WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 08:18 PM EDT

PDB ID	:	1IXE
Title	:	Crystal structure of citrate synthase from Thermus thermophilus HB8
Authors	:	Murakami, M.; Kanamori, E.; Kawaguchi, S.; Kuramitsu, S.; Kouyama, T.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-06-20
Resolution	:	2.30 Å(reported)

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

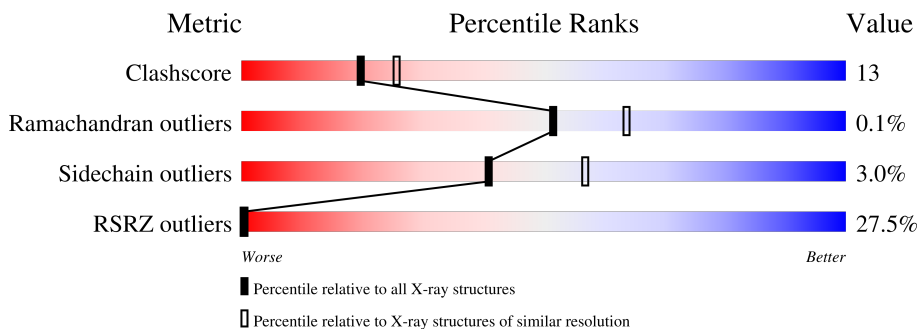|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1   Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		3.0%
RSRZ outliers		27.5%

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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	377	26% / 72% 25% ··
1	B	377	22% / 72% 24% ··
1	C	377	34% / 69% 26% ·
1	D	377	25% / 69% 26% ··

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

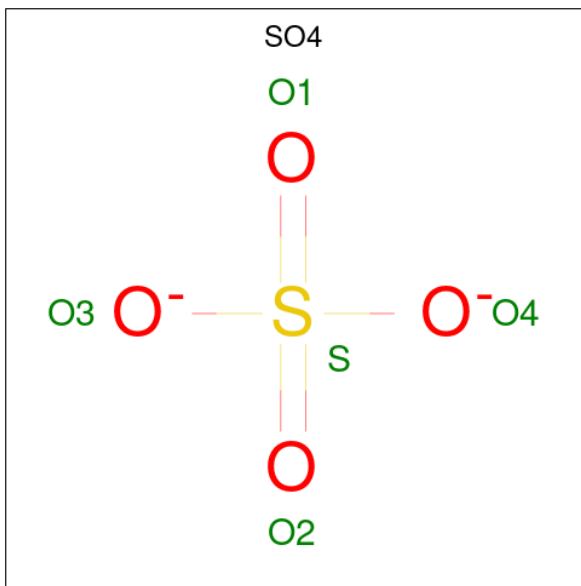| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	390	-	-	-	X
3	COA	D	404	-	-	-	X
4	CIT	D	408	-	X	X	-
5	GOL	C	413	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 12452 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	371	Total	C	N	O	S	0	0	0
			2920	1870	508	532	10			
1	B	370	Total	C	N	O	S	0	0	0
			2922	1871	507	534	10			
1	C	366	Total	C	N	O	S	0	0	0
			2887	1851	499	527	10			
1	D	366	Total	C	N	O	S	0	0	0
			2888	1851	501	526	10			

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

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		

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
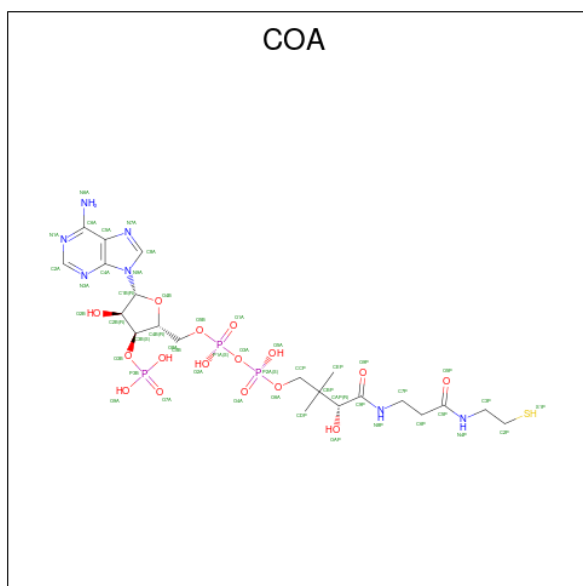
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
3	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
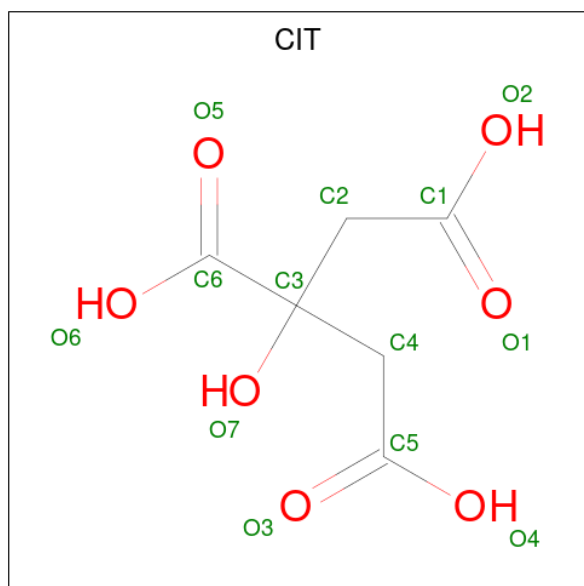
CIT

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0
4	B	1	Total 13	C 6	O 7	0	0
4	C	1	Total 13	C 6	O 7	0	0
4	D	1	Total 13	C 6	O 7	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total 125	O 125	0	0
6	B	138	Total 138	O 138	0	0
6	C	120	Total 120	O 120	0	0
6	D	134	Total 134	O 134	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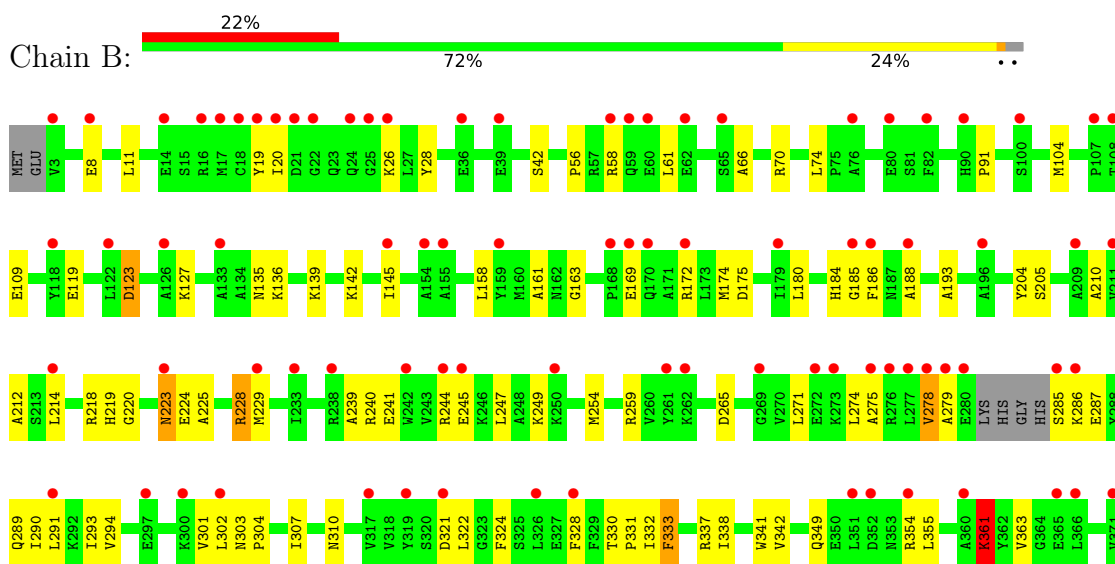 graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates 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.
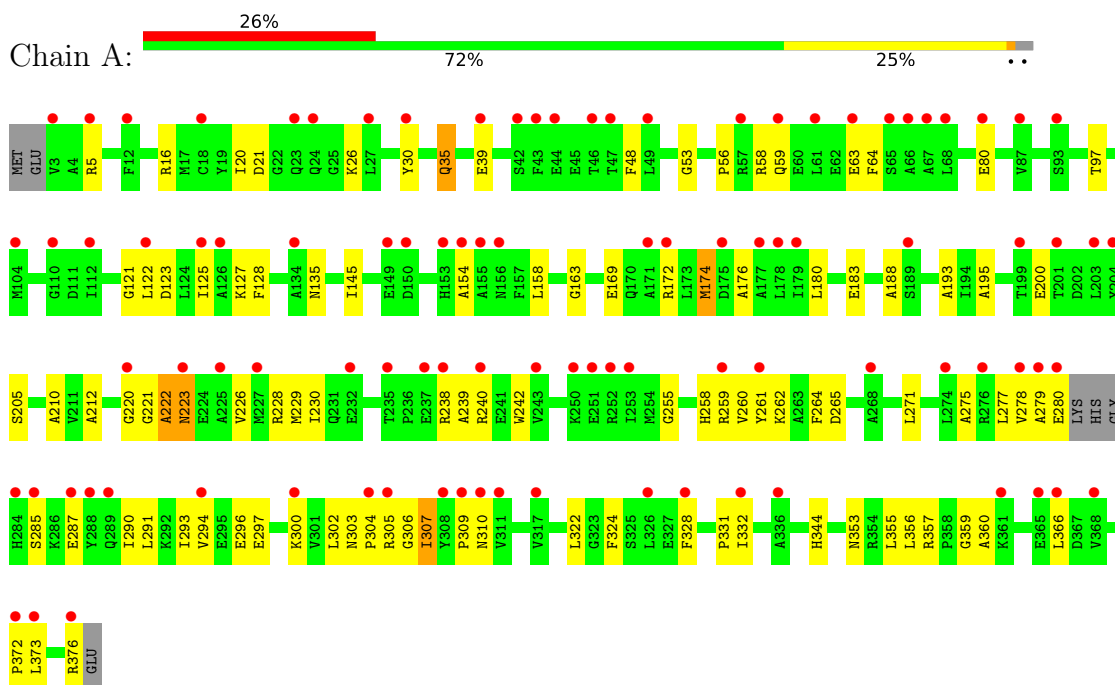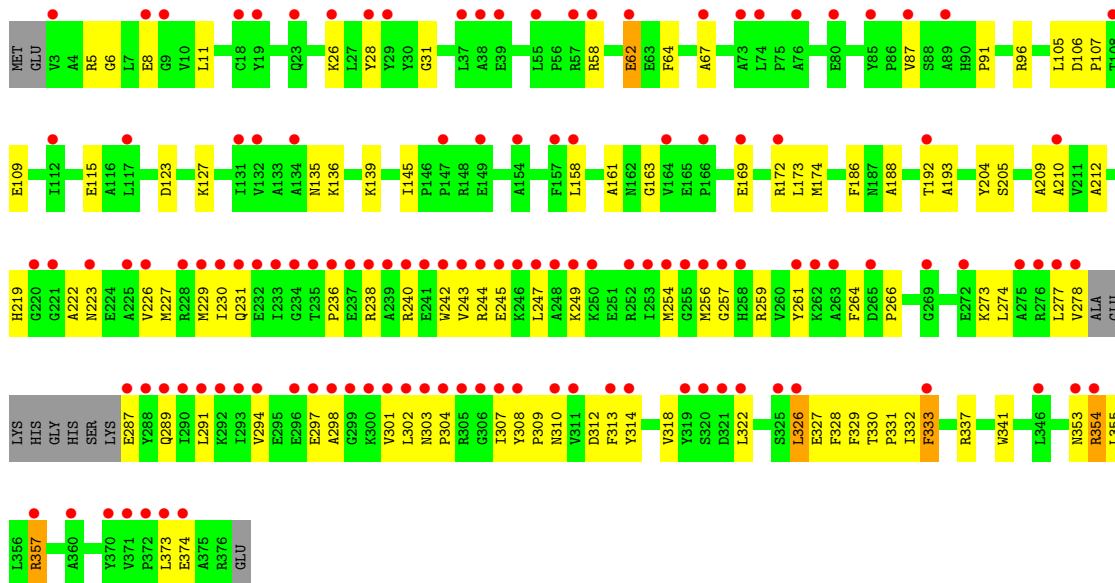
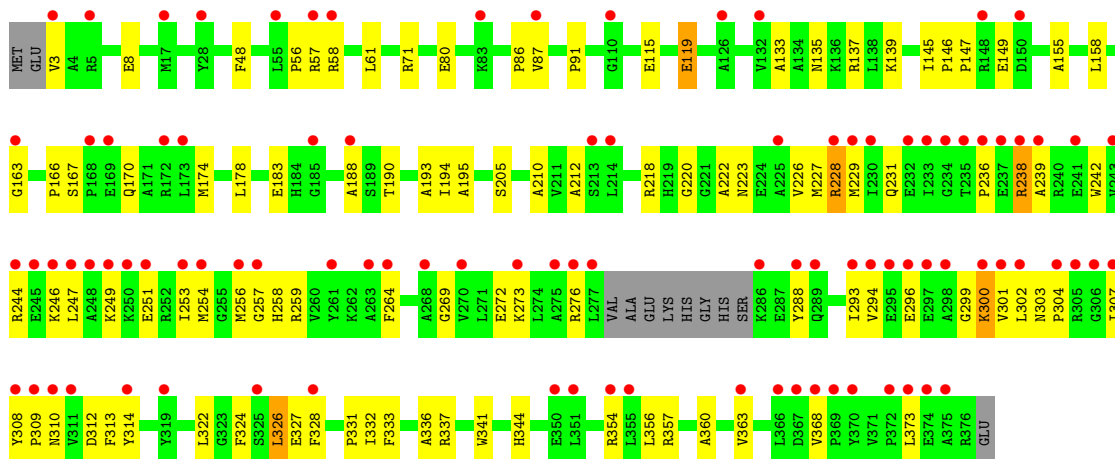• Molecule 1: citrate synthase

• Molecule 1: citrate synthase

E374 A375 R376 GLU

• Molecule 1: citrate synthase

Chain C:

34%

69% 26%

• Molecule 1: citrate synthase

Chain D:

25%

69% 26%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.01Å 110.63Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.79 – 2.30 14.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (14.79-2.30) 90.7 (14.79-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.217 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.6	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12452	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: GOL, COA, SO4, CIT

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	0.33	0/2986	0.47	0/4036
1	B	0.37	0/2987	0.51	0/4035
1	C	0.34	0/2952	0.48	0/3990
1	D	0.41	0/2953	0.54	0/3990
All	All	0.36	0/11878	0.50	0/16051

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	LYS	Mainchain

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	2920	0	2911	81	0
1	B	2922	0	2924	76	0
1	C	2887	0	2884	87	0
1	D	2888	0	2888	89	0
2	A	10	0	0	0	0
2	B	15	0	0	2	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	1	0
3	C	48	0	32	1	0
3	D	48	0	32	11	0
4	A	13	0	5	1	0
4	B	13	0	5	1	0
4	C	13	0	5	0	0
4	D	13	0	5	6	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	125	0	0	1	0
6	B	138	0	0	6	0
6	C	120	0	0	1	0
6	D	134	0	0	3	0
All	All	12452	0	11787	302	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 13.

All (302) 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)
3:D:404:COA:H21	4:D:408:CIT:O4	1.53	1.06
3:D:404:COA:H21	4:D:408:CIT:C5	1.94	0.97
1:A:35:GLN:H	1:A:35:GLN:HE21	1.16	0.88
1:A:35:GLN:H	1:A:35:GLN:NE2	1.73	0.87
3:D:404:COA:C2P	4:D:408:CIT:O4	2.26	0.83
1:C:236:PRO:HG3	1:C:289:GLN:NE2	1.92	0.83
1:C:229:MET:HE1	1:C:254:MET:N	1.93	0.82
1:B:169:GLU:HG3	1:B:172:ARG:HH22	1.45	0.81
1:C:236:PRO:HG3	1:C:289:GLN:HE21	1.46	0.81
1:C:229:MET:HE1	1:C:254:MET:H	1.45	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:HD13	1:B:301:VAL:HG21	1.64	0.78
1:B:169:GLU:HG3	1:B:172:ARG:NH2	2.00	0.76
1:A:20:ILE:HG21	1:A:260:VAL:HG21	1.67	0.76
1:C:355:LEU:HD23	3:D:404:COA:H132	1.68	0.75
1:D:246:LYS:HE2	1:D:251:GLU:HB2	1.71	0.72
1:B:123:ASP:O	1:B:127:LYS:HG3	1.88	0.72
1:B:274:LEU:O	1:B:278:VAL:HG12	1.92	0.70
1:C:245:GLU:O	1:C:249:LYS:HD3	1.91	0.70
1:C:169:GLU:HG3	1:C:172:ARG:NH1	2.07	0.70
1:D:229:MET:HE1	1:D:254:MET:N	2.08	0.69
1:C:58:ARG:HA	1:D:373:LEU:HD11	1.74	0.68
1:A:200:GLU:HG3	1:B:218:ARG:HG3	1.76	0.67
1:C:357:ARG:HB3	1:D:259:ARG:HG2	1.75	0.67
1:B:142:LYS:HE3	6:B:896:HOH:O	1.94	0.67
1:C:205:SER:HB3	1:D:212:ALA:HB1	1.76	0.67
1:C:169:GLU:HG3	1:C:172:ARG:HH12	1.58	0.66
1:A:258:HIS:CE1	1:A:260:VAL:HG22	2.30	0.66
1:D:310:ASN:ND2	3:D:404:COA:H31	2.11	0.66
1:C:328:PHE:C	1:C:331:PRO:HD2	2.16	0.65
1:A:58:ARG:HH22	1:B:374:GLU:HA	1.62	0.65
1:B:193:ALA:HB2	1:B:210:ALA:HB2	1.79	0.65
1:B:229:MET:HE1	1:B:254:MET:H	1.62	0.64
1:A:222:ALA:HB2	3:A:401:COA:H31	1.79	0.64
1:C:354:ARG:HH11	1:C:354:ARG:HB2	1.63	0.64
1:D:149:GLU:HG3	6:D:589:HOH:O	1.97	0.64
1:D:324:PHE:CG	1:D:332:ILE:HD11	2.33	0.63
3:D:404:COA:C3P	4:D:408:CIT:O4	2.46	0.63
3:B:402:COA:H21	6:B:601:HOH:O	1.99	0.63
1:C:26:LYS:HE2	1:C:28:TYR:OH	1.99	0.63
1:D:363:VAL:HG12	1:D:363:VAL:O	1.98	0.63
1:A:5:ARG:NE	1:B:354:ARG:HH11	1.96	0.62
1:B:285:SER:O	1:B:289:GLN:HG3	2.00	0.62
1:D:8:GLU:HG3	1:D:259:ARG:HD2	1.80	0.62
1:A:174:MET:HG2	1:A:322:LEU:HD13	1.82	0.62
1:D:174:MET:HE2	1:D:322:LEU:HD13	1.82	0.62
3:D:404:COA:H22	6:D:801:HOH:O	2.00	0.62
1:D:294:VAL:HG23	1:D:313:PHE:HZ	1.64	0.61
1:B:302:LEU:HB3	1:B:307:ILE:HB	1.82	0.61
1:A:35:GLN:HE21	1:A:35:GLN:N	1.93	0.61
1:A:328:PHE:C	1:A:331:PRO:HD2	2.21	0.60
1:B:328:PHE:C	1:B:331:PRO:HD2	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:O	1:A:300:LYS:HG2	2.00	0.60
1:D:222:ALA:O	1:D:226:VAL:HG23	2.02	0.60
1:A:324:PHE:CG	1:A:332:ILE:HD11	2.37	0.60
1:D:167:SER:OG	1:D:170:GLN:HG3	2.02	0.60
1:C:259:ARG:HG2	1:D:357:ARG:HB3	1.83	0.59
1:B:158:LEU:HD21	1:B:174:MET:HE2	1.83	0.59
1:D:246:LYS:HE2	1:D:251:GLU:CB	2.31	0.59
1:B:241:GLU:HG2	6:B:696:HOH:O	2.03	0.58
1:B:278:VAL:HG21	1:B:321:ASP:HB2	1.86	0.58
1:D:228:ARG:HB3	1:D:228:ARG:NH2	2.18	0.58
1:A:212:ALA:HB1	1:B:205:SER:HB3	1.86	0.57
1:A:145:ILE:CD1	1:A:163:GLY:HA2	2.33	0.57
1:B:66:ALA:O	1:B:70:ARG:HG3	2.04	0.57
1:C:5:ARG:HG2	1:D:354:ARG:HD3	1.86	0.57
1:B:275:ALA:O	1:B:278:VAL:HG13	2.04	0.57
1:B:245:GLU:O	1:B:249:LYS:HG2	2.05	0.57
1:B:337:ARG:HG3	1:B:341:TRP:CE2	2.40	0.57
1:D:308:TYR:HB3	1:D:309:PRO:HD2	1.87	0.57
1:A:303:ASN:N	1:A:304:PRO:HD2	2.20	0.56
1:D:229:MET:HE1	1:D:254:MET:H	1.69	0.56
1:C:226:VAL:O	1:C:229:MET:HB3	2.05	0.56
1:B:42:SER:HA	1:B:175:ASP:OD2	2.05	0.56
1:A:372:PRO:O	1:A:376:ARG:HG3	2.06	0.56
1:B:109:GLU:HG3	1:B:204:TYR:CD1	2.41	0.56
1:C:212:ALA:HB1	1:D:205:SER:HB3	1.88	0.56
1:D:190:THR:O	1:D:194:ILE:HG12	2.05	0.56
1:D:56:PRO:HG3	1:D:61:LEU:HD13	1.88	0.56
1:D:326:LEU:HD13	1:D:327:GLU:H	1.70	0.56
1:B:8:GLU:HG3	1:B:259:ARG:HD2	1.86	0.56
1:B:225:ALA:HB1	1:B:254:MET:HG3	1.87	0.56
1:D:299:GLY:O	1:D:303:ASN:HB2	2.06	0.55
1:B:229:MET:HE1	1:B:254:MET:N	2.21	0.55
1:D:276:ARG:HG3	1:D:288:TYR:CZ	2.42	0.55
1:A:302:LEU:O	1:A:307:ILE:HG23	2.06	0.55
1:C:373:LEU:HD23	1:D:58:ARG:HH11	1.72	0.55
1:A:275:ALA:O	1:A:278:VAL:HG22	2.06	0.55
1:D:91:PRO:HB2	1:D:331:PRO:HG2	1.88	0.55
1:C:222:ALA:HB3	1:C:312:ASP:OD1	2.06	0.54
1:D:247:LEU:HD13	1:D:301:VAL:HG11	1.88	0.54
1:A:305:ARG:HG2	1:A:305:ARG:HH21	1.71	0.54
1:D:220:GLY:O	1:D:223:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ALA:HB2	1:D:210:ALA:HB2	1.89	0.54
1:B:174:MET:HE2	1:B:322:LEU:HD13	1.90	0.54
1:C:226:VAL:O	1:C:230:ILE:HG13	2.07	0.54
1:C:11:LEU:O	1:D:3:VAL:HB	2.08	0.53
1:D:87:VAL:HG23	1:D:139:LYS:HA	1.90	0.53
1:A:183:GLU:OE1	1:A:344:HIS:NE2	2.35	0.53
1:A:353:ASN:ND2	1:B:218:ARG:HH12	2.06	0.53
1:D:183:GLU:OE1	1:D:344:HIS:NE2	2.36	0.53
1:A:264:PHE:CE2	1:A:309:PRO:HG2	2.43	0.53
1:D:326:LEU:HD13	1:D:327:GLU:N	2.23	0.53
1:C:173:LEU:HD11	1:C:318:VAL:HG13	1.91	0.53
1:A:324:PHE:CD1	1:A:332:ILE:HD11	2.44	0.53
1:C:223:ASN:HD21	1:C:333:PHE:HD2	1.56	0.53
1:C:223:ASN:HD22	1:C:330:THR:HA	1.73	0.53
1:C:257:GLY:N	1:C:307:ILE:HG23	2.24	0.53
1:D:87:VAL:CG2	1:D:139:LYS:HA	2.39	0.52
1:C:87:VAL:CG2	1:C:139:LYS:HA	2.39	0.52
1:D:158:LEU:HD21	1:D:174:MET:HE2	1.92	0.52
3:D:404:COA:H32	4:D:408:CIT:O4	2.08	0.52
1:D:229:MET:CE	1:D:254:MET:H	2.22	0.52
1:B:290:ILE:O	1:B:294:VAL:HG23	2.08	0.52
1:B:324:PHE:CG	1:B:332:ILE:HD11	2.45	0.52
1:A:226:VAL:O	1:A:230:ILE:HG13	2.10	0.52
1:C:337:ARG:HG3	1:C:341:TRP:CE2	2.45	0.52
1:B:214:LEU:HA	1:B:219:HIS:CD2	2.45	0.51
1:C:115:GLU:CD	1:C:115:GLU:H	2.14	0.51
1:C:193:ALA:HB2	1:C:210:ALA:HB2	1.93	0.51
1:C:8:GLU:OE1	1:D:354:ARG:NH2	2.42	0.51
1:C:303:ASN:N	1:C:304:PRO:HD2	2.25	0.51
1:A:205:SER:HB3	1:B:212:ALA:HB1	1.92	0.51
1:C:374:GLU:CD	1:C:374:GLU:H	2.14	0.51
1:B:145:ILE:CD1	1:B:163:GLY:HA2	2.41	0.51
1:A:35:GLN:O	1:A:39:GLU:HG3	2.11	0.50
1:D:303:ASN:N	1:D:304:PRO:HD2	2.25	0.50
1:C:109:GLU:HG3	1:C:204:TYR:CD1	2.46	0.50
1:C:247:LEU:HD13	1:C:301:VAL:HG11	1.93	0.50
1:C:326:LEU:HD23	1:C:327:GLU:N	2.26	0.50
1:A:265:ASP:HB2	1:A:310:ASN:HA	1.92	0.50
1:C:145:ILE:CD1	1:C:163:GLY:HA2	2.41	0.50
1:D:145:ILE:CD1	1:D:163:GLY:HA2	2.41	0.50
1:C:123:ASP:O	1:C:127:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLU:O	1:D:300:LYS:HD2	2.12	0.50
1:C:256:MET:HB3	1:C:307:ILE:CG2	2.42	0.50
3:D:404:COA:C2P	4:D:408:CIT:C5	2.81	0.50
1:A:20:ILE:HD12	2:B:382:SO4:O3	2.11	0.49
1:A:305:ARG:HH11	3:A:401:COA:H4B	1.77	0.49
1:C:136:LYS:HD3	1:C:161:ALA:HB1	1.94	0.49
1:A:80:GLU:OE2	1:D:80:GLU:OE1	2.30	0.49
1:A:240:ARG:NH2	1:A:296:GLU:OE2	2.46	0.49
1:A:359:GLY:O	1:B:11:LEU:HA	2.11	0.49
1:C:291:LEU:HD21	1:C:313:PHE:O	2.12	0.49
1:B:303:ASN:N	1:B:304:PRO:HD2	2.28	0.49
1:C:222:ALA:O	1:C:226:VAL:HG23	2.12	0.49
1:C:326:LEU:HD23	1:C:327:GLU:H	1.76	0.49
1:C:223:ASN:HB3	1:C:329:PHE:HB3	1.94	0.49
1:D:227:MET:O	1:D:231:GLN:HG3	2.13	0.48
1:D:302:LEU:HB3	1:D:307:ILE:HB	1.95	0.48
1:A:169:GLU:HG3	1:A:172:ARG:HH12	1.77	0.48
1:B:286:LYS:O	1:B:290:ILE:HG13	2.13	0.48
1:A:5:ARG:HB3	1:B:354:ARG:NE	2.28	0.48
1:A:5:ARG:HB3	1:B:354:ARG:HE	1.79	0.48
1:B:136:LYS:HE2	6:B:719:HOH:O	2.14	0.48
1:C:91:PRO:HB2	1:C:331:PRO:HG2	1.95	0.48
1:C:96:ARG:NH1	1:D:205:SER:OG	2.44	0.48
1:D:269:GLY:O	1:D:273:LYS:HG3	2.14	0.48
1:C:294:VAL:O	1:C:298:ALA:HB3	2.14	0.48
1:A:357:ARG:HB3	1:B:259:ARG:HG2	1.96	0.47
1:C:291:LEU:HD23	1:C:314:TYR:CD1	2.49	0.47
1:D:337:ARG:HG3	1:D:341:TRP:CE2	2.49	0.47
1:A:59:GLN:O	1:A:63:GLU:HG3	2.15	0.47
1:B:328:PHE:O	1:B:332:ILE:HG13	2.14	0.47
1:D:300:LYS:CA	1:D:300:LYS:HE3	2.45	0.47
1:A:373:LEU:HD11	1:B:58:ARG:HA	1.96	0.47
1:B:180:LEU:HD13	1:B:271:LEU:HG	1.97	0.47
1:B:240:ARG:O	1:B:244:ARG:HG2	2.15	0.47
1:B:275:ALA:HA	1:B:278:VAL:CG1	2.45	0.46
1:C:373:LEU:HD23	1:D:58:ARG:NH1	2.29	0.46
1:D:239:ALA:HB3	1:D:293:ILE:HG13	1.97	0.46
1:C:243:VAL:HG21	1:C:297:GLU:CB	2.45	0.46
1:C:353:ASN:ND2	1:D:218:ARG:HH12	2.13	0.46
1:D:228:ARG:HB3	1:D:228:ARG:CZ	2.45	0.46
1:B:26:LYS:HD3	1:B:28:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:VAL:HG23	1:C:313:PHE:HZ	1.79	0.46
1:C:302:LEU:HD13	1:C:307:ILE:HG21	1.97	0.46
1:A:221:GLY:O	1:A:223:ASN:N	2.48	0.46
1:A:302:LEU:HD13	1:A:307:ILE:CD1	2.46	0.46
1:B:279:ALA:O	1:B:285:SER:HB3	2.15	0.46
1:C:355:LEU:HD11	1:D:188:ALA:HB2	1.98	0.46
1:C:240:ARG:HA	1:C:297:GLU:HG3	1.97	0.46
1:A:21:ASP:HB3	1:A:26:LYS:HB2	1.98	0.46
1:A:258:HIS:ND1	1:A:260:VAL:HG22	2.30	0.46
1:C:328:PHE:O	1:C:332:ILE:HG13	2.16	0.46
1:D:195:ALA:HA	1:D:356:LEU:HD12	1.98	0.46
1:C:210:ALA:HB1	1:C:341:TRP:CE2	2.51	0.46
1:D:71:ARG:HH21	1:D:119:GLU:CD	2.19	0.46
1:A:279:ALA:O	1:A:285:SER:OG	2.25	0.46
1:A:290:ILE:O	1:A:294:VAL:HG23	2.16	0.46
1:D:328:PHE:C	1:D:331:PRO:HD2	2.37	0.46
1:B:136:LYS:HA	1:B:328:PHE:CZ	2.51	0.45
1:B:224:GLU:OE1	1:B:228:ARG:NH1	2.49	0.45
1:C:174:MET:HE2	1:C:322:LEU:HD13	1.98	0.45
1:A:64:PHE:CE1	1:A:122:LEU:HD21	2.52	0.45
1:A:366:LEU:HD21	1:B:19:TYR:CG	2.52	0.45
1:A:220:GLY:H	4:A:405:CIT:C5	2.29	0.45
1:B:265:ASP:HB2	1:B:310:ASN:HA	1.98	0.45
1:A:277:LEU:O	1:A:280:GLU:HG2	2.16	0.45
1:A:58:ARG:NH2	1:B:374:GLU:HA	2.29	0.45
1:B:136:LYS:HD3	1:B:161:ALA:HB1	1.99	0.45
1:C:227:MET:O	1:C:231:GLN:HG3	2.16	0.45
1:A:58:ARG:NH2	1:A:58:ARG:HB2	2.31	0.45
1:B:330:THR:O	1:B:333:PHE:HB3	2.17	0.45
1:C:354:ARG:HB2	1:C:354:ARG:NH1	2.29	0.45
1:B:91:PRO:HB2	1:B:331:PRO:HG2	1.99	0.44
1:B:219:HIS:CE1	4:B:406:CIT:H41	2.52	0.44
1:D:294:VAL:HG23	1:D:313:PHE:CZ	2.50	0.44
1:A:188:ALA:HB2	1:B:355:LEU:HD11	1.98	0.44
1:A:193:ALA:HB2	1:A:210:ALA:HB2	1.99	0.44
1:A:355:LEU:HD11	1:B:188:ALA:HB2	2.00	0.44
1:B:56:PRO:HG3	1:B:61:LEU:HD13	1.99	0.44
1:C:264:PHE:CE1	1:C:309:PRO:HG2	2.52	0.44
1:A:200:GLU:HG2	6:A:820:HOH:O	2.17	0.44
1:C:31:GLY:HA3	1:D:368:VAL:HG23	1.99	0.44
1:D:236:PRO:O	1:D:293:ILE:HD11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:TRP:CH2	1:D:246:LYS:HD2	2.53	0.44
1:C:62:GLU:OE1	1:C:62:GLU:HA	2.17	0.44
1:A:123:ASP:CG	1:A:127:LYS:HE2	2.38	0.43
1:B:74:LEU:HD23	1:B:127:LYS:HD3	2.00	0.43
1:D:249:LYS:HG3	1:D:251:GLU:HG2	2.00	0.43
1:D:300:LYS:HE3	1:D:300:LYS:N	2.33	0.43
1:C:238:ARG:O	1:C:242:TRP:HB2	2.18	0.43
1:B:338:ILE:O	1:B:342:VAL:HG23	2.17	0.43
1:C:58:ARG:HD3	1:D:373:LEU:HD21	2.01	0.43
1:C:307:ILE:N	1:C:307:ILE:HD12	2.33	0.43
1:A:302:LEU:HD13	1:A:307:ILE:HD11	1.99	0.43
1:B:220:GLY:O	1:B:223:ASN:HB2	2.18	0.43
1:A:123:ASP:O	1:A:127:LYS:HG3	2.19	0.43
1:A:305:ARG:HG2	1:A:305:ARG:NH2	2.33	0.43
1:C:308:TYR:HB3	1:C:309:PRO:HD2	2.00	0.43
1:C:6:GLY:HA2	1:D:356:LEU:HD23	1.99	0.43
1:A:121:GLY:O	1:A:125:ILE:HG13	2.19	0.43
1:C:158:LEU:HD21	1:C:174:MET:HE2	2.00	0.43
1:D:272:GLU:HG2	1:D:314:TYR:CZ	2.54	0.43
1:A:260:VAL:HG23	1:A:261:TYR:N	2.33	0.42
1:D:155:ALA:HA	1:D:166:PRO:HG3	2.01	0.42
1:C:273:LYS:O	1:C:277:LEU:HG	2.18	0.42
1:D:229:MET:HE2	1:D:242:TRP:HH2	1.84	0.42
1:D:300:LYS:HE3	1:D:300:LYS:HA	1.99	0.42
1:A:20:ILE:HG21	1:A:260:VAL:CG2	2.44	0.42
1:A:195:ALA:HA	1:A:356:LEU:HD12	2.01	0.42
1:A:287:GLU:H	1:A:287:GLU:HG2	1.69	0.42
1:A:158:LEU:HD21	1:A:174:MET:HG2	2.01	0.42
1:A:176:ALA:O	1:A:180:LEU:HG	2.19	0.42
1:D:178:LEU:O	1:D:336:ALA:HB1	2.20	0.42
1:A:30:TYR:CD1	1:A:53:GLY:HA2	2.55	0.42
1:C:186:PHE:CE2	1:D:360:ALA:HB2	2.55	0.42
1:C:302:LEU:HB3	1:C:307:ILE:HB	2.02	0.42
1:A:48:PHE:CG	1:A:56:PRO:HB3	2.54	0.42
1:B:239:ALA:HB3	1:B:293:ILE:HG21	2.02	0.42
1:B:361:LYS:HD3	1:B:361:LYS:C	2.40	0.42
1:C:355:LEU:CD2	3:D:404:COA:H132	2.45	0.42
1:D:210:ALA:HB1	1:D:341:TRP:CE2	2.55	0.42
1:A:262:LYS:HA	1:A:306:GLY:O	2.19	0.42
1:B:349:GLN:HG3	6:B:683:HOH:O	2.19	0.42
1:A:154:ALA:HB1	1:A:174:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:HE2	6:B:451:HOH:O	2.20	0.42
1:D:236:PRO:C	1:D:238:ARG:H	2.23	0.42
1:D:276:ARG:HG3	1:D:288:TYR:CE1	2.54	0.42
1:C:192:THR:HG22	1:C:209:ALA:HB1	2.02	0.41
1:D:48:PHE:CD1	1:D:48:PHE:C	2.93	0.41
1:C:249:LYS:HD2	1:C:249:LYS:N	2.35	0.41
1:C:274:LEU:O	1:C:278:VAL:HG23	2.20	0.41
1:C:310:ASN:ND2	3:C:403:COA:H31	2.35	0.41
1:D:115:GLU:H	1:D:115:GLU:CD	2.23	0.41
1:D:258:HIS:HA	3:D:404:COA:S1P	2.61	0.41
1:B:123:ASP:OD1	1:B:127:LYS:HE2	2.20	0.41
1:A:229:MET:HG3	1:A:242:TRP:CH2	2.55	0.41
1:D:139:LYS:HE2	6:D:662:HOH:O	2.21	0.41
1:D:246:LYS:HG2	1:D:253:ILE:HG12	2.01	0.41
1:D:324:PHE:CD2	1:D:332:ILE:HD11	2.56	0.41
1:C:91:PRO:HG3	1:C:139:LYS:HE3	2.01	0.41
1:D:174:MET:CE	1:D:322:LEU:HD13	2.50	0.41
1:D:257:GLY:CA	1:D:307:ILE:HG23	2.50	0.41
1:A:35:GLN:NE2	1:A:35:GLN:N	2.54	0.41
1:A:16:ARG:HG2	1:B:363:VAL:HG23	2.03	0.41
1:B:20:ILE:HD13	1:B:184:HIS:CE1	2.55	0.41
1:B:286:LYS:H	1:B:286:LYS:HD2	1.84	0.41
1:C:87:VAL:HG22	1:C:139:LYS:HA	2.02	0.41
1:C:106:ASP:HA	1:C:107:PRO:HD2	1.93	0.41
1:D:146:PRO:HA	1:D:147:PRO:HD3	1.91	0.41
1:D:264:PHE:CE1	1:D:309:PRO:HG2	2.56	0.41
1:A:5:ARG:HG3	1:B:354:ARG:NH1	2.35	0.41
1:A:48:PHE:CD1	1:A:56:PRO:HB3	2.56	0.41
1:A:360:ALA:HB2	1:B:186:PHE:CE2	2.56	0.41
1:B:185:GLY:HA3	2:B:383:SO4:O3	2.20	0.41
1:C:136:LYS:HA	1:C:328:PHE:CZ	2.56	0.41
1:C:261:TYR:CZ	1:C:266:PRO:HD2	2.55	0.41
1:C:287:GLU:N	6:C:572:HOH:O	2.53	0.41
1:D:226:VAL:HG21	1:D:312:ASP:O	2.21	0.41
1:C:105:LEU:HD23	1:D:86:PRO:HG2	2.02	0.41
1:C:64:PHE:O	1:C:67:ALA:HB3	2.21	0.40
1:D:256:MET:HG2	1:D:309:PRO:HA	2.03	0.40
1:A:97:THR:HG21	1:B:104:MET:CE	2.51	0.40
1:A:180:LEU:HD13	1:A:271:LEU:HG	2.02	0.40
1:C:188:ALA:HB3	1:C:219:HIS:CD2	2.56	0.40
1:C:243:VAL:HG21	1:C:297:GLU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HG21	1:B:104:MET:HE2	2.03	0.40
1:A:255:GLY:O	1:A:309:PRO:HA	2.21	0.40
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.90	0.40
1:A:239:ALA:HB3	1:A:293:ILE:HG21	2.04	0.40
1:D:133:ALA:O	1:D:137:ARG:HG2	2.21	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	367/377 (97%)	356 (97%)	10 (3%)	1 (0%)	41	50
1	B	366/377 (97%)	356 (97%)	10 (3%)	0	100	100
1	C	362/377 (96%)	349 (96%)	13 (4%)	0	100	100
1	D	362/377 (96%)	350 (97%)	12 (3%)	0	100	100
All	All	1457/1508 (97%)	1411 (97%)	45 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ALA

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	298/307 (97%)	288 (97%)	10 (3%)	37	51
1	B	300/307 (98%)	290 (97%)	10 (3%)	38	53
1	C	296/307 (96%)	289 (98%)	7 (2%)	49	66
1	D	296/307 (96%)	287 (97%)	9 (3%)	41	57
All	All	1190/1228 (97%)	1154 (97%)	36 (3%)	41	57

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	128	PHE
1	A	135	ASN
1	A	174	MET
1	A	223	ASN
1	A	228	ARG
1	A	238	ARG
1	A	259	ARG
1	A	291	LEU
1	A	307	ILE
1	B	119	GLU
1	B	123	ASP
1	B	135	ASN
1	B	223	ASN
1	B	228	ARG
1	B	278	VAL
1	B	287	GLU
1	B	291	LEU
1	B	333	PHE
1	B	361	LYS
1	C	62	GLU
1	C	135	ASN
1	C	244	ARG
1	C	326	LEU
1	C	333	PHE
1	C	354	ARG
1	C	357	ARG
1	D	57	ARG
1	D	119	GLU
1	D	135	ASN
1	D	228	ARG
1	D	238	ARG
1	D	244	ARG

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Mol	Chain	Res	Type
1	D	300	LYS
1	D	326	LEU
1	D	333	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	59	GLN
1	A	162	ASN
1	A	170	GLN
1	A	223	ASN
1	A	231	GLN
1	B	23	GLN
1	B	289	GLN
1	C	23	GLN
1	C	289	GLN
1	D	353	ASN

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 ⓘ

22 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	B	382	-	4,4,4	0.25	0	6,6,6	0.10	0
3	COA	C	403	-	41,50,50	1.89	10 (24%)	52,75,75	1.68	10 (19%)
3	COA	A	401	-	41,50,50	1.89	9 (21%)	52,75,75	1.66	10 (19%)
2	SO4	A	391	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	387	-	4,4,4	0.24	0	6,6,6	0.10	0
5	GOL	B	412	-	5,5,5	0.81	0	5,5,5	0.30	0
2	SO4	B	385	-	4,4,4	0.28	0	6,6,6	0.09	0
4	CIT	B	406	-	12,12,12	1.58	2 (16%)	17,17,17	3.27	6 (35%)
5	GOL	C	413	-	5,5,5	0.88	0	5,5,5	0.59	0
2	SO4	B	383	-	4,4,4	0.28	0	6,6,6	0.07	0
4	CIT	D	408	-	12,12,12	1.93	2 (16%)	17,17,17	2.74	7 (41%)
2	SO4	C	390	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	C	388	-	4,4,4	0.26	0	6,6,6	0.10	0
5	GOL	D	414	-	5,5,5	0.73	0	5,5,5	0.20	0
2	SO4	D	386	-	4,4,4	0.27	0	6,6,6	0.14	0
4	CIT	C	407	-	12,12,12	1.76	2 (16%)	17,17,17	3.23	7 (41%)
2	SO4	D	389	-	4,4,4	0.25	0	6,6,6	0.10	0
4	CIT	A	405	-	12,12,12	2.02	3 (25%)	17,17,17	3.01	8 (47%)
3	COA	B	402	-	41,50,50	1.83	11 (26%)	52,75,75	1.60	10 (19%)
2	SO4	C	381	-	4,4,4	0.19	0	6,6,6	0.12	0
5	GOL	A	411	-	5,5,5	0.80	0	5,5,5	0.20	0
3	COA	D	404	-	41,50,50	2.32	13 (31%)	52,75,75	1.82	14 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	D	408	-	-	9/16/16/16	-
4	CIT	C	407	-	-	6/16/16/16	-
5	GOL	B	412	-	-	0/4/4/4	-
3	COA	C	403	-	-	2/44/64/64	0/3/3/3
5	GOL	C	413	-	-	0/4/4/4	-
4	CIT	A	405	-	-	4/16/16/16	-
3	COA	B	402	-	-	9/44/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	B	406	-	-	2/16/16/16	-
5	GOL	D	414	-	-	2/4/4/4	-
3	COA	A	401	-	-	5/44/64/64	0/3/3/3
5	GOL	A	411	-	-	0/4/4/4	-
3	COA	D	404	-	-	17/44/64/64	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	COA	O4B-C1B	6.65	1.50	1.41
3	A	401	COA	P3B-O3B	5.71	1.70	1.59
3	C	403	COA	P3B-O3B	5.52	1.69	1.59
3	D	404	COA	O9P-C9P	5.34	1.34	1.23
4	D	408	CIT	C2-C3	5.09	1.60	1.53
3	B	402	COA	P3B-O3B	5.00	1.68	1.59
4	C	407	CIT	C2-C3	4.85	1.59	1.53
4	A	405	CIT	C2-C3	4.78	1.59	1.53
3	D	404	COA	P3B-O3B	4.64	1.68	1.59
3	C	403	COA	O9P-C9P	4.38	1.32	1.23
3	A	401	COA	O9P-C9P	4.21	1.31	1.23
4	B	406	CIT	C2-C3	4.11	1.58	1.53
3	D	404	COA	C2B-C1B	-3.97	1.47	1.53
3	B	402	COA	O9P-C9P	3.82	1.31	1.23
3	D	404	COA	C3B-C4B	3.67	1.62	1.52
3	D	404	COA	P3B-O7A	3.60	1.62	1.50
3	C	403	COA	C2A-N1A	3.58	1.40	1.33
3	B	402	COA	O4B-C1B	3.45	1.45	1.41
3	B	402	COA	P3B-O7A	3.42	1.61	1.50
3	A	401	COA	C2A-N1A	3.41	1.40	1.33
3	A	401	COA	O4B-C1B	3.39	1.45	1.41
3	B	402	COA	C2A-N1A	3.35	1.40	1.33
4	A	405	CIT	C4-C3	3.35	1.58	1.53
3	A	401	COA	P3B-O7A	3.26	1.61	1.50
3	C	403	COA	P3B-O7A	3.22	1.60	1.50
3	C	403	COA	O4B-C1B	3.13	1.45	1.41
3	C	403	COA	C4A-N3A	2.84	1.39	1.35
3	D	404	COA	P2A-O4A	2.82	1.60	1.50
3	D	404	COA	C2A-N1A	2.80	1.39	1.33
3	D	404	COA	O2B-C2B	2.75	1.49	1.43
3	D	404	COA	C4A-N3A	2.75	1.39	1.35
3	A	401	COA	C2B-C1B	-2.71	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	COA	OAP-CAP	2.68	1.47	1.42
3	D	404	COA	CEP-CBP	2.65	1.59	1.53
3	A	401	COA	O4B-C4B	2.64	1.50	1.45
4	D	408	CIT	C4-C3	2.61	1.57	1.53
4	A	405	CIT	C3-C6	2.45	1.56	1.53
3	C	403	COA	C2B-C1B	-2.44	1.50	1.53
3	D	404	COA	C8A-N7A	-2.37	1.30	1.34
3	B	402	COA	O5P-C5P	2.37	1.28	1.23
3	C	403	COA	O5P-C5P	2.36	1.28	1.23
3	B	402	COA	O4B-C4B	2.31	1.50	1.45
4	C	407	CIT	C4-C3	2.31	1.56	1.53
3	B	402	COA	C2B-C1B	-2.27	1.50	1.53
3	C	403	COA	O4B-C4B	2.26	1.50	1.45
3	A	401	COA	C2A-N3A	2.26	1.35	1.32
3	B	402	COA	C4A-N3A	2.25	1.38	1.35
3	C	403	COA	C2A-N3A	2.25	1.35	1.32
3	B	402	COA	C3P-N4P	2.21	1.51	1.46
3	A	401	COA	O5P-C5P	2.08	1.27	1.23
3	B	402	COA	C2A-N3A	2.08	1.35	1.32
4	B	406	CIT	C4-C3	2.03	1.56	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	CIT	C3-C4-C5	8.15	133.54	113.81
4	B	406	CIT	C3-C4-C5	7.84	132.80	113.81
4	C	407	CIT	C3-C4-C5	7.47	131.91	113.81
4	B	406	CIT	C4-C3-C6	-6.79	95.53	110.11
4	C	407	CIT	C4-C3-C6	-6.11	96.98	110.11
4	D	408	CIT	C4-C3-C6	-5.36	98.59	110.11
4	B	406	CIT	C3-C2-C1	5.10	126.16	113.81
4	D	408	CIT	C3-C4-C5	4.61	124.97	113.81
4	D	408	CIT	C3-C2-C1	4.60	124.96	113.81
4	A	405	CIT	C4-C3-C6	-4.45	100.55	110.11
4	C	407	CIT	C3-C2-C1	4.42	124.51	113.81
3	D	404	COA	CEP-CBP-CAP	4.37	116.40	108.82
3	A	401	COA	O8A-P3B-O3B	-4.26	86.89	105.99
3	C	403	COA	O8A-P3B-O3B	-4.22	87.10	105.99
4	C	407	CIT	O7-C3-C6	-4.15	103.04	108.86
3	B	402	COA	O8A-P3B-O3B	-4.06	87.79	105.99
3	D	404	COA	O8A-P3B-O3B	-3.91	88.46	105.99
3	C	403	COA	P1A-O5B-C5B	3.81	144.05	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	COA	P1A-O5B-C5B	3.81	144.04	121.68
4	C	407	CIT	O6-C6-C3	3.81	119.67	113.05
3	B	402	COA	N3A-C2A-N1A	-3.81	122.73	128.68
4	D	408	CIT	O6-C6-C3	3.80	119.64	113.05
4	A	405	CIT	O6-C6-C3	3.73	119.53	113.05
3	D	404	COA	P1A-O5B-C5B	3.70	143.36	121.68
3	C	403	COA	CEP-CBP-CAP	3.65	115.16	108.82
4	B	406	CIT	O7-C3-C4	3.63	117.91	109.40
3	D	404	COA	C7P-N8P-C9P	-3.63	116.12	122.59
3	D	404	COA	N3A-C2A-N1A	-3.61	123.03	128.68
3	A	401	COA	CEP-CBP-CAP	3.58	115.02	108.82
4	D	408	CIT	O7-C3-C6	-3.55	103.89	108.86
3	B	402	COA	P1A-O5B-C5B	3.52	142.32	121.68
4	A	405	CIT	C3-C2-C1	3.51	122.32	113.81
3	A	401	COA	O3B-C3B-C4B	3.47	122.62	110.08
3	D	404	COA	O3B-C3B-C4B	3.47	122.61	110.08
3	C	403	COA	N3A-C2A-N1A	-3.44	123.30	128.68
3	B	402	COA	CEP-CBP-CAP	3.37	114.67	108.82
3	A	401	COA	O4B-C1B-C2B	-3.34	102.04	106.93
4	C	407	CIT	O7-C3-C4	3.32	117.18	109.40
3	C	403	COA	CDP-CBP-CAP	3.24	114.44	108.82
3	B	402	COA	O3B-C3B-C4B	3.19	121.63	110.08
3	A	401	COA	N3A-C2A-N1A	-3.19	123.69	128.68
3	B	402	COA	CDP-CBP-CAP	3.16	114.30	108.82
3	C	403	COA	O3B-C3B-C4B	3.15	121.46	110.08
3	C	403	COA	O4B-C1B-C2B	-3.14	102.33	106.93
3	A	401	COA	CDP-CBP-CAP	3.12	114.23	108.82
4	B	406	CIT	O6-C6-C3	3.11	118.44	113.05
4	A	405	CIT	O7-C3-C6	-3.09	104.53	108.86
4	D	408	CIT	O7-C3-C4	2.89	116.16	109.40
4	B	406	CIT	O7-C3-C6	-2.87	104.83	108.86
3	D	404	COA	O4B-C1B-C2B	-2.68	103.01	106.93
3	D	404	COA	CDP-CBP-CAP	2.62	113.37	108.82
3	D	404	COA	O2B-C2B-C1B	-2.49	101.65	110.85
4	A	405	CIT	O6-C6-O5	-2.45	116.03	123.82
3	D	404	COA	C2A-N1A-C6A	2.43	122.91	118.75
3	B	402	COA	C6P-C7P-N8P	-2.42	107.00	111.90
3	C	403	COA	C2A-N1A-C6A	2.40	122.86	118.75
3	B	402	COA	O4B-C1B-C2B	-2.40	103.42	106.93
4	A	405	CIT	O7-C3-C4	2.38	114.97	109.40
3	C	403	COA	C7P-N8P-C9P	-2.37	118.36	122.59
3	C	403	COA	C6P-C7P-N8P	-2.36	107.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	401	COA	C7P-N8P-C9P	-2.33	118.43	122.59
3	D	404	COA	C4A-C5A-N7A	2.33	111.83	109.40
3	D	404	COA	C6P-C7P-N8P	-2.26	107.33	111.90
4	A	405	CIT	C4-C3-C2	2.22	114.95	109.16
3	A	401	COA	C6P-C7P-N8P	-2.21	107.44	111.90
3	D	404	COA	CDP-CBP-CCP	2.20	111.82	108.23
4	D	408	CIT	O6-C6-O5	-2.13	117.04	123.82
3	B	402	COA	C7P-N8P-C9P	-2.12	118.80	122.59
3	A	401	COA	C2A-N1A-C6A	2.09	122.33	118.75
3	D	404	COA	C5B-C4B-C3B	2.09	121.33	114.40
4	C	407	CIT	O6-C6-O5	-2.04	117.31	123.82
3	B	402	COA	C2A-N1A-C6A	2.00	122.18	118.75

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	COA	C4B-C3B-O3B-P3B
3	A	401	COA	C6P-C5P-N4P-C3P
3	D	404	COA	C4B-C3B-O3B-P3B
3	D	404	COA	C5B-O5B-P1A-O2A
3	D	404	COA	C5B-O5B-P1A-O3A
3	D	404	COA	CEP-CBP-CCP-O6A
3	D	404	COA	CAP-CBP-CCP-O6A
3	D	404	COA	OAP-CAP-CBP-CCP
3	D	404	COA	C9P-CAP-CBP-CCP
3	D	404	COA	OAP-CAP-CBP-CDP
3	D	404	COA	OAP-CAP-CBP-CEP
3	D	404	COA	C9P-CAP-CBP-CEP
4	A	405	CIT	C2-C3-C4-C5
4	A	405	CIT	O7-C3-C4-C5
4	A	405	CIT	C6-C3-C4-C5
4	C	407	CIT	C2-C3-C6-O5
4	C	407	CIT	C2-C3-C6-O6
4	D	408	CIT	C2-C3-C6-O5
4	D	408	CIT	C2-C3-C6-O6
4	D	408	CIT	O7-C3-C6-O6
5	D	414	GOL	O1-C1-C2-C3
3	A	401	COA	O5P-C5P-N4P-C3P
3	B	402	COA	C4B-C3B-O3B-P3B
3	C	403	COA	C4B-C3B-O3B-P3B
3	D	404	COA	C2B-C3B-O3B-P3B

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Mol	Chain	Res	Type	Atoms
3	D	404	COA	CDP-CBP-CCP-O6A
4	D	408	CIT	C4-C3-C6-O6
5	D	414	GOL	O1-C1-C2-O2
4	D	408	CIT	O7-C3-C4-C5
4	C	407	CIT	O7-C3-C6-O6
4	B	406	CIT	C2-C3-C4-C5
3	B	402	COA	O4B-C4B-C5B-O5B
3	D	404	COA	C9P-CAP-CBP-CDP
3	D	404	COA	C3B-O3B-P3B-O9A
4	C	407	CIT	C4-C3-C6-O5
4	C	407	CIT	C4-C3-C6-O6
4	D	408	CIT	C4-C3-C6-O5
3	B	402	COA	C3B-C4B-C5B-O5B
3	C	403	COA	C2B-C3B-O3B-P3B
3	A	401	COA	O9P-C9P-N8P-C7P
3	D	404	COA	O9P-C9P-N8P-C7P
3	A	401	COA	CAP-C9P-N8P-C7P
3	D	404	COA	CAP-C9P-N8P-C7P
4	B	406	CIT	C6-C3-C4-C5
4	C	407	CIT	O7-C3-C6-O5
4	D	408	CIT	O7-C3-C6-O5
4	D	408	CIT	C2-C3-C4-C5
3	B	402	COA	C2B-C3B-O3B-P3B
4	A	405	CIT	C4-C3-C6-O6
3	B	402	COA	C3B-O3B-P3B-O8A
3	B	402	COA	CCP-O6A-P2A-O3A
3	B	402	COA	P2A-O3A-P1A-O1A
3	B	402	COA	P2A-O3A-P1A-O2A
3	D	404	COA	CBP-CCP-O6A-P2A
3	B	402	COA	C5B-O5B-P1A-O1A
4	D	408	CIT	C6-C3-C4-C5

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	382	SO4	1	0
3	C	403	COA	1	0
3	A	401	COA	2	0
4	B	406	CIT	1	0
2	B	383	SO4	1	0
4	D	408	CIT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	CIT	1	0
3	B	402	COA	1	0
3	D	404	COA	11	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 COA C 403

Ligand COA A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand COA B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand COA D 404

Bond lengths

Bond angles

Torsions

Rings
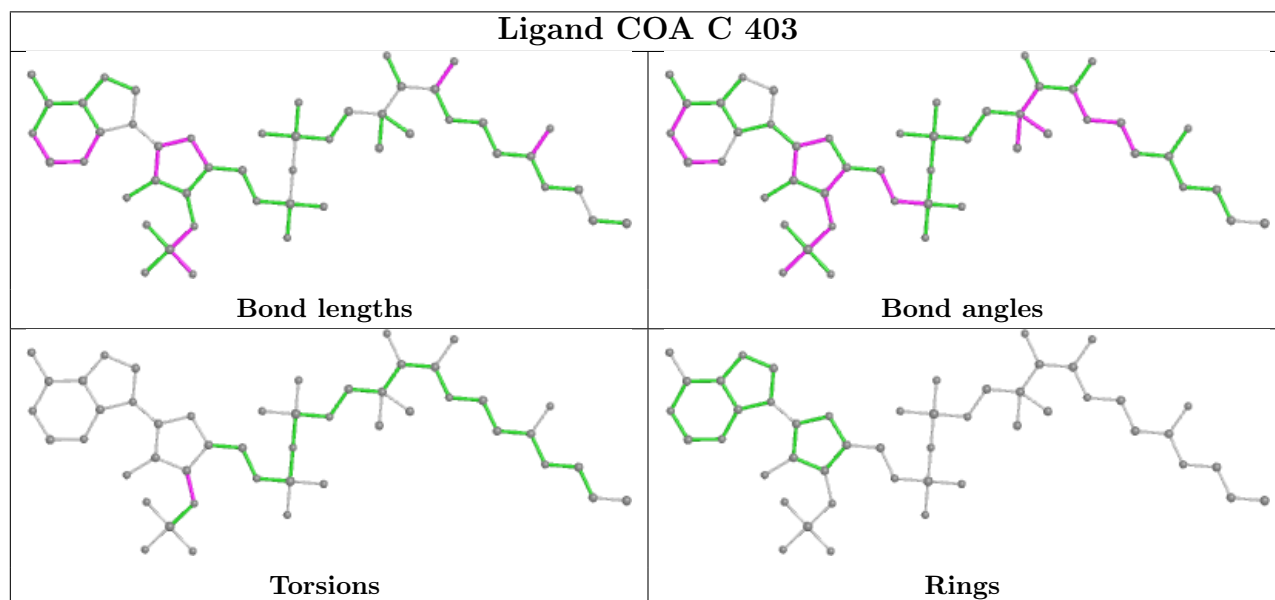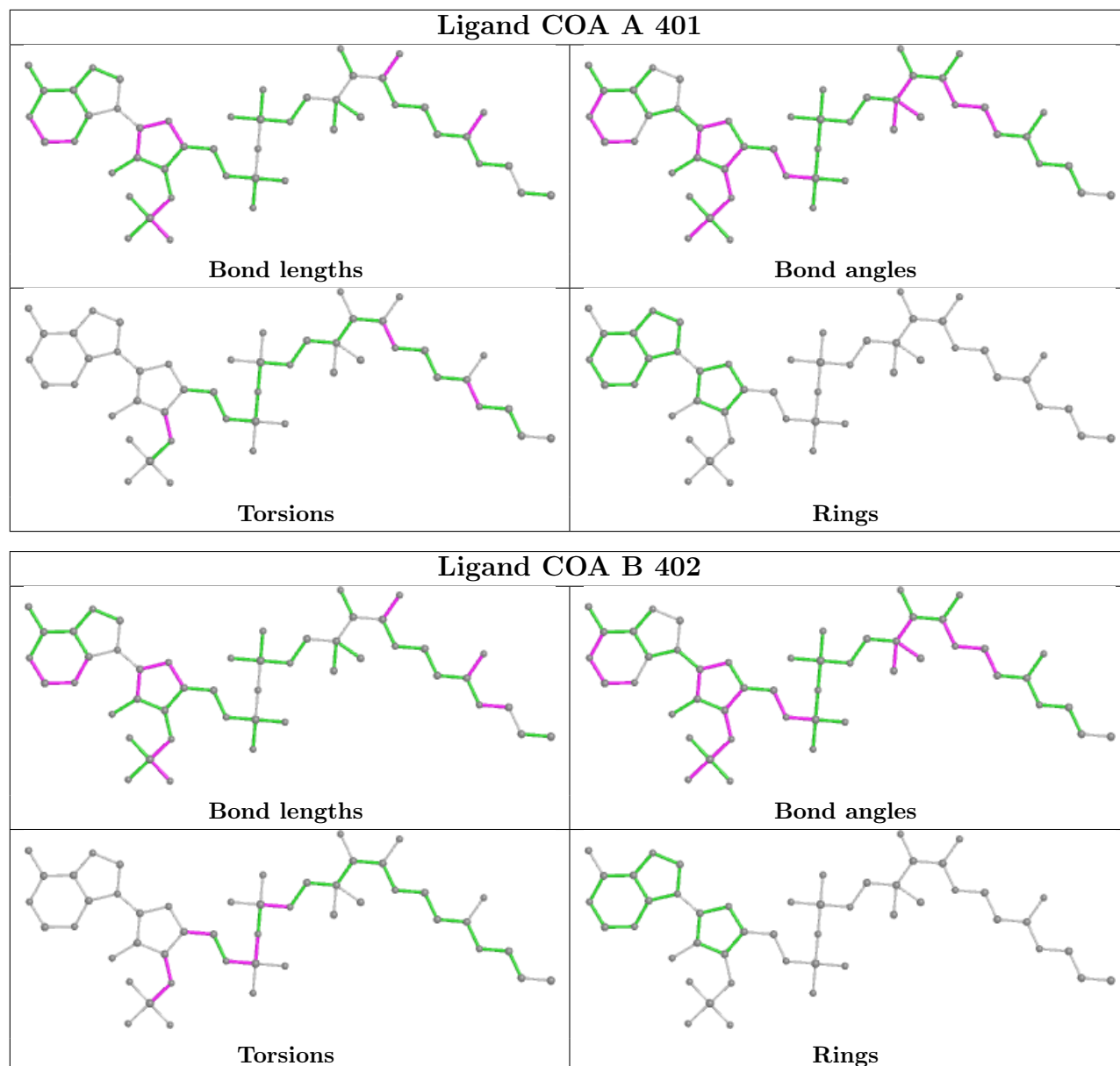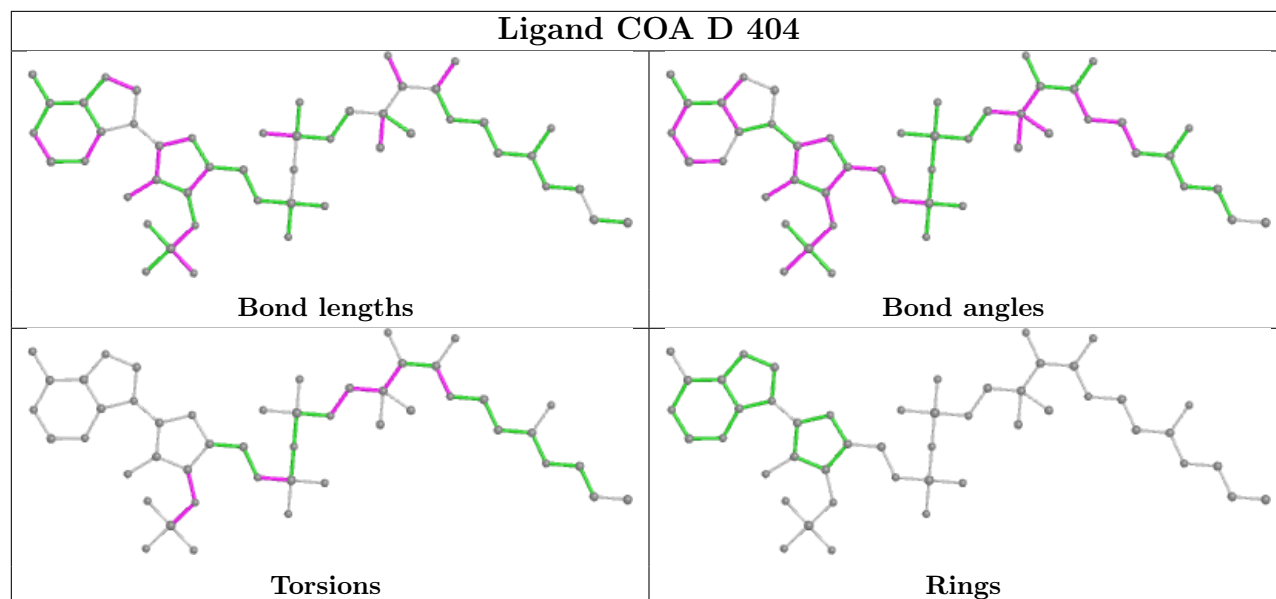
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	371/377 (98%)	1.62	97 (26%)	0	0	8, 21, 39, 57	21 (5%)
1	B	370/377 (98%)	1.49	84 (22%)	0	1	10, 21, 39, 55	24 (6%)
1	C	366/377 (97%)	1.86	128 (34%)	0	0	10, 25, 65, 79	30 (8%)
1	D	366/377 (97%)	1.66	96 (26%)	0	0	10, 23, 52, 64	28 (7%)
All	All	1473/1508 (97%)	1.66	405 (27%)	0	0	8, 22, 51, 79	103 (6%)

All (405) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	15.8
1	C	288	TYR	9.4
1	C	278	VAL	8.7
1	C	247	LEU	8.5
1	C	302	LEU	8.2
1	A	44	GLU	8.0
1	D	248	ALA	7.5
1	D	250	LYS	7.2
1	D	228	ARG	6.9
1	A	284	HIS	6.8
1	D	305	ARG	6.5
1	D	294	VAL	6.4
1	D	244	ARG	6.3
1	C	287	GLU	6.1
1	C	242	TRP	6.1
1	D	245	GLU	6.0
1	C	248	ALA	5.7
1	A	42	SER	5.7
1	A	279	ALA	5.6
1	C	245	GLU	5.5
1	C	250	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	306	GLY	5.4
1	C	303	ASN	5.3
1	C	254	MET	5.3
1	C	262	LYS	5.2
1	B	169	GLU	5.2
1	D	237	GLU	5.2
1	C	231	GLN	5.2
1	A	46	THR	5.1
1	C	314	TYR	5.1
1	D	301	VAL	5.1
1	C	297	GLU	5.0
1	C	232	GLU	5.0
1	C	298	ALA	5.0
1	D	293	ILE	5.0
1	C	293	ILE	4.9
1	A	156	ASN	4.9
1	C	9	GLY	4.9
1	A	178	LEU	4.8
1	C	249	LYS	4.8
1	B	280	GLU	4.8
1	C	237	GLU	4.8
1	D	249	LYS	4.8
1	A	153	HIS	4.8
1	C	238	ARG	4.5
1	A	23	GLN	4.5
1	D	286	LYS	4.4
1	D	110	GLY	4.3
1	A	285	SER	4.3
1	C	244	ARG	4.2
1	C	354	ARG	4.2
1	D	300	LYS	4.2
1	A	3	VAL	4.2
1	A	68	LEU	4.2
1	C	300	LYS	4.2
1	A	154	ALA	4.1
1	C	291	LEU	4.1
1	A	289	GLN	4.0
1	C	220	GLY	4.0
1	D	350	GLU	4.0
1	B	24	GLN	4.0
1	D	251	GLU	4.0
1	D	304	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	253	ILE	4.0
1	C	169	GLU	3.9
1	A	125	ILE	3.9
1	D	275	ALA	3.9
1	C	325	SER	3.9
1	A	220	GLY	3.8
1	C	301	VAL	3.8
1	C	307	ILE	3.8
1	D	308	TYR	3.8
1	D	289	GLN	3.8
1	B	36	GLU	3.7
1	A	250	LYS	3.7
1	C	28	TYR	3.7
1	A	238	ARG	3.6
1	B	168	PRO	3.6
1	A	59	GLN	3.6
1	D	373	LEU	3.6
1	C	246	LYS	3.6
1	D	375	ALA	3.6
1	D	233	ILE	3.6
1	C	172	ARG	3.6
1	D	311	VAL	3.5
1	B	275	ALA	3.5
1	A	287	GLU	3.5
1	B	20	ILE	3.5
1	C	87	VAL	3.5
1	D	254	MET	3.5
1	A	310	ASN	3.5
1	C	353	ASN	3.5
1	A	150	ASP	3.5
1	D	230	ILE	3.4
1	D	247	LEU	3.4
1	B	279	ALA	3.4
1	C	313	PHE	3.4
1	B	300	LYS	3.4
1	D	276	ARG	3.4
1	B	126	ALA	3.4
1	C	236	PRO	3.4
1	B	273	LYS	3.4
1	C	374	GLU	3.3
1	C	230	ILE	3.3
1	C	265	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	369	PRO	3.3
1	A	373	LEU	3.3
1	B	250	LYS	3.3
1	D	172	ARG	3.3
1	C	360	ALA	3.3
1	C	269	GLY	3.3
1	D	17	MET	3.3
1	A	61	LEU	3.3
1	D	263	ALA	3.3
1	A	308	TYR	3.3
1	D	246	LYS	3.3
1	C	23	GLN	3.2
1	D	277	LEU	3.2
1	A	300	LYS	3.2
1	B	302	LEU	3.2
1	B	277	LEU	3.2
1	B	262	LYS	3.2
1	C	57	ARG	3.2
1	A	126	ALA	3.2
1	A	63	GLU	3.2
1	D	297	GLU	3.2
1	B	58	ARG	3.2
1	B	133	ALA	3.2
1	B	326	LEU	3.2
1	A	328	PHE	3.1
1	C	19	TYR	3.1
1	C	304	PRO	3.1
1	A	259	ARG	3.1
1	C	308	TYR	3.1
1	A	372	PRO	3.1
1	A	232	GLU	3.1
1	A	110	GLY	3.1
1	C	234	GLY	3.1
1	D	243	VAL	3.1
1	A	223	ASN	3.1
1	A	65	SER	3.0
1	B	100	SER	3.0
1	D	295	GLU	3.0
1	B	360	ALA	3.0
1	C	239	ALA	3.0
1	B	276	ARG	3.0
1	A	280	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	261	TYR	3.0
1	B	244	ARG	3.0
1	C	276	ARG	3.0
1	C	310	ASN	3.0
1	A	376	ARG	3.0
1	C	290	ILE	3.0
1	A	87	VAL	3.0
1	D	302	LEU	2.9
1	A	227	MET	2.9
1	D	256	MET	2.9
1	C	3	VAL	2.9
1	C	256	MET	2.9
1	B	19	TYR	2.9
1	A	175	ASP	2.9
1	A	361	LYS	2.9
1	D	173	LEU	2.9
1	D	355	LEU	2.9
1	B	261	TYR	2.9
1	C	166	PRO	2.9
1	C	80	GLU	2.9
1	B	285	SER	2.9
1	A	268	ALA	2.9
1	C	225	ALA	2.9
1	D	28	TYR	2.9
1	A	311	VAL	2.9
1	C	18	CYS	2.9
1	C	134	ALA	2.8
1	B	39	GLU	2.8
1	A	278	VAL	2.8
1	A	317	VAL	2.8
1	D	238	ARG	2.8
1	B	76	ALA	2.8
1	D	298	ALA	2.8
1	A	18	CYS	2.8
1	D	351	LEU	2.8
1	C	289	GLN	2.8
1	A	57	ARG	2.8
1	D	5	ARG	2.8
1	D	325	SER	2.8
1	A	240	ARG	2.8
1	A	177	ALA	2.8
1	A	326	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	26	LYS	2.8
1	A	30	TYR	2.8
1	B	278	VAL	2.8
1	D	257	GLY	2.8
1	D	314	TYR	2.8
1	B	26	LYS	2.8
1	C	243	VAL	2.7
1	C	235	THR	2.7
1	C	294	VAL	2.7
1	C	321	ASP	2.7
1	B	159	TYR	2.7
1	B	272	GLU	2.7
1	C	241	GLU	2.7
1	A	225	ALA	2.7
1	B	319	TYR	2.7
1	C	132	VAL	2.7
1	B	179	ILE	2.7
1	A	67	ALA	2.7
1	C	221	GLY	2.7
1	B	80	GLU	2.6
1	B	25	GLY	2.6
1	D	372	PRO	2.6
1	D	354	ARG	2.6
1	A	366	LEU	2.6
1	B	62	GLU	2.6
1	C	296	GLU	2.6
1	C	319	TYR	2.6
1	C	131	ILE	2.6
1	D	268	ALA	2.6
1	C	157	PHE	2.6
1	A	5	ARG	2.6
1	B	90	HIS	2.6
1	C	76	ALA	2.6
1	B	291	LEU	2.6
1	C	346	LEU	2.6
1	C	229	MET	2.6
1	B	59	GLN	2.6
1	B	18	CYS	2.6
1	C	58	ARG	2.6
1	C	372	PRO	2.6
1	B	371	VAL	2.6
1	D	264	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	257	GLY	2.6
1	C	37	LEU	2.5
1	C	311	VAL	2.5
1	B	352	ASP	2.5
1	B	8	GLU	2.5
1	A	305	ARG	2.5
1	A	332	ILE	2.5
1	B	17	MET	2.5
1	D	58	ARG	2.5
1	C	89	ALA	2.5
1	C	333	PHE	2.5
1	D	368	VAL	2.5
1	D	213	SER	2.5
1	B	22	GLY	2.5
1	A	368	VAL	2.5
1	D	261	TYR	2.5
1	A	179	ILE	2.5
1	A	24	GLN	2.5
1	C	252	ARG	2.5
1	D	236	PRO	2.5
1	C	253	ILE	2.5
1	C	299	GLY	2.5
1	D	163	GLY	2.5
1	C	277	LEU	2.5
1	B	186	PHE	2.4
1	C	164	VAL	2.4
1	C	272	GLU	2.4
1	D	241	GLU	2.4
1	D	309	PRO	2.4
1	A	288	TYR	2.4
1	B	269	GLY	2.4
1	A	251	GLU	2.4
1	D	214	LEU	2.4
1	D	225	ALA	2.4
1	C	108	THR	2.4
1	B	211	VAL	2.4
1	C	371	VAL	2.4
1	C	8	GLU	2.4
1	D	57	ARG	2.4
1	B	145	ILE	2.4
1	B	223	ASN	2.4
1	A	66	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	292	LYS	2.4
1	C	320	SER	2.4
1	C	74	LEU	2.4
1	A	276	ARG	2.4
1	B	286	LYS	2.4
1	B	82	PHE	2.4
1	D	363	VAL	2.4
1	C	29	TYR	2.4
1	D	307	ILE	2.4
1	D	367	ASP	2.4
1	A	309	PRO	2.4
1	D	132	VAL	2.4
1	A	172	ARG	2.3
1	A	112	ILE	2.3
1	B	196	ALA	2.3
1	C	263	ALA	2.3
1	D	126	ALA	2.3
1	B	229	MET	2.3
1	B	16	ARG	2.3
1	C	370	TYR	2.3
1	D	288	TYR	2.3
1	D	319	TYR	2.3
1	D	239	ALA	2.3
1	B	108	THR	2.3
1	B	238	ARG	2.3
1	D	150	ASP	2.3
1	D	185	GLY	2.3
1	A	304	PRO	2.3
1	A	252	ARG	2.3
1	C	223	ASN	2.3
1	C	373	LEU	2.3
1	D	234	GLY	2.3
1	B	60	GLU	2.3
1	B	365	GLU	2.3
1	D	232	GLU	2.3
1	D	374	GLU	2.3
1	A	203	LEU	2.3
1	C	305	ARG	2.3
1	B	209	ALA	2.3
1	C	357	ARG	2.3
1	C	112	ILE	2.3
1	C	154	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	2.2
1	C	55	LEU	2.2
1	D	270	VAL	2.2
1	A	47	THR	2.2
1	A	171	ALA	2.2
1	A	253	ILE	2.2
1	C	73	ALA	2.2
1	D	273	LYS	2.2
1	A	49	LEU	2.2
1	C	258	HIS	2.2
1	B	170	GLN	2.2
1	C	228	ARG	2.2
1	B	14	GLU	2.2
1	D	366	LEU	2.2
1	A	261	TYR	2.2
1	B	118	TYR	2.2
1	B	21	ASP	2.2
1	C	275	ALA	2.2
1	A	365	GLU	2.2
1	B	65	SER	2.2
1	C	85	TYR	2.2
1	D	370	TYR	2.2
1	B	154	ALA	2.2
1	B	122	LEU	2.2
1	A	104	MET	2.2
1	B	321	ASP	2.2
1	B	328	PHE	2.1
1	A	199	THR	2.1
1	C	67	ALA	2.1
1	D	235	THR	2.1
1	B	242	TRP	2.1
1	D	306	GLY	2.1
1	B	354	ARG	2.1
1	A	336	ALA	2.1
1	B	155	ALA	2.1
1	D	328	PHE	2.1
1	B	172	ARG	2.1
1	B	297	GLU	2.1
1	C	39	GLU	2.1
1	B	3	VAL	2.1
1	C	38	ALA	2.1
1	C	210	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	3	VAL	2.1
1	A	149	GLU	2.1
1	C	233	ILE	2.1
1	B	214	LEU	2.1
1	C	226	VAL	2.1
1	A	80	GLU	2.1
1	C	62	GLU	2.1
1	D	296	GLU	2.1
1	C	147	PRO	2.1
1	A	27	LEU	2.1
1	A	122	LEU	2.1
1	C	149	GLU	2.1
1	B	188	ALA	2.1
1	D	188	ALA	2.1
1	D	310	ASN	2.1
1	A	243	VAL	2.1
1	B	317	VAL	2.1
1	B	366	LEU	2.1
1	C	158	LEU	2.1
1	C	326	LEU	2.1
1	D	169	GLU	2.1
1	D	148	ARG	2.1
1	A	201	THR	2.1
1	C	192	THR	2.1
1	A	155	ALA	2.1
1	A	294	VAL	2.1
1	A	12	PHE	2.1
1	A	204	TYR	2.1
1	B	107	PRO	2.1
1	A	237	GLU	2.0
1	B	233	ILE	2.0
1	C	117	LEU	2.0
1	D	55	LEU	2.0
1	D	83	LYS	2.0
1	A	93	SER	2.0
1	C	255	GLY	2.0
1	D	87	VAL	2.0
1	D	168	PRO	2.0
1	A	274	LEU	2.0
1	D	229	MET	2.0
1	A	39	GLU	2.0
1	B	245	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	THR	2.0
1	A	134	ALA	2.0
1	C	240	ARG	2.0
1	B	351	LEU	2.0
1	C	322	LEU	2.0
1	A	189	SER	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
3	COA	D	404	48/48	0.47	0.43	82,86,89,90	0
5	GOL	B	412	6/6	0.59	0.37	35,39,40,42	0
3	COA	C	403	48/48	0.60	0.35	63,73,81,82	0
5	GOL	C	413	6/6	0.62	0.57	43,47,50,51	0
3	COA	A	401	48/48	0.65	0.32	42,52,62,65	0
4	CIT	D	408	13/13	0.69	0.30	32,39,47,49	0
5	GOL	D	414	6/6	0.70	0.27	59,61,62,62	0
4	CIT	C	407	13/13	0.71	0.30	36,43,51,53	0
4	CIT	B	406	13/13	0.77	0.33	22,31,42,43	0
4	CIT	A	405	13/13	0.78	0.28	22,28,42,45	0
3	COA	B	402	48/48	0.79	0.22	18,25,43,45	0
2	SO4	C	390	5/5	0.79	0.52	80,82,83,83	0
5	GOL	A	411	6/6	0.80	0.40	22,30,31,36	0
2	SO4	B	383	5/5	0.83	0.50	59,62,63,64	0
2	SO4	D	386	5/5	0.83	0.22	42,43,44,45	0
2	SO4	D	389	5/5	0.85	0.39	70,70,72,73	0
2	SO4	A	387	5/5	0.89	0.31	42,43,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	382	5/5	0.90	0.23	52,55,56,58	0
2	SO4	C	388	5/5	0.91	0.14	49,50,51,53	0
2	SO4	B	385	5/5	0.92	0.25	43,43,44,45	0
2	SO4	C	381	5/5	0.95	0.14	25,26,27,29	0
2	SO4	A	391	5/5	0.96	0.14	15,16,17,19	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 COA D 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
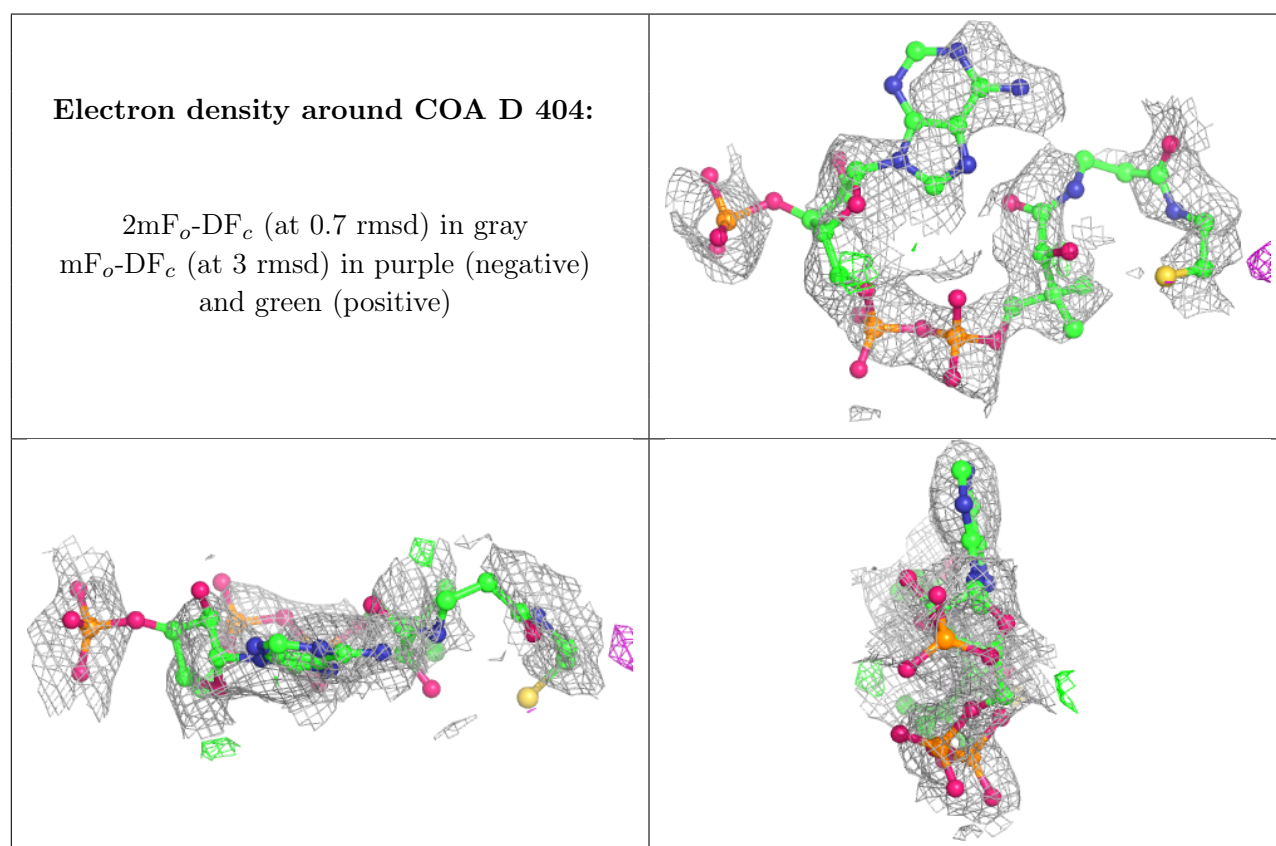
Electron density around COA C 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
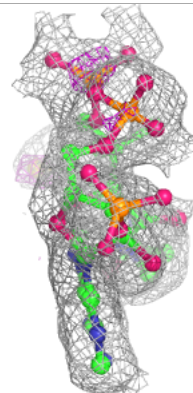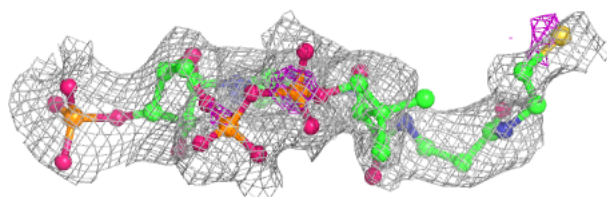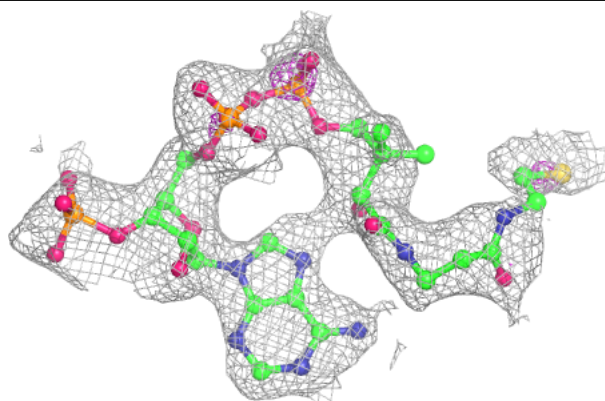and green (positive)
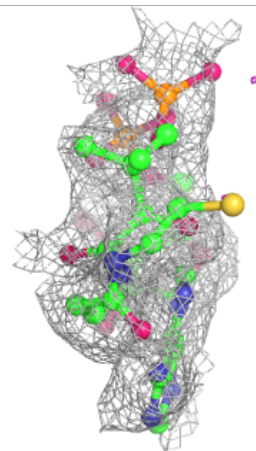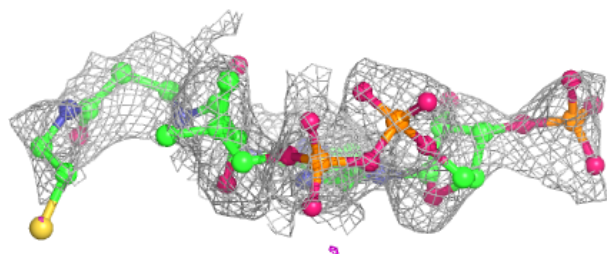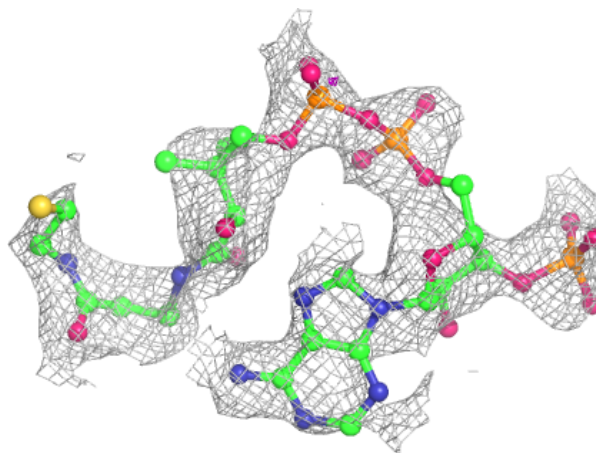
Electron density around COA A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
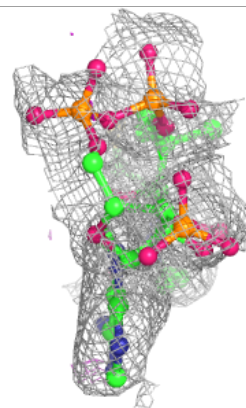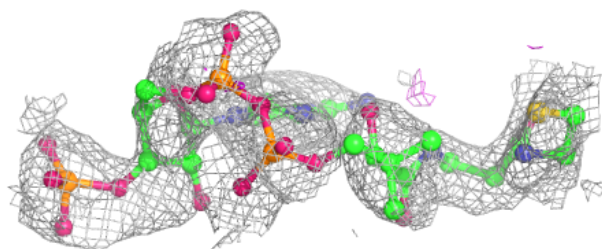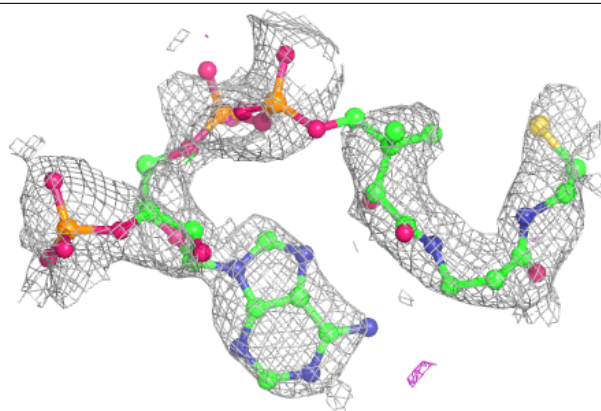
Electron density around COA B 402:

$2mF_o$-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 ⓘ

There are no such residues in this entry.