



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:01 AM UTC

PDB ID : 6LPF / pdb_00006lpf
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 : 2020-01-10
Resolution : 2.49 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

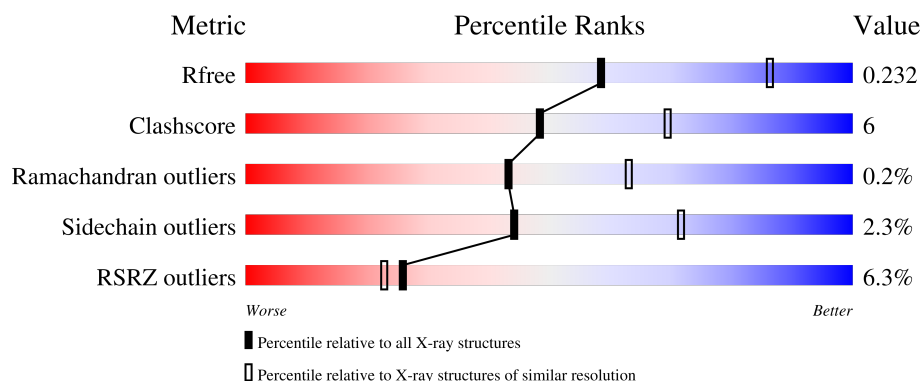
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	
1	B	1092	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16988 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	1002	Total	C	N	O	S	0	0	0
			8088	5204	1343	1488	53			
1	B	1006	Total	C	N	O	S	0	0	0
			8124	5226	1351	1492	55			

There are 44 discrepancies between the modelled and reference sequences:

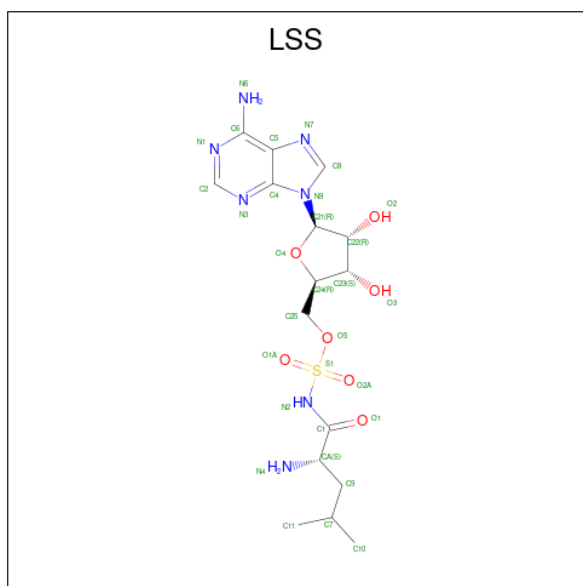
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q9P2J5
A	-20	GLY	-	expression tag	UNP Q9P2J5
A	-19	HIS	-	expression tag	UNP Q9P2J5
A	-18	HIS	-	expression tag	UNP Q9P2J5
A	-17	HIS	-	expression tag	UNP Q9P2J5
A	-16	HIS	-	expression tag	UNP Q9P2J5
A	-15	HIS	-	expression tag	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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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).

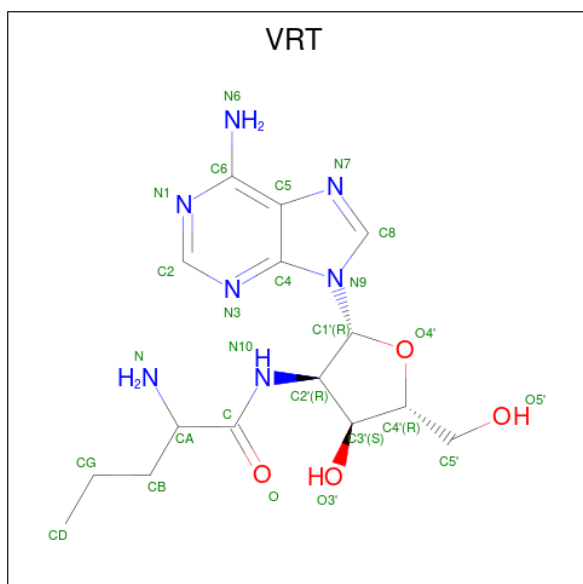


- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2'-(L-NORVALYL)AMINO-2'-DEOXYADENOSINE (CCD ID: VRT) (formula: $C_{15}H_{23}N_7O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			26	15	7	4		

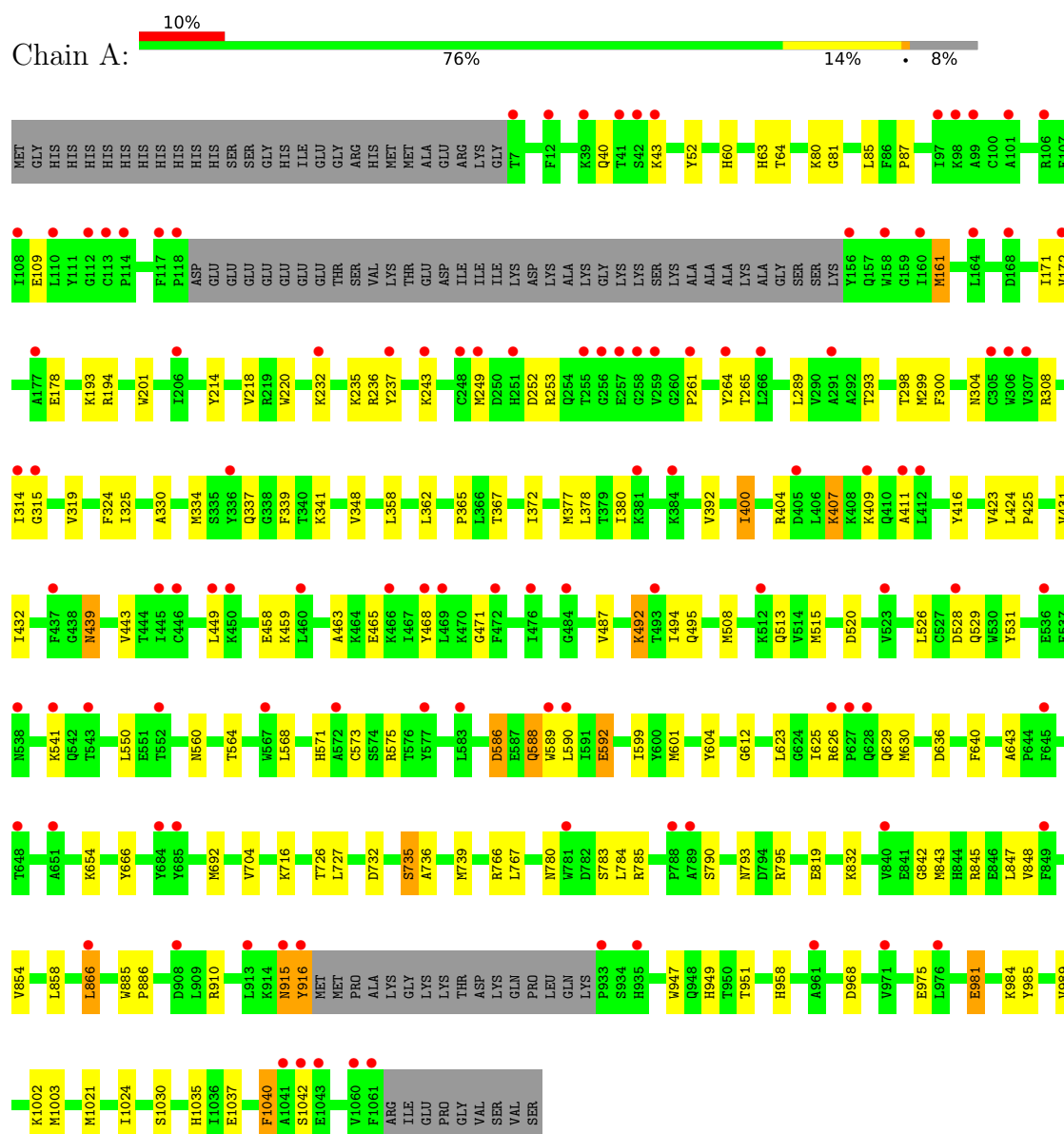
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	89	Total 89	O 89	0	0
5	B	593	Total 593	O 593	0	0

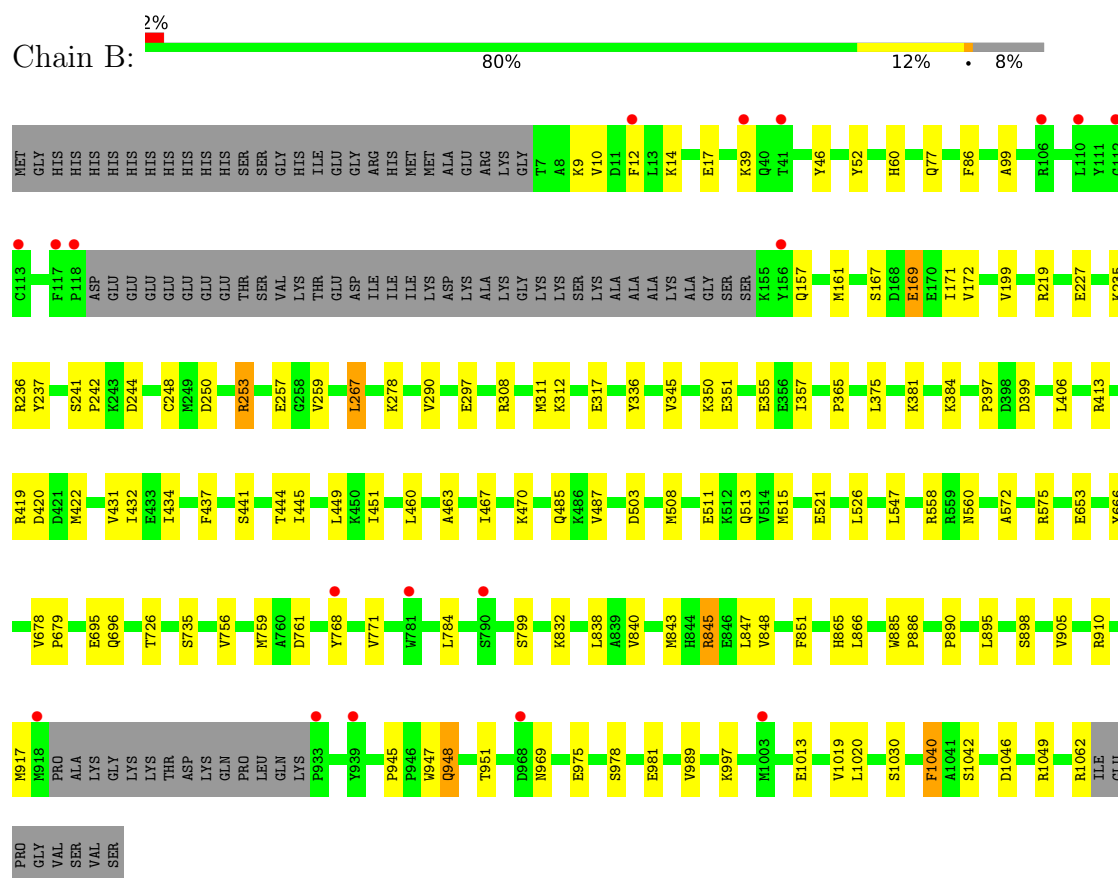
3 Residue-property plots [i](#)

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: 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	88.22Å 94.68Å 680.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 2.49 49.08 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.08-2.49) 97.3 (49.08-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.199 , 0.242 (Not available) , 0.232	Depositor DCC
R_{free} test set	4888 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16988	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: GOL, LSS, VRT

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	0.14	0/8288	0.33	0/11203
1	B	0.20	0/8324	0.40	0/11248
All	All	0.17	0/16612	0.37	0/22451

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	8088	0	8046	103	0
1	B	8124	0	8090	76	0
2	A	31	0	25	2	0
2	B	31	0	25	1	0
3	B	6	0	8	1	0
4	B	26	0	0	3	0
5	A	89	0	0	12	0
5	B	593	0	0	12	0
All	All	16988	0	16194	179	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 6.

All (179) 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:A:1200:LSS:O4	2:A:1200:LSS:C24	1.63	1.30
4:B:1103:VRT:C4'	4:B:1103:VRT:O4'	1.65	1.07
1:A:739:MET:N	5:A:1301:HOH:O	1.96	0.97
1:B:445:ILE:HD12	1:B:463:ALA:HB1	1.54	0.87
1:A:735:SER:O	5:A:1301:HOH:O	1.96	0.82
1:B:945:PRO:HG2	1:B:948:GLN:HG3	1.66	0.77
1:A:400:ILE:HD12	1:A:443:VAL:HG22	1.70	0.72
1:A:439:ASN:OD1	1:A:439:ASN:N	2.25	0.69
1:B:236:ARG:NH1	5:B:1207:HOH:O	2.24	0.69
1:A:80:LYS:NZ	5:A:1306:HOH:O	2.28	0.66
1:A:308:ARG:NH1	1:A:378:LEU:O	2.28	0.66
1:A:400:ILE:HD11	1:A:404:ARG:HE	1.62	0.65
1:B:419:ARG:NH2	5:B:1216:HOH:O	2.29	0.65
1:A:293:THR:HG21	1:A:299:MET:HE3	1.79	0.64
1:A:736:ALA:O	5:A:1301:HOH:O	2.15	0.64
1:B:99:ALA:O	5:B:1201:HOH:O	2.16	0.63
1:B:969:ASN:OD1	1:B:997:LYS:NZ	2.30	0.63
1:B:485:GLN:NE2	5:B:1221:HOH:O	2.31	0.62
1:A:43:LYS:HE2	1:A:81:GLY:HA3	1.81	0.62
1:A:337:GLN:NE2	1:A:508:MET:O	2.32	0.62
1:A:949:HIS:CE1	1:B:890:PRO:HG3	2.34	0.61
1:A:736:ALA:C	5:A:1301:HOH:O	2.43	0.60
1:A:261:PRO:HB2	1:A:508:MET:HE3	1.82	0.60
1:A:314:ILE:HG23	1:A:348:VAL:HG13	1.84	0.60
1:A:586:ASP:HB3	1:A:589:TRP:HD1	1.68	0.59
1:B:397:PRO:HG3	1:B:445:ILE:HD11	1.84	0.59
1:A:541:LYS:NZ	5:A:1314:HOH:O	2.35	0.59
1:A:915:ASN:HD22	1:A:916:TYR:HD1	1.51	0.59
1:A:60:HIS:HA	1:A:726:THR:HA	1.87	0.57
1:B:12:PHE:HB3	1:B:768:TYR:OH	2.05	0.56
1:A:358:LEU:HD13	1:A:416:TYR:HB3	1.86	0.56
1:A:407:LYS:HD3	1:A:423:VAL:HG12	1.88	0.56
1:A:785:ARG:NH2	1:A:842:GLY:O	2.39	0.56
1:B:278:LYS:HE2	1:B:350:LYS:HE2	1.88	0.56
1:B:449:LEU:HD12	1:B:463:ALA:HB2	1.86	0.55
1:B:771:VAL:HG21	1:B:866:LEU:HD11	1.86	0.55
1:B:419:ARG:HE	1:B:422:MET:HE3	1.69	0.55
1:A:64:THR:HG21	1:A:727:LEU:HD13	1.87	0.55
1:B:60:HIS:HA	1:B:726:THR:HA	1.89	0.55
1:A:40:GLN:NE2	5:A:1321:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:THR:N	5:A:1302:HOH:O	2.13	0.54
1:A:984:LYS:HE3	1:B:1013:GLU:HA	1.89	0.54
1:B:951:THR:HG21	1:B:989:VAL:HG23	1.88	0.54
1:A:626:ARG:HB2	1:A:629:GLN:HB2	1.90	0.54
1:A:784:LEU:HB2	1:A:845:ARG:HB2	1.90	0.54
1:A:243:LYS:HD2	1:A:520:ASP:HB2	1.89	0.53
1:B:832:LYS:HB2	1:B:851:PHE:CZ	2.43	0.53
1:B:312:LYS:HE3	1:B:351:GLU:HG2	1.90	0.53
1:B:431:VAL:HG12	1:B:432:ILE:HG13	1.90	0.53
1:B:399:ASP:OD2	4:B:1103:VRT:N	2.42	0.52
1:A:431:VAL:HG12	1:A:432:ILE:HG13	1.91	0.52
1:A:289:LEU:HD23	1:A:325:ILE:HB	1.91	0.52
1:A:471:GLY:O	1:A:487:VAL:HG21	2.09	0.51
1:B:345:VAL:HA	3:B:1102:GOL:H2	1.92	0.51
1:A:409:LYS:HE2	1:A:411:ALA:HB3	1.92	0.51
1:A:193:LYS:HE2	1:A:201:TRP:CD1	2.46	0.51
1:A:780:ASN:HB3	1:A:783:SER:HB2	1.93	0.51
1:A:843:MET:HE2	1:A:848:VAL:HG22	1.93	0.50
1:A:910:ARG:NH1	1:A:1030:SER:OG	2.39	0.50
1:A:264:TYR:HB3	5:A:1302:HOH:O	2.10	0.50
1:A:449:LEU:HD12	1:A:463:ALA:HB2	1.94	0.50
1:B:397:PRO:HD3	1:B:467:ILE:HD11	1.92	0.50
1:A:1035:HIS:CD2	1:A:1037:GLU:HG2	2.47	0.49
1:A:465:GLU:HA	1:A:468:TYR:HB2	1.94	0.49
1:A:232:LYS:HB3	1:A:531:TYR:CZ	2.48	0.48
1:B:308:ARG:HB3	1:B:311:MET:HE3	1.95	0.48
1:B:885:TRP:CD2	1:B:886:PRO:HD2	2.48	0.48
1:B:905:VAL:HG11	1:B:1020:LEU:HD21	1.95	0.48
1:A:220:TRP:NE1	1:A:636:ASP:OD1	2.45	0.48
1:A:235:LYS:HA	1:A:528:ASP:HA	1.94	0.48
1:A:298:THR:HB	1:A:392:VAL:HG11	1.95	0.48
1:B:365:PRO:HG3	1:B:503:ASP:HB3	1.95	0.48
1:B:898:SER:HB2	1:B:1019:VAL:HG21	1.95	0.47
1:A:237:TYR:CE1	1:A:526:LEU:HB2	2.49	0.47
1:B:547:LEU:O	1:B:558:ARG:NH2	2.47	0.47
1:A:319:VAL:HG23	1:A:341:LYS:HA	1.96	0.47
1:A:640:PHE:HB2	1:A:643:ALA:HB2	1.97	0.47
1:B:241:SER:HB3	1:B:244:ASP:HB2	1.96	0.47
1:B:248:CYS:O	1:B:253:ARG:NH2	2.48	0.47
1:B:381:LYS:HB2	1:B:384:LYS:HG2	1.96	0.47
1:A:293:THR:O	5:A:1302:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:O	1:A:590:LEU:N	2.40	0.47
1:A:885:TRP:CD2	1:A:886:PRO:HD2	2.50	0.46
1:B:761:ASP:OD2	5:B:1202:HOH:O	2.20	0.46
1:A:790:SER:O	1:A:795:ARG:NH2	2.48	0.46
1:B:910:ARG:NH1	1:B:1030:SER:OG	2.41	0.46
1:A:194:ARG:NH2	1:A:732:ASP:OD1	2.39	0.46
1:B:678:VAL:HB	1:B:679:PRO:HD3	1.98	0.46
1:A:601:MET:O	1:A:604:TYR:HB2	2.15	0.46
1:A:315:GLY:HA2	1:A:324:PHE:O	2.16	0.46
1:B:843:MET:HE2	1:B:848:VAL:HG22	1.98	0.46
1:B:696:GLN:NE2	5:B:1253:HOH:O	2.49	0.45
1:B:167:SER:O	1:B:171:ILE:HG13	2.16	0.45
1:B:17:GLU:HG2	1:B:865:HIS:CG	2.52	0.45
1:A:588:GLN:H	1:A:588:GLN:CD	2.25	0.45
1:B:572:ALA:O	1:B:575:ARG:NH2	2.50	0.45
1:A:161:MET:HB3	1:A:171:ILE:HD13	1.98	0.45
1:B:444:THR:HG22	5:B:1759:HOH:O	2.14	0.45
1:A:625:ILE:HG21	1:A:630:MET:HE2	1.99	0.45
1:A:265:THR:N	5:A:1302:HOH:O	2.48	0.45
1:A:599:ILE:HD13	1:A:692:MET:HG3	1.99	0.45
1:B:784:LEU:HB2	1:B:845:ARG:HG3	1.99	0.45
1:A:573:CYS:HA	1:A:592:GLU:HG2	1.99	0.45
1:A:981:GLU:CG	1:B:895:LEU:HD13	2.47	0.45
1:B:375:LEU:HD13	1:B:406:LEU:HD23	1.98	0.45
1:B:267:LEU:O	1:B:290:VAL:HA	2.18	0.44
1:B:947:TRP:O	1:B:951:THR:HG23	2.17	0.44
1:A:847:LEU:HD12	1:A:847:LEU:HA	1.79	0.44
1:B:513:GLN:NE2	1:B:515:MET:SD	2.90	0.44
1:A:85:LEU:HG	1:A:87:PRO:HD3	1.99	0.44
1:A:236:ARG:HH11	1:A:236:ARG:HA	1.83	0.44
1:A:300:PHE:HE2	1:A:494:ILE:HD13	1.83	0.44
1:A:832:LYS:HE3	1:A:832:LYS:HB3	1.91	0.44
1:B:237:TYR:CD2	1:B:508:MET:HE3	2.52	0.44
1:B:242:PRO:HB3	1:B:336:TYR:OH	2.17	0.44
2:B:1101:LSS:H11A	2:B:1101:LSS:HA	1.80	0.44
1:A:304:ASN:HA	1:A:372:ILE:HB	2.00	0.43
1:B:9:LYS:HB3	1:B:768:TYR:CE2	2.53	0.43
1:A:866:LEU:HD23	1:A:866:LEU:HA	1.75	0.43
1:B:521:GLU:OE2	5:B:1203:HOH:O	2.21	0.43
1:B:39:LYS:HB2	5:B:1648:HOH:O	2.18	0.43
1:B:169:GLU:O	1:B:172:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1046:ASP:OD1	1:B:1049:ARG:NH1	2.43	0.43
1:B:434:ILE:HB	1:B:437:PHE:HB2	1.99	0.43
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.88	0.43
1:B:1040:PHE:O	1:B:1042:SER:N	2.48	0.43
1:B:219:ARG:HD3	5:B:1328:HOH:O	2.17	0.43
1:B:441:SER:O	1:B:445:ILE:HG12	2.19	0.43
1:A:407:LYS:HE2	1:A:407:LYS:HB2	1.85	0.43
1:B:317:GLU:OE2	5:B:1204:HOH:O	2.22	0.43
1:A:1002:LYS:HG3	1:A:1003:MET:HG2	2.00	0.43
1:A:252:ASP:OD1	1:A:252:ASP:N	2.51	0.42
1:A:377:MET:HB3	1:A:380:ILE:HD11	2.01	0.42
1:B:297:GLU:HG3	1:B:487:VAL:HG13	2.01	0.42
1:A:249:MET:O	1:A:253:ARG:HG3	2.19	0.42
1:B:46:TYR:CE2	1:B:77:GLN:HG3	2.54	0.42
1:B:259:VAL:HG13	1:B:511:GLU:HB2	2.00	0.42
1:A:958:HIS:NE2	1:A:975:GLU:OE1	2.41	0.42
1:A:513:GLN:HE21	1:A:515:MET:HE2	1.84	0.42
1:A:550:LEU:HD11	1:A:704:VAL:HG23	2.02	0.42
1:A:495:GLN:HE21	1:A:495:GLN:HB3	1.63	0.42
1:A:1021:MET:O	1:A:1024:ILE:HG12	2.20	0.42
1:B:86:PHE:O	1:B:199:VAL:HA	2.20	0.42
1:A:409:LYS:O	5:A:1303:HOH:O	2.22	0.42
1:B:695:GLU:OE2	5:B:1205:HOH:O	2.22	0.42
1:A:236:ARG:HA	1:A:236:ARG:NH1	2.35	0.42
1:A:334:MET:HB3	1:A:339:PHE:CG	2.55	0.42
1:B:250:ASP:HB3	1:B:257:GLU:HG2	2.02	0.41
1:A:1040:PHE:C	1:A:1042:SER:H	2.27	0.41
1:B:756:VAL:HG12	1:B:759:MET:H	1.85	0.41
1:A:289:LEU:HD12	1:A:362:LEU:HD11	2.02	0.41
1:A:214:TYR:O	1:A:218:VAL:HG23	2.21	0.41
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.84	0.41
1:B:235:LYS:HG2	1:B:526:LEU:HG	2.01	0.41
1:A:564:THR:O	1:A:568:LEU:HB2	2.20	0.41
1:A:571:HIS:NE2	1:A:592:GLU:OE2	2.39	0.41
1:A:458:GLU:HG2	1:A:459:LYS:H	1.86	0.41
1:A:716:LYS:HD3	1:A:716:LYS:HA	1.76	0.41
1:A:985:TYR:O	1:A:989:VAL:HG23	2.20	0.41
1:B:470:LYS:HA	1:B:470:LYS:HD3	1.81	0.41
1:A:330:ALA:O	1:A:334:MET:HG3	2.20	0.41
1:A:365:PRO:O	1:A:367:THR:N	2.53	0.41
1:A:63:HIS:NE2	2:A:1200:LSS:O2A	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LYS:HB3	1:A:531:TYR:CE1	2.56	0.41
1:A:289:LEU:HD12	1:A:362:LEU:HD21	2.03	0.41
1:A:588:GLN:HG2	1:A:589:TRP:CD1	2.56	0.41
1:A:947:TRP:O	1:A:951:THR:HG23	2.21	0.41
1:B:975:GLU:O	1:B:978:SER:OG	2.32	0.41
1:A:424:LEU:HB2	1:A:425:PRO:HD3	2.02	0.41
1:A:854:VAL:O	1:A:858:LEU:HG	2.21	0.40
1:B:384:LYS:NZ	4:B:1103:VRT:O5'	2.48	0.40
1:B:413:ARG:NH1	1:B:420:ASP:OD1	2.39	0.40
1:B:838:LEU:O	1:B:840:VAL:N	2.53	0.40
1:A:767:LEU:HD22	1:A:866:LEU:HD12	2.02	0.40
1:B:451:ILE:HD13	1:B:460:LEU:HD23	2.04	0.40
1:A:623:LEU:HB3	1:A:654:LYS:HD2	2.04	0.40
1:B:10:VAL:HG12	1:B:14:LYS:HD3	2.03	0.40
1:A:916:TYR:HD1	1:A:916:TYR:H	1.69	0.40
1:B:157:GLN:O	1:B:161:MET:HG2	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	859/1092 (79%)	809 (94%)	48 (6%)	2 (0%)	43	63
1	B	1000/1092 (92%)	963 (96%)	36 (4%)	1 (0%)	48	68
All	All	1859/2184 (85%)	1772 (95%)	84 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	612	GLY

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	883/958 (92%)	859 (97%)	24 (3%)	39	67
1	B	887/958 (93%)	870 (98%)	17 (2%)	50	76
All	All	1770/1916 (92%)	1729 (98%)	41 (2%)	44	72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	TYR
1	A	109	GLU
1	A	161	MET
1	A	172	VAL
1	A	178	GLU
1	A	400	ILE
1	A	407	LYS
1	A	439	ASN
1	A	492	LYS
1	A	529	GLN
1	A	560	ASN
1	A	586	ASP
1	A	588	GLN
1	A	592	GLU
1	A	666	TYR
1	A	766	ARG
1	A	793	ASN
1	A	819	GLU
1	A	866	LEU
1	A	915	ASN
1	A	916	TYR
1	A	968	ASP

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Mol	Chain	Res	Type
1	A	981	GLU
1	A	1040	PHE
1	B	52	TYR
1	B	169	GLU
1	B	227	GLU
1	B	253	ARG
1	B	267	LEU
1	B	355	GLU
1	B	357	ILE
1	B	560	ASN
1	B	653	GLU
1	B	666	TYR
1	B	799	SER
1	B	845	ARG
1	B	917	MET
1	B	948	GLN
1	B	981	GLU
1	B	1040	PHE
1	B	1062	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	HIS
1	A	254	GLN
1	A	304	ASN
1	A	410	GLN
1	A	452	GLN
1	A	495	GLN
1	A	529	GLN
1	A	545	GLN
1	A	588	GLN
1	A	696	GLN
1	A	900	GLN
1	A	915	ASN
1	A	949	HIS
1	B	40	GLN
1	B	254	GLN
1	B	343	ASN
1	B	549	ASN
1	B	560	ASN
1	B	618	GLN

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Mol	Chain	Res	Type
1	B	657	GLN
1	B	696	GLN
1	B	829	GLN
1	B	855	GLN
1	B	882	ASN
1	B	935	HIS
1	B	1023	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1101	-	32,33,33	5.21	17 (53%)	43,49,49	2.12	11 (25%)
2	LSS	A	1200	-	32,33,33	5.66	18 (56%)	43,49,49	2.08	10 (23%)
3	GOL	B	1102	-	5,5,5	1.31	0	5,5,5	0.85	0
4	VRT	B	1103	-	28,28,28	3.60	11 (39%)	35,40,40	1.96	8 (22%)

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	1101	-	-	4/22/39/39	0/3/3/3
2	LSS	A	1200	-	-	5/22/39/39	0/3/3/3
3	GOL	B	1102	-	-	2/4/4/4	-
4	VRT	B	1103	-	-	12/17/33/33	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	LSS	O1A-S1	15.57	1.56	1.42
2	B	1101	LSS	O1A-S1	13.82	1.54	1.42
2	A	1200	LSS	C1-N2	11.78	1.58	1.37
2	A	1200	LSS	S1-N2	11.08	1.78	1.59
2	B	1101	LSS	C1-N2	10.71	1.56	1.37
4	B	1103	VRT	C3'-C4'	-9.82	1.28	1.53
2	B	1101	LSS	S1-N2	9.75	1.76	1.59
4	B	1103	VRT	O4'-C4'	9.02	1.65	1.45
2	A	1200	LSS	C4-N9	8.79	1.55	1.37
2	A	1200	LSS	C8-N7	8.56	1.48	1.31
2	B	1101	LSS	C8-N7	8.54	1.48	1.31
2	A	1200	LSS	O4-C24	8.51	1.63	1.45
2	B	1101	LSS	C4-N9	8.25	1.54	1.37
2	B	1101	LSS	O4-C24	7.86	1.62	1.45
2	A	1200	LSS	C2-N3	7.61	1.47	1.33
2	B	1101	LSS	C2-N3	7.47	1.47	1.33
2	B	1101	LSS	C5-N7	6.76	1.51	1.39
2	A	1200	LSS	C5-N7	6.66	1.51	1.39
4	B	1103	VRT	C-N10	5.85	1.46	1.34
4	B	1103	VRT	O4'-C1'	-5.70	1.28	1.42
2	A	1200	LSS	O5-S1	5.57	1.71	1.60
2	A	1200	LSS	C5-C4	5.41	1.48	1.39
2	A	1200	LSS	C5-C6	5.39	1.56	1.41
4	B	1103	VRT	O-C	5.32	1.33	1.23
2	B	1101	LSS	C5-C6	5.27	1.55	1.41
2	B	1101	LSS	C5-C4	5.23	1.48	1.39
2	A	1200	LSS	O2A-S1	4.96	1.46	1.42
2	B	1101	LSS	O5-S1	4.80	1.69	1.60
2	A	1200	LSS	O4-C21	4.63	1.52	1.42
2	A	1200	LSS	C6-N6	4.61	1.46	1.34
2	B	1101	LSS	C6-N6	4.49	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	VRT	C2-N3	4.42	1.41	1.33
4	B	1103	VRT	C2'-N10	-4.22	1.39	1.45
4	B	1103	VRT	O3'-C3'	4.20	1.53	1.43
2	B	1101	LSS	O4-C21	3.97	1.51	1.42
2	B	1101	LSS	O2A-S1	3.74	1.45	1.42
2	A	1200	LSS	C4-N3	2.83	1.39	1.34
4	B	1103	VRT	C5-C6	2.62	1.48	1.41
2	B	1101	LSS	C4-N3	2.55	1.39	1.34
2	B	1101	LSS	C8-N9	2.51	1.41	1.37
2	A	1200	LSS	C2-N1	2.39	1.38	1.33
2	A	1200	LSS	C8-N9	2.29	1.41	1.37
4	B	1103	VRT	C4-N3	2.18	1.38	1.34
4	B	1103	VRT	CG-CB	2.15	1.63	1.51
2	A	1200	LSS	CA-N4	-2.10	1.38	1.48
2	B	1101	LSS	CA-N4	-2.10	1.38	1.48

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	LSS	O2A-S1-O1A	-6.36	111.32	120.85
2	A	1200	LSS	O2A-S1-O1A	-6.36	111.33	120.85
2	A	1200	LSS	C5-C4-N3	-5.52	119.12	126.72
2	B	1101	LSS	C5-C4-N3	-5.19	119.57	126.72
4	B	1103	VRT	C5-C4-N3	-5.03	119.78	126.72
4	B	1103	VRT	N3-C2-N1	-4.69	121.48	128.58
2	B	1101	LSS	N3-C4-N9	4.36	134.58	127.17
2	A	1200	LSS	N3-C4-N9	4.35	134.57	127.17
2	A	1200	LSS	N3-C2-N1	-3.95	122.61	128.58
4	B	1103	VRT	N9-C8-N7	-3.86	108.46	113.94
2	B	1101	LSS	N3-C2-N1	-3.74	122.92	128.58
4	B	1103	VRT	C2-N3-C4	3.50	120.39	111.83
4	B	1103	VRT	C5-N7-C8	3.48	108.92	103.45
2	A	1200	LSS	C2-N3-C4	3.48	120.32	111.83
4	B	1103	VRT	N3-C4-N9	3.42	132.99	127.17
2	B	1101	LSS	C4-N9-C8	3.36	109.26	105.74
2	B	1101	LSS	C2-N3-C4	3.31	119.91	111.83
2	B	1101	LSS	N9-C8-N7	-3.27	109.30	113.94
2	A	1200	LSS	C5-N7-C8	3.21	108.50	103.45
4	B	1103	VRT	C4-C5-N7	-3.20	106.93	110.58
2	A	1200	LSS	C4-C5-N7	-3.17	106.95	110.58
2	A	1200	LSS	N9-C8-N7	-3.02	109.65	113.94
2	B	1101	LSS	C5-N7-C8	2.91	108.02	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1200	LSS	C4-N9-C8	2.71	108.59	105.74
2	B	1101	LSS	C4-C5-N7	-2.64	107.56	110.58
4	B	1103	VRT	C4-N9-C8	2.60	108.47	105.74
2	B	1101	LSS	C1-N2-S1	-2.41	115.26	124.07
2	B	1101	LSS	O1-C1-CA	2.26	125.03	120.28
2	A	1200	LSS	C1-N2-S1	-2.00	116.75	124.07

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1200	LSS	C25-O5-S1-N2
2	B	1101	LSS	C25-O5-S1-N2
4	B	1103	VRT	O-C-CA-N
4	B	1103	VRT	N10-C-CA-N
4	B	1103	VRT	O4'-C4'-C5'-O5'
4	B	1103	VRT	C3'-C4'-C5'-O5'
3	B	1102	GOL	C1-C2-C3-O3
4	B	1103	VRT	C-CA-CB-CG
2	B	1101	LSS	C25-O5-S1-O1A
4	B	1103	VRT	O-C-CA-CB
4	B	1103	VRT	CA-CB-CG-CD
3	B	1102	GOL	O2-C2-C3-O3
2	B	1101	LSS	C25-O5-S1-O2A
4	B	1103	VRT	C2'-C1'-N9-C8
4	B	1103	VRT	N-CA-CB-CG
4	B	1103	VRT	O4'-C1'-N9-C8
2	A	1200	LSS	C25-O5-S1-O2A
4	B	1103	VRT	C2'-C1'-N9-C4
4	B	1103	VRT	N10-C-CA-CB
2	B	1101	LSS	O4-C24-C25-O5
2	A	1200	LSS	O1-C1-CA-N4
2	A	1200	LSS	N2-C1-CA-N4
2	A	1200	LSS	C25-O5-S1-O1A

There are no ring outliers.

4 monomers are involved in 7 short contacts:

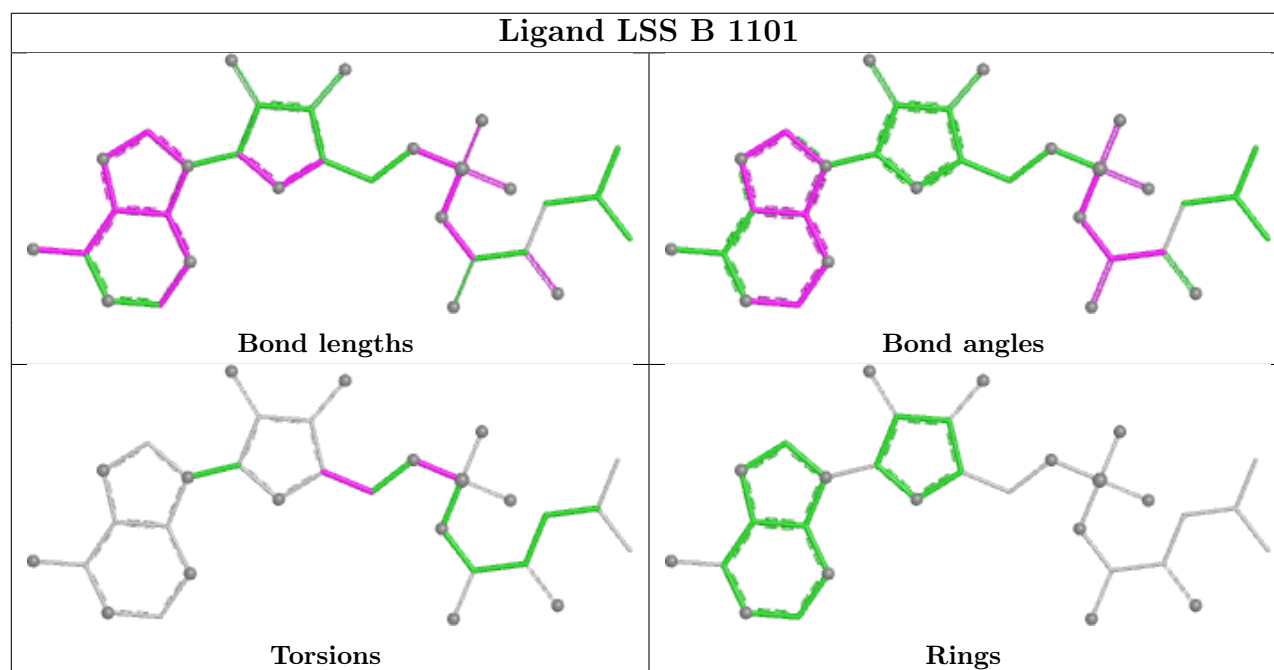
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	LSS	1	0
2	A	1200	LSS	2	0

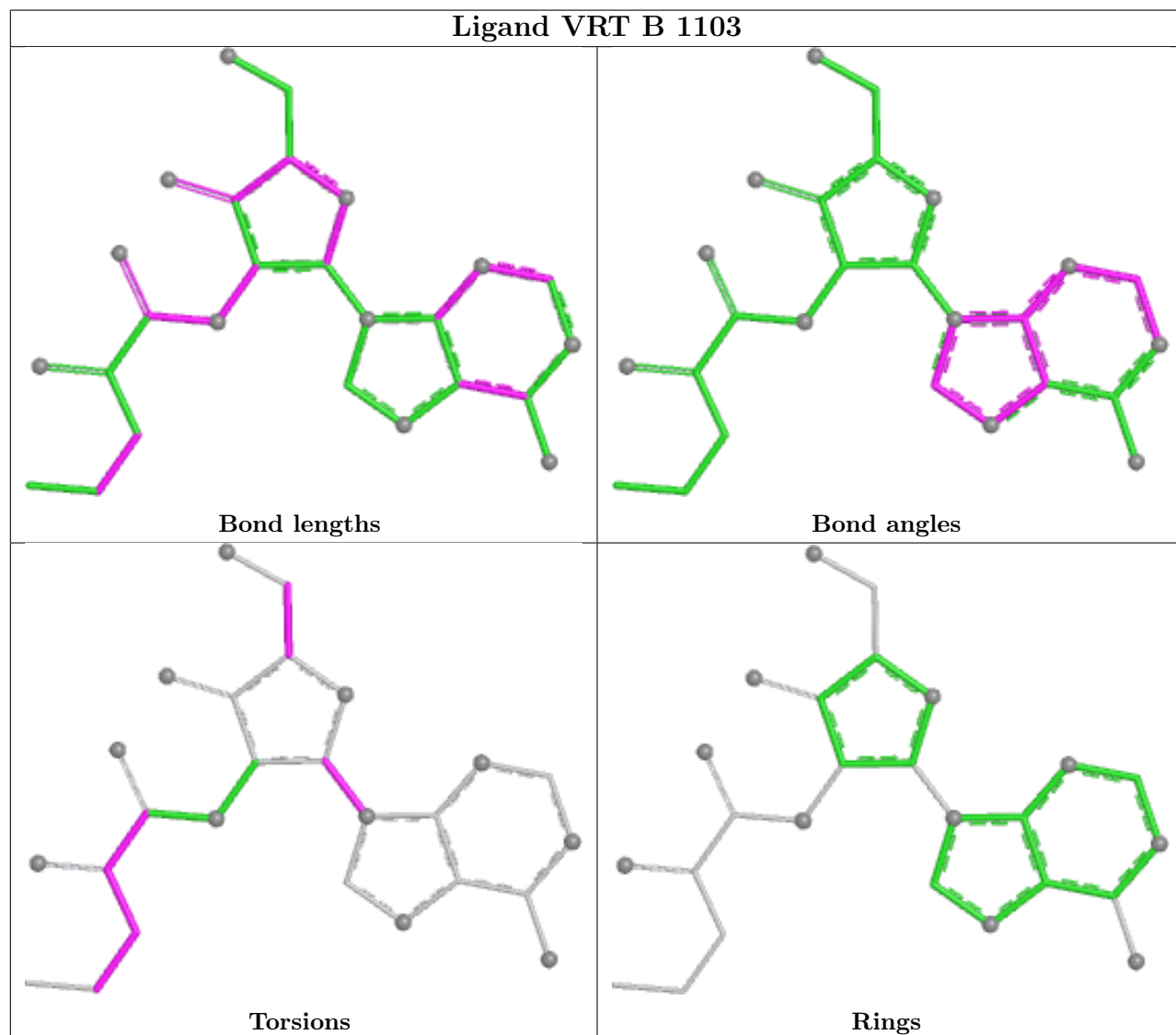
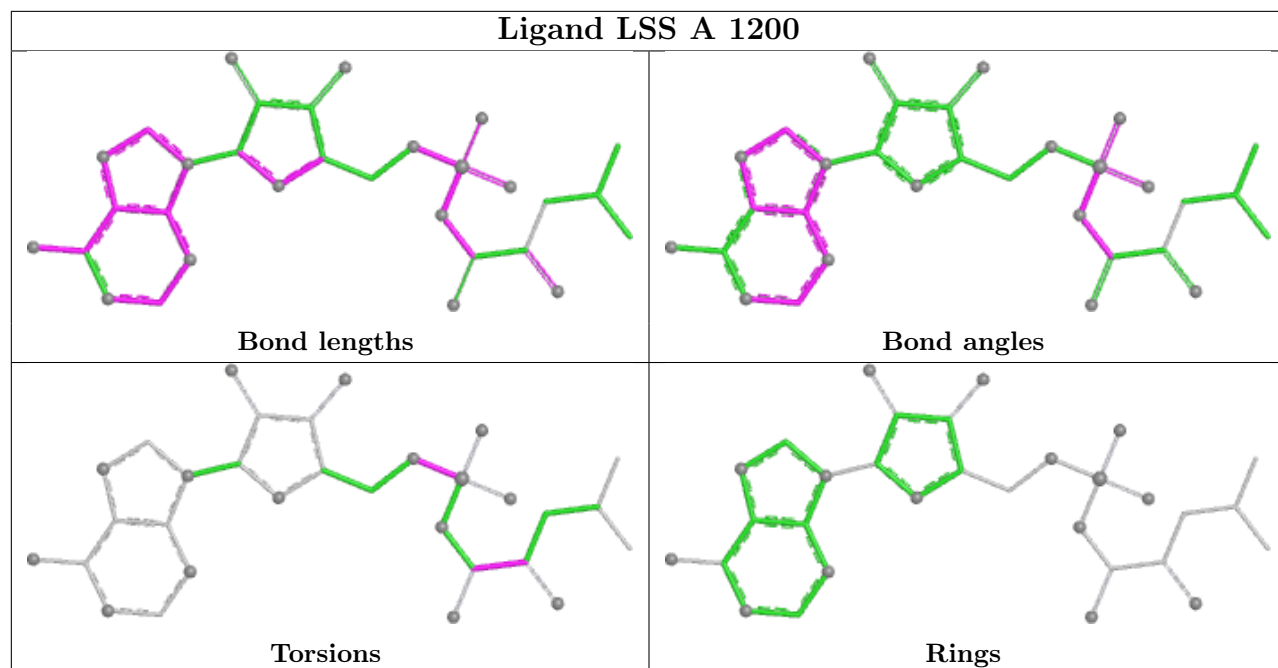
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1102	GOL	1	0
4	B	1103	VRT	3	0

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	1002/1092 (91%)	0.96	108 (10%) 11 9	38, 65, 88, 107	0
1	B	1006/1092 (92%)	-0.08	18 (1%) 67 64	8, 30, 70, 100	0
All	All	2008/2184 (91%)	0.44	126 (6%) 26 23	8, 51, 85, 107	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ILE	5.3
1	A	567	TRP	4.2
1	A	156	TYR	4.1
1	A	110	LEU	3.9
1	A	172	VAL	3.6
1	A	41	THR	3.6
1	A	412	LEU	3.5
1	A	849	PHE	3.5
1	A	468	TYR	3.4
1	A	472	PHE	3.4
1	B	41	THR	3.2
1	A	469	LEU	3.1
1	A	291	ALA	3.1
1	B	918	MET	3.0
1	A	117	PHE	3.0
1	A	97	ILE	3.0
1	A	118	PRO	3.0
1	A	916	TYR	3.0
1	A	98	LYS	3.0
1	A	572	ALA	2.9
1	A	43	LYS	2.9
1	B	118	PRO	2.9
1	A	42	SER	2.8
1	A	114	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	645	PHE	2.8
1	B	781	TRP	2.8
1	A	538	ASN	2.8
1	A	933	PRO	2.8
1	A	536	GLU	2.8
1	A	411	ALA	2.8
1	A	101	ALA	2.7
1	A	249	MET	2.7
1	A	314	ILE	2.7
1	B	768	TYR	2.7
1	A	264	TYR	2.7
1	A	651	ALA	2.7
1	B	12	PHE	2.7
1	B	106	ARG	2.6
1	A	961	ALA	2.6
1	A	446	CYS	2.6
1	B	113	CYS	2.6
1	A	259	VAL	2.6
1	A	255	THR	2.6
1	A	384	LYS	2.6
1	B	1003	MET	2.6
1	A	684	TYR	2.6
1	B	933	PRO	2.6
1	A	409	LYS	2.6
1	A	315	GLY	2.5
1	A	257	GLU	2.5
1	A	781	TRP	2.5
1	A	12	PHE	2.5
1	B	39	LYS	2.5
1	A	99	ALA	2.5
1	A	112	GLY	2.5
1	A	583	LEU	2.5
1	A	866	LEU	2.5
1	A	168	ASP	2.4
1	A	626	ARG	2.4
1	A	493	THR	2.4
1	A	476	ILE	2.4
1	A	237	TYR	2.4
1	A	266	LEU	2.4
1	A	232	LYS	2.4
1	A	512	LYS	2.4
1	A	256	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	445	ILE	2.4
1	A	528	ASP	2.4
1	A	164	LEU	2.4
1	A	840	VAL	2.4
1	A	789	ALA	2.4
1	B	110	LEU	2.4
1	B	156	TYR	2.4
1	A	177	ALA	2.4
1	A	589	TRP	2.4
1	A	628	GLN	2.3
1	A	437	PHE	2.3
1	A	523	VAL	2.3
1	A	158	TRP	2.3
1	A	484	GLY	2.3
1	A	7	THR	2.3
1	A	935	HIS	2.3
1	A	261	PRO	2.3
1	A	39	LYS	2.2
1	A	449	LEU	2.2
1	A	908	ASP	2.2
1	A	1043	GLU	2.2
1	A	460	LEU	2.2
1	A	1041	ALA	2.2
1	A	305	CYS	2.2
1	A	206	ILE	2.2
1	A	307	VAL	2.2
1	A	915	ASN	2.2
1	A	590	LEU	2.2
1	B	117	PHE	2.2
1	A	543	THR	2.1
1	B	968	ASP	2.1
1	A	466	LYS	2.1
1	A	251	HIS	2.1
1	A	552	THR	2.1
1	A	108	ILE	2.1
1	A	450	LYS	2.1
1	A	788	PRO	2.1
1	A	976	LEU	2.1
1	A	648	THR	2.1
1	B	112	GLY	2.1
1	A	243	LYS	2.1
1	A	113	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	336	TYR	2.1
1	A	405	ASP	2.1
1	A	248	CYS	2.1
1	A	627	PRO	2.1
1	A	1060	VAL	2.0
1	A	106	ARG	2.0
1	A	258	GLY	2.0
1	A	381	LYS	2.0
1	A	685	TYR	2.0
1	A	1042	SER	2.0
1	A	971	VAL	2.0
1	A	1061	PHE	2.0
1	A	913	LEU	2.0
1	A	541	LYS	2.0
1	A	306	TRP	2.0
1	A	577	TYR	2.0
1	B	790	SER	2.0
1	B	939	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](#)

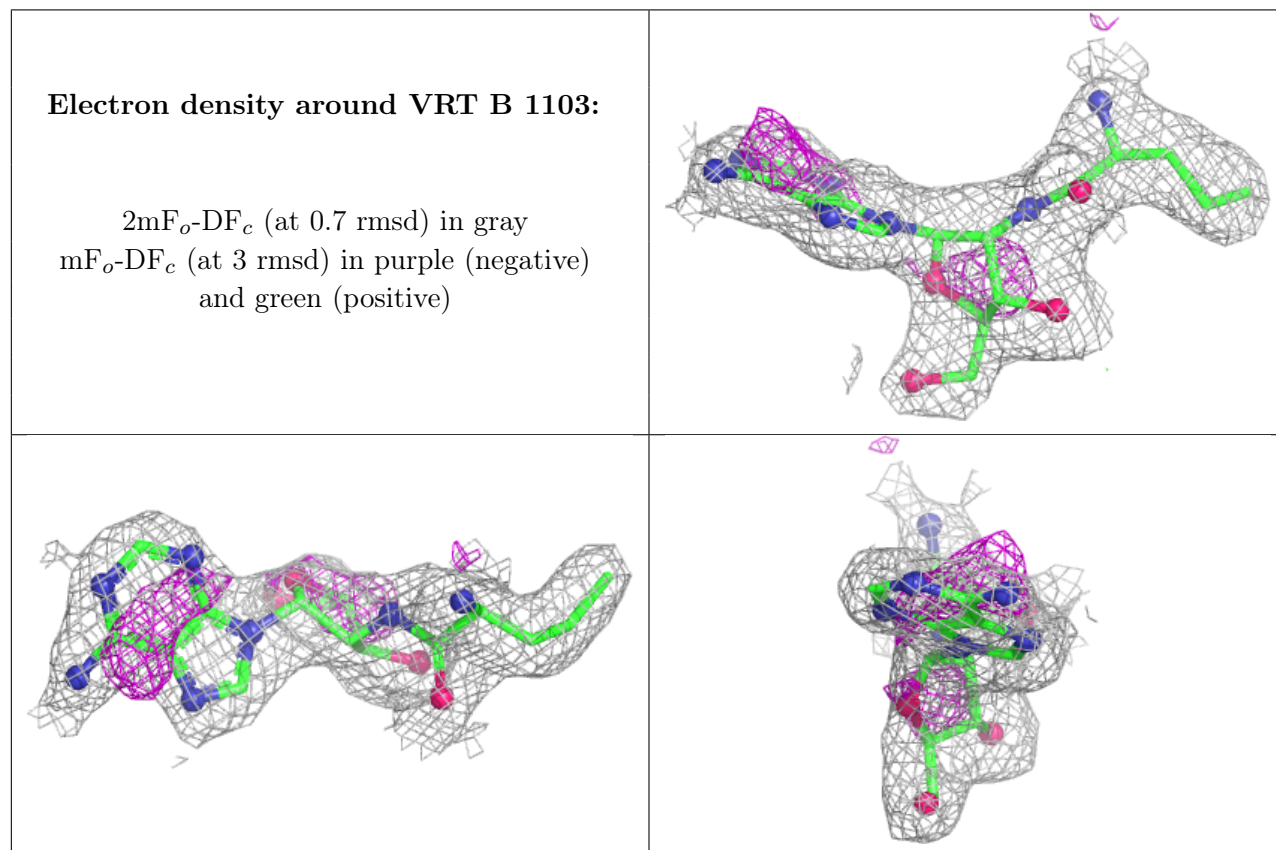
There are no oligosaccharides in this entry.

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, 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.

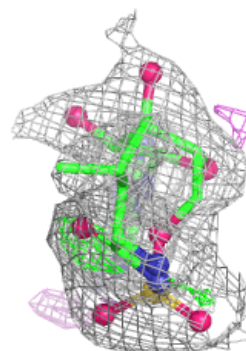
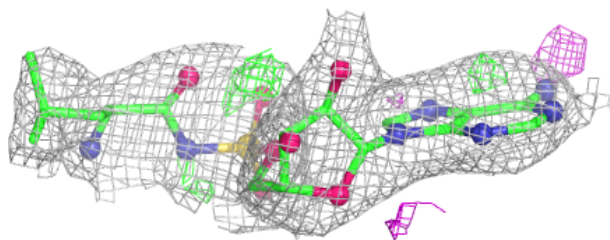
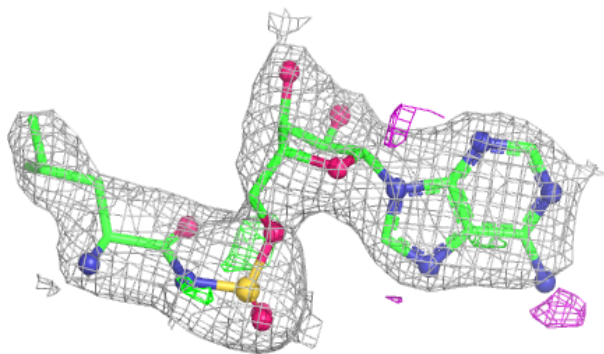
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1102	6/6	0.82	0.23	33,37,39,41	0
4	VRT	B	1103	26/26	0.89	0.10	27,40,47,48	0
2	LSS	A	1200	31/31	0.93	0.12	40,44,51,52	0
2	LSS	B	1101	31/31	0.98	0.07	7,11,16,24	0

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.

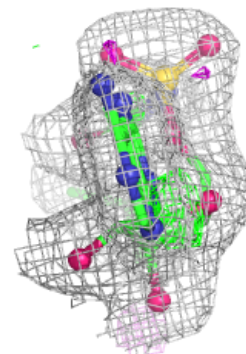
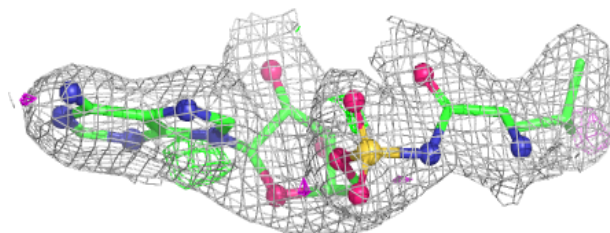
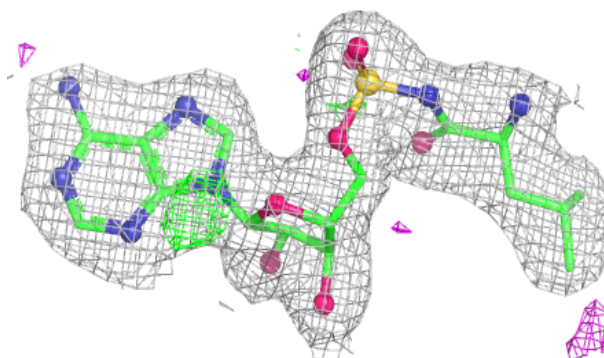


Electron density around LSS A 1200:

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

**Electron density around LSS B 1101:**

$2mF_o-DF_c$ (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.