



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:02 pm BST

PDB ID : 1IM2  
Title : HslU, Haemophilus Influenzae, Selenomethionine Variant  
Authors : Trame, C.B.; McKay, D.B.  
Deposited on : 2001-05-09  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

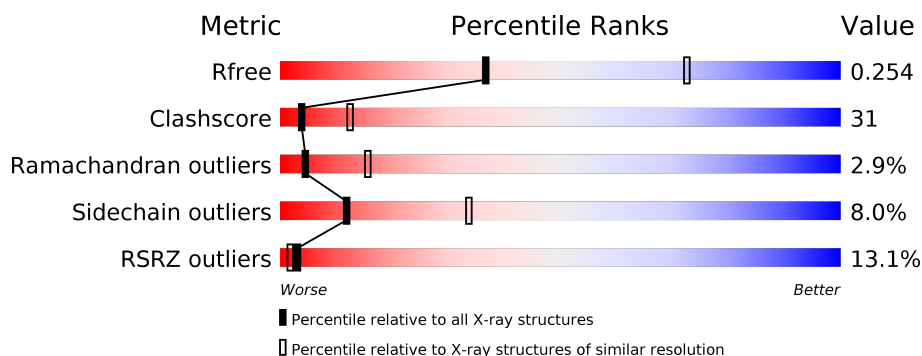
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	444	

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	A	600	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2729 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 ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	Se	0	0	0
			2697	1684	480	523	1	9			

There are 15 discrepancies between the modelled and reference sequences:

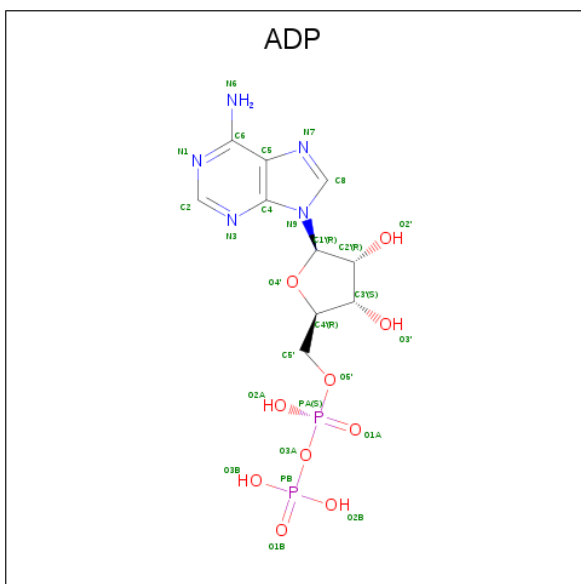
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	4	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	38	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	55	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	108	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	183	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	188	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	193	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	196	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	217	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	297	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	360	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	400	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	404	MSE	MET	MODIFIED RESIDUE	UNP P43773
A	414	MSE	MET	MODIFIED RESIDUE	UNP P43773

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.83Å 109.83Å 313.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.90 – 2.80 37.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.6 (37.90-2.80) 85.3 (37.90-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.79 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.233 , 0.250 0.240 , 0.254	Depositor DCC
$R_{free}$ test set	4235 reflections (9.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	2729	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP

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	0.41	0/2718	0.63	0/3649

There are no bond length outliers.

There are no bond angle outliers.

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	2697	0	2749	169	0
2	A	5	0	0	2	0
3	A	27	0	12	3	0
All	All	2729	0	2761	169	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 31.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:THR:HG22	1:A:373:ALA:H	1.16	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:HB	3:A:450:ADP:O1A	1.65	0.96
1:A:20:GLN:HA	1:A:20:GLN:HE21	1.33	0.93
1:A:120:ARG:HA	1:A:233:LYS:HZ1	1.37	0.89
1:A:104:THR:HA	1:A:248:VAL:HG21	1.55	0.85
1:A:279:GLN:HE22	1:A:320:ILE:H	1.20	0.84
1:A:370:THR:HB	1:A:422:ASP:HA	1.60	0.84
1:A:111:VAL:O	1:A:115:GLU:HB2	1.80	0.82
1:A:20:GLN:HE22	1:A:334:THR:H	1.28	0.78
1:A:27:VAL:HB	1:A:70:LEU:HD22	1.66	0.78
1:A:108:MSE:HA	1:A:108:MSE:HE3	1.64	0.77
1:A:370:THR:HG22	1:A:373:ALA:N	1.97	0.77
1:A:370:THR:HG21	2:A:600:SO4:O1	1.85	0.76
1:A:34:ARG:O	1:A:38:MSE:HG2	1.89	0.73
1:A:108:MSE:CE	1:A:240:LEU:HG	2.20	0.72
1:A:227:ILE:HG12	1:A:228:ASP:H	1.54	0.71
1:A:313:VAL:HG23	1:A:314:ALA:H	1.55	0.71
1:A:20:GLN:CA	1:A:20:GLN:HE21	2.04	0.71
1:A:283:LEU:HB3	1:A:284:PRO:HD3	1.73	0.69
1:A:91:TYR:OH	1:A:95:GLU:HB3	1.91	0.69
1:A:116:ILE:O	1:A:120:ARG:HD3	1.93	0.68
1:A:279:GLN:NE2	1:A:320:ILE:H	1.89	0.68
1:A:4:MSE:HE2	1:A:9:ILE:HA	1.76	0.68
1:A:23:ALA:HA	1:A:331:VAL:HG21	1.76	0.68
1:A:227:ILE:HG12	1:A:228:ASP:N	2.10	0.67
1:A:101:ARG:CG	1:A:293:THR:HG22	2.23	0.67
1:A:262:ILE:C	1:A:275:ARG:HB3	2.15	0.67
1:A:294:LYS:HE3	1:A:295:HIS:HE1	1.60	0.66
1:A:407:ILE:HD11	1:A:419:VAL:HG11	1.78	0.66
1:A:372:ASP:O	1:A:376:LYS:HG2	1.96	0.65
1:A:227:ILE:HG23	1:A:228:ASP:N	2.11	0.65
1:A:279:GLN:HB3	1:A:323:LEU:CD2	2.28	0.64
1:A:120:ARG:HD2	1:A:123:ALA:HB2	1.79	0.63
1:A:227:ILE:HG23	1:A:228:ASP:H	1.64	0.63
1:A:230:GLU:O	1:A:233:LYS:HG3	1.99	0.62
1:A:101:ARG:HG3	1:A:293:THR:HG22	1.82	0.62
1:A:290:THR:HG22	1:A:297:MSE:HE2	1.81	0.62
1:A:436:ASN:CG	1:A:439:LEU:HD13	2.20	0.62
1:A:63:LYS:HD2	1:A:308:SER:HB2	1.81	0.61
1:A:120:ARG:C	1:A:122:ARG:H	2.04	0.61
1:A:367:ILE:HG22	1:A:419:VAL:HB	1.83	0.61
1:A:122:ARG:HH21	1:A:125:ASP:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ALA:HB2	1:A:248:VAL:HG23	1.83	0.60
1:A:370:THR:CG2	1:A:373:ALA:H	2.04	0.60
1:A:279:GLN:HB3	1:A:323:LEU:HD22	1.84	0.59
1:A:359:LEU:O	1:A:362:THR:HB	2.02	0.59
1:A:274:SER:O	1:A:278:VAL:HG23	2.03	0.58
1:A:436:ASN:OD1	1:A:439:LEU:HD13	2.03	0.58
1:A:107:ALA:CB	1:A:248:VAL:HG23	2.34	0.57
1:A:101:ARG:HG2	1:A:293:THR:HG22	1.84	0.57
1:A:123:ALA:HB1	1:A:227:ILE:HD11	1.87	0.57
1:A:44:LEU:HA	1:A:47:GLU:HB2	1.87	0.56
1:A:326:ARG:C	1:A:328:PRO:HD3	2.26	0.56
1:A:108:MSE:HE1	1:A:240:LEU:HG	1.87	0.55
1:A:326:ARG:HE	1:A:326:ARG:HA	1.70	0.55
1:A:110:LEU:O	1:A:114:GLN:HB3	2.07	0.55
1:A:264:LYS:HD2	1:A:264:LYS:C	2.26	0.55
1:A:124:GLU:HG3	1:A:125:ASP:OD2	2.06	0.55
1:A:35:TRP:O	1:A:39:GLN:HG2	2.06	0.54
1:A:123:ALA:HB1	1:A:227:ILE:CD1	2.36	0.54
1:A:313:VAL:HG23	1:A:314:ALA:N	2.22	0.54
1:A:17:ILE:N	1:A:17:ILE:HD12	2.22	0.54
1:A:373:ALA:O	1:A:377:ILE:HG13	2.06	0.54
1:A:403:LEU:HD11	1:A:426:VAL:HG22	1.90	0.54
1:A:404:MSE:O	1:A:408:SER:HB2	2.07	0.54
1:A:390:ASN:ND2	1:A:392:GLY:H	2.06	0.54
1:A:322:GLU:OE1	1:A:322:GLU:N	2.34	0.54
1:A:228:ASP:C	1:A:230:GLU:H	2.11	0.53
1:A:343:ARG:O	1:A:347:GLU:HG3	2.08	0.53
1:A:120:ARG:HA	1:A:233:LYS:NZ	2.15	0.53
1:A:277:GLY:O	1:A:280:ARG:HB2	2.09	0.52
1:A:233:LYS:C	1:A:235:ILE:H	2.13	0.52
1:A:279:GLN:NE2	1:A:320:ILE:HG12	2.24	0.52
1:A:94:LYS:HB3	1:A:98:SER:HB3	1.90	0.52
1:A:292:SER:OG	1:A:297:MSE:HE3	2.09	0.52
1:A:257:ASP:OD2	1:A:258:GLU:HG2	2.09	0.52
1:A:78:PHE:CG	1:A:79:ILE:N	2.78	0.52
1:A:128:GLU:HG3	1:A:129:GLU:H	1.75	0.51
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.74	0.51
1:A:233:LYS:HD2	1:A:233:LYS:O	2.10	0.51
1:A:294:LYS:HE3	1:A:295:HIS:CE1	2.43	0.51
1:A:262:ILE:O	1:A:275:ARG:HB3	2.11	0.51
1:A:122:ARG:HH21	1:A:125:ASP:CB	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:HG22	1:A:441:ARG:NH1	2.27	0.50
1:A:78:PHE:O	1:A:79:ILE:HB	2.12	0.50
1:A:407:ILE:HG13	1:A:425:TYR:OH	2.11	0.50
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.25	0.49
1:A:110:LEU:O	1:A:114:GLN:CB	2.60	0.49
1:A:16:HIS:HB2	1:A:17:ILE:HD12	1.95	0.49
1:A:276:GLU:O	1:A:280:ARG:HG2	2.13	0.49
1:A:107:ALA:O	1:A:111:VAL:HG23	2.12	0.49
1:A:70:LEU:O	1:A:73:LEU:HG	2.12	0.48
1:A:79:ILE:C	1:A:79:ILE:HD13	2.33	0.48
1:A:128:GLU:C	1:A:130:ARG:H	2.17	0.48
1:A:78:PHE:CZ	1:A:255:PHE:HB2	2.48	0.48
1:A:270:GLY:C	1:A:272:ASP:H	2.15	0.48
1:A:120:ARG:HG3	1:A:120:ARG:O	2.14	0.48
1:A:235:ILE:O	1:A:236:ASN:HB3	2.13	0.48
1:A:356:TYR:CD1	1:A:404:MSE:HG3	2.49	0.48
1:A:292:SER:CA	1:A:297:MSE:HE3	2.44	0.47
1:A:294:LYS:HG3	1:A:295:HIS:ND1	2.29	0.47
1:A:107:ALA:HB2	1:A:248:VAL:CG2	2.45	0.47
1:A:341:PHE:CE1	1:A:393:ALA:HA	2.50	0.47
1:A:37:ARG:HD2	1:A:48:VAL:O	2.15	0.47
1:A:243:LYS:O	1:A:247:ALA:N	2.48	0.47
1:A:4:MSE:CE	1:A:9:ILE:HA	2.44	0.47
1:A:52:ASN:O	1:A:328:PRO:HD2	2.15	0.47
1:A:17:ILE:HD11	1:A:69:ARG:HG3	1.97	0.47
1:A:58:PRO:HG2	1:A:61:VAL:HG11	1.97	0.46
1:A:410:SER:O	1:A:414:MSE:HG3	2.15	0.46
1:A:294:LYS:HG3	1:A:295:HIS:HD1	1.80	0.46
1:A:83:ALA:HB1	1:A:262:ILE:HD13	1.98	0.46
1:A:18:ILE:O	3:A:450:ADP:N6	2.43	0.46
1:A:384:VAL:HG12	1:A:395:ARG:HE	1.81	0.46
1:A:258:GLU:HB3	1:A:261:LYS:HD2	1.97	0.45
1:A:347:GLU:O	1:A:348:PRO:C	2.53	0.45
1:A:242:GLN:NE2	1:A:246:ASP:HB2	2.31	0.45
1:A:363:GLU:HG3	1:A:411:ALA:HB3	1.99	0.45
1:A:120:ARG:C	1:A:122:ARG:N	2.68	0.45
1:A:283:LEU:HB3	1:A:284:PRO:CD	2.44	0.45
1:A:341:PHE:HB2	1:A:378:ALA:HB1	1.98	0.45
1:A:125:ASP:HA	1:A:129:GLU:OE2	2.17	0.45
1:A:108:MSE:C	1:A:110:LEU:H	2.20	0.44
1:A:82:GLU:O	1:A:85:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HD12	1:A:300:THR:HG22	1.99	0.44
1:A:112:ARG:O	1:A:115:GLU:N	2.49	0.44
1:A:263:CYS:O	1:A:275:ARG:HD2	2.16	0.44
1:A:387:LYS:HE2	1:A:387:LYS:HB3	1.82	0.44
1:A:128:GLU:OE1	1:A:128:GLU:HA	2.18	0.44
1:A:279:GLN:HE22	1:A:320:ILE:N	1.99	0.44
1:A:54:LEU:HA	1:A:307:ALA:O	2.18	0.44
1:A:279:GLN:HE21	1:A:320:ILE:HG12	1.82	0.44
1:A:60:GLY:HA3	1:A:392:GLY:HA3	1.99	0.44
1:A:5:THR:OG1	1:A:8:GLU:HG3	2.18	0.44
1:A:16:HIS:CB	1:A:17:ILE:HD12	2.47	0.43
1:A:395:ARG:HD3	1:A:395:ARG:HA	1.84	0.43
1:A:422:ASP:HB2	2:A:600:SO4:O1	2.18	0.43
1:A:333:LEU:HD12	1:A:333:LEU:N	2.33	0.43
1:A:370:THR:CB	1:A:422:ASP:HA	2.40	0.43
1:A:326:ARG:O	1:A:328:PRO:HD3	2.18	0.43
1:A:123:ALA:O	1:A:227:ILE:HD12	2.18	0.43
1:A:420:ASN:HA	1:A:420:ASN:HD22	1.63	0.43
1:A:65:GLU:HB2	3:A:450:ADP:O2A	2.19	0.43
1:A:264:LYS:HE2	1:A:318:ASP:HB3	2.01	0.42
1:A:20:GLN:NE2	1:A:20:GLN:CA	2.77	0.42
1:A:119:ASN:O	1:A:119:ASN:OD1	2.36	0.42
1:A:227:ILE:CG1	1:A:228:ASP:H	2.22	0.42
1:A:227:ILE:CG2	1:A:228:ASP:H	2.28	0.42
1:A:108:MSE:HE2	1:A:240:LEU:HG	2.01	0.42
1:A:262:ILE:HA	1:A:275:ARG:HD3	2.02	0.42
1:A:9:ILE:HD13	1:A:31:LEU:HD23	2.02	0.42
1:A:413:ASP:N	1:A:413:ASP:OD2	2.53	0.42
1:A:124:GLU:O	1:A:125:ASP:HB2	2.19	0.41
1:A:74:ALA:O	1:A:75:ASN:C	2.59	0.41
1:A:387:LYS:NZ	1:A:435:GLU:HA	2.35	0.41
1:A:58:PRO:HG2	1:A:61:VAL:CG1	2.51	0.41
1:A:120:ARG:O	1:A:122:ARG:N	2.54	0.41
1:A:283:LEU:HD11	1:A:322:GLU:HB3	2.02	0.41
1:A:227:ILE:HG13	1:A:230:GLU:HB3	2.03	0.41
1:A:38:MSE:HE2	1:A:38:MSE:HA	2.03	0.41
1:A:88:GLU:O	1:A:89:VAL:C	2.60	0.41
1:A:19:GLY:O	1:A:24:LYS:HE3	2.21	0.40
1:A:227:ILE:HG23	1:A:228:ASP:OD2	2.20	0.40
1:A:428:ASP:OD1	1:A:429:ALA:N	2.55	0.40
1:A:124:GLU:HG3	1:A:125:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:O	1:A:262:ILE:HG12	2.20	0.40
1:A:54:LEU:HD12	1:A:307:ALA:O	2.21	0.40
1:A:118:LYS:C	1:A:120:ARG:H	2.24	0.40
1:A:256:ILE:HD13	1:A:282:LEU:HD21	2.03	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	340/444 (77%)	283 (83%)	47 (14%)	10 (3%)	4	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	227	ILE
1	A	235	ILE
1	A	44	LEU
1	A	89	VAL
1	A	121	ALA
1	A	234	LEU
1	A	93	GLY
1	A	262	ILE
1	A	92	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/358 (81%)	266 (92%)	23 (8%)	12	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	20	GLN
1	A	59	THR
1	A	79	ILE
1	A	81	VAL
1	A	82	GLU
1	A	84	THR
1	A	95	GLU
1	A	97	ASP
1	A	233	LYS
1	A	250	GLN
1	A	264	LYS
1	A	286	VAL
1	A	301	ASP
1	A	304	LEU
1	A	323	LEU
1	A	326	ARG
1	A	345	LEU
1	A	370	THR
1	A	389	GLU
1	A	390	ASN
1	A	413	ASP
1	A	428	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	236	ASN
1	A	242	GLN
1	A	279	GLN
1	A	295	HIS
1	A	385	ASN
1	A	390	ASN

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Mol	Chain	Res	Type
1	A	420	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	600	-	4,4,4	0.62	0	6,6,6	0.17	0
3	ADP	A	450	-	24,29,29	1.26	2 (8%)	29,45,45	0.95	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
3	ADP	A	450	-	-	1/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	ADP	C8-N7	-3.53	1.28	1.34
3	A	450	ADP	C2-N3	2.48	1.36	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

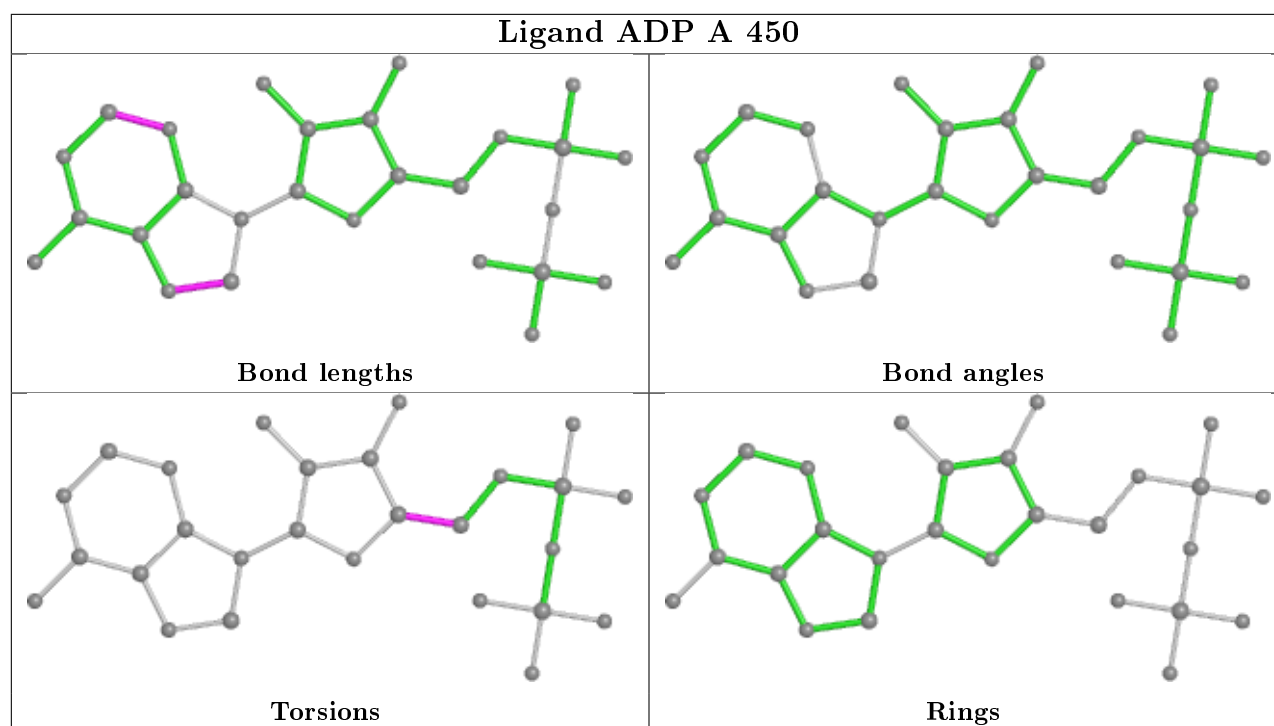
Mol	Chain	Res	Type	Atoms
3	A	450	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	SO4	2	0
3	A	450	ADP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	337/444 (75%)	0.44	44 (13%) 3 2	10, 39, 160, 198	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	GLY	10.8
1	A	232	ALA	10.1
1	A	128	GLU	9.4
1	A	269	SER	9.2
1	A	267	GLU	8.6
1	A	124	GLU	8.0
1	A	268	TYR	7.9
1	A	226	LEU	7.8
1	A	116	ILE	7.7
1	A	119	ASN	7.6
1	A	127	ALA	7.2
1	A	92	VAL	6.9
1	A	130	ARG	6.9
1	A	228	ASP	6.6
1	A	121	ALA	6.6
1	A	125	ASP	6.5
1	A	123	ALA	6.2
1	A	231	ALA	6.1
1	A	122	ARG	6.0
1	A	270	GLY	6.0
1	A	229	ASP	5.6
1	A	271	ALA	5.2
1	A	234	LEU	5.1
1	A	90	GLY	4.8
1	A	126	VAL	4.7
1	A	112	ARG	4.6
1	A	235	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	94	LYS	3.8
1	A	295	HIS	3.7
1	A	117	ALA	3.7
1	A	240	LEU	3.6
1	A	89	VAL	3.6
1	A	129	GLU	3.2
1	A	241	LYS	3.2
1	A	236	ASN	3.0
1	A	227	ILE	3.0
1	A	245	ILE	3.0
1	A	91	TYR	2.7
1	A	120	ARG	2.7
1	A	238	GLU	2.6
1	A	88	GLU	2.3
1	A	272	ASP	2.2
1	A	237	PRO	2.1
1	A	230	GLU	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

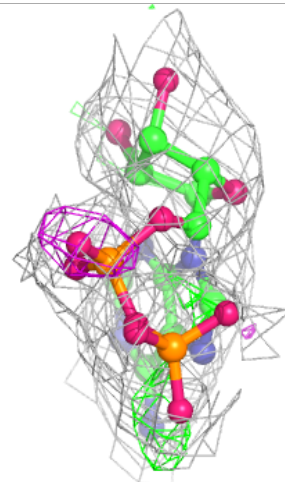
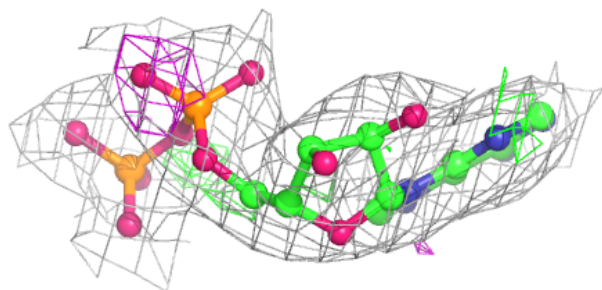
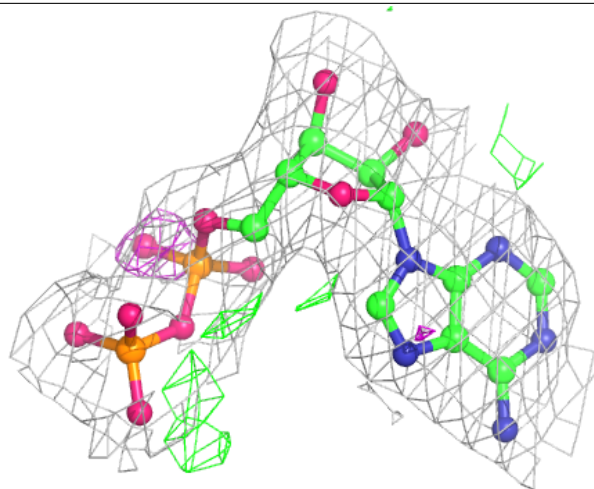
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	ADP	A	450	27/27	0.93	0.23	32,35,54,66	0
2	SO4	A	600	5/5	0.97	0.13	41,41,41,41	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 ADP A 450:**

$2mF_o-DF_c$  (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.