Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 02:07 PM UTC

PDB ID	:	6ZA5 / pdb_00006za5
Title	:	M. tuberculosis salicylate synthase MbtI in complex with salicylate and Mg2+
Authors	:	Mori, M.; Villa, S.; Meneghetti, F.; Bellinzoni, M.
Deposited on	:	2020-06-04
Resolution	:	2.11 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 (i) 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 (i)) were used in the production of this report:

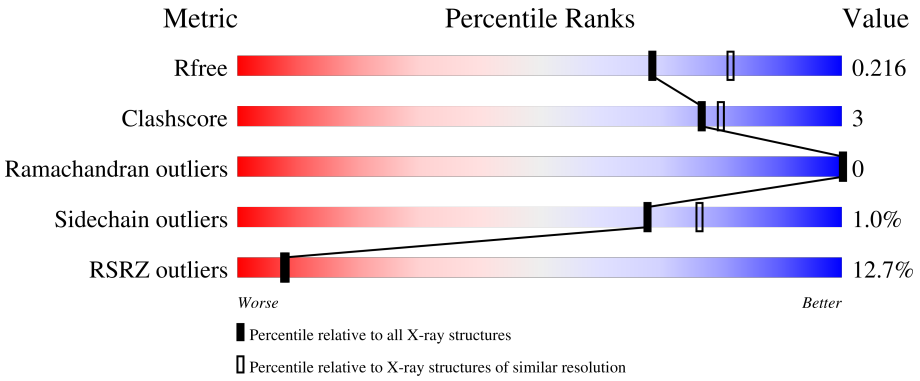
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.11 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	452	4% 94%
1	B	452	5% 90% 7%
1	C	452	30% 85% 11%
1	D	452	10% 91% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	501	-	-	X	-
4	ACT	A	520	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14227 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.

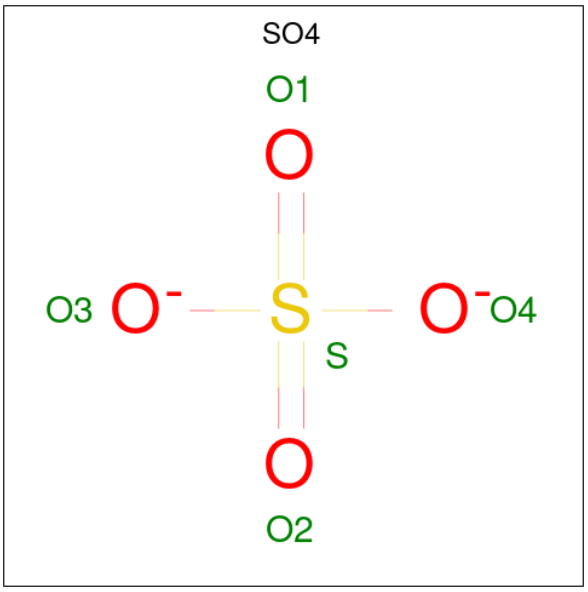
- Molecule 1 is a protein called Salicylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	8	0
			3401	2133	612	646	10			
1	B	440	Total	C	N	O	S	0	1	0
			3310	2077	603	620	10			
1	C	435	Total	C	N	O	S	0	6	0
			3245	2042	588	605	10			
1	D	436	Total	C	N	O	S	0	1	0
			3276	2056	594	616	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P9WFX1
A	0	HIS	-	expression tag	UNP P9WFX1
B	-1	GLY	-	expression tag	UNP P9WFX1
B	0	HIS	-	expression tag	UNP P9WFX1
C	-1	GLY	-	expression tag	UNP P9WFX1
C	0	HIS	-	expression tag	UNP P9WFX1
D	-1	GLY	-	expression tag	UNP P9WFX1
D	0	HIS	-	expression tag	UNP P9WFX1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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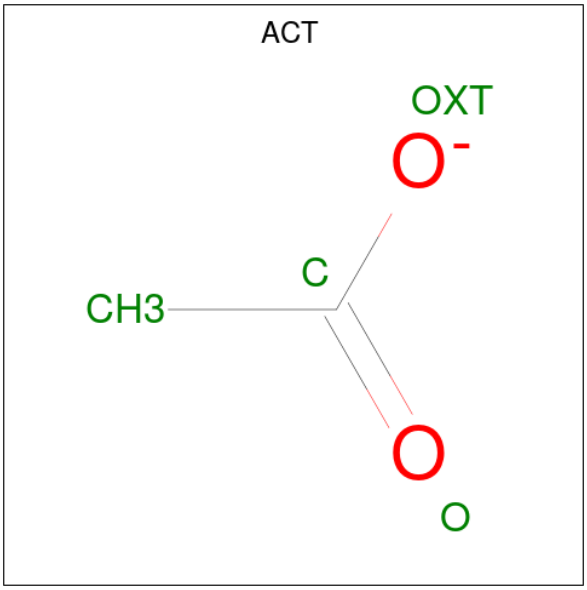
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

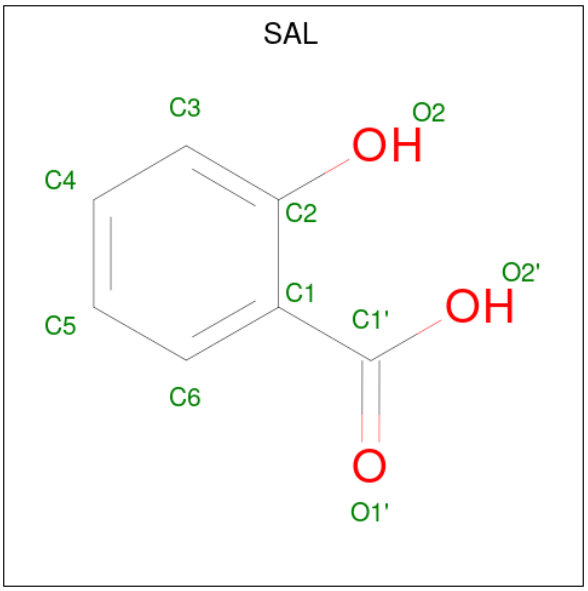
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $C_7H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 10 7 3	0	0
5	D	1	Total C O 10 7 3	0	0

- Molecule 6 is water.

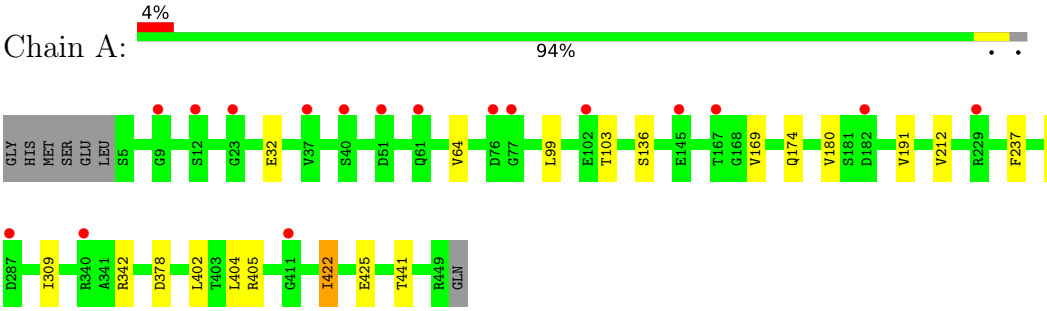
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	331	Total O 331 331	0	0
6	B	214	Total O 214 214	0	0
6	C	123	Total O 123 123	0	0
6	D	129	Total O 129 129	0	0

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.

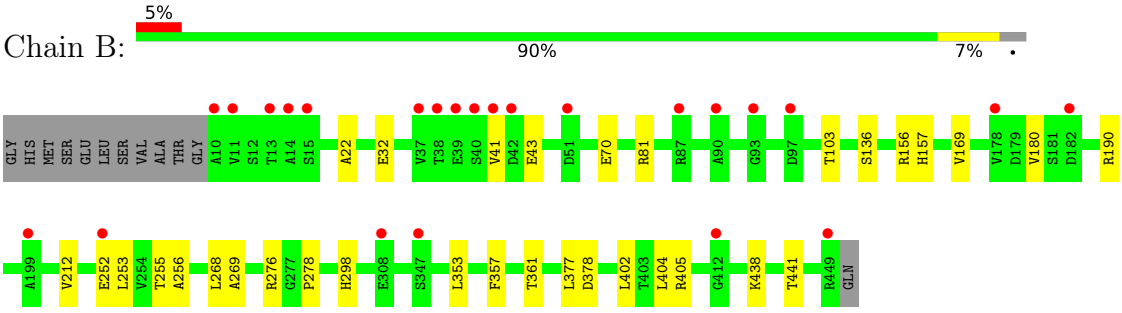
• Molecule 1: Salicylate synthase

Chain A:



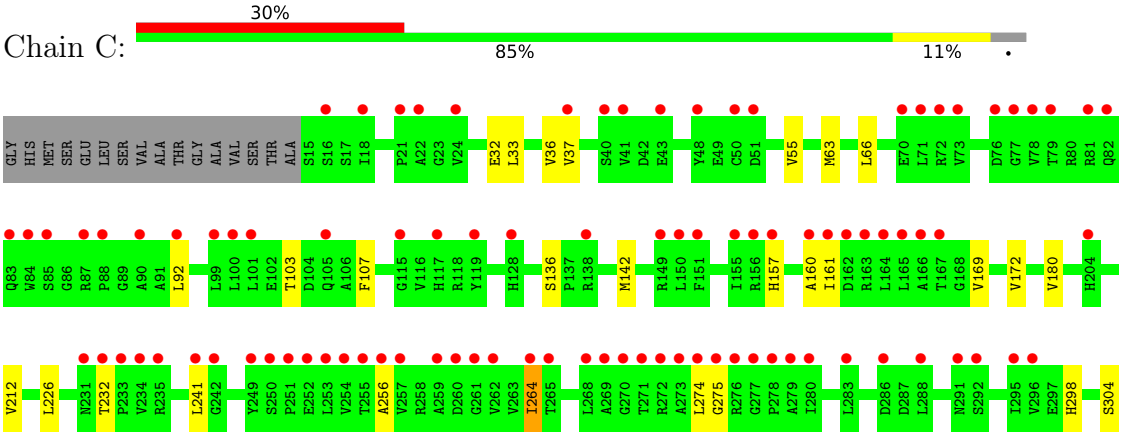
• Molecule 1: Salicylate synthase

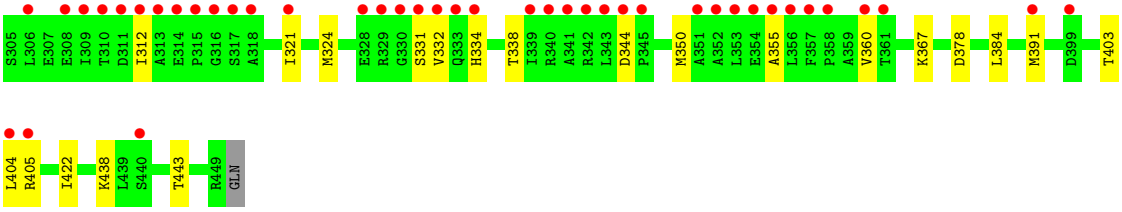
Chain B:



• Molecule 1: Salicylate synthase

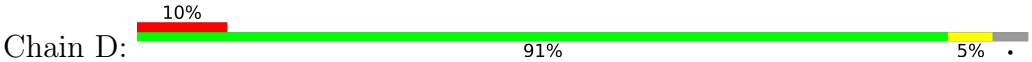
Chain C:

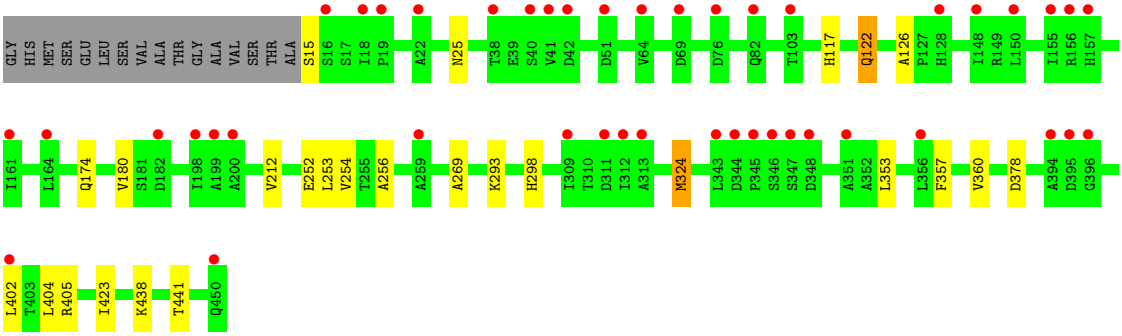




• Molecule 1: Salicylate synthase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	193.97Å 193.97Å 257.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.83 – 2.11 154.83 – 2.11	Depositor EDS
% Data completeness (in resolution range)	93.9 (154.83-2.11) 93.3 (154.83-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.195 , 0.217 (Not available) , 0.216	Depositor DCC
R_{free} test set	6600 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	43.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14227	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: SAL, MG, ACT, 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	0.75	1/3480 (0.0%)	0.96	0/4731
1	B	0.71	0/3371	0.95	1/4584 (0.0%)
1	C	0.76	1/3309 (0.0%)	0.99	1/4511 (0.0%)
1	D	0.67	0/3337	0.96	3/4539 (0.1%)
All	All	0.72	2/13497 (0.0%)	0.97	5/18365 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	422	ILE	CG1-CD1	-5.36	1.30	1.51
1	A	422	ILE	CG1-CD1	-5.17	1.31	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	344	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	22	ALA	N-CA-C	5.75	118.01	111.11
1	D	360	VAL	CA-C-N	5.68	128.16	120.38
1	D	360	VAL	C-N-CA	5.68	128.16	120.38
1	D	254	VAL	N-CA-C	-5.28	105.56	110.53

There are no chirality outliers.

There are no planarity outliers.

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	3401	0	3420	13	0
1	B	3310	0	3301	16	0
1	C	3245	0	3174	36	0
1	D	3276	0	3252	13	0
2	A	85	0	0	0	0
2	B	25	0	0	1	0
2	C	20	0	0	2	0
2	D	40	0	0	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	3	3	0
5	B	10	0	4	0	0
5	D	10	0	4	0	0
6	A	331	0	0	1	0
6	B	214	0	0	0	0
6	C	123	0	0	2	0
6	D	129	0	0	0	0
All	All	14227	0	13158	77	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 3.

All (77) 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:D:298:HIS:CD2	1:D:324:MET:HG2	2.24	0.73
1:C:332:VAL:HG23	1:C:334:HIS:HE1	1.55	0.72
1:C:312:ILE:CG1	1:C:355:ALA:HB2	2.21	0.70
1:C:298:HIS:CD2	1:C:324:MET:HG2	2.28	0.69
1:C:312:ILE:HG12	1:C:355:ALA:HB2	1.79	0.64
1:C:332:VAL:HG23	1:C:334:HIS:CE1	2.33	0.62
1:C:304:SER:HB3	1:C:360:VAL:HG21	1.82	0.62
1:B:268:LEU:H	1:B:361:THR:HG21	1.66	0.59
1:C:36:VAL:HG12	1:C:160:ALA:HB1	1.84	0.58
1:C:312:ILE:HG13	1:C:355:ALA:HB2	1.84	0.58
1:C:63:MET:HE1	1:C:241:LEU:HD11	1.84	0.58
1:A:103:THR:HG21	1:A:136:SER:HB2	1.86	0.58
1:C:37:VAL:HG13	1:C:157:HIS:HD2	1.69	0.57
1:C:274:LEU:HD13	1:C:275:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:THR:CB	1:C:331:SER:H	2.17	0.57
1:A:174:GLN:H	1:A:174:GLN:CD	2.12	0.56
1:C:107:PHE:HE2	1:C:391:MET:HE2	1.71	0.55
1:B:438:LYS:HD3	2:B:503:SO4:O4	2.07	0.55
1:C:37:VAL:HG13	1:C:157:HIS:CD2	2.42	0.54
1:A:405:ARG:HH21	4:A:520:ACT:H3	1.73	0.54
1:D:174:GLN:CD	1:D:174:GLN:H	2.15	0.54
1:B:103:THR:HG21	1:B:136:SER:HB2	1.90	0.54
1:B:190:ARG:HD2	1:B:377:LEU:O	2.08	0.52
1:C:321:ILE:HG13	1:C:338:THR:HB	1.90	0.52
1:B:353:LEU:O	1:B:357:PHE:HB2	2.10	0.51
1:D:293:LYS:HG2	1:D:423:ILE:HD11	1.90	0.51
1:C:384:LEU:HG	1:C:403:THR:HG21	1.93	0.50
1:D:353:LEU:O	1:D:357:PHE:HB2	2.11	0.50
1:C:33:LEU:HD21	1:C:161:ILE:HG12	1.93	0.50
1:C:55:VAL:HG22	1:C:142:MET:HG2	1.94	0.49
1:C:404:LEU:HB3	2:C:501:SO4:O4	2.11	0.49
1:C:103:THR:HG21	1:C:136:SER:HB2	1.92	0.49
1:D:402:LEU:HG	1:D:404:LEU:HG	1.94	0.49
1:C:438:LYS:HD3	2:C:501:SO4:O3	2.13	0.48
1:B:402:LEU:HG	1:B:404:LEU:HG	1.95	0.48
1:D:438:LYS:HD3	2:D:504:SO4:O2	2.13	0.48
1:A:260:ASP:O	1:A:342:ARG:NH1	2.48	0.47
1:D:180:VAL:HG12	1:D:212:VAL:HG11	1.95	0.47
1:A:180:VAL:HG12	1:A:212:VAL:HG11	1.97	0.46
1:A:404:LEU:HD13	4:A:520:ACT:H3	1.96	0.46
1:C:274:LEU:HG	6:C:659:HOH:O	2.15	0.46
1:C:180:VAL:HG11	1:C:443:THR:HG21	1.97	0.46
1:C:274:LEU:HD13	1:C:275:GLY:H	1.80	0.46
1:C:180:VAL:HG12	1:C:212:VAL:HG11	1.98	0.45
1:D:253:LEU:HD13	1:D:256:ALA:HB2	1.98	0.45
1:B:180:VAL:HG12	1:B:212:VAL:HG11	1.97	0.45
1:B:405:ARG:HB3	1:B:441:THR:HG21	1.99	0.45
1:D:405:ARG:HB3	1:D:441:THR:HG21	1.98	0.45
1:C:66:LEU:HD22	1:C:92:LEU:HB2	1.98	0.45
1:B:41:VAL:HG12	1:B:43:GLU:HB3	1.97	0.44
1:A:405:ARG:HB3	1:A:441:THR:HG21	1.99	0.44
1:D:298:HIS:HD2	1:D:324:MET:HG2	1.80	0.44
1:C:312:ILE:HG13	1:C:355:ALA:CB	2.46	0.44
1:C:332:VAL:CG2	1:C:334:HIS:CE1	2.99	0.44
1:C:32:GLU:HG3	1:C:169:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PRO:HG3	1:D:126:ALA:HB3	2.00	0.43
1:C:256:ALA:HB3	1:C:264:ILE:HG13	1.99	0.43
1:A:191:VAL:HG22	1:A:422:ILE:HD11	2.01	0.43
1:B:253:LEU:HD13	1:B:256:ALA:HB2	1.99	0.43
1:D:269:ALA:HB3	1:D:298:HIS:HA	2.01	0.43
1:A:32:GLU:HG3	1:A:169:VAL:HB	2.01	0.43
1:C:92:LEU:HD23	1:C:350:MET:CE	2.50	0.42
1:A:405:ARG:HH21	4:A:520:ACT:CH3	2.31	0.42
1:A:237:PHE:HE1	6:A:619:HOH:O	2.03	0.42
1:B:269:ALA:HB3	1:B:298:HIS:HA	2.02	0.42
1:C:107:PHE:CE2	1:C:391:MET:HE2	2.53	0.42
1:C:360:VAL:HB	1:C:367:LYS:HD2	2.02	0.42
1:B:32:GLU:HG3	1:B:169:VAL:HB	2.02	0.41
1:C:312:ILE:CG1	1:C:355:ALA:CB	2.97	0.41
1:A:402:LEU:HG	1:A:404:LEU:HG	2.01	0.41
1:B:70:GLU:OE1	1:B:81:ARG:NH2	2.54	0.41
1:B:156:ARG:NH1	1:B:157:HIS:CE1	2.89	0.41
1:D:117:HIS:HA	1:D:122:GLN:HE21	1.85	0.41
1:B:252:GLU:HB3	1:B:268:LEU:HD22	2.02	0.40
1:C:172:VAL:HG11	1:C:226:LEU:HB2	2.03	0.40
1:A:64:VAL:HG23	1:A:99:LEU:HD11	2.04	0.40
1:C:405:ARG:HB3	6:C:624:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	451/452 (100%)	445 (99%)	6 (1%)	0	100	100
1	B	439/452 (97%)	434 (99%)	5 (1%)	0	100	100
1	C	439/452 (97%)	427 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	435/452 (96%)	430 (99%)	5 (1%)	0	100	100
All	All	1764/1808 (98%)	1736 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	356/359 (99%)	353 (99%)	3 (1%)	73	81
1	B	337/359 (94%)	334 (99%)	3 (1%)	70	78
1	C	321/359 (89%)	319 (99%)	2 (1%)	78	86
1	D	333/359 (93%)	327 (98%)	6 (2%)	51	60
All	All	1347/1436 (94%)	1333 (99%)	14 (1%)	68	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ILE
1	A	378	ASP
1	A	425	GLU
1	B	255	THR
1	B	276	ARG
1	B	378	ASP
1	C	264	ILE
1	C	378	ASP
1	D	15	SER
1	D	25	ASN
1	D	122	GLN
1	D	252	GLU
1	D	324	MET
1	D	378	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	409	GLN
1	B	123	GLN
1	B	409	GLN
1	C	157	HIS
1	C	334	HIS
1	D	82	GLN
1	D	122	GLN
1	D	409	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 4 are monoatomic - leaving 37 for Mogul analysis.

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	503	-	4,4,4	0.40	0	6,6,6	0.38	0
2	SO4	B	504	-	4,4,4	0.17	0	6,6,6	0.37	0
2	SO4	A	510	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	B	507	-	4,4,4	0.28	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	D	505	-	4,4,4	0.27	0	6,6,6	0.39	0
2	SO4	B	503	-	4,4,4	0.40	0	6,6,6	0.33	0
2	SO4	A	506	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	A	502	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	A	504	-	4,4,4	0.61	0	6,6,6	0.15	0
2	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	C	501	-	4,4,4	0.53	0	6,6,6	0.69	0
2	SO4	A	512	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	D	509	-	4,4,4	0.27	0	6,6,6	0.08	0
4	ACT	A	520	-	3,3,3	1.13	0	3,3,3	0.55	0
5	SAL	B	502	3	10,10,10	0.75	0	13,13,13	0.82	1 (7%)
2	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	A	516	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SAL	D	502	3	10,10,10	0.70	0	13,13,13	1.00	2 (15%)
2	SO4	A	517	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	A	514	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	D	503	-	4,4,4	0.21	0	6,6,6	0.16	0
2	SO4	D	508	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	A	515	-	4,4,4	0.26	0	6,6,6	0.28	0
2	SO4	B	506	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	D	507	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	A	513	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	D	504	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	A	505	-	4,4,4	0.29	0	6,6,6	0.37	0
2	SO4	A	511	-	4,4,4	0.33	0	6,6,6	0.17	0
2	SO4	D	506	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	A	507	-	4,4,4	0.50	0	6,6,6	0.50	0
2	SO4	D	510	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	A	501	3	4,4,4	0.23	0	6,6,6	0.46	0
2	SO4	C	504	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	A	508	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	A	509	-	4,4,4	0.27	0	6,6,6	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAL	D	502	3	-	0/4/4/4	0/1/1/1
5	SAL	B	502	3	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	502	SAL	C2-C1-C1'	2.19	122.25	120.00
5	B	502	SAL	C2-C1-C1'	2.19	122.25	120.00
5	D	502	SAL	O1'-C1'-C1	-2.01	117.18	121.97

There are no chirality outliers.

There are no torsion outliers.

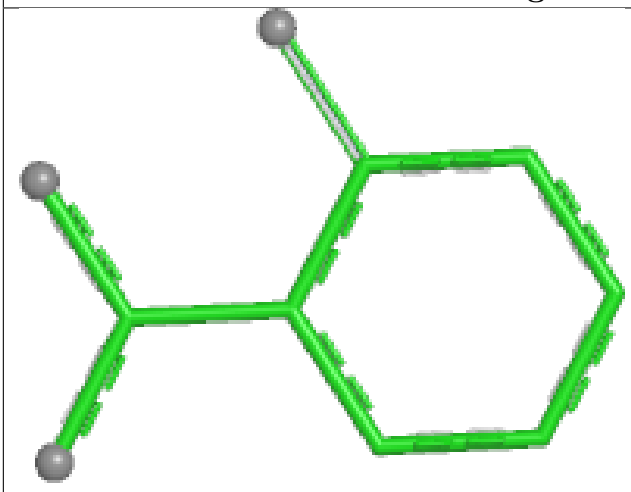
There are no ring outliers.

4 monomers are involved in 7 short contacts:

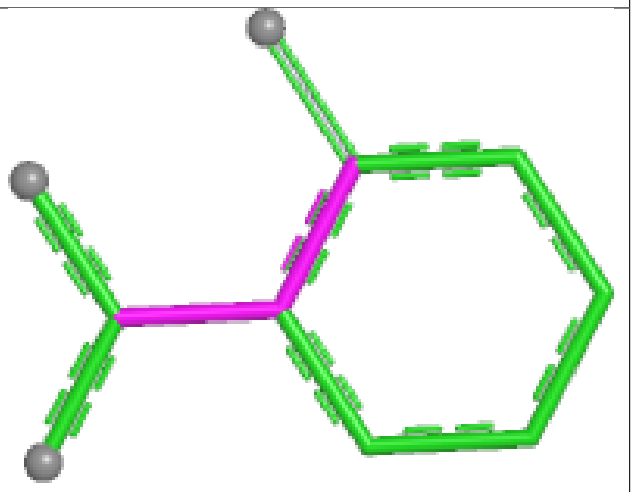
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	SO4	1	0
2	C	501	SO4	2	0
4	A	520	ACT	3	0
2	D	504	SO4	1	0

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.

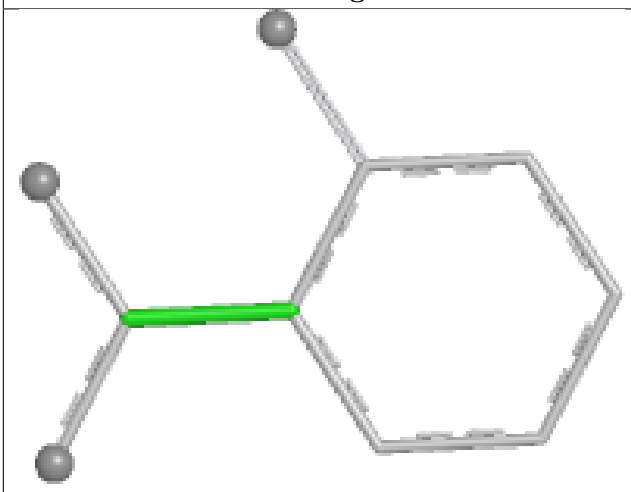
Ligand SAL B 502



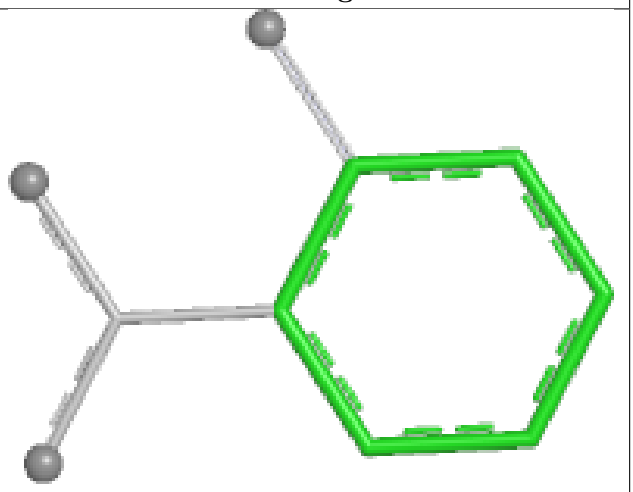
Bond lengths



Bond angles

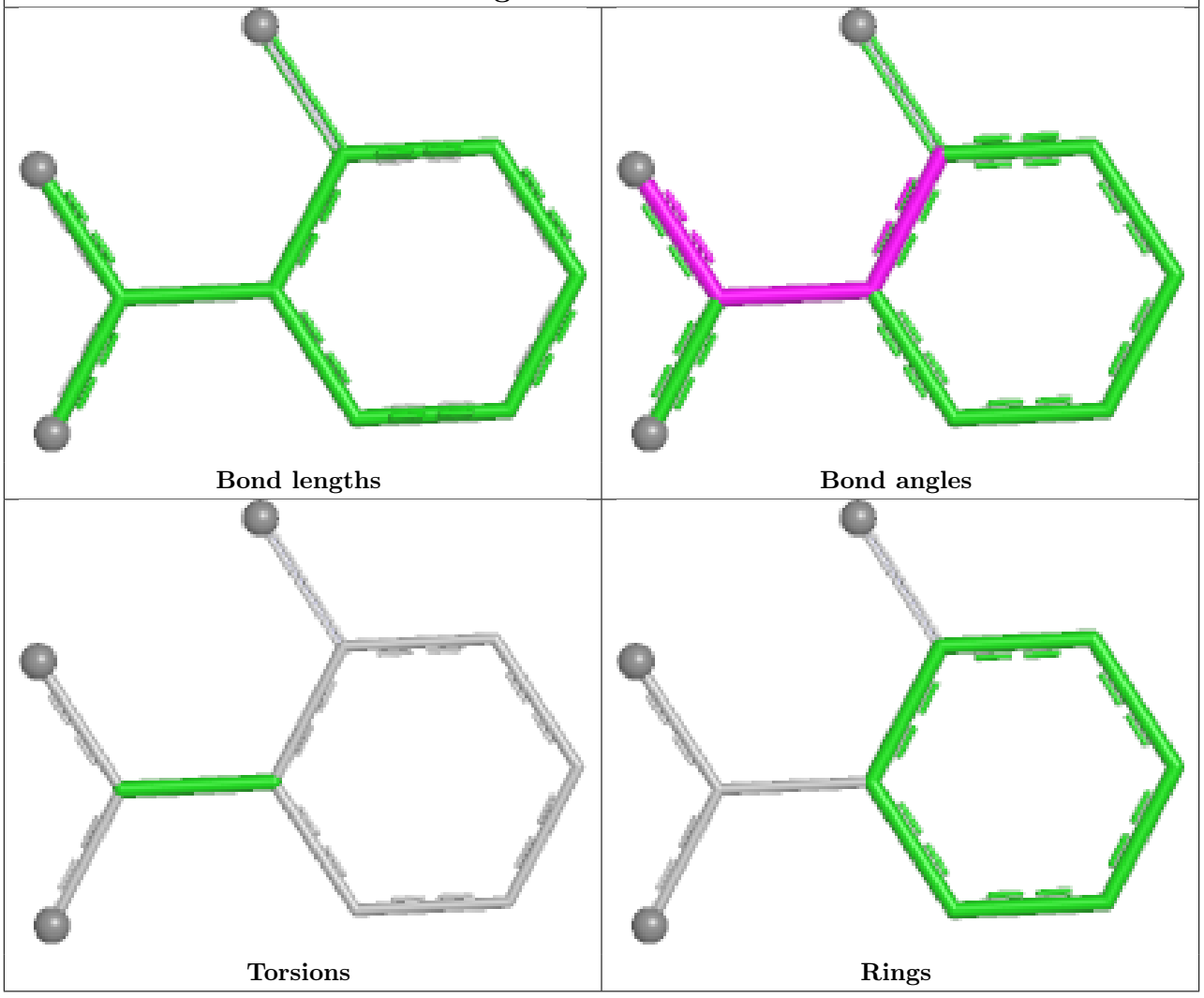


Torsions



Rings

Ligand SAL D 502



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	445/452 (98%)	0.24	18 (4%) 42 44	20, 38, 56, 79	8 (1%)
1	B	440/452 (97%)	0.52	24 (5%) 30 32	25, 45, 63, 84	1 (0%)
1	C	435/452 (96%)	1.54	137 (31%) 1 1	21, 59, 90, 101	6 (1%)
1	D	436/452 (96%)	0.86	44 (10%) 12 13	25, 59, 85, 97	1 (0%)
All	All	1756/1808 (97%)	0.79	223 (12%) 8 8	20, 48, 84, 101	16 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	VAL	7.7
1	C	355	ALA	7.3
1	C	315[A]	PRO	5.9
1	C	332	VAL	5.8
1	C	357	PHE	5.8
1	B	41	VAL	5.6
1	C	356	LEU	5.2
1	C	233	PRO	5.2
1	C	232	THR	5.2
1	C	253	LEU	5.0
1	C	251	PRO	5.0
1	C	345	PRO	4.9
1	C	273	ALA	4.7
1	C	269	ALA	4.6
1	C	41	VAL	4.5
1	C	312	ILE	4.4
1	C	254	VAL	4.4
1	D	396	GLY	4.4
1	C	329	ARG	4.4
1	C	310	THR	4.4
1	D	347	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	308	GLU	4.3
1	B	11	VAL	4.3
1	C	40	SER	4.3
1	C	274	LEU	4.2
1	C	343	LEU	4.2
1	C	242	GLY	4.2
1	C	288	LEU	4.2
1	C	164	LEU	4.1
1	C	358	PRO	4.1
1	D	16	SER	4.1
1	D	199	ALA	3.9
1	B	10	ALA	3.9
1	B	38	THR	3.9
1	D	182	ASP	3.8
1	A	37	VAL	3.8
1	C	309	ILE	3.8
1	C	100	LEU	3.8
1	C	48	TYR	3.7
1	C	255	THR	3.7
1	C	286	ASP	3.7
1	C	353	LEU	3.7
1	C	313[A]	ALA	3.7
1	C	276	ARG	3.7
1	C	283	LEU	3.6
1	C	316[A]	GLY	3.6
1	C	331	SER	3.6
1	C	92	LEU	3.6
1	B	40	SER	3.6
1	C	268	LEU	3.6
1	C	278	PRO	3.6
1	C	22	ALA	3.6
1	C	82	GLN	3.6
1	C	344	ASP	3.5
1	C	84	TRP	3.4
1	C	78	VAL	3.4
1	C	259	ALA	3.4
1	B	13	THR	3.4
1	C	272	ARG	3.4
1	A	145	GLU	3.4
1	C	231	ASN	3.3
1	A	76	ASP	3.3
1	D	164	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	87	ARG	3.3
1	C	279	ALA	3.3
1	D	42	ASP	3.3
1	C	76	ASP	3.2
1	C	70	GLU	3.2
1	C	360	VAL	3.2
1	C	354	GLU	3.2
1	C	257	VAL	3.2
1	C	166	ALA	3.2
1	C	163	ARG	3.2
1	C	73	VAL	3.1
1	C	264	ILE	3.1
1	C	399	ASP	3.1
1	D	259	ALA	3.1
1	C	71	LEU	3.1
1	C	249	TYR	3.1
1	C	85	SER	3.1
1	D	348	ASP	3.1
1	C	275	GLY	3.0
1	C	151	PHE	3.0
1	C	314[A]	GLU	3.0
1	C	50	CYS	3.0
1	D	150	LEU	3.0
1	C	88	PRO	3.0
1	B	42	ASP	3.0
1	A	229	ARG	2.9
1	A	102	GLU	2.9
1	C	317	SER	2.9
1	C	328	GLU	2.9
1	C	115	GLY	2.9
1	C	334	HIS	2.9
1	C	21	PRO	2.9
1	C	321	ILE	2.9
1	D	18	ILE	2.9
1	B	449	ARG	2.9
1	D	312	ILE	2.9
1	C	292	SER	2.9
1	D	346	SER	2.9
1	C	256	ALA	2.9
1	C	277	GLY	2.9
1	D	155	ILE	2.8
1	C	77	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	291	ASN	2.8
1	D	128	HIS	2.8
1	D	41	VAL	2.8
1	C	83	GLN	2.8
1	D	351	ALA	2.8
1	C	280	ILE	2.8
1	C	16	SER	2.7
1	C	405	ARG	2.7
1	C	295	ILE	2.7
1	C	333	GLN	2.7
1	C	204[A]	HIS	2.7
1	C	261	GLY	2.7
1	C	79	THR	2.7
1	C	262	VAL	2.7
1	C	311	ASP	2.7
1	C	306	LEU	2.7
1	C	250	SER	2.7
1	C	161	ILE	2.7
1	D	344	ASP	2.7
1	C	128	HIS	2.6
1	C	18	ILE	2.6
1	C	72	ARG	2.6
1	C	165	LEU	2.6
1	C	81	ARG	2.6
1	C	342	ARG	2.6
1	C	260	ASP	2.6
1	C	37	VAL	2.5
1	D	198	ILE	2.5
1	C	330	GLY	2.5
1	A	40	SER	2.5
1	C	24	VAL	2.5
1	D	161	ILE	2.5
1	C	51	ASP	2.5
1	C	162	ASP	2.5
1	C	90	ALA	2.5
1	D	22	ALA	2.5
1	D	200	ALA	2.5
1	C	296	VAL	2.5
1	C	157	HIS	2.5
1	C	235	ARG	2.5
1	D	395	ASP	2.4
1	B	14	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	318	ALA	2.4
1	C	391	MET	2.4
1	A	182	ASP	2.4
1	C	271	THR	2.4
1	C	117[A]	HIS	2.4
1	D	356	LEU	2.4
1	B	97	ASP	2.4
1	D	76	ASP	2.4
1	C	339	ILE	2.4
1	C	440	SER	2.4
1	D	343	LEU	2.4
1	D	311	ASP	2.4
1	A	340[A]	ARG	2.4
1	D	82	GLN	2.3
1	D	38	THR	2.3
1	C	341	ALA	2.3
1	A	9	GLY	2.3
1	C	340	ARG	2.3
1	B	308	GLU	2.3
1	D	19	PRO	2.3
1	C	351	ALA	2.3
1	A	51	ASP	2.3
1	C	43	GLU	2.3
1	D	345	PRO	2.3
1	B	90	ALA	2.3
1	A	23	GLY	2.3
1	C	150	LEU	2.3
1	D	51	ASP	2.2
1	D	313	ALA	2.2
1	C	99	LEU	2.2
1	B	252	GLU	2.2
1	B	87	ARG	2.2
1	C	138	ARG	2.2
1	C	265	THR	2.2
1	D	309	ILE	2.2
1	A	411	GLY	2.2
1	B	412	GLY	2.2
1	C	252	GLU	2.2
1	C	404	LEU	2.2
1	D	402	LEU	2.2
1	C	149	ARG	2.2
1	A	167	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	51	ASP	2.2
1	C	101	LEU	2.2
1	A	275	GLY	2.1
1	B	199	ALA	2.1
1	A	287	ASP	2.1
1	C	361	THR	2.1
1	A	61	GLN	2.1
1	B	93	GLY	2.1
1	D	157	HIS	2.1
1	C	160	ALA	2.1
1	B	15	SER	2.1
1	D	40	SER	2.1
1	B	39	GLU	2.1
1	C	167	THR	2.1
1	D	103	THR	2.1
1	B	37	VAL	2.1
1	D	394	ALA	2.1
1	A	12	SER	2.1
1	B	347	SER	2.1
1	C	156	ARG	2.1
1	C	155	ILE	2.1
1	D	148	ILE	2.1
1	B	178	VAL	2.1
1	D	64	VAL	2.1
1	B	182	ASP	2.0
1	D	450	GLN	2.0
1	D	156	ARG	2.0
1	C	270	GLY	2.0
1	C	352	ALA	2.0
1	C	105	GLN	2.0
1	C	241	LEU	2.0
1	D	69	ASP	2.0
1	A	77	GLY	2.0
1	C	119	TYR	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 (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	D	509	5/5	0.58	0.15	125,125,125,125	0
2	SO4	A	502	5/5	0.64	0.11	109,109,109,109	0
2	SO4	A	510	5/5	0.67	0.12	119,119,119,119	0
2	SO4	A	513	5/5	0.70	0.16	143,143,143,143	0
2	SO4	D	507	5/5	0.71	0.13	121,121,121,121	0
2	SO4	D	508	5/5	0.71	0.14	144,144,144,144	0
2	SO4	A	511	5/5	0.71	0.15	105,105,106,106	0
2	SO4	B	507	5/5	0.74	0.14	127,127,127,127	0
2	SO4	A	512	5/5	0.75	0.11	128,128,128,128	0
2	SO4	A	514	5/5	0.77	0.14	105,105,105,105	0
2	SO4	A	515	5/5	0.78	0.10	86,86,86,86	0
2	SO4	A	509	5/5	0.78	0.12	116,116,116,116	0
2	SO4	C	504	5/5	0.78	0.09	114,114,114,114	0
2	SO4	A	517	5/5	0.79	0.10	136,136,136,136	0
2	SO4	A	506	5/5	0.81	0.11	97,97,97,97	0
2	SO4	A	516	5/5	0.81	0.11	113,113,113,113	0
2	SO4	B	506	5/5	0.83	0.13	147,147,147,147	0
2	SO4	B	505	5/5	0.84	0.10	105,106,106,106	0
2	SO4	C	502	5/5	0.84	0.12	121,121,122,122	0
2	SO4	A	504	5/5	0.86	0.17	54,54,54,54	5
2	SO4	A	507	5/5	0.87	0.13	59,59,60,60	5
2	SO4	A	505	5/5	0.89	0.11	64,65,65,66	5
5	SAL	B	502	10/10	0.89	0.14	56,59,59,60	0
4	ACT	A	520	4/4	0.90	0.14	35,37,38,39	0
2	SO4	D	510	5/5	0.90	0.11	157,157,157,157	0
5	SAL	D	502	10/10	0.90	0.13	52,52,53,55	0
2	SO4	D	506	5/5	0.91	0.10	88,89,89,89	0
2	SO4	A	508	5/5	0.92	0.14	84,85,85,85	0
2	SO4	A	503	5/5	0.92	0.10	55,56,57,57	0
2	SO4	C	503	5/5	0.92	0.18	36,36,37,38	5
2	SO4	C	501	5/5	0.94	0.10	44,45,46,46	5
2	SO4	D	505	5/5	0.95	0.09	51,51,52,52	5

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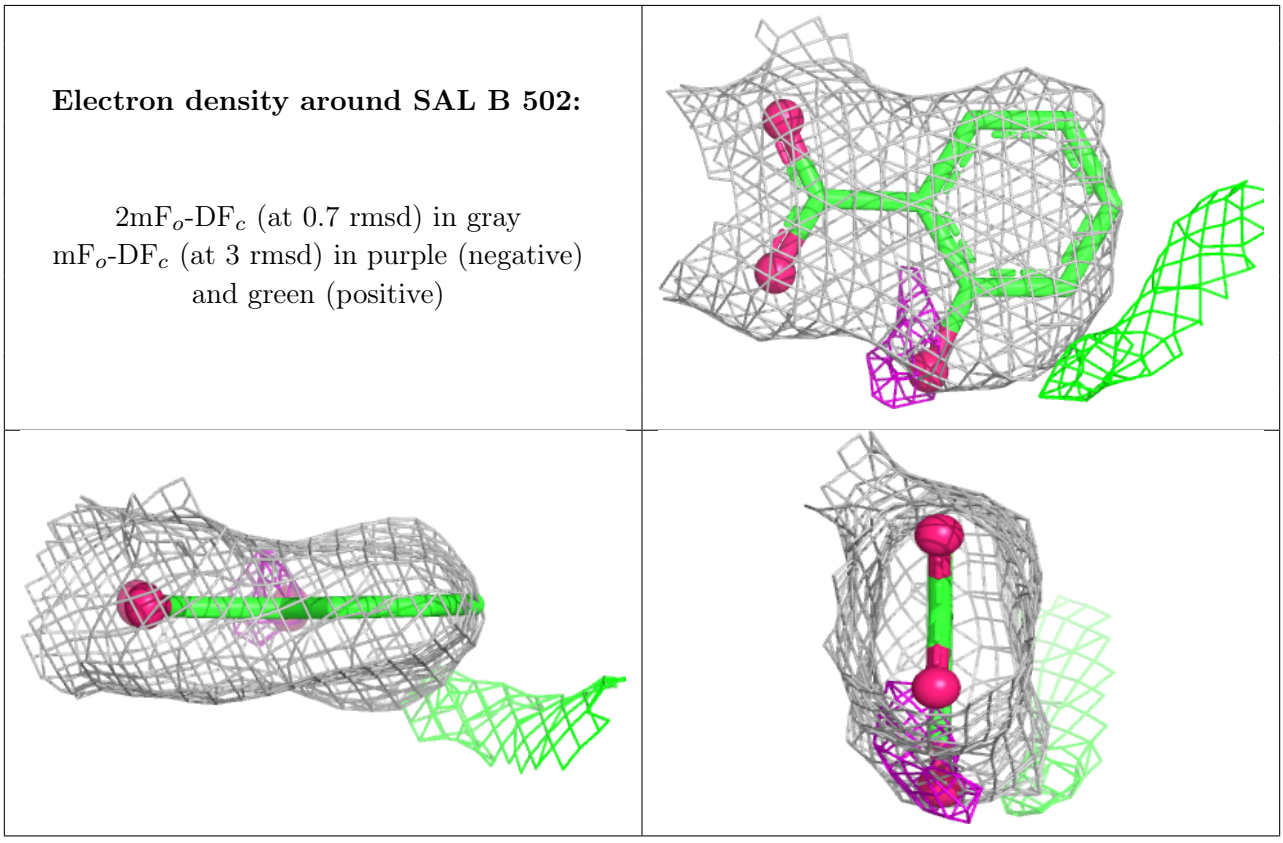
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	503	5/5	0.95	0.08	58,58,59,59	0
2	SO4	D	504	5/5	0.95	0.09	57,57,58,58	0
2	SO4	B	504	5/5	0.96	0.07	68,68,69,69	0
2	SO4	B	503	5/5	0.97	0.07	45,45,45,45	5
2	SO4	A	501	5/5	0.97	0.07	37,39,39,39	5
3	MG	D	501	1/1	0.98	0.04	50,50,50,50	0
3	MG	B	501	1/1	0.98	0.04	55,55,55,55	0
3	MG	A	519	1/1	0.99	0.10	36,36,36,36	0
3	MG	A	518	1/1	0.99	0.04	44,44,44,44	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.

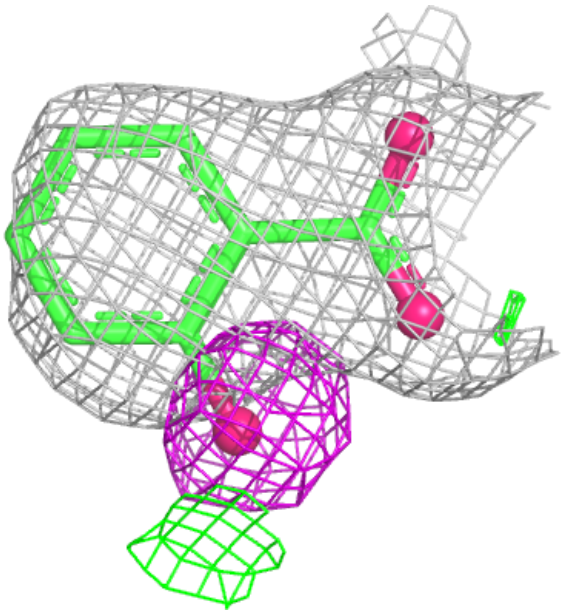
Electron density around SAL B 502:

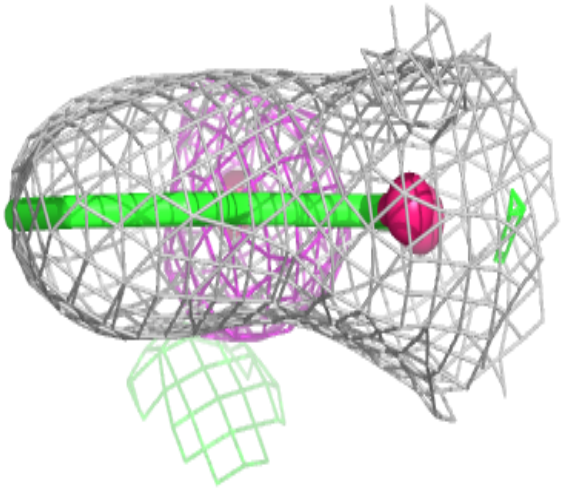
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

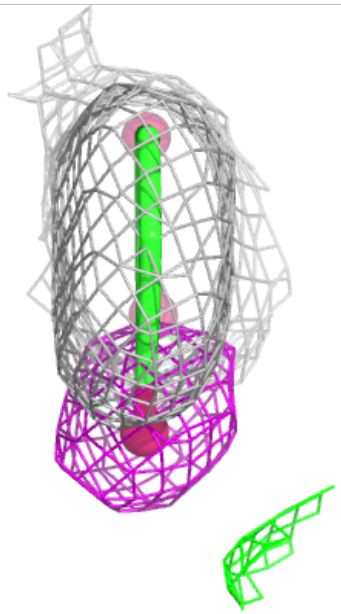


Electron density around SAL D 502:

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

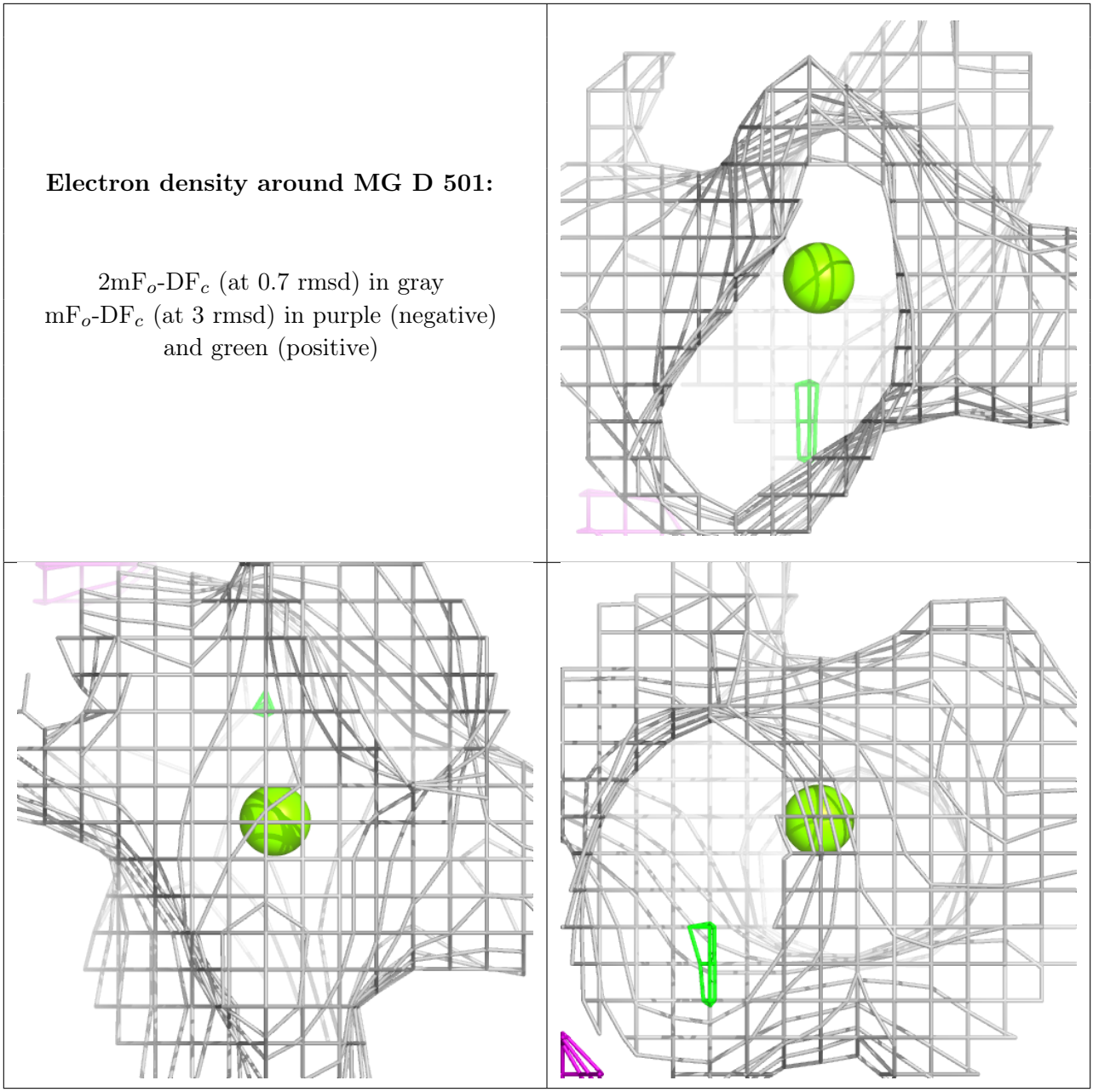






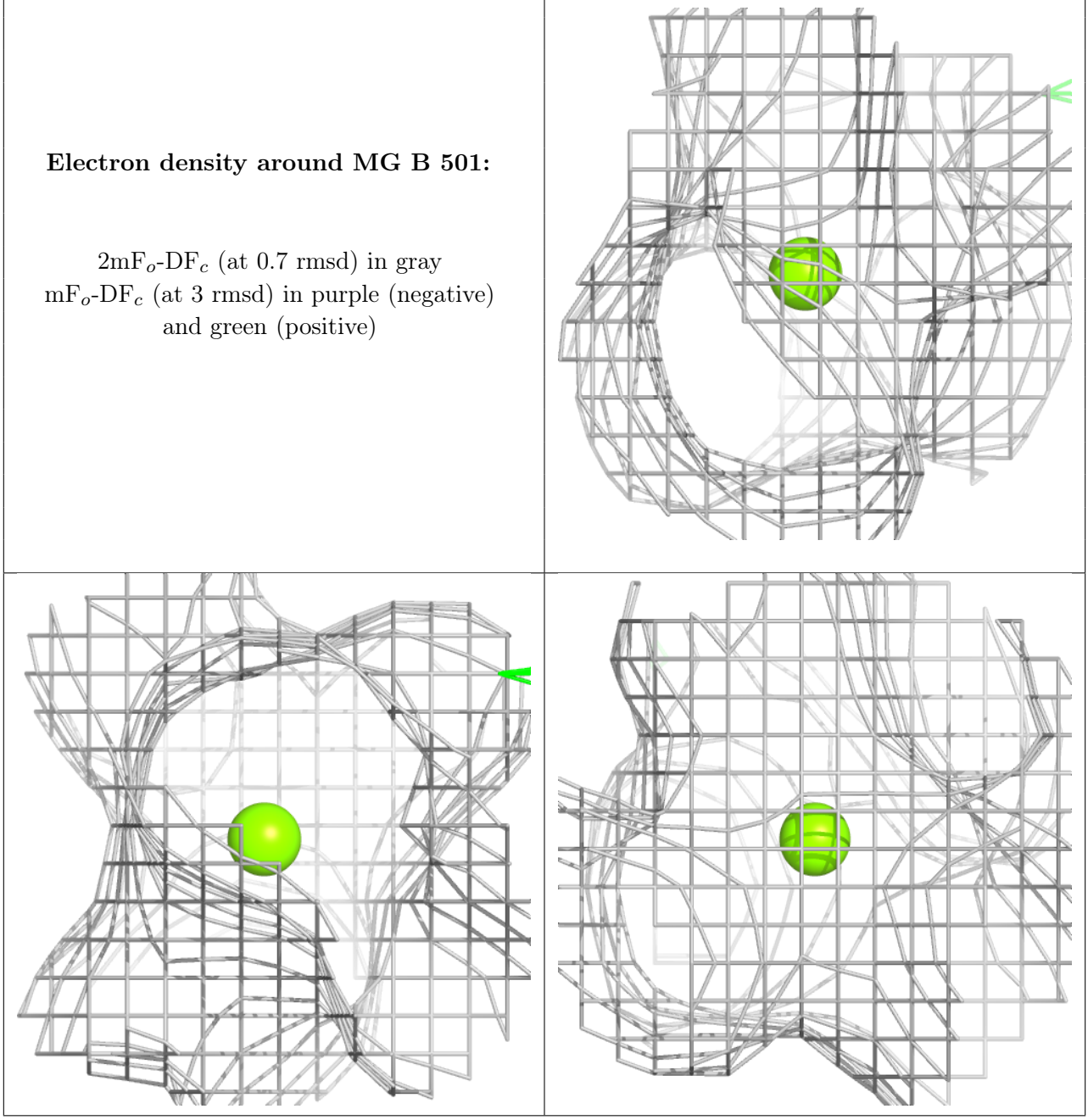
Electron density around MG D 501:

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



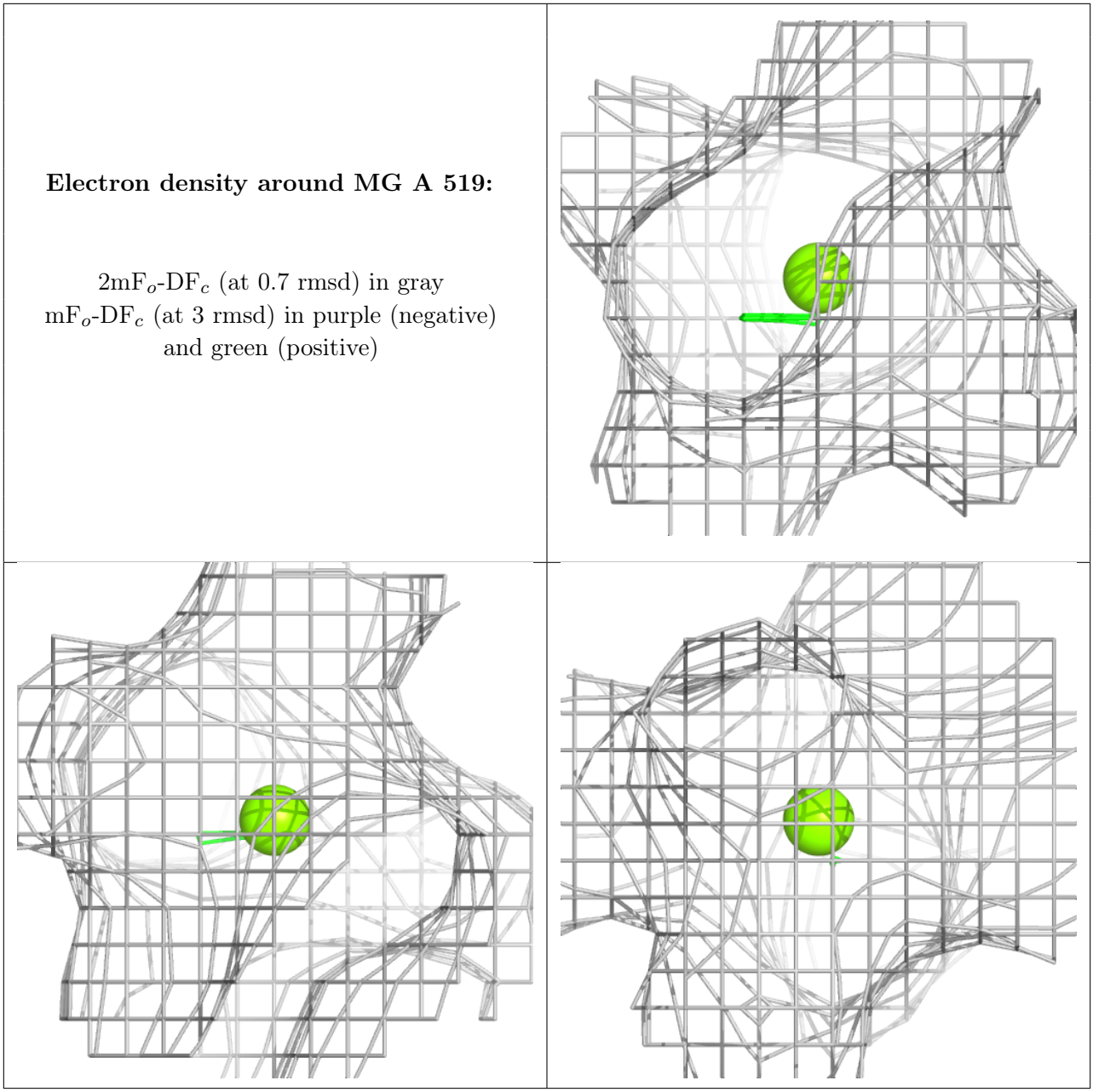
Electron density around MG B 501:

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



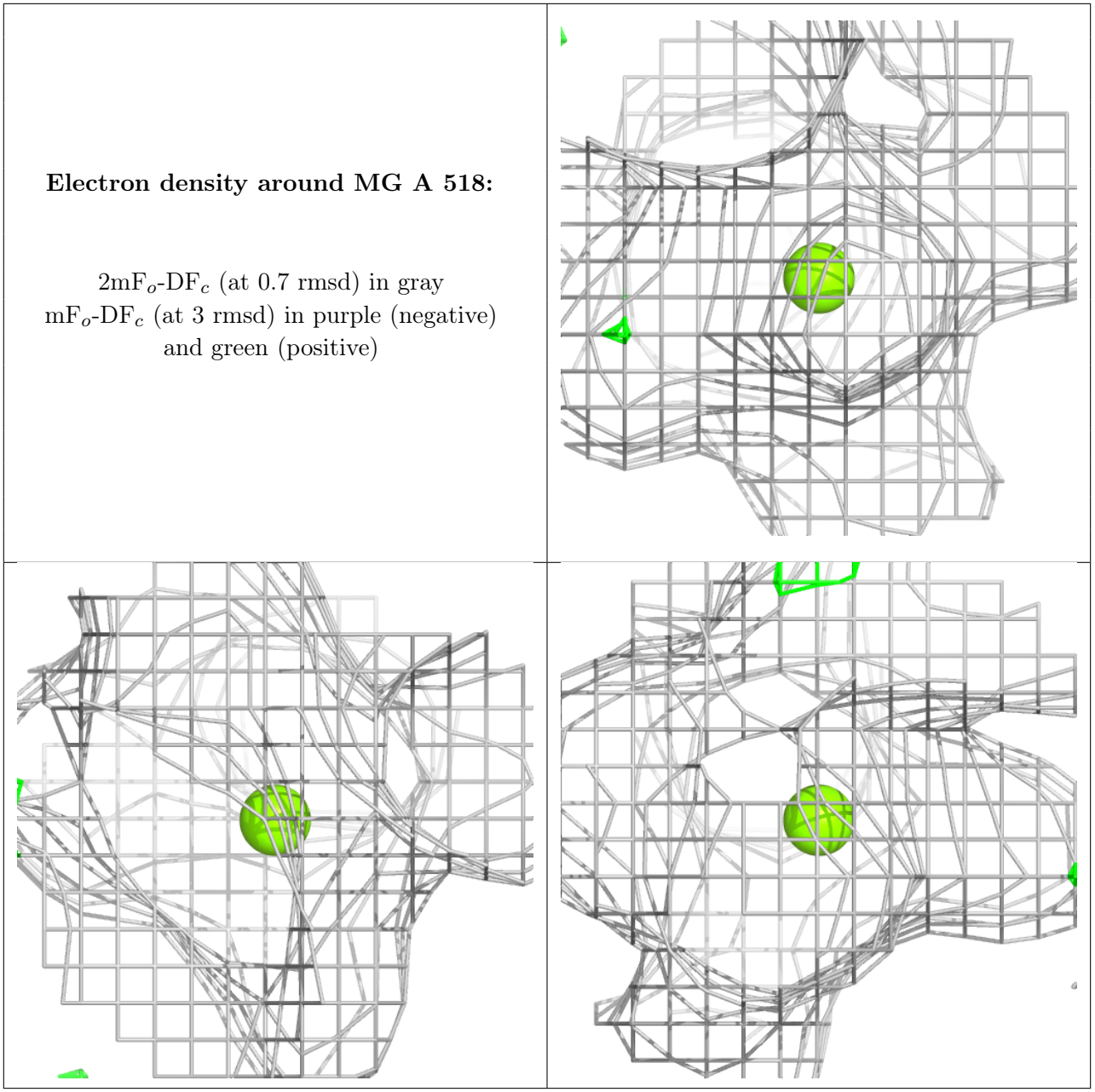
Electron density around MG A 519:

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



Electron density around MG A 518:

$2mF_o$-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.