Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:34 AM EDT

PDB ID	:	8WZU / pdb_00008wzu
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:

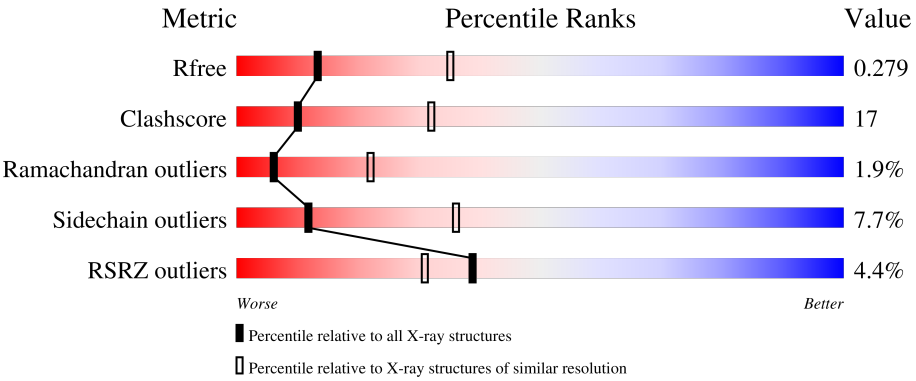
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 <=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	3% 63% 21% • • 11%
1	B	698	5% 60% 24% 5% 10%

2 Entry composition

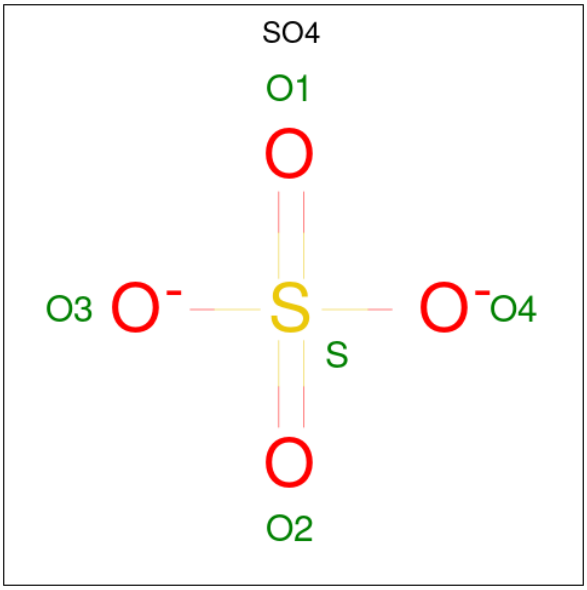
There are 3 unique types of molecules in this entry. The entry contains 9578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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.

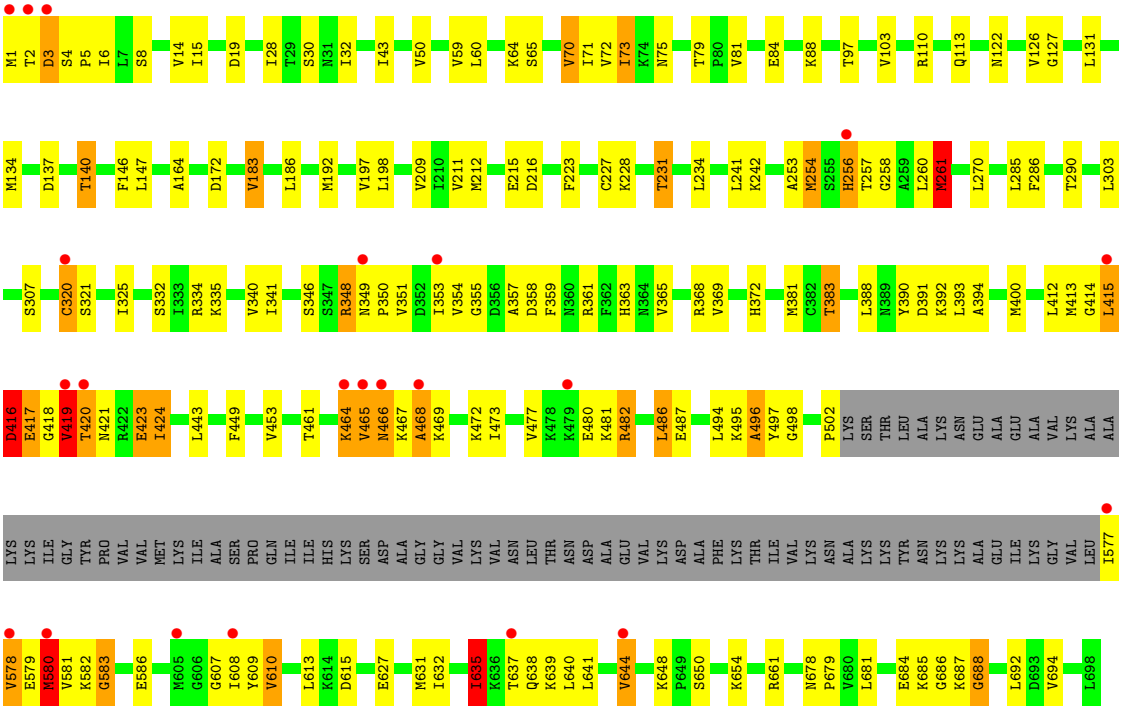
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	51	Total O 51 51	0	0
3	B	32	Total O 32 32	0	0

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.

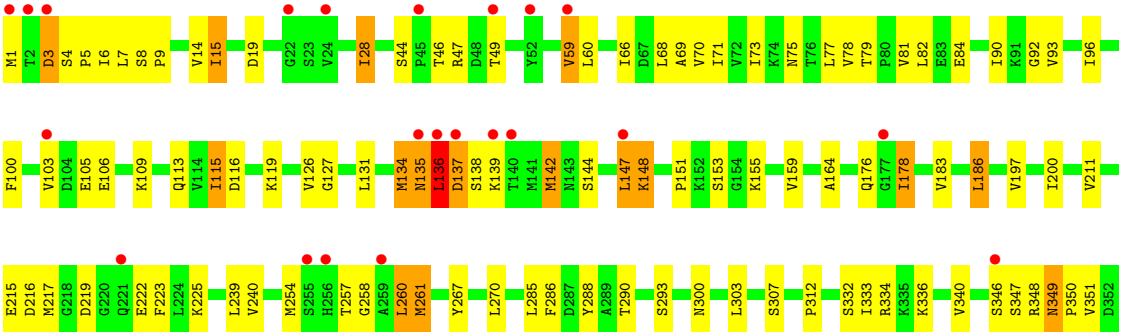
• Molecule 1: 4-hydroxybutyrate--CoA ligase [ADP-forming]

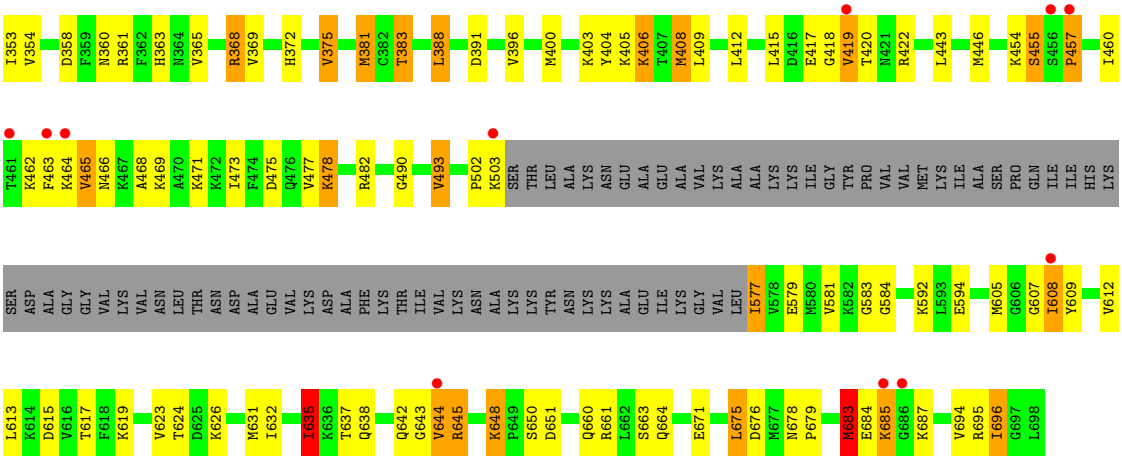
Chain A:



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

Chain B:




I353 V354 D358 F359 N360 R361 F362 H363 N364 V365 R368 V369 H372 V375 M381 C382 T383 L388 D391 V396 M400 K403 Y404 K405 K406 T407 M408 L409 L412 L415 D416 E417 G418 V419 T420 N421 R422 L443 M446 K454 S455 S456 P457 I460
T461 K462 F463 K464 V465 N466 K467 A468 K469 A470 K471 K472 I473 F474 D475 Q476 V477 K478 R482 G490 V493 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 G583 G584 K592 L593 E594 M605 G606 G607 I608 Y609 V612
L613 K614 D615 V616 T617 F618 K619 V623 T624 D625 K626 M631 I632 T635 K636 T637 Q638 Q642 G643 V644 R645 K648 P649 S650 D651 Q660 R661 L662 S663 Q664 E671 L675 D676 M677 N678 P679 M683 E684 K685 G686 K687 V694 R695 I696 G697 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)	24.88 – 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
$< I/\sigma(I) >$ [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	2992 reflections (6.23%)	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]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

[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	0.62	2/4805 (0.0%)	0.97	7/6466 (0.1%)
1	B	0.65	4/4808 (0.1%)	0.97	5/6469 (0.1%)
All	All	0.64	6/9613 (0.1%)	0.97	12/12935 (0.1%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	MET	SD-CE	-6.73	1.62	1.79
1	B	683	MET	SD-CE	-6.11	1.64	1.79
1	B	381	MET	SD-CE	-5.96	1.64	1.79
1	A	212	MET	SD-CE	-5.69	1.65	1.79
1	B	28	ILE	CG1-CD1	-5.58	1.29	1.51
1	A	261	MET	SD-CE	-5.14	1.66	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	414	GLY	N-CA-C	8.19	121.09	110.45
1	A	496	ALA	N-CA-C	-7.96	100.06	110.33
1	A	419	VAL	N-CA-C	6.60	123.06	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	454	LYS	N-CA-C	6.52	119.71	111.69
1	B	19	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	3	ASP	N-CA-C	6.12	116.51	107.88
1	B	463	PHE	CA-CB-CG	6.10	119.90	113.80
1	B	635	ILE	N-CA-CB	5.84	117.49	110.31
1	A	635	ILE	N-CA-CB	5.55	117.14	110.31
1	A	146	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	19	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	455	SER	N-CA-C	5.20	116.98	108.76

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
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 (i)

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	148	0
1	B	4744	0	5009	201	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	337	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 17.

All (337) 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:B:134:MET:HE1	1:B:151:PRO:HD2	1.24	1.08
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	0.91
1:B:136:LEU:HD22	1:B:136:LEU:C	1.94	0.91
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: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
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:134:MET:HE1	1:B:151:PRO:CD	2.09	0.80
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: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:C	1:B:136:LEU:H	1.97	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:135:ASN:CG	1:B:138:SER:OG	2.35	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: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:A:615:ASP:OD2	1:A:637:THR:HG23	1.97	0.64
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:134:MET:C	1:B:136:LEU:N	2.53	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:B:3:ASP:C	1:B:5:PRO:HD2	2.25	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:O	1:B:136:LEU:C	2.43	0.61
1:B:135:ASN:OD1	1:B:137:ASP:O	2.19	0.61
1:B:15:ILE:C	1:B:15:ILE:HD12	2.26	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:465:VAL:CG2	1:A:497:TYR:C	2.75	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:ILE:HD13	1:B:115:ILE:C	2.28	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:B:651:ASP:OD2	1:B:687:LYS:C	2.48	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: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: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
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:494:LEU:C	1:A:496:ALA:O	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:HG23	1:A:497:TYR:C	2.33	0.53
1:B:155:LYS:HE3	1:B:293:SER:O	2.08	0.53
1:B:409:LEU:HD11	1:B:446:MET:HE1	1.91	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:134:MET:HG3	1:B:135:ASN:H	1.73	0.53
1:A:216:ASP:HB3	1:A:261:MET:HE3	1.91	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:155:LYS:NZ	3:B:808:HOH:O	2.39	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:312:PRO:HB2	1:B:381:MET:HE2	1.91	0.52
1:A:415:LEU:HD23	1:A:415:LEU:C	2.34	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:A:502:PRO:C	1:A:579:GLU:CD	2.77	0.52
1:A:241:LEU:C	1:A:241:LEU:HD23	2.35	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:496:ALA:C	1:A:498:GLY:H	2.18	0.51
1:B:136:LEU:C	1:B:136:LEU:CD2	2.64	0.51
1:A:137:ASP:HB2	1:A:140:THR:HG23	1.91	0.51
1:B:79:THR:HA	1:B:82:LEU:HD21	1.91	0.51
1:A:502:PRO:C	1:A:579:GLU:OE1	2.54	0.51
1:B:71:ILE:HG21	1:B:78:VAL:HG13	1.91	0.51
1:A:685:LYS:O	1:A:687:LYS:HG2	2.10	0.51
1:B:75:ASN:O	1:B:78:VAL:HG23	2.11	0.51
1:B:134:MET:O	1:B:135:ASN:C	2.53	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:B:135:ASN:CG	1:B:138:SER:HA	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:O	1:B:103:VAL:HG13	2.12	0.50
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: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:695:ARG:C	1:B:696:ILE:HD12	2.37	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:B:651:ASP:OD2	1:B:687:LYS:O	2.31	0.49
1:B:312:PRO:CB	1:B:381:MET:HE2	2.43	0.48
1:B:609:TYR:HA	1:B:612:VAL:HG12	1.95	0.48
1:A:391:ASP:CG	1:A:420:THR:HG22	2.39	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:A:579:GLU:O	1:A:580:MET:C	2.55	0.48
1:B:15:ILE:HD12	1:B:15:ILE:O	2.13	0.48
1:A:227:CYS:O	1:A:231:THR:OG1	2.29	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:B:348:ARG:HD3	1:B:348:ARG:C	2.39	0.47
1:A:394:ALA:HB3	1:A:424:ILE:HD11	1.96	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASP:C	1:A:5:PRO:HD2	2.39	0.47
1:A:211:VAL:HG13	1:A:285:LEU:HD22	1.97	0.47
1:A:348:ARG:O	1:A:350:PRO:C	2.58	0.47
1:A:481:LYS:O	1:A:481:LYS:CD	2.58	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:B:28:ILE:HD11	1:B:144:SER:C	2.40	0.46
1:A:164:ALA:CB	1:B:383:THR:HG21	2.46	0.46
1:B:404:TYR:O	1:B:405:LYS:C	2.56	0.46
1:B:577:ILE:HG23	1:B:577:ILE:O	2.15	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:A:419:VAL:HG11	1:A:423:GLU:CD	2.40	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:363:HIS:CE1	1:B:400:MET:HE1	2.51	0.45
1:B:685:LYS:HD2	1:B:685:LYS:N	2.32	0.45
1:A:363:HIS:CD2	1:A:400:MET:HE3	2.51	0.45
1:B:462:LYS:HE2	1:B:661:ARG:CG	2.41	0.45
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:B:607:GLY:C	1:B:609:TYR:H	2.25	0.45
1:A:650:SER:HA	1:A:684:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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:A:242:LYS:HE2	1:A:261:MET:HE1	2.01	0.42
1:A:495:LYS:C	1:A:496:ALA:O	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASN:HA	1:B:350:PRO:C	2.45	0.42
1:B:490:GLY:HA2	1:B:493:VAL:CG2	2.50	0.42
1:B:684:GLU:OE1	1:B:687:LYS:CG	2.68	0.42
1:A:215:GLU:O	1:A:261:MET:CE	2.68	0.42
1:B:75:ASN:C	1:B:78:VAL:HG23	2.44	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:138:SER:HB3	1:B:153:SER:OG	2.19	0.42
1:B:223:PHE:CD1	1:B:223:PHE:C	2.97	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:223:PHE:CD1	1:A:223:PHE:C	2.97	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:70:VAL:C	1:B:71:ILE:HD12	2.45	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: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: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:HD12	1:B:71:ILE:N	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
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:241:LEU:C	1:A:241:LEU:CD2	2.94	0.41
1:A:467:LYS:HD3	1:A:469:LYS:HD2	2.03	0.41
1:B:7:LEU:C	1:B:9:PRO:HD3	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:LYS:HZ1	1:A:261:MET:HE1	1.86	0.40
1:A:358:ASP:OD1	1:A:358:ASP:C	2.65	0.40
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:A:464:LYS:C	1:A:466:ASN:N	2.78	0.40
1:A:486:LEU:O	1:A:487:GLU:C	2.65	0.40
1:B:592:LYS:HD2	1:B:594:GLU:OE2	2.22	0.40
1:B:643:GLY:O	1:B:644:VAL:C	2.64	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
1:B:408:MET:HE3	1:B:408:MET:HB3	1.97	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%)	7 27
1	B	621/698 (89%)	580 (93%)	27 (4%)	14 (2%)	5 18
All	All	1242/1396 (89%)	1161 (94%)	57 (5%)	24 (2%)	6 22

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 (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	531/589 (90%)	487 (92%)	44 (8%)	10 32
1	B	531/589 (90%)	492 (93%)	39 (7%)	13 38
All	All	1062/1178 (90%)	979 (92%)	83 (8%)	12 35

All (83) 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	43	ILE
1	A	50	VAL
1	A	59	VAL
1	A	70	VAL
1	A	72	VAL
1	A	73	ILE
1	A	97	THR
1	A	103	VAL
1	A	140	THR
1	A	183	VAL
1	A	198	LEU
1	A	209	VAL
1	A	231	THR
1	A	234	LEU
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	369	VAL
1	A	383	THR
1	A	415	LEU
1	A	416	ASP
1	A	419	VAL
1	A	420	THR
1	A	421	ASN
1	A	423	GLU
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	586	GLU
1	A	608	ILE
1	A	610	VAL
1	A	631	MET
1	A	635	ILE

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Mol	Chain	Res	Type
1	A	644	VAL
1	B	1	MET
1	B	3	ASP
1	B	14	VAL
1	B	15	ILE
1	B	59	VAL
1	B	115	ILE
1	B	136	LEU
1	B	142	MET
1	B	147	LEU
1	B	178	ILE
1	B	186	LEU
1	B	225	LYS
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	396	VAL
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	619	LYS
1	B	631	MET
1	B	635	ILE
1	B	637	THR
1	B	648	LYS
1	B	671	GLU
1	B	675	LEU
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	75	ASN
1	A	122	ASN
1	A	124	GLN
1	A	349	ASN
1	A	363	HIS
1	A	364	ASN
1	A	638	GLN
1	B	112	GLN
1	B	389	ASN
1	B	429	ASN
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	0.31	0	6,6,6	0.12	0
2	SO4	B	701	-	4,4,4	0.32	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

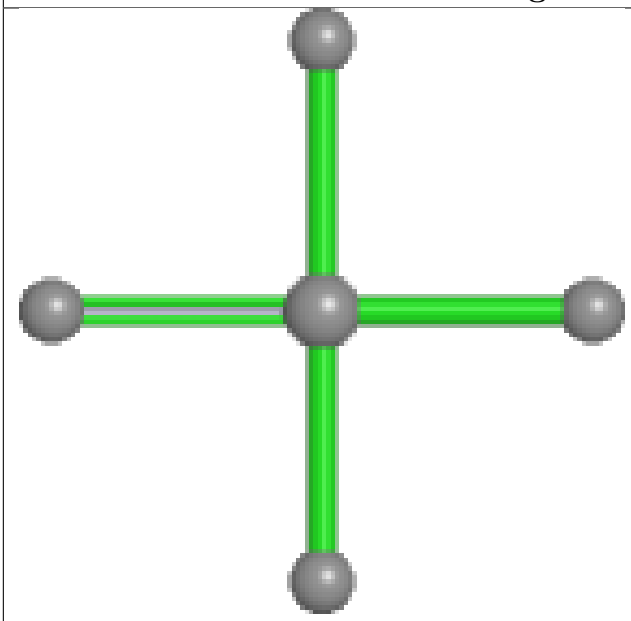
There are no torsion outliers.

There are no ring outliers.

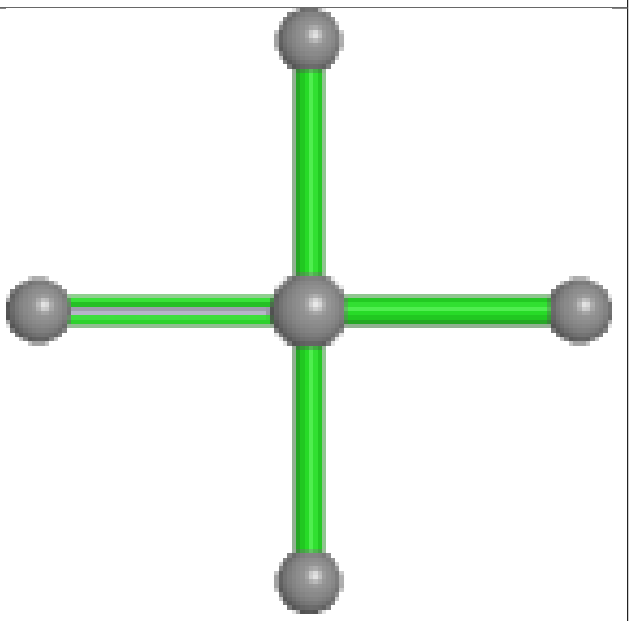
No monomer is involved in short contacts.

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 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.

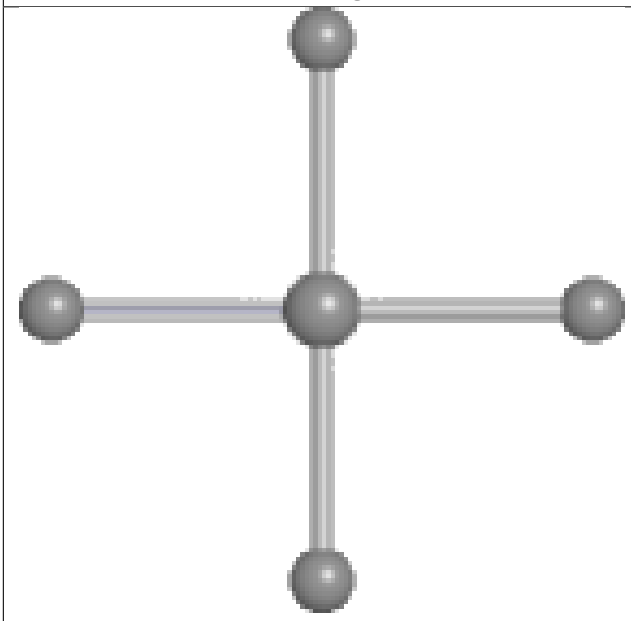
Ligand SO4 A 701



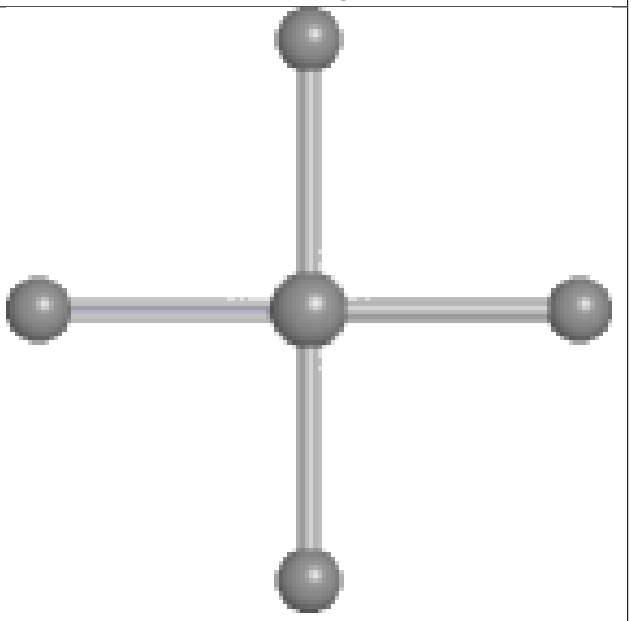
Bond lengths



Bond angles

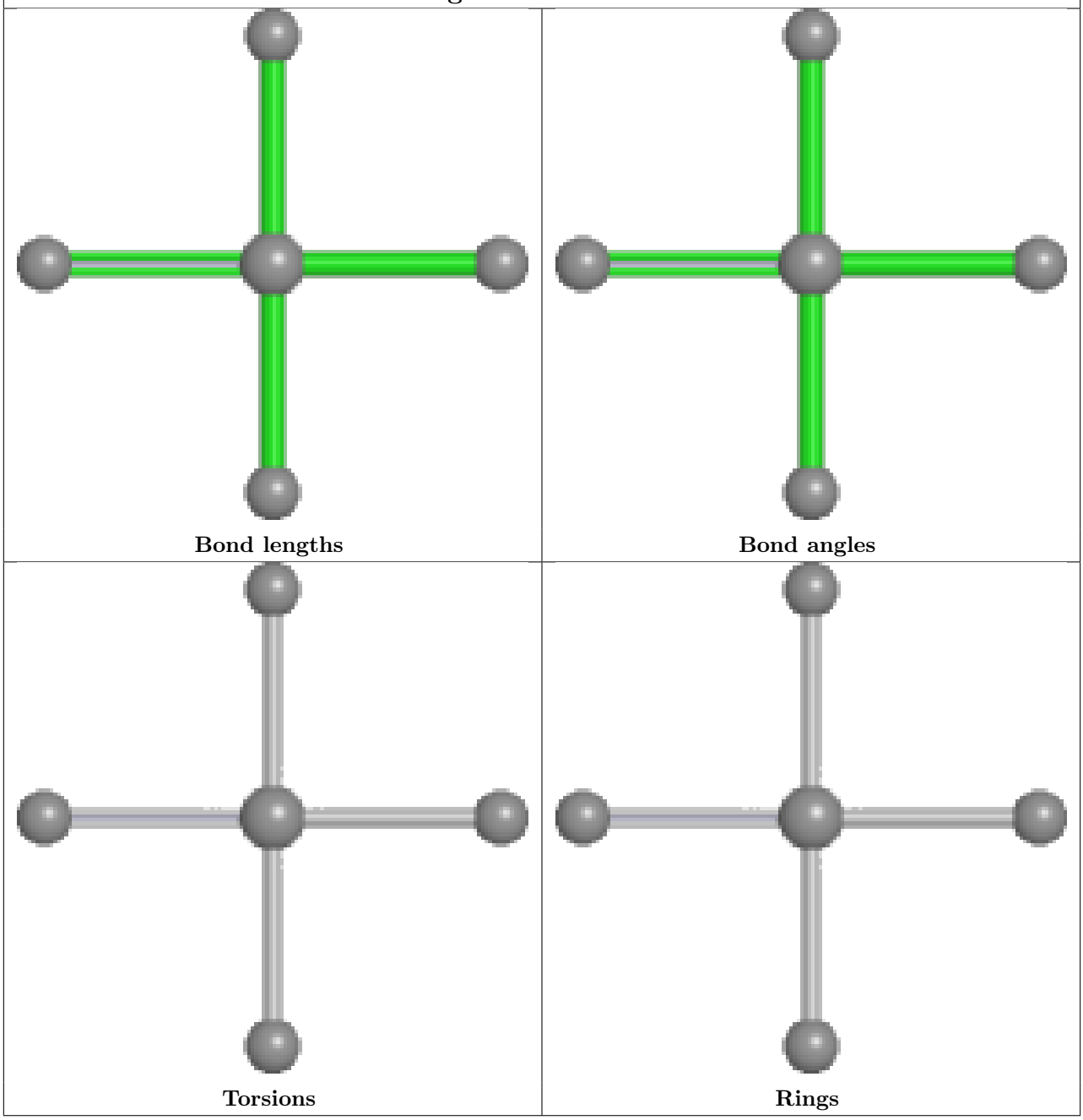


Torsions



Rings

Ligand SO4 B 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%)	0.10	22 (3%)	47	38	18, 57, 101, 153	1 (0%)
1	B	625/698 (89%)	0.35	33 (5%)	32	24	31, 66, 113, 160	0
All	All	1249/1396 (89%)	0.23	55 (4%)	39	31	18, 61, 110, 160	1 (0%)

All (55) 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	5.6
1	B	463	PHE	5.2
1	B	1	MET	5.1
1	B	135	ASN	5.1
1	B	3	ASP	4.9
1	A	2	THR	4.2
1	B	685	LYS	4.0
1	A	320[A]	CYS	3.9
1	B	137	ASP	3.8
1	A	465	VAL	3.7
1	A	578	VAL	3.6
1	A	1	MET	3.5
1	A	644	VAL	3.4
1	A	580	MET	3.4
1	B	256	HIS	3.3
1	B	608	ILE	3.2
1	B	259	ALA	3.2
1	B	419	VAL	3.2
1	B	140	THR	3.0
1	B	103	VAL	2.9
1	A	256	HIS	2.9
1	B	686	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	644	VAL	2.9
1	B	221	GLN	2.8
1	B	464	LYS	2.8
1	B	136	LEU	2.8
1	A	608	ILE	2.7
1	B	503	LYS	2.7
1	A	420	THR	2.6
1	A	353	ILE	2.6
1	A	464	LYS	2.6
1	A	468	ALA	2.6
1	B	139	LYS	2.5
1	B	59	VAL	2.5
1	B	255	SER	2.5
1	A	479	LYS	2.5
1	A	415	LEU	2.5
1	A	577	ILE	2.5
1	A	637	THR	2.4
1	B	461	THR	2.4
1	B	147	LEU	2.3
1	B	457	PRO	2.3
1	B	346	SER	2.3
1	A	3	ASP	2.2
1	B	45	PRO	2.2
1	B	52	TYR	2.2
1	B	456	SER	2.2
1	A	349	ASN	2.1
1	B	24	VAL	2.1
1	B	22	GLY	2.1
1	B	177	GLY	2.1
1	A	605	MET	2.0
1	B	49	THR	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

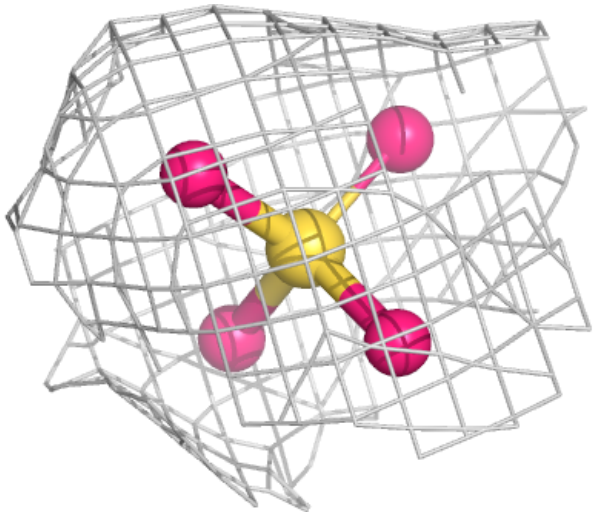
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

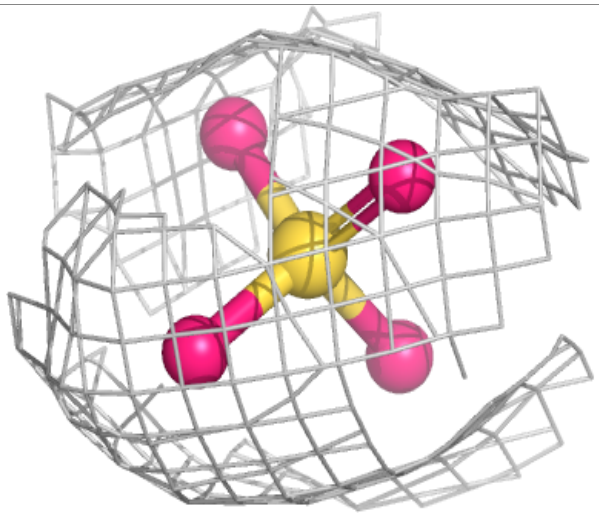
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	701	5/5	0.88	0.10	67,70,72,75	0
2	SO4	A	701	5/5	0.97	0.09	50,61,63,64	0

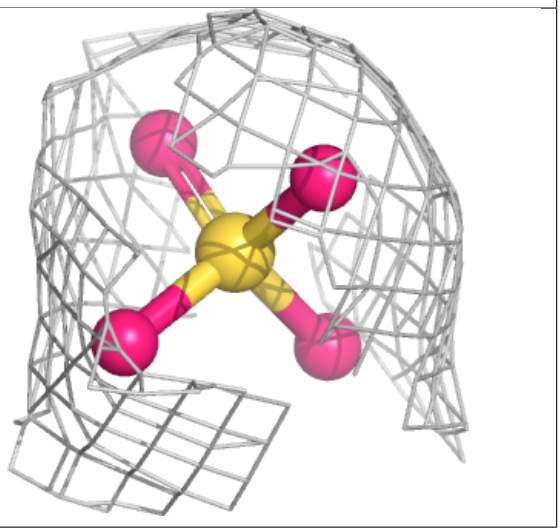
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

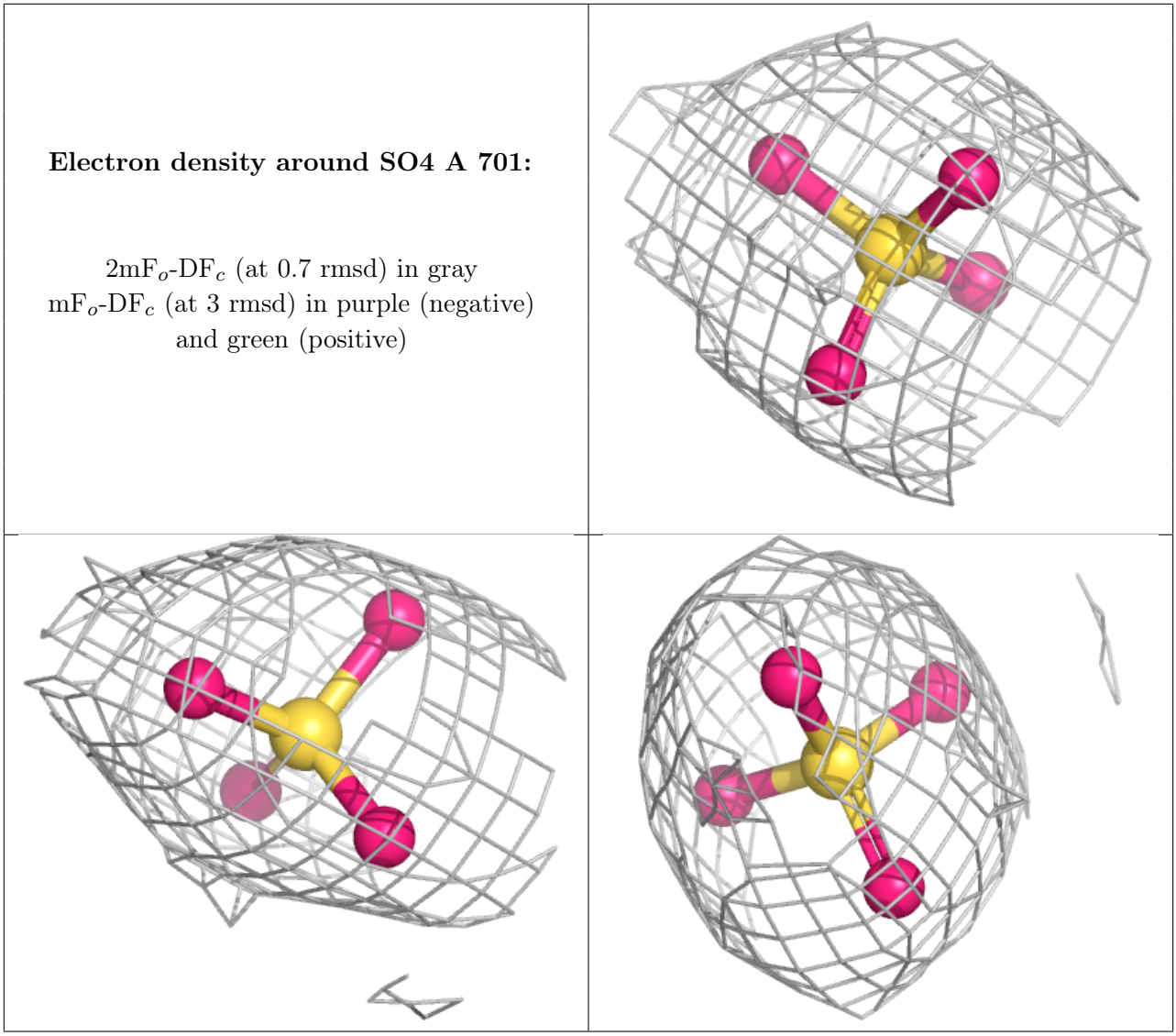






Electron density around SO4 A 701:

$2mF_o$-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

There are no such residues in this entry.