



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:38 PM UTC

PDB ID : 6LR6 / pdb_00006lr6
Title : The crystal structure of human cytoplasmic LRS
Authors : Liu, R.J.; Long, T.; Li, H.; Li, J.; Zhao, J.H.; Lin, J.Z.; Palencia, A.; Wang, M.Z.; Cusack, S.; Wang, E.D.
Deposited on : 2020-01-15
Resolution : 3.01 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

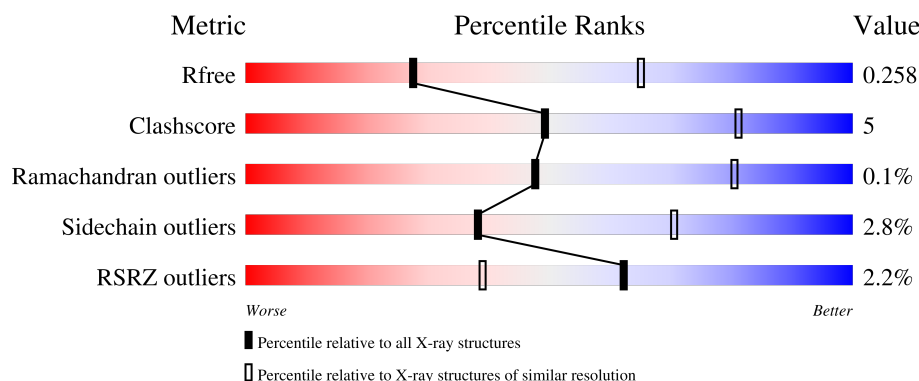
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

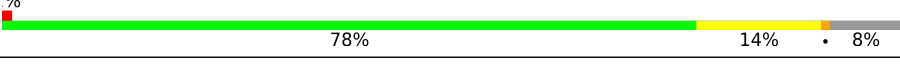
The reported resolution of this entry is 3.01 Å.

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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1092	 3% 76% 15% 8%
1	B	1092	 % 78% 14% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16358 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 Leucine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1003	Total	C	N	O	S	0	0	0
			8097	5210	1345	1489	53			
1	B	1005	Total	C	N	O	S	0	0	0
			8113	5220	1347	1491	55			

There are 44 discrepancies between the modelled and reference sequences:

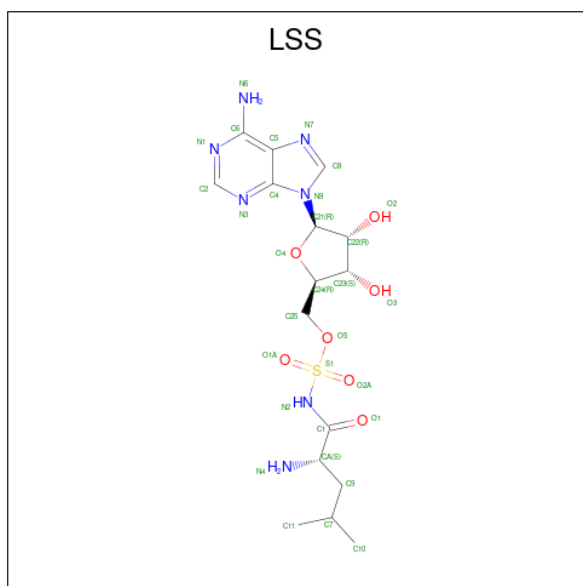
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q9P2J5
A	-20	GLY	-	expression tag	UNP Q9P2J5
A	-19	HIS	-	expression tag	UNP Q9P2J5
A	-18	HIS	-	expression tag	UNP Q9P2J5
A	-17	HIS	-	expression tag	UNP Q9P2J5
A	-16	HIS	-	expression tag	UNP Q9P2J5
A	-15	HIS	-	expression tag	UNP Q9P2J5
A	-14	HIS	-	expression tag	UNP Q9P2J5
A	-13	HIS	-	expression tag	UNP Q9P2J5
A	-12	HIS	-	expression tag	UNP Q9P2J5
A	-11	HIS	-	expression tag	UNP Q9P2J5
A	-10	HIS	-	expression tag	UNP Q9P2J5
A	-9	SER	-	expression tag	UNP Q9P2J5
A	-8	SER	-	expression tag	UNP Q9P2J5
A	-7	GLY	-	expression tag	UNP Q9P2J5
A	-6	HIS	-	expression tag	UNP Q9P2J5
A	-5	ILE	-	expression tag	UNP Q9P2J5
A	-4	GLU	-	expression tag	UNP Q9P2J5
A	-3	GLY	-	expression tag	UNP Q9P2J5
A	-2	ARG	-	expression tag	UNP Q9P2J5
A	-1	HIS	-	expression tag	UNP Q9P2J5
A	0	MET	-	expression tag	UNP Q9P2J5
B	-21	MET	-	expression tag	UNP Q9P2J5
B	-20	GLY	-	expression tag	UNP Q9P2J5
B	-19	HIS	-	expression tag	UNP Q9P2J5

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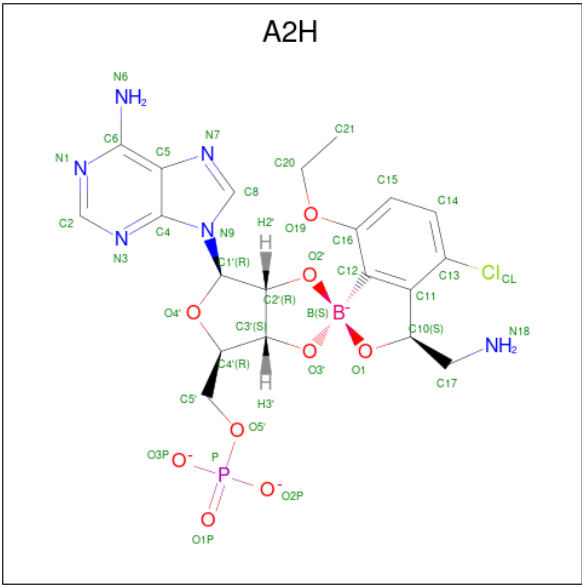
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q9P2J5
B	-17	HIS	-	expression tag	UNP Q9P2J5
B	-16	HIS	-	expression tag	UNP Q9P2J5
B	-15	HIS	-	expression tag	UNP Q9P2J5
B	-14	HIS	-	expression tag	UNP Q9P2J5
B	-13	HIS	-	expression tag	UNP Q9P2J5
B	-12	HIS	-	expression tag	UNP Q9P2J5
B	-11	HIS	-	expression tag	UNP Q9P2J5
B	-10	HIS	-	expression tag	UNP Q9P2J5
B	-9	SER	-	expression tag	UNP Q9P2J5
B	-8	SER	-	expression tag	UNP Q9P2J5
B	-7	GLY	-	expression tag	UNP Q9P2J5
B	-6	HIS	-	expression tag	UNP Q9P2J5
B	-5	ILE	-	expression tag	UNP Q9P2J5
B	-4	GLU	-	expression tag	UNP Q9P2J5
B	-3	GLY	-	expression tag	UNP Q9P2J5
B	-2	ARG	-	expression tag	UNP Q9P2J5
B	-1	HIS	-	expression tag	UNP Q9P2J5
B	0	MET	-	expression tag	UNP Q9P2J5

- Molecule 2 is 5'-O-(L-leucylsulfamoyl)adenosine (CCD ID: LSS) (formula: C₁₆H₂₅N₇O₇S).



- Molecule 3 is 4-Chloro-3-aminomethyl-7-[ethoxy]-3H-benzo[C][1,2]oxaborol-1-ol modified adenosine (CCD ID: A2H) (formula: C₂₀H₂₂BClN₆O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	B	C	Cl	N	O	P		
3	A	1	38	1	20	1	6	9	1	0	0
3	B	1	38	1	20	1	6	9	1	0	0

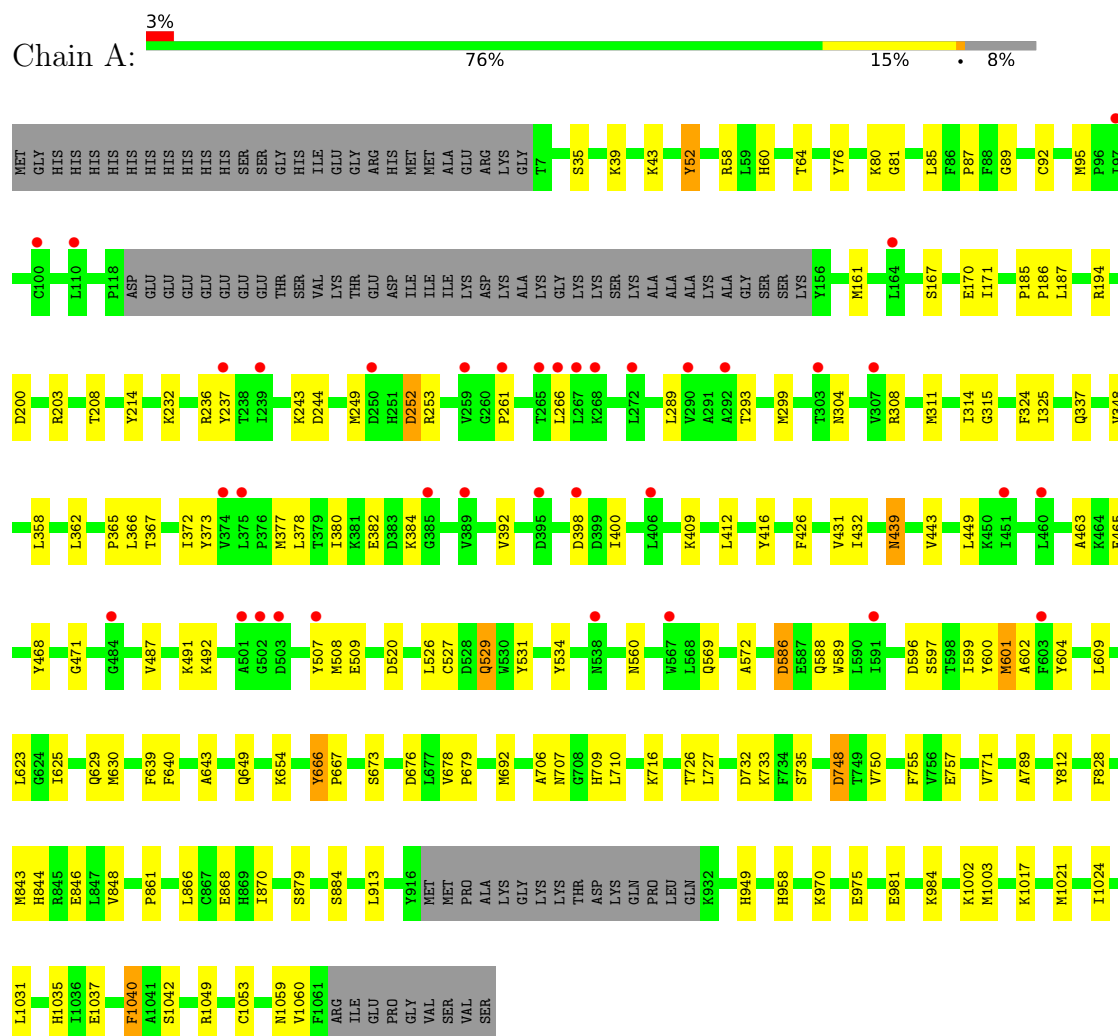
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	10	Total O 10 10	0	0

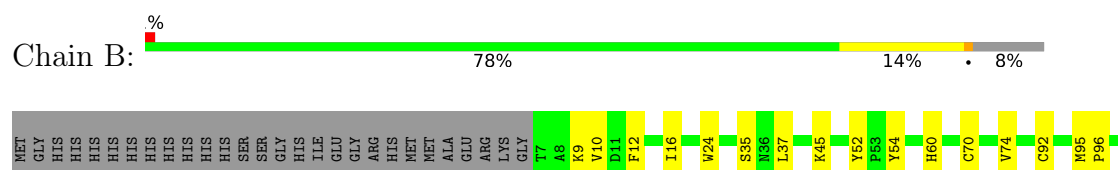
3 Residue-property plots

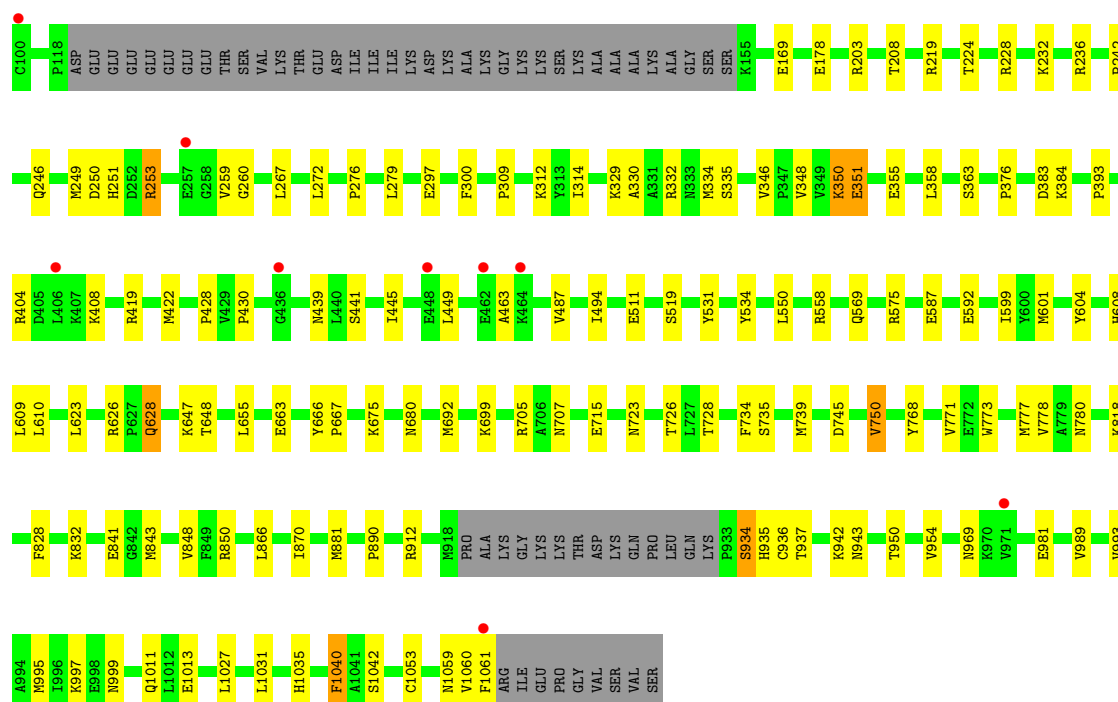
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Leucine-tRNA ligase, cytoplasmic



• Molecule 1: Leucine-tRNA ligase, cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.85Å 95.80Å 682.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 3.01 49.41 – 3.01	Depositor EDS
% Data completeness (in resolution range)	74.6 (49.41-3.01) 74.5 (49.41-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.211 , 0.260 0.211 , 0.258	Depositor DCC
R_{free} test set	2245 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16358	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: LSS, A2H

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	0.13	0/8297	0.31	0/11215
1	B	0.17	0/8313	0.38	0/11234
All	All	0.15	0/16610	0.35	0/22449

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	8097	0	8058	97	0
1	B	8113	0	8077	81	0
2	A	31	0	25	3	0
2	B	31	0	25	1	0
3	A	38	0	0	3	0
3	B	38	0	0	0	0
4	B	10	0	0	2	0
All	All	16358	0	16185	177	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 5.

All (177) 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)
2:B:1200:LSS:O4	2:B:1200:LSS:C24	1.63	1.41
2:A:1200:LSS:O4	2:A:1200:LSS:C24	1.64	1.28
1:B:445:ILE:HD12	1:B:463:ALA:HB1	1.58	0.85
1:A:43:LYS:HE2	1:A:81:GLY:HA3	1.70	0.73
1:A:337:GLN:NE2	1:A:508:MET:O	2.21	0.72
1:A:384:LYS:O	3:A:1201:A2H:N6	2.24	0.70
1:B:419:ARG:HE	1:B:422:MET:HE3	1.56	0.70
1:A:311:MET:HE2	1:A:382:GLU:HG2	1.76	0.67
1:B:219:ARG:NH2	1:B:587:GLU:OE2	2.28	0.66
1:A:64:THR:HG21	1:A:727:LEU:HD13	1.78	0.66
1:B:745:ASP:O	1:B:818:LYS:NZ	2.30	0.65
1:A:439:ASN:OD1	1:A:439:ASN:N	2.28	0.62
1:B:550:LEU:O	1:B:558:ARG:NH2	2.30	0.62
1:A:58:ARG:HE	1:A:187:LEU:HB3	1.63	0.62
1:A:400:ILE:HD12	1:A:443:VAL:HG22	1.81	0.61
1:A:431:VAL:HG12	1:A:432:ILE:HG13	1.83	0.61
1:A:599:ILE:HD13	1:A:692:MET:HG3	1.83	0.61
1:A:625:ILE:HG21	1:A:630:MET:HE2	1.82	0.60
1:A:299:MET:HB2	1:A:366:LEU:HD12	1.84	0.60
1:A:449:LEU:HD12	1:A:463:ALA:HB2	1.83	0.59
1:A:308:ARG:NH1	1:A:378:LEU:O	2.34	0.59
1:B:350:LYS:HE3	1:B:351:GLU:H	1.68	0.59
1:A:409:LYS:HE2	1:A:412:LEU:HG	1.85	0.59
1:B:912:ARG:NH2	1:B:1059:ASN:OD1	2.34	0.58
1:A:35:SER:O	1:A:39:LYS:NZ	2.28	0.58
1:B:300:PHE:HE1	1:B:494:ILE:HD13	1.70	0.57
1:A:60:HIS:HA	1:A:726:THR:HA	1.86	0.56
1:B:771:VAL:HG21	1:B:866:LEU:HD11	1.87	0.56
1:A:623:LEU:HB3	1:A:654:LYS:HD2	1.88	0.56
1:B:54:TYR:OH	1:B:251:HIS:ND1	2.23	0.56
1:A:358:LEU:HD13	1:A:416:TYR:HB3	1.88	0.56
1:B:943:ASN:OD1	1:B:1011:GLN:NE2	2.37	0.56
1:B:430:PRO:HB3	1:B:439:ASN:HB3	1.87	0.55
1:A:200:ASP:OD2	1:A:203:ARG:NH2	2.40	0.55
1:B:449:LEU:HD12	1:B:463:ALA:HB2	1.88	0.54
1:B:599:ILE:HD13	1:B:692:MET:HG3	1.90	0.54
1:A:315:GLY:HA2	1:A:324:PHE:O	2.07	0.54
1:B:934:SER:O	1:B:934:SER:OG	2.25	0.53
1:B:276:PRO:HD2	1:B:279:LEU:HD12	1.91	0.53
1:A:748:ASP:OD1	1:A:748:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:NH2	1:A:732:ASP:OD1	2.38	0.52
1:B:771:VAL:HG22	1:B:870:ILE:HD11	1.91	0.52
1:B:203:ARG:HG2	1:B:608:HIS:HB3	1.91	0.52
1:B:675:LYS:HD3	1:B:750:VAL:HG12	1.92	0.52
1:B:969:ASN:OD1	1:B:997:LYS:NZ	2.33	0.52
1:A:249:MET:HE3	1:A:572:ALA:HB3	1.92	0.51
1:B:329:LYS:NZ	1:B:383:ASP:O	2.43	0.51
1:A:289:LEU:HD23	1:A:325:ILE:HB	1.91	0.51
1:A:601:MET:O	1:A:604:TYR:HB2	2.11	0.50
1:A:1040:PHE:O	1:A:1042:SER:N	2.39	0.50
1:B:60:HIS:HA	1:B:726:THR:HA	1.94	0.50
1:A:293:THR:HG21	1:A:299:MET:HE3	1.94	0.49
1:A:1021:MET:HA	1:A:1024:ILE:HG23	1.93	0.49
1:B:297:GLU:HG3	1:B:487:VAL:HG13	1.95	0.49
1:A:89:GLY:N	1:A:604:TYR:OH	2.45	0.49
1:A:76:TYR:OH	1:A:80:LYS:HD2	2.13	0.49
1:B:9:LYS:HB3	1:B:768:TYR:CE1	2.48	0.48
1:A:586:ASP:OD2	1:A:588:GLN:NE2	2.46	0.48
1:B:601:MET:HA	1:B:604:TYR:CD2	2.47	0.48
1:A:237:TYR:CE1	1:A:526:LEU:HB2	2.48	0.48
1:A:868:GLU:OE2	1:A:879:SER:OG	2.19	0.48
1:B:242:PRO:HG2	1:B:332:ARG:NH2	2.28	0.48
1:A:710:LEU:HD11	1:A:755:PHE:HB2	1.96	0.48
1:B:663:GLU:OE1	1:B:699:LYS:NZ	2.42	0.48
1:B:249:MET:HG2	1:B:575:ARG:HH22	1.78	0.48
1:A:214:TYR:OH	1:A:596:ASP:O	2.28	0.48
1:A:949:HIS:NE2	1:B:890:PRO:HG3	2.29	0.47
1:B:95:MET:SD	1:B:246:GLN:NE2	2.86	0.47
1:A:249:MET:O	1:A:253:ARG:HG3	2.14	0.47
1:A:666:TYR:CD2	1:A:667:PRO:HA	2.49	0.47
1:B:1040:PHE:O	1:B:1042:SER:N	2.41	0.47
1:B:253:ARG:NH1	1:B:259:VAL:O	2.47	0.47
1:B:12:PHE:HB3	1:B:768:TYR:OH	2.15	0.47
1:A:289:LEU:HD12	1:A:362:LEU:HD11	1.97	0.47
1:A:733:LYS:NZ	1:A:757:GLU:OE2	2.39	0.47
1:B:609:LEU:HD13	1:B:623:LEU:HD11	1.96	0.47
1:B:843:MET:HE2	1:B:848:VAL:HG22	1.97	0.47
1:A:167:SER:O	1:A:171:ILE:HG13	2.14	0.47
1:A:771:VAL:HG22	1:A:870:ILE:HD11	1.95	0.47
1:A:266:LEU:HD22	1:A:507:TYR:HB2	1.97	0.47
1:A:1002:LYS:HG3	1:A:1003:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:PHE:CE2	1:B:16:ILE:HD11	2.50	0.46
1:B:92:CYS:HB2	1:B:208:THR:HG23	1.96	0.46
1:B:705:ARG:NH1	4:B:1301:HOH:O	2.48	0.46
1:B:935:HIS:CD2	1:B:1035:HIS:HB3	2.50	0.46
1:A:1042:SER:HA	1:A:1049:ARG:HH11	1.80	0.46
1:B:314:ILE:HD12	1:B:348:VAL:HG22	1.98	0.46
1:A:465:GLU:HA	1:A:468:TYR:HB2	1.96	0.46
1:B:297:GLU:OE1	1:B:297:GLU:N	2.43	0.46
1:B:1027:LEU:O	1:B:1031:LEU:HB2	2.16	0.46
1:A:167:SER:HB2	1:A:170:GLU:HG3	1.99	0.45
1:A:392:VAL:HB	3:A:1201:A2H:CL	2.53	0.45
1:A:491:LYS:HE3	1:A:491:LYS:HB2	1.76	0.45
1:B:236:ARG:HD3	1:B:236:ARG:HA	1.72	0.45
1:B:178:GLU:H	1:B:178:GLU:CD	2.24	0.45
1:B:355:GLU:HA	1:B:358:LEU:HG	1.98	0.45
1:A:844:HIS:HE1	1:A:846:GLU:HB2	1.81	0.45
1:B:24:TRP:CZ2	1:B:881:MET:HE3	2.52	0.45
1:B:330:ALA:O	1:B:334:MET:HG3	2.17	0.45
1:A:984:LYS:HE3	1:B:1013:GLU:HA	1.99	0.44
1:B:715:GLU:HB2	1:B:723:ASN:HD21	1.82	0.44
1:A:95:MET:HE1	1:A:244:ASP:CG	2.43	0.44
1:A:373:TYR:HD2	1:A:426:PHE:HE2	1.66	0.44
1:A:1017:LYS:O	1:A:1021:MET:HG2	2.18	0.44
1:B:832:LYS:HE3	1:B:832:LYS:HB3	1.72	0.44
1:B:250:ASP:HA	1:B:253:ARG:HD3	2.00	0.44
1:A:92:CYS:HB2	1:A:208:THR:HG23	2.00	0.43
1:B:335:SER:HB3	1:B:346:VAL:HG22	2.00	0.43
1:B:419:ARG:NE	1:B:422:MET:HE3	2.30	0.43
1:A:314:ILE:HG23	1:A:348:VAL:HG13	2.01	0.43
1:B:260:GLY:O	1:B:511:GLU:HG3	2.18	0.43
1:B:558:ARG:NH1	4:B:1302:HOH:O	2.51	0.43
1:B:950:THR:O	1:B:954:VAL:HG23	2.18	0.43
1:A:678:VAL:HB	1:A:679:PRO:HD3	2.00	0.43
1:A:716:LYS:HD3	1:A:716:LYS:HA	1.78	0.43
1:A:365:PRO:O	1:A:367:THR:N	2.47	0.43
1:A:243:LYS:HD2	1:A:520:ASP:HB2	2.00	0.43
1:A:586:ASP:HB3	1:A:589:TRP:HD1	1.84	0.43
1:B:942:LYS:HE3	1:B:1040:PHE:CZ	2.53	0.43
1:A:844:HIS:CE1	1:A:846:GLU:HB2	2.54	0.43
1:B:70:CYS:O	1:B:74:VAL:HG22	2.19	0.43
1:B:534:TYR:HB2	1:B:569:GLN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HD21	1:B:363:SER:HB2	2.01	0.43
1:B:936:CYS:SG	1:B:937:THR:N	2.92	0.43
1:B:224:THR:O	1:B:228:ARG:HG3	2.19	0.42
1:B:232:LYS:HB2	1:B:531:TYR:CZ	2.54	0.42
1:B:95:MET:N	1:B:96:PRO:CD	2.82	0.42
1:B:312:LYS:HE3	1:B:351:GLU:HG2	2.00	0.42
1:A:236:ARG:HA	1:A:236:ARG:NH1	2.33	0.42
1:A:958:HIS:NE2	1:A:975:GLU:OE1	2.47	0.42
1:A:252:ASP:OD1	1:A:252:ASP:N	2.48	0.42
1:B:626:ARG:HB3	1:B:628:GLN:HE21	1.84	0.42
1:A:261:PRO:HB2	1:A:508:MET:HE3	2.01	0.42
1:A:812:TYR:OH	1:A:861:PRO:HG2	2.20	0.42
1:B:995:MET:O	1:B:999:ASN:ND2	2.39	0.42
1:A:629:GLN:NE2	1:A:649:GLN:HB2	2.35	0.42
1:A:52:TYR:O	2:A:1200:LSS:N4	2.53	0.42
1:A:949:HIS:CE1	1:B:890:PRO:HG3	2.55	0.42
1:A:232:LYS:HB3	1:A:531:TYR:CZ	2.55	0.42
1:A:602:ALA:HB1	1:A:639:PHE:CE1	2.54	0.42
1:A:185:PRO:HB2	1:A:186:PRO:HD3	2.02	0.42
1:A:471:GLY:O	1:A:487:VAL:HG21	2.19	0.42
1:B:45:LYS:NZ	1:B:667:PRO:O	2.52	0.42
1:A:377:MET:HB3	1:A:380:ILE:HD11	2.02	0.41
1:A:970:LYS:HE3	1:A:970:LYS:HB3	1.76	0.41
1:B:259:VAL:HG13	1:B:511:GLU:HB2	2.02	0.41
1:B:393:PRO:HB2	1:B:428:PRO:HG3	2.02	0.41
1:A:304:ASN:HA	1:A:372:ILE:HB	2.02	0.41
1:B:404:ARG:O	1:B:408:LYS:HB2	2.20	0.41
1:B:734:PHE:O	1:B:735:SER:OG	2.31	0.41
1:A:308:ARG:HD3	1:A:311:MET:HE3	2.02	0.41
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.86	0.41
1:A:676:ASP:HB3	1:A:709:HIS:HE2	1.85	0.41
1:A:600:TYR:CE1	1:A:601:MET:HE3	2.55	0.41
1:A:609:LEU:HD13	1:A:623:LEU:HD11	2.03	0.41
1:B:989:VAL:O	1:B:993:VAL:HG23	2.21	0.41
1:A:866:LEU:HD23	1:A:866:LEU:HA	1.73	0.41
1:B:773:TRP:NE1	1:B:777:MET:HE3	2.35	0.41
1:A:673:SER:O	1:A:706:ALA:HA	2.20	0.41
1:A:913:LEU:HD22	1:A:1031:LEU:HD13	2.03	0.41
1:A:1021:MET:O	1:A:1024:ILE:HG12	2.21	0.41
1:B:309:PRO:HG3	1:B:376:PRO:HB3	2.03	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LYS:HA	1:B:384:LYS:HE2	2.02	0.41
1:B:739:MET:HE2	1:B:739:MET:HB3	2.01	0.41
1:A:1035:HIS:CD2	1:A:1037:GLU:HG2	2.56	0.41
1:A:534:TYR:HB2	1:A:569:GLN:O	2.21	0.40
1:A:597:SER:OG	2:A:1200:LSS:H11	2.21	0.40
1:A:527:CYS:O	1:A:529:GLN:NE2	2.53	0.40
1:A:85:LEU:HG	1:A:87:PRO:HD3	2.04	0.40
1:A:789:ALA:HB2	1:A:844:HIS:CD2	2.56	0.40
1:A:237:TYR:CE1	1:A:508:MET:HG3	2.57	0.40
1:A:384:LYS:HD3	3:A:1201:A2H:P	2.61	0.40
1:A:491:LYS:HG3	1:A:492:LYS:N	2.36	0.40
1:A:640:PHE:HB2	1:A:643:ALA:HB2	2.03	0.40
1:A:843:MET:HE2	1:A:848:VAL:HG22	2.02	0.40
1:B:441:SER:O	1:B:445:ILE:HG12	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	997/1092 (91%)	945 (95%)	51 (5%)	1 (0%)	48	80
1	B	999/1092 (92%)	946 (95%)	52 (5%)	1 (0%)	48	80
All	All	1996/2184 (91%)	1891 (95%)	103 (5%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	735	SER
1	B	934	SER

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	884/958 (92%)	863 (98%)	21 (2%)	43	73
1	B	886/958 (92%)	857 (97%)	29 (3%)	33	67
All	All	1770/1916 (92%)	1720 (97%)	50 (3%)	38	70

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TYR
1	A	161	MET
1	A	252	ASP
1	A	398	ASP
1	A	439	ASN
1	A	509	GLU
1	A	529	GLN
1	A	560	ASN
1	A	586	ASP
1	A	601	MET
1	A	666	TYR
1	A	707	ASN
1	A	748	ASP
1	A	750	VAL
1	A	828	PHE
1	A	884	SER
1	A	981	GLU
1	A	1040	PHE
1	A	1053	CYS
1	A	1059	ASN
1	A	1060	VAL
1	B	10	VAL
1	B	35	SER
1	B	52	TYR
1	B	169	GLU
1	B	253	ARG
1	B	267	LEU

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Mol	Chain	Res	Type
1	B	350	LYS
1	B	351	GLU
1	B	519	SER
1	B	592	GLU
1	B	610	LEU
1	B	628	GLN
1	B	647	LYS
1	B	648	THR
1	B	666	TYR
1	B	680	ASN
1	B	707	ASN
1	B	728	THR
1	B	750	VAL
1	B	778	VAL
1	B	780	ASN
1	B	828	PHE
1	B	841	GLU
1	B	850	ARG
1	B	981	GLU
1	B	1040	PHE
1	B	1053	CYS
1	B	1060	VAL
1	B	1061	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	HIS
1	A	254	GLN
1	A	302	GLN
1	A	614	ASN
1	A	869	HIS
1	A	999	ASN
1	A	1035	HIS
1	B	190	GLN
1	B	211	ASN
1	B	560	ASN
1	B	707	ASN
1	B	713	ASN
1	B	729	GLN
1	B	829	GLN
1	B	855	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 ⓘ

4 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	LSS	B	1200	-	32,33,33	5.70	18 (56%)	43,49,49	2.23	11 (25%)
3	A2H	B	1201	-	41,43,43	0.90	3 (7%)	48,67,67	1.97	13 (27%)
2	LSS	A	1200	-	32,33,33	5.76	18 (56%)	43,49,49	2.17	10 (23%)
3	A2H	A	1201	-	41,43,43	0.91	3 (7%)	48,67,67	1.95	13 (27%)

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
2	LSS	B	1200	-	-	8/22/39/39	0/3/3/3
3	A2H	B	1201	-	-	7/14/56/56	0/6/6/6
2	LSS	A	1200	-	-	5/22/39/39	0/3/3/3
3	A2H	A	1201	-	-	7/14/56/56	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	LSS	O1A-S1	15.80	1.56	1.42
2	A	1200	LSS	O1A-S1	15.74	1.56	1.42
2	A	1200	LSS	C1-N2	12.18	1.59	1.37
2	B	1200	LSS	C1-N2	12.15	1.59	1.37
2	A	1200	LSS	S1-N2	11.63	1.79	1.59
2	B	1200	LSS	S1-N2	11.45	1.78	1.59
2	A	1200	LSS	C4-N9	8.87	1.56	1.37
2	B	1200	LSS	C4-N9	8.75	1.55	1.37
2	A	1200	LSS	C8-N7	8.63	1.48	1.31
2	A	1200	LSS	O4-C24	8.53	1.64	1.45
2	B	1200	LSS	O4-C24	8.52	1.63	1.45
2	B	1200	LSS	C8-N7	8.49	1.48	1.31
2	A	1200	LSS	C2-N3	7.70	1.47	1.33
2	B	1200	LSS	C2-N3	7.54	1.47	1.33
2	A	1200	LSS	C5-N7	6.87	1.51	1.39
2	B	1200	LSS	C5-N7	6.73	1.51	1.39
2	A	1200	LSS	O5-S1	5.73	1.71	1.60
2	B	1200	LSS	O5-S1	5.63	1.71	1.60
2	A	1200	LSS	C5-C6	5.52	1.56	1.41
2	B	1200	LSS	C5-C6	5.43	1.56	1.41
2	A	1200	LSS	C5-C4	5.40	1.48	1.39
2	B	1200	LSS	C5-C4	5.16	1.48	1.39
2	A	1200	LSS	O2A-S1	4.76	1.46	1.42
2	A	1200	LSS	C6-N6	4.76	1.46	1.34
2	B	1200	LSS	C6-N6	4.68	1.46	1.34
2	B	1200	LSS	O4-C21	4.61	1.52	1.42
2	A	1200	LSS	O4-C21	4.58	1.52	1.42
2	B	1200	LSS	O2A-S1	4.52	1.46	1.42
2	A	1200	LSS	C4-N3	2.90	1.39	1.34
2	B	1200	LSS	C4-N3	2.80	1.39	1.34
3	B	1201	A2H	C13-CL	2.67	1.79	1.73
3	A	1201	A2H	C13-CL	2.61	1.79	1.73
2	A	1200	LSS	C2-N1	2.42	1.38	1.33
2	A	1200	LSS	C8-N9	2.32	1.41	1.37
2	B	1200	LSS	C2-N1	2.28	1.38	1.33
3	B	1201	A2H	C5-N7	-2.14	1.35	1.39
3	A	1201	A2H	C8-N7	2.13	1.35	1.31
2	A	1200	LSS	CA-N4	-2.12	1.37	1.48
2	B	1200	LSS	CA-N4	-2.11	1.38	1.48
2	B	1200	LSS	C8-N9	2.07	1.41	1.37
3	A	1201	A2H	C5-N7	-2.07	1.35	1.39
3	B	1201	A2H	C8-N7	2.01	1.35	1.31

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	LSS	O2A-S1-O1A	-7.78	109.21	120.85
2	A	1200	LSS	O2A-S1-O1A	-7.21	110.06	120.85
2	B	1200	LSS	C5-C4-N3	-5.68	118.89	126.72
3	B	1201	A2H	C5-C4-N3	-5.68	118.90	126.72
2	A	1200	LSS	C5-C4-N3	-5.56	119.06	126.72
3	A	1201	A2H	C5-C4-N3	-5.27	119.46	126.72
3	A	1201	A2H	N3-C2-N1	-5.02	120.98	128.58
3	B	1201	A2H	N3-C2-N1	-4.67	121.51	128.58
2	A	1200	LSS	N3-C4-N9	4.42	134.68	127.17
2	B	1200	LSS	N3-C4-N9	4.40	134.65	127.17
3	B	1201	A2H	O1-C10-C11	-4.27	99.13	103.58
3	A	1201	A2H	O1-C10-C11	-4.03	99.39	103.58
2	B	1200	LSS	N3-C2-N1	-3.80	122.83	128.58
2	A	1200	LSS	N3-C2-N1	-3.77	122.88	128.58
3	B	1201	A2H	N3-C4-N9	3.58	133.25	127.17
3	B	1201	A2H	C2-N3-C4	3.57	120.54	111.83
3	B	1201	A2H	O1-B-O2'	-3.54	102.27	108.36
3	A	1201	A2H	C2-N3-C4	3.47	120.31	111.83
3	A	1201	A2H	N3-C4-N9	3.46	133.05	127.17
2	B	1200	LSS	C2-N3-C4	3.43	120.21	111.83
2	A	1200	LSS	C2-N3-C4	3.39	120.12	111.83
2	B	1200	LSS	C4-C5-N7	-3.36	106.74	110.58
3	A	1201	A2H	N9-C8-N7	-3.36	109.17	113.94
2	B	1200	LSS	C5-N7-C8	3.29	108.62	103.45
3	B	1201	A2H	N9-C8-N7	-3.24	109.34	113.94
2	A	1200	LSS	C5-N7-C8	3.23	108.52	103.45
2	A	1200	LSS	C4-C5-N7	-3.18	106.95	110.58
2	A	1200	LSS	N9-C8-N7	-3.12	109.52	113.94
2	B	1200	LSS	N9-C8-N7	-3.11	109.53	113.94
3	B	1201	A2H	C4-C5-N7	-3.01	107.14	110.58
3	B	1201	A2H	C14-C13-C11	-2.96	118.46	122.38
2	A	1200	LSS	C4-N9-C8	2.88	108.76	105.74
3	A	1201	A2H	C14-C13-C11	-2.81	118.66	122.38
2	B	1200	LSS	C4-N9-C8	2.78	108.65	105.74
3	B	1201	A2H	C5-N7-C8	2.68	107.66	103.45
3	A	1201	A2H	C4-C5-N7	-2.57	107.64	110.58
3	A	1201	A2H	O1-B-O2'	-2.53	104.01	108.36
3	A	1201	A2H	C5-N7-C8	2.53	107.42	103.45
3	A	1201	A2H	C4-N9-C8	2.42	108.28	105.74
3	A	1201	A2H	O3P-P-O5'	-2.34	100.56	106.67
3	B	1201	A2H	O19-C16-C15	-2.32	118.88	123.95
2	A	1200	LSS	C23-C22-C21	2.27	105.75	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1201	A2H	C4-N9-C8	2.16	108.00	105.74
2	B	1200	LSS	C24-O4-C21	-2.13	104.76	109.47
2	B	1200	LSS	C22-C21-N9	-2.09	108.11	113.30
3	A	1201	A2H	O3P-P-O2P	2.08	115.60	107.80
3	B	1201	A2H	C15-C16-C12	-2.04	118.62	122.66

There are no chirality outliers.

All (27) torsion outliers are listed below:

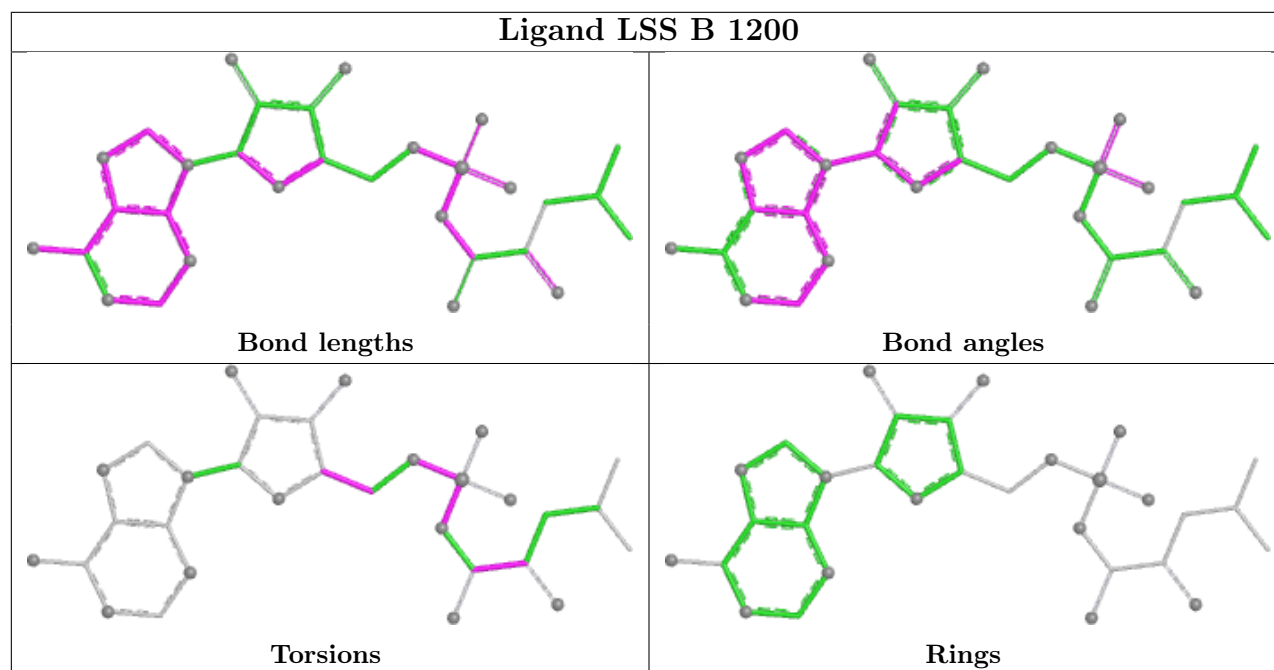
Mol	Chain	Res	Type	Atoms
2	A	1200	LSS	C25-O5-S1-N2
2	B	1200	LSS	C25-O5-S1-N2
2	B	1200	LSS	C25-O5-S1-O1A
2	B	1200	LSS	O4-C24-C25-O5
2	B	1200	LSS	C23-C24-C25-O5
3	A	1201	A2H	C5'-O5'-P-O1P
3	A	1201	A2H	C5'-O5'-P-O2P
3	A	1201	A2H	C5'-O5'-P-O3P
3	B	1201	A2H	C5'-O5'-P-O1P
3	B	1201	A2H	C5'-O5'-P-O2P
3	B	1201	A2H	C5'-O5'-P-O3P
2	A	1200	LSS	C10-C7-C9-CA
2	A	1200	LSS	C11-C7-C9-CA
3	A	1201	A2H	C21-C20-O19-C16
2	B	1200	LSS	C25-O5-S1-O2A
3	B	1201	A2H	C21-C20-O19-C16
2	B	1200	LSS	C1-N2-S1-O2A
2	A	1200	LSS	C25-O5-S1-O2A
3	A	1201	A2H	C2'-C1'-N9-C8
3	B	1201	A2H	C2'-C1'-N9-C8
3	B	1201	A2H	C2'-C1'-N9-C4
2	A	1200	LSS	C25-O5-S1-O1A
3	A	1201	A2H	O4'-C1'-N9-C8
2	B	1200	LSS	O1-C1-CA-N4
2	B	1200	LSS	N2-C1-CA-N4
3	B	1201	A2H	O4'-C1'-N9-C8
3	A	1201	A2H	C2'-C1'-N9-C4

There are no ring outliers.

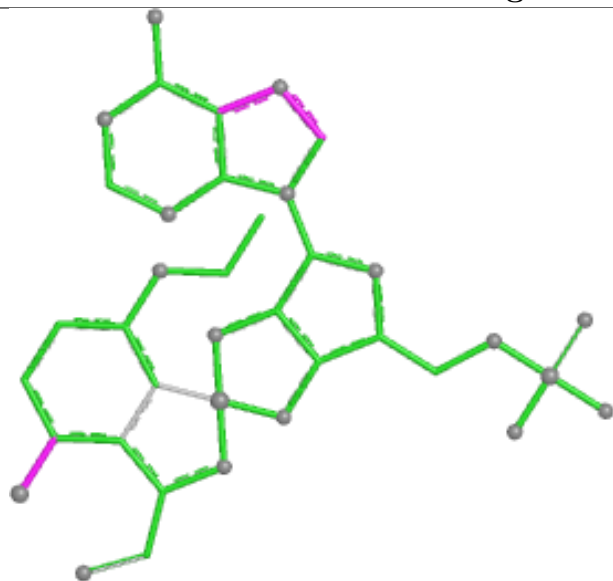
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1200	LSS	1	0
2	A	1200	LSS	3	0
3	A	1201	A2H	3	0

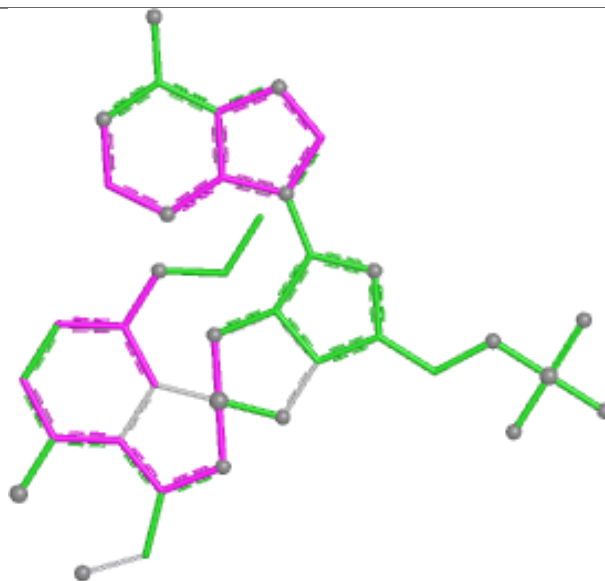
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



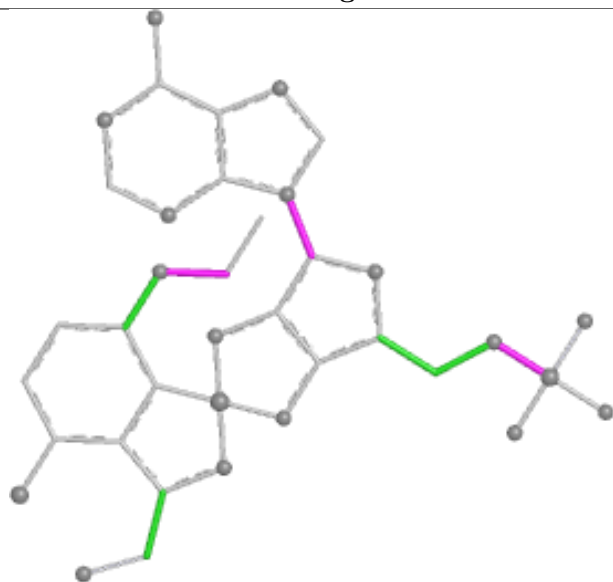
Ligand A2H B 1201



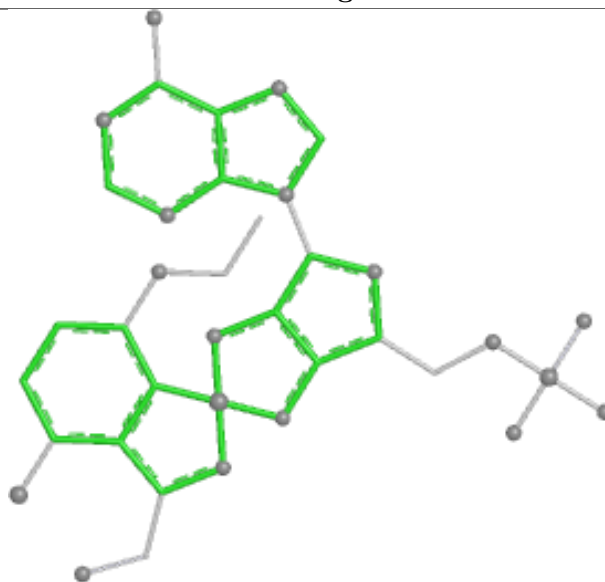
Bond lengths



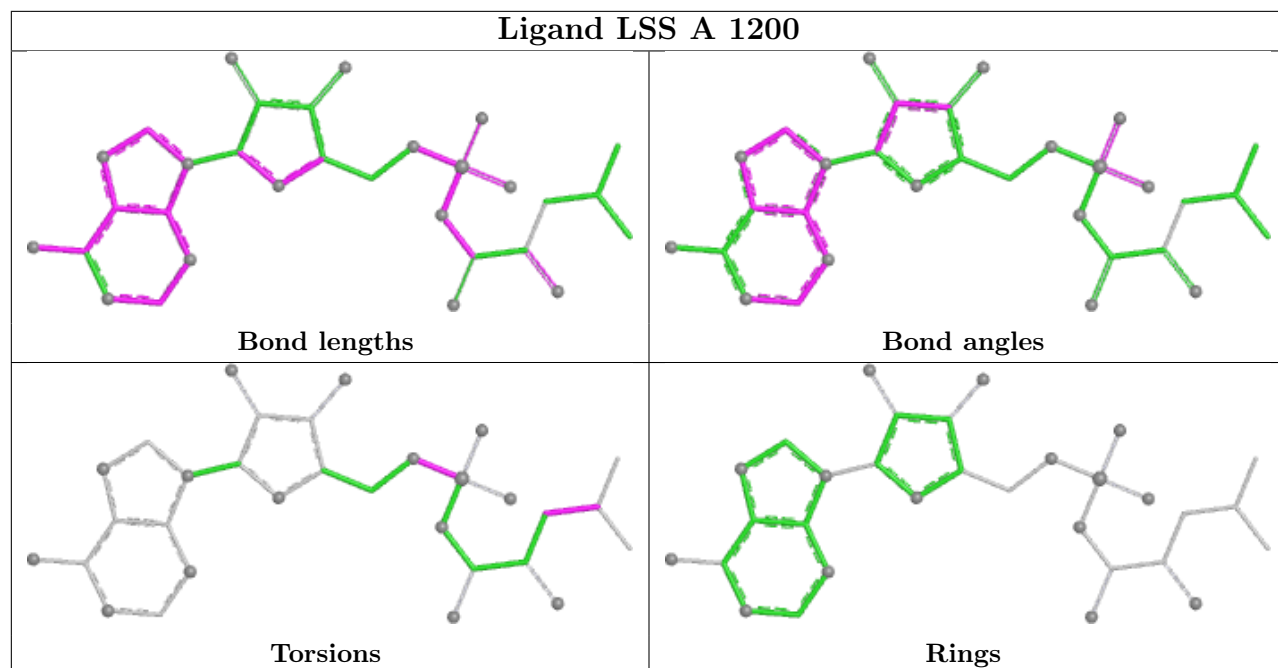
Bond angles

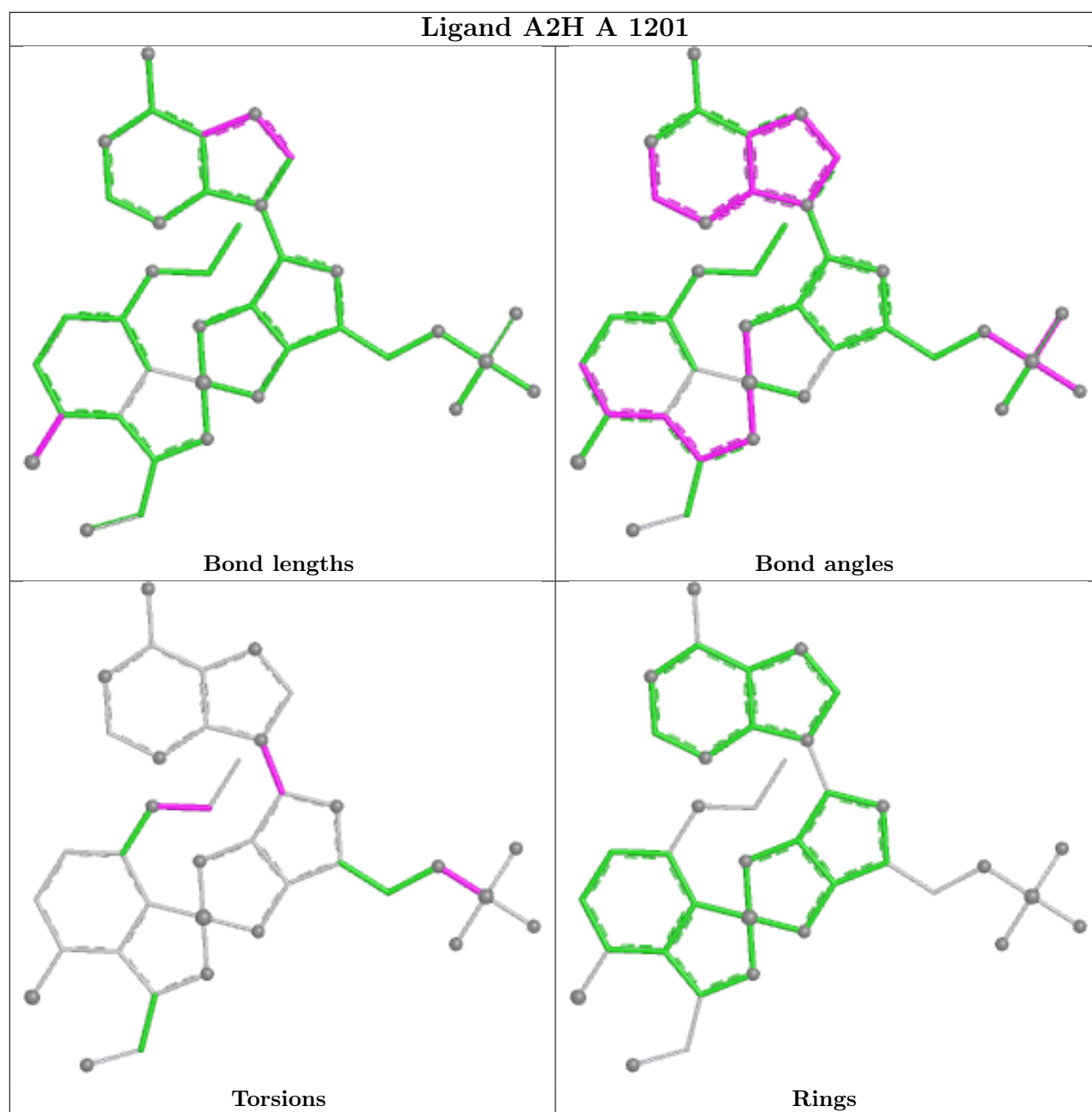


Torsions



Rings





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	1003/1092 (91%)	0.42	36 (3%) 46 26	38, 80, 113, 129	0
1	B	1005/1092 (92%)	-0.23	9 (0%) 81 61	9, 34, 79, 118	0
All	All	2008/2184 (91%)	0.10	45 (2%) 62 39	9, 58, 107, 129	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	5.7
1	A	385	GLY	4.0
1	A	97	ILE	3.7
1	A	406	LEU	3.5
1	A	567	TRP	3.4
1	A	266	LEU	3.1
1	A	265	THR	3.1
1	A	307	VAL	3.1
1	A	250	ASP	3.1
1	A	290	VAL	3.0
1	A	110	LEU	3.0
1	A	268	LYS	3.0
1	B	971	VAL	3.0
1	A	501	ALA	2.9
1	A	259	VAL	2.7
1	B	436	GLY	2.7
1	A	502	GLY	2.6
1	A	484	GLY	2.5
1	A	292	ALA	2.5
1	A	503	ASP	2.5
1	B	448	GLU	2.5
1	A	591	ILE	2.4
1	B	100	CYS	2.4
1	A	100	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	603	PHE	2.3
1	B	257	GLU	2.3
1	A	374	VAL	2.3
1	A	237	TYR	2.2
1	B	462	GLU	2.2
1	A	303	THR	2.2
1	B	406	LEU	2.2
1	A	460	LEU	2.1
1	A	389	VAL	2.1
1	A	538	ASN	2.1
1	B	1061	PHE	2.1
1	A	272	LEU	2.1
1	A	261	PRO	2.1
1	A	164	LEU	2.1
1	A	398	ASP	2.1
1	A	507	TYR	2.1
1	A	451	ILE	2.0
1	B	464	LYS	2.0
1	A	375	LEU	2.0
1	A	239	ILE	2.0
1	A	395	ASP	2.0

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

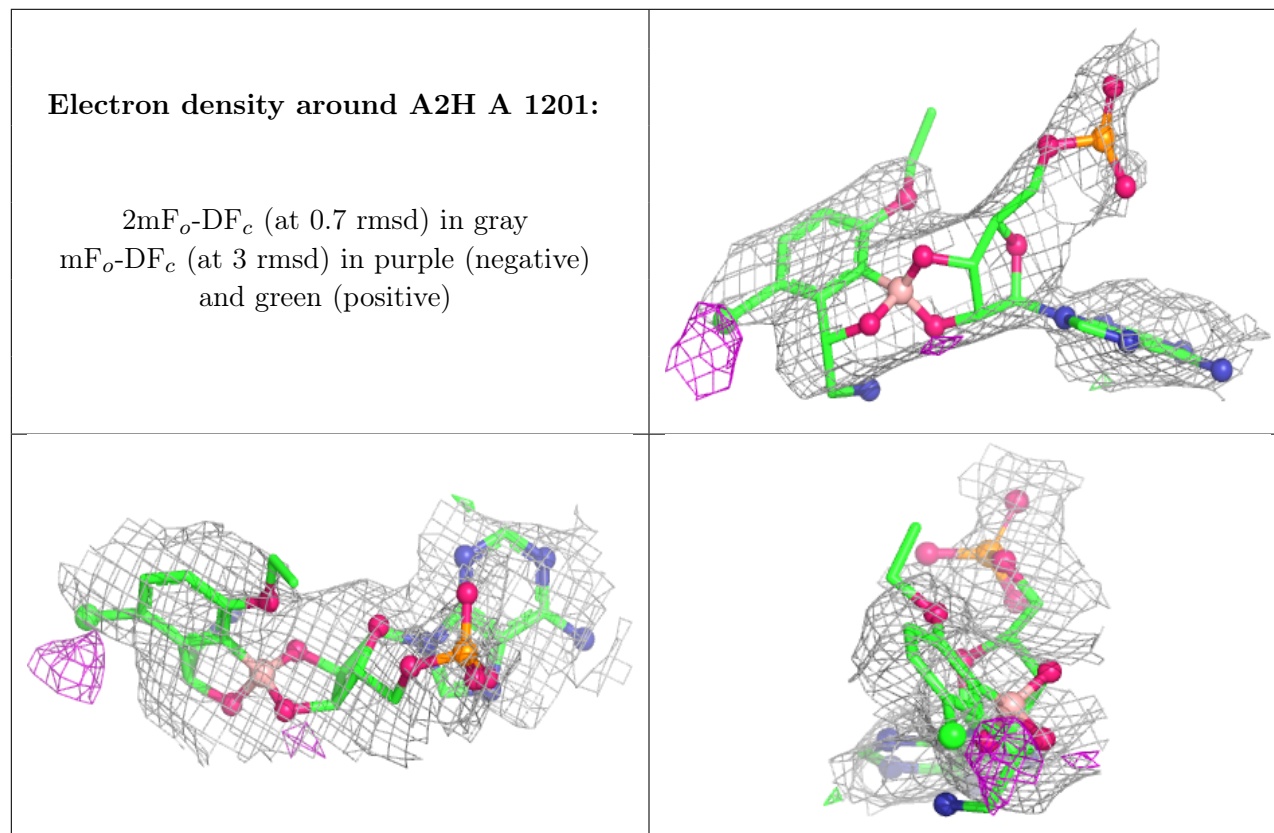
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A2H	A	1201	38/38	0.79	0.14	93,103,110,124	0
2	LSS	A	1200	31/31	0.93	0.13	50,59,67,73	0

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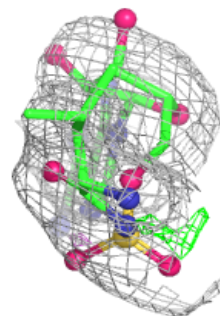
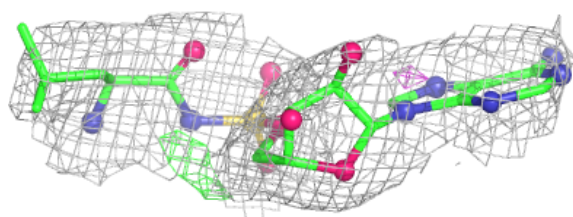
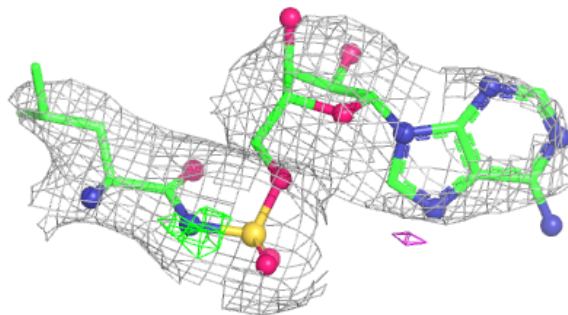
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A2H	B	1201	38/38	0.94	0.09	31,42,62,70	0
2	LSS	B	1200	31/31	0.96	0.10	8,14,19,23	0

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.

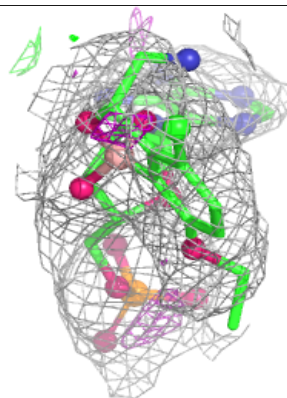
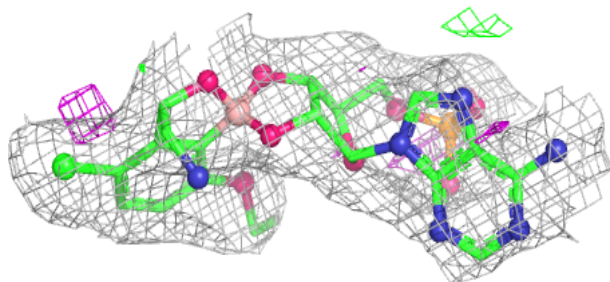
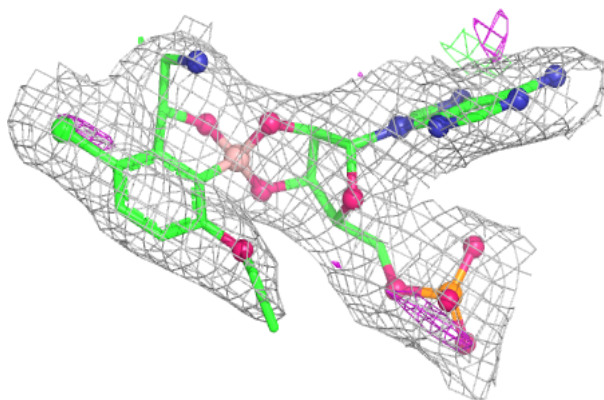


Electron density around LSS A 1200:

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

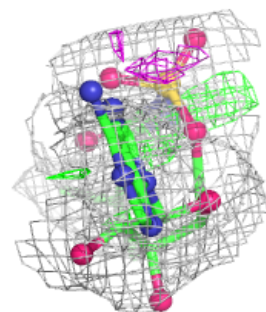
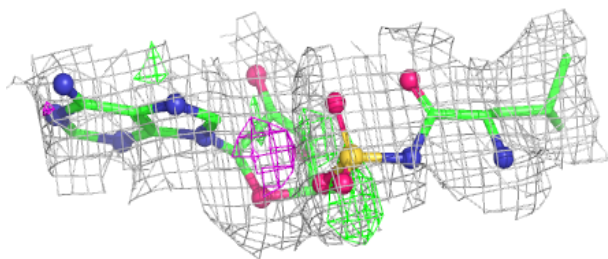
**Electron density around A2H B 1201:**

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



Electron density around LSS B 1200:

$2mF_o-DF_c$ (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.