Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 06:09 PM JST

PDB ID	:	8IUP
Title	:	4-hydroxybutyryl-CoA Synthetase (ADP-forming) from Nitrosopumilus maritimus.
Authors	:	Johnson, J.; Demirci, H.
Deposited on	:	2023-03-24
Resolution	:	2.69 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

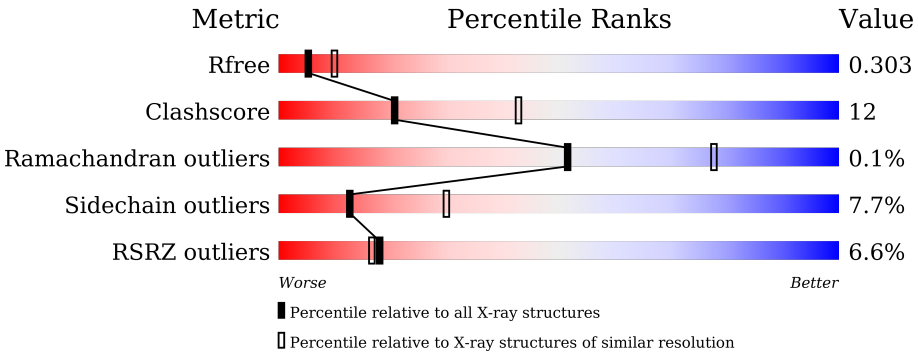
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	698	4% 65% 23% • 11%
1	B	698	8% 59% 27% • 10%

2 Entry composition

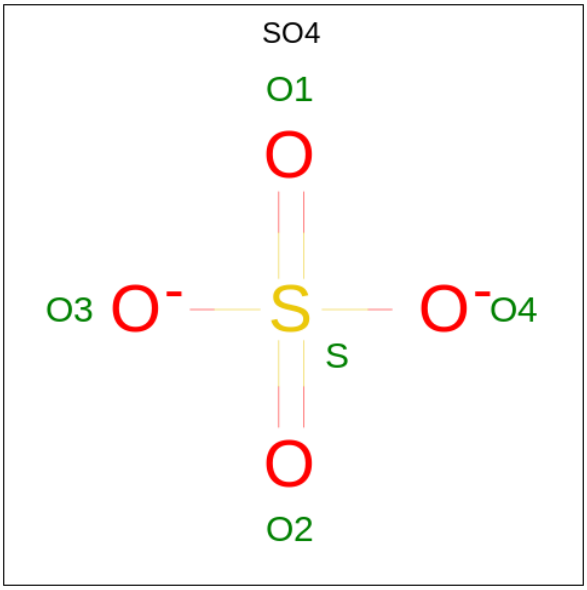
There are 3 unique types of molecules in this entry. The entry contains 9538 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-hydroxybutyrate--CoA ligase [ADP-forming].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	1	0
			4679	2975	780	891	33			
1	B	625	Total	C	N	O	S	0	0	0
			4718	3005	788	893	32			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

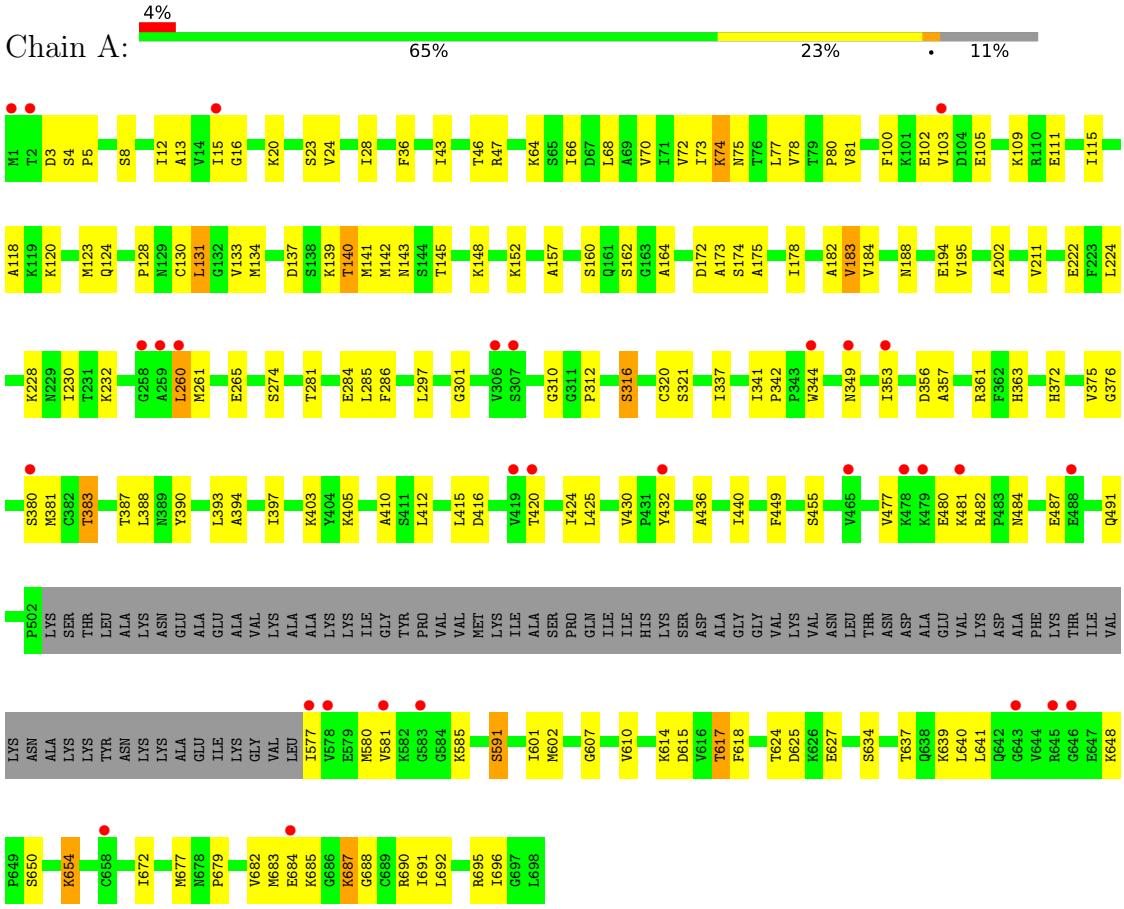
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	B	54	Total O 54 54	0	0

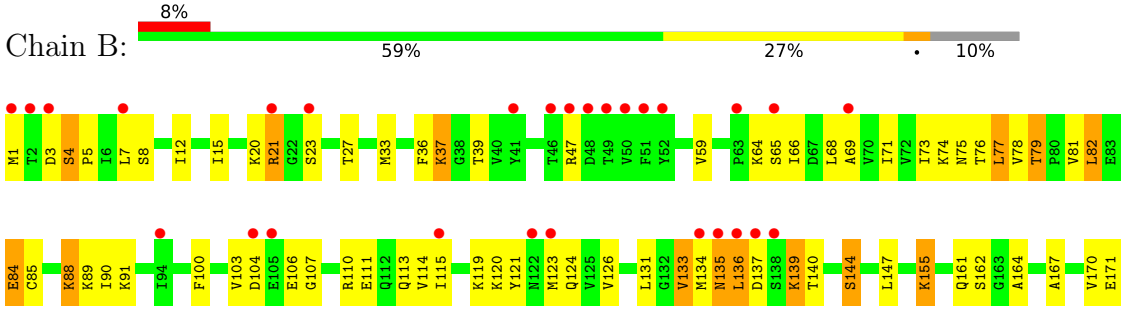
3 Residue-property plots (i)

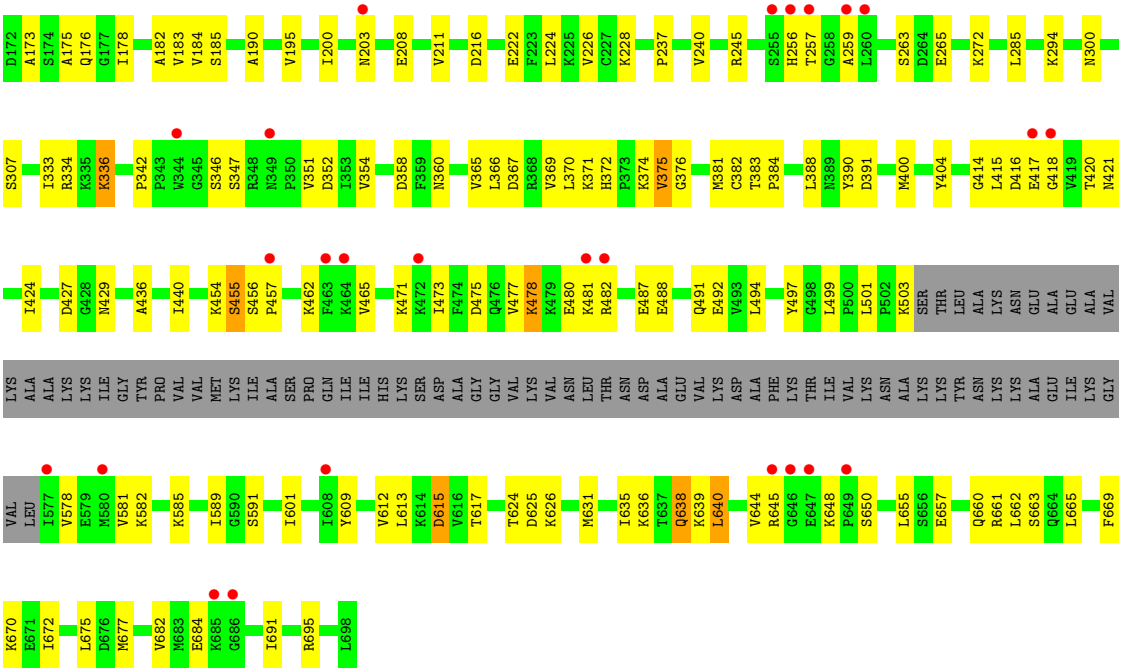
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-hydroxybutyrate--CoA ligase [ADP-forming]



• Molecule 1: 4-hydroxybutyrate--CoA ligase [ADP-forming]




D172 A173 S174 A175 Q176 G177 I178 A182 V183 V184 S185 A190 V195 I200 N203 E208 V211 D216 E222 F223 L224 K225 V226 C227 K228 P237 V240 R245 S255 H256 T257 G258 A259 L260 S263 D264 E265 K272 L285 K294 N300
S307 I333 R334 K335 K336 P342 P343 W344 G345 S346 S347 R348 N349 P350 V351 D352 I353 V354 D358 F359 N360 V365 L366 D367 R368 V369 L370 K371 H372 P373 K374 V375 G376 M381 C382 T383 P384 L388 N389 Y390 D391 M400 Y404 G414 L415 D416 E417 G418 V419 T420 N421
I424 D427 G428 N429 A436 I440 K454 S455 S456 P457 K462 F463 K464 V465 K471 K472 I473 F474 D475 Q476 V477 K478 K479 E480 K481 R482 E487 E488 Q491 E492 V493 L494 Y497 G498 L499 P500 L501 P502 K503 SER THR LEU ALA LYS ASN GLU ALA GLU ALA VAL
LYS ALA ALA LYS LYS ILE GLY TYR PRO VAL VAL MET LYS ILE ALA SER PRO GLN ILE ILE HIS LYS SER ASP ALA GLY GLY VAL LYS VAL ASN LEU THR ASN ASP ALA GLU VAL LYS ASP ALA PHE LYS THR ILE VAL LYS ASN ALA LYS LYS TYR ASN LYS LYS ALA GLU ILE LYS GLY
VAL LEU I577 V578 E579 M580 V581 K582 K585 I589 G590 S591 I601 I608 Y609 V612 L613 K614 D615 V616 T617 T624 D625 K626 M631 I635 K636 T637 Q638 K639 L640 V644 R645 G646 E647 K648 P649 S650 L655 S656 E657 Q660 R661 L662 S663 Q664 L665 F669
K670 E671 I672 L675 D676 M677 V682 M683 E684 K685 G686 I691 R695 L698

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	356.98Å 70.40Å 75.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.87 – 2.69 24.87 – 2.69	Depositor EDS
% Data completeness (in resolution range)	88.3 (24.87-2.69) 88.4 (24.87-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.84 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.304 0.255 , 0.303	Depositor DCC
R_{free} test set	2007 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/4741	0.48	0/6389
1	B	0.26	0/4782	0.50	0/6438
All	All	0.26	0/9523	0.49	0/12827

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	136	LEU	Peptide

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	4679	0	4848	103	0
1	B	4718	0	4946	144	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	77	0	0	6	0
3	B	54	0	0	3	0
All	All	9538	0	9794	236	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 12.

All (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HG21	1:A:81:VAL:HG11	1.56	0.85
1:A:134:MET:HB2	1:A:183:VAL:HG13	1.60	0.82
1:A:639:LYS:HB3	1:B:612:VAL:HG12	1.62	0.80
1:B:20:LYS:HB3	1:B:23:SER:HB3	1.65	0.78
1:A:412:LEU:H	1:A:432:TYR:HE1	1.30	0.77
1:A:172:ASP:HA	1:B:415:LEU:HB2	1.67	0.76
1:A:195:VAL:HG11	1:A:222:GLU:HB3	1.69	0.74
1:B:294:LYS:HE2	1:B:429:ASN:HA	1.70	0.74
1:B:4:SER:O	1:B:8:SER:N	2.16	0.74
1:B:257:THR:HG23	1:B:259:ALA:H	1.53	0.73
1:A:388:LEU:HD11	1:A:393:LEU:HD22	1.70	0.72
1:B:7:LEU:HD12	1:B:136:LEU:HG	1.72	0.72
1:B:136:LEU:HD11	1:B:184:VAL:HG22	1.71	0.71
1:B:4:SER:HA	1:B:7:LEU:HB3	1.73	0.70
1:B:100:PHE:HB3	1:B:111:GLU:HB2	1.74	0.69
1:A:173:ALA:HB1	1:A:178:ILE:HB	1.75	0.68
1:A:174:SER:OG	1:B:416:ASP:OD2	2.11	0.68
1:A:312:PRO:O	1:A:316:SER:OG	2.12	0.68
1:B:15:ILE:HD11	1:B:71:ILE:HG23	1.74	0.68
1:B:91:LYS:NZ	1:B:121:TYR:O	2.26	0.68
1:B:73:ILE:HD12	1:B:77:LEU:HD13	1.77	0.67
1:A:650:SER:HA	1:A:684:GLU:HA	1.77	0.66
1:A:78:VAL:HG21	1:A:100:PHE:CZ	2.32	0.65
1:B:74:LYS:NZ	3:B:805:HOH:O	2.27	0.65
1:B:120:LYS:NZ	3:B:807:HOH:O	2.29	0.65
1:B:640:LEU:HA	1:B:645:ARG:HD2	1.79	0.64
1:B:591:SER:HB2	1:B:601:ILE:HG22	1.81	0.63
1:B:455:SER:OG	1:B:626:LYS:NZ	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HD12	1:B:400:MET:HG3	1.82	0.61
1:A:13:ALA:HB2	1:A:66:ILE:HD13	1.83	0.61
1:A:15:ILE:HA	1:A:43:ILE:HB	1.83	0.60
1:B:195:VAL:HG11	1:B:222:GLU:HG3	1.83	0.60
1:B:418:GLY:HA2	1:B:421:ASN:HD21	1.67	0.60
1:A:577:ILE:N	3:A:808:HOH:O	2.33	0.60
1:A:47:ARG:NH2	3:A:809:HOH:O	2.34	0.59
1:B:134:MET:HB3	1:B:183:VAL:HB	1.84	0.59
1:A:20:LYS:HB3	1:A:23:SER:HB2	1.85	0.59
1:B:110:ARG:O	1:B:114:VAL:HG23	2.03	0.58
1:B:59:VAL:HG21	1:B:90:ILE:HD11	1.85	0.58
1:B:475:ASP:HA	1:B:478:LYS:HE3	1.86	0.58
1:A:16:GLY:HA2	1:A:73:ILE:HG23	1.85	0.57
1:B:134:MET:HE2	1:B:135:ASN:HB2	1.87	0.57
1:A:4:SER:HB3	1:A:8:SER:HB2	1.86	0.57
1:A:124:GLN:NE2	3:A:814:HOH:O	2.38	0.57
1:A:356:ASP:OD1	1:A:361:ARG:NH1	2.36	0.57
1:A:232:LYS:NZ	1:A:455:SER:OG	2.38	0.57
1:B:367:ASP:OD1	1:B:404:TYR:OH	2.14	0.56
1:B:78:VAL:O	1:B:81:VAL:HG12	2.05	0.56
1:A:100:PHE:HB3	1:A:111:GLU:HB2	1.87	0.56
1:B:161:GLN:NE2	1:B:216:ASP:OD1	2.30	0.56
1:A:194:GLU:OE2	3:A:802:HOH:O	2.18	0.56
1:B:372:HIS:HE1	1:B:374:LYS:HB2	1.69	0.56
1:A:211:VAL:HG13	1:A:285:LEU:HD22	1.88	0.56
1:B:471:LYS:HD3	1:B:669:PHE:HE1	1.71	0.56
1:B:7:LEU:HA	1:B:136:LEU:HD23	1.88	0.55
1:A:640:LEU:HG	1:B:612:VAL:HG11	1.88	0.55
1:B:657:GLU:O	1:B:661:ARG:HG3	2.06	0.55
1:B:144:SER:O	1:B:144:SER:OG	2.25	0.55
1:B:384:PRO:HG3	1:B:414:GLY:HA3	1.88	0.55
1:A:131:LEU:HD22	1:A:145:THR:HB	1.89	0.55
1:A:173:ALA:HB2	1:A:286:PHE:CE2	2.43	0.54
1:B:333:ILE:HA	1:B:336:LYS:HD3	1.89	0.54
1:B:672:ILE:HG23	1:B:675:LEU:HD23	1.89	0.53
1:B:644:VAL:HG12	1:B:644:VAL:O	2.08	0.53
1:B:372:HIS:CE1	1:B:374:LYS:HB2	2.43	0.53
1:A:585:LYS:HD2	1:A:640:LEU:O	2.09	0.53
1:B:78:VAL:HG11	1:B:100:PHE:HZ	1.73	0.53
1:A:390:TYR:OH	3:A:801:HOH:O	2.17	0.53
1:B:366:LEU:HB3	1:B:400:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:LEU:HD12	1:B:640:LEU:H	1.73	0.53
1:B:457:PRO:HB3	1:B:626:LYS:HG3	1.91	0.52
1:B:37:LYS:HD2	1:B:37:LYS:H	1.74	0.52
1:A:301:GLY:H	1:A:376:GLY:HA3	1.73	0.52
1:B:106:GLU:HG3	1:B:110:ARG:NH2	2.24	0.52
1:B:635:ILE:HD12	1:B:638:GLN:HG2	1.91	0.52
1:A:137:ASP:HB2	1:A:140:THR:HG23	1.91	0.52
1:A:78:VAL:HG21	1:A:100:PHE:HZ	1.72	0.52
1:A:357:ALA:O	1:A:387:THR:OG1	2.25	0.52
1:A:381:MET:HE1	1:A:436:ALA:HB1	1.92	0.52
1:A:4:SER:N	1:A:5:PRO:HD2	2.25	0.51
1:B:347:SER:HB3	1:B:352:ASP:H	1.76	0.51
1:B:12:ILE:HG12	1:B:68:LEU:HD23	1.92	0.51
1:B:134:MET:CE	1:B:135:ASN:HB2	2.40	0.51
1:A:310:GLY:HA3	1:B:256:HIS:CE1	2.46	0.51
1:A:137:ASP:HB3	1:A:139:LYS:HD3	1.93	0.51
1:A:342:PRO:HB2	1:A:344:TRP:HD1	1.75	0.50
1:B:79:THR:HG21	1:B:113:GLN:HB3	1.93	0.50
1:B:211:VAL:HG13	1:B:285:LEU:HD22	1.94	0.50
1:A:78:VAL:HG21	1:A:100:PHE:CE2	2.47	0.50
1:B:78:VAL:HG11	1:B:100:PHE:CZ	2.46	0.50
1:B:488:GLU:O	1:B:492:GLU:HG2	2.12	0.50
1:B:147:LEU:HD13	1:B:170:VAL:HG11	1.93	0.49
1:B:585:LYS:NZ	1:B:640:LEU:O	2.38	0.49
1:B:133:VAL:HG13	1:B:136:LEU:HD13	1.93	0.49
1:B:457:PRO:HB2	1:B:624:THR:HB	1.95	0.49
1:A:260:LEU:HD23	1:A:261:MET:H	1.76	0.49
1:B:85:CYS:SG	1:B:90:ILE:HD12	2.52	0.49
1:B:195:VAL:HG13	1:B:226:VAL:HG21	1.93	0.49
1:B:103:VAL:O	1:B:107:GLY:N	2.45	0.49
1:A:585:LYS:HB2	1:A:682:VAL:HG13	1.93	0.48
1:B:487:GLU:O	1:B:491:GLN:HG2	2.12	0.48
1:A:100:PHE:CD1	1:A:128:PRO:HB3	2.48	0.48
1:A:637:THR:C	1:A:639:LYS:H	2.16	0.48
1:A:118:ALA:HA	1:A:123:MET:HB2	1.96	0.48
1:B:82:LEU:HA	1:B:85:CYS:HB2	1.95	0.48
1:A:100:PHE:O	1:A:188:ASN:ND2	2.47	0.48
1:B:390:TYR:CD2	1:B:417:GLU:HB2	2.49	0.48
1:B:69:ALA:HB2	1:B:90:ILE:HD13	1.95	0.47
1:B:263:SER:OG	1:B:265:GLU:HG3	2.14	0.47
1:A:133:VAL:HG13	1:A:184:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LYS:C	1:A:641:LEU:H	2.16	0.47
1:A:480:GLU:OE1	1:A:482:ARG:NH1	2.48	0.47
1:B:103:VAL:HB	1:B:107:GLY:H	1.79	0.47
1:B:21:ARG:H	1:B:21:ARG:HD3	1.79	0.47
1:A:224:LEU:O	1:A:228:LYS:HB2	2.13	0.47
1:B:37:LYS:HD2	1:B:37:LYS:N	2.30	0.47
1:A:602:MET:HG3	1:A:618:PHE:CE2	2.49	0.47
1:A:74:LYS:H	1:A:74:LYS:HD2	1.79	0.47
1:A:685:LYS:HD2	1:A:685:LYS:HA	1.72	0.47
1:A:111:GLU:O	1:A:115:ILE:HG23	2.15	0.46
1:A:342:PRO:HB2	1:A:344:TRP:CD1	2.50	0.46
1:B:81:VAL:O	1:B:84:GLU:HG3	2.15	0.46
1:B:672:ILE:CG2	1:B:675:LEU:HD23	2.45	0.46
1:B:147:LEU:HD21	1:B:167:ALA:HA	1.96	0.46
1:B:176:GLN:HB2	1:B:178:ILE:HD11	1.97	0.46
1:B:351:VAL:HG11	1:B:365:VAL:HG11	1.98	0.46
1:A:624:THR:OG1	1:A:627:GLU:HG3	2.16	0.46
1:B:503:LYS:O	1:B:578:VAL:HA	2.16	0.46
1:B:609:TYR:HB3	1:B:613:LEU:HD12	1.97	0.46
1:A:581:VAL:HG11	1:A:690:ARG:HG3	1.97	0.46
1:B:74:LYS:HD2	1:B:76:THR:H	1.80	0.46
1:A:157:ALA:HA	1:A:182:ALA:O	2.16	0.46
1:B:121:TYR:HB2	1:B:123:MET:HG3	1.98	0.46
1:B:499:LEU:O	1:B:501:LEU:HD12	2.16	0.46
1:B:589:ILE:O	1:B:677:MET:HB2	2.16	0.46
1:B:137:ASP:HB2	1:B:139:LYS:O	2.16	0.45
1:A:139:LYS:HD2	1:A:139:LYS:N	2.30	0.45
1:A:137:ASP:O	1:A:141:MET:HG2	2.15	0.45
1:A:337:ILE:O	1:A:341:ILE:HG12	2.16	0.45
1:A:591:SER:HB2	1:A:601:ILE:HD13	1.97	0.45
1:B:639:LYS:HD2	1:B:639:LYS:HA	1.75	0.45
1:B:119:LYS:HE2	1:B:119:LYS:HB2	1.89	0.45
1:B:480:GLU:O	1:B:481:LYS:HG2	2.16	0.45
1:A:477:VAL:HG22	1:A:482:ARG:NH2	2.31	0.45
1:A:672:ILE:HG23	1:A:696:ILE:HG23	1.98	0.45
1:A:415:LEU:HB2	1:B:171:GLU:O	2.17	0.45
1:B:358:ASP:HB2	1:B:360:ASN:OD1	2.17	0.45
1:A:380:SER:O	1:A:410:ALA:HA	2.17	0.45
1:B:421:ASN:HA	1:B:424:ILE:HD12	1.98	0.45
1:A:164:ALA:HB1	1:B:383:THR:HG21	1.98	0.44
1:A:316:SER:HB3	1:A:440:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:HZ3	1:B:65:SER:H	1.63	0.44
1:B:307:SER:HA	1:B:381:MET:O	2.17	0.44
1:B:334:ARG:NH2	1:B:346:SER:O	2.51	0.44
1:B:173:ALA:HA	1:B:178:ILE:HD13	1.99	0.44
1:B:462:LYS:HZ1	1:B:660:GLN:HB3	1.82	0.44
1:B:615:ASP:OD1	1:B:636:LYS:N	2.47	0.44
1:A:75:ASN:O	1:A:78:VAL:HG22	2.17	0.44
1:A:105:GLU:HG2	1:A:109:LYS:NZ	2.33	0.44
1:B:334:ARG:HA	1:B:334:ARG:HD2	1.84	0.44
1:B:155:LYS:HB3	1:B:208:GLU:HG3	2.00	0.44
1:B:436:ALA:O	1:B:440:ILE:HG12	2.17	0.44
1:B:462:LYS:HB2	1:B:465:VAL:HG23	1.98	0.44
1:A:36:PHE:CD1	1:A:142:MET:HB2	2.52	0.44
1:A:152:LYS:HB2	1:A:152:LYS:HE3	1.54	0.44
1:A:265:GLU:H	1:A:265:GLU:HG2	1.64	0.44
1:B:333:ILE:CA	1:B:336:LYS:HD3	2.48	0.44
1:B:475:ASP:O	1:B:478:LYS:HD2	2.18	0.44
1:B:473:ILE:O	1:B:477:VAL:HG23	2.17	0.44
1:B:365:VAL:O	1:B:369:VAL:HG13	2.17	0.43
1:A:383:THR:HG21	1:B:164:ALA:HB1	1.99	0.43
1:A:679:PRO:HG2	1:A:692:LEU:HB2	2.01	0.43
1:B:650:SER:HA	1:B:684:GLU:HB2	2.01	0.43
1:B:115:ILE:HG22	1:B:190:ALA:HB1	1.99	0.43
1:A:607:GLY:O	1:A:610:VAL:HG12	2.18	0.43
1:B:111:GLU:O	1:B:115:ILE:HG23	2.19	0.43
1:B:88:LYS:O	1:B:89:LYS:HG2	2.18	0.43
1:B:640:LEU:HD23	1:B:645:ARG:NH2	2.34	0.43
1:B:224:LEU:O	1:B:228:LYS:HB2	2.18	0.43
1:A:160:SER:OG	1:A:162:SER:O	2.34	0.43
1:A:615:ASP:OD2	1:A:637:THR:HG23	2.19	0.43
1:B:136:LEU:HD12	1:B:136:LEU:HA	1.55	0.42
1:B:415:LEU:HD23	1:B:415:LEU:HA	1.82	0.42
1:A:64:LYS:HA	1:A:64:LYS:HD2	1.76	0.42
1:A:687:LYS:H	1:A:687:LYS:HG3	1.42	0.42
1:B:391:ASP:OD1	1:B:420:THR:HB	2.19	0.42
1:A:173:ALA:HA	1:A:178:ILE:HD12	2.01	0.42
1:B:382:CYS:HG	1:B:390:TYR:HE1	1.66	0.42
1:B:7:LEU:HA	1:B:136:LEU:HB3	2.02	0.42
1:B:333:ILE:HA	1:B:336:LYS:HZ3	1.84	0.42
1:B:342:PRO:HB2	1:B:354:VAL:HG21	2.02	0.42
1:A:394:ALA:HB1	1:A:425:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASP:O	1:B:371:LYS:HG3	2.19	0.42
1:A:677:MET:HG2	1:A:691:ILE:HG21	2.01	0.42
1:B:3:ASP:OD2	1:B:124:GLN:HG3	2.19	0.42
1:A:344:TRP:CD1	1:A:344:TRP:N	2.88	0.42
1:B:126:VAL:HG21	1:B:133:VAL:HG21	2.01	0.42
1:B:388:LEU:HA	3:B:820:HOH:O	2.20	0.42
1:B:591:SER:HA	1:B:601:ILE:HA	2.02	0.42
1:A:297:LEU:HD21	1:A:449:PHE:HD2	1.84	0.41
1:A:625:ASP:N	1:A:625:ASP:OD1	2.53	0.41
1:B:7:LEU:HD13	1:B:200:ILE:HG22	2.02	0.41
1:B:66:ILE:CD1	1:B:90:ILE:HG12	2.51	0.41
1:A:102:GLU:OE2	3:A:803:HOH:O	2.22	0.41
1:B:162:SER:OG	2:B:701:SO4:O1	2.31	0.41
1:B:462:LYS:HG3	1:B:661:ARG:HG2	2.01	0.41
1:B:617:THR:HG21	1:B:631:MET:O	2.20	0.41
1:B:677:MET:HG2	1:B:691:ILE:HG21	2.02	0.41
1:A:281:THR:OG1	1:A:284:GLU:HG3	2.20	0.41
1:A:353:ILE:CG2	1:A:361:ARG:HD2	2.51	0.41
1:A:397:ILE:HG22	1:A:430:VAL:HG21	2.02	0.41
1:A:372:HIS:HB3	1:A:375:VAL:HG23	2.02	0.41
1:B:457:PRO:HB3	1:B:626:LYS:CG	2.49	0.41
1:B:300:ASN:OD1	1:B:376:GLY:HA3	2.20	0.41
1:A:134:MET:HG2	1:A:143:ASN:HA	2.02	0.41
1:A:654:LYS:HG2	1:A:688:GLY:HA3	2.03	0.41
1:A:175:ALA:HB3	1:B:415:LEU:HB3	2.03	0.41
1:A:310:GLY:HA3	1:B:256:HIS:HE1	1.86	0.41
1:A:415:LEU:HA	1:B:175:ALA:HB2	2.02	0.41
1:A:648:LYS:HE2	1:A:684:GLU:CD	2.41	0.41
1:B:4:SER:N	1:B:5:PRO:HD2	2.35	0.41
1:B:36:PHE:HA	1:B:140:THR:O	2.21	0.41
1:B:135:ASN:O	1:B:182:ALA:HA	2.21	0.41
1:A:77:LEU:C	1:A:80:PRO:HD2	2.42	0.41
1:A:202:ALA:HB2	1:A:230:ILE:HD11	2.03	0.41
1:B:88:LYS:HA	1:B:88:LYS:HD2	1.90	0.41
1:B:176:GLN:HB2	1:B:178:ILE:CD1	2.52	0.40
1:B:589:ILE:HG22	1:B:662:LEU:HD22	2.03	0.40
1:A:224:LEU:HD12	1:A:274:SER:HB3	2.04	0.40
1:B:655:LEU:HD13	1:B:682:VAL:HG21	2.04	0.40
1:A:487:GLU:O	1:A:491:GLN:HG3	2.20	0.40
1:B:372:HIS:HB3	1:B:375:VAL:HG13	2.04	0.40
1:B:497:TYR:CE2	1:B:665:LEU:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HG12	1:A:68:LEU:HD23	2.04	0.40
1:A:617:THR:HG21	1:A:634:SER:HB2	2.03	0.40
1:B:477:VAL:HG22	1:B:482:ARG:HH22	1.87	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	621/698 (89%)	602 (97%)	19 (3%)	0	100 100
1	B	621/698 (89%)	591 (95%)	29 (5%)	1 (0%)	47 73
All	All	1242/1396 (89%)	1193 (96%)	48 (4%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	512/589 (87%)	475 (93%)	37 (7%)	14 34
1	B	523/589 (89%)	479 (92%)	44 (8%)	11 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1035/1178 (88%)	954 (92%)	81 (8%)	13 29

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	24	VAL
1	A	28	ILE
1	A	46	THR
1	A	70	VAL
1	A	72	VAL
1	A	74	LYS
1	A	103	VAL
1	A	120	LYS
1	A	130	CYS
1	A	131	LEU
1	A	140	THR
1	A	148	LYS
1	A	183	VAL
1	A	260	LEU
1	A	316	SER
1	A	320[A]	CYS
1	A	320[B]	CYS
1	A	321	SER
1	A	349	ASN
1	A	363	HIS
1	A	383	THR
1	A	403	LYS
1	A	405	LYS
1	A	416	ASP
1	A	420	THR
1	A	424	ILE
1	A	481	LYS
1	A	484	ASN
1	A	580	MET
1	A	591	SER
1	A	614	LYS
1	A	617	THR
1	A	654	LYS
1	A	683	MET
1	A	687	LYS
1	A	695	ARG

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Mol	Chain	Res	Type
1	B	1	MET
1	B	4	SER
1	B	21	ARG
1	B	27	THR
1	B	33	MET
1	B	37	LYS
1	B	39	THR
1	B	47	ARG
1	B	75	ASN
1	B	77	LEU
1	B	79	THR
1	B	82	LEU
1	B	84	GLU
1	B	88	LYS
1	B	104	ASP
1	B	131	LEU
1	B	135	ASN
1	B	139	LYS
1	B	144	SER
1	B	155	LYS
1	B	185	SER
1	B	203	ASN
1	B	237	PRO
1	B	240	VAL
1	B	245	ARG
1	B	272	LYS
1	B	336	LYS
1	B	375	VAL
1	B	427	ASP
1	B	454	LYS
1	B	455	SER
1	B	456	SER
1	B	478	LYS
1	B	494	LEU
1	B	581	VAL
1	B	582	LYS
1	B	615	ASP
1	B	625	ASP
1	B	638	GLN
1	B	640	LEU
1	B	648	LYS
1	B	663	SER

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Mol	Chain	Res	Type
1	B	670	LYS
1	B	695	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	B	122	ASN
1	B	204	HIS
1	B	421	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	701	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	701	-	4,4,4	0.14	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

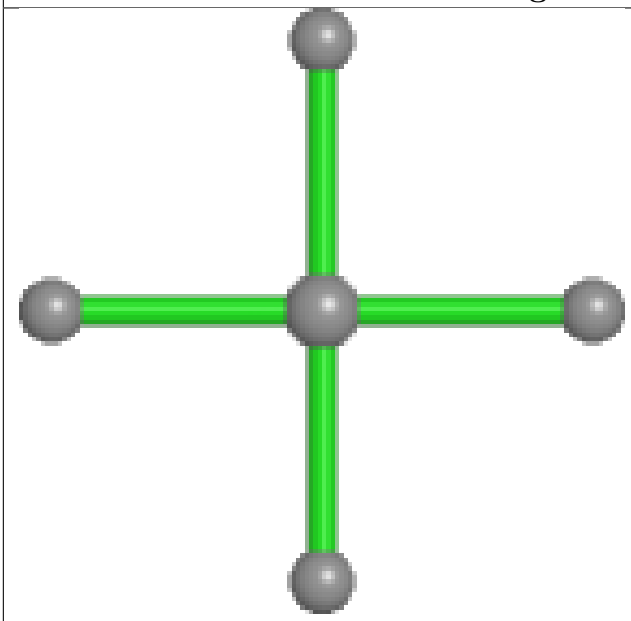
There are no ring outliers.

1 monomer is involved in 1 short contact:

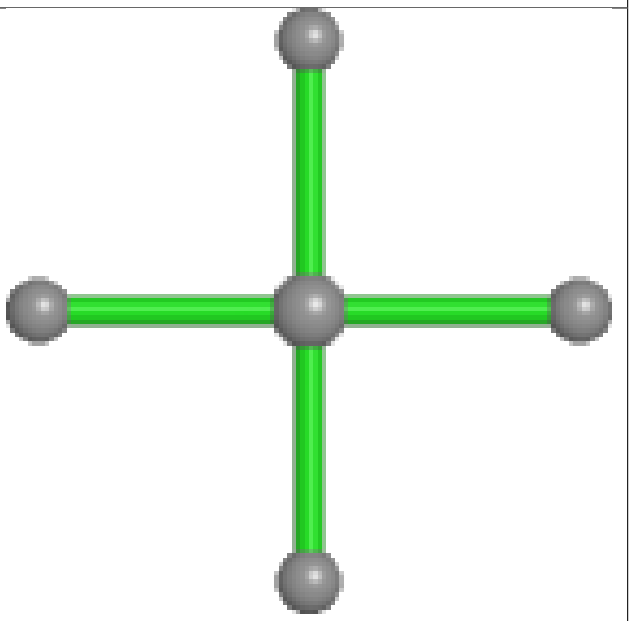
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	SO4	1	0

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 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.

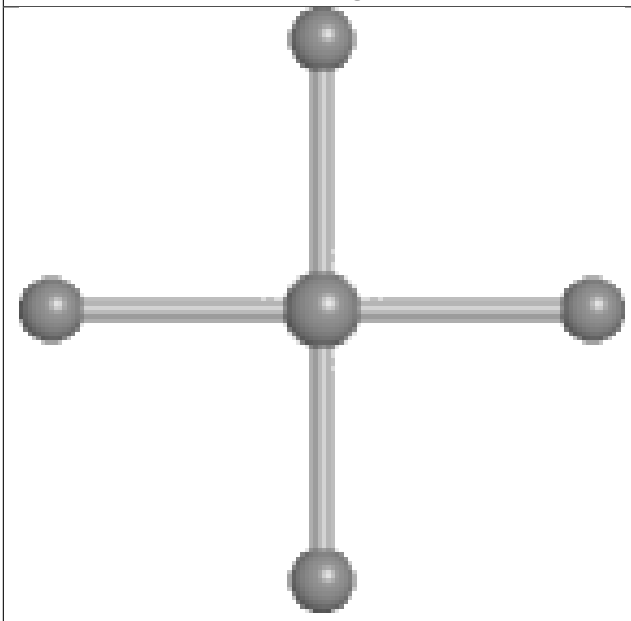
Ligand SO4 B 701



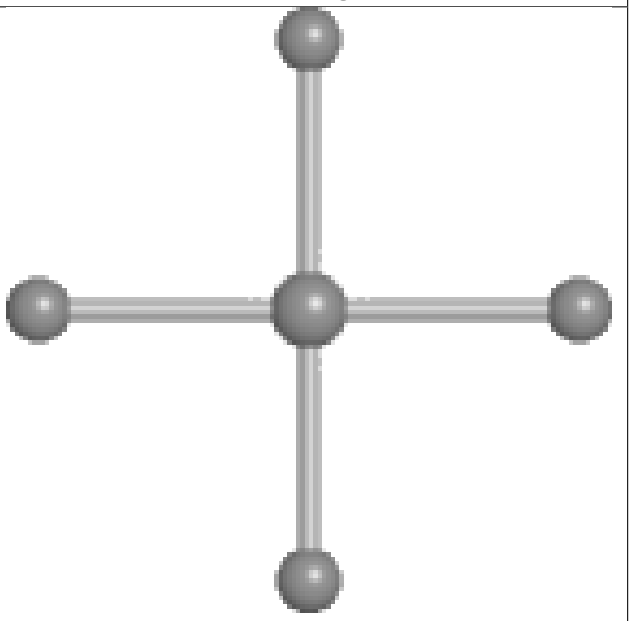
Bond lengths



Bond angles

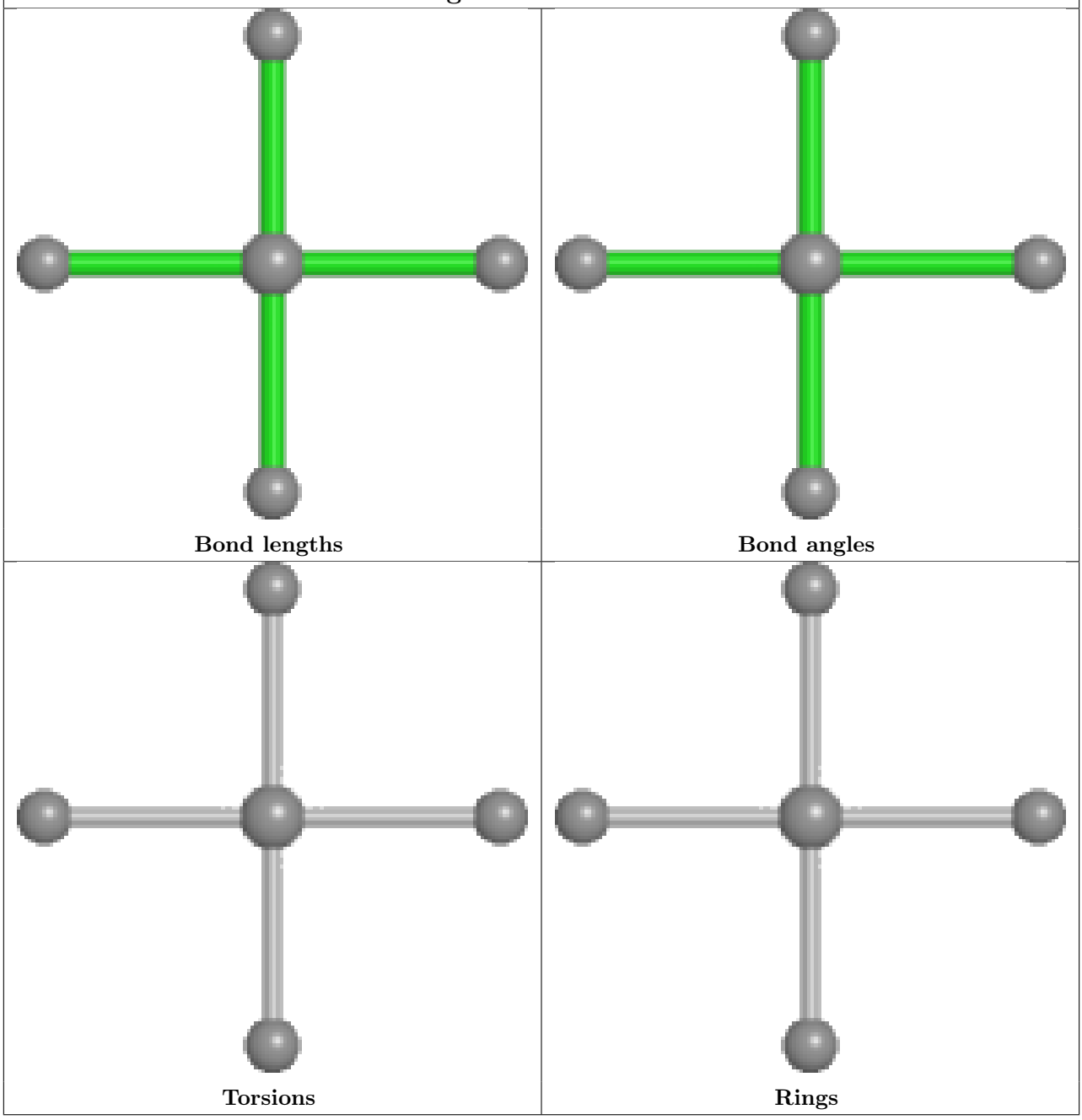


Torsions



Rings

Ligand SO4 A 701



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, 95^{th} 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	624/698 (89%)	0.16	30 (4%) 30 28	22, 51, 87, 132	0
1	B	625/698 (89%)	0.44	53 (8%) 10 9	20, 60, 95, 136	0
All	All	1249/1396 (89%)	0.30	83 (6%) 18 16	20, 55, 92, 136	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	14.8
1	B	2	THR	9.4
1	A	2	THR	8.6
1	B	136	LEU	7.1
1	A	1	MET	6.9
1	B	418	GLY	6.9
1	B	645	ARG	6.4
1	A	646	GLY	6.1
1	B	646	GLY	6.0
1	B	685	LYS	5.8
1	B	65	SER	5.5
1	B	135	ASN	5.4
1	A	577	ILE	5.2
1	A	419	VAL	5.2
1	A	259	ALA	4.6
1	B	463	PHE	4.4
1	B	48	ASP	4.2
1	B	686	GLY	4.1
1	A	465	VAL	4.1
1	B	608	ILE	3.9
1	A	103	VAL	3.9
1	A	349	ASN	3.8
1	A	578	VAL	3.7
1	B	104	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	684	GLU	3.6
1	B	649	PRO	3.5
1	B	647	GLU	3.5
1	B	69	ALA	3.5
1	B	259	ALA	3.3
1	B	457	PRO	3.3
1	A	658	CYS	3.2
1	B	257	THR	3.2
1	B	123	MET	3.1
1	A	258	GLY	3.0
1	B	46	THR	3.0
1	B	481	LYS	3.0
1	A	581	VAL	2.9
1	B	41	TYR	2.9
1	B	52	TYR	2.9
1	B	134	MET	2.9
1	A	488	GLU	2.9
1	A	306	VAL	2.8
1	B	47	ARG	2.8
1	A	432	TYR	2.8
1	B	482	ARG	2.7
1	A	478	LYS	2.7
1	A	344	TRP	2.7
1	B	577	ILE	2.7
1	B	21	ARG	2.6
1	B	115	ILE	2.6
1	B	256	HIS	2.6
1	A	260	LEU	2.5
1	B	138	SER	2.5
1	A	15	ILE	2.5
1	B	63	PRO	2.5
1	B	7	LEU	2.5
1	B	50	VAL	2.5
1	A	380	SER	2.4
1	B	203	ASN	2.4
1	B	49	THR	2.4
1	B	344	TRP	2.4
1	B	255	SER	2.4
1	B	137	ASP	2.4
1	B	349	ASN	2.3
1	A	481	LYS	2.3
1	B	94	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	307	SER	2.3
1	B	260	LEU	2.2
1	B	464	LYS	2.2
1	A	353	ILE	2.2
1	A	583	GLY	2.2
1	B	23	SER	2.2
1	B	122	ASN	2.1
1	A	420	THR	2.1
1	A	643	GLY	2.1
1	B	472	LYS	2.1
1	B	417	GLU	2.1
1	B	51	PHE	2.1
1	B	105	GLU	2.1
1	B	3	ASP	2.1
1	A	479	LYS	2.0
1	B	580	MET	2.0
1	A	645	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

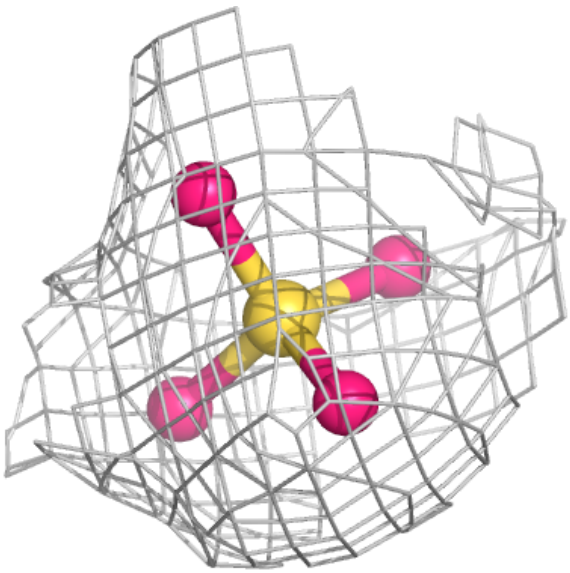
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

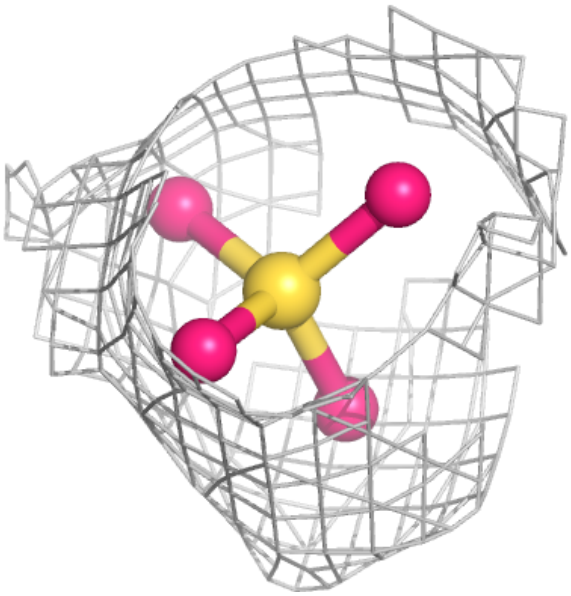
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	701	5/5	0.97	0.10	52,58,73,74	0
2	SO4	A	701	5/5	0.99	0.08	40,52,64,80	0

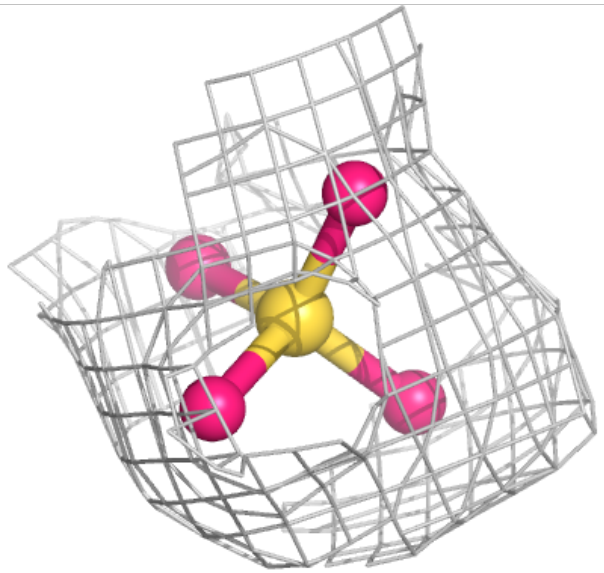
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SO4 B 701:

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

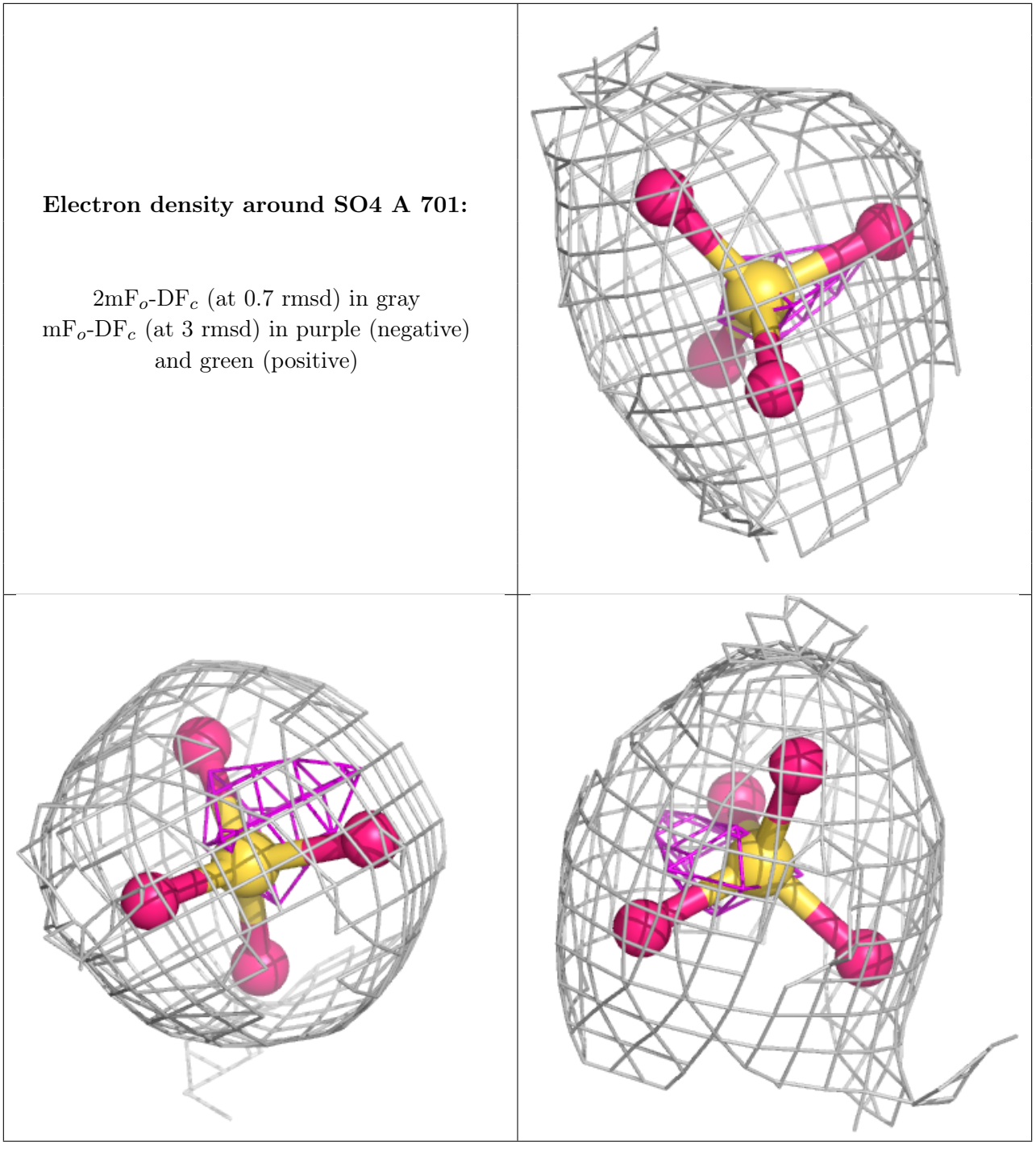






Electron density around SO4 A 701:

$2mF_o$-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.