



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 4JAE / pdb_00004jae
Title : STRUCTURAL DETERMINATION OF THE A50T:S279G:S280K:V281
K: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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

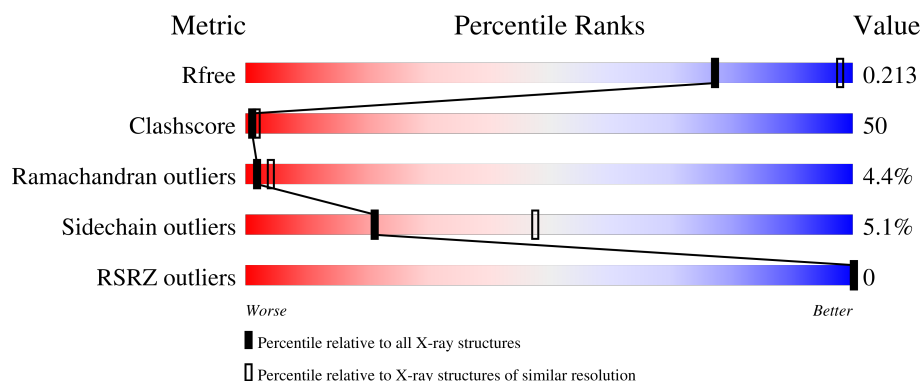
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

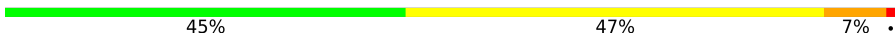
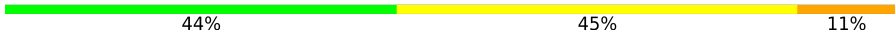
The reported resolution of this entry is 2.70 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	426	
1	B	426	

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	C	N	O	S	0	0	0
			3365	2132	578	630	25			
1	B	426	Total	C	N	O	S	0	0	0
			3365	2132	578	630	25			

There are 14 discrepancies between the modelled and reference sequences:

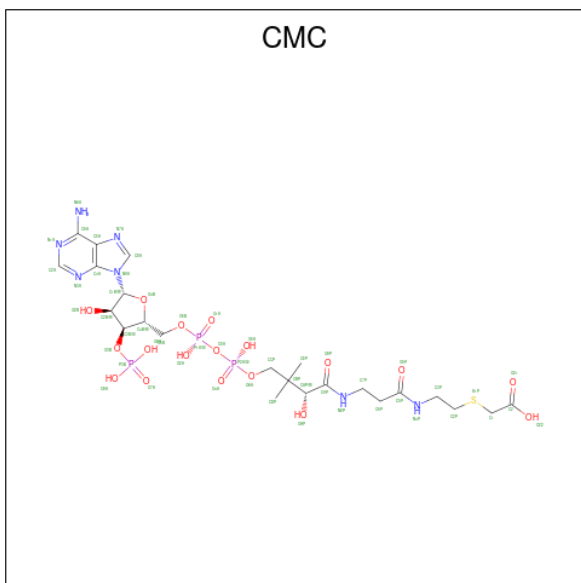
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ASP	ASN	SEE REMARK 999	UNP P0ABH7
A	50	THR	ALA	engineered mutation	UNP P0ABH7
A	279	GLY	SER	engineered mutation	UNP P0ABH7
A	280	LYS	SER	engineered mutation	UNP P0ABH7
A	281	LYS	VAL	engineered mutation	UNP P0ABH7
A	282	GLU	LYS	engineered mutation	UNP 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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CARBOXYMETHYL COENZYME *A (CCD ID: CMC) (formula: C₂₃H₃₈N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			52	23	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			52	23	7	18	3	1		

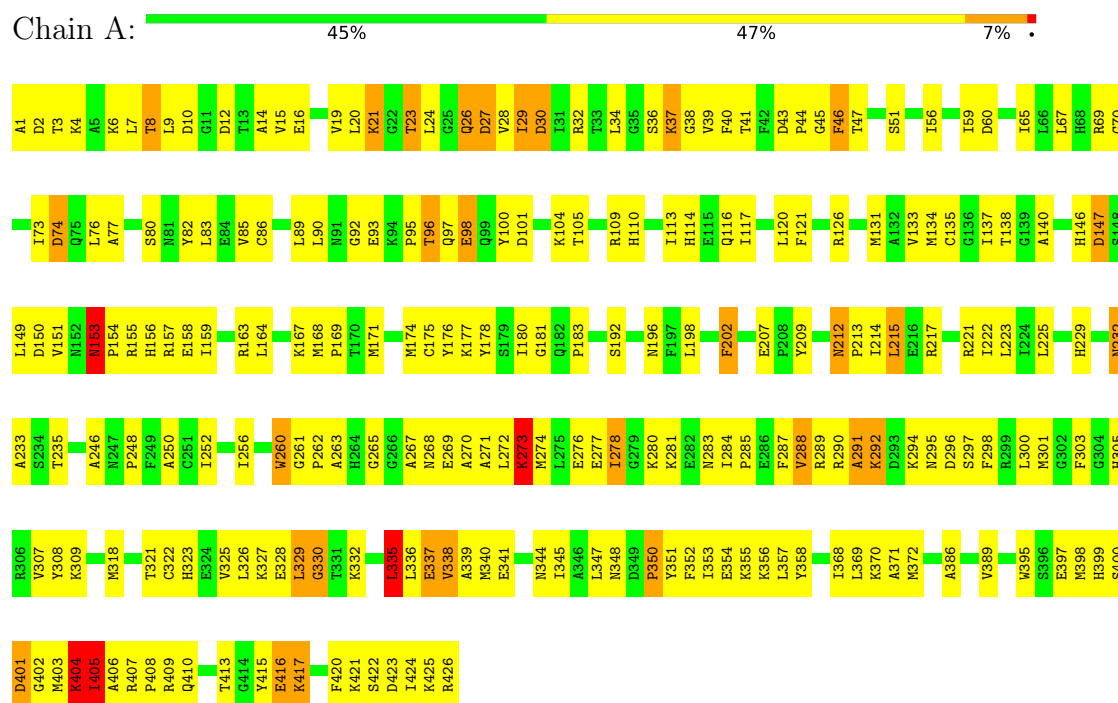
- Molecule 4 is water.

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

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



• Molecule 1: Citrate synthase



H1247	D1312	M1247
P1248	P1313	P1248
F1249	M1318	F1249
I1256	R1319	I1256
A1257	E1320	A1257
S1258	T1321	S1258
L1259	E1324	L1259
W1260	V1325	W1260
G1261	L1326	G1261
P1262	K1327	P1262
A1263	E1328	A1263
H1264	L1329	H1264
G1265	G1330	G1265
G1266	K1332	G1266
A1267	D1333	A1267
N1268	D1334	N1268
E1269	L1335	E1269
N1270	L1336	N1270
A1271	E1337	A1271
L1272	V1338	L1272
K1273	A1339	K1273
M1274	M1340	M1274
L1275	E1341	L1275
E1276	L1342	E1276
E1277	E1343	E1277
I1278	E1344	I1278
G1279	I1345	G1279
K1280	A1346	K1280
K1281	D1349	K1281
E1282	P1350	E1282
N1283	Y1351	N1283
I1284	F1352	I1284
P1285	K1355	P1285
E1286	K1356	E1286
F1287	L1357	F1287
V1288	Y1358	V1288
R1289	F1363	R1289
R1290	Y1364	R1290
A1291	I1367	A1291
K1292	I1368	K1292
D1293	L1369	D1293
K1294	K1370	K1294
N1295	A1371	N1295
D1296	M1378	D1296
S1297	F1379	S1297
F1298	T1380	F1298
R1299	V1381	R1299
L1300	T1388	L1300
M1301	I1392	M1301
G1302	A1393	G1302
F1303		F1303
G1304		G1304
H1305		H1305
R1306		R1306
V1307		V1307
Y1308		Y1308
K1309		K1309
N1310		N1310
Y1311		Y1311

H1394	E1416
W1395	K1417
M1398	R1418
H1399	D1419
S1400	F1420
K1404	K1425
T1405	R1426
A1406	
R1407	
P1408	
R1409	
Y1412	

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 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.70) 98.2 (30.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	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.*

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

5.1 Standard geometry

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

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	0.50	0/3441	1.03	15/4649 (0.3%)
1	B	0.50	0/3441	1.04	23/4649 (0.5%)
All	All	0.50	0/6882	1.04	38/9298 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	GLU	N-CA-C	-11.07	98.46	113.18
1	B	1355	LYS	CA-C-N	-7.89	110.48	122.08
1	B	1355	LYS	C-N-CA	-7.89	110.48	122.08
1	B	1416	GLU	N-CA-C	-7.40	100.98	110.53
1	A	332	LYS	N-CA-C	-7.39	103.22	114.16
1	A	339	ALA	N-CA-C	-7.06	103.20	111.03
1	B	1400	SER	N-CA-C	-7.02	104.85	113.41
1	B	1202	PHE	N-CA-C	6.85	122.74	113.97
1	B	1290	ARG	N-CA-C	-6.80	104.24	112.54
1	B	1096	THR	N-CA-C	-6.66	100.10	110.42
1	B	1294	LYS	N-CA-C	6.61	121.19	111.34
1	A	202	PHE	N-CA-C	6.59	122.81	114.31
1	A	291	ALA	N-CA-C	-6.28	105.58	113.18
1	B	1269	GLU	N-CA-C	-6.09	106.18	113.97
1	B	1167	LYS	N-CA-C	5.93	120.67	112.90
1	B	1028	VAL	N-CA-C	5.90	117.21	108.65
1	B	1052	CYS	N-CA-C	5.90	116.88	108.74
1	B	1295	ASN	CA-C-N	-5.79	113.66	121.71
1	B	1295	ASN	C-N-CA	-5.79	113.66	121.71
1	B	1335	LEU	N-CA-C	-5.77	104.96	112.23
1	A	46	PHE	N-CA-C	-5.63	104.14	111.74
1	A	273	LYS	N-CA-C	-5.62	105.24	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	VAL	N-CA-C	-5.54	104.28	112.04
1	B	1342	LEU	N-CA-C	-5.49	104.94	111.03
1	B	1012	ASP	N-CA-C	-5.47	107.85	114.75
1	A	229	HIS	N-CA-C	5.45	117.85	110.06
1	A	335	LEU	N-CA-C	-5.41	105.38	111.28
1	B	1271	ALA	N-CA-C	-5.32	104.37	112.04
1	A	23	THR	N-CA-C	-5.32	106.63	113.01
1	B	1333	ASP	N-CA-C	5.26	121.99	110.80
1	A	153	ASN	CA-C-N	5.18	124.68	119.19
1	A	153	ASN	C-N-CA	5.18	124.68	119.19
1	A	260	TRP	N-CA-C	-5.17	108.24	114.75
1	B	1010	ASP	N-CA-C	5.12	117.71	107.62
1	B	1296	ASP	N-CA-C	-5.10	100.67	110.56
1	B	1027	ASP	N-CA-C	-5.08	103.23	110.59
1	A	250	ALA	N-CA-C	-5.04	105.87	111.36
1	B	1276	GLU	N-CA-C	-5.02	107.11	113.43

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	359	0
1	B	3365	0	3312	366	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	52	0	33	15	0
3	B	52	0	33	15	0
4	A	104	0	0	7	0
4	B	123	0	0	10	0
All	All	7081	0	6693	673	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 50.

All (673) 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: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:298:PHE:HA	1:A:301:MET:HE2	1.57	0.86
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
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:A:403:MET:C	1:A:405:ILE:H	1.83	0.84
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:1134:MET:HE2	1:B:1381:VAL:HG13	1.59	0.82
1:B:1329:LEU:HB3	1:B:1332:LYS:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:ARG:HH21	1:A:217:ARG:HG3	1.48	0.78
1:B:1271:ALA:C	1:B:1273:LYS:H	1.92	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:328:GLU:C	1:A:330:GLY:H	1.93	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:1318:MET:HE2	1:B:1368:ILE:HD12	1.69	0.74
1:A:134:MET:HE3	1:A:168:MET:HE1	1.68	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1272:LEU:HD21	1:B:1300:LEU:C	2.17	0.70
1:A:318:MET:HE2	1:A:368:ILE:CD1	2.21	0.70
1:A:318:MET:HE2	1:A:368:ILE:HD12	1.74	0.70
1:A:417:LYS:HD3	1:A:417:LYS:C	2.17	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: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:A:15:VAL:HG13	1:A:37:LYS:HZ3	1.56	0.69
1:B:1281:LYS:H	1:B:1281:LYS:HD2	1.57	0.68
1:A:153:ASN:HD22	1:A:153:ASN:C	1.99	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:212:ASN:C	1:A:212:ASN:HD22	2.00	0.68
1:A:405:ILE:HG23	1:A:407:ARG:CZ	2.25	0.67
1:B:1081:ASN:C	1:B:1081:ASN:HD22	1.98	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: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:B:1035:GLY:C	1:B:1037:LYS:H	2.03	0.66
1:B:1318:MET:HE3	1:B:1318:MET:HA	1.77	0.66
1:A:6:LYS:HB2	1:A:16:GLU:OE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1330:GLY:C	1:B:1332:LYS:H	2.04	0.64
1:A:36:SER:C	1:A:38:GLY:H	2.05	0.64
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:117:ILE:O	1:A:120:LEU:HB2	1.98	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:134:MET:HE3	1:A:168:MET:CE	2.28	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:1176:TYR:HB2	1:B:1378:MET:HE2	1.82	0.61
1:A:28:VAL:C	1:A:29:ILE:HD12	2.25	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:270:ALA:HA	1:A:273:LYS:HZ2	1.63	0.60
1:B:1318:MET:HE2	1:B:1368:ILE:CD1	2.32	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:1338:VAL:O	1:B:1342:LEU:HG	2.01	0.59
1:A:215:LEU:HD13	1:A:372:MET:HE2	1.85	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CD2	1:A:403:MET:HE1	2.38	0.59
1:B:1346:ALA:HA	1:B:1352:PHE:CD2	2.38	0.59
1:A:408:PRO:CB	1:B:1051:SER:HB3	2.30	0.59
1:A:416:GLU:O	1:A:417:LYS:C	2.45	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:A:212:ASN:HD21	1:A:214:ILE:HG12	1.68	0.58
1:B:1087:TYR:CD1	1:B:1087:TYR:C	2.81	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:328:GLU:C	1:A:330:GLY:N	2.60	0.58
1:A:277:GLU:HG3	1:A:278:ILE:N	2.18	0.58
1:B:1134:MET:CE	1:B:1381:VAL:HG13	2.33	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:1131:MET:HE3	1:B:1256:ILE:HG23	1.86	0.57
1:B:1129:HIS:CD2	1:B:1131:MET:H	2.20	0.57
1:B:1153:ASN:C	1:B:1153:ASN:HD22	2.12	0.57
1:A:278:ILE:CD1	1:A:283:ASN:CG	2.78	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:B:1355:LYS:O	1:B:1356:LYS:C	2.43	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: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:110:HIS:CE1	3:A:503:CMC:H142	2.39	0.56
1:A:297:SER:O	1:A:301:MET:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:MET:HA	1:A:318:MET:HE3	1.86	0.56
1:B:1417:LYS:HD3	1:B:1417:LYS:C	2.30	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
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:B:1131:MET:HE3	1:B:1256:ILE:CG2	2.36	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:278:ILE:HD11	1:A:283:ASN:CG	2.31	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:A:413:THR:HG22	1:A:413:THR:O	2.05	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:1081:ASN:ND2	1:B:1081:ASN:C	2.63	0.55
1:B:1286:GLU:O	1:B:1288:VAL:HG23	2.05	0.55
1:B:1035:GLY:C	1:B:1037:LYS:N	2.65	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:403:MET:C	1:A:405:ILE:N	2.57	0.54
1:B:1271:ALA:C	1:B:1273:LYS:N	2.61	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
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:212:ASN:C	1:A:212:ASN:ND2	2.65	0.53
1:A:20:LEU:HB2	1:A:28:VAL:CG2	2.38	0.53
1:A:36:SER:C	1:A:38:GLY:N	2.66	0.53
1:A:271:ALA:HA	1:A:274:MET:CB	2.39	0.53
1:B:1096:THR:O	1:B:1097:GLN:C	2.51	0.53
1:B:1145:TYR:CB	1:B:1163:ARG:NH2	2.65	0.53
1:A:335:LEU:HD23	1:A:335:LEU:N	2.20	0.53
1:A:177:LYS:HZ1	1:A:202:PHE:HA	1.74	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:167:LYS:NZ	3:A:503:CMC:O2A	2.40	0.53
1:A:273:LYS:O	1:A:277:GLU:HG2	2.09	0.53
1:A:284:ILE:HG22	1:A:341:GLU:HG2	1.90	0.53
1:A:113:ILE:HD11	1:A:174:MET:HE1	1.91	0.53
1:A:270:ALA:O	1:A:274:MET:HB2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1230:GLU:HG2	1:B:1231:GLN:N	2.07	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:2:ASP:C	1:A:4:LYS:H	2.17	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:A:406:ALA:C	1:A:407:ARG:HD2	2.34	0.52
1:B:1007:LEU:CD1	1:B:1017:LEU:HB2	2.39	0.52
1:B:1293:ASP:CG	1:B:1298:PHE:HE2	2.17	0.52
1:B:1293:ASP:C	1:B:1294:LYS:HD2	2.35	0.52
1:A:153:ASN:ND2	1:A:153:ASN:C	2.65	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: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
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:A:350:PRO:O	1:A:351:TYR:C	2.54	0.51
1:B:1119:ARG:HD3	1:B:1119:ARG:N	2.26	0.51
1:B:1298:PHE:C	1:B:1300:LEU:H	2.18	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:B:1331:THR:C	1:B:1332:LYS:HG2	2.34	0.51
1:A:268:ASN:O	1:A:272:LEU:N	2.44	0.51
1:A:273:LYS:O	1:A:274:MET:C	2.53	0.51
1:A:370:LYS:C	1:A:372:MET:N	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:426:ARG:CD	1:B:1101:ASP:OD1	2.60	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
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:1271:ALA:HB1	1:B:1301:MET:HE2	1.94	0.49
1:B:1330:GLY:C	1:B:1332:LYS:N	2.70	0.49
1:B:1369:LEU:C	1:B:1371:ALA:H	2.19	0.49
1:A:270:ALA:HA	1:A:273:LYS:HZ3	1.76	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: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:A:278:ILE:CG2	1:A:289:ARG:HD3	2.43	0.48
1:B:1273:LYS:C	1:B:1275:LEU:H	2.21	0.48
1:A:157:ARG:HE	1:A:399:HIS:CG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:ASN:C	1:A:288:VAL:HB	2.38	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:1104:LYS:NZ	4:B:2121:HOH:O	2.43	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:297:SER:C	1:A:301:MET:HE2	2.39	0.47
1:B:1349:ASP:OD1	1:B:1351:TYR:HB3	2.14	0.47
1:B:1265:GLY:H	1:B:1268:ASN:CG	2.21	0.47
1:A:6:LYS:O	1:A:7:LEU:HD23	2.14	0.47
1:A:274:MET:HA	1:A:277:GLU:CD	2.39	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
1:A:271:ALA:HB3	1:A:297:SER:OG	2.14	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:B:1137:ILE:O	1:B:1138:THR:C	2.57	0.47
1:B:1369:LEU:C	1:B:1371:ALA:N	2.71	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:A:399:HIS:C	1:A:401:ASP:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:CE2	1:A:86:CYS:SG	3.08	0.47
1:A:417:LYS:C	1:A:417:LYS:CD	2.88	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: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:A:9:LEU:HD12	1:B:1008:THR:C	2.40	0.46
1:A:120:LEU:O	1:A:121:PHE:C	2.57	0.46
1:B:1153:ASN:C	1:B:1155:ARG:H	2.23	0.46
1:A:51:SER:HB3	1:B:1046:PHE:HZ	1.81	0.46
1:A:267:ALA:HB1	1:A:295:ASN:CG	2.41	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: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:292:LYS:HB2	1:A:292:LYS:NZ	2.31	0.46
1:A:421:LYS:HD2	4:A:606:HOH:O	2.14	0.46
1:B:1033:THR:O	1:B:1034:LEU:C	2.59	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: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:370:LYS:C	1:A:372:MET:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1153:ASN:C	1:B:1155:ARG:N	2.74	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:1153:ASN:ND2	1:B:1153:ASN:C	2.73	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:A:399:HIS:C	1:A:401:ASP:H	2.25	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:B:1189:ASN:C	1:B:1191:LEU:H	2.24	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
1:B:1268:ASN:O	1:B:1300:LEU:HD12	2.17	0.45
1:B:1344:ASN:O	1:B:1345:ILE:C	2.59	0.45
1:A:305:HIS:HB3	1:A:358:TYR:OH	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:298:PHE:CA	1:A:301:MET:HE2	2.39	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:B:1326:LEU:O	1:B:1327:LYS:C	2.61	0.44
1:A:300:LEU:HD22	1:A:300:LEU:H	1.83	0.44
1:B:1282:GLU:HB3	1:B:1286:GLU:CD	2.43	0.44
1:B:1296:ASP:O	1:B:1298:PHE:CD1	2.71	0.44
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: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: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
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: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:A:97:GLN:HB3	4:A:638:HOH:O	2.18	0.43
1:A:221:ARG:O	1:A:222:ILE:C	2.61	0.42
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:318:MET:HE3	1:A:321:THR:HB	2.00	0.42
1:A:369:LEU:O	1:A:372:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1285:PRO:O	1:B:1286:GLU:C	2.63	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:113:ILE:CD1	1:A:174:MET:HE1	2.49	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:B:1135:CYS:O	1:B:1136:GLY:C	2.61	0.42
1:A:223:LEU:HD23	1:A:386:ALA:HB2	2.02	0.42
1:A:289:ARG:NH2	1:A:289:ARG:C	2.77	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:A:24:LEU:HB2	1:B:1412:TYR:HD1	1.85	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
1:A:43:ASP:HB2	1:B:1031:ILE:CG1	2.50	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:B:1398:MET:HE3	1:B:1398:MET:HB3	1.71	0.42
1:B:1007:LEU:HD23	1:B:1007:LEU:H	1.85	0.41
1:A:15:VAL:HG13	1:A:37:LYS:NZ	2.32	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:1088:ILE:O	1:B:1089:LEU:C	2.62	0.41
1:B:1159:ILE:HG23	3:B:2003:CMC:OAP	2.21	0.41
1:B:1288:VAL:C	1:B:1290:ARG:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:SER:CB	1:B:1046:PHE:HZ	2.33	0.41
1:A:95:PRO:C	1:A:96:THR:O	2.61	0.41
1:B:1337:GLU:C	1:B:1339:ALA:H	2.27	0.41
1:A:155:ARG:C	1:A:158:GLU:HB3	2.43	0.41
1:A:398:MET:SD	1:A:398:MET:C	3.04	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: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: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: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:138:THR:C	1:A:140:ALA:H	2.29	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: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:30:ASP:OD1	1:A:30:ASP:C	2.64	0.41
1:A:192:SER:O	1:A:196:ASN:CB	2.69	0.41
1:A:278:ILE:C	1:A:278:ILE:HD13	2.45	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:CD2	1:A:325:VAL:HG13	2.51	0.40
1:A:215:LEU:HB3	1:A:372:MET:CE	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LYS:C	1:A:405:ILE:CG2	2.94	0.40
1:B:1080:SER:OG	1:B:1081:ASN:N	2.50	0.40
1:B:1417:LYS:C	1:B:1417:LYS:CD	2.92	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:1334:ASP:C	1:B:1337:GLU:HG2	2.47	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:A:336:LEU:O	1:A:340:MET:HE1	2.21	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%)	2	5
1	B	424/426 (100%)	341 (80%)	63 (15%)	20 (5%)	2	3
All	All	848/852 (100%)	687 (81%)	124 (15%)	37 (4%)	2	4

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ASP

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

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	361/361 (100%)	339 (94%)	22 (6%)	17	40
1	B	361/361 (100%)	346 (96%)	15 (4%)	26	55
All	All	722/722 (100%)	685 (95%)	37 (5%)	21	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	21	LYS
1	A	26	GLN
1	A	27	ASP
1	A	29	ILE
1	A	74	ASP
1	A	83	LEU
1	A	98	GLU
1	A	105	THR
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	335	LEU
1	A	404	LYS
1	A	405	ILE
1	A	416	GLU
1	B	1004	LYS
1	B	1006	LYS
1	B	1007	LEU
1	B	1020	LEU
1	B	1040	PHE
1	B	1081	ASN
1	B	1134	MET
1	B	1153	ASN
1	B	1204	THR
1	B	1223	LEU
1	B	1292	LYS

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Mol	Chain	Res	Type
1	B	1306	ARG
1	B	1326	LEU
1	B	1398	MET
1	B	1409	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	91	ASN
1	A	99	GLN
1	A	110	HIS
1	A	153	ASN
1	A	182	GLN
1	A	196	ASN
1	A	199	ASN
1	A	212	ASN
1	A	231	GLN
1	A	232	ASN
1	A	283	ASN
1	A	348	ASN
1	B	1081	ASN
1	B	1097	GLN
1	B	1114	HIS
1	B	1122	HIS
1	B	1129	HIS
1	B	1146	HIS
1	B	1156	HIS
1	B	1231	GLN
1	B	1232	ASN
1	B	1268	ASN
1	B	1305	HIS
1	B	1323	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	CMC	B	2003	-	52,54,54	1.01	3 (5%)	75,80,80	1.45	12 (16%)
2	SO4	B	2002	-	4,4,4	0.79	0	6,6,6	0.43	0
2	SO4	A	502	-	4,4,4	0.79	0	6,6,6	0.47	0
2	SO4	A	501	-	4,4,4	0.78	0	6,6,6	0.45	0
3	CMC	A	503	-	52,54,54	0.99	3 (5%)	75,80,80	1.44	9 (12%)
2	SO4	B	2001	-	4,4,4	0.87	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CMC	B	2003	-	-	14/52/68/68	0/3/3/3
3	CMC	A	503	-	-	15/52/68/68	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	CMC	C5A-N7A	-3.15	1.33	1.39
3	B	2003	CMC	C5A-N7A	-3.07	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2003	CMC	C8A-N9A	-2.33	1.33	1.37
3	A	503	CMC	C8A-N9A	-2.28	1.33	1.37
3	B	2003	CMC	C4A-N9A	-2.08	1.33	1.37
3	A	503	CMC	C4A-N9A	-2.07	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2003	CMC	C5A-C4A-N3A	-5.42	119.25	126.72
3	A	503	CMC	C5A-C4A-N3A	-5.21	119.54	126.72
3	B	2003	CMC	N3A-C2A-N1A	-4.69	121.48	128.58
3	A	503	CMC	N3A-C2A-N1A	-4.63	121.57	128.58
3	B	2003	CMC	N3A-C4A-N9A	3.92	133.84	127.17
3	A	503	CMC	N3A-C4A-N9A	3.78	133.59	127.17
3	B	2003	CMC	C2A-N3A-C4A	3.71	120.89	111.83
3	A	503	CMC	C2A-N3A-C4A	3.60	120.62	111.83
3	A	503	CMC	N9A-C8A-N7A	-3.15	109.46	113.94
3	B	2003	CMC	N9A-C8A-N7A	-2.97	109.72	113.94
3	A	503	CMC	C5A-N7A-C8A	2.81	107.87	103.45
3	A	503	CMC	C4A-C5A-N7A	-2.66	107.54	110.58
3	B	2003	CMC	C5A-N7A-C8A	2.63	107.58	103.45
3	B	2003	CMC	C4A-C5A-N7A	-2.56	107.66	110.58
3	A	503	CMC	C4A-N9A-C8A	2.41	108.27	105.74
3	B	2003	CMC	O21-C2-C1	-2.33	116.55	122.85
3	B	2003	CMC	C4A-N9A-C8A	2.29	108.14	105.74
3	B	2003	CMC	C5B-C4B-C3B	-2.27	106.83	114.38
3	B	2003	CMC	O4B-C1B-N9A	2.23	112.36	108.09
3	A	503	CMC	O21-C2-C1	-2.17	116.99	122.85
3	B	2003	CMC	C2B-C1B-N9A	-2.10	108.09	113.30

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	CMC	C5B-O5B-P1A-O1A
3	A	503	CMC	C5B-O5B-P1A-O3A
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

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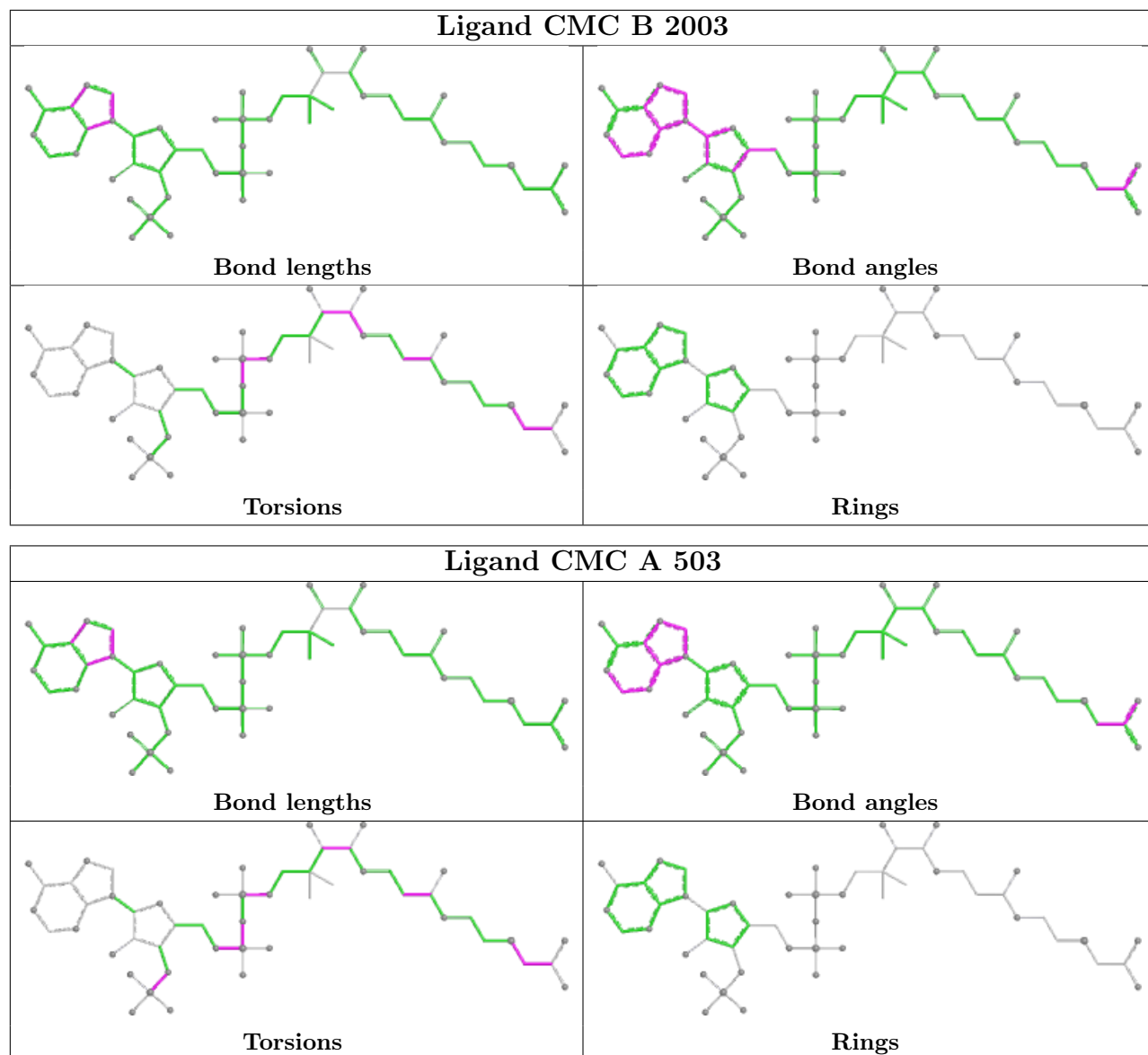
Mol	Chain	Res	Type	Atoms
3	B	2003	CMC	N8P-C9P-CAP-OAP
3	B	2003	CMC	CAP-C9P-N8P-C7P
3	B	2003	CMC	O9P-C9P-N8P-C7P
3	A	503	CMC	O9P-C9P-CAP-OAP
3	B	2003	CMC	O9P-C9P-CAP-OAP
3	B	2003	CMC	N8P-C9P-CAP-CBP
3	A	503	CMC	C2-C1-S1P-C2P
3	B	2003	CMC	C2-C1-S1P-C2P
3	B	2003	CMC	O5P-C5P-C6P-C7P
3	B	2003	CMC	P1A-O3A-P2A-O4A
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
3	A	503	CMC	C3B-O3B-P3B-O9A
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
3	B	2003	CMC	P1A-O3A-P2A-O5A

There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2003	CMC	15	0
3	A	503	CMC	15	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	426/426 (100%)	-1.63	0 100 100	19, 41, 98, 117	0
1	B	426/426 (100%)	-1.61	0 100 100	21, 39, 105, 111	0
All	All	852/852 (100%)	-1.62	0 100 100	19, 40, 104, 117	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

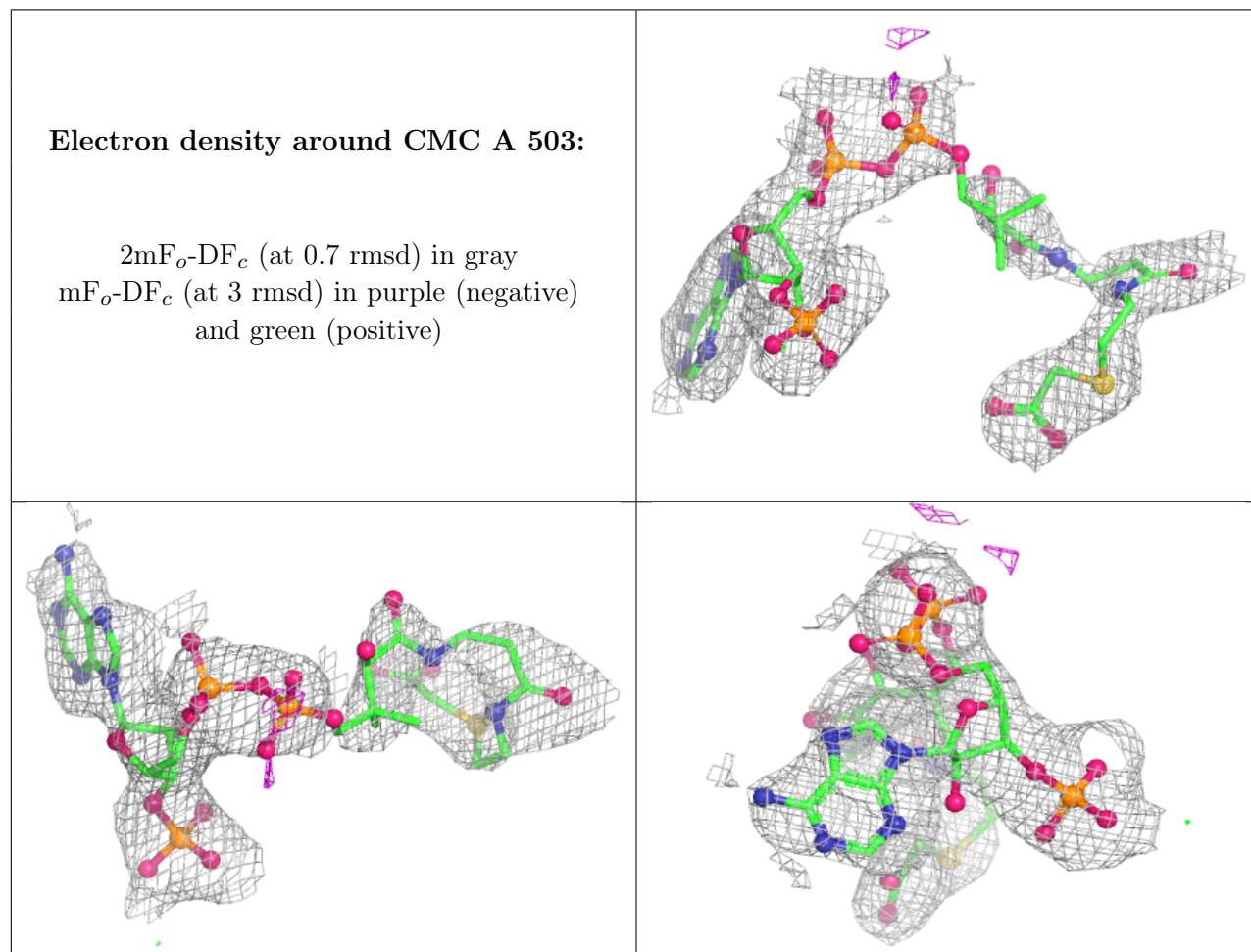
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

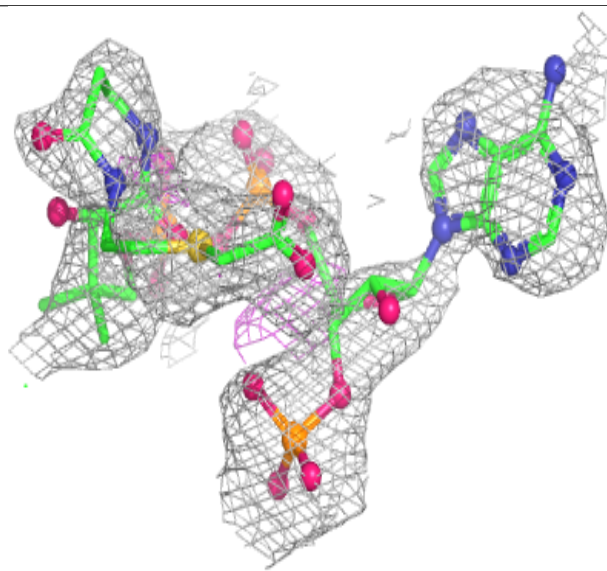
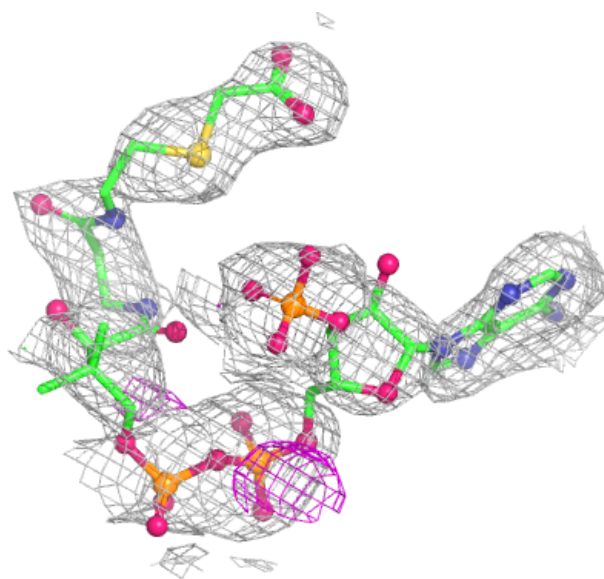
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	502	5/5	0.99	0.04	80,80,81,81	0
2	SO4	B	2002	5/5	0.99	0.03	63,63,64,64	0
3	CMC	A	503	52/52	0.99	0.04	69,74,78,78	0
3	CMC	B	2003	52/52	0.99	0.05	67,73,76,77	0
2	SO4	B	2001	5/5	1.00	0.03	43,43,43,44	0
2	SO4	A	501	5/5	1.00	0.03	53,53,54,54	0

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)



6.5 Other polymers [i](#)

There are no such residues in this entry.