



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:07 AM UTC

PDB ID : 1IXE / pdb_00001ixe
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)

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

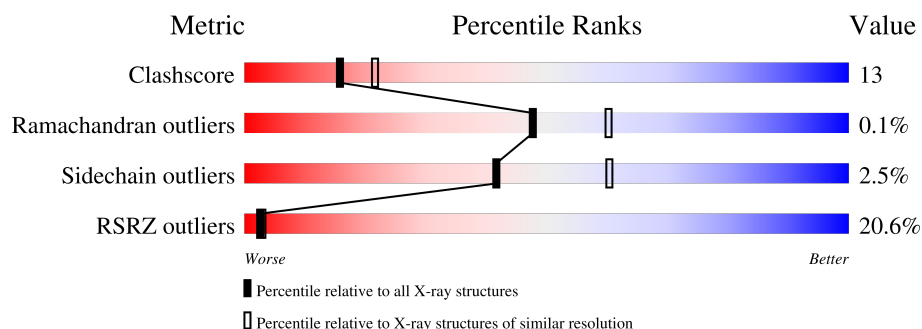
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	377	17% 70% 27% ..
1	B	377	14% 72% 24% ..
1	C	377	27% 68% 28% ..
1	D	377	23% 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
4	CIT	D	408	-	-	X	-

2 Entry composition [i](#)

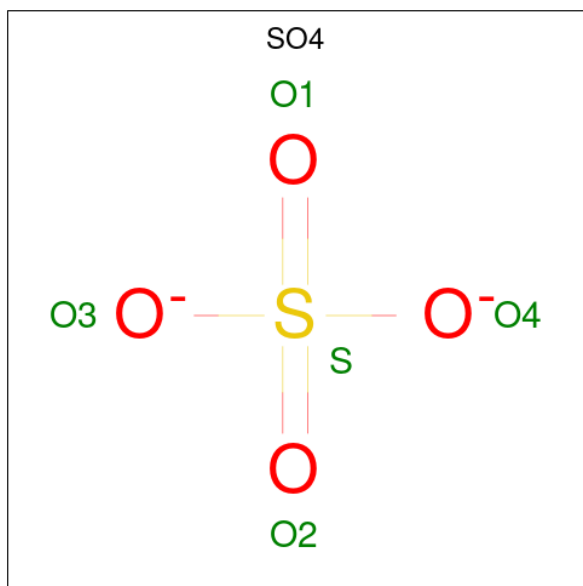
There are 6 unique types of molecules in this entry. The entry contains 12452 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



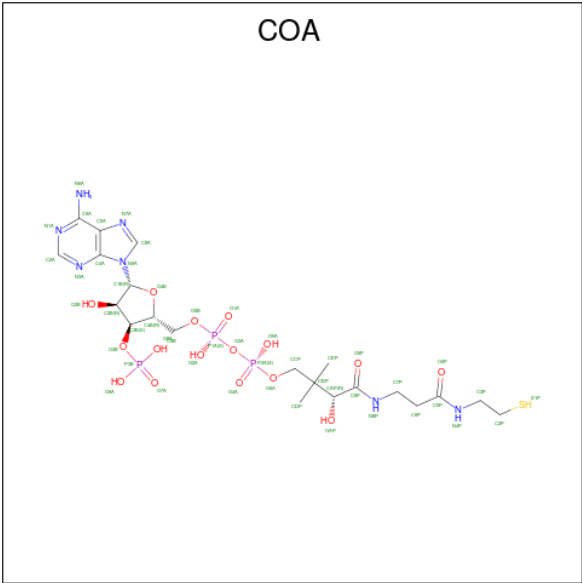
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



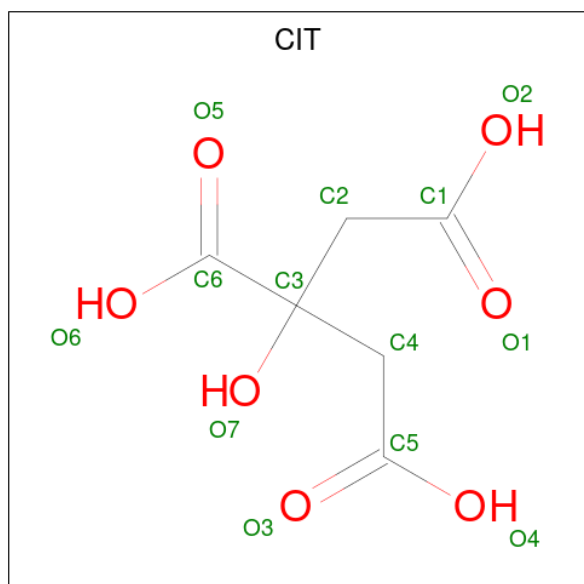
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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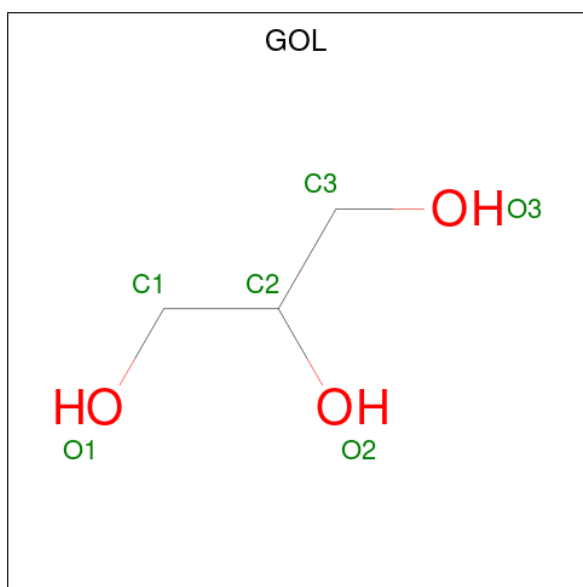
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

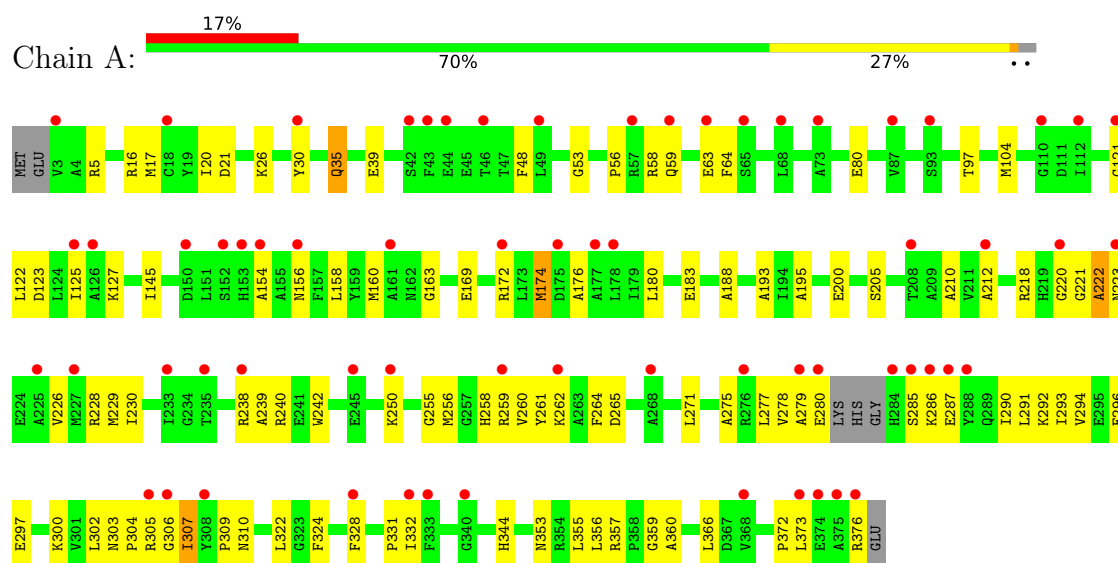
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	138	Total	O	0	0
			138	138		
6	C	120	Total	O	0	0
			120	120		
6	D	134	Total	O	0	0
			134	134		

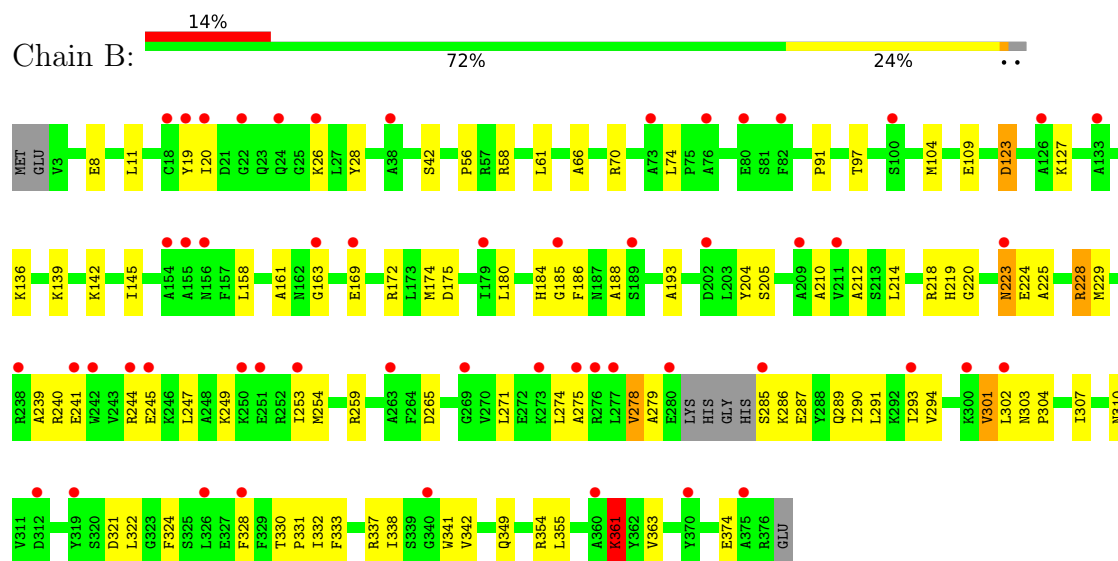
3 Residue-property plots

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.

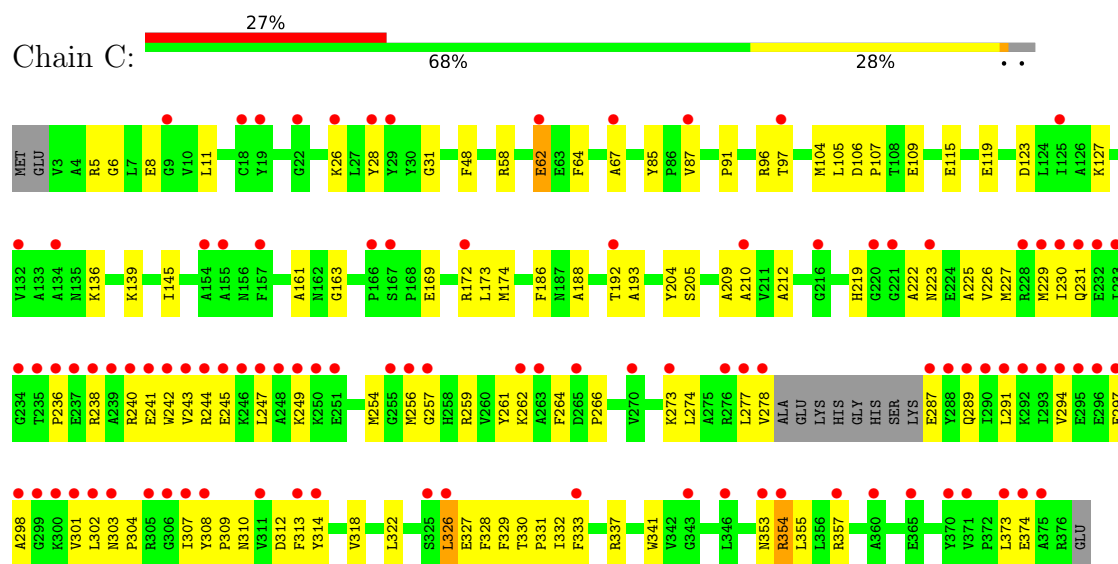
• Molecule 1: citrate synthase



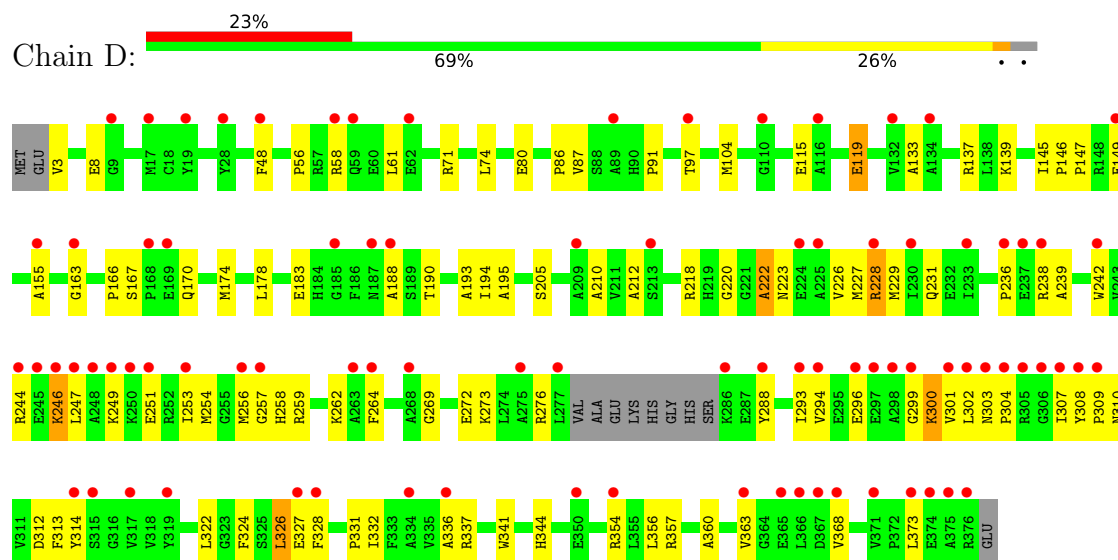
• Molecule 1: citrate synthase



• Molecule 1: citrate synthase



• Molecule 1: citrate synthase



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) 88.4 (14.79-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.217 0.183 , (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)	0.37 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

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, COA, GOL, 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	0.40	0/2986	0.71	0/4036
1	B	0.46	0/2987	0.77	0/4035
1	C	0.40	0/2952	0.74	1/3990 (0.0%)
1	D	0.50	0/2953	0.79	4/3990 (0.1%)
All	All	0.44	0/11878	0.75	5/16051 (0.0%)

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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	LYS	N-CA-C	-6.13	105.11	112.59
1	D	262	LYS	N-CA-C	-5.85	105.45	112.59
1	D	222	ALA	N-CA-C	-5.64	105.66	112.54
1	D	74	LEU	CA-C-N	-5.36	114.43	119.85
1	D	74	LEU	C-N-CA	-5.36	114.43	119.85

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	87	0
1	B	2922	0	2924	77	0
1	C	2887	0	2884	95	0
1	D	2888	0	2888	91	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	315	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 (315) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:247:LEU:HD13	1:B:301:VAL:HG21	1.64	0.78
1:D:174:MET:HE2	1:D:322:LEU:HD13	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:229:MET:HE1	1:D:254:MET:N	2.03	0.73
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:C:225:ALA:HB1	1:C:254:MET:HE3	1.70	0.71
1:C:328:PHE:C	1:C:331:PRO:HD2	2.16	0.70
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:C:58:ARG:HA	1:D:373:LEU:HD11	1.74	0.68
1:C:229:MET:HE1	1:C:254:MET:N	2.09	0.67
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:174:MET:HE2	1:C:322:LEU:HD13	1.78	0.65
1:A:58:ARG:HH22	1:B:374:GLU:HA	1.62	0.65
1:A:328:PHE:C	1:A:331:PRO:HD2	2.21	0.65
1:B:193:ALA:HB2	1:B:210:ALA:HB2	1.79	0.65
1:A:222:ALA:HB2	3:A:401:COA:H31	1.79	0.64
1:A:256:MET:HE3	1:A:309:PRO:HD3	1.80	0.64
1:B:328:PHE:C	1:B:331:PRO:HD2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:404:COA:H22	6:D:801:HOH:O	2.00	0.62
1:A:97:THR:HG21	1:B:104:MET:HE2	1.80	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: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:D:229:MET:HE1	1:D:254:MET:H	1.65	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:97:THR:HG21	1:D:104:MET:HE2	1.83	0.59
1:C:259:ARG:HG2	1:D:357:ARG:HB3	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:174:MET:HE2	1:B:322:LEU:HD13	1.85	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:C:229:MET:HE1	1:C:254:MET:H	1.67	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:B:229:MET:HE1	1:B:253:ILE:HG23	1.87	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: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:C:115:GLU:CD	1:C:115:GLU:H	2.14	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:C:374:GLU:CD	1:C:374:GLU:H	2.14	0.56
1:D:56:PRO:HG3	1:D:61:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:193:ALA:HB2	1:D:210:ALA:HB2	1.89	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:B:158:LEU:HD21	1:B:174:MET:HE2	1.90	0.52
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:229:MET:CE	1:C:254:MET:H	2.23	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:D:71:ARG:HH21	1:D:119:GLU:CD	2.19	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:328:PHE:C	1:D:331:PRO:HD2	2.37	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
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:A:123:ASP:CG	1:A:127:LYS:HE2	2.38	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:A:156:ASN:ND2	1:A:160:MET:HE2	2.28	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:C:225:ALA:CB	1:C:254:MET:HE3	2.42	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:A:104:MET:HE2	1:B:97:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:LYS:HD3	1:B:361:LYS:C	2.40	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:D:236:PRO:C	1:D:238:ARG:H	2.23	0.46
1:B:26:LYS:HD3	1:B:28:TYR:OH	2.15	0.46
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:D:48:PHE:CD1	1:D:48:PHE:C	2.93	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:D:115:GLU:H	1:D:115:GLU:CD	2.23	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:48:PHE:CD1	1:C:48:PHE:C	2.95	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
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:C:229:MET:HE2	1:C:242:TRP:CH2	2.53	0.44
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:B:374:GLU:H	1:B:374:GLU:CD	2.26	0.43
1:D:229:MET:HE2	1:D:242:TRP:HH2	1.83	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:85:TYR:CG	1:D:104:MET:HE1	2.54	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:A:17:MET:HE2	1:A:17:MET:HB3	1.96	0.43
1:D:272:GLU:HG2	1:D:314:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:221:GLY:O	1:A:222:ALA:C	2.62	0.42
1:C:273:LYS:O	1:C:277:LEU:HG	2.18	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:B:158:LEU:HD21	1:B:174:MET:CE	2.50	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: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
1:A:222:ALA:O	1:A:223:ASN:C	2.62	0.42
1:B:139:LYS:HE2	6:B:451:HOH:O	2.20	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: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: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: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:286:LYS:O	1:A:287:GLU:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:85:TYR:CD2	1:D:104:MET:HE1	2.56	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:104:MET:HE2	1:D:97:THR:HG21	2.03	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: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
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	367/377 (97%)	356 (97%)	10 (3%)	1 (0%)	36 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	48	60

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%)	32	49
1	B	300/307 (98%)	292 (97%)	8 (3%)	39	58
1	C	296/307 (96%)	290 (98%)	6 (2%)	48	67
1	D	296/307 (96%)	290 (98%)	6 (2%)	48	67
All	All	1190/1228 (97%)	1160 (98%)	30 (2%)	42	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	174	MET
1	A	218	ARG
1	A	228	ARG
1	A	238	ARG
1	A	250	LYS
1	A	259	ARG
1	A	291	LEU
1	A	292	LYS
1	A	307	ILE

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Mol	Chain	Res	Type
1	B	123	ASP
1	B	223	ASN
1	B	228	ARG
1	B	278	VAL
1	B	287	GLU
1	B	291	LEU
1	B	301	VAL
1	B	361	LYS
1	C	62	GLU
1	C	119	GLU
1	C	241	GLU
1	C	244	ARG
1	C	326	LEU
1	C	354	ARG
1	D	119	GLU
1	D	228	ARG
1	D	244	ARG
1	D	246	LYS
1	D	300	LYS
1	D	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	59	GLN
1	A	162	ASN
1	A	231	GLN
1	A	303	ASN
1	B	23	GLN
1	B	24	GLN
1	B	289	GLN
1	C	23	GLN
1	C	289	GLN
1	C	353	ASN
1	D	223	ASN
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 oligosaccharides 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	$\# Z > 2$
4	CIT	B	406	-	12,12,12	1.56	1 (8%)	17,17,17	3.05	6 (35%)
5	GOL	D	414	-	5,5,5	0.77	0	5,5,5	0.23	0
2	SO4	A	391	-	4,4,4	0.35	0	6,6,6	0.12	0
3	COA	B	402	-	47,50,50	1.91	13 (27%)	69,75,75	1.57	12 (17%)
3	COA	D	404	-	47,50,50	2.12	15 (31%)	69,75,75	1.81	15 (21%)
2	SO4	C	388	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	A	387	-	4,4,4	0.35	0	6,6,6	0.11	0
4	CIT	D	408	-	12,12,12	1.91	2 (16%)	17,17,17	2.58	7 (41%)
5	GOL	C	413	-	5,5,5	0.94	0	5,5,5	0.61	0
4	CIT	A	405	-	12,12,12	2.00	3 (25%)	17,17,17	2.79	9 (52%)
2	SO4	D	386	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	B	385	-	4,4,4	0.39	0	6,6,6	0.10	0
2	SO4	B	382	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	C	390	-	4,4,4	0.34	0	6,6,6	0.10	0
5	GOL	B	412	-	5,5,5	0.86	0	5,5,5	0.29	0
3	COA	A	401	-	47,50,50	1.99	9 (19%)	69,75,75	1.65	16 (23%)
2	SO4	B	383	-	4,4,4	0.39	0	6,6,6	0.06	0
4	CIT	C	407	-	12,12,12	1.74	2 (16%)	17,17,17	3.03	7 (41%)
3	COA	C	403	-	47,50,50	2.04	11 (23%)	69,75,75	1.62	13 (18%)
5	GOL	A	411	-	5,5,5	0.85	0	5,5,5	0.21	0
2	SO4	C	381	-	4,4,4	0.31	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	389	-	4,4,4	0.36	0	6,6,6	0.11	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
4	CIT	C	407	-	-	6/16/16/16	-
4	CIT	B	406	-	-	2/16/16/16	-
5	GOL	D	414	-	-	2/4/4/4	-
3	COA	C	403	-	-	3/48/64/64	0/3/3/3
3	COA	B	402	-	-	9/48/64/64	0/3/3/3
5	GOL	B	412	-	-	0/4/4/4	-
4	CIT	D	408	-	-	8/16/16/16	-
3	COA	A	401	-	-	5/48/64/64	0/3/3/3
5	GOL	A	411	-	-	0/4/4/4	-
5	GOL	C	413	-	-	0/4/4/4	-
4	CIT	A	405	-	-	5/16/16/16	-
3	COA	D	404	-	-	17/48/64/64	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	COA	P3B-O3B	6.03	1.70	1.59
3	C	403	COA	P3B-O3B	5.83	1.69	1.59
3	D	404	COA	O9P-C9P	5.53	1.34	1.23
3	C	403	COA	P2A-O3A	5.36	1.65	1.59
3	A	401	COA	P2A-O3A	5.33	1.65	1.59
3	B	402	COA	P3B-O3B	5.27	1.68	1.59
4	D	408	CIT	C2-C3	5.01	1.60	1.54
3	D	404	COA	P3B-O3B	4.87	1.68	1.59
4	C	407	CIT	C2-C3	4.77	1.59	1.54
4	A	405	CIT	C2-C3	4.70	1.59	1.54
3	C	403	COA	O9P-C9P	4.53	1.32	1.23
3	A	401	COA	O9P-C9P	4.35	1.31	1.23
4	B	406	CIT	C2-C3	4.02	1.58	1.54
3	B	402	COA	O9P-C9P	3.96	1.31	1.23
3	B	402	COA	P2A-O3A	3.81	1.63	1.59
3	D	404	COA	C3B-C4B	3.79	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	COA	P3B-O7A	3.75	1.62	1.50
3	C	403	COA	C2A-N1A	3.74	1.40	1.33
3	D	404	COA	O4B-C1B	3.62	1.50	1.42
3	D	404	COA	P2A-O3A	3.58	1.63	1.59
3	B	402	COA	P3B-O7A	3.57	1.61	1.50
3	A	401	COA	C2A-N1A	3.55	1.40	1.33
3	B	402	COA	C2A-N1A	3.50	1.40	1.33
3	A	401	COA	P3B-O7A	3.40	1.61	1.50
3	C	403	COA	P3B-O7A	3.36	1.60	1.50
4	A	405	CIT	C4-C3	3.26	1.58	1.54
3	C	403	COA	C5A-C6A	3.26	1.50	1.41
3	A	401	COA	C5A-C6A	3.18	1.49	1.41
3	B	402	COA	C5A-C6A	3.13	1.49	1.41
3	D	404	COA	C2A-N1A	2.92	1.39	1.33
3	D	404	COA	P2A-O4A	2.91	1.60	1.50
3	D	404	COA	CEP-CBP	2.83	1.59	1.53
3	D	404	COA	OAP-CAP	2.78	1.47	1.42
3	C	403	COA	C4A-N3A	2.76	1.39	1.34
3	B	402	COA	P1A-O3A	-2.72	1.56	1.59
3	D	404	COA	C5A-C6A	2.70	1.48	1.41
3	D	404	COA	C4A-N3A	2.69	1.39	1.34
3	A	401	COA	O4B-C4B	2.66	1.50	1.45
3	C	403	COA	C8A-N9A	2.64	1.42	1.37
3	C	403	COA	C5A-C4A	2.63	1.43	1.39
3	D	404	COA	O2B-C2B	2.63	1.49	1.43
4	D	408	CIT	C4-C3	2.51	1.57	1.54
3	B	402	COA	C5A-C4A	2.45	1.43	1.39
3	B	402	COA	O5P-C5P	2.43	1.28	1.23
3	C	403	COA	O5P-C5P	2.43	1.28	1.23
4	A	405	CIT	C3-C6	2.40	1.56	1.53
3	B	402	COA	O4B-C4B	2.33	1.50	1.45
3	B	402	COA	C4A-N3A	2.32	1.38	1.34
3	B	402	COA	C8A-N9A	2.28	1.41	1.37
3	C	403	COA	O4B-C4B	2.28	1.50	1.45
3	B	402	COA	C3P-N4P	2.25	1.51	1.46
4	C	407	CIT	C4-C3	2.21	1.56	1.54
3	D	404	COA	C8A-N9A	2.16	1.41	1.37
3	A	401	COA	C5A-C4A	2.15	1.42	1.39
3	A	401	COA	O5P-C5P	2.14	1.27	1.23
3	D	404	COA	P3B-O9A	2.02	1.62	1.54

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	CIT	C3-C4-C5	7.17	133.54	113.92
4	B	406	CIT	C3-C4-C5	6.90	132.80	113.92
4	C	407	CIT	C3-C4-C5	6.58	131.91	113.92
4	B	406	CIT	C4-C3-C6	-6.56	95.53	110.03
4	C	407	CIT	C4-C3-C6	-5.90	96.98	110.03
4	D	408	CIT	C4-C3-C6	-5.17	98.59	110.03
3	D	404	COA	O4B-C1B-N9A	-5.04	98.41	108.09
3	A	401	COA	O8A-P3B-O3B	-4.86	86.89	105.85
3	C	403	COA	O8A-P3B-O3B	-4.81	87.10	105.85
3	B	402	COA	O8A-P3B-O3B	-4.63	87.79	105.85
3	D	404	COA	CEP-CBP-CAP	4.48	116.40	108.77
4	B	406	CIT	C3-C2-C1	4.47	126.16	113.92
3	D	404	COA	O8A-P3B-O3B	-4.46	88.46	105.85
4	A	405	CIT	C4-C3-C6	-4.29	100.55	110.03
4	C	407	CIT	O7-C3-C6	-4.17	103.04	108.96
4	D	408	CIT	C3-C4-C5	4.04	124.97	113.92
4	D	408	CIT	C3-C2-C1	4.04	124.96	113.92
3	C	403	COA	P1A-O5B-C5B	3.96	144.05	121.35
3	A	401	COA	P1A-O5B-C5B	3.96	144.04	121.35
4	C	407	CIT	C3-C2-C1	3.87	124.51	113.92
3	B	402	COA	N3A-C2A-N1A	-3.87	122.73	128.58
3	D	404	COA	P1A-O5B-C5B	3.84	143.36	121.35
3	C	403	COA	CEP-CBP-CAP	3.75	115.16	108.77
4	B	406	CIT	O7-C3-C4	3.74	117.91	109.38
3	A	401	COA	CEP-CBP-CAP	3.67	115.02	108.77
3	D	404	COA	N3A-C2A-N1A	-3.67	123.03	128.58
3	B	402	COA	P1A-O5B-C5B	3.66	142.32	121.35
3	D	404	COA	C7P-N8P-C9P	-3.58	116.12	122.55
4	D	408	CIT	O7-C3-C6	-3.58	103.89	108.96
3	A	401	COA	O3B-C3B-C4B	3.57	122.62	110.03
3	D	404	COA	O3B-C3B-C4B	3.57	122.61	110.03
3	C	403	COA	N3A-C2A-N1A	-3.49	123.30	128.58
3	B	402	COA	CEP-CBP-CAP	3.46	114.67	108.77
4	C	407	CIT	O7-C3-C4	3.42	117.18	109.38
4	C	407	CIT	O6-C6-C3	3.40	119.67	113.14
4	D	408	CIT	O6-C6-C3	3.39	119.64	113.14
3	B	402	COA	O4B-C1B-N9A	-3.37	101.62	108.09
4	A	405	CIT	O6-C6-C3	3.33	119.53	113.14
3	C	403	COA	CDP-CBP-CAP	3.32	114.44	108.77
3	B	402	COA	O3B-C3B-C4B	3.29	121.63	110.03
3	C	403	COA	O3B-C3B-C4B	3.24	121.46	110.03
3	B	402	COA	CDP-CBP-CAP	3.24	114.30	108.77
3	A	401	COA	N3A-C2A-N1A	-3.23	123.69	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	COA	CDP-CBP-CAP	3.21	114.23	108.77
4	A	405	CIT	O7-C3-C6	-3.12	104.53	108.96
4	A	405	CIT	C3-C2-C1	3.07	122.32	113.92
3	C	403	COA	O5A-P2A-O3A	3.06	115.54	107.27
4	D	408	CIT	O7-C3-C4	2.98	116.16	109.38
4	B	406	CIT	O7-C3-C6	-2.91	104.83	108.96
3	C	403	COA	O4B-C1B-N9A	-2.85	102.61	108.09
4	B	406	CIT	O6-C6-C3	2.76	118.44	113.14
3	A	401	COA	O4B-C1B-N9A	-2.74	102.83	108.09
3	D	404	COA	CDP-CBP-CAP	2.70	113.37	108.77
3	B	402	COA	O5A-P2A-O3A	2.65	114.44	107.27
3	D	404	COA	O5A-P2A-O3A	2.63	114.39	107.27
3	A	401	COA	N9A-C8A-N7A	-2.62	110.21	113.94
3	A	401	COA	O5A-P2A-O3A	2.59	114.27	107.27
3	D	404	COA	C2A-N1A-C6A	2.55	122.91	118.73
3	B	402	COA	C2B-C1B-N9A	-2.54	107.00	113.30
3	A	401	COA	C2B-C1B-N9A	-2.52	107.03	113.30
3	C	403	COA	C2A-N1A-C6A	2.51	122.86	118.73
3	D	404	COA	O2B-C2B-C1B	-2.46	101.65	110.10
4	A	405	CIT	O7-C3-C4	2.45	114.97	109.38
4	A	405	CIT	O6-C6-O5	-2.45	116.03	123.86
3	C	403	COA	C2B-C1B-N9A	-2.35	107.46	113.30
3	B	402	COA	C6P-C7P-N8P	-2.35	107.00	112.00
3	C	403	COA	C7P-N8P-C9P	-2.33	118.36	122.55
3	A	401	COA	C5A-C4A-N9A	-2.31	103.30	105.81
3	A	401	COA	C7P-N8P-C9P	-2.29	118.43	122.55
3	C	403	COA	C6P-C7P-N8P	-2.29	107.12	112.00
4	A	405	CIT	C4-C3-C2	2.20	114.95	109.31
3	A	401	COA	C2A-N1A-C6A	2.19	122.33	118.73
3	D	404	COA	C6P-C7P-N8P	-2.19	107.33	112.00
3	D	404	COA	CDP-CBP-CCP	2.18	111.82	108.22
3	A	401	COA	C6P-C7P-N8P	-2.14	107.44	112.00
3	A	401	COA	O4B-C1B-C2B	-2.14	102.04	106.62
4	D	408	CIT	O6-C6-O5	-2.13	117.04	123.86
3	B	402	COA	C2A-N1A-C6A	2.10	122.18	118.73
3	D	404	COA	C6A-C5A-C4A	-2.09	114.33	117.18
3	D	404	COA	C5B-C4B-C3B	2.09	121.33	114.38
3	B	402	COA	C7P-N8P-C9P	-2.09	118.80	122.55
4	C	407	CIT	O6-C6-O5	-2.05	117.31	123.86
3	A	401	COA	O3B-P3B-O7A	2.02	116.54	109.33
4	A	405	CIT	O4-C5-C4	2.00	120.70	114.35
3	C	403	COA	O4B-C1B-C2B	-2.00	102.33	106.62

There are no chirality outliers.

All (57) 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	CDP-CBP-CCP-O6A
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	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
4	A	405	CIT	O7-C3-C4-C5
3	B	402	COA	C4B-C3B-O3B-P3B
3	C	403	COA	C4B-C3B-O3B-P3B
3	D	404	COA	C2B-C3B-O3B-P3B
5	D	414	GOL	O1-C1-C2-O2
4	C	407	CIT	O7-C3-C6-O6
4	D	408	CIT	C4-C3-C6-O6
4	B	406	CIT	C2-C3-C4-C5
4	D	408	CIT	O7-C3-C4-C5
3	B	402	COA	O4B-C4B-C5B-O5B
3	D	404	COA	C9P-CAP-CBP-CDP
4	C	407	CIT	C4-C3-C6-O6
3	B	402	COA	C3B-C4B-C5B-O5B
3	B	402	COA	S1P-C2P-C3P-N4P
3	C	403	COA	S1P-C2P-C3P-N4P
3	B	402	COA	C5B-O5B-P1A-O1A
3	B	402	COA	CCP-O6A-P2A-O3A
3	C	403	COA	C2B-C3B-O3B-P3B

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Mol	Chain	Res	Type	Atoms
3	A	401	COA	CAP-C9P-N8P-C7P
3	D	404	COA	CAP-C9P-N8P-C7P
4	C	407	CIT	O7-C3-C6-O5
4	D	408	CIT	O7-C3-C6-O5
3	D	404	COA	O9P-C9P-N8P-C7P
4	C	407	CIT	C4-C3-C6-O5
4	D	408	CIT	C4-C3-C6-O5
3	A	401	COA	O9P-C9P-N8P-C7P
4	B	406	CIT	C6-C3-C4-C5
4	A	405	CIT	C4-C3-C6-O6
3	B	402	COA	C2B-C3B-O3B-P3B
3	B	402	COA	P2A-O3A-P1A-O1A
3	B	402	COA	P2A-O3A-P1A-O2A
4	A	405	CIT	C2-C3-C6-O6
3	D	404	COA	CBP-CCP-O6A-P2A
3	D	404	COA	S1P-C2P-C3P-N4P
4	D	408	CIT	C2-C3-C4-C5

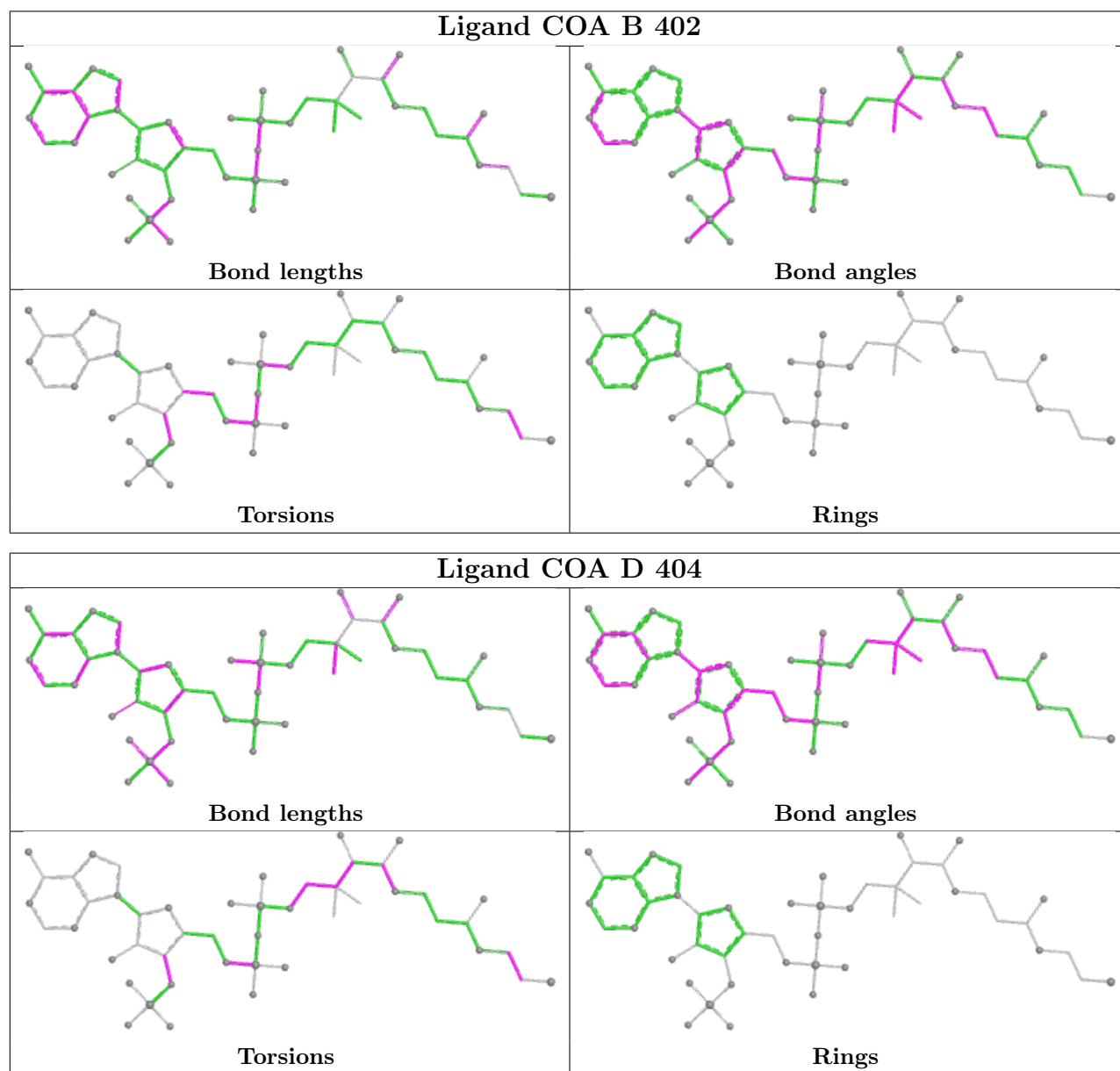
There are no ring outliers.

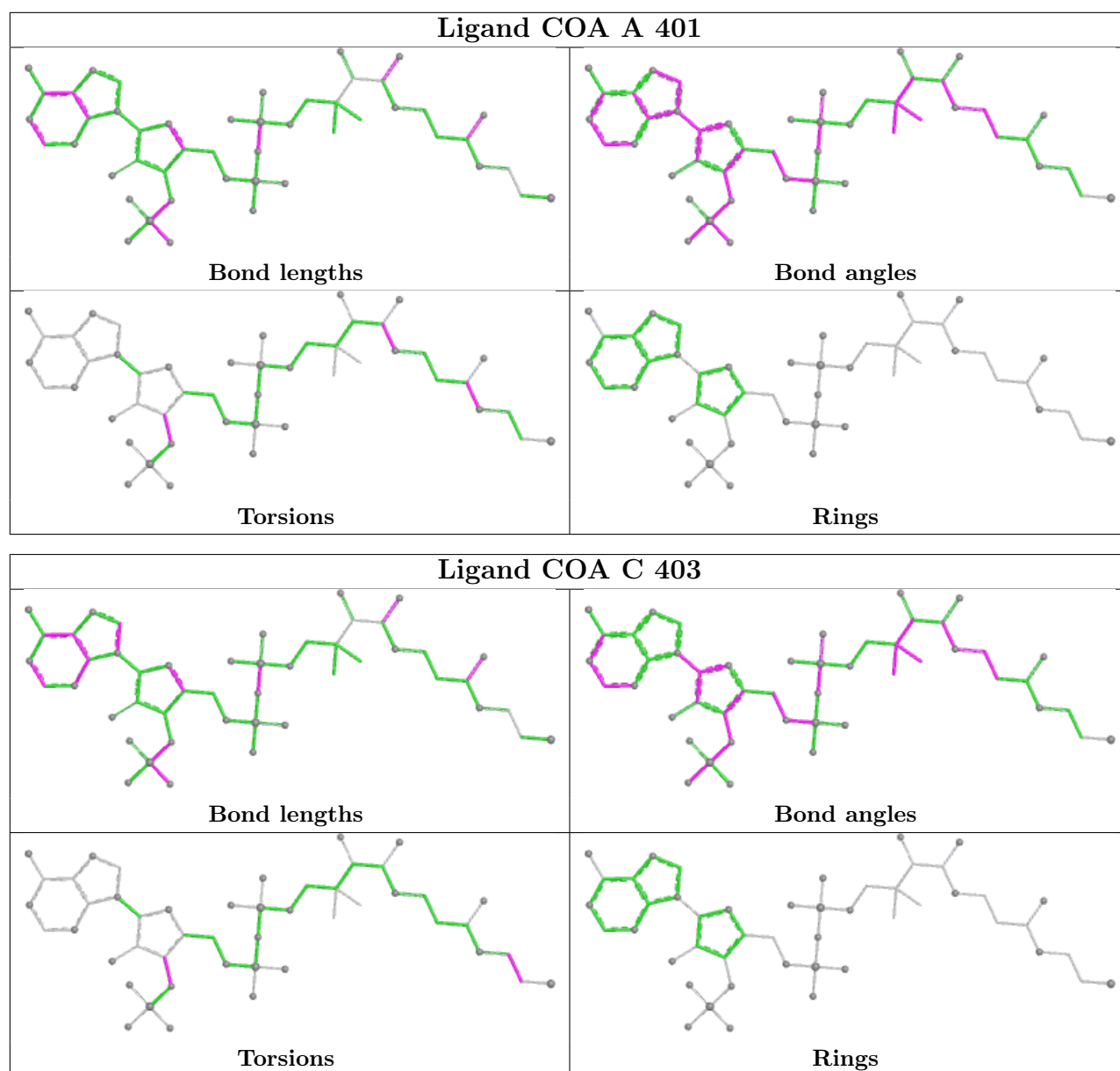
9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	406	CIT	1	0
3	B	402	COA	1	0
3	D	404	COA	11	0
4	D	408	CIT	6	0
4	A	405	CIT	1	0
2	B	382	SO4	1	0
3	A	401	COA	2	0
2	B	383	SO4	1	0
3	C	403	COA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	371/377 (98%)	1.58	65 (17%) 4 4	8, 21, 38, 49	21 (5%)
1	B	370/377 (98%)	1.42	53 (14%) 6 7	10, 21, 36, 55	24 (6%)
1	C	366/377 (97%)	1.71	100 (27%) 1 1	10, 25, 64, 79	30 (8%)
1	D	366/377 (97%)	1.55	86 (23%) 2 2	10, 23, 50, 64	28 (7%)
All	All	1473/1508 (97%)	1.56	304 (20%) 2 3	8, 22, 49, 79	103 (6%)

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	18.7
1	A	44	GLU	9.9
1	C	288	TYR	7.5
1	D	249	LYS	7.3
1	A	280	GLU	7.2
1	C	287	GLU	6.7
1	B	285	SER	6.5
1	A	284	HIS	6.3
1	B	280	GLU	6.2
1	D	277	LEU	6.2
1	C	278	VAL	5.7
1	A	153	HIS	5.5
1	A	156	ASN	5.4
1	A	42	SER	5.3
1	A	46	THR	5.3
1	A	178	LEU	4.9
1	C	247	LEU	4.9
1	D	286	LYS	4.8
1	D	293	ILE	4.8
1	D	248	ALA	4.7
1	C	248	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	244	ARG	4.6
1	C	220	GLY	4.5
1	C	249	LYS	4.4
1	A	125	ILE	4.0
1	D	228	ARG	4.0
1	C	298	ALA	3.9
1	C	306	GLY	3.9
1	C	251	GLU	3.8
1	C	277	LEU	3.7
1	A	3	VAL	3.7
1	D	303	ASN	3.7
1	C	303	ASN	3.7
1	C	302	LEU	3.6
1	D	298	ALA	3.6
1	C	238	ARG	3.6
1	C	293	ILE	3.6
1	C	262	LYS	3.5
1	C	300	LYS	3.5
1	D	250	LYS	3.5
1	C	314	TYR	3.5
1	C	297	GLU	3.5
1	C	244	ARG	3.5
1	C	236	PRO	3.4
1	C	235	THR	3.4
1	A	285	SER	3.4
1	C	240	ARG	3.4
1	A	18	CYS	3.4
1	C	290	ILE	3.3
1	C	242	TRP	3.3
1	C	241	GLU	3.3
1	C	301	VAL	3.3
1	C	234	GLY	3.3
1	C	250	LYS	3.3
1	A	172	ARG	3.2
1	C	228	ARG	3.2
1	C	354	ARG	3.2
1	C	154	ALA	3.2
1	C	237	GLU	3.2
1	B	375	ALA	3.2
1	C	245	GLU	3.2
1	D	294	VAL	3.2
1	D	302	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	232	GLU	3.1
1	A	177	ALA	3.1
1	A	368	VAL	3.1
1	B	100	SER	3.1
1	C	307	ILE	3.1
1	A	63	GLU	3.1
1	A	306	GLY	3.1
1	A	65	SER	3.0
1	D	263	ALA	3.0
1	C	291	LEU	3.0
1	C	296	GLU	3.0
1	D	301	VAL	3.0
1	B	126	ALA	3.0
1	D	253	ILE	3.0
1	B	244	ARG	3.0
1	A	175	ASP	3.0
1	C	360	ALA	2.9
1	C	18	CYS	2.9
1	C	230	ILE	2.9
1	D	308	TYR	2.9
1	A	223	ASN	2.9
1	A	227	MET	2.9
1	D	350	GLU	2.9
1	B	209	ALA	2.9
1	C	87	VAL	2.9
1	D	238	ARG	2.9
1	D	314	TYR	2.9
1	C	246	LYS	2.9
1	A	154	ALA	2.9
1	B	326	LEU	2.9
1	D	247	LEU	2.9
1	A	112	ILE	2.9
1	B	22	GLY	2.9
1	C	255	GLY	2.9
1	D	237	GLU	2.9
1	D	110	GLY	2.8
1	C	305	ARG	2.8
1	D	304	PRO	2.8
1	B	24	GLN	2.8
1	A	68	LEU	2.8
1	B	277	LEU	2.8
1	B	302	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	163	GLY	2.8
1	D	306	GLY	2.8
1	A	225	ALA	2.8
1	A	340	GLY	2.7
1	A	279	ALA	2.7
1	C	134	ALA	2.7
1	D	225	ALA	2.7
1	A	328	PHE	2.7
1	C	233	ILE	2.7
1	C	308	TYR	2.7
1	A	220	GLY	2.7
1	D	233	ILE	2.7
1	A	238	ARG	2.7
1	A	373	LEU	2.7
1	C	311	VAL	2.7
1	C	22	GLY	2.7
1	C	221	GLY	2.7
1	D	299	GLY	2.7
1	B	189	SER	2.7
1	D	89	ALA	2.6
1	D	246	LYS	2.6
1	C	223	ASN	2.6
1	C	353	ASN	2.6
1	B	269	GLY	2.6
1	C	276	ARG	2.6
1	A	49	LEU	2.6
1	C	28	TYR	2.6
1	C	265	ASP	2.6
1	C	243	VAL	2.6
1	A	59	GLN	2.6
1	B	202	ASP	2.6
1	C	333	PHE	2.6
1	C	373	LEU	2.6
1	D	366	LEU	2.6
1	C	374	GLU	2.6
1	A	126	ALA	2.6
1	A	375	ALA	2.6
1	B	76	ALA	2.6
1	B	275	ALA	2.6
1	D	116	ALA	2.6
1	D	48	PHE	2.6
1	B	370	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	251	GLU	2.5
1	B	133	ALA	2.5
1	C	313	PHE	2.5
1	C	371	VAL	2.5
1	B	319	TYR	2.5
1	A	287	GLU	2.5
1	B	245	GLU	2.5
1	D	296	GLU	2.5
1	D	188	ALA	2.5
1	D	245	GLU	2.5
1	D	374	GLU	2.5
1	A	305	ARG	2.5
1	C	346	LEU	2.5
1	C	229	MET	2.5
1	C	263	ALA	2.5
1	A	259	ARG	2.5
1	B	238	ARG	2.5
1	C	132	VAL	2.5
1	D	363	VAL	2.5
1	A	268	ALA	2.5
1	C	9	GLY	2.5
1	D	257	GLY	2.5
1	B	155	ALA	2.4
1	B	18	CYS	2.4
1	B	211	VAL	2.4
1	D	230	ILE	2.4
1	B	26	LYS	2.4
1	C	256	MET	2.4
1	D	373	LEU	2.4
1	B	241	GLU	2.4
1	B	154	ALA	2.4
1	C	325	SER	2.4
1	B	273	LYS	2.4
1	B	328	PHE	2.4
1	B	276	ARG	2.4
1	A	93	SER	2.4
1	D	251	GLU	2.4
1	C	370	TYR	2.3
1	B	300	LYS	2.3
1	C	299	GLY	2.3
1	C	155	ALA	2.3
1	C	97	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	376	ARG	2.3
1	A	30	TYR	2.3
1	A	250	LYS	2.3
1	C	19	TYR	2.3
1	C	26	LYS	2.3
1	C	29	TYR	2.3
1	C	343	GLY	2.3
1	D	336	ALA	2.3
1	A	57	ARG	2.3
1	B	293	ILE	2.3
1	D	307	ILE	2.3
1	C	62	GLU	2.3
1	D	169	GLU	2.3
1	D	317	VAL	2.3
1	B	223	ASN	2.3
1	D	168	PRO	2.3
1	C	67	ALA	2.3
1	C	239	ALA	2.3
1	D	209	ALA	2.3
1	D	268	ALA	2.3
1	A	376	ARG	2.3
1	D	224	GLU	2.3
1	C	294	VAL	2.3
1	D	371	VAL	2.3
1	B	156	ASN	2.3
1	D	309	PRO	2.3
1	C	216	GLY	2.3
1	A	308	TYR	2.3
1	B	19	TYR	2.3
1	D	28	TYR	2.3
1	C	295	GLU	2.3
1	C	375	ALA	2.2
1	A	208	THR	2.2
1	C	231	GLN	2.2
1	A	332	ILE	2.2
1	A	87	VAL	2.2
1	B	312	ASP	2.2
1	B	163	GLY	2.2
1	B	185	GLY	2.2
1	A	374	GLU	2.2
1	D	297	GLU	2.2
1	B	73	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	292	LYS	2.2
1	D	288	TYR	2.2
1	B	179	ILE	2.2
1	D	132	VAL	2.2
1	D	58	ARG	2.2
1	D	236	PRO	2.2
1	A	286	LYS	2.2
1	A	161	ALA	2.2
1	A	212	ALA	2.2
1	B	360	ALA	2.2
1	D	275	ALA	2.2
1	A	152	SER	2.2
1	A	233	ILE	2.2
1	B	253	ILE	2.2
1	A	276	ARG	2.2
1	D	17	MET	2.2
1	D	256	MET	2.2
1	A	110	GLY	2.2
1	C	257	GLY	2.2
1	D	185	GLY	2.2
1	B	38	ALA	2.2
1	D	155	ALA	2.2
1	D	315	SER	2.2
1	B	20	ILE	2.1
1	D	242	TRP	2.1
1	B	80	GLU	2.1
1	D	365	GLU	2.1
1	D	375	ALA	2.1
1	D	354	ARG	2.1
1	C	273	LYS	2.1
1	D	149	GLU	2.1
1	C	270	VAL	2.1
1	C	172	ARG	2.1
1	D	213	SER	2.1
1	D	62	GLU	2.1
1	D	59	GLN	2.1
1	C	157	PHE	2.1
1	B	340	GLY	2.1
1	D	9	GLY	2.1
1	C	357	ARG	2.1
1	A	235	THR	2.1
1	C	192	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	97	THR	2.1
1	A	262	LYS	2.1
1	B	250	LYS	2.1
1	A	245	GLU	2.1
1	C	365	GLU	2.1
1	A	150	ASP	2.1
1	C	125	ILE	2.1
1	D	187	ASN	2.1
1	A	288	TYR	2.1
1	C	166	PRO	2.1
1	D	264	PHE	2.1
1	D	328	PHE	2.1
1	B	242	TRP	2.1
1	D	305	ARG	2.1
1	A	73	ALA	2.0
1	B	169	GLU	2.0
1	C	210	ALA	2.0
1	C	326	LEU	2.0
1	D	367	ASP	2.0
1	D	19	TYR	2.0
1	D	319	TYR	2.0
1	D	368	VAL	2.0
1	A	121	GLY	2.0
1	A	333	PHE	2.0
1	B	82	PHE	2.0
1	C	167	SER	2.0
1	D	327	GLU	2.0
1	B	263	ALA	2.0
1	D	134	ALA	2.0
1	D	334	ALA	2.0
1	C	289	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

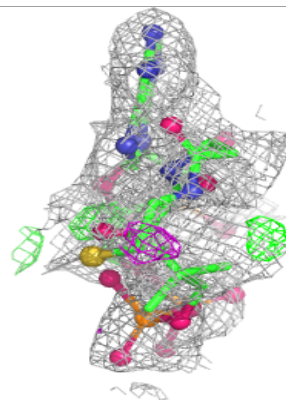
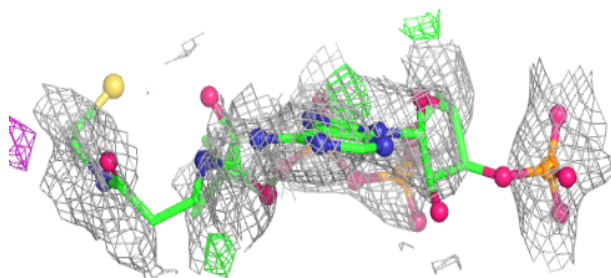
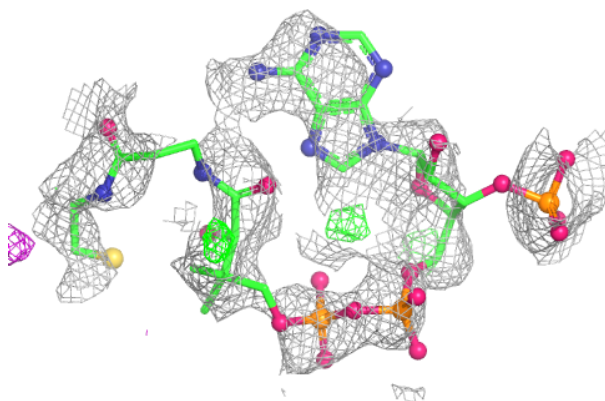
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.41	0.26	82,86,89,90	0
5	GOL	A	411	6/6	0.53	0.28	22,30,31,36	0
3	COA	C	403	48/48	0.55	0.20	63,73,81,82	0
5	GOL	C	413	6/6	0.55	0.30	43,47,50,51	0
3	COA	A	401	48/48	0.61	0.18	42,52,62,65	0
4	CIT	D	408	13/13	0.62	0.18	32,39,47,49	0
4	CIT	A	405	13/13	0.64	0.23	22,28,42,45	0
4	CIT	C	407	13/13	0.66	0.16	36,43,51,53	0
5	GOL	B	412	6/6	0.67	0.19	35,39,40,42	0
2	SO4	C	390	5/5	0.67	0.42	80,82,83,83	0
5	GOL	D	414	6/6	0.68	0.15	59,61,62,62	0
2	SO4	B	383	5/5	0.69	0.38	59,62,63,64	0
4	CIT	B	406	13/13	0.74	0.25	22,31,42,43	0
2	SO4	D	386	5/5	0.75	0.17	42,43,44,45	0
2	SO4	D	389	5/5	0.76	0.30	70,70,72,73	0
2	SO4	A	387	5/5	0.77	0.21	42,43,43,46	0
3	COA	B	402	48/48	0.77	0.14	18,25,43,45	0
2	SO4	B	382	5/5	0.81	0.24	52,55,56,58	0
2	SO4	B	385	5/5	0.87	0.21	43,43,44,45	0
2	SO4	C	388	5/5	0.88	0.12	49,50,51,53	0
2	SO4	C	381	5/5	0.91	0.14	25,26,27,29	0
2	SO4	A	391	5/5	0.94	0.10	15,16,17,19	0

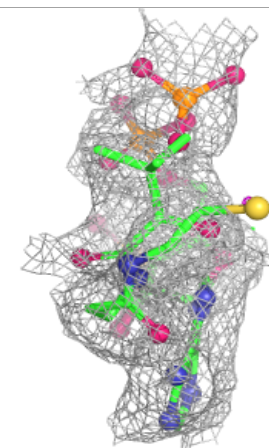
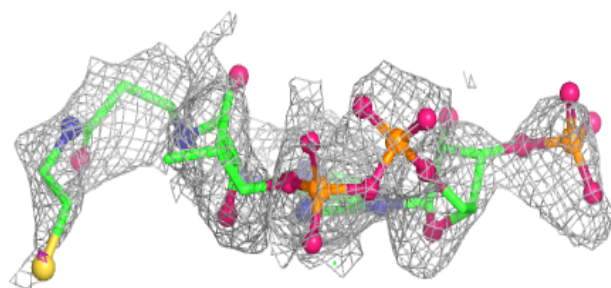
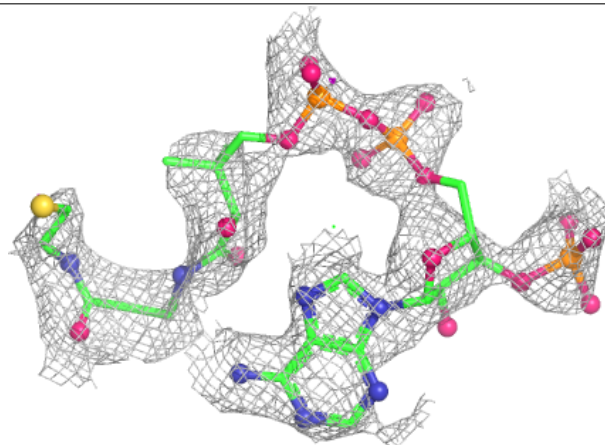
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 404:

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

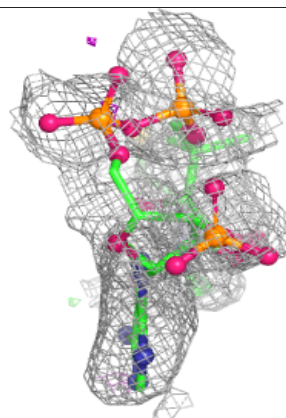
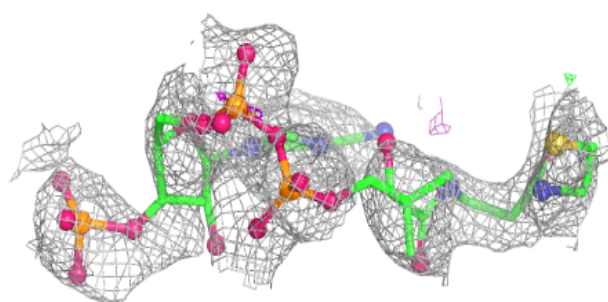
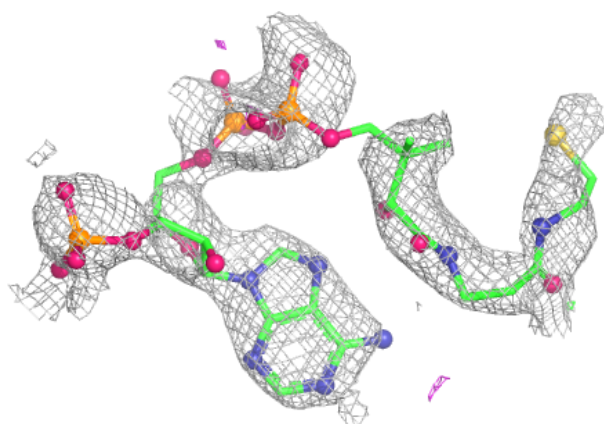
**Electron density around COA C 403:**

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

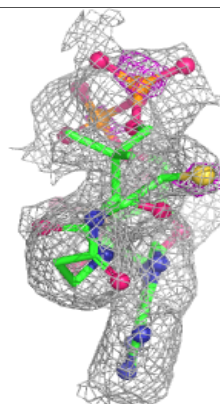
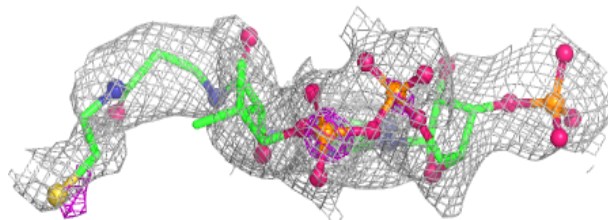
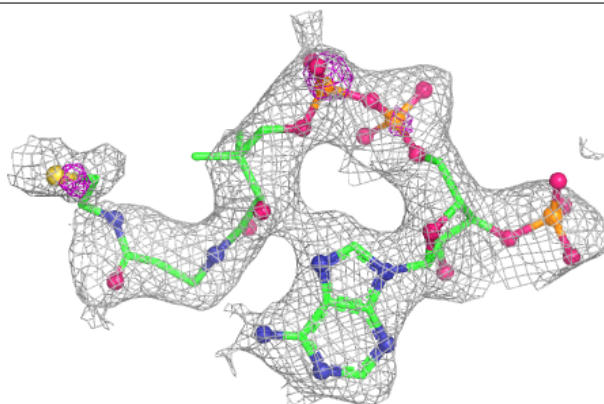


Electron density around COA A 401:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.