



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:50 PM UTC

PDB ID : 3HY1 / pdb_00003hy1
Title : Crystal Structure of catalytic fragment of E. coli AlaRS G237A in complex with SerSA
Authors : Guo, M.; Yang, X.-L.; Schimmel, P.
Deposited on : 2009-06-22
Resolution : 2.79 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

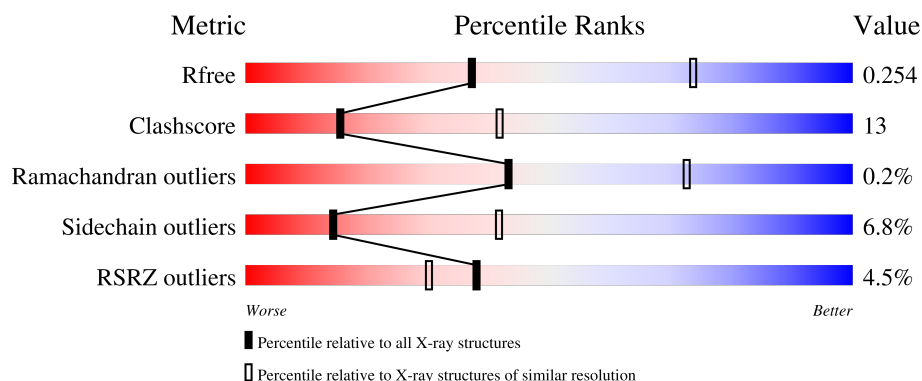
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

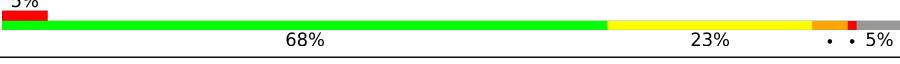
The reported resolution of this entry is 2.79 Å.

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 $\leq 5\%$. 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	441	 4% 75% 22% ..
1	B	441	 5% 68% 23% .. 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6988 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.

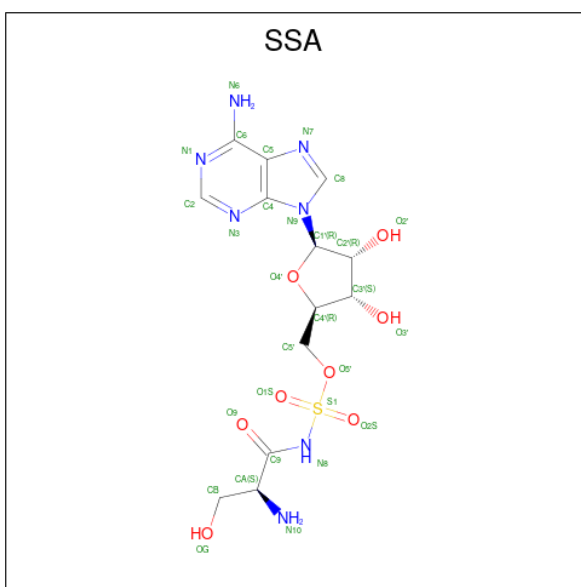
- Molecule 1 is a protein called Alanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3505	2210	617	663	15			
1	B	420	Total	C	N	O	S	0	0	0
			3355	2122	591	627	15			

There are 8 discrepancies between the modelled and reference sequences:

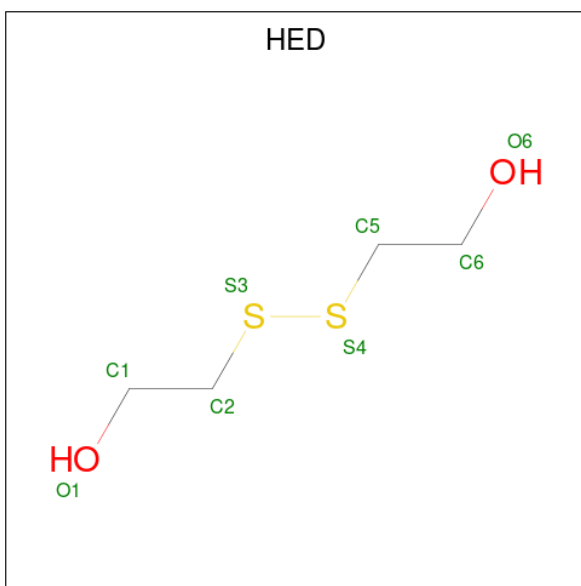
Chain	Residue	Modelled	Actual	Comment	Reference
A	104	LEU	HIS	engineered mutation	UNP P00957
A	108	LEU	GLN	engineered mutation	UNP P00957
A	112	LEU	GLU	engineered mutation	UNP P00957
A	237	ALA	GLY	engineered mutation	UNP P00957
B	104	LEU	HIS	engineered mutation	UNP P00957
B	108	LEU	GLN	engineered mutation	UNP P00957
B	112	LEU	GLU	engineered mutation	UNP P00957
B	237	ALA	GLY	engineered mutation	UNP P00957

- Molecule 2 is 5'-O-(N-(L-SERYL)-SULFAMOYL)ADENOSINE (CCD ID: SSA) (formula: C₁₃H₁₉N₇O₈S).



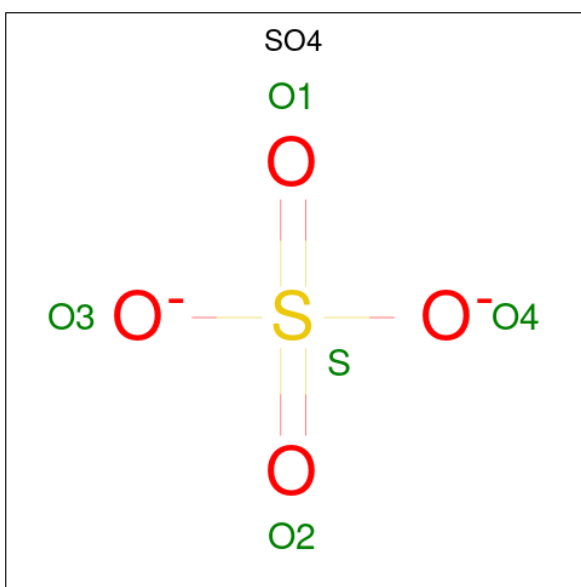
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	13	7	8	1		

- Molecule 3 is 2-HYDROXYETHYL DISULFIDE (CCD ID: HED) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

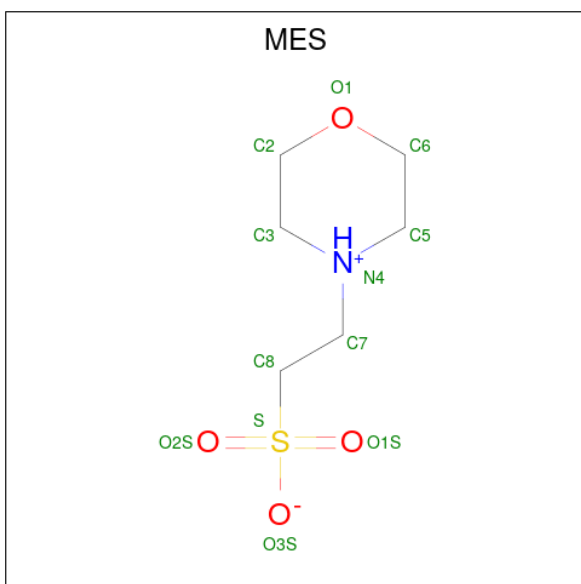


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

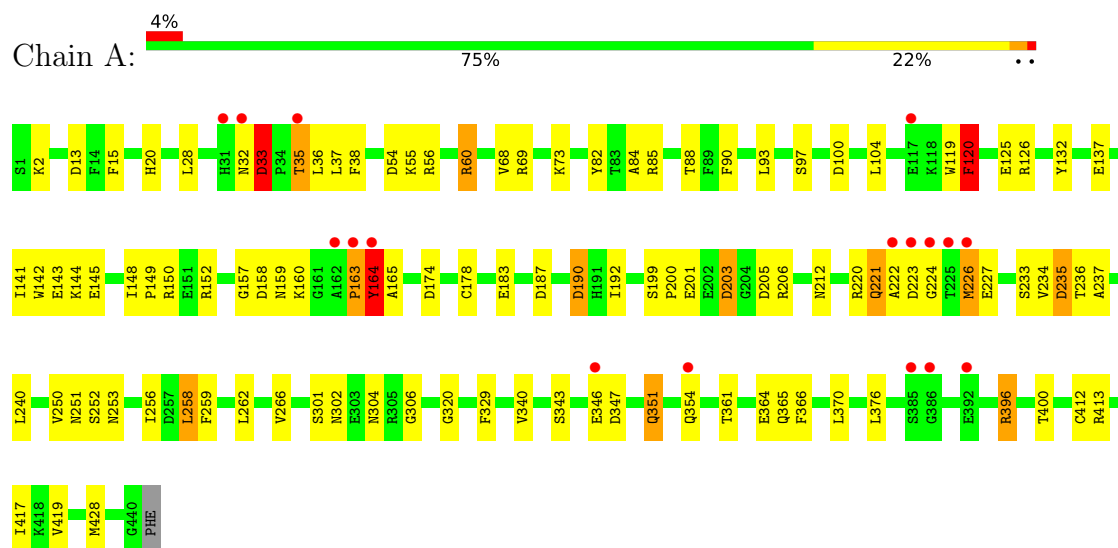
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	45	Total	O	0	0
			45	45		
7	B	28	Total	O	0	0
			28	28		

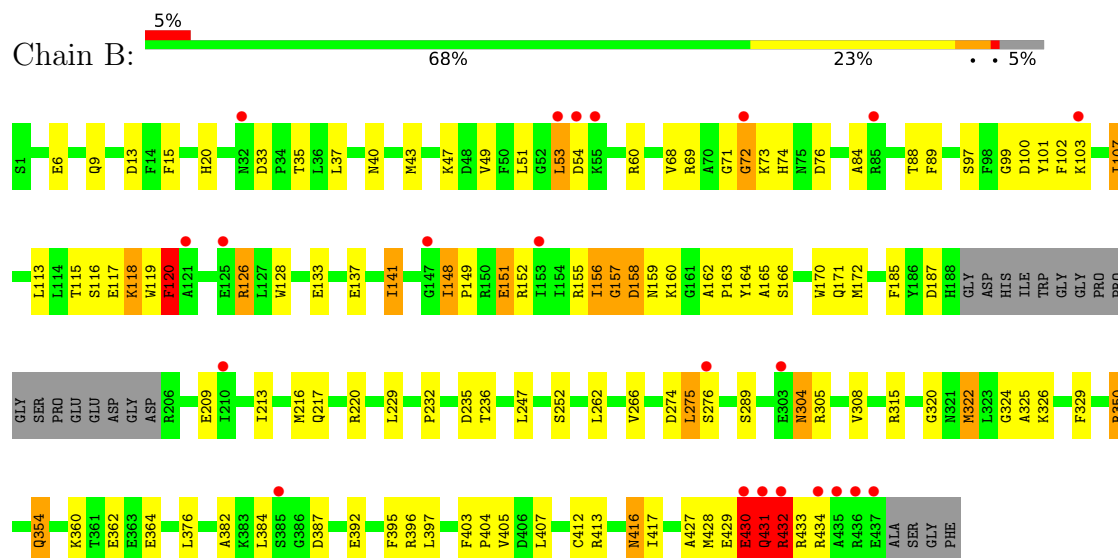
3 Residue-property plots [i](#)

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: Alanyl-tRNA synthetase



• Molecule 1: Alanyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.31Å 117.09Å 150.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.47 – 2.79 46.47 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.47-2.79) 99.8 (46.47-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.266 0.222 , 0.254	Depositor DCC
R_{free} test set	1727 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6988	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 3.37% 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: MES, SSA, SO4, HED, MG

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	0.44	3/3583 (0.1%)	0.85	11/4844 (0.2%)
1	B	0.42	2/3426 (0.1%)	0.82	6/4629 (0.1%)
All	All	0.43	5/7009 (0.1%)	0.83	17/9473 (0.2%)

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	0	2
1	B	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	GLY	N-CA	8.59	1.53	1.45
1	A	163	PRO	C-O	7.25	1.32	1.23
1	A	164	TYR	N-CA	7.06	1.55	1.46
1	A	163	PRO	C-N	6.16	1.42	1.33
1	B	72	GLY	CA-C	-5.46	1.47	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	GLY	N-CA-C	-14.31	94.61	111.36
1	A	221	GLN	N-CA-C	10.97	123.31	111.36
1	A	33	ASP	CA-C-N	9.58	129.24	119.56
1	A	33	ASP	C-N-CA	9.58	129.24	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	ARG	N-CA-C	-8.93	102.51	113.50
1	B	431	GLN	N-CA-C	-8.66	101.81	111.07
1	A	163	PRO	CA-C-N	-8.16	105.96	121.54
1	A	163	PRO	C-N-CA	-8.16	105.96	121.54
1	B	430	GLU	N-CA-C	-6.85	102.66	111.02
1	A	304	ASN	CB-CA-C	-6.33	109.28	116.63
1	B	304	ASN	CB-CA-C	-5.62	110.11	116.63
1	A	304	ASN	N-CA-C	5.41	117.21	108.08
1	A	119	TRP	CA-C-N	-5.28	115.32	122.77
1	A	119	TRP	C-N-CA	-5.28	115.32	122.77
1	B	120	PHE	N-CA-C	-5.27	103.52	110.43
1	A	100	ASP	CB-CA-C	-5.23	109.54	117.07
1	A	163	PRO	O-C-N	5.21	129.22	122.91

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	PHE	Peptide
1	A	163	PRO	Peptide
1	B	430	GLU	Peptide
1	B	431	GLN	Peptide
1	B	434	ARG	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	3505	0	3396	75	0
1	B	3355	0	3270	111	0
2	A	29	0	19	3	0
3	A	8	0	10	0	0
4	A	5	0	0	0	0
5	A	1	0	0	0	0
6	B	12	0	12	1	0
7	A	45	0	0	2	0
7	B	28	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6988	0	6707	183	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (183) 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:103:LYS:HE3	1:B:137:GLU:HB3	1.24	1.10
1:A:158:ASP:OD2	1:A:164:TYR:HB3	1.50	1.08
1:B:350:ARG:HG3	1:B:350:ARG:HH11	1.14	1.04
1:B:350:ARG:HH11	1:B:350:ARG:CG	1.73	1.02
1:B:47:LYS:HG3	1:B:172:MET:CE	1.89	1.01
1:B:47:LYS:HG3	1:B:172:MET:HE3	1.47	0.96
1:A:235:ASP:OD1	2:A:442:SSA:OG	1.86	0.94
1:B:49:VAL:HA	1:B:54:ASP:O	1.71	0.91
1:B:47:LYS:CG	1:B:172:MET:CE	2.52	0.88
1:B:43:MET:HB3	1:B:235:ASP:OD1	1.74	0.87
1:B:350:ARG:HG3	1:B:350:ARG:NH1	1.86	0.86
1:B:102:PHE:HZ	1:B:217:GLN:HG2	1.43	0.83
1:A:33:ASP:HB3	1:A:35:THR:OG1	1.79	0.83
1:A:97:SER:O	1:A:233:SER:HB3	1.82	0.79
1:B:53:LEU:N	1:B:53:LEU:HD23	1.97	0.79
1:B:118:LYS:O	1:B:118:LYS:HD3	1.83	0.79
1:B:128:TRP:CD2	1:B:152:ARG:HG2	2.16	0.79
1:A:158:ASP:OD2	1:A:164:TYR:CB	2.29	0.77
1:B:128:TRP:CE3	1:B:152:ARG:HG2	2.19	0.77
1:B:69:ARG:HB3	1:B:74:HIS:O	1.83	0.77
1:B:103:LYS:HE3	1:B:137:GLU:CB	2.11	0.76
1:B:103:LYS:CE	1:B:137:GLU:HB3	2.11	0.73
1:B:47:LYS:HG3	1:B:172:MET:HE1	1.70	0.73
1:A:160:LYS:HB2	1:A:165:ALA:CB	2.21	0.70
1:B:133:GLU:HG2	1:B:155:ARG:HB3	1.72	0.70
1:B:60:ARG:NE	1:B:100:ASP:OD1	2.21	0.70
1:B:47:LYS:CG	1:B:172:MET:HE1	2.21	0.70
1:A:125:GLU:O	1:A:152:ARG:NH1	2.26	0.69
1:A:160:LYS:HB2	1:A:165:ALA:HB1	1.75	0.69
1:B:171:GLN:HG2	1:B:220:ARG:HH22	1.57	0.68
1:A:120:PHE:O	1:A:120:PHE:HD2	1.75	0.67
1:B:137:GLU:O	1:B:141:ILE:HG12	1.95	0.67
1:A:235:ASP:OD1	1:A:235:ASP:C	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:ALA:O	1:B:431:GLN:HB2	1.95	0.66
1:B:149:PRO:HB2	1:B:151:GLU:HG2	1.77	0.66
1:A:20:HIS:CD2	1:A:60:ARG:HB2	2.31	0.66
1:A:104:LEU:HD11	1:A:145:GLU:HG2	1.79	0.65
1:B:274:ASP:CG	1:B:276:SER:OG	2.40	0.65
1:A:354:GLN:HG3	7:A:459:HOH:O	1.96	0.64
1:A:85:ARG:NH1	1:A:203:ASP:O	2.24	0.64
1:B:427:ALA:O	1:B:431:GLN:CB	2.46	0.64
1:B:304:ASN:CG	1:B:305:ARG:H	2.05	0.63
1:A:126:ARG:HD2	1:A:187:ASP:O	1.99	0.63
1:A:54:ASP:OD1	1:A:54:ASP:C	2.43	0.62
1:A:54:ASP:OD2	1:A:56:ARG:NH2	2.22	0.62
1:A:221:GLN:HE21	1:A:227:GLU:CD	2.07	0.62
1:B:120:PHE:CD1	1:B:120:PHE:N	2.67	0.61
1:B:118:LYS:O	1:B:118:LYS:CD	2.48	0.61
1:B:102:PHE:CZ	1:B:217:GLN:HG2	2.31	0.61
1:A:142:TRP:CE3	1:A:148:ILE:HD12	2.37	0.60
1:A:2:LYS:NZ	1:B:9:GLN:OE1	2.34	0.60
1:B:315:ARG:HA	1:B:407:LEU:HD13	1.84	0.60
1:B:69:ARG:NH1	1:B:76:ASP:OD2	2.35	0.59
1:B:430:GLU:O	1:B:431:GLN:C	2.46	0.59
1:B:157:GLY:O	1:B:159:ASN:N	2.31	0.59
1:B:97:SER:HB3	1:B:101:TYR:CE2	2.38	0.58
1:A:120:PHE:O	1:A:120:PHE:CD2	2.55	0.58
1:B:432:ARG:NE	1:B:432:ARG:HA	2.18	0.58
1:B:162:ALA:HB1	1:B:163:PRO:HD2	1.85	0.58
1:B:350:ARG:CG	1:B:350:ARG:NH1	2.44	0.57
1:B:69:ARG:HH11	1:B:76:ASP:CG	2.12	0.57
1:A:361:THR:O	1:A:365:GLN:HG3	2.05	0.57
1:B:185:PHE:CE2	1:B:209:GLU:HG2	2.39	0.57
1:A:220:ARG:HG3	7:A:489:HOH:O	2.06	0.56
1:B:47:LYS:HG2	1:B:172:MET:CE	2.34	0.56
1:A:68:VAL:HA	1:A:88:THR:O	2.05	0.56
1:B:97:SER:HB2	1:B:100:ASP:HB3	1.86	0.56
1:A:157:GLY:O	1:A:159:ASN:N	2.39	0.55
1:B:274:ASP:CG	1:B:276:SER:HG	2.15	0.55
1:B:416:ASN:O	1:B:416:ASN:ND2	2.36	0.55
1:B:158:ASP:OD2	1:B:164:TYR:N	2.22	0.55
1:B:103:LYS:HE2	1:B:141:ILE:HD11	1.89	0.54
1:A:262:LEU:O	1:A:266:VAL:HG23	2.08	0.54
1:B:37:LEU:HD21	1:B:308:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:O	1:B:120:PHE:O	2.26	0.54
1:B:304:ASN:CG	1:B:305:ARG:N	2.66	0.53
1:A:158:ASP:HB3	1:A:164:TYR:HA	1.89	0.53
1:A:412:CYS:HB3	1:A:417:ILE:HB	1.91	0.53
1:B:47:LYS:CG	1:B:172:MET:HE3	2.25	0.53
1:A:159:ASN:OD1	1:A:159:ASN:C	2.51	0.53
1:B:156:ILE:HG22	1:B:157:GLY:H	1.74	0.53
1:B:429:GLU:CD	1:B:433:ARG:HD3	2.34	0.53
1:A:158:ASP:OD2	1:A:164:TYR:CA	2.57	0.53
1:A:235:ASP:CG	2:A:442:SSA:OG	2.51	0.52
1:A:15:PHE:O	1:A:20:HIS:HB2	2.09	0.52
1:B:113:LEU:HD12	1:B:119:TRP:HB3	1.92	0.52
1:A:237:ALA:HB3	2:A:442:SSA:H5'1	1.92	0.52
1:A:343:SER:OG	1:B:6:GLU:OE2	2.22	0.52
1:B:275:LEU:CD2	1:B:275:LEU:N	2.72	0.52
1:A:190:ASP:OD1	1:A:190:ASP:N	2.39	0.51
1:B:53:LEU:N	1:B:53:LEU:CD2	2.62	0.51
1:B:118:LYS:CD	1:B:118:LYS:C	2.83	0.51
1:B:320:GLY:HA3	1:B:329:PHE:CZ	2.45	0.51
1:A:36:LEU:HD12	1:A:37:LEU:H	1.75	0.51
1:B:416:ASN:HD22	1:B:416:ASN:C	2.19	0.51
1:A:396:ARG:NH1	1:A:400:THR:OG1	2.44	0.51
1:B:429:GLU:O	1:B:430:GLU:C	2.52	0.51
1:A:258:LEU:HD23	1:A:259:PHE:N	2.25	0.51
1:A:132:TYR:OH	1:A:158:ASP:OD2	2.27	0.50
1:B:158:ASP:HA	1:B:166:SER:HB2	1.92	0.50
1:A:301:SER:OG	1:A:302:ASN:N	2.45	0.50
1:A:301:SER:HB3	1:A:306:GLY:HA3	1.94	0.50
1:B:387:ASP:O	1:B:417:ILE:HG23	2.11	0.50
1:B:53:LEU:CD2	1:B:53:LEU:H	2.22	0.49
1:B:213:ILE:HG23	1:B:236:THR:HG22	1.94	0.49
1:A:320:GLY:HA3	1:A:329:PHE:CZ	2.47	0.49
1:A:343:SER:O	1:A:346:GLU:HG3	2.12	0.49
1:B:160:LYS:HB2	1:B:165:ALA:O	2.13	0.49
1:B:120:PHE:HB3	1:B:247:LEU:HD21	1.94	0.49
1:A:164:TYR:CD2	1:A:164:TYR:N	2.72	0.48
1:B:382:ALA:C	1:B:384:LEU:H	2.21	0.48
1:A:143:GLU:OE2	1:A:144:LYS:HE3	2.14	0.48
1:A:143:GLU:OE1	1:A:150:ARG:NE	2.39	0.48
1:B:126:ARG:HG2	1:B:187:ASP:O	2.13	0.48
1:B:274:ASP:OD2	1:B:276:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HB2	1:A:340:VAL:HB	1.95	0.47
1:A:84:ALA:HB1	1:A:252:SER:HA	1.95	0.47
1:B:84:ALA:HB1	1:B:252:SER:HA	1.95	0.47
1:B:116:SER:HB3	1:B:119:TRP:HD1	1.80	0.47
1:A:253:ASN:O	1:A:256:ILE:HG12	2.15	0.47
1:B:118:LYS:HD3	1:B:118:LYS:C	2.35	0.47
1:A:54:ASP:OD1	1:A:55:LYS:N	2.48	0.47
1:A:178:CYS:SG	1:A:226:MET:HE2	2.55	0.47
1:B:47:LYS:HG2	1:B:172:MET:HE1	1.94	0.47
6:B:442:MES:H32	6:B:442:MES:H82	1.55	0.47
1:A:33:ASP:OD2	1:A:33:ASP:N	2.48	0.46
1:B:148:ILE:HG12	1:B:149:PRO:HD2	1.98	0.46
1:B:69:ARG:NH1	1:B:76:ASP:CG	2.73	0.46
1:A:36:LEU:HD12	1:A:37:LEU:N	2.31	0.46
1:B:53:LEU:HD23	1:B:53:LEU:H	1.75	0.46
1:B:156:ILE:HG22	1:B:157:GLY:N	2.31	0.46
1:B:158:ASP:OD1	1:B:158:ASP:N	2.46	0.46
1:B:354:GLN:H	1:B:354:GLN:CD	2.23	0.46
1:A:220:ARG:NH1	1:A:224:GLY:O	2.45	0.46
1:B:412:CYS:HB3	1:B:417:ILE:HB	1.98	0.45
1:B:99:GLY:HA2	1:B:232:PRO:O	2.16	0.45
1:A:351:GLN:H	1:A:351:GLN:HG2	1.53	0.45
1:B:88:THR:OG1	1:B:289:SER:OG	2.34	0.45
1:A:160:LYS:HB2	1:A:165:ALA:HB3	1.99	0.45
1:B:274:ASP:C	1:B:276:SER:N	2.74	0.45
1:B:71:GLY:O	1:B:72:GLY:C	2.60	0.45
1:B:89:PHE:CD2	1:B:89:PHE:C	2.95	0.45
1:A:366:PHE:CE2	1:A:370:LEU:HD13	2.52	0.44
1:B:395:PHE:CE2	1:B:431:GLN:HG2	2.52	0.44
1:B:404:PRO:O	1:B:407:LEU:HB3	2.18	0.44
1:A:69:ARG:HG3	1:A:90:PHE:HE2	1.82	0.44
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.83	0.44
1:A:148:ILE:HG23	1:A:149:PRO:HD2	1.99	0.44
1:B:9:GLN:NE2	1:B:13:ASP:OD1	2.51	0.44
1:B:387:ASP:OD1	1:B:387:ASP:N	2.51	0.44
1:A:37:LEU:O	1:A:38:PHE:CD1	2.70	0.44
1:A:158:ASP:OD2	1:A:164:TYR:HA	2.17	0.44
1:A:82:TYR:CE2	1:A:413:ARG:NH1	2.86	0.44
1:A:85:ARG:HD3	1:A:205:ASP:OD1	2.18	0.44
1:B:33:ASP:OD1	1:B:35:THR:OG1	2.34	0.43
1:B:431:GLN:HG3	1:B:432:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LYS:O	1:B:364:GLU:HB2	2.18	0.43
1:A:93:LEU:HD21	1:A:240:LEU:HD13	2.00	0.43
1:B:216:MET:O	1:B:229:LEU:HD12	2.18	0.43
1:A:137:GLU:O	1:A:141:ILE:HG13	2.18	0.43
1:B:396:ARG:NH1	7:B:468:HOH:O	2.51	0.43
1:A:13:ASP:OD2	1:B:13:ASP:HB2	2.19	0.42
1:A:250:VAL:C	1:A:251:ASN:HD22	2.27	0.42
1:A:97:SER:HB3	1:A:234:VAL:HB	2.02	0.42
1:B:107:ILE:HD11	1:B:141:ILE:HG22	2.02	0.42
1:A:199:SER:O	1:A:200:PRO:C	2.63	0.42
1:B:170:TRP:C	1:B:171:GLN:HG3	2.45	0.42
1:A:221:GLN:NE2	1:A:227:GLU:OE1	2.53	0.42
1:B:429:GLU:OE2	1:B:433:ARG:HD3	2.20	0.41
1:A:13:ASP:OD2	1:B:13:ASP:CB	2.68	0.41
1:A:28:LEU:HD22	1:A:68:VAL:HG23	2.01	0.41
1:B:324:GLY:O	1:B:325:ALA:C	2.63	0.41
1:B:15:PHE:O	1:B:20:HIS:HB2	2.20	0.41
1:B:68:VAL:HA	1:B:88:THR:O	2.20	0.41
1:B:429:GLU:OE1	1:B:433:ARG:HD3	2.20	0.41
1:B:427:ALA:O	1:B:431:GLN:HB3	2.20	0.41
1:B:428:MET:O	1:B:432:ARG:HB2	2.21	0.41
1:A:258:LEU:O	1:A:262:LEU:HB2	2.22	0.40
1:B:262:LEU:O	1:B:266:VAL:HG23	2.22	0.40
1:A:183:GLU:HG3	1:A:212:ASN:ND2	2.36	0.40
1:B:397:LEU:O	1:B:403:PHE:HB2	2.21	0.40
1:A:192:ILE:HB	1:A:206:ARG:HB2	2.03	0.40
1:B:322:MET:HG3	7:B:466:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	438/441 (99%)	421 (96%)	15 (3%)	2 (0%)	24	55
1	B	416/441 (94%)	394 (95%)	22 (5%)	0	100	100
All	All	854/882 (97%)	815 (95%)	37 (4%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	ALA
1	A	164	TYR

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	368/369 (100%)	345 (94%)	23 (6%)	16	45
1	B	352/369 (95%)	326 (93%)	26 (7%)	13	37
All	All	720/738 (98%)	671 (93%)	49 (7%)	14	42

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	ASP
1	A	35	THR
1	A	60	ARG
1	A	73	LYS
1	A	120	PHE
1	A	164	TYR
1	A	174	ASP
1	A	190	ASP
1	A	201	GLU
1	A	203	ASP
1	A	223	ASP
1	A	226	MET
1	A	235	ASP

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Mol	Chain	Res	Type
1	A	236	THR
1	A	258	LEU
1	A	347	ASP
1	A	351	GLN
1	A	364	GLU
1	A	376	LEU
1	A	396	ARG
1	A	419	VAL
1	A	428	MET
1	B	40	ASN
1	B	53	LEU
1	B	73	LYS
1	B	107	ILE
1	B	115	THR
1	B	117	GLU
1	B	118	LYS
1	B	120	PHE
1	B	126	ARG
1	B	141	ILE
1	B	148	ILE
1	B	151	GLU
1	B	156	ILE
1	B	158	ASP
1	B	275	LEU
1	B	322	MET
1	B	326	LYS
1	B	350	ARG
1	B	354	GLN
1	B	362	GLU
1	B	376	LEU
1	B	392	GLU
1	B	405	VAL
1	B	413	ARG
1	B	416	ASN
1	B	432	ARG

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	16	HIS
1	A	32	ASN
1	A	40	ASN

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Mol	Chain	Res	Type
1	A	221	GLN
1	A	253	ASN
1	A	351	GLN
1	B	44	ASN
1	B	74	HIS
1	B	217	GLN
1	B	221	GLN
1	B	251	ASN
1	B	253	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	HED	A	443	-	7,7,7	0.27	0	6,6,6	0.77	0
6	MES	B	442	-	12,12,12	2.33	1 (8%)	15,16,16	2.38	5 (33%)
4	SO4	A	444	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SSA	A	442	-	30,31,31	1.51	5 (16%)	41,46,46	2.17	9 (21%)

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
3	HED	A	443	-	-	3/5/5/5	-
6	MES	B	442	-	-	3/6/14/14	0/1/1/1
2	SSA	A	442	-	-	5/20/37/37	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	442	MES	C8-S	-7.80	1.66	1.77
2	A	442	SSA	C5-C4	4.67	1.47	1.39
2	A	442	SSA	C9-N8	-2.70	1.32	1.37
2	A	442	SSA	C5-C6	2.65	1.48	1.41
2	A	442	SSA	C5-N7	-2.31	1.34	1.39
2	A	442	SSA	C8-N7	2.28	1.36	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	442	SSA	O2S-S1-O1S	-7.42	109.74	120.85
2	A	442	SSA	C5-C4-N3	-5.76	118.78	126.72
6	B	442	MES	C5-N4-C3	5.24	120.12	108.84
2	A	442	SSA	N3-C4-N9	4.65	135.07	127.17
2	A	442	SSA	C2-N3-C4	3.65	120.74	111.83
6	B	442	MES	C7-N4-C3	3.41	120.32	111.24
6	B	442	MES	C6-C5-N4	-3.31	105.10	110.12
2	A	442	SSA	C4-C5-N7	-3.26	106.86	110.58
2	A	442	SSA	N3-C2-N1	-3.23	123.69	128.58
6	B	442	MES	C7-N4-C5	3.12	119.56	111.24
6	B	442	MES	C2-C3-N4	-2.81	105.85	110.12
2	A	442	SSA	C4-N9-C8	2.67	108.55	105.74
2	A	442	SSA	C9-N8-S1	-2.56	114.72	124.07
2	A	442	SSA	C5-N7-C8	2.44	107.28	103.45

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	442	SSA	N10-CA-CB-OG

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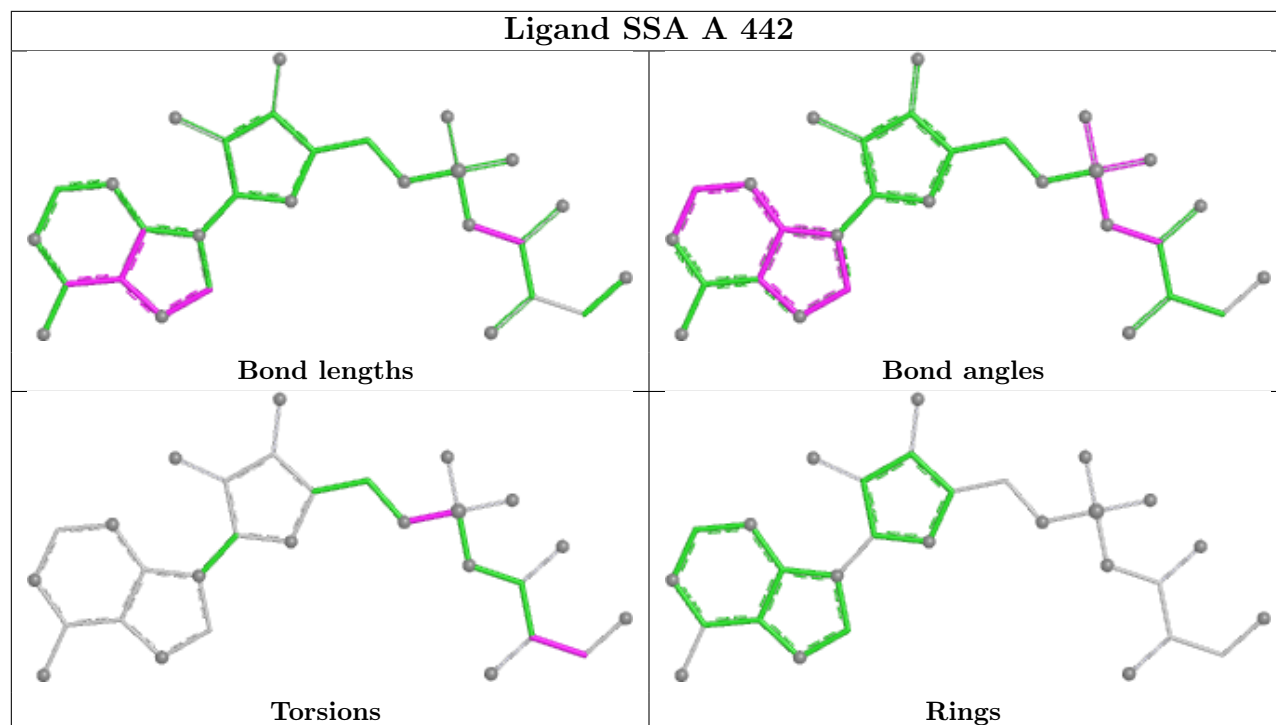
Mol	Chain	Res	Type	Atoms
2	A	442	SSA	C9-CA-CB-OG
2	A	442	SSA	C5'-O5'-S1-N8
3	A	443	HED	O1-C1-C2-S3
3	A	443	HED	C2-S3-S4-C5
6	B	442	MES	C8-C7-N4-C3
2	A	442	SSA	C5'-O5'-S1-O2S
6	B	442	MES	C7-C8-S-O3S
6	B	442	MES	C7-C8-S-O1S
2	A	442	SSA	C5'-O5'-S1-O1S
3	A	443	HED	C6-C5-S4-S3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	442	MES	1	0
2	A	442	SSA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/441 (99%)	0.22	17 (3%) 43 34	32, 48, 73, 81	0
1	B	420/441 (95%)	0.47	22 (5%) 33 25	37, 54, 75, 91	0
All	All	860/882 (97%)	0.34	39 (4%) 38 30	32, 52, 74, 91	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ASP	5.2
1	B	435	ALA	5.1
1	B	385	SER	5.0
1	B	437	GLU	4.5
1	B	103	LYS	4.2
1	B	436	ARG	3.9
1	A	163	PRO	3.5
1	A	117	GLU	3.3
1	A	225	THR	3.2
1	A	222	ALA	3.2
1	B	432	ARG	3.1
1	B	72	GLY	3.0
1	A	385	SER	2.9
1	B	55	LYS	2.8
1	A	346	GLU	2.7
1	B	85	ARG	2.7
1	B	121	ALA	2.6
1	A	226	MET	2.6
1	A	386	GLY	2.6
1	B	431	GLN	2.4
1	B	147	GLY	2.4
1	B	434	ARG	2.3
1	A	162	ALA	2.3
1	A	164	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	31	HIS	2.3
1	A	35	THR	2.3
1	B	430	GLU	2.3
1	B	153	ILE	2.3
1	B	303	GLU	2.2
1	A	392	GLU	2.2
1	B	32	ASN	2.2
1	B	125	GLU	2.1
1	A	223	ASP	2.1
1	B	210	ILE	2.1
1	A	354	GLN	2.1
1	B	276	SER	2.1
1	B	53	LEU	2.1
1	A	224	GLY	2.1
1	A	32	ASN	2.1

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.

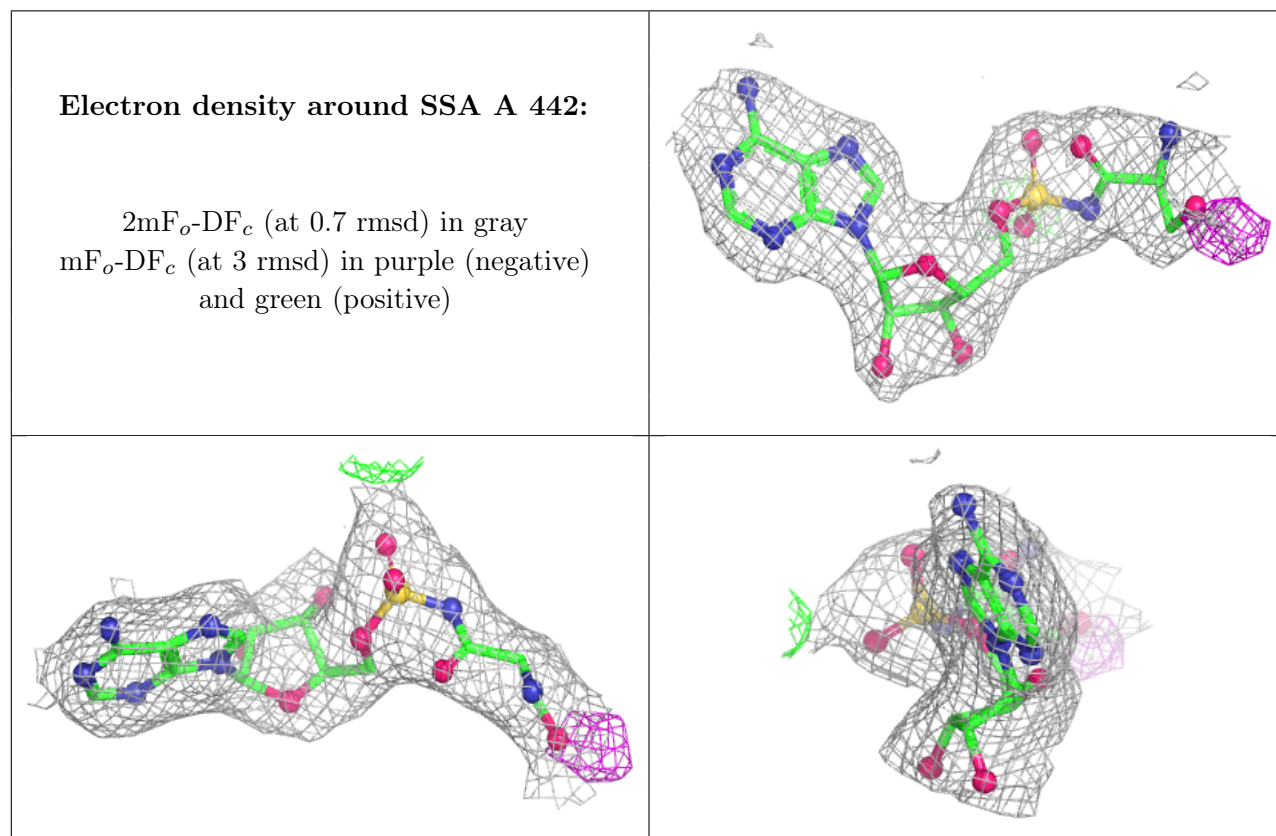
6.4 Ligands [i](#)

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, 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($\text{\AA}^2$)	Q<0.9
5	MG	A	445	1/1	0.63	0.40	64,64,64,64	0
3	HED	A	443	8/8	0.82	0.19	60,62,63,63	0
6	MES	B	442	12/12	0.91	0.13	64,64,66,66	0
4	SO4	A	444	5/5	0.92	0.09	66,67,67,67	0
2	SSA	A	442	29/29	0.96	0.07	39,40,42,45	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.