ASN:HD22	1:A:154:PRO:N	1.75	0.84
1:A:269:GLU:O	1:A:273:LYS:HD3	1.78	0.83
1:B:1329:LEU:HB3	1:B:1332:LYS:HB2	1.60	0.82
1:B:1409:ARG:CZ	1:B:1409:ARG:HA	2.10	0.82
1:A:268:ASN:HA	1:A:297:SER:HB3	1.61	0.82
1:A:405:ILE:CG1	1:A:406:ALA:H	1.94	0.81
1:B:1007:LEU:HD13	1:B:1029:ILE:HD13	1.61	0.80
1:B:1263:ALA:HA	1:B:1268:ASN:HD22	1.45	0.80
1:A:425:LYS:H	1:B:1097:GLN:NE2	1.79	0.80
1:B:1113:ILE:HD11	1:B:1171:MET:HG3	1.63	0.80
1:A:309:LYS:O	1:A:356:LYS:HD3	1.82	0.79
1:B:1149:LEU:HD22	1:B:1247:ASN:HB2	1.63	0.79
1:A:403:MET:C	1:A:405:ILE:H	1.83	0.79
1:A:217:ARG:HH21	1:A:217:ARG:HG3	1.48	0.78
1:A:405:ILE:HG23	1:A:407:ARG:NH1	1.99	0.78
1:A:283:ASN:HA	1:A:288:VAL:HB	1.64	0.77
1:A:335:LEU:HD23	1:A:335:LEU:H	1.47	0.77
1:B:1335:LEU:H	1:B:1335:LEU:HD23	1.49	0.77
1:A:155:ARG:O	1:A:158:GLU:HB3	1.84	0.77
1:B:1278:ILE:HG23	1:B:1280:LYS:CE	2.15	0.76
1:B:1284:ILE:HB	1:B:1285:PRO:HD3	1.65	0.76
1:A:298:PHE:HA	1:A:301:MET:CE	2.15	0.76
1:B:1081:ASN:ND2	1:B:1084:GLU:H	1.83	0.76
1:A:246:ALA:HB2	1:B:1258:SER:HA	1.66	0.75
1:A:110:HIS:NE2	3:A:503:CMC:H142	2.00	0.75
1:A:44:PRO:HA	1:B:1404:LYS:HE2	1.67	0.75
3:A:503:CMC:HN8	3:A:503:CMC:H131	1.50	0.75
1:A:153:ASN:ND2	1:A:155:ARG:H	1.84	0.74
1:A:289:ARG:HH12	1:A:290:ARG:CG	1.99	0.74
1:B:1273:LYS:HG3	1:B:1277:GLU:OE2	1.86	0.74
1:A:352:PHE:HA	1:A:357:LEU:CD2	2.17	0.74
1:B:1271:ALA:C	1:B:1273:LYS:H	1.92	0.73
1:A:268:ASN:HA	1:A:297:SER:CB	2.18	0.73
1:A:337:GLU:HA	1:A:340:MET:SD	2.28	0.73
1:A:355:LYS:HB3	1:A:357:LEU:HD21	1.70	0.73
1:A:368:ILE:O	1:A:372:MET:HG3	1.88	0.73
1:A:404:LYS:HD3	1:A:404:LYS:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:HIS:HD2	1:B:1131:MET:H	1.37	0.73
1:A:45:GLY:N	1:B:1404:LYS:HE2	2.03	0.72
1:A:270:ALA:HA	1:A:273:LYS:NZ	2.05	0.72
1:A:283:ASN:CA	1:A:288:VAL:HB	2.20	0.72
1:B:1164:LEU:O	1:B:1168:MET:HG2	1.90	0.71
1:B:1231:GLN:HE22	1:B:1239:ARG:HD2	1.56	0.71
1:A:7:LEU:HD22	1:B:1010:ASP:O	1.91	0.71
1:A:233:ALA:HB1	1:B:1244:SER:HB3	1.71	0.70
1:A:283:ASN:HA	1:A:288:VAL:CB	2.21	0.70
1:B:1285:PRO:HG2	1:B:1286:GLU:H	1.56	0.70
1:B:1007:LEU:HD11	1:B:1029:ILE:HG23	1.74	0.70
1:A:7:LEU:HD22	1:B:1011:GLY:HA2	1.74	0.69
1:A:283:ASN:HA	1:A:288:VAL:CG2	2.22	0.69
1:B:1034:LEU:HB3	1:B:1039:VAL:HG13	1.73	0.69
1:A:328:GLU:C	1:A:330:GLY:H	1.93	0.69
1:B:1106:THR:O	1:B:1110:HIS:HD2	1.75	0.69
1:B:1034:LEU:HB3	1:B:1039:VAL:O	1.91	0.69
1:B:1290:ARG:N	1:B:1290:ARG:HE	1.90	0.69
1:B:1326:LEU:HD13	1:B:1333:ASP:HB2	1.74	0.69
1:B:1281:LYS:H	1:B:1281:LYS:HD2	1.57	0.68
1:A:45:GLY:H	1:B:1404:LYS:CE	2.05	0.68
1:A:150:ASP:HB3	1:A:156:HIS:CE1	2.27	0.68
1:B:1318:MET:HG2	1:B:1364:TYR:HB2	1.74	0.68
1:A:405:ILE:HG23	1:A:407:ARG:CZ	2.25	0.67
1:A:420:PHE:HB2	1:B:1071:PHE:CD2	2.29	0.67
1:B:1034:LEU:HD22	1:B:1039:VAL:HG11	1.75	0.67
1:A:86:CYS:HA	1:A:389:VAL:HG21	1.76	0.67
1:B:1007:LEU:HD13	1:B:1029:ILE:CD1	2.24	0.67
1:A:284:ILE:N	1:A:285:PRO:HD2	2.10	0.67
1:A:405:ILE:HG12	1:A:406:ALA:H	1.58	0.67
1:A:289:ARG:HH22	1:A:290:ARG:CG	2.09	0.66
1:A:29:ILE:HD12	1:A:29:ILE:N	2.10	0.66
1:A:153:ASN:HD22	1:A:154:PRO:CD	2.08	0.66
1:A:15:VAL:HG13	1:A:37:LYS:HZ3	1.60	0.66
1:A:21:LYS:HE2	1:A:21:LYS:N	2.05	0.66
1:B:1231:GLN:HE22	1:B:1239:ARG:CD	2.08	0.66
1:B:1278:ILE:O	1:B:1284:ILE:HD11	1.96	0.66
1:A:6:LYS:HB2	1:A:16:GLU:OE2	1.95	0.66
1:A:1:ALA:HA	1:A:4:LYS:CD	2.24	0.65
1:B:1020:LEU:O	1:B:1027:ASP:HB3	1.96	0.65
1:A:289:ARG:HH22	1:A:290:ARG:HG2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1272:LEU:HD21	1:B:1300:LEU:C	2.17	0.65
1:A:417:LYS:HD3	1:A:417:LYS:C	2.17	0.65
1:B:1370:LYS:HG3	1:B:1379:PHE:CZ	2.32	0.65
1:A:426:ARG:HB3	1:B:1100:TYR:HE1	1.61	0.65
1:B:1326:LEU:HD12	1:B:1337:GLU:OE2	1.96	0.65
1:A:104:LYS:HD3	1:B:1426:ARG:CD	2.27	0.65
1:B:1188:ARG:HB2	1:B:1191:LEU:HD12	1.77	0.65
1:B:1269:GLU:O	1:B:1273:LYS:HE2	1.97	0.65
1:B:1081:ASN:HD21	1:B:1084:GLU:H	1.44	0.64
1:B:1285:PRO:HA	1:B:1290:ARG:NH1	2.12	0.64
1:B:1275:LEU:HG	1:B:1301:MET:HG2	1.79	0.64
1:A:77:ALA:HB2	1:A:225:LEU:HD21	1.80	0.64
1:A:426:ARG:CZ	1:B:1104:LYS:HD3	2.28	0.64
1:B:1272:LEU:HD21	1:B:1300:LEU:O	1.97	0.64
1:A:150:ASP:HB3	1:A:156:HIS:ND1	2.13	0.63
1:B:1338:VAL:HG23	1:B:1338:VAL:O	1.96	0.63
1:B:1153:ASN:ND2	1:B:1155:ARG:HB3	2.13	0.63
1:B:1164:LEU:HD21	1:B:1249:PHE:HD2	1.64	0.63
1:B:1290:ARG:HH22	1:B:1345:ILE:HD13	1.63	0.63
1:B:1008:THR:HG22	1:B:1010:ASP:OD1	1.99	0.63
1:A:212:ASN:C	1:A:212:ASN:HD22	2.00	0.63
1:A:117:ILE:O	1:A:120:LEU:HB2	1.98	0.63
1:A:270:ALA:HA	1:A:273:LYS:HZ3	1.61	0.63
1:B:1284:ILE:O	1:B:1288:VAL:HB	1.99	0.63
1:A:290:ARG:HH12	1:A:303:PHE:HE2	1.47	0.62
1:A:153:ASN:HD22	1:A:153:ASN:C	1.99	0.62
1:B:1081:ASN:C	1:B:1081:ASN:HD22	1.98	0.62
1:A:217:ARG:HD3	1:A:221:ARG:NH2	2.15	0.62
1:A:284:ILE:HD12	1:A:338:VAL:HB	1.80	0.62
1:B:1417:LYS:HD3	1:B:1418:ARG:N	2.15	0.62
1:A:183:PRO:HG2	4:A:608:HOH:O	1.98	0.62
1:A:280:LYS:H	1:A:283:ASN:HD22	1.47	0.62
1:A:423:ASP:OD2	1:B:1094:LYS:HE3	1.99	0.62
1:B:1337:GLU:OE1	1:B:1337:GLU:CA	2.48	0.62
1:A:4:LYS:HD3	1:A:21:LYS:HB3	1.81	0.62
1:A:43:ASP:OD2	1:A:47:THR:HB	1.99	0.62
1:A:289:ARG:HH21	1:A:289:ARG:HG2	1.65	0.62
1:B:1077:ALA:HA	1:B:1224:ILE:HG21	1.82	0.62
3:A:503:CMC:H141	3:A:503:CMC:N8P	2.14	0.61
1:B:1280:LYS:HG3	1:B:1283:ASN:HB3	1.81	0.61
1:B:1188:ARG:CB	1:B:1191:LEU:HD12	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HB	1:B:1031:ILE:HD13	1.82	0.61
1:A:336:LEU:O	1:A:340:MET:SD	2.58	0.61
1:B:1284:ILE:HB	1:B:1285:PRO:CD	2.30	0.61
3:A:503:CMC:H131	3:A:503:CMC:N8P	2.15	0.61
1:B:1035:GLY:C	1:B:1037:LYS:H	2.03	0.61
1:B:1370:LYS:HG3	1:B:1379:PHE:HZ	1.63	0.61
1:A:404:LYS:H	1:A:404:LYS:CD	1.97	0.61
1:A:408:PRO:HB2	1:B:1051:SER:CB	2.28	0.61
1:A:271:ALA:O	1:A:274:MET:HB3	2.01	0.61
1:B:1230:GLU:CG	1:B:1231:GLN:H	2.08	0.61
1:A:150:ASP:HB3	1:A:156:HIS:HD1	1.66	0.61
1:A:217:ARG:HG3	1:A:217:ARG:NH2	2.16	0.61
1:A:284:ILE:CG1	1:A:289:ARG:HH11	2.03	0.61
1:A:233:ALA:HB1	1:B:1244:SER:CB	2.30	0.60
1:B:1113:ILE:CD1	1:B:1171:MET:HG3	2.30	0.60
1:B:1158:GLU:HG3	4:B:2178:HOH:O	2.00	0.60
1:A:289:ARG:NH2	1:A:290:ARG:HG2	2.15	0.60
1:B:1106:THR:O	1:B:1110:HIS:CD2	2.54	0.60
1:B:1276:GLU:HB2	1:B:1370:LYS:HE2	1.83	0.60
1:A:426:ARG:HB3	1:B:1100:TYR:CE1	2.36	0.60
1:B:1062:ASP:HA	1:B:1309:LYS:CB	2.31	0.60
1:B:1062:ASP:HA	1:B:1309:LYS:HB2	1.82	0.60
1:B:1269:GLU:HB3	4:B:2193:HOH:O	2.01	0.60
1:A:426:ARG:HD2	1:B:1101:ASP:OD1	2.01	0.60
1:B:1272:LEU:HD23	1:B:1301:MET:CG	2.32	0.60
1:B:1381:VAL:HG23	4:B:2146:HOH:O	2.02	0.60
1:A:9:LEU:HD11	1:B:1007:LEU:HD12	1.84	0.60
1:A:212:ASN:ND2	1:A:214:ILE:H	2.00	0.60
1:A:289:ARG:CZ	1:A:290:ARG:HG2	2.31	0.59
1:A:405:ILE:HG13	1:A:406:ALA:H	1.63	0.59
1:B:1330:GLY:C	1:B:1332:LYS:H	2.04	0.59
1:B:1338:VAL:O	1:B:1342:LEU:HG	2.01	0.59
1:A:415:TYR:HE2	1:B:1093:GLU:OE2	1.85	0.59
1:B:1104:LYS:O	1:B:1108:THR:HG23	2.02	0.59
1:A:36:SER:C	1:A:38:GLY:H	2.05	0.59
1:A:355:LYS:HB3	1:A:357:LEU:CD2	2.32	0.59
1:B:1163:ARG:NH1	3:B:2003:CMC:H133	2.14	0.59
1:B:1230:GLU:HG2	1:B:1231:GLN:N	2.07	0.59
1:A:110:HIS:CG	3:A:503:CMC:H10	2.38	0.59
1:B:1009:LEU:HD21	1:B:1039:VAL:HG21	1.83	0.59
1:B:1346:ALA:HA	1:B:1352:PHE:CD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PRO:CB	1:B:1051:SER:HB3	2.30	0.59
3:A:503:CMC:HN8	3:A:503:CMC:H141	1.66	0.59
1:B:1334:ASP:HA	1:B:1337:GLU:HG2	1.84	0.59
1:A:405:ILE:CG1	1:A:406:ALA:N	2.59	0.58
1:B:1363:PHE:CZ	1:B:1367:ILE:HD11	2.38	0.58
1:B:1243:SER:HB2	1:B:1404:LYS:O	2.02	0.58
1:B:1318:MET:CG	1:B:1364:TYR:HB2	2.32	0.58
1:B:1289:ARG:CA	1:B:1292:LYS:HB3	2.24	0.58
1:B:1134:MET:CE	1:B:1381:VAL:HG13	2.33	0.58
1:A:212:ASN:HD21	1:A:214:ILE:HG12	1.68	0.58
1:B:1420:PHE:HA	4:B:2115:HOH:O	2.02	0.58
1:A:289:ARG:HH22	1:A:290:ARG:CD	2.16	0.58
1:A:289:ARG:CZ	1:A:289:ARG:HB3	2.34	0.58
1:B:1297:SER:O	1:B:1298:PHE:CD2	2.57	0.58
1:A:277:GLU:HG3	1:A:278:ILE:N	2.18	0.58
1:B:1156:HIS:HA	1:B:1159:ILE:HD12	1.86	0.57
1:B:1276:GLU:OE2	1:B:1370:LYS:HG2	2.04	0.57
1:B:1292:LYS:O	1:B:1292:LYS:HD3	2.03	0.57
1:A:407:ARG:N	1:A:407:ARG:HD2	2.19	0.57
1:B:1129:HIS:CD2	1:B:1131:MET:H	2.20	0.57
3:A:503:CMC:H11	3:A:503:CMC:H72	1.85	0.57
1:B:1020:LEU:HD21	1:B:1030:ASP:HB2	1.86	0.57
1:A:403:MET:C	1:A:405:ILE:N	2.57	0.57
1:B:1177:LYS:HE3	1:B:1185:VAL:HG23	1.86	0.57
1:A:100:TYR:HE1	1:B:1426:ARG:HB3	1.69	0.57
1:A:323:HIS:NE2	1:A:327:LYS:HD2	2.20	0.57
1:A:283:ASN:HA	1:A:288:VAL:HG21	1.87	0.57
1:B:1162:PHE:HB2	3:B:2003:CMC:H61	1.85	0.57
1:B:1346:ALA:HA	1:B:1352:PHE:CG	2.39	0.57
1:B:1355:LYS:O	1:B:1356:LYS:C	2.43	0.57
1:A:10:ASP:HB3	1:A:14:ALA:HA	1.86	0.57
1:B:1009:LEU:HB3	1:B:1015:VAL:HB	1.86	0.57
1:A:413:THR:HG22	1:A:413:THR:O	2.05	0.56
1:A:110:HIS:CE1	3:A:503:CMC:H142	2.39	0.56
1:A:28:VAL:C	1:A:29:ILE:HD12	2.25	0.56
1:A:413:THR:HA	1:B:1023:THR:HG23	1.86	0.56
1:B:1335:LEU:H	1:B:1335:LEU:CD2	2.18	0.56
1:A:4:LYS:HE3	1:A:27:ASP:OD1	2.06	0.56
1:B:1034:LEU:HD22	1:B:1039:VAL:CG1	2.35	0.56
1:A:34:LEU:HB3	1:A:39:VAL:HB	1.87	0.56
1:B:1034:LEU:CB	1:B:1039:VAL:HG13	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1119:ARG:HD3	1:B:1119:ARG:H	1.71	0.56
1:B:1290:ARG:NH2	1:B:1345:ILE:HD13	2.20	0.56
3:B:2003:CMC:O9P	3:B:2003:CMC:H121	2.04	0.56
1:A:322:CYS:O	1:A:326:LEU:HG	2.05	0.56
1:A:164:LEU:HD13	1:A:252:ILE:HG12	1.87	0.56
1:A:328:GLU:OE2	1:A:328:GLU:HA	2.06	0.56
1:A:329:LEU:HD12	1:A:371:ALA:HB1	1.88	0.56
1:A:409:ARG:HB3	1:A:409:ARG:CZ	2.35	0.56
1:B:1131:MET:HG2	1:B:1260:TRP:CG	2.40	0.56
1:A:329:LEU:HD13	1:A:371:ALA:O	2.06	0.55
1:B:1340:MET:O	1:B:1344:ASN:HB2	2.06	0.55
1:B:1069:ARG:HD2	1:B:1092:GLY:HA2	1.86	0.55
1:B:1286:GLU:O	1:B:1288:VAL:HG23	2.05	0.55
1:A:157:ARG:HH11	1:A:399:HIS:CD2	2.24	0.55
1:A:405:ILE:HG12	1:A:406:ALA:N	2.21	0.55
1:B:1153:ASN:ND2	1:B:1155:ARG:H	2.04	0.55
1:A:101:ASP:HA	1:B:1426:ARG:HH21	1.71	0.55
1:A:284:ILE:CD1	1:A:338:VAL:HB	2.36	0.55
1:B:1388:THR:O	1:B:1392:ILE:HG13	2.06	0.55
1:A:168:MET:N	1:A:169:PRO:HD2	2.22	0.55
1:B:1149:LEU:HD22	1:B:1247:ASN:CB	2.36	0.55
1:A:177:LYS:HZ1	1:A:202:PHE:HA	1.72	0.55
1:A:347:LEU:O	1:A:353:ILE:HD11	2.07	0.55
1:B:1290:ARG:HH22	1:B:1345:ILE:CD1	2.19	0.55
1:A:296:ASP:O	1:A:301:MET:HE1	2.07	0.55
1:A:415:TYR:CE2	1:B:1093:GLU:OE2	2.59	0.55
1:A:40:PHE:HB2	1:B:1028:VAL:HG12	1.89	0.55
1:B:1118:THR:HB	1:B:1119:ARG:HH21	1.72	0.55
1:A:73:ILE:HG23	1:A:74:ASP:N	2.22	0.54
1:A:110:HIS:CD2	3:A:503:CMC:H10	2.42	0.54
1:A:350:PRO:O	1:A:354:GLU:HG3	2.06	0.54
1:B:1115:GLU:O	1:B:1119:ARG:HD3	2.06	0.54
1:B:1281:LYS:H	1:B:1281:LYS:CD	2.20	0.54
1:A:36:SER:O	1:A:38:GLY:N	2.41	0.54
1:A:100:TYR:CE1	1:B:1426:ARG:HB3	2.43	0.54
1:B:1007:LEU:HD11	1:B:1017:LEU:HB2	1.88	0.54
1:A:296:ASP:HB2	1:A:298:PHE:CD2	2.42	0.54
1:B:1110:HIS:CE1	3:B:2003:CMC:O9P	2.59	0.54
1:A:416:GLU:O	1:A:417:LYS:C	2.45	0.54
1:B:1067:LEU:HD23	1:B:1072:PRO:HA	1.89	0.54
1:B:1286:GLU:HG2	1:B:1287:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1069:ARG:CD	1:B:1092:GLY:HA2	2.37	0.54
1:B:1289:ARG:HB2	1:B:1290:ARG:HH11	1.73	0.54
1:B:1289:ARG:HG3	1:B:1292:LYS:HB3	1.88	0.54
1:B:1081:ASN:HA	1:B:1224:ILE:HD11	1.90	0.54
1:A:294:LYS:H	1:A:294:LYS:HD2	1.72	0.54
1:B:1097:GLN:HG3	1:B:1101:ASP:OD2	2.07	0.54
1:B:1288:VAL:HG12	1:B:1289:ARG:HD3	1.90	0.54
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.38	0.53
1:A:271:ALA:HA	1:A:274:MET:CB	2.39	0.53
1:B:1087:TYR:CD1	1:B:1087:TYR:C	2.81	0.53
1:B:1145:TYR:CB	1:B:1163:ARG:NH2	2.65	0.53
1:A:328:GLU:C	1:A:330:GLY:N	2.60	0.53
1:A:335:LEU:HD23	1:A:335:LEU:N	2.20	0.53
1:A:281:LYS:HE2	1:A:337:GLU:HB3	1.90	0.53
1:B:1145:TYR:CZ	1:B:1167:LYS:HE3	2.43	0.53
1:B:1370:LYS:HE3	1:B:1379:PHE:HE1	1.74	0.53
1:A:273:LYS:O	1:A:277:GLU:HG2	2.09	0.53
1:A:278:ILE:CD1	1:A:283:ASN:CG	2.78	0.53
1:A:284:ILE:HG22	1:A:341:GLU:HG2	1.90	0.53
1:A:270:ALA:O	1:A:274:MET:HB2	2.08	0.53
1:B:1153:ASN:C	1:B:1153:ASN:HD22	2.12	0.53
1:A:67:LEU:HD22	1:A:70:GLY:O	2.09	0.52
1:A:217:ARG:HD3	1:A:221:ARG:CZ	2.39	0.52
1:A:403:MET:O	1:A:405:ILE:N	2.41	0.52
1:B:1284:ILE:HG22	1:B:1289:ARG:HE	1.73	0.52
1:A:214:ILE:HG12	4:A:665:HOH:O	2.10	0.52
1:B:1204:THR:HG22	1:B:1206:CYS:N	2.17	0.52
1:B:1417:LYS:HD3	1:B:1417:LYS:C	2.30	0.52
1:A:59:ILE:HG21	1:A:307:VAL:HG11	1.91	0.52
1:A:198:LEU:HD22	1:A:202:PHE:HE1	1.74	0.52
1:A:287:PHE:O	1:A:291:ALA:HB2	2.09	0.52
1:B:1163:ARG:NH1	3:B:2003:CMC:O6A	2.43	0.52
1:A:44:PRO:CA	1:B:1404:LYS:HE2	2.37	0.52
1:A:133:VAL:O	1:A:137:ILE:HG12	2.10	0.52
1:A:278:ILE:HG23	1:A:278:ILE:O	2.10	0.52
1:B:1007:LEU:CD1	1:B:1017:LEU:HB2	2.39	0.52
1:B:1425:LYS:HA	1:B:1425:LYS:CE	2.29	0.52
1:A:30:ASP:OD2	1:A:32:ARG:HD3	2.10	0.52
1:A:167:LYS:NZ	3:A:503:CMC:O2A	2.40	0.52
1:A:352:PHE:CD2	1:A:357:LEU:HB2	2.45	0.51
1:A:157:ARG:HE	1:A:399:HIS:CB	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1081:ASN:ND2	1:B:1081:ASN:C	2.63	0.51
1:B:1163:ARG:O	1:B:1167:LYS:HG3	2.11	0.51
1:B:1272:LEU:HD23	1:B:1301:MET:HG2	1.92	0.51
1:B:1290:ARG:N	1:B:1290:ARG:NE	2.58	0.51
1:B:1119:ARG:HD3	1:B:1119:ARG:N	2.26	0.51
1:A:209:TYR:HB2	4:A:625:HOH:O	2.09	0.51
1:A:278:ILE:HG22	1:A:289:ARG:HD3	1.92	0.51
1:A:405:ILE:HG21	1:A:407:ARG:NH2	2.25	0.51
1:A:261:GLY:N	1:A:262:PRO:HD2	2.26	0.51
1:A:46:PHE:CG	1:B:1408:PRO:HG3	2.43	0.51
1:A:60:ASP:HB3	1:A:65:ILE:HG12	1.92	0.51
1:A:335:LEU:HG	1:A:336:LEU:HD13	1.92	0.51
1:A:268:ASN:O	1:A:272:LEU:N	2.44	0.51
1:B:1151:VAL:HG12	1:B:1248:PRO:HD3	1.93	0.51
1:A:110:HIS:CD2	3:A:503:CMC:H121	2.45	0.51
1:A:114:HIS:CE1	1:A:116:GLN:HB2	2.46	0.51
1:A:280:LYS:HB2	1:A:283:ASN:HD21	1.76	0.51
1:B:1232:ASN:HD22	1:B:1234:SER:H	1.58	0.51
1:B:1271:ALA:O	1:B:1275:LEU:HD23	2.10	0.51
1:A:278:ILE:HD11	1:A:283:ASN:CG	2.31	0.51
1:B:1288:VAL:HG12	1:B:1289:ARG:N	2.26	0.51
1:A:9:LEU:HA	1:B:1008:THR:O	2.10	0.50
1:A:114:HIS:HB3	1:A:117:ILE:HG13	1.93	0.50
1:A:176:TYR:O	1:A:180:ILE:HG12	2.11	0.50
1:B:1299:ARG:HG3	1:B:1299:ARG:O	2.11	0.50
1:B:1272:LEU:HD23	1:B:1301:MET:HG3	1.93	0.50
1:B:1333:ASP:O	1:B:1336:LEU:N	2.45	0.50
1:A:370:LYS:C	1:A:372:MET:N	2.65	0.50
1:A:426:ARG:OXT	1:A:426:ARG:HG2	2.11	0.50
1:A:420:PHE:HB2	1:B:1071:PHE:HD2	1.73	0.50
1:B:1060:ASP:HB3	1:B:1065:ILE:HB	1.93	0.50
1:B:1096:THR:HG22	4:B:2202:HOH:O	2.12	0.50
1:B:1286:GLU:HG2	1:B:1287:PHE:CE2	2.47	0.50
1:B:1303:PHE:CE1	1:B:1346:ALA:HB2	2.47	0.50
1:B:1399:HIS:CE1	4:B:2109:HOH:O	2.65	0.50
1:A:212:ASN:C	1:A:212:ASN:ND2	2.65	0.49
1:A:426:ARG:CD	1:B:1101:ASP:OD1	2.60	0.49
1:B:1271:ALA:C	1:B:1273:LYS:N	2.61	0.49
1:B:1329:LEU:HB3	1:B:1332:LYS:CB	2.35	0.49
1:A:131:MET:HG2	1:A:260:TRP:CD1	2.47	0.49
1:B:1007:LEU:HD22	1:B:1029:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HD3	1:B:1426:ARG:HG2	1.94	0.49
1:B:1096:THR:HG21	1:B:1098:GLU:OE1	2.12	0.49
1:B:1239:ARG:NH1	1:B:1394:HIS:ND1	2.60	0.49
1:A:403:MET:O	1:A:403:MET:HG3	2.12	0.49
1:B:1134:MET:HE2	1:B:1381:VAL:HG13	1.94	0.49
1:B:1280:LYS:HE3	1:B:1283:ASN:ND2	2.28	0.49
1:B:1289:ARG:HG3	1:B:1292:LYS:CG	2.42	0.49
1:B:1305:HIS:HD2	1:B:1306:ARG:N	2.11	0.49
1:B:1409:ARG:HA	1:B:1409:ARG:NE	2.28	0.49
1:A:280:LYS:HB2	1:A:283:ASN:ND2	2.28	0.49
1:A:410:GLN:HA	1:B:1052:CYS:O	2.12	0.49
1:A:7:LEU:CD2	1:B:1011:GLY:HA2	2.40	0.49
1:A:268:ASN:O	1:A:272:LEU:HG	2.13	0.49
1:A:212:ASN:HD22	1:A:213:PRO:N	2.10	0.49
1:A:350:PRO:HB3	1:A:354:GLU:OE1	2.13	0.49
1:A:355:LYS:O	1:A:355:LYS:HG2	2.13	0.49
1:B:1153:ASN:O	1:B:1155:ARG:N	2.46	0.49
1:B:1096:THR:O	1:B:1097:GLN:C	2.51	0.48
1:A:278:ILE:CG2	1:A:289:ARG:HD3	2.43	0.48
1:A:153:ASN:ND2	1:A:153:ASN:C	2.65	0.48
1:A:157:ARG:HE	1:A:399:HIS:CG	2.32	0.48
1:A:292:LYS:HD3	1:A:294:LYS:HE2	1.96	0.48
1:A:399:HIS:O	1:A:401:ASP:N	2.47	0.48
1:A:29:ILE:N	1:A:29:ILE:CD1	2.76	0.48
1:A:305:HIS:CD2	1:A:307:VAL:H	2.31	0.48
1:A:405:ILE:CG2	1:A:407:ARG:CZ	2.92	0.48
1:A:335:LEU:H	1:A:335:LEU:CD2	2.19	0.48
1:B:1040:PHE:N	1:B:1040:PHE:CD1	2.81	0.48
1:B:1406:ALA:HB2	4:B:2108:HOH:O	2.14	0.48
1:B:1331:THR:O	1:B:1331:THR:HG22	2.13	0.48
1:B:1020:LEU:N	1:B:1028:VAL:O	2.46	0.48
1:B:1289:ARG:HG2	1:B:1289:ARG:HH21	1.78	0.48
1:B:1007:LEU:HD11	1:B:1029:ILE:CG2	2.42	0.48
1:B:1153:ASN:HD21	1:B:1155:ARG:HB3	1.79	0.48
1:A:36:SER:C	1:A:38:GLY:N	2.66	0.47
1:B:1349:ASP:OD1	1:B:1351:TYR:HB3	2.14	0.47
1:A:2:ASP:C	1:A:4:LYS:H	2.17	0.47
1:B:1293:ASP:CG	1:B:1298:PHE:HE2	2.17	0.47
1:A:6:LYS:O	1:A:7:LEU:HD23	2.14	0.47
1:B:1155:ARG:O	1:B:1159:ILE:HG13	2.15	0.47
1:A:69:ARG:N	4:A:685:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:HB3	1:A:297:SER:OG	2.14	0.47
1:A:406:ALA:C	1:A:407:ARG:HD2	2.34	0.47
1:B:1293:ASP:C	1:B:1294:LYS:HD2	2.35	0.47
1:A:73:ILE:HG23	1:A:74:ASP:H	1.78	0.47
1:A:153:ASN:HB3	1:A:156:HIS:CG	2.49	0.47
1:A:157:ARG:HH11	1:A:399:HIS:HB3	1.80	0.47
1:B:1096:THR:HB	1:B:1098:GLU:HG2	1.97	0.47
1:B:1131:MET:O	1:B:1134:MET:HB3	2.15	0.47
3:B:2003:CMC:OAP	3:B:2003:CMC:H71	2.14	0.47
1:A:104:LYS:HD3	1:B:1426:ARG:NE	2.30	0.47
1:A:20:LEU:HB2	1:A:28:VAL:HG23	1.96	0.47
1:A:135:CYS:SG	1:A:256:ILE:HG22	2.55	0.47
1:A:138:THR:HG22	1:A:171:MET:SD	2.55	0.47
1:A:289:ARG:HH22	1:A:290:ARG:HD3	1.79	0.47
1:A:289:ARG:HH21	1:A:289:ARG:CG	2.26	0.47
1:B:1035:GLY:O	1:B:1037:LYS:N	2.47	0.47
1:B:1064:GLY:O	1:B:1313:PRO:HB3	2.15	0.47
1:A:6:LYS:HD2	1:A:16:GLU:OE2	2.15	0.47
1:A:82:TYR:CE2	1:A:86:CYS:SG	3.08	0.47
1:A:422:SER:OG	1:A:424:ILE:HG12	2.15	0.47
1:B:1087:TYR:CD1	1:B:1095:PRO:HD3	2.50	0.47
1:B:1154:PRO:HG3	1:B:1157:ARG:NH1	2.20	0.47
1:A:76:LEU:O	1:A:80:SER:HB3	2.14	0.47
1:A:92:GLY:O	1:A:93:GLU:HG2	2.15	0.47
1:A:126:ARG:HH21	1:A:181:GLY:HA2	1.80	0.47
1:A:350:PRO:O	1:A:351:TYR:C	2.54	0.47
1:B:1204:THR:CG2	1:B:1206:CYS:SG	3.03	0.47
1:B:1273:LYS:O	1:B:1277:GLU:HB3	2.15	0.47
1:B:1341:GLU:O	1:B:1345:ILE:HG13	2.14	0.47
1:B:1298:PHE:C	1:B:1300:LEU:H	2.18	0.46
1:A:51:SER:HB3	1:B:1046:PHE:HZ	1.81	0.46
1:A:284:ILE:HD12	1:A:338:VAL:CG1	2.45	0.46
1:B:1329:LEU:CB	1:B:1332:LYS:HB2	2.39	0.46
1:B:1409:ARG:HA	1:B:1409:ARG:NH2	2.30	0.46
1:A:159:ILE:HG23	3:A:503:CMC:H133	1.96	0.46
1:A:270:ALA:HA	1:A:273:LYS:HZ2	1.79	0.46
1:B:1129:HIS:HD2	1:B:1131:MET:N	2.08	0.46
1:B:1271:ALA:O	1:B:1273:LYS:N	2.45	0.46
1:A:157:ARG:HH11	1:A:399:HIS:HD2	1.64	0.46
1:A:273:LYS:O	1:A:274:MET:C	2.53	0.46
1:A:292:LYS:HB2	1:A:292:LYS:NZ	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LYS:HD2	4:A:606:HOH:O	2.14	0.46
1:B:1035:GLY:C	1:B:1037:LYS:N	2.65	0.46
1:A:60:ASP:HB3	1:A:65:ILE:CG1	2.45	0.46
1:A:138:THR:CG2	1:A:171:MET:SD	3.04	0.46
1:A:284:ILE:HD12	1:A:338:VAL:CB	2.44	0.46
1:A:85:VAL:O	1:A:89:LEU:HB2	2.15	0.46
1:A:252:ILE:O	1:A:256:ILE:HG13	2.16	0.46
1:B:1020:LEU:N	1:B:1020:LEU:HD22	2.31	0.46
1:B:1119:ARG:N	1:B:1119:ARG:CD	2.77	0.46
1:B:1331:THR:C	1:B:1332:LYS:HG2	2.34	0.46
1:A:56:ILE:HG13	1:A:397:GLU:OE2	2.16	0.46
1:B:1114:HIS:CD2	1:B:1116:GLN:H	2.32	0.46
1:B:1281:LYS:HD2	1:B:1281:LYS:N	2.25	0.46
1:B:1305:HIS:HD2	1:B:1306:ARG:H	1.63	0.46
1:A:405:ILE:CG2	1:A:407:ARG:NH2	2.79	0.46
1:B:1114:HIS:HD2	1:B:1116:GLN:CB	2.29	0.46
1:B:1145:TYR:HB3	1:B:1163:ARG:HH22	1.74	0.46
1:B:1231:GLN:HE22	1:B:1239:ARG:NE	2.14	0.46
1:B:1278:ILE:HG21	1:B:1283:ASN:OD1	2.16	0.46
1:A:153:ASN:HD21	1:A:155:ARG:H	1.58	0.46
1:B:1131:MET:HG2	1:B:1260:TRP:CD2	2.51	0.46
1:B:1221:ARG:NH2	1:B:1321:THR:OG1	2.45	0.46
1:B:1285:PRO:HB2	1:B:1345:ILE:HD11	1.98	0.46
1:A:357:LEU:N	1:A:357:LEU:HD22	2.31	0.45
1:B:1059:ILE:HA	1:B:1065:ILE:O	2.16	0.45
1:A:271:ALA:HA	1:A:274:MET:HB2	1.99	0.45
1:A:298:PHE:HB3	1:A:303:PHE:CB	2.37	0.45
1:B:1006:LYS:O	1:B:1006:LYS:HG2	2.17	0.45
1:B:1204:THR:HG23	1:B:1205:PRO:HD2	1.98	0.45
1:B:1208:PRO:HA	4:B:2124:HOH:O	2.16	0.45
1:B:1339:ALA:O	1:B:1342:LEU:N	2.49	0.45
1:B:1113:ILE:CD1	1:B:1171:MET:CG	2.95	0.45
1:A:23:THR:O	1:A:24:LEU:HG	2.16	0.45
1:A:109:ARG:HB3	1:A:110:HIS:CE1	2.52	0.45
1:A:277:GLU:CG	1:A:278:ILE:N	2.78	0.45
1:B:1064:GLY:HA2	1:B:1308:TYR:CD1	2.51	0.45
1:A:214:ILE:HG21	1:A:328:GLU:HG2	1.98	0.45
1:B:1007:LEU:CD2	1:B:1029:ILE:HG12	2.47	0.45
1:B:1229:HIS:HE1	1:B:1305:HIS:CE1	2.35	0.45
1:B:1285:PRO:HA	1:B:1290:ARG:CZ	2.46	0.45
1:B:1330:GLY:N	1:B:1333:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1268:ASN:O	1:B:1300:LEU:HD12	2.17	0.45
1:B:1369:LEU:C	1:B:1371:ALA:H	2.19	0.45
1:A:305:HIS:HB3	1:A:358:TYR:OH	2.17	0.45
1:B:1330:GLY:C	1:B:1332:LYS:N	2.70	0.45
1:B:1042:PHE:CZ	1:B:1044:PRO:HG2	2.52	0.45
1:B:1330:GLY:O	1:B:1332:LYS:N	2.49	0.45
1:A:337:GLU:CA	1:A:340:MET:SD	3.01	0.44
1:A:407:ARG:N	1:A:407:ARG:CD	2.79	0.44
1:B:1177:LYS:HE2	1:B:1200:MET:O	2.17	0.44
1:B:1275:LEU:HD22	1:B:1289:ARG:HH12	1.81	0.44
1:A:41:THR:CB	1:B:1031:ILE:HD13	2.46	0.44
1:A:126:ARG:NH2	1:A:181:GLY:HA2	2.32	0.44
1:A:198:LEU:CD2	1:A:202:PHE:HE1	2.31	0.44
1:A:273:LYS:HB2	1:A:273:LYS:HE2	1.77	0.44
1:B:1289:ARG:HG2	1:B:1289:ARG:NH2	2.32	0.44
1:A:7:LEU:O	1:A:8:THR:HG23	2.18	0.44
1:B:1162:PHE:CB	3:B:2003:CMC:H61	2.47	0.44
1:A:28:VAL:HB	1:B:1042:PHE:HB2	1.99	0.44
1:B:1035:GLY:O	1:B:1038:GLY:N	2.51	0.44
1:A:146:HIS:O	1:A:149:LEU:HD12	2.18	0.44
1:A:271:ALA:HA	1:A:274:MET:HB3	2.00	0.44
1:A:410:GLN:OE1	1:B:1054:SER:HB3	2.18	0.44
1:B:1266:GLY:O	1:B:1270:ALA:HB2	2.17	0.44
1:B:1293:ASP:HB2	1:B:1297:SER:HB2	2.00	0.44
1:A:300:LEU:HD22	1:A:300:LEU:H	1.83	0.44
1:B:1296:ASP:O	1:B:1298:PHE:CD1	2.71	0.44
1:A:15:VAL:HG13	1:A:37:LYS:NZ	2.32	0.43
1:A:159:ILE:HA	3:A:503:CMC:H61	1.99	0.43
1:A:300:LEU:HD22	1:A:300:LEU:N	2.33	0.43
1:B:1051:SER:O	1:B:1404:LYS:HE3	2.18	0.43
1:B:1273:LYS:C	1:B:1275:LEU:H	2.21	0.43
1:B:1335:LEU:HD23	1:B:1335:LEU:N	2.25	0.43
1:A:7:LEU:HG	1:A:19:VAL:CG2	2.48	0.43
1:A:104:LYS:NZ	1:B:1426:ARG:HG2	2.32	0.43
1:A:283:ASN:C	1:A:288:VAL:HB	2.38	0.43
1:A:45:GLY:H	1:B:1404:LYS:NZ	2.15	0.43
1:A:232:ASN:N	1:A:232:ASN:HD22	2.15	0.43
1:B:1110:HIS:CD2	3:B:2003:CMC:HN8	2.37	0.43
1:B:1114:HIS:HD2	1:B:1116:GLN:HB3	1.83	0.43
1:B:1304:GLY:N	1:B:1358:TYR:O	2.51	0.43
1:A:155:ARG:HA	1:A:158:GLU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:HG21	4:A:692:HOH:O	2.19	0.43
1:B:1263:ALA:O	1:B:1264:HIS:CD2	2.71	0.43
1:B:1288:VAL:CG1	1:B:1289:ARG:HD3	2.48	0.43
1:B:1369:LEU:C	1:B:1371:ALA:N	2.71	0.43
1:A:12:ASP:HB2	1:B:1003:THR:O	2.19	0.43
1:A:104:LYS:HD3	1:B:1426:ARG:CG	2.49	0.43
1:B:1333:ASP:O	1:B:1336:LEU:HB3	2.19	0.43
1:A:214:ILE:HB	1:A:328:GLU:HG2	2.01	0.43
1:B:1008:THR:HA	1:B:1015:VAL:O	2.19	0.43
1:B:1265:GLY:H	1:B:1268:ASN:CG	2.21	0.43
1:A:97:GLN:HB3	4:A:638:HOH:O	2.18	0.43
1:A:157:ARG:NH1	1:A:399:HIS:HB3	2.35	0.42
1:B:1199:ASN:OD1	1:B:1209:TYR:HB3	2.19	0.42
1:A:369:LEU:O	1:A:372:MET:HB2	2.19	0.42
1:B:1137:ILE:O	1:B:1138:THR:C	2.57	0.42
1:B:1285:PRO:HG2	1:B:1286:GLU:N	2.31	0.42
1:A:163:ARG:NE	3:A:503:CMC:O4A	2.53	0.42
1:A:274:MET:HA	1:A:277:GLU:CD	2.39	0.42
1:A:284:ILE:HG22	1:A:341:GLU:CG	2.49	0.42
1:A:341:GLU:HG3	1:A:345:ILE:CD1	2.49	0.42
1:B:1110:HIS:ND1	3:B:2003:CMC:H52A	2.33	0.42
1:B:1320:GLU:O	1:B:1324:GLU:HG3	2.19	0.42
1:B:1395:TRP:CZ2	1:B:1399:HIS:CE1	3.07	0.42
1:A:110:HIS:CD2	3:A:503:CMC:O3A	2.73	0.42
1:A:112:MET:O	1:A:167:LYS:NZ	2.53	0.42
1:A:274:MET:O	1:A:277:GLU:HG2	2.19	0.42
1:B:1147:ASP:OD2	1:B:1147:ASP:N	2.46	0.42
3:B:2003:CMC:O9P	3:B:2003:CMC:H142	2.19	0.42
1:A:77:ALA:CB	1:A:225:LEU:HD21	2.48	0.42
1:A:121:PHE:HE1	1:A:175:CYS:SG	2.43	0.42
1:A:164:LEU:O	1:A:168:MET:HG2	2.19	0.42
1:A:399:HIS:C	1:A:401:ASP:N	2.73	0.42
1:A:223:LEU:HD23	1:A:386:ALA:HB2	2.02	0.42
1:A:305:HIS:HD2	1:A:307:VAL:H	1.66	0.42
1:A:308:TYR:HB2	1:A:358:TYR:OH	2.20	0.42
1:B:1105:THR:HG22	3:B:2003:CMC:O21	2.19	0.42
1:B:1131:MET:HE1	1:B:1256:ILE:HG23	2.02	0.42
1:A:24:LEU:HB2	1:B:1412:TYR:HD1	1.85	0.42
1:A:370:LYS:C	1:A:372:MET:H	2.23	0.42
1:B:1103:PHE:O	1:B:1107:VAL:HG23	2.20	0.42
1:B:1280:LYS:N	1:B:1338:VAL:HG11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD12	1:B:1008:THR:C	2.40	0.42
1:A:43:ASP:HB2	1:B:1031:ILE:CG1	2.50	0.42
1:A:120:LEU:O	1:A:121:PHE:C	2.57	0.42
1:B:1033:THR:O	1:B:1036:SER:N	2.53	0.42
1:B:1286:GLU:O	1:B:1287:PHE:CD1	2.73	0.42
1:B:1289:ARG:HA	1:B:1292:LYS:CB	2.25	0.42
1:A:214:ILE:CB	1:A:328:GLU:HG2	2.50	0.42
1:A:248:PRO:HB3	1:A:395:TRP:CZ2	2.55	0.42
1:B:1274:MET:SD	1:B:1289:ARG:HD2	2.60	0.42
1:A:110:HIS:HE2	3:A:503:CMC:H142	1.83	0.41
1:B:1007:LEU:HD23	1:B:1007:LEU:H	1.85	0.41
1:A:26:GLN:HE21	1:A:26:GLN:HB2	1.57	0.41
1:A:126:ARG:HD3	1:A:178:TYR:O	2.21	0.41
1:A:292:LYS:CD	1:A:294:LYS:HE2	2.50	0.41
1:B:1159:ILE:HG23	3:B:2003:CMC:OAP	2.21	0.41
1:B:1153:ASN:C	1:B:1155:ARG:H	2.23	0.41
1:A:51:SER:CB	1:B:1046:PHE:HZ	2.33	0.41
1:B:1033:THR:O	1:B:1034:LEU:C	2.59	0.41
1:B:1210:GLU:HA	1:B:1210:GLU:OE1	2.21	0.41
1:A:232:ASN:ND2	1:A:235:THR:H	2.18	0.41
1:A:344:ASN:OD1	1:A:348:ASN:ND2	2.53	0.41
1:B:1153:ASN:C	1:B:1155:ARG:N	2.74	0.41
1:B:1153:ASN:O	1:B:1156:HIS:N	2.43	0.41
1:B:1248:PRO:HG3	1:B:1395:TRP:CH2	2.56	0.41
1:A:51:SER:CB	1:B:1046:PHE:CZ	3.03	0.41
1:A:101:ASP:HA	1:B:1426:ARG:NH2	2.35	0.41
1:A:116:GLN:NE2	1:B:1123:ALA:O	2.54	0.41
1:A:284:ILE:N	1:A:285:PRO:CD	2.82	0.41
1:B:1308:TYR:HB3	1:B:1311:TYR:O	2.20	0.41
1:A:86:CYS:O	1:A:90:LEU:N	2.51	0.41
1:A:267:ALA:HB1	1:A:295:ASN:CG	2.41	0.41
1:A:289:ARG:NH2	1:A:289:ARG:CG	2.81	0.41
1:A:323:HIS:CE1	1:A:327:LYS:HD2	2.55	0.41
1:B:1167:LYS:HZ1	3:B:2003:CMC:P1A	2.44	0.41
1:A:24:LEU:HD12	1:B:1412:TYR:CE1	2.55	0.41
1:A:104:LYS:HD3	1:B:1426:ARG:HD3	2.01	0.41
1:A:263:ALA:O	1:A:272:LEU:HD11	2.20	0.41
1:A:288:VAL:O	1:A:291:ALA:HB3	2.21	0.41
1:B:1009:LEU:N	1:B:1015:VAL:O	2.45	0.41
1:B:1034:LEU:HD13	1:B:1039:VAL:HG22	2.01	0.41
1:B:1189:ASN:C	1:B:1191:LEU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1278:ILE:HD12	1:B:1280:LYS:CE	2.51	0.41
3:B:2003:CMC:O9P	3:B:2003:CMC:CCP	2.69	0.41
1:A:192:SER:O	1:A:196:ASN:CB	2.69	0.41
1:A:215:LEU:HB3	1:A:372:MET:HE2	2.03	0.41
1:A:297:SER:HA	1:A:300:LEU:HD23	2.03	0.41
1:B:1281:LYS:HD2	1:B:1338:VAL:HG12	2.04	0.41
1:B:1297:SER:O	1:B:1298:PHE:HD2	2.04	0.41
1:A:98:GLU:O	1:A:98:GLU:HG2	2.20	0.40
1:A:215:LEU:HB3	1:A:372:MET:CE	2.51	0.40
1:A:215:LEU:CD2	1:A:325:VAL:HG13	2.51	0.40
1:A:399:HIS:C	1:A:401:ASP:H	2.25	0.40
1:B:1133:VAL:HG21	4:B:2148:HOH:O	2.21	0.40
1:B:1280:LYS:HG3	1:B:1283:ASN:CB	2.51	0.40
1:A:24:LEU:HD12	1:B:1412:TYR:HE1	1.86	0.40
1:A:30:ASP:OD1	1:A:32:ARG:HB2	2.21	0.40
1:A:214:ILE:HG21	1:A:328:GLU:CB	2.51	0.40
1:B:1080:SER:OG	1:B:1081:ASN:N	2.50	0.40
1:B:1153:ASN:ND2	1:B:1153:ASN:C	2.73	0.40
1:A:155:ARG:HA	1:A:158:GLU:HB3	2.02	0.40
1:A:246:ALA:HB2	1:B:1258:SER:CA	2.43	0.40
1:B:1144:PHE:O	1:B:1146:HIS:N	2.54	0.40
1:B:1273:LYS:HD3	1:B:1273:LYS:HA	1.93	0.40
1:B:1355:LYS:HB3	1:B:1357:LEU:HG	2.04	0.40
1:B:1425:LYS:O	1:B:1426:ARG:HB3	2.22	0.40
1:A:287:PHE:O	1:A:291:ALA:N	2.55	0.40
1:B:1368:ILE:O	1:B:1371:ALA:HB3	2.21	0.40
1:A:278:ILE:CD1	1:A:283:ASN:ND2	2.85	0.40
1:B:1059:ILE:HG21	1:B:1307:VAL:HG11	2.03	0.40
1:B:1064:GLY:HA2	1:B:1308:TYR:HD1	1.86	0.40
1:B:1395:TRP:CZ2	1:B:1399:HIS:HE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	424/426 (100%)	346 (82%)	61 (14%)	17 (4%)	3	6
1	B	424/426 (100%)	341 (80%)	63 (15%)	20 (5%)	2	4
All	All	848/852 (100%)	687 (81%)	124 (15%)	37 (4%)	2	5

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ASP
1	A	405	ILE
1	A	30	ASP
1	A	37	LYS
1	A	147	ASP
1	A	400	SER
1	B	1036	SER
1	B	1261	GLY
1	B	1285	PRO
1	B	1286	GLU
1	B	1299	ARG
1	B	1330	GLY
1	B	1334	ASP
1	B	1404	LYS
1	A	3	THR
1	A	402	GLY
1	A	404	LYS
1	A	417	LYS
1	B	1038	GLY
1	B	1231	GLN
1	B	1264	HIS
1	B	1272	LEU
1	B	1331	THR
1	A	96	THR
1	B	1263	ALA
1	A	276	GLU
1	A	329	LEU
1	A	350	PRO
1	B	1154	PRO
1	B	1283	ASN
1	B	1328	GLU
1	A	288	VAL
1	B	1274	MET

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Mol	Chain	Res	Type
1	B	1031	ILE
1	B	1061	GLY
1	A	265	GLY
1	A	330	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/361 (100%)	340 (94%)	21 (6%)	20	43
1	B	361/361 (100%)	347 (96%)	14 (4%)	32	61
All	All	722/722 (100%)	687 (95%)	35 (5%)	25	53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	12	ASP
1	A	21	LYS
1	A	26	GLN
1	A	27	ASP
1	A	74	ASP
1	A	129	HIS
1	A	147	ASP
1	A	153	ASN
1	A	207	GLU
1	A	212	ASN
1	A	215	LEU
1	A	232	ASN
1	A	273	LYS
1	A	278	ILE
1	A	292	LYS
1	A	296	ASP
1	A	335	LEU
1	A	340	MET

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Mol	Chain	Res	Type
1	A	404	LYS
1	A	416	GLU
1	B	1004	LYS
1	B	1006	LYS
1	B	1007	LEU
1	B	1040	PHE
1	B	1081	ASN
1	B	1134	MET
1	B	1153	ASN
1	B	1156	HIS
1	B	1232	ASN
1	B	1289	ARG
1	B	1292	LYS
1	B	1306	ARG
1	B	1326	LEU
1	B	1398	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	99	GLN
1	A	110	HIS
1	A	153	ASN
1	A	182	GLN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	283	ASN
1	A	305	HIS
1	A	399	HIS
1	B	1081	ASN
1	B	1091	ASN
1	B	1097	GLN
1	B	1114	HIS
1	B	1129	HIS
1	B	1146	HIS
1	B	1231	GLN
1	B	1232	ASN
1	B	1268	ASN
1	B	1305	HIS
1	B	1399	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	501	-	4,4,4	0.72	0	6,6,6	0.44	0
2	SO4	B	2002	-	4,4,4	0.72	0	6,6,6	0.41	0
2	SO4	B	2001	-	4,4,4	0.81	0	6,6,6	0.38	0
2	SO4	A	502	-	4,4,4	0.72	0	6,6,6	0.45	0
3	CMC	B	2003	-	46,54,54	0.87	1 (2%)	58,80,80	1.13	4 (6%)
3	CMC	A	503	-	46,54,54	0.85	1 (2%)	58,80,80	1.20	3 (5%)

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	CMC	A	503	-	-	15/48/68/68	0/3/3/3
3	CMC	B	2003	-	-	13/48/68/68	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2003	CMC	O4B-C1B	2.32	1.44	1.41
3	A	503	CMC	O4B-C1B	2.24	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	CMC	P2A-O3A-P1A	-4.74	116.56	132.83
3	B	2003	CMC	N3A-C2A-N1A	-4.60	121.48	128.68
3	A	503	CMC	N3A-C2A-N1A	-4.55	121.57	128.68
3	B	2003	CMC	P2A-O3A-P1A	-4.41	117.70	132.83
3	B	2003	CMC	O21-C2-C1	-2.29	116.55	122.82
3	B	2003	CMC	C5B-C4B-C3B	-2.28	106.83	114.40
3	A	503	CMC	O21-C2-C1	-2.13	116.99	122.82

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	CMC	C3B-O3B-P3B-O9A
3	A	503	CMC	C5B-O5B-P1A-O1A
3	A	503	CMC	CCP-O6A-P2A-O3A
3	A	503	CMC	O9P-C9P-CAP-CBP
3	A	503	CMC	N8P-C9P-CAP-CBP
3	A	503	CMC	N8P-C9P-CAP-OAP
3	B	2003	CMC	CCP-O6A-P2A-O3A
3	B	2003	CMC	O9P-C9P-CAP-CBP
3	B	2003	CMC	N8P-C9P-CAP-CBP
3	B	2003	CMC	N8P-C9P-CAP-OAP
3	B	2003	CMC	CAP-C9P-N8P-C7P
3	B	2003	CMC	O9P-C9P-N8P-C7P
3	A	503	CMC	C2-C1-S1P-C2P
3	B	2003	CMC	C2-C1-S1P-C2P
3	A	503	CMC	O9P-C9P-CAP-OAP
3	B	2003	CMC	O9P-C9P-CAP-OAP
3	B	2003	CMC	O5P-C5P-C6P-C7P
3	A	503	CMC	C5B-O5B-P1A-O3A
3	B	2003	CMC	P1A-O3A-P2A-O4A
3	A	503	CMC	C5B-O5B-P1A-O2A
3	A	503	CMC	O5P-C5P-C6P-C7P
3	A	503	CMC	N4P-C5P-C6P-C7P
3	B	2003	CMC	S1P-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
3	B	2003	CMC	N4P-C5P-C6P-C7P
3	A	503	CMC	S1P-C1-C2-O21
3	B	2003	CMC	S1P-C1-C2-O22
3	A	503	CMC	P2A-O3A-P1A-O2A
3	A	503	CMC	S1P-C1-C2-O22

There are no ring outliers.

2 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2003	CMC	16	0
3	A	503	CMC	16	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 CMC B 2003

Bond lengths

Bond angles

Torsions

Rings

Ligand CMC A 503	
Bond lengths	Bond angles
Torsions	Rings
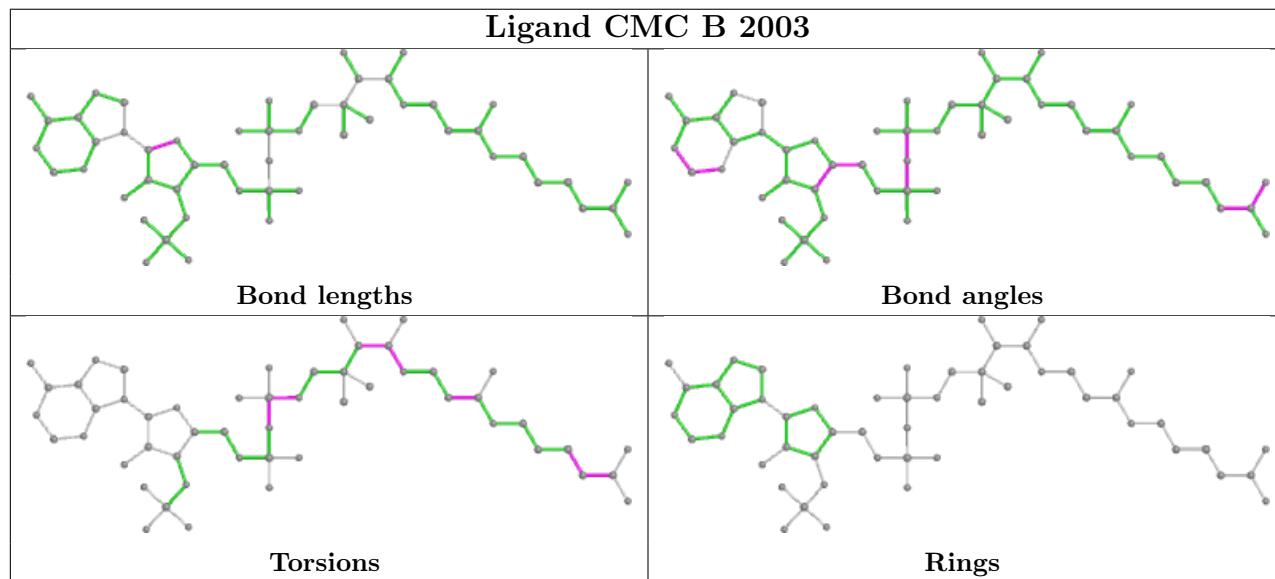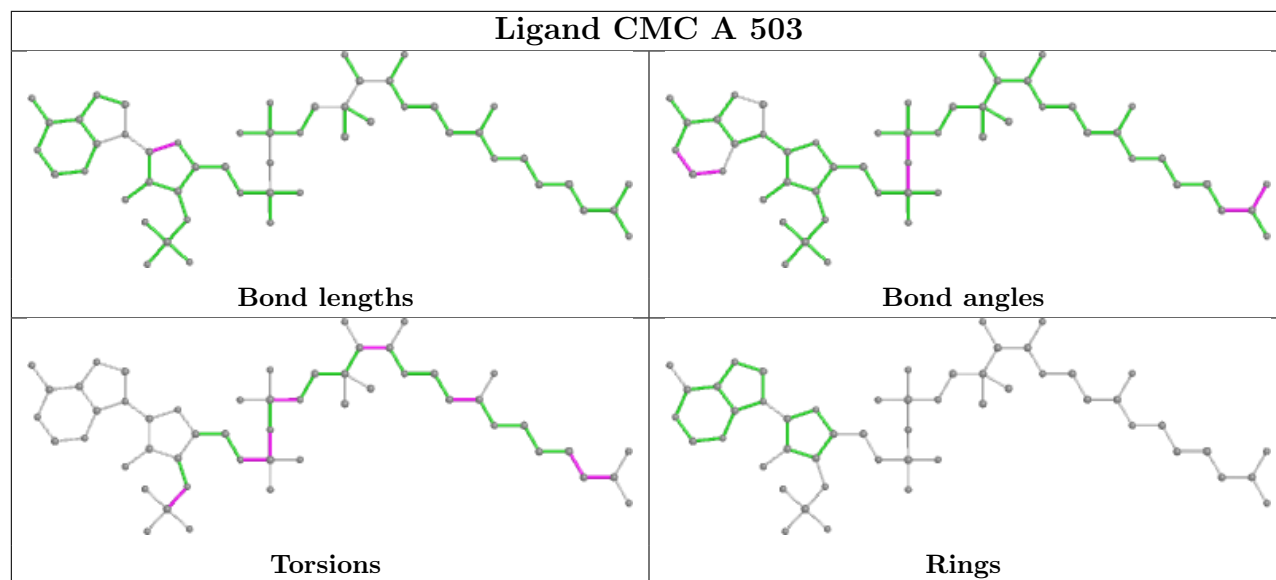
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

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	426/426 (100%)	0.11	18 (4%)	36	35	19, 41, 98, 117	0
1	B	426/426 (100%)	0.09	17 (3%)	38	37	21, 39, 105, 111	0
All	All	852/852 (100%)	0.10	35 (4%)	37	36	19, 40, 104, 117	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1007	LEU	6.0
1	A	290	ARG	5.2
1	A	1	ALA	5.1
1	B	1001	ALA	4.5
1	B	1004	LYS	4.1
1	B	1275	LEU	3.4
1	A	265	GLY	3.4
1	B	1274	MET	3.3
1	A	3	THR	3.0
1	B	1271	ALA	2.9
1	B	1017	LEU	2.8
1	A	149	LEU	2.8
1	B	1289	ARG	2.7
1	A	4	LYS	2.7
1	B	1009	LEU	2.7
1	A	271	ALA	2.6
1	A	284	ILE	2.6
1	B	1267	ALA	2.6
1	A	17	LEU	2.5
1	B	1284	ILE	2.5
1	A	298	PHE	2.5
1	A	288	VAL	2.5
1	B	1002	ASP	2.4
1	A	148	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	2.3
1	A	406	ALA	2.3
1	B	1426	ARG	2.2
1	A	2	ASP	2.2
1	A	275	LEU	2.2
1	B	1404	LYS	2.2
1	B	1287	PHE	2.2
1	A	9	LEU	2.1
1	A	272	LEU	2.1
1	B	1278	ILE	2.0
1	B	1149	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	502	5/5	0.90	0.16	80,80,81,81	0
3	CMC	B	2003	52/52	0.91	0.23	67,73,76,77	0
3	CMC	A	503	52/52	0.93	0.20	69,74,78,78	0
2	SO4	B	2002	5/5	0.96	0.17	63,63,64,64	0
2	SO4	A	501	5/5	0.98	0.17	53,53,54,54	0
2	SO4	B	2001	5/5	0.99	0.18	43,43,43,44	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 CMC B 2003:

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

Electron density around CMC A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
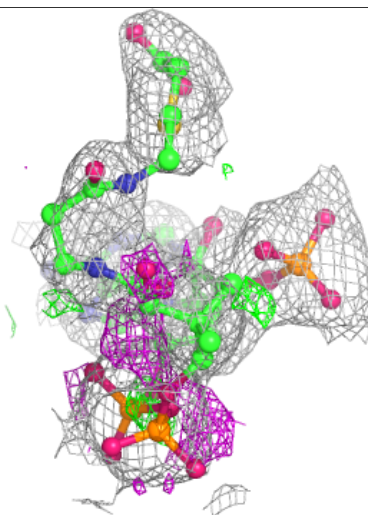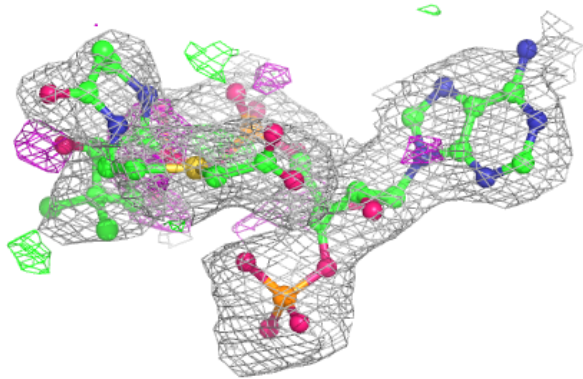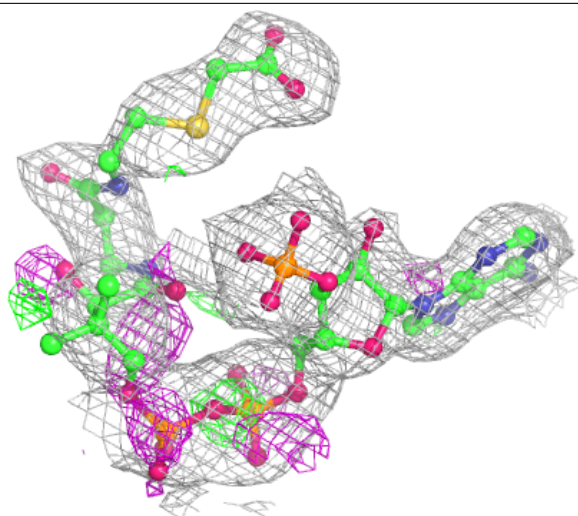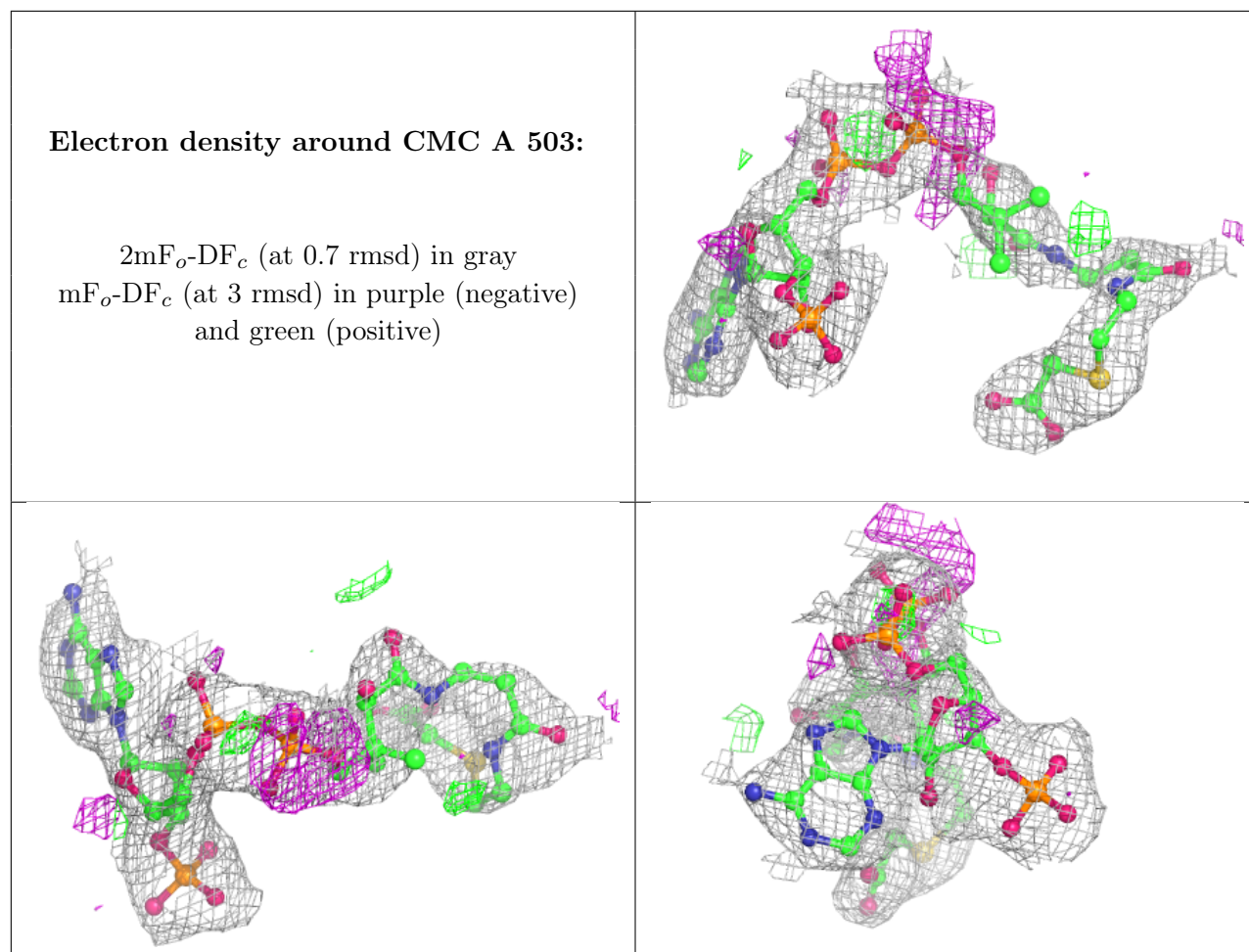
6.5   Other polymers (i)

There are no such residues in this entry.