



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2025 – 08:09 PM JST

PDB ID : 8WZU
Title : 4-hydroxybutyryl-CoA Synthetase (ADP-forming) from *Nitrosopumilus maritimus*.
Authors : Johnson, J.; Demirci, H.
Deposited on : 2023-11-02
Resolution : 2.80 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)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

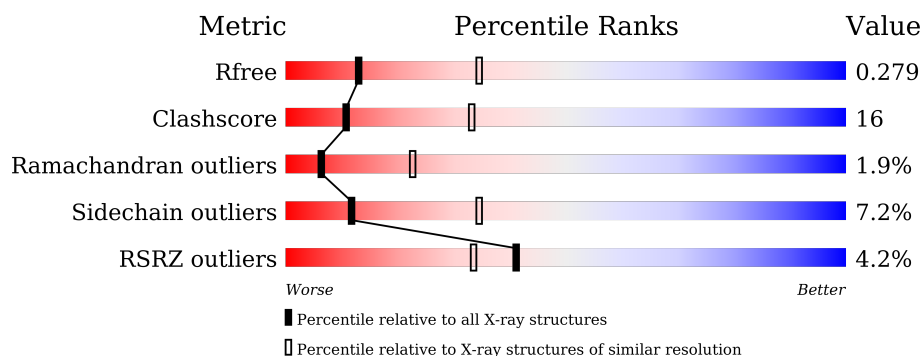
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	698	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	698	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>23%</div> <div>5%</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

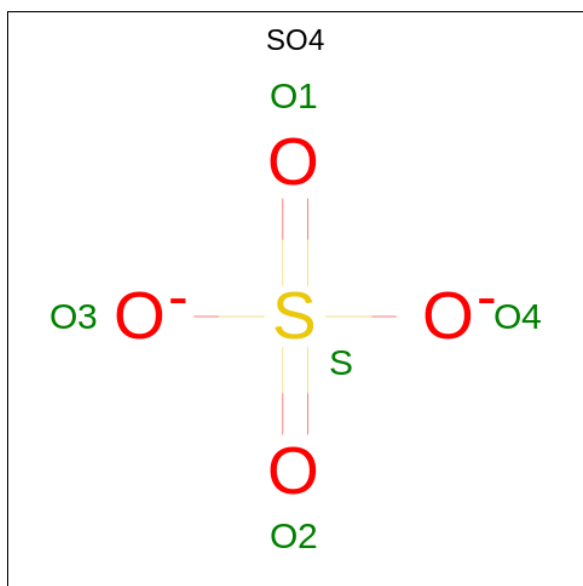
There are 3 unique types of molecules in this entry. The entry contains 9578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4741	3019	793	896	33			
1	B	625	Total	C	N	O	S	0	0	0
			4744	3022	794	896	32			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (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		

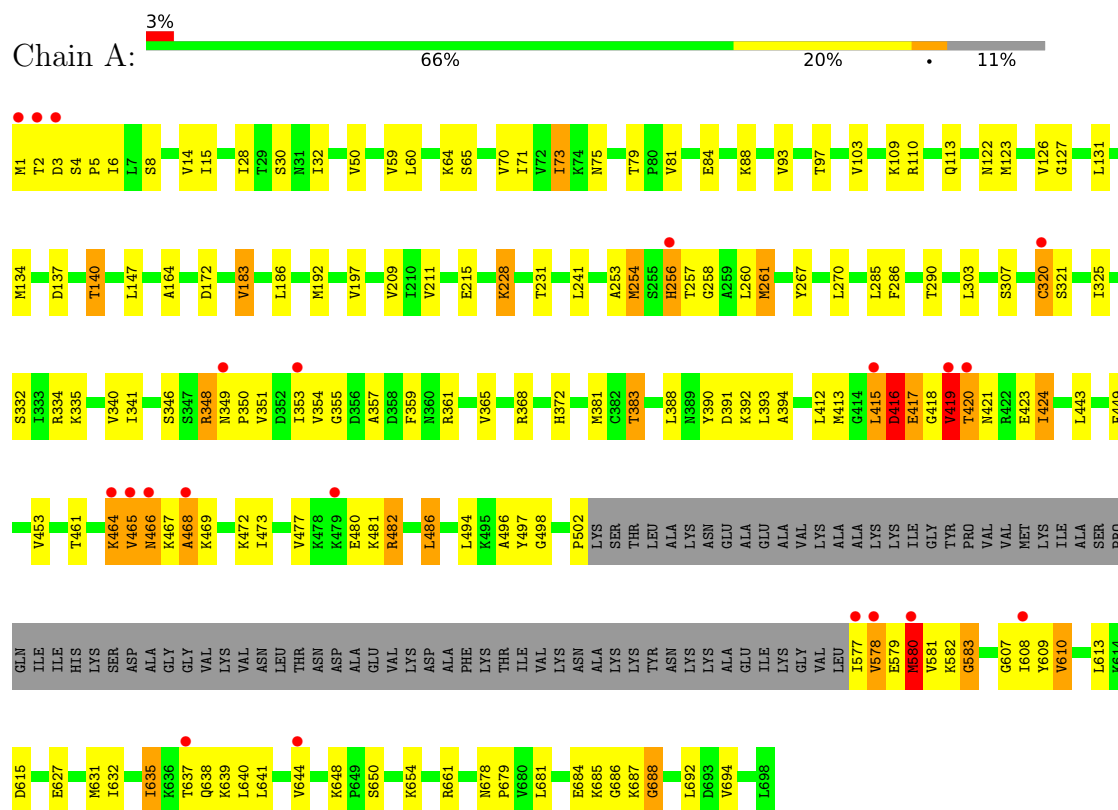
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	32	Total 32	O 32	0	0

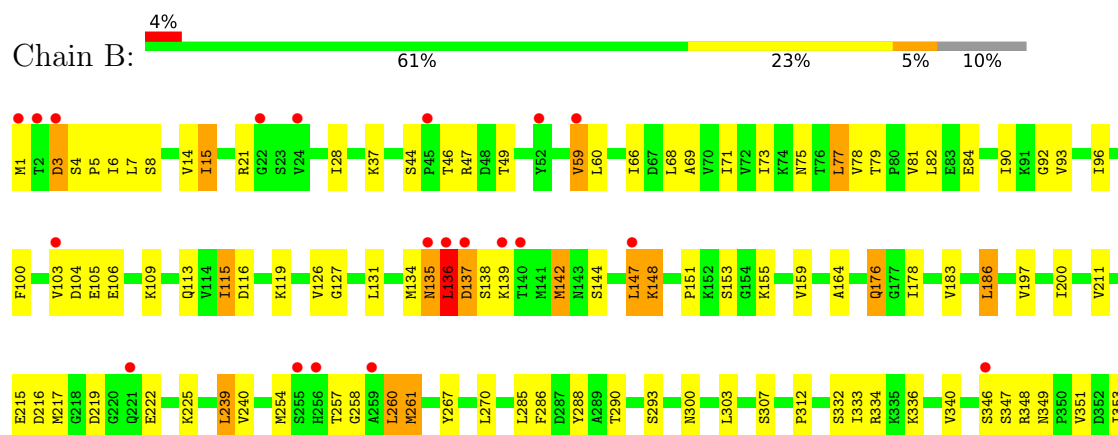
3 Residue-property plots

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



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





4 Data and refinement statistics

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)	24.88 – 2.80 24.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.4 (24.88-2.80) 91.4 (24.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.80Å)	Xtriage
Refinement program	REFMAC v5.5	Depositor
R, R_{free}	0.236 , 0.280 0.239 , 0.279	Depositor DCC
R_{free} test set	3536 reflections (6.78%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9578	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.17% 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

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	0.39	0/4805	0.63	0/6466
1	B	0.40	0/4808	0.63	0/6469
All	All	0.39	0/9613	0.63	0/12935

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	A	1	6
1	B	0	6
All	All	1	12

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	419	VAL	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	ARG	Sidechain
1	A	349	ASN	Peptide
1	A	368	ARG	Sidechain
1	A	416	ASP	Peptide
1	A	468	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	482	ARG	Sidechain
1	B	368	ARG	Sidechain
1	B	412	LEU	Peptide
1	B	417	GLU	Peptide
1	B	422	ARG	Sidechain
1	B	645	ARG	Sidechain
1	B	683	MET	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	4741	0	5000	139	0
1	B	4744	0	5009	193	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	51	0	0	5	0
3	B	32	0	0	5	0
All	All	9578	0	10009	320	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 16.

All (320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HG	1:B:136:LEU:HD23	1.24	1.13
1:A:419:VAL:HG21	1:A:423:GLU:HG2	1.38	1.01
1:B:136:LEU:HD13	1:B:136:LEU:O	1.63	0.97
1:B:134:MET:CE	1:B:151:PRO:HD2	1.98	0.94
1:B:134:MET:O	1:B:136:LEU:N	2.05	0.90
1:B:460:ILE:HD12	1:B:660:GLN:OE1	1.73	0.89
1:B:136:LEU:HD22	1:B:136:LEU:C	1.94	0.87
1:B:134:MET:HE1	1:B:151:PRO:HD2	1.56	0.85
1:B:131:LEU:HD21	1:B:147:LEU:CD2	2.06	0.84
1:B:7:LEU:HD12	1:B:136:LEU:HB2	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:OE1	1:A:256:HIS:CD2	2.31	0.83
1:B:347:SER:HA	1:B:351:VAL:HA	1.61	0.82
1:A:419:VAL:CG2	1:A:423:GLU:HG2	2.09	0.82
1:A:494:LEU:HD22	1:A:694:VAL:HG21	1.62	0.81
1:B:7:LEU:CG	1:B:136:LEU:HD23	2.11	0.79
1:B:462:LYS:HE2	1:B:661:ARG:HG3	1.64	0.79
1:B:581:VAL:O	3:B:801:HOH:O	2.01	0.78
1:A:640:LEU:CD1	1:B:612:VAL:HG21	2.13	0.78
1:B:333:ILE:HA	1:B:336:LYS:CE	2.15	0.77
1:A:215:GLU:O	1:A:261:MET:HE1	1.86	0.76
1:B:135:ASN:OD1	1:B:138:SER:HA	1.87	0.74
1:B:136:LEU:HD22	1:B:137:ASP:N	2.03	0.73
1:A:481:LYS:HD2	1:A:481:LYS:O	1.88	0.73
1:B:333:ILE:HA	1:B:336:LYS:HE2	1.69	0.73
1:B:134:MET:HE2	1:B:151:PRO:HD2	1.69	0.72
1:A:303:LEU:HD22	1:A:325:ILE:HD11	1.71	0.72
1:B:78:VAL:O	1:B:81:VAL:HG12	1.89	0.72
1:B:115:ILE:HD13	1:B:116:ASP:N	2.04	0.72
1:B:131:LEU:HD21	1:B:147:LEU:HD21	1.72	0.72
1:B:457:PRO:HB3	1:B:626:LYS:HB2	1.71	0.71
1:A:607:GLY:O	1:A:610:VAL:HG12	1.91	0.71
1:B:455:SER:N	3:B:803:HOH:O	2.23	0.70
1:B:3:ASP:HB2	1:B:200:ILE:HG12	1.74	0.70
1:B:147:LEU:O	1:B:148:LYS:HG2	1.91	0.70
1:A:480:GLU:OE1	1:A:482:ARG:NH1	2.24	0.69
1:A:466:ASN:OD1	1:A:468:ALA:HB2	1.93	0.69
1:A:415:LEU:HD23	1:A:416:ASP:N	2.08	0.69
1:B:675:LEU:CD2	1:B:696:ILE:HG13	2.23	0.69
1:B:609:TYR:HB3	1:B:613:LEU:HD12	1.75	0.69
1:B:134:MET:HB3	1:B:183:VAL:HB	1.75	0.68
1:B:134:MET:C	1:B:136:LEU:H	1.97	0.68
1:A:390:TYR:OH	3:A:801:HOH:O	2.10	0.68
1:B:66:ILE:HD11	1:B:90:ILE:HD11	1.75	0.67
1:A:413:MET:O	3:A:801:HOH:O	2.10	0.67
1:A:640:LEU:HD12	1:B:612:VAL:HG21	1.77	0.67
1:B:615:ASP:OD1	3:B:802:HOH:O	2.13	0.66
1:B:469:LYS:O	1:B:473:ILE:HD12	1.95	0.66
1:A:15:ILE:HG21	1:A:81:VAL:HG11	1.78	0.65
1:B:135:ASN:ND2	1:B:138:SER:OG	2.29	0.65
1:B:135:ASN:CG	1:B:138:SER:OG	2.35	0.65
1:A:615:ASP:OD2	1:A:637:THR:HG23	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:SER:N	1:B:5:PRO:HD2	2.13	0.63
1:A:71:ILE:HG23	1:A:73:ILE:CD1	2.29	0.63
1:B:457:PRO:HG2	1:B:624:THR:HG21	1.80	0.62
1:A:469:LYS:O	1:A:472:LYS:HG2	1.99	0.62
1:A:465:VAL:HG21	1:A:498:GLY:HA3	1.80	0.62
1:A:494:LEU:O	1:A:496:ALA:O	2.18	0.62
1:A:64:LYS:NZ	1:A:65:SER:OG	2.32	0.62
1:A:467:LYS:HD2	1:A:469:LYS:H	1.64	0.62
1:B:147:LEU:O	1:B:148:LYS:CG	2.48	0.61
1:B:135:ASN:OD1	1:B:137:ASP:O	2.19	0.61
1:B:78:VAL:HG21	1:B:100:PHE:HZ	1.65	0.61
1:B:28:ILE:HD13	1:B:96:ILE:CD1	2.31	0.60
1:B:47:ARG:HG3	1:B:49:THR:H	1.67	0.59
1:A:134:MET:HB2	1:A:183:VAL:HG13	1.82	0.59
1:B:643:GLY:O	1:B:645:ARG:HG3	2.02	0.59
1:A:391:ASP:OD2	1:A:420:THR:HG22	2.03	0.58
1:B:71:ILE:HD13	1:B:93:VAL:HG13	1.85	0.58
1:B:388:LEU:HA	3:B:819:HOH:O	2.04	0.58
1:A:684:GLU:O	1:A:685:LYS:HG2	2.04	0.58
1:B:405:LYS:O	1:B:406:LYS:O	2.22	0.58
1:B:3:ASP:C	1:B:5:PRO:HD2	2.25	0.57
1:B:75:ASN:HA	1:B:78:VAL:CG2	2.35	0.57
1:B:469:LYS:O	1:B:473:ILE:CD1	2.52	0.57
1:A:609:TYR:HB3	1:A:613:LEU:HD12	1.86	0.57
1:A:641:LEU:N	1:A:641:LEU:HD12	2.19	0.57
1:B:135:ASN:O	1:B:136:LEU:C	2.43	0.57
1:B:78:VAL:O	1:B:82:LEU:HD23	2.05	0.56
1:A:654:LYS:HG2	1:A:688:GLY:HA3	1.86	0.56
1:A:419:VAL:HG21	1:A:423:GLU:CG	2.25	0.56
1:B:15:ILE:C	1:B:15:ILE:HD12	2.26	0.56
1:B:155:LYS:NZ	3:B:808:HOH:O	2.39	0.56
1:A:632:ILE:O	1:A:635:ILE:CD1	2.54	0.56
1:B:632:ILE:O	1:B:635:ILE:CD1	2.54	0.56
1:A:15:ILE:HG21	1:A:81:VAL:CG1	2.36	0.55
1:A:353:ILE:CG2	1:A:361:ARG:HD2	2.36	0.55
1:B:59:VAL:HG23	1:B:66:ILE:HD11	1.88	0.55
1:A:416:ASP:O	1:A:417:GLU:O	2.25	0.55
1:A:419:VAL:CB	1:A:423:GLU:HG2	2.36	0.55
1:A:639:LYS:HB3	1:B:612:VAL:HG23	1.88	0.55
1:B:254:MET:SD	1:B:260:LEU:HA	2.46	0.55
1:A:71:ILE:HG23	1:A:73:ILE:HD11	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:CG2	1:A:357:ALA:HB2	2.37	0.55
1:B:684:GLU:OE1	1:B:687:LYS:HG3	2.07	0.55
1:B:468:ALA:O	1:B:471:LYS:HG2	2.07	0.54
1:A:228:LYS:NZ	1:A:627:GLU:OE2	2.38	0.54
1:A:465:VAL:CG2	1:A:497:TYR:C	2.75	0.54
1:A:578:VAL:HG12	1:A:579:GLU:H	1.73	0.54
1:B:115:ILE:HG12	1:B:119:LYS:HE2	1.90	0.54
1:B:134:MET:CG	1:B:135:ASN:N	2.71	0.54
1:B:361:ARG:O	1:B:365:VAL:HG23	2.07	0.54
1:B:409:LEU:HD11	1:B:446:MET:HE1	1.90	0.54
1:B:178:ILE:N	1:B:178:ILE:HD12	2.23	0.53
1:B:457:PRO:HB2	1:B:624:THR:HB	1.90	0.53
1:B:608:ILE:HD13	1:B:608:ILE:H	1.73	0.53
1:B:136:LEU:O	1:B:136:LEU:CD1	2.47	0.53
1:B:215:GLU:O	1:B:261:MET:SD	2.66	0.53
1:A:172:ASP:HA	1:B:415:LEU:HB2	1.90	0.53
1:A:215:GLU:OE1	1:A:256:HIS:NE2	2.40	0.53
1:A:341:ILE:HG22	1:A:361:ARG:HD3	1.89	0.53
1:B:155:LYS:HE3	1:B:293:SER:O	2.08	0.53
1:B:73:ILE:HD12	1:B:77:LEU:HD12	1.90	0.53
1:B:502:PRO:HB2	1:B:579:GLU:HB3	1.90	0.53
1:B:115:ILE:HD13	1:B:115:ILE:C	2.28	0.53
1:B:134:MET:HG3	1:B:135:ASN:H	1.73	0.53
1:A:256:HIS:CD2	1:A:257:THR:HG23	2.43	0.53
1:A:361:ARG:O	1:A:365:VAL:HG23	2.08	0.53
1:B:134:MET:C	1:B:136:LEU:N	2.53	0.53
1:B:186:LEU:HD11	1:B:197:VAL:HG21	1.89	0.53
1:B:353:ILE:HG21	1:B:365:VAL:HG21	1.90	0.53
1:A:303:LEU:HD22	1:A:325:ILE:CD1	2.36	0.53
1:B:694:VAL:HG22	1:B:696:ILE:CD1	2.39	0.53
1:B:651:ASP:OD2	1:B:687:LYS:C	2.48	0.52
1:A:685:LYS:O	1:A:687:LYS:N	2.43	0.52
1:B:475:ASP:HA	1:B:478:LYS:HE2	1.91	0.52
1:B:136:LEU:O	1:B:137:ASP:O	2.26	0.52
1:B:136:LEU:HD12	1:B:142:MET:HB3	1.92	0.52
1:A:137:ASP:HB2	1:A:140:THR:HG23	1.91	0.51
1:B:312:PRO:HB2	1:B:381:MET:HE2	1.93	0.51
1:B:79:THR:HA	1:B:82:LEU:HD21	1.91	0.51
1:B:71:ILE:HG21	1:B:78:VAL:HG13	1.91	0.51
1:B:136:LEU:C	1:B:136:LEU:CD2	2.64	0.51
1:A:685:LYS:O	1:A:687:LYS:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:O	1:B:78:VAL:HG23	2.11	0.51
1:A:73:ILE:HD13	1:A:73:ILE:H	1.75	0.50
1:B:4:SER:O	1:B:8:SER:N	2.44	0.50
1:B:159:VAL:CG1	1:B:186:LEU:HD21	2.41	0.50
1:B:60:LEU:CD1	1:B:84:GLU:HB2	2.40	0.50
1:A:353:ILE:HG23	1:A:361:ARG:CD	2.41	0.50
1:A:353:ILE:HG12	1:A:365:VAL:HG21	1.93	0.50
1:B:6:ILE:HG21	1:B:126:VAL:CG2	2.41	0.50
1:B:73:ILE:HD12	1:B:77:LEU:CD1	2.42	0.50
1:B:333:ILE:CA	1:B:336:LYS:HE2	2.39	0.50
1:B:103:VAL:O	1:B:103:VAL:HG13	2.12	0.50
1:A:494:LEU:C	1:A:496:ALA:O	2.50	0.49
1:A:127:GLY:CA	3:A:814:HOH:O	2.60	0.49
1:B:638:GLN:HG3	1:B:642:GLN:HE21	1.77	0.49
1:B:675:LEU:HD13	1:B:676:ASP:N	2.27	0.49
1:B:675:LEU:HD23	1:B:696:ILE:HG13	1.94	0.49
1:A:637:THR:OG1	1:A:638:GLN:N	2.46	0.49
1:B:176:GLN:HB2	1:B:178:ILE:CD1	2.42	0.49
1:B:254:MET:O	1:B:258:GLY:N	2.45	0.49
1:A:261:MET:HE2	1:A:267:TYR:CE2	2.47	0.49
1:A:581:VAL:HG21	1:A:692:LEU:CD2	2.43	0.49
1:A:186:LEU:HD21	1:A:197:VAL:HG21	1.94	0.49
1:B:60:LEU:HD11	1:B:84:GLU:HB2	1.94	0.49
1:B:303:LEU:HD13	1:B:443:LEU:CD2	2.43	0.49
1:B:334:ARG:NE	1:B:347:SER:OG	2.46	0.49
1:A:465:VAL:HG23	1:A:497:TYR:C	2.33	0.49
1:B:651:ASP:OD2	1:B:687:LYS:O	2.31	0.49
1:B:609:TYR:HA	1:B:612:VAL:HG12	1.95	0.48
1:B:103:VAL:HG13	1:B:106:GLU:HB3	1.96	0.48
1:B:584:GLY:HA3	1:B:683:MET:CE	2.43	0.48
1:A:303:LEU:CD2	1:A:325:ILE:HD11	2.40	0.48
1:B:403:LYS:HE2	1:B:404:TYR:OH	2.13	0.48
1:B:15:ILE:HD12	1:B:15:ILE:O	2.13	0.48
1:B:136:LEU:HD22	1:B:137:ASP:HB2	1.95	0.48
1:B:372:HIS:HB3	1:B:375:VAL:HG13	1.96	0.48
1:B:490:GLY:HA2	1:B:493:VAL:HG22	1.95	0.48
1:A:383:THR:HG21	1:B:164:ALA:HA	1.96	0.47
1:A:417:GLU:HG2	1:A:420:THR:OG1	2.14	0.47
1:A:394:ALA:HB3	1:A:424:ILE:HD11	1.96	0.47
1:A:415:LEU:HD23	1:A:415:LEU:C	2.34	0.47
1:B:312:PRO:CB	1:B:381:MET:HE2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:MET:HG3	1:B:135:ASN:N	2.29	0.47
1:B:372:HIS:HB3	1:B:375:VAL:CG1	2.43	0.47
1:B:403:LYS:HE2	1:B:404:TYR:CZ	2.49	0.47
1:A:353:ILE:HG22	1:A:357:ALA:HB2	1.96	0.47
1:A:131:LEU:HD21	1:A:147:LEU:HD11	1.96	0.47
1:A:241:LEU:C	1:A:241:LEU:HD23	2.35	0.47
1:B:79:THR:HA	1:B:82:LEU:CD2	2.45	0.47
1:B:239:LEU:HD22	1:B:288:TYR:HB2	1.96	0.47
1:B:336:LYS:HB3	1:B:368:ARG:HD3	1.97	0.47
1:B:477:VAL:HG22	1:B:482:ARG:HH22	1.79	0.47
1:A:211:VAL:HG13	1:A:285:LEU:HD22	1.97	0.47
1:A:481:LYS:O	1:A:481:LYS:CD	2.58	0.47
1:A:496:ALA:C	1:A:498:GLY:H	2.18	0.47
1:A:482:ARG:HH21	1:A:486:LEU:HD13	1.80	0.47
1:A:413:MET:N	3:A:801:HOH:O	2.48	0.46
1:A:164:ALA:CB	1:B:383:THR:HG21	2.46	0.46
1:A:502:PRO:C	1:A:579:GLU:OE1	2.54	0.46
1:B:577:ILE:HG23	1:B:577:ILE:O	2.15	0.46
1:B:134:MET:O	1:B:135:ASN:C	2.53	0.46
1:B:216:ASP:OD2	1:B:257:THR:HG21	2.15	0.46
1:B:465:VAL:HG21	1:B:664:GLN:NE2	2.31	0.46
1:B:219:ASP:OD2	1:B:222:GLU:N	2.40	0.46
1:B:475:ASP:O	1:B:478:LYS:HG2	2.16	0.46
1:B:3:ASP:OD1	1:B:3:ASP:N	2.49	0.46
1:B:15:ILE:HD12	1:B:73:ILE:HG23	1.98	0.46
1:A:4:SER:O	1:A:8:SER:N	2.45	0.46
1:A:254:MET:O	1:A:258:GLY:N	2.46	0.46
1:B:135:ASN:CG	1:B:138:SER:HA	2.36	0.46
1:B:159:VAL:HG13	1:B:186:LEU:HD21	1.97	0.46
1:B:211:VAL:HG13	1:B:285:LEU:HD22	1.98	0.46
1:B:365:VAL:O	1:B:369:VAL:HG13	2.16	0.46
1:A:681:LEU:HD11	1:A:692:LEU:HD11	1.97	0.45
1:B:75:ASN:HA	1:B:78:VAL:HG23	1.98	0.45
1:A:388:LEU:HD11	1:A:393:LEU:HD22	1.98	0.45
1:A:88:LYS:O	1:A:88:LYS:HG3	2.16	0.45
1:A:164:ALA:HB1	1:B:383:THR:HG21	1.97	0.45
1:B:648:LYS:N	1:B:648:LYS:HD2	2.31	0.45
1:A:303:LEU:HD13	1:A:443:LEU:CD2	2.47	0.45
1:B:685:LYS:HD2	1:B:685:LYS:N	2.32	0.45
1:B:695:ARG:C	1:B:696:ILE:HD12	2.37	0.45
1:B:462:LYS:HE2	1:B:661:ARG:CG	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ALA:HA	1:B:383:THR:HG21	1.99	0.45
1:A:412:LEU:HD12	1:A:412:LEU:N	2.32	0.45
1:A:354:VAL:HG12	1:A:355:GLY:N	2.32	0.45
1:B:8:SER:OG	1:B:136:LEU:HD21	2.16	0.45
1:B:68:LEU:CD2	1:B:142:MET:CE	2.95	0.45
1:B:217:MET:CE	1:B:267:TYR:HD1	2.30	0.45
1:A:650:SER:HA	1:A:684:GLU:HA	1.99	0.44
1:B:176:GLN:CB	1:B:178:ILE:CD1	2.95	0.44
1:B:307:SER:HA	1:B:381:MET:O	2.17	0.44
1:B:136:LEU:CD1	1:B:142:MET:HB3	2.47	0.44
1:B:312:PRO:HB3	1:B:381:MET:CE	2.48	0.44
1:B:332:SER:HB2	1:B:372:HIS:HE2	1.81	0.44
1:B:391:ASP:OD1	1:B:420:THR:HB	2.17	0.44
1:B:66:ILE:CD1	1:B:90:ILE:HD11	2.44	0.44
1:A:334:ARG:HG3	1:A:335:LYS:N	2.32	0.44
1:A:579:GLU:O	1:A:580:MET:C	2.55	0.44
1:A:640:LEU:HD13	1:B:612:VAL:HG21	1.96	0.44
1:A:126:VAL:HG22	1:A:192:MET:CE	2.48	0.44
1:B:137:ASP:OD1	1:B:139:LYS:HB2	2.17	0.44
1:B:147:LEU:O	1:B:148:LYS:CB	2.65	0.44
1:A:75:ASN:HD21	1:A:110:ARG:HD2	1.81	0.43
1:A:383:THR:HG21	1:B:164:ALA:HB1	2.00	0.43
1:A:391:ASP:CG	1:A:420:THR:HG22	2.39	0.43
1:B:105:GLU:O	1:B:109:LYS:HG2	2.17	0.43
1:A:253:ALA:O	1:A:257:THR:HG23	2.18	0.43
1:A:320[A]:CYS:HB2	1:A:325:ILE:HG12	1.99	0.43
1:A:464:LYS:O	1:A:466:ASN:N	2.51	0.43
1:B:6:ILE:HD13	1:B:92:GLY:HA2	2.00	0.43
1:A:417:GLU:CG	1:A:420:THR:OG1	2.67	0.43
1:A:473:ILE:O	1:A:477:VAL:HG23	2.19	0.43
1:A:648:LYS:HE3	1:A:684:GLU:HG2	2.00	0.43
1:A:578:VAL:HG12	1:A:579:GLU:N	2.32	0.43
1:B:270:LEU:O	1:B:270:LEU:HD23	2.18	0.43
1:B:336:LYS:HB3	1:B:368:ARG:CD	2.48	0.43
1:B:404:TYR:O	1:B:405:LYS:C	2.56	0.43
1:A:79:THR:HG21	1:A:113:GLN:OE1	2.17	0.43
1:A:353:ILE:HG23	1:A:361:ARG:HD3	2.01	0.43
1:A:359:PHE:CE2	1:A:392:LYS:HD3	2.53	0.43
1:B:348:ARG:HD3	1:B:348:ARG:C	2.39	0.43
1:A:254:MET:SD	1:A:260:LEU:HA	2.59	0.43
1:A:383:THR:HG21	1:B:164:ALA:CA	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:HG23	1:A:73:ILE:HD13	1.98	0.42
1:A:307:SER:HA	1:A:381:MET:O	2.19	0.42
1:A:320[A]:CYS:SG	1:A:321:SER:N	2.92	0.42
1:B:286:PHE:O	1:B:290:THR:HG23	2.17	0.42
1:B:696:ILE:HD12	1:B:696:ILE:N	2.33	0.42
1:A:502:PRO:C	1:A:579:GLU:CD	2.77	0.42
1:B:155:LYS:CE	1:B:293:SER:O	2.67	0.42
1:B:44:SER:OG	1:B:46:THR:HG22	2.20	0.42
1:A:412:LEU:N	1:A:412:LEU:CD1	2.83	0.42
1:A:415:LEU:HD23	1:A:416:ASP:CA	2.48	0.42
1:B:490:GLY:HA2	1:B:493:VAL:CG2	2.50	0.42
1:A:3:ASP:C	1:A:5:PRO:HD2	2.39	0.42
1:B:684:GLU:OE1	1:B:687:LYS:CG	2.68	0.42
1:B:79:THR:HG21	1:B:113:GLN:OE1	2.19	0.42
1:A:383:THR:HG21	1:B:164:ALA:CB	2.49	0.42
1:B:6:ILE:HG21	1:B:126:VAL:HG23	2.02	0.42
1:B:28:ILE:HD11	1:B:144:SER:C	2.40	0.42
1:B:138:SER:HB3	1:B:153:SER:OG	2.19	0.42
1:B:632:ILE:O	1:B:635:ILE:HD12	2.20	0.42
1:A:60:LEU:CD2	1:A:84:GLU:HB3	2.50	0.42
1:A:93:VAL:HG21	1:A:123:MET:HE2	2.00	0.42
1:A:286:PHE:O	1:A:290:THR:HG23	2.20	0.42
1:B:473:ILE:O	1:B:477:VAL:HG23	2.20	0.42
1:A:465:VAL:HB	3:A:826:HOH:O	2.20	0.41
1:A:641:LEU:N	1:A:641:LEU:CD1	2.82	0.41
1:A:678:ASN:HA	1:A:679:PRO:HA	1.80	0.41
1:B:103:VAL:O	1:B:103:VAL:CG1	2.67	0.41
1:B:650:SER:HA	1:B:684:GLU:HB2	2.02	0.41
1:A:348:ARG:O	1:A:350:PRO:C	2.58	0.41
1:A:465:VAL:HG21	1:A:661:ARG:NH1	2.35	0.41
1:B:69:ALA:HB2	1:B:90:ILE:HD13	2.02	0.41
1:B:418:GLY:O	1:B:420:THR:N	2.53	0.41
1:A:340:VAL:O	1:A:340:VAL:HG22	2.20	0.41
1:A:419:VAL:HG11	1:A:423:GLU:CD	2.40	0.41
1:A:32:ILE:CD1	1:A:70:VAL:HG11	2.51	0.41
1:A:346:SER:O	1:A:351:VAL:HA	2.20	0.41
1:B:71:ILE:N	1:B:71:ILE:HD12	2.35	0.41
1:B:462:LYS:HB2	1:B:465:VAL:HG23	2.02	0.41
1:B:623:VAL:HG22	1:B:663:SER:HB2	2.01	0.41
1:B:340:VAL:HG22	1:B:340:VAL:O	2.19	0.41
1:A:449:PHE:O	1:A:453:VAL:HG13	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:HG23	1:A:497:TYR:CA	2.51	0.41
1:B:358:ASP:OD2	1:B:360:ASN:HB2	2.21	0.41
1:A:1:MET:CE	1:A:122:ASN:HD21	2.33	0.41
1:A:467:LYS:HD3	1:A:469:LYS:HD2	2.03	0.41
1:A:6:ILE:HD12	1:A:6:ILE:H	1.85	0.41
1:A:14:VAL:HA	1:A:70:VAL:HG13	2.02	0.41
1:A:581:VAL:HG21	1:A:692:LEU:HD22	2.02	0.41
1:B:134:MET:HE2	1:B:151:PRO:CD	2.46	0.41
1:B:409:LEU:CD1	1:B:409:LEU:N	2.84	0.41
1:B:678:ASN:HA	1:B:679:PRO:HA	1.79	0.41
1:B:683:MET:H	1:B:683:MET:HG2	1.76	0.41
1:B:7:LEU:HD12	1:B:136:LEU:CB	2.40	0.41
1:A:332:SER:HB2	1:A:372:HIS:HE2	1.85	0.40
1:A:582:LYS:HG3	1:A:583:GLY:N	2.36	0.40
1:A:640:LEU:HA	1:A:644:VAL:CG1	2.51	0.40
1:B:131:LEU:HD11	1:B:147:LEU:HD22	2.04	0.40
1:B:609:TYR:N	1:B:609:TYR:CD1	2.89	0.40
1:A:581:VAL:HG21	1:A:692:LEU:HD21	2.04	0.40
1:B:464:LYS:O	1:B:466:ASN:N	2.54	0.40
1:A:4:SER:N	1:A:5:PRO:CD	2.84	0.40
1:B:592:LYS:HD2	1:B:594:GLU:OE2	2.22	0.40
1:A:353:ILE:HG21	1:A:357:ALA:HB2	2.02	0.40
1:A:424:ILE:HD13	1:A:424:ILE:HG21	1.85	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%)	581 (94%)	30 (5%)	10 (2%)	8	27
1	B	621/698 (89%)	580 (93%)	27 (4%)	14 (2%)	5	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1242/1396 (89%)	1161 (94%)	57 (5%)	24 (2%)	6	23

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	ASP
1	A	417	GLU
1	A	419	VAL
1	B	135	ASN
1	B	137	ASP
1	B	346	SER
1	B	406	LYS
1	B	419	VAL
1	A	466	ASN
1	A	583	GLY
1	A	686	GLY
1	A	688	GLY
1	B	127	GLY
1	B	349	ASN
1	B	354	VAL
1	B	148	LYS
1	B	457	PRO
1	A	580	MET
1	B	136	LEU
1	A	418	GLY
1	B	644	VAL
1	B	465	VAL
1	A	578	VAL
1	B	583	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	531/589 (90%)	495 (93%)	36 (7%)	13	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	531/589 (90%)	490 (92%)	41 (8%)	10	31
All	All	1062/1178 (90%)	985 (93%)	77 (7%)	12	34

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	28	ILE
1	A	30	SER
1	A	50	VAL
1	A	59	VAL
1	A	73	ILE
1	A	97	THR
1	A	103	VAL
1	A	109	LYS
1	A	140	THR
1	A	183	VAL
1	A	209	VAL
1	A	228	LYS
1	A	231	THR
1	A	254	MET
1	A	256	HIS
1	A	261	MET
1	A	270	LEU
1	A	320[A]	CYS
1	A	320[B]	CYS
1	A	383	THR
1	A	415	LEU
1	A	419	VAL
1	A	420	THR
1	A	421	ASN
1	A	424	ILE
1	A	461	THR
1	A	464	LYS
1	A	465	VAL
1	A	486	LEU
1	A	577	ILE
1	A	580	MET
1	A	608	ILE
1	A	610	VAL
1	A	631	MET
1	A	635	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1	MET
1	B	3	ASP
1	B	14	VAL
1	B	15	ILE
1	B	21	ARG
1	B	37	LYS
1	B	59	VAL
1	B	77	LEU
1	B	104	ASP
1	B	115	ILE
1	B	136	LEU
1	B	142	MET
1	B	147	LEU
1	B	176	GLN
1	B	186	LEU
1	B	225	LYS
1	B	239	LEU
1	B	240	VAL
1	B	260	LEU
1	B	261	MET
1	B	300	ASN
1	B	375	VAL
1	B	383	THR
1	B	388	LEU
1	B	408	MET
1	B	419	VAL
1	B	478	LYS
1	B	493	VAL
1	B	503	LYS
1	B	577	ILE
1	B	605	MET
1	B	608	ILE
1	B	617	THR
1	B	631	MET
1	B	635	ILE
1	B	637	THR
1	B	648	LYS
1	B	671	GLU
1	B	683	MET
1	B	685	LYS
1	B	696	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	122	ASN
1	B	112	GLN
1	B	300	ASN
1	B	389	ASN
1	B	429	ASN
1	B	638	GLN
1	B	642	GLN

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 oligosaccharides 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	A	701	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	701	-	4,4,4	0.37	0	6,6,6	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

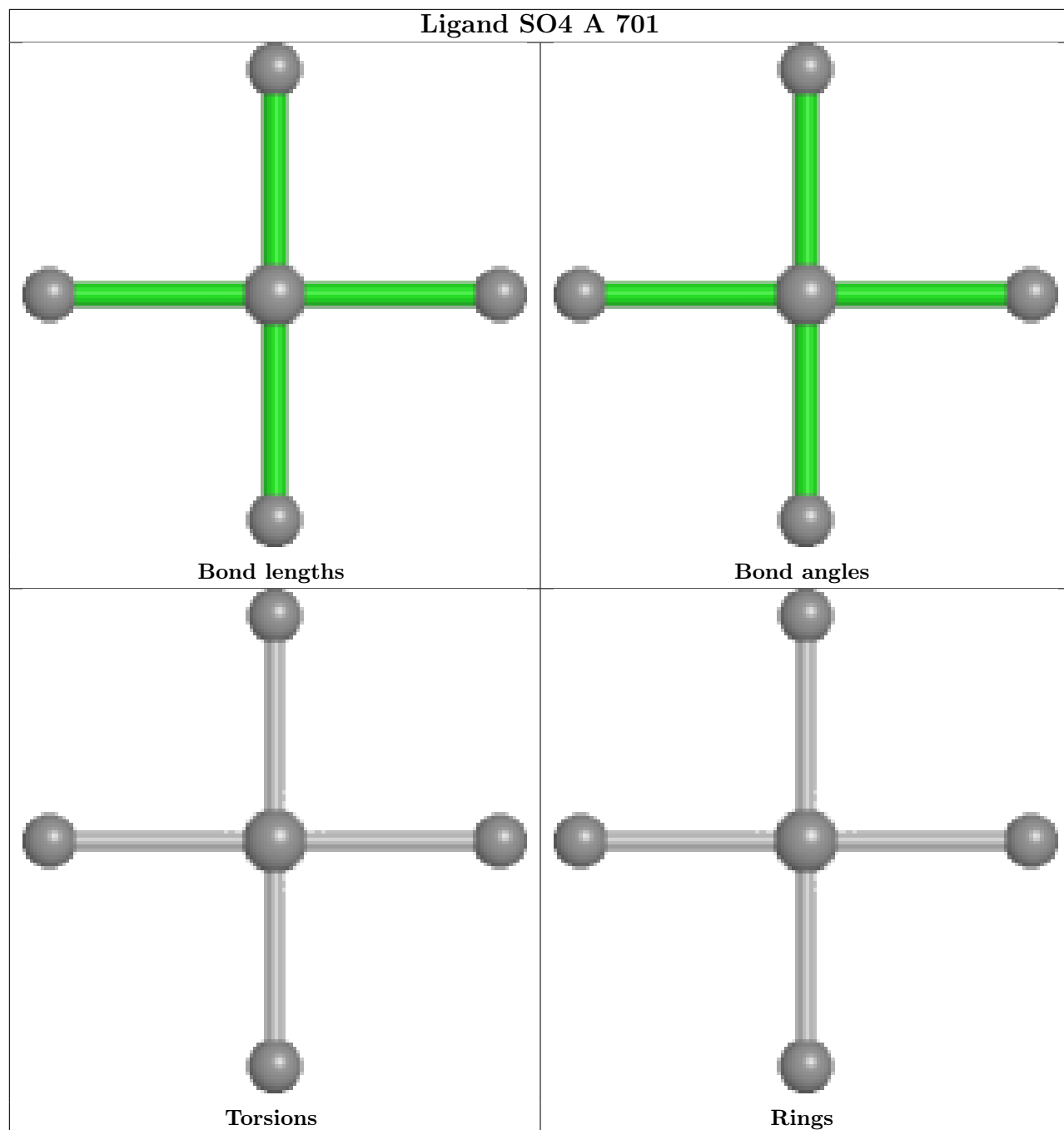
There are no chirality outliers.

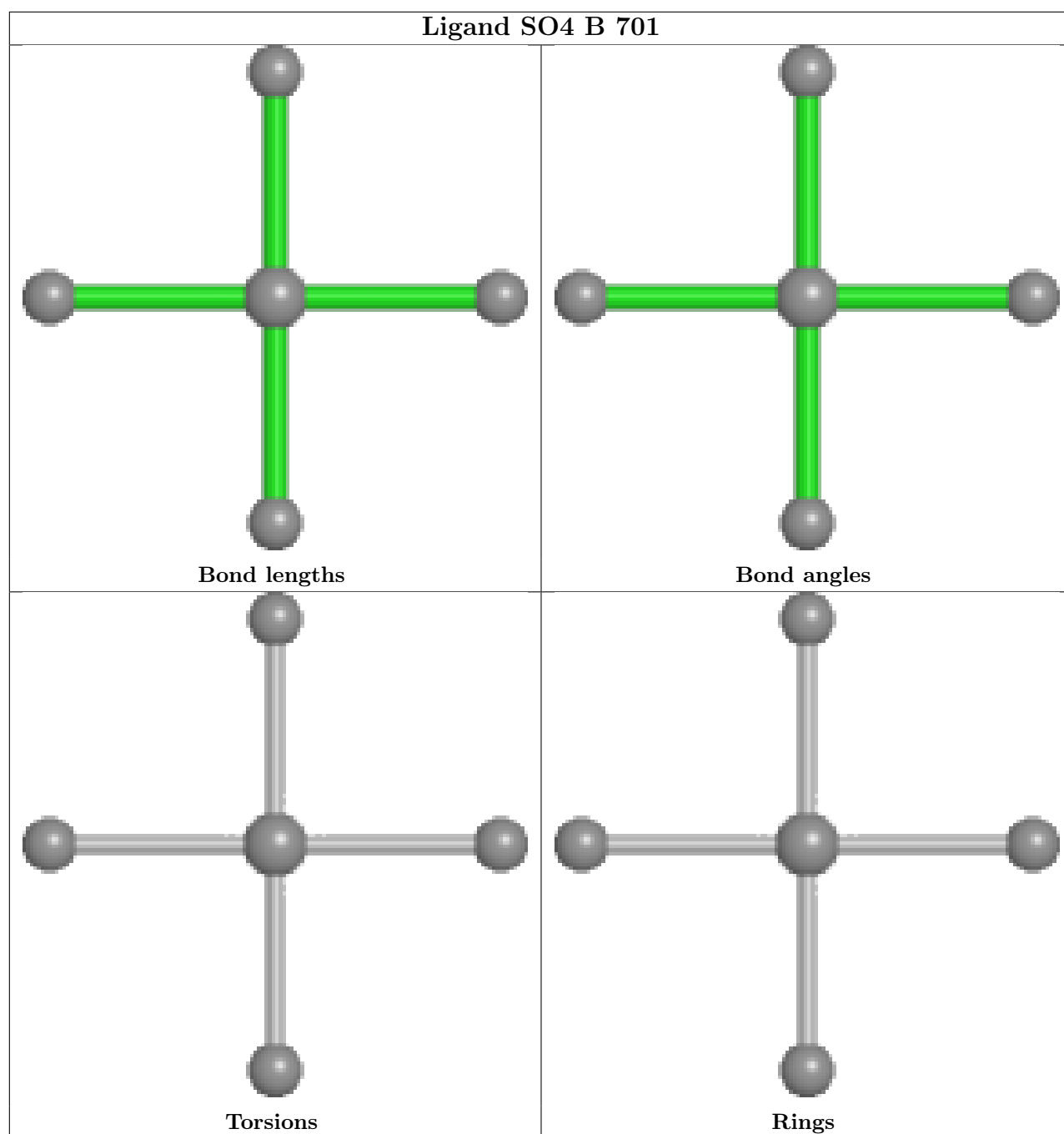
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	624/698 (89%)	-0.04	21 (3%)	48 40	18, 57, 101, 153	1 (0%)
1	B	625/698 (89%)	0.21	31 (4%)	35 28	31, 66, 113, 160	0
All	All	1249/1396 (89%)	0.08	52 (4%)	41 33	18, 61, 110, 160	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	6.6
1	A	466	ASN	6.1
1	A	419	VAL	5.5
1	B	135	ASN	5.1
1	B	1	MET	5.0
1	B	463	PHE	5.0
1	B	3	ASP	4.8
1	A	2	THR	4.1
1	B	685	LYS	3.9
1	A	320[A]	CYS	3.7
1	B	137	ASP	3.7
1	A	465	VAL	3.7
1	A	578	VAL	3.5
1	A	1	MET	3.4
1	A	644	VAL	3.4
1	A	580	MET	3.3
1	B	256	HIS	3.2
1	B	608	ILE	3.1
1	B	259	ALA	3.1
1	B	419	VAL	3.1
1	B	140	THR	2.9
1	B	103	VAL	2.8
1	A	256	HIS	2.8
1	B	221	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	644	VAL	2.8
1	B	686	GLY	2.8
1	B	464	LYS	2.7
1	B	503	LYS	2.7
1	B	136	LEU	2.6
1	A	608	ILE	2.6
1	A	464	LYS	2.5
1	A	420	THR	2.5
1	A	353	ILE	2.5
1	A	468	ALA	2.5
1	B	139	LYS	2.5
1	B	59	VAL	2.4
1	A	479	LYS	2.4
1	B	255	SER	2.4
1	A	415	LEU	2.4
1	A	577	ILE	2.4
1	A	637	THR	2.3
1	B	461	THR	2.3
1	B	147	LEU	2.2
1	B	457	PRO	2.2
1	B	346	SER	2.2
1	A	3	ASP	2.1
1	B	45	PRO	2.1
1	B	456	SER	2.0
1	A	349	ASN	2.0
1	B	24	VAL	2.0
1	B	52	TYR	2.0
1	B	22	GLY	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,

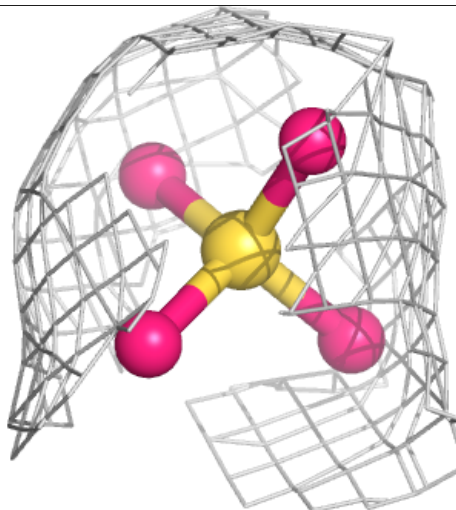
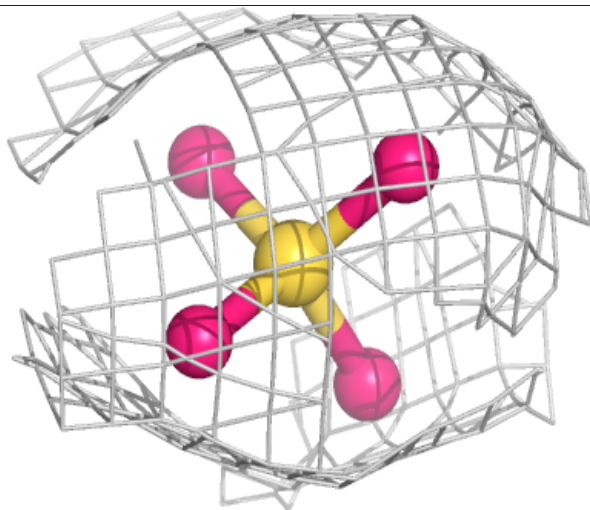
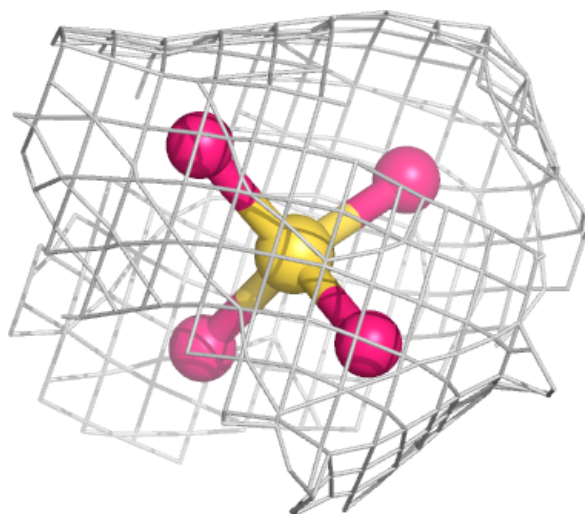
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	701	5/5	0.88	0.10	67,70,72,75	0
2	SO4	A	701	5/5	0.97	0.09	50,61,63,64	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.

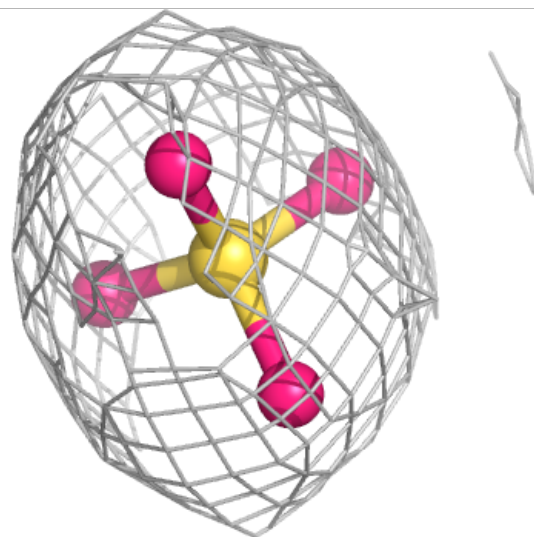
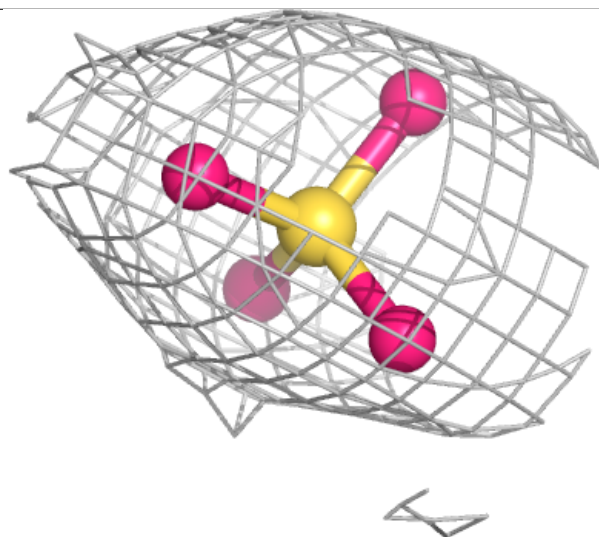
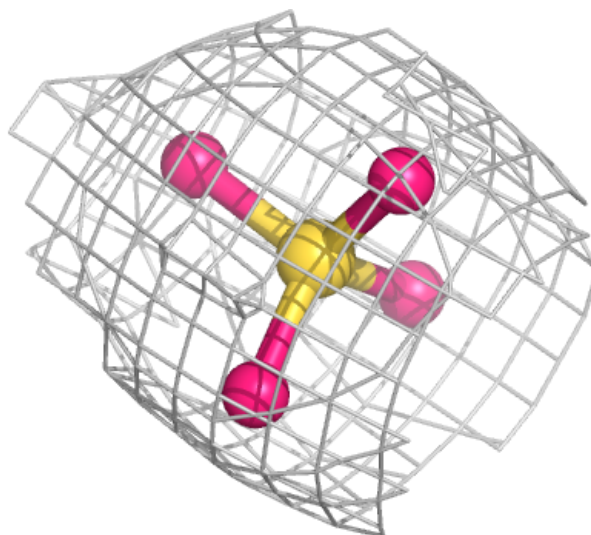
Electron density around SO4 B 701:

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.