Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 04:50 PM JST

PDB ID	:	6LPF
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

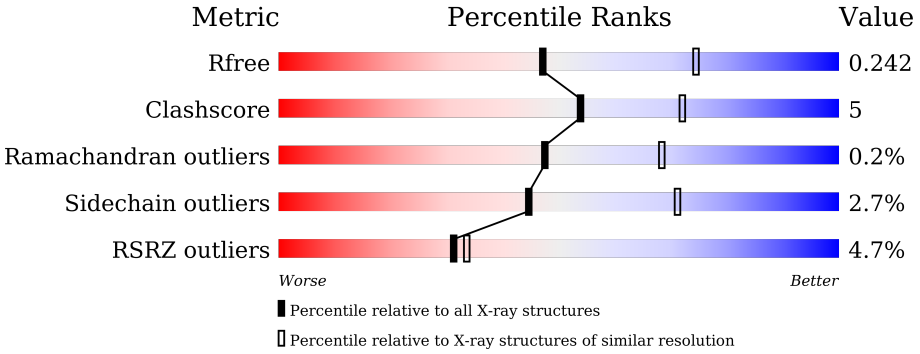
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	7% 76% 14% • 8%
1	B	1092	2% 80% 12% • 8%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1002	8088	5204	1343	1488	53	0	0	0
1	B	1006	8124	5226	1351	1492	55	0	0	0

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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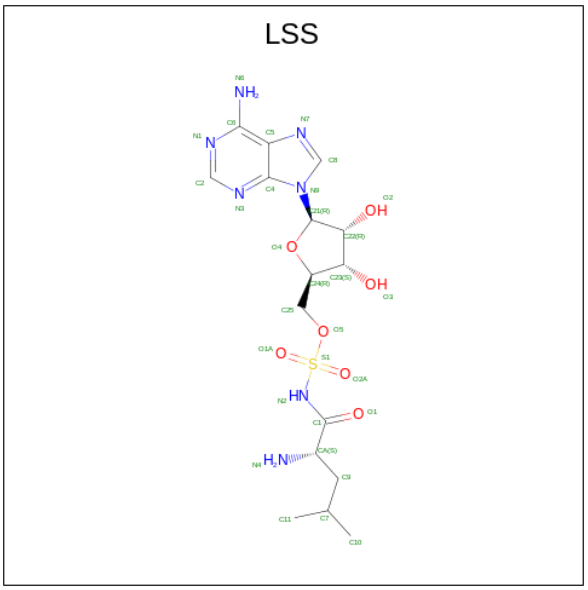
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q9P2J5
B	-17	HIS	-	expression tag	UNP Q9P2J5
B	-16	HIS	-	expression tag	UNP Q9P2J5
B	-15	HIS	-	expression tag	UNP Q9P2J5
B	-14	HIS	-	expression tag	UNP Q9P2J5
B	-13	HIS	-	expression tag	UNP Q9P2J5
B	-12	HIS	-	expression tag	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 (three-letter code: LSS) (formula: $C_{16}H_{25}N_7O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	31	16	7	7	1	0	0

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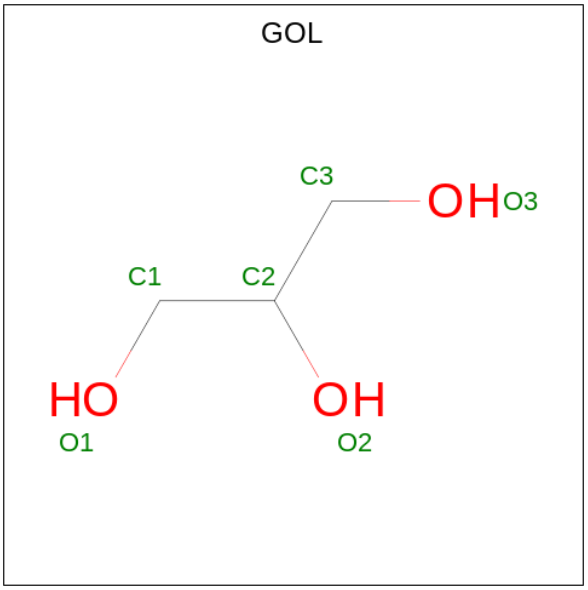
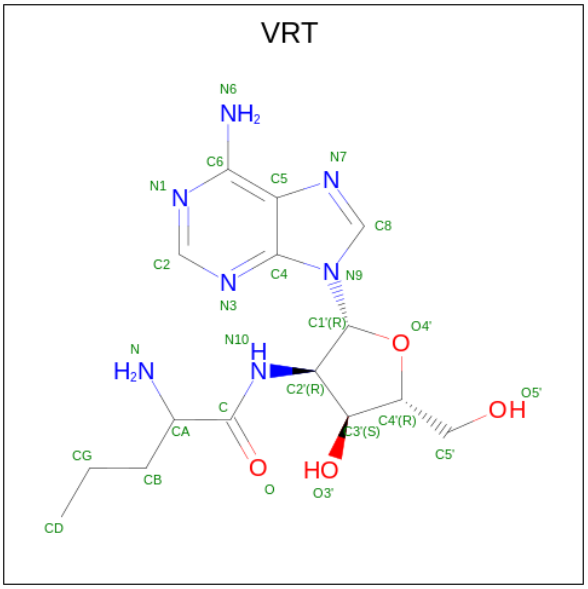
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	31	16	7	7	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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



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

- Molecule 5 is water.

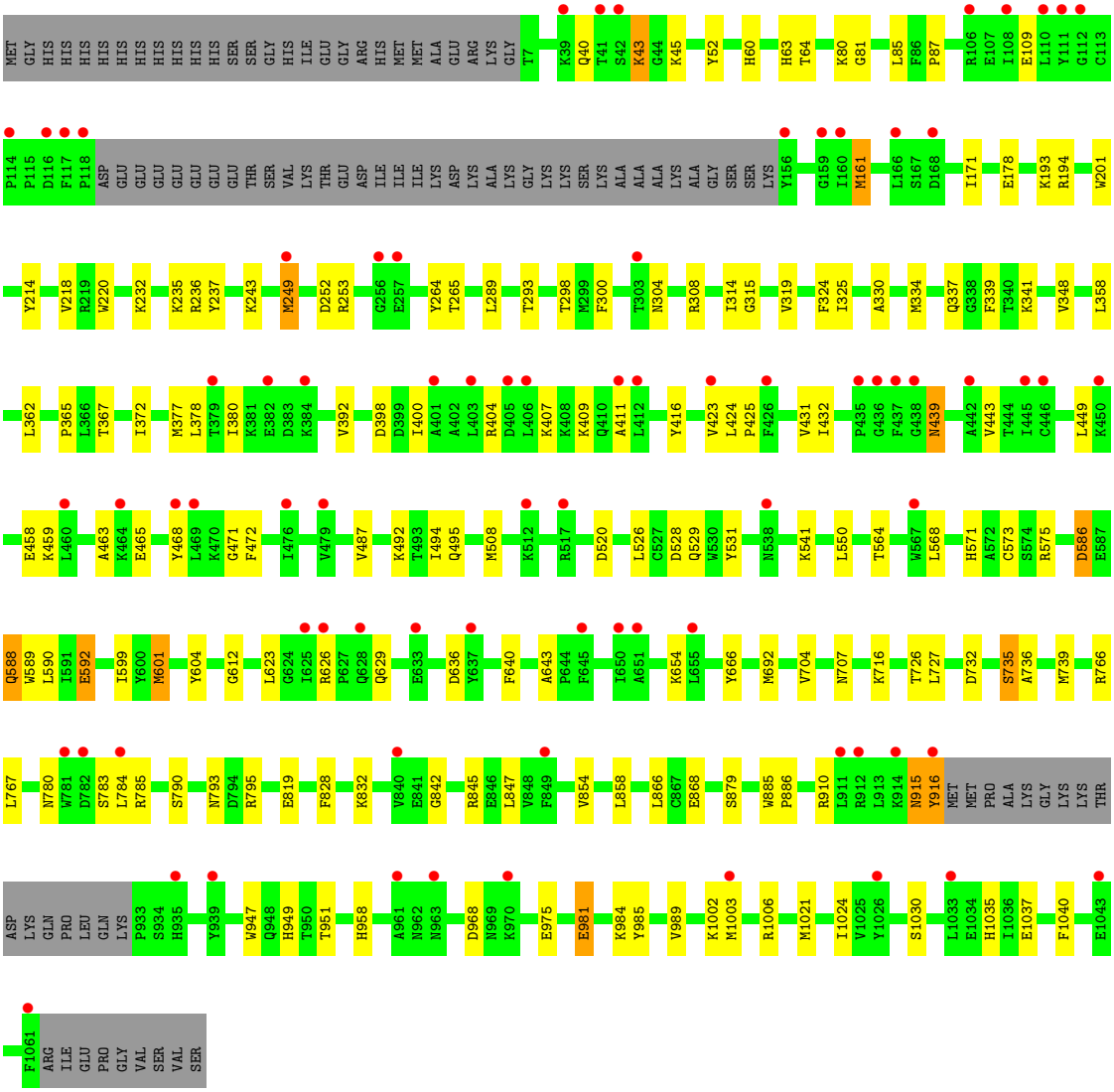
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	89	89	89	0	0
5	B	593	Total	O	0	0
			593	593		

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

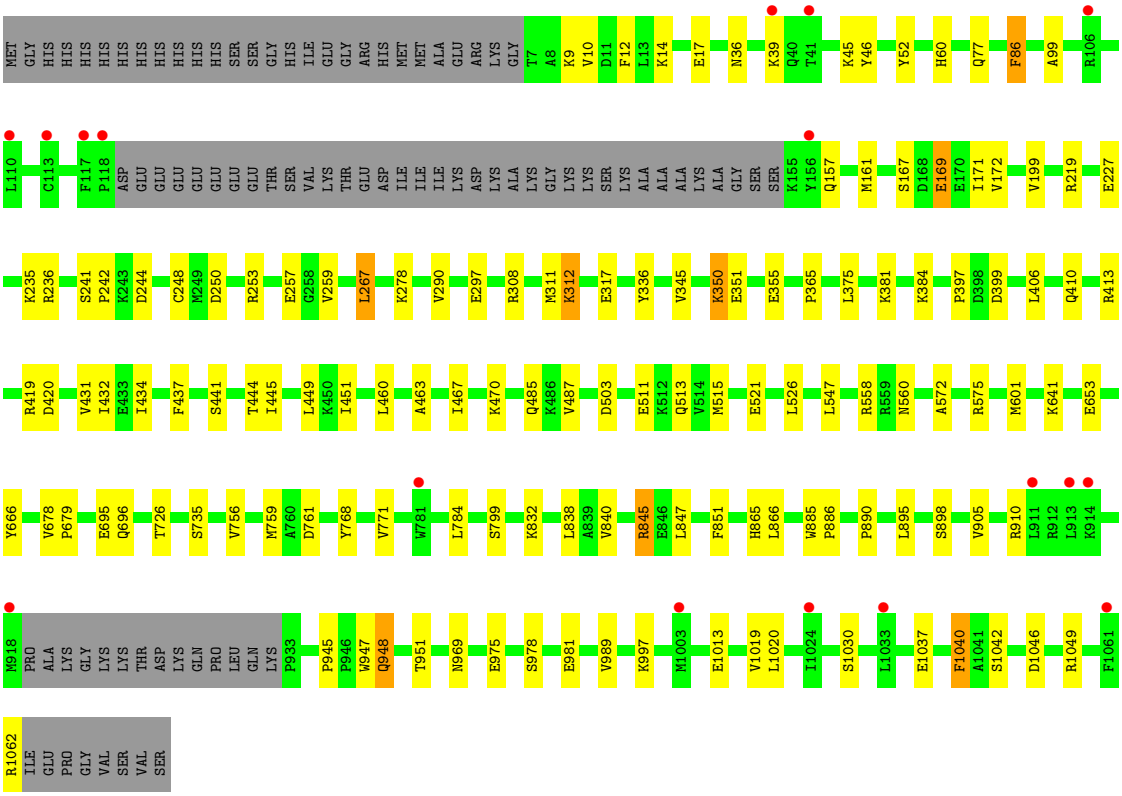
Chain A: 7% 76% 14% • 8%



- Molecule 1: Leucine–tRNA ligase, cytoplasmic

Chain B:

2%
80%
12%
8%


MET GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY ARG HIS MET MET ALA GLU ARG LYS GLY T7 A8 K9 V10 D11 F12 L13 K14 E17 N36 K39 Q40 T41 K45 Y46 Y52 H60 Q77 F86 A99 R106
L110 C113 F117 P118 ASP GLU GLU GLU GLU GLU GLU GLU THR SER VAL LYS THR GLU ASP ILE ILE ILE LYS ASP LYS ALA LYS GLY LYS LYS SER LYS ALA ALA ALA LYS ALA GLY SER SER K155 Y156 Q157 M161 S167 D168 E169 E170 I171 V172 V199 R219 E227
K235 R236 S241 P242 K243 D244 C248 M249 D250 R253 E257 G258 V259 L267 K278 V290 E297 R308 M311 K312 E317 Y336 V345 K350 E351 E355 P365 L375 K381 K384 P397 D398 D399 L406 Q410 R413
R419 D420 V431 I432 E433 I434 F437 S441 T444 I445 L449 K450 I451 L460 A463 I467 K470 Q485 K486 V487 D503 E511 K512 Q513 V514 M515 E521 L526 L547 R558 R559 N560 A572 R575 M601 K641 E653
Y666 V678 P679 E695 Q696 T726 S735 V756 M759 A760 D761 Y768 V771 W781 L784 S799 K832 L838 A839 V840 R845 E846 L847 F851 H865 L866 W885 P886 P890 L895 S898 V905 R910 L911 R912 L913 K914
M918 PRO ALA LYS GLY LYS LYS THR ASP LYS GLN PRO LEU GLN LYS P933 P945 P946 W947 Q948 T951 N969 E975 S978 E981 V989 K997 M1003 E1013 V1019 L1020 I1024 S1030 L1033 E1037 F1040 A1041 S1042 D1046 R1049 F1061
R1062 ILE GLU PRO GLY VAL SER VAL SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.92 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.199 , 0.242 0.199 , 0.242	Depositor DCC
R_{free} test set	4888 reflections (5.00%)	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 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, VRT, LSS

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	0.26	0/8288	0.42	0/11203
1	B	0.30	0/8324	0.47	0/11248
All	All	0.28	0/16612	0.45	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 (i)

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	99	0
1	B	8124	0	8090	72	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	2	0
5	A	89	0	0	12	0
5	B	593	0	0	12	0
All	All	16988	0	16194	171	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 (171) 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: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: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:314:ILE:HG23	1:A:348:VAL:HG13	1.84	0.60
1:A:377:MET:HE3	1:A:398:ASP:HB3	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:B:308:ARG:HH11	1:B:311:MET:HE2	1.67	0.57
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:736:ALA:C	5:A:1301:HOH:O	2.43	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:A:64:THR:HG21	1:A:727:LEU:HD13	1.87	0.55
1:B:969:ASN:OD1	1:B:997:LYS:NZ	2.30	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
1:A:293:THR:N	5:A:1302:HOH:O	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:868:GLU:OE2	1:A:879:SER:OG	2.24	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:588:GLN:H	1:A:588:GLN:CD	2.25	0.40
1:A:854:VAL:O	1:A:858:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	996/1092 (91%)	941 (94%)	52 (5%)	3 (0%)	41	61
1	B	1000/1092 (92%)	963 (96%)	36 (4%)	1 (0%)	51	73
All	All	1996/2184 (91%)	1904 (95%)	88 (4%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	735	SER
1	B	735	SER
1	A	249	MET
1	A	612	GLY

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	883/958 (92%)	858 (97%)	25 (3%)	43	70
1	B	887/958 (93%)	864 (97%)	23 (3%)	46	72
All	All	1770/1916 (92%)	1722 (97%)	48 (3%)	44	71

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	45	LYS
1	A	52	TYR
1	A	109	GLU
1	A	161	MET
1	A	178	GLU
1	A	439	ASN
1	A	472	PHE
1	A	529	GLN
1	A	586	ASP
1	A	588	GLN
1	A	592	GLU
1	A	601	MET
1	A	666	TYR
1	A	707	ASN
1	A	766	ARG
1	A	793	ASN
1	A	819	GLU
1	A	828	PHE
1	A	915	ASN
1	A	916	TYR
1	A	968	ASP
1	A	981	GLU
1	A	1006	ARG
1	A	1040	PHE
1	B	36	ASN
1	B	45	LYS
1	B	52	TYR
1	B	86	PHE
1	B	169	GLU
1	B	227	GLU
1	B	267	LEU
1	B	312	LYS

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Mol	Chain	Res	Type
1	B	350	LYS
1	B	355	GLU
1	B	410	GLN
1	B	560	ASN
1	B	601	MET
1	B	641	LYS
1	B	653	GLU
1	B	666	TYR
1	B	799	SER
1	B	845	ARG
1	B	948	GLN
1	B	981	GLU
1	B	1037	GLU
1	B	1040	PHE
1	B	1062	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	A	452	GLN
1	A	495	GLN
1	A	529	GLN
1	A	588	GLN
1	A	900	GLN
1	A	915	ASN
1	B	254	GLN
1	B	328	GLN
1	B	696	GLN

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 monosaccharides 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	A	1200	-	30,33,33	5.50	16 (53%)	33,49,49	1.77	5 (15%)
4	VRT	B	1103	-	25,28,28	4.05	10 (40%)	23,40,40	1.29	2 (8%)
2	LSS	B	1101	-	30,33,33	5.00	15 (50%)	33,49,49	1.90	4 (12%)
3	GOL	B	1102	-	5,5,5	1.24	0	5,5,5	0.79	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
2	LSS	A	1200	-	-	4/18/39/39	0/3/3/3
4	VRT	B	1103	-	-	9/13/33/33	0/3/3/3
2	LSS	B	1101	-	-	4/18/39/39	0/3/3/3
3	GOL	B	1102	-	-	2/4/4/4	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	LSS	O1A-S1	16.07	1.56	1.42
2	B	1101	LSS	O1A-S1	14.26	1.54	1.42
2	A	1200	LSS	C1-N2	11.24	1.58	1.37
2	A	1200	LSS	S1-N2	10.34	1.78	1.59
2	B	1101	LSS	C1-N2	10.22	1.56	1.37
4	B	1103	VRT	C3'-C4'	-9.75	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	LSS	C2-N3	9.51	1.47	1.32
2	B	1101	LSS	C2-N3	9.35	1.47	1.32
2	B	1101	LSS	S1-N2	9.08	1.76	1.59
4	B	1103	VRT	O4'-C4'	8.97	1.65	1.45
4	B	1103	VRT	O4'-C1'	-8.79	1.28	1.41
2	A	1200	LSS	O4-C24	8.46	1.63	1.45
2	A	1200	LSS	O4-C21	8.32	1.52	1.41
2	B	1101	LSS	O4-C24	7.82	1.62	1.45
2	A	1200	LSS	C8-N7	7.54	1.48	1.34
2	B	1101	LSS	C8-N7	7.51	1.48	1.34
2	B	1101	LSS	O4-C21	7.24	1.51	1.41
4	B	1103	VRT	C2-N3	6.00	1.41	1.32
4	B	1103	VRT	C-N10	5.69	1.46	1.34
2	A	1200	LSS	O5-S1	5.53	1.71	1.59
4	B	1103	VRT	O-C	5.14	1.33	1.23
2	A	1200	LSS	O2A-S1	5.10	1.46	1.42
2	B	1101	LSS	O5-S1	4.79	1.69	1.59
4	B	1103	VRT	O3'-C3'	4.41	1.53	1.43
4	B	1103	VRT	C2'-N10	-4.12	1.39	1.45
2	B	1101	LSS	O2A-S1	3.84	1.45	1.42
2	A	1200	LSS	C6-C5	3.43	1.56	1.43
2	B	1101	LSS	C6-C5	3.33	1.55	1.43
2	A	1200	LSS	C6-N6	3.27	1.46	1.34
2	B	1101	LSS	C5-N7	3.22	1.51	1.39
2	B	1101	LSS	C6-N6	3.19	1.45	1.34
2	A	1200	LSS	C5-N7	3.18	1.51	1.39
2	A	1200	LSS	C5-C4	2.95	1.48	1.40
2	A	1200	LSS	C4-N3	2.94	1.39	1.35
2	B	1101	LSS	C5-C4	2.83	1.48	1.40
2	B	1101	LSS	C4-N3	2.56	1.39	1.35
2	A	1200	LSS	C2-N1	2.30	1.38	1.33
2	A	1200	LSS	CA-N4	-2.09	1.38	1.48
2	B	1101	LSS	CA-N4	-2.09	1.38	1.48
4	B	1103	VRT	CG-CB	2.08	1.63	1.51
4	B	1103	VRT	C4-N3	2.06	1.38	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	LSS	O2A-S1-O1A	-6.06	111.32	120.76
2	A	1200	LSS	O2A-S1-O1A	-6.05	111.33	120.76
2	B	1101	LSS	C1-N2-S1	-5.78	115.26	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1200	LSS	C1-N2-S1	-4.85	116.75	124.61
4	B	1103	VRT	N3-C2-N1	-4.61	121.48	128.68
2	A	1200	LSS	N3-C2-N1	-3.88	122.61	128.68
2	B	1101	LSS	N3-C2-N1	-3.68	122.92	128.68
4	B	1103	VRT	C4-C5-N7	-2.37	106.93	109.40
2	A	1200	LSS	C23-C22-C21	2.37	104.55	100.98
2	A	1200	LSS	C4-C5-N7	-2.35	106.95	109.40
2	B	1101	LSS	O1-C1-CA	2.29	125.03	120.18

There are no chirality outliers.

All (19) 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'
4	B	1103	VRT	CA-CB-CG-CD
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
3	B	1102	GOL	O2-C2-C3-O3
2	B	1101	LSS	C25-O5-S1-O2A
4	B	1103	VRT	N-CA-CB-CG
2	A	1200	LSS	O1-C1-CA-N4
2	A	1200	LSS	N2-C1-CA-N4
4	B	1103	VRT	N10-C-CA-CB
2	B	1101	LSS	O4-C24-C25-O5
2	A	1200	LSS	C25-O5-S1-O2A

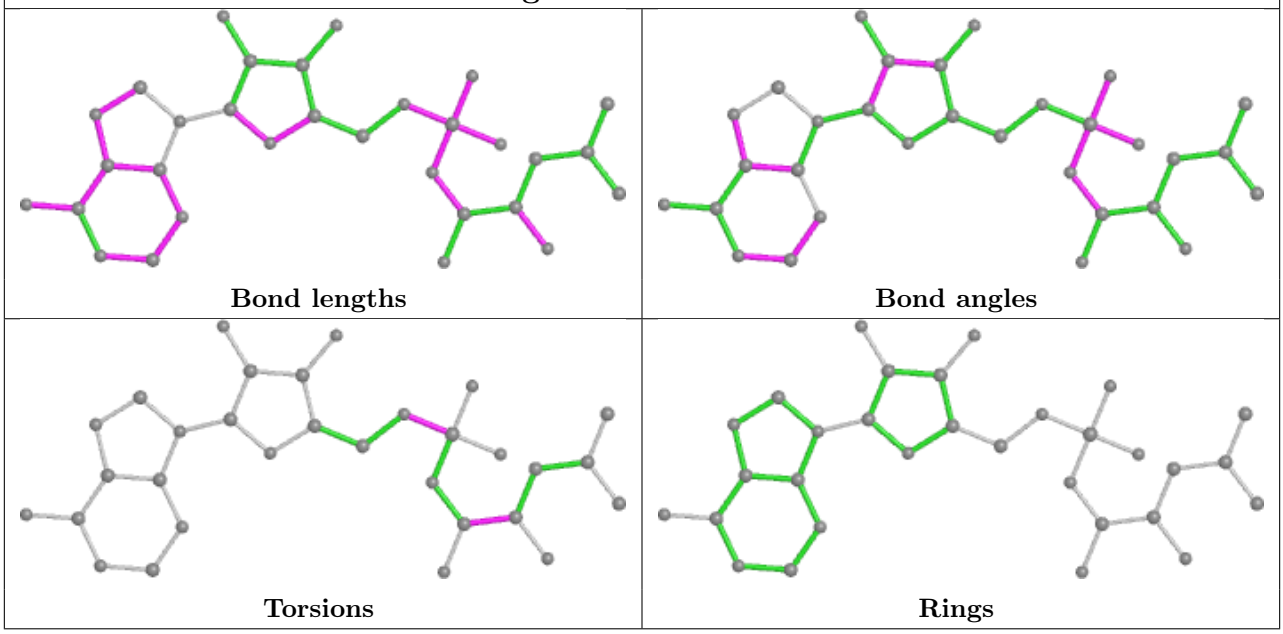
There are no ring outliers.

4 monomers are involved in 6 short contacts:

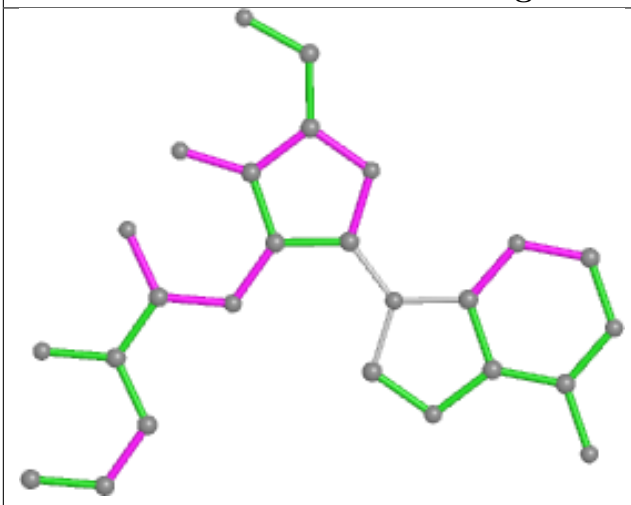
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1200	LSS	2	0
4	B	1103	VRT	2	0
2	B	1101	LSS	1	0
3	B	1102	GOL	1	0

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

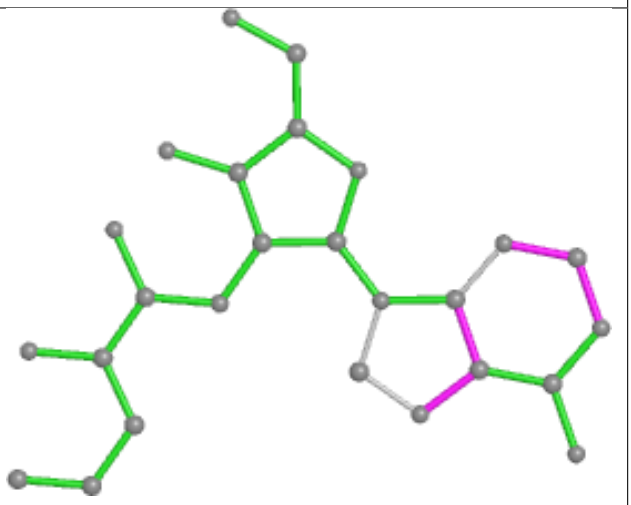
Ligand LSS A 1200



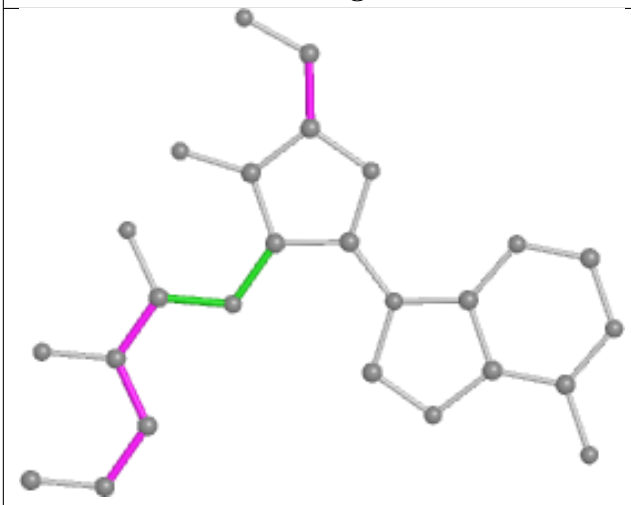
Ligand VRT B 1103



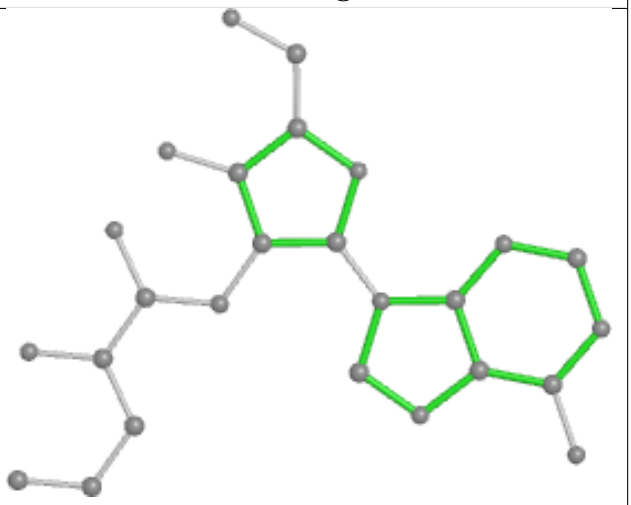
Bond lengths



Bond angles

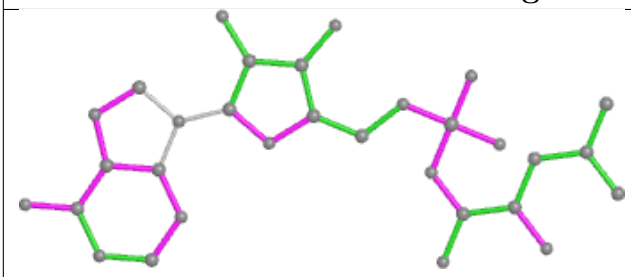


Torsions

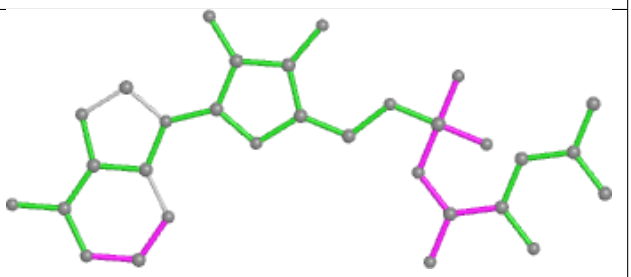


Rings

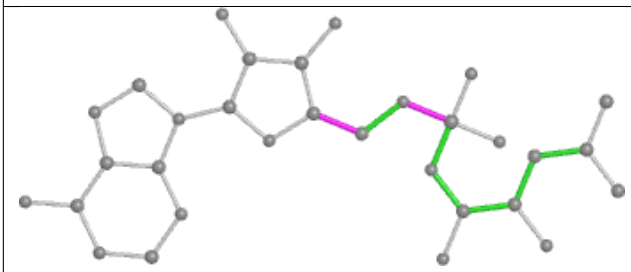
Ligand LSS B 1101



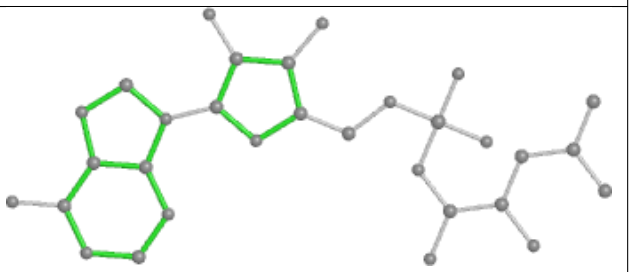
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.53	78 (7%)	13	13	38, 65, 88, 107	0
1	B	1006/1092 (92%)	0.08	17 (1%)	70	72	8, 30, 70, 100	0
All	All	2008/2184 (91%)	0.31	95 (4%)	31	33	8, 51, 85, 107	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	PHE	7.1
1	A	156	TYR	5.3
1	A	412	LEU	4.7
1	A	110	LEU	4.6
1	A	114	PRO	4.5
1	A	476	ILE	4.4
1	B	913	LEU	4.3
1	A	1061	PHE	4.1
1	A	411	ALA	4.0
1	A	468	TYR	3.9
1	A	916	TYR	3.9
1	A	256	GLY	3.8
1	A	106	ARG	3.7
1	A	567	TRP	3.7
1	B	106	ARG	3.7
1	A	479	VAL	3.7
1	A	512	LYS	3.6
1	A	784	LEU	3.6
1	B	113	CYS	3.5
1	A	446	CYS	3.4
1	B	39	LYS	3.4
1	A	436	GLY	3.2
1	A	108	ILE	3.2
1	B	1061	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	PHE	3.1
1	A	303	THR	3.1
1	A	382	GLU	3.0
1	B	1003	MET	3.0
1	A	645	PHE	3.0
1	B	1033	LEU	3.0
1	A	384	LYS	2.9
1	A	112	GLY	2.9
1	A	963	ASN	2.9
1	A	405	ASP	2.9
1	A	655	LEU	2.9
1	B	781	TRP	2.8
1	A	961	ALA	2.8
1	A	406	LEU	2.8
1	A	469	LEU	2.8
1	A	935	HIS	2.8
1	A	460	LEU	2.7
1	A	160	ILE	2.7
1	B	156	TYR	2.7
1	A	116	ASP	2.6
1	A	257	GLU	2.6
1	A	628	GLN	2.6
1	A	626	ARG	2.6
1	A	401	ALA	2.5
1	A	849	PHE	2.5
1	A	118	PRO	2.4
1	A	1033	LEU	2.4
1	A	637	TYR	2.4
1	A	781	TRP	2.4
1	A	1043	GLU	2.4
1	A	166	LEU	2.4
1	A	625	ILE	2.4
1	A	42	SER	2.4
1	A	970	LYS	2.4
1	A	650	ILE	2.4
1	B	918	MET	2.3
1	B	1024	ILE	2.3
1	B	117	PHE	2.3
1	A	1003	MET	2.3
1	A	168	ASP	2.3
1	A	450	LYS	2.3
1	A	445	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	914	LYS	2.3
1	B	110	LEU	2.3
1	B	118	PRO	2.2
1	A	633	GLU	2.2
1	A	159	GLY	2.2
1	A	438	GLY	2.2
1	A	912	ARG	2.2
1	A	111	TYR	2.2
1	A	782	ASP	2.2
1	A	840	VAL	2.2
1	A	517	ARG	2.2
1	A	426	PHE	2.2
1	B	911	LEU	2.2
1	A	911	LEU	2.1
1	A	39	LYS	2.1
1	A	435	PRO	2.1
1	A	41	THR	2.1
1	A	403	LEU	2.1
1	A	651	ALA	2.1
1	A	939	TYR	2.1
1	A	914	LYS	2.1
1	A	423	VAL	2.0
1	A	464	LYS	2.0
1	B	41	THR	2.0
1	A	538	ASN	2.0
1	A	1026	TYR	2.0
1	A	249	MET	2.0
1	A	442	ALA	2.0
1	A	379	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

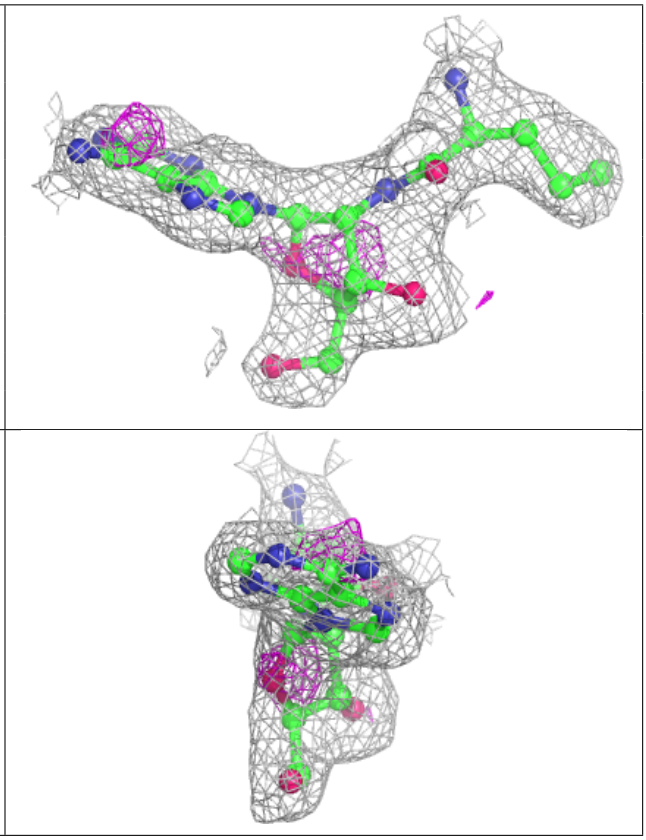
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1102	6/6	0.88	0.32	33,37,39,41	0
4	VRT	B	1103	26/26	0.91	0.22	27,40,47,48	0
2	LSS	A	1200	31/31	0.95	0.20	40,44,51,52	0
2	LSS	B	1101	31/31	0.98	0.20	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.

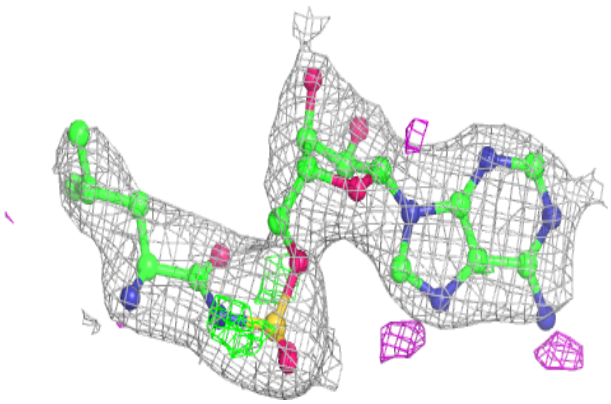
Electron density around VRT B 1103:

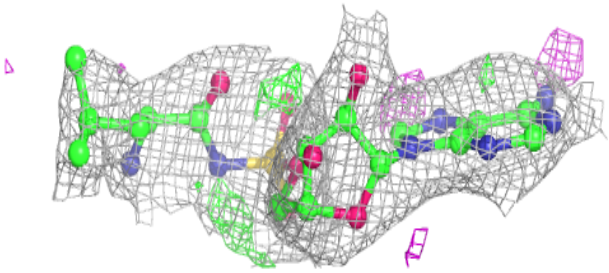
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

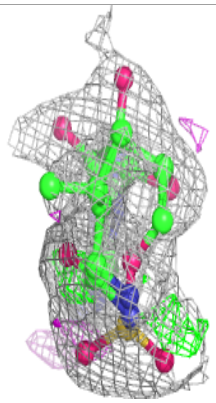


Electron density around LSS A 1200:

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

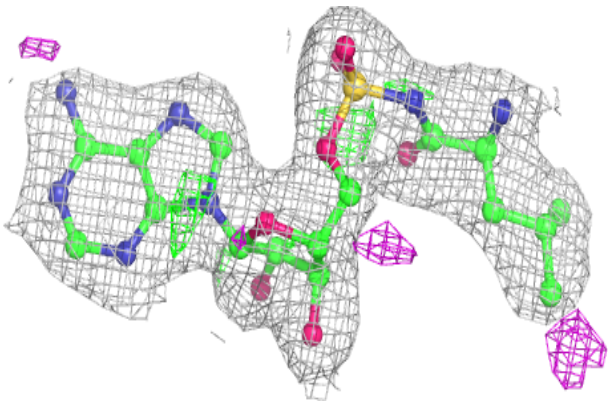


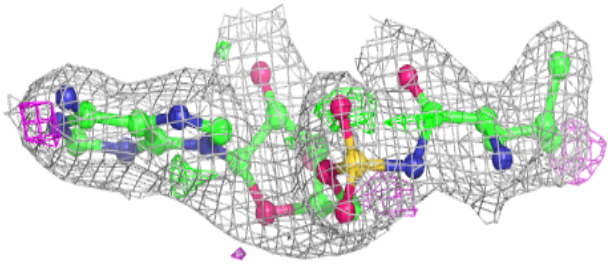


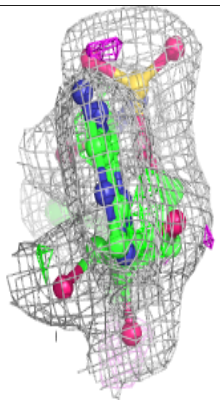


Electron density around LSS B 1101:

$2mF_o$-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.