Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 02:09 PM EST

PDB ID	:	8TLC
Title	:	Human mitochondrial serine hydroxymethyltransferase (SHMT2) in complex with PLP, glycine and tri-glutamate AGF347 inhibitor
Authors	:	Katinas, J.M.; Dann III, C.E.
Deposited on	:	2023-07-26
Resolution	:	2.72 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:

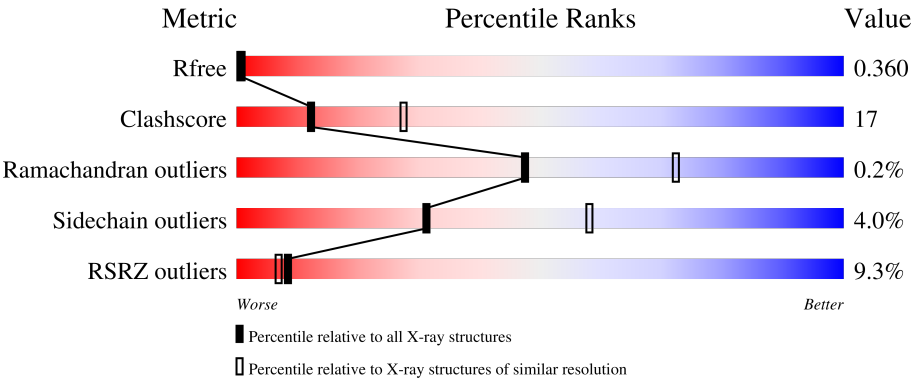
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	493	3% 65% 27% · 8%
1	B	493	14% 57% 32% · 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7003 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	P	S	0	0	0
			3540	2228	633	662	1	16			
1	B	450	Total	C	N	O	P	S	0	1	0
			3401	2142	599	644	1	15			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	UNP P34897
A	19	HIS	-	expression tag	UNP P34897
A	20	HIS	-	expression tag	UNP P34897
A	21	HIS	-	expression tag	UNP P34897
A	22	SER	-	expression tag	UNP P34897
A	23	SER	-	expression tag	UNP P34897
A	24	GLY	-	expression tag	UNP P34897
A	25	LEU	-	expression tag	UNP P34897
A	26	VAL	-	expression tag	UNP P34897
A	27	PRO	-	expression tag	UNP P34897
A	28	ARG	-	expression tag	UNP P34897
B	12	MET	-	initiating methionine	UNP P34897
B	13	GLY	-	expression tag	UNP P34897
B	14	SER	-	expression tag	UNP P34897
B	15	SER	-	expression tag	UNP P34897
B	16	HIS	-	expression tag	UNP P34897
B	17	HIS	-	expression tag	UNP P34897
B	18	HIS	-	expression tag	UNP P34897
B	19	HIS	-	expression tag	UNP P34897

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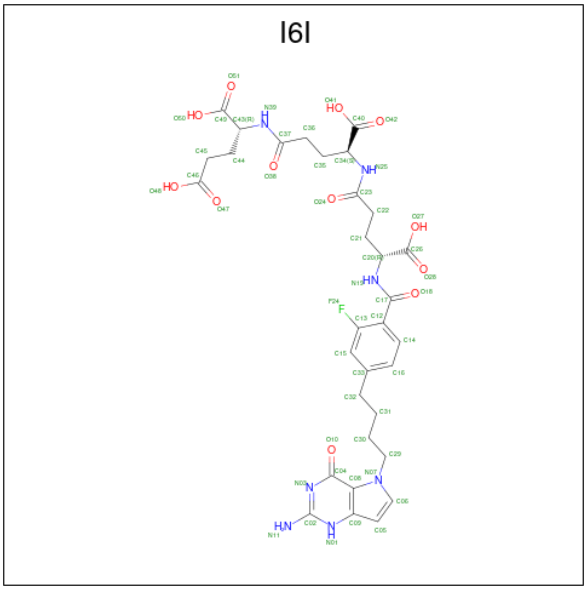
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	HIS	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	22	SER	-	expression tag	UNP P34897
B	23	SER	-	expression tag	UNP P34897
B	24	GLY	-	expression tag	UNP P34897
B	25	LEU	-	expression tag	UNP P34897
B	26	VAL	-	expression tag	UNP P34897
B	27	PRO	-	expression tag	UNP P34897
B	28	ARG	-	expression tag	UNP P34897

- Molecule 2 is N-{4-[4-(2-amino-4-oxo-1,4-dihydro-5H-pyrrolo[3,2-d]pyrimidin-5-yl)butyl]-2-fluorobenzoyl}-D-gamma-glutamyl-L-gamma-glutamyl-D-glutamic acid (three-letter code: I6I) (formula: $C_{32}H_{38}FN_7O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			52	32	1	7	12		

- Molecule 3 is water.

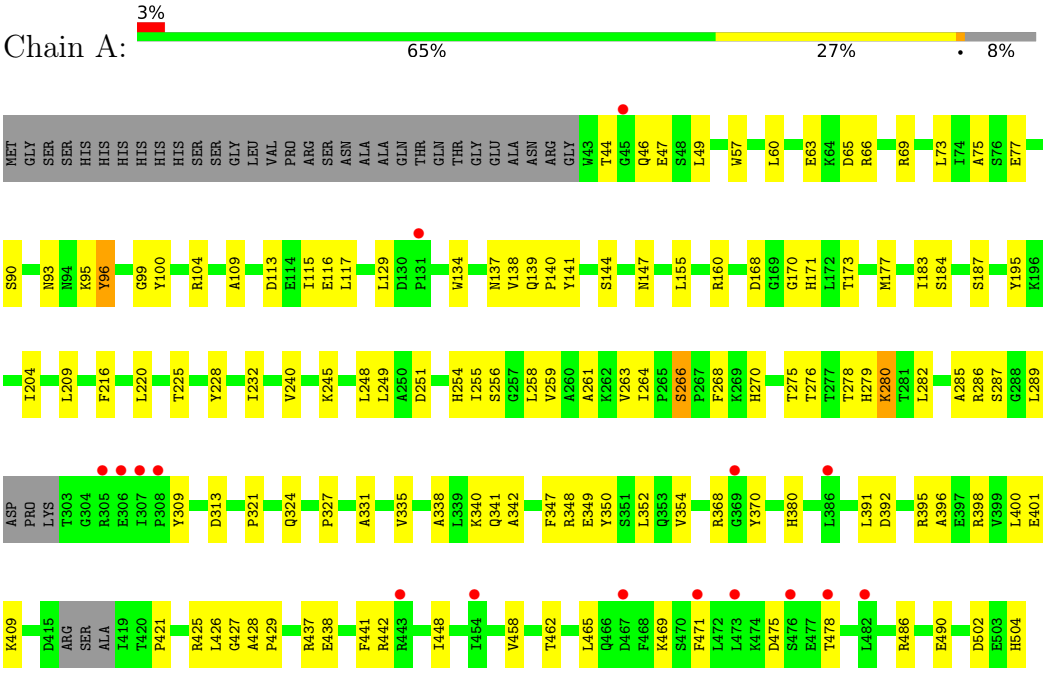
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		

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.

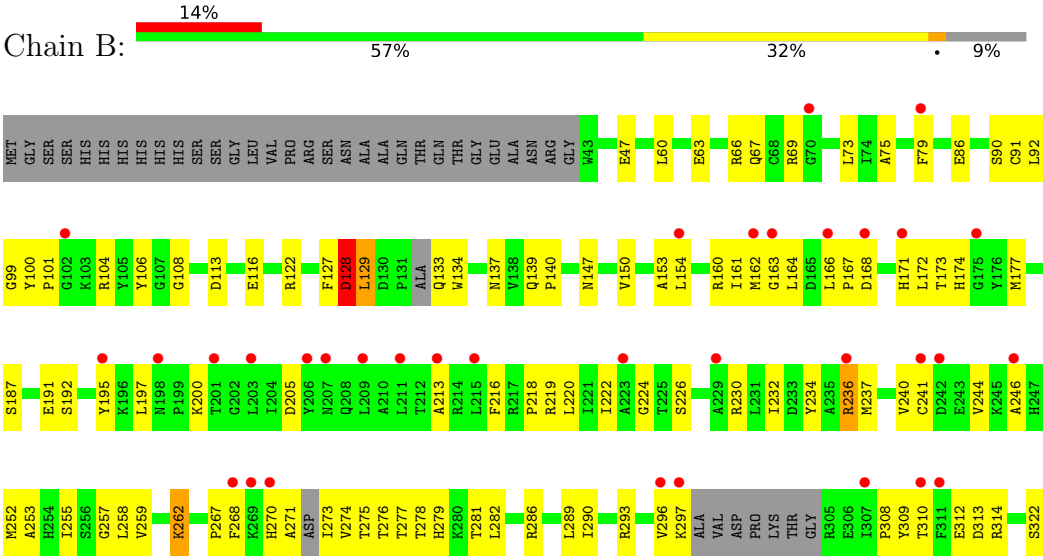
• Molecule 1: Serine hydroxymethyltransferase, mitochondrial

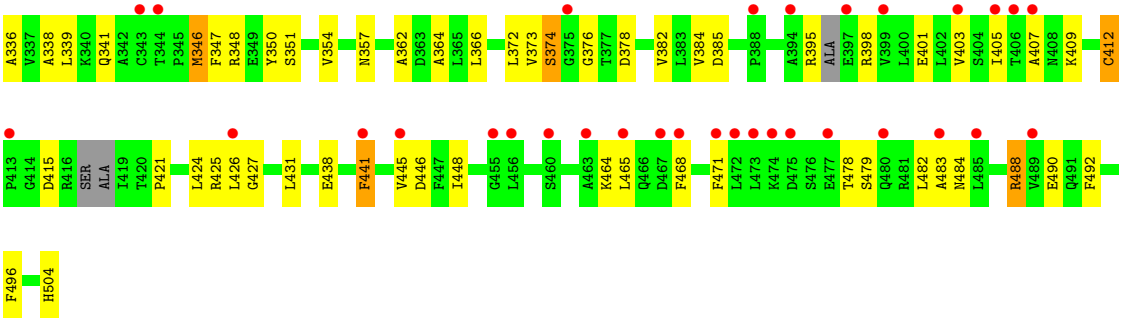
Chain A:



• Molecule 1: Serine hydroxymethyltransferase, mitochondrial

Chain B:




A336 V337 A338 L339 K340 Q341 A342 C343 T344 P345 M346 F347 R348 E349 Y350 S351 V354 N357 A362 D363 A364 L365 L366 L372 V373 S374 G375 G376 T377 D378 V382 L383 V384 D385 P388 A394 R395 ALA E397 R398 V399 L400 E401 L402 V403 S404 I405 T406 A407 N408 K409 C412
P413 G414 D415 R416 SER ALA I419 T420 P421 L424 R425 L426 G427 L431 E438 F441 V445 D446 F447 I448 G455 L456 S460 A463 K464 L465 Q466 D467 F468 F471 L472 L473 K474 D475 S476 E477 T478 S479 Q480 R481 L482 A483 N484 L485 R488 V489 E490 Q491 F492
F496 H504

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	158.72Å 158.72Å 207.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.71 – 2.72 48.71 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.71-2.72) 99.7 (48.71-2.72)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.306 , 0.359 0.306 , 0.360	Depositor DCC
R_{free} test set	2050 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	7003	wwPDB-VP
Average B, all atoms (Å^2)	63.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, I6I

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	0.27	0/3585	0.48	0/4850
1	B	0.28	0/3441	0.53	1/4665 (0.0%)
All	All	0.28	0/7026	0.51	1/9515 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	488	ARG	NE-CZ-NH1	-5.16	117.72	120.30

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	3540	0	3484	101	0
1	B	3401	0	3205	149	0
2	A	52	0	0	1	0
3	A	10	0	0	0	0
All	All	7003	0	6689	233	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 17.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD23	1:A:204:ILE:HA	1.46	0.96
1:B:163:GLY:HA2	1:B:222:ILE:HG13	1.61	0.82
1:B:171:HIS:H	1:B:174:HIS:CE1	1.98	0.81
1:A:225:THR:HG21	1:A:228:TYR:HB3	1.65	0.79
1:B:312:GLU:HG3	1:B:313:ASP:H	1.48	0.78
1:B:213:ALA:HB1	1:B:244:VAL:HG21	1.66	0.77
1:B:73:LEU:HB3	1:B:426:LEU:HD12	1.68	0.76
1:A:141:TYR:H	1:A:324:GLN:HE22	1.33	0.75
1:B:162:MET:HE3	1:B:218:PRO:HG3	1.69	0.75
1:B:331:ALA:O	1:B:335:VAL:HG13	1.86	0.74
1:A:225:THR:CG2	1:A:228:TYR:HB3	2.22	0.70
1:A:197:LEU:CD2	1:A:204:ILE:HA	2.20	0.70
1:B:222:ILE:HA	1:B:249:LEU:O	1.92	0.69
1:B:255:ILE:HG22	1:B:258:LEU:HD12	1.73	0.69
1:B:232:ILE:HB	1:B:234:TYR:HE2	1.57	0.69
1:A:96:TYR:OH	1:B:279:HIS:NE2	2.26	0.68
1:B:296:VAL:HA	1:B:308:PRO:HA	1.74	0.68
1:A:475:ASP:HB3	1:A:478:THR:HG22	1.74	0.68
1:A:198:ASN:HB3	1:A:201:THR:HB	1.75	0.67
1:B:122:ARG:HB3	1:B:339:LEU:HB3	1.75	0.66
1:A:170:GLY:O	2:A:601:I6I:N03	2.27	0.66
1:B:226:SER:O	1:B:425:ARG:NH1	2.28	0.66
1:B:232:ILE:HB	1:B:234:TYR:CE2	2.29	0.66
1:A:66:ARG:HA	1:A:69:ARG:HB3	1.78	0.66
1:B:197:LEU:HA	1:B:205:ASP:H	1.60	0.66
1:B:250:ALA:H	1:B:274:VAL:HG22	1.62	0.65
1:A:66:ARG:HH22	1:B:95:LYS:HD3	1.62	0.65
1:B:484:ASN:O	1:B:488:ARG:NH1	2.30	0.65
1:B:407:ALA:HB1	1:B:424:LEU:HD13	1.78	0.64
1:B:465:LEU:HA	1:B:468:PHE:HB3	1.79	0.64
1:B:177:MET:HG2	1:B:187:SER:HB2	1.79	0.64
1:A:44:THR:HG23	1:A:46:GLN:H	1.61	0.63
1:B:484:ASN:CG	1:B:488:ARG:HH12	2.03	0.62
1:A:398:ARG:NH1	1:A:401:GLU:OE2	2.31	0.62
1:A:49:LEU:HD12	1:A:57:TRP:HE3	1.65	0.61
1:B:278:THR:HG21	1:B:335:VAL:CG1	2.30	0.61
1:A:141:TYR:H	1:A:324:GLN:NE2	1.98	0.61
1:A:141:TYR:N	1:A:324:GLN:HE22	1.99	0.61
1:B:372:LEU:HD13	1:B:373:VAL:O	2.00	0.61
1:A:65:ASP:O	1:A:69:ARG:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:HIS:CD2	1:B:222:ILE:HD13	2.35	0.60
1:A:321:PRO:HB2	1:B:172:LEU:HD13	1.84	0.59
1:B:336:ALA:HA	1:B:339:LEU:HB2	1.82	0.59
1:A:66:ARG:NH1	1:B:108:GLY:O	2.36	0.59
1:B:113:ASP:O	1:B:116:GLU:HB3	2.02	0.59
1:B:409:LYS:HB3	1:B:421:PRO:HG2	1.83	0.59
1:A:259:VAL:HG13	1:A:266:SER:HB2	1.85	0.58
1:B:445:VAL:HA	1:B:448:ILE:HD12	1.85	0.58
1:B:382:VAL:HG12	1:B:426:LEU:HB2	1.84	0.58
1:A:183:ILE:HG13	1:A:184:SER:N	2.19	0.57
1:A:380:HIS:HB2	1:A:429:PRO:HD3	1.85	0.57
1:B:128:ASP:O	1:B:129:LEU:HB2	2.05	0.56
1:B:160:ARG:NH1	1:B:216:PHE:O	2.38	0.56
1:B:150:VAL:HG11	1:B:249:LEU:HD22	1.88	0.56
1:B:278:THR:HG21	1:B:335:VAL:HG12	1.87	0.56
1:B:253:ALA:HA	1:B:277:THR:HG22	1.87	0.56
1:A:350:TYR:O	1:A:354:VAL:HG23	2.06	0.56
1:A:184:SER:HA	1:B:322:SER:HA	1.87	0.56
1:B:163:GLY:O	1:B:195:TYR:N	2.36	0.56
1:A:113:ASP:O	1:A:117:LEU:HD12	2.05	0.55
1:B:403:VAL:HG12	1:B:405:ILE:HD12	1.88	0.55
1:B:395:ARG:HH11	1:B:465:LEU:HD21	1.71	0.55
1:B:99:GLY:HA3	1:B:104:ARG:HA	1.89	0.55
1:A:90:SER:HB2	1:B:60:LEU:HD21	1.89	0.55
1:B:164:LEU:HA	1:B:195:TYR:O	2.07	0.55
1:B:166:LEU:HD13	1:B:172:LEU:HG	1.89	0.55
1:A:171:HIS:HB2	1:A:280:LLP:H2'3	1.89	0.54
1:B:60:LEU:HD22	1:B:504:HIS:HB2	1.88	0.54
1:B:372:LEU:HD23	1:B:384:VAL:HA	1.89	0.54
1:B:154:LEU:HA	1:B:314:ARG:HH12	1.72	0.54
1:A:177:MET:HG2	1:A:187:SER:HB2	1.90	0.54
1:A:95:LYS:O	1:B:286:ARG:NH2	2.41	0.54
1:B:362:ALA:O	1:B:366:LEU:N	2.39	0.54
1:B:73:LEU:HD22	1:B:426:LEU:HB3	1.88	0.54
1:A:95:LYS:HD3	1:B:66:ARG:HH22	1.74	0.53
1:A:115:ILE:HG13	1:A:116:GLU:N	2.22	0.53
1:B:364:ALA:HB3	1:B:445:VAL:HG21	1.89	0.53
1:A:100:TYR:OH	1:A:137:ASN:ND2	2.40	0.53
1:B:153:ALA:O	1:B:314:ARG:NH1	2.41	0.53
1:B:350:TYR:O	1:B:354:VAL:HG13	2.09	0.52
1:A:486:ARG:O	1:A:490:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:HB3	1:B:268:PHE:CE1	2.44	0.52
1:A:400:LEU:HD21	1:A:448:ILE:HG23	1.90	0.52
1:B:234:TYR:CE1	1:B:267:PRO:HB3	2.45	0.52
1:B:234:TYR:HB3	1:B:270:HIS:HB2	1.92	0.52
1:B:160:ARG:HA	1:B:191:GLU:O	2.10	0.52
1:B:161:ILE:HA	1:B:220:LEU:O	2.10	0.51
1:B:166:LEU:HD12	1:B:171:HIS:HA	1.92	0.51
1:B:271:ALA:O	1:B:293:ARG:NH2	2.41	0.51
1:B:161:ILE:O	1:B:192:SER:HB2	2.09	0.51
1:B:438:GLU:HA	1:B:441:PHE:HB2	1.91	0.51
1:B:73:LEU:HD23	1:B:427:GLY:O	2.10	0.51
1:B:147:ASN:ND2	1:B:173:THR:OG1	2.36	0.51
1:B:230:ARG:HH21	1:B:376:GLY:N	2.08	0.51
1:A:75:ALA:HA	1:A:427:GLY:HA3	1.92	0.51
1:A:278:THR:OG1	1:A:285:ALA:O	2.23	0.51
1:A:396:ALA:O	1:A:400:LEU:HD12	2.10	0.51
1:B:75:ALA:HA	1:B:427:GLY:HA3	1.92	0.50
1:B:249:LEU:HD12	1:B:273:ILE:O	2.10	0.50
1:A:398:ARG:HG2	1:A:469:LYS:HG2	1.93	0.50
1:B:160:ARG:HB2	1:B:218:PRO:HA	1.92	0.50
1:B:230:ARG:HG2	1:B:374:SER:OG	2.12	0.50
1:A:280:LLP:H4'1	1:B:96:TYR:OH	2.12	0.50
1:A:502:ASP:N	1:A:502:ASP:OD1	2.44	0.50
1:B:63:GLU:HG3	1:B:67:GLN:HE21	1.77	0.50
1:B:312:GLU:HG3	1:B:313:ASP:N	2.22	0.50
1:B:90:SER:OG	1:B:91:CYS:N	2.45	0.50
1:B:482:LEU:HD12	1:B:483:ALA:N	2.27	0.49
1:A:327:PRO:O	1:B:286:ARG:NH1	2.46	0.49
1:B:279:HIS:CE1	1:B:286:ARG:HA	2.48	0.49
1:B:154:LEU:HA	1:B:314:ARG:NH1	2.28	0.49
1:B:278:THR:O	1:B:282:LEU:HB3	2.13	0.49
1:A:100:TYR:H	1:A:104:ARG:HG2	1.78	0.48
1:A:147:ASN:ND2	1:A:173:THR:OG1	2.40	0.48
1:A:438:GLU:O	1:A:442:ARG:HG3	2.14	0.48
1:B:47:GLU:OE1	1:B:47:GLU:N	2.46	0.48
1:A:391:LEU:HD23	1:A:392:ASP:O	2.14	0.48
1:A:96:TYR:HA	1:B:286:ARG:NH2	2.28	0.48
1:A:331:ALA:O	1:A:335:VAL:HG13	2.14	0.48
1:B:100:TYR:HB3	1:B:101:PRO:HD2	1.96	0.47
1:B:262:LYS:HE3	1:B:348:ARG:HH11	1.80	0.47
1:B:241:CYS:SG	1:B:248:LEU:HB2	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:MET:HB2	1:B:276:THR:HB	1.96	0.47
1:B:297:LYS:HA	1:B:309:TYR:CE2	2.49	0.47
1:A:255:ILE:HB	1:A:264:ILE:HD11	1.96	0.47
1:B:171:HIS:N	1:B:174:HIS:HD1	2.13	0.47
1:A:73:LEU:HD13	1:A:426:LEU:HD12	1.97	0.46
1:A:129:LEU:HB3	1:A:134:TRP:HB2	1.96	0.46
1:A:255:ILE:HG22	1:A:258:LEU:HD12	1.98	0.46
1:A:279:HIS:ND1	1:A:286:ARG:HA	2.30	0.46
1:A:96:TYR:OH	1:B:279:HIS:CD2	2.68	0.46
1:A:256:SER:HB3	1:A:276:THR:OG1	2.16	0.46
1:B:63:GLU:OE1	1:B:67:GLN:NE2	2.49	0.46
1:B:293:ARG:HD2	1:B:309:TYR:CE2	2.50	0.46
1:B:373:VAL:HG13	1:B:385:ASP:HB2	1.96	0.46
1:B:63:GLU:O	1:B:67:GLN:HG3	2.14	0.46
1:A:49:LEU:HD12	1:A:57:TRP:CE3	2.48	0.46
1:B:275:THR:HG22	1:B:290:ILE:HG12	1.97	0.46
1:B:279:HIS:ND1	1:B:286:ARG:HA	2.30	0.46
1:A:138:VAL:HG12	1:A:289:LEU:HD22	1.97	0.46
1:A:263:VAL:HG12	1:A:264:ILE:HG23	1.97	0.46
1:B:338:ALA:HA	1:B:341:GLN:HB3	1.98	0.46
1:B:351:SER:O	1:B:354:VAL:HG22	2.16	0.45
1:B:255:ILE:O	1:B:259:VAL:HG13	2.15	0.45
1:A:403:VAL:O	1:A:404:SER:HB2	2.17	0.45
1:B:219:ARG:HD2	1:B:219:ARG:HA	1.73	0.45
1:A:63:GLU:HG2	1:B:92:LEU:HD23	1.98	0.45
1:A:254:HIS:HB3	1:A:380:HIS:NE2	2.31	0.45
1:B:63:GLU:OE1	1:B:66:ARG:NH2	2.50	0.45
1:B:382:VAL:CG1	1:B:426:LEU:HB2	2.47	0.45
1:A:209:LEU:HD13	1:A:240:VAL:HG11	1.97	0.45
1:B:69:ARG:O	1:B:490:GLU:HA	2.17	0.45
1:A:256:SER:HB2	1:A:282:LEU:HG	1.98	0.45
1:A:380:HIS:H	1:A:380:HIS:CD2	2.34	0.45
1:A:73:LEU:O	1:A:427:GLY:N	2.47	0.44
1:B:133:GLN:HG2	1:B:134:TRP:HD1	1.82	0.44
1:B:166:LEU:HB3	1:B:167:PRO:HD3	2.00	0.44
1:A:144:SER:HA	1:A:173:THR:HG21	1.99	0.44
1:A:504:HIS:NE2	1:B:86:GLU:O	2.50	0.44
1:A:99:GLY:HA3	1:A:104:ARG:HA	1.99	0.44
1:B:133:GLN:HG2	1:B:134:TRP:CD1	2.53	0.44
1:B:192:SER:HA	1:B:216:PHE:CZ	2.53	0.44
1:B:346:MET:SD	1:B:347:PHE:N	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:PHE:HE2	1:B:496:PHE:HE2	1.65	0.44
1:A:249:LEU:HD11	1:A:275:THR:HG23	2.00	0.44
1:A:342:ALA:HA	1:A:347:PHE:CG	2.53	0.44
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.53	0.43
1:A:261:ALA:HB1	1:A:348:ARG:HA	2.00	0.43
1:A:409:LYS:HB2	1:A:421:PRO:HG2	2.00	0.43
1:B:67:GLN:HB3	1:B:79:PHE:HE1	1.83	0.43
1:B:479:SER:HA	1:B:482:LEU:HG	2.00	0.43
1:A:137:ASN:OD1	1:A:140:PRO:HD3	2.18	0.43
1:A:195:TYR:CB	1:A:209:LEU:HD23	2.49	0.43
1:B:137:ASN:OD1	1:B:140:PRO:HD3	2.18	0.43
1:B:412:CYS:SG	1:B:415:ASP:CB	3.06	0.43
1:A:47:GLU:OE1	1:A:47:GLU:N	2.47	0.43
1:A:338:ALA:O	1:A:341:GLN:HG2	2.18	0.43
1:B:267:PRO:HB2	1:B:271:ALA:HB3	2.00	0.43
1:B:127:PHE:HB3	1:B:268:PHE:HE1	1.82	0.43
1:A:129:LEU:HD11	1:A:268:PHE:HB3	2.00	0.43
1:A:368:ARG:HB2	1:A:370:TYR:CD2	2.54	0.42
1:B:63:GLU:CG	1:B:67:GLN:HE21	2.31	0.42
1:B:257:GLY:HA3	1:B:347:PHE:HZ	1.84	0.42
1:A:141:TYR:O	1:A:287:SER:HA	2.19	0.42
1:A:395:ARG:HG3	1:A:465:LEU:HD12	2.00	0.42
1:A:428:ALA:N	1:A:429:PRO:HD2	2.34	0.42
1:B:310:THR:HB	1:B:314:ARG:HH21	1.84	0.42
1:A:139:GLN:N	1:A:140:PRO:CD	2.82	0.42
1:B:275:THR:HG22	1:B:290:ILE:HG23	2.00	0.42
1:A:82:ARG:NE	1:A:86:GLU:OE2	2.44	0.42
1:A:245:LYS:O	1:A:245:LYS:HG3	2.20	0.42
1:B:139:GLN:N	1:B:140:PRO:CD	2.83	0.42
1:B:129:LEU:HD13	1:B:129:LEU:HA	1.92	0.42
1:B:241:CYS:HB3	1:B:246:ALA:O	2.20	0.42
1:A:60:LEU:HD13	1:A:504:HIS:HE1	1.85	0.42
1:B:147:ASN:O	1:B:150:VAL:HG12	2.19	0.42
1:A:155:LEU:HD11	1:A:220:LEU:HB2	2.02	0.41
1:B:478:THR:O	1:B:482:LEU:HG	2.20	0.41
1:A:104:ARG:NE	1:A:113:ASP:OD1	2.40	0.41
1:B:236:ARG:O	1:B:240:VAL:HG23	2.20	0.41
1:B:268:PHE:N	1:B:268:PHE:CD2	2.88	0.41
1:A:458:VAL:O	1:A:462:THR:HG22	2.20	0.41
1:B:398:ARG:NH2	1:B:401:GLU:OE2	2.45	0.41
1:A:82:ARG:HD3	1:B:47:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:CD2	1:A:204:ILE:CA	2.97	0.41
1:B:412:CYS:SG	1:B:415:ASP:HB2	2.60	0.41
1:A:69:ARG:HG3	1:A:490:GLU:OE2	2.20	0.41
1:B:171:HIS:N	1:B:174:HIS:ND1	2.68	0.41
1:A:75:ALA:HB3	1:A:425:ARG:NH1	2.35	0.41
1:A:248:LEU:HD23	1:A:270:HIS:O	2.21	0.41
1:A:349:GLU:HA	1:A:352:LEU:HD12	2.02	0.41
1:A:95:LYS:HZ3	1:A:109:ALA:HA	1.86	0.41
1:B:218:PRO:HD2	1:B:244:VAL:CG1	2.51	0.41
1:B:335:VAL:O	1:B:339:LEU:N	2.54	0.41
1:A:96:TYR:HH	1:B:279:HIS:CD2	2.31	0.41
1:A:297:LYS:HE2	1:A:309:TYR:CE1	2.56	0.41
1:B:237:MET:HB3	1:B:248:LEU:HD22	2.02	0.41
1:B:249:LEU:HD11	1:B:275:THR:HG23	2.02	0.41
1:B:279:HIS:O	1:B:281:THR:N	2.55	0.40
1:B:357:ASN:HB3	1:B:441:PHE:CZ	2.55	0.40
1:B:412:CYS:SG	1:B:415:ASP:HB3	2.61	0.40
1:B:395:ARG:NH1	1:B:465:LEU:HD21	2.35	0.40
1:A:77:GLU:HG3	1:B:96:TYR:HB2	2.03	0.40
1:A:368:ARG:HB2	1:A:370:TYR:HD2	1.87	0.40
1:B:100:TYR:H	1:B:104:ARG:HG2	1.86	0.40
1:B:172:LEU:HB3	1:B:184:SER:HB2	2.04	0.40
1:B:224:GLY:HA2	1:B:251:ASP:H	1.86	0.40
1:B:252:MET:HB2	1:B:276:THR:CB	2.52	0.40
1:A:129:LEU:HD12	1:A:134:TRP:CD1	2.57	0.40
1:A:225:THR:OG1	1:A:232:ILE:HD11	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	447/493 (91%)	405 (91%)	42 (9%)	0	100 100
1	B	437/493 (89%)	394 (90%)	41 (9%)	2 (0%)	29 53
All	All	884/986 (90%)	799 (90%)	83 (9%)	2 (0%)	47 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	LEU
1	B	128	ASP

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	367/404 (91%)	357 (97%)	10 (3%)	44 72
1	B	335/404 (83%)	317 (95%)	18 (5%)	22 45
All	All	702/808 (87%)	674 (96%)	28 (4%)	31 58

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	96	TYR
1	A	168	ASP
1	A	251	ASP
1	A	266	SER
1	A	313	ASP
1	A	340	LYS
1	A	437	ARG
1	A	441	PHE
1	A	471	PHE
1	B	96	TYR
1	B	106	TYR
1	B	128	ASP
1	B	168	ASP

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Mol	Chain	Res	Type
1	B	200	LYS
1	B	236	ARG
1	B	251	ASP
1	B	262	LYS
1	B	289	LEU
1	B	346	MET
1	B	374	SER
1	B	378	ASP
1	B	412	CYS
1	B	431	LEU
1	B	441	PHE
1	B	446	ASP
1	B	464	LYS
1	B	471	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	B	174	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LLP	A	280	1	23,24,25	2.59	6 (26%)	25,32,34	1.44	3 (12%)

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
1	LLP	A	280	1	-	7/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	LLP	C4-C4'	7.97	1.61	1.46
1	A	280	LLP	C4'-NZ	4.93	1.43	1.27
1	A	280	LLP	C4-C5	-4.08	1.36	1.42
1	A	280	LLP	C2'-C2	3.54	1.56	1.50
1	A	280	LLP	C6-N1	2.94	1.40	1.34
1	A	280	LLP	C5'-C5	2.12	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	LLP	OP4-C5'-C5	3.43	115.89	109.35
1	A	280	LLP	C4-C4'-NZ	-3.24	109.44	124.31
1	A	280	LLP	CE-NZ-C4'	-2.97	109.79	118.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	LLP	C4-C4'-NZ-CE
1	A	280	LLP	C5'-OP4-P-OP2
1	A	280	LLP	C5'-OP4-P-OP3
1	A	280	LLP	O-C-CA-CB
1	A	280	LLP	C5'-OP4-P-OP1
1	A	280	LLP	CD-CE-NZ-C4'
1	A	280	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	LLP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	I6I	A	601	-	52,54,54	2.46	14 (26%)	64,74,74	1.30	5 (7%)

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	I6I	A	601	-	-	16/50/50/50	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	I6I	C23-N25	6.81	1.48	1.34
2	A	601	I6I	C17-N19	6.42	1.48	1.34
2	A	601	I6I	C37-N39	6.31	1.47	1.34
2	A	601	I6I	C09-N01	5.53	1.49	1.39
2	A	601	I6I	C02-N03	5.08	1.45	1.33
2	A	601	I6I	C02-N11	4.83	1.45	1.34
2	A	601	I6I	C02-N01	3.85	1.47	1.37
2	A	601	I6I	C06-N07	-3.49	1.33	1.38
2	A	601	I6I	O10-C04	-2.88	1.18	1.23
2	A	601	I6I	C12-C17	2.83	1.56	1.50
2	A	601	I6I	C36-C37	2.34	1.55	1.51
2	A	601	I6I	C04-N03	2.32	1.43	1.39
2	A	601	I6I	O18-C17	-2.02	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	I6I	O38-C37	-2.02	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	I6I	C15-C13-C12	-3.29	120.02	123.53
2	A	601	I6I	C14-C12-C13	2.85	119.91	116.67
2	A	601	I6I	C36-C37-N39	2.84	120.76	115.83
2	A	601	I6I	C13-C12-C17	-2.57	119.15	125.09
2	A	601	I6I	C22-C23-N25	2.12	119.52	115.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	I6I	C13-C12-C17-N19
2	A	601	I6I	C36-C37-N39-C43
2	A	601	I6I	N25-C34-C35-C36
2	A	601	I6I	O38-C37-N39-C43
2	A	601	I6I	C20-C21-C22-C23
2	A	601	I6I	C40-C34-C35-C36
2	A	601	I6I	N39-C43-C49-O50
2	A	601	I6I	N39-C43-C49-O51
2	A	601	I6I	C13-C12-C17-O18
2	A	601	I6I	C29-C30-C31-C32
2	A	601	I6I	C34-C35-C36-C37
2	A	601	I6I	C44-C45-C46-O47
2	A	601	I6I	C44-C45-C46-O48
2	A	601	I6I	C43-C44-C45-C46
2	A	601	I6I	C31-C32-C33-C16
2	A	601	I6I	C31-C32-C33-C15

There are no ring outliers.

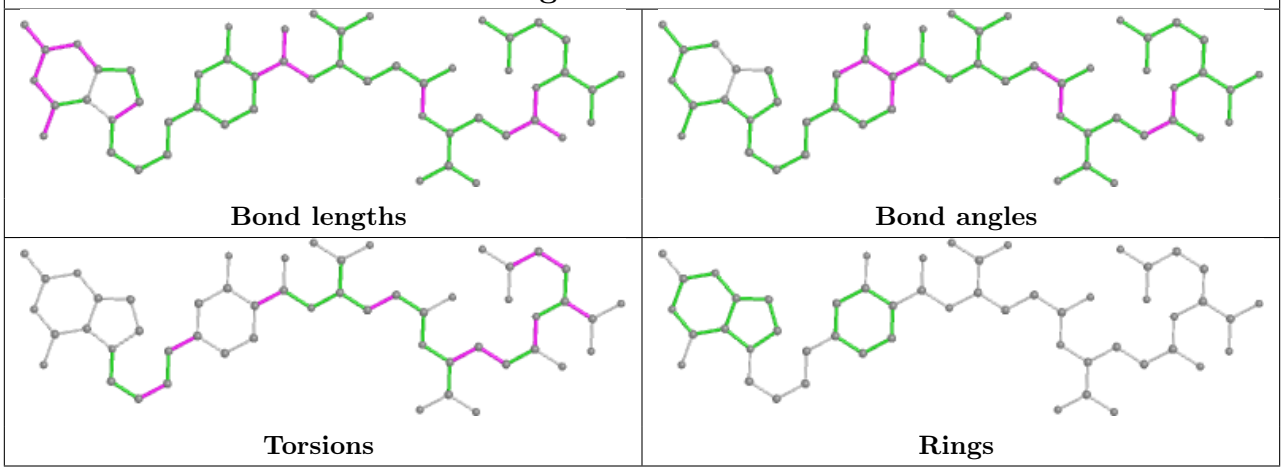
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	I6I	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 I6I A 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	453/493 (91%)	0.39	16 (3%) 44 44	15, 48, 80, 102	0
1	B	449/493 (91%)	0.99	68 (15%) 2 1	35, 78, 108, 127	0
All	All	902/986 (91%)	0.69	84 (9%) 8 7	15, 61, 102, 127	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	6.4
1	B	399	VAL	4.8
1	B	413	PRO	4.7
1	B	211	LEU	4.6
1	B	246	ALA	4.5
1	B	483	ALA	4.2
1	B	455	GLY	3.9
1	B	472	LEU	3.8
1	B	215	LEU	3.7
1	B	480	GLN	3.7
1	A	306	GLU	3.7
1	B	460	SER	3.7
1	B	471	PHE	3.6
1	B	180	VAL	3.6
1	B	474	LYS	3.5
1	B	223	ALA	3.4
1	B	388	PRO	3.4
1	B	405	ILE	3.4
1	A	482	LEU	3.4
1	B	375	GLY	3.4
1	B	201	THR	3.3
1	A	307	ILE	3.2
1	B	209	LEU	3.0
1	B	307	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	242	ASP	3.0
1	B	456	LEU	3.0
1	B	441	PHE	2.9
1	B	229	ALA	2.9
1	B	403	VAL	2.8
1	B	473	LEU	2.8
1	B	207	ASN	2.8
1	B	241	CYS	2.7
1	B	195	TYR	2.7
1	B	344	THR	2.7
1	A	443	ARG	2.7
1	A	386	LEU	2.6
1	B	485	LEU	2.6
1	B	407	ALA	2.6
1	B	213	ALA	2.6
1	B	296	VAL	2.6
1	B	102	GLY	2.6
1	B	463	ALA	2.5
1	B	343	CYS	2.5
1	A	478	THR	2.5
1	A	476	SER	2.5
1	A	467	ASP	2.5
1	A	454	ILE	2.4
1	B	468	PHE	2.4
1	B	163	GLY	2.4
1	B	475	ASP	2.4
1	B	270	HIS	2.4
1	B	175	GLY	2.4
1	B	198	ASN	2.4
1	A	131	PRO	2.3
1	B	96	TYR	2.3
1	B	406	THR	2.3
1	B	467	ASP	2.3
1	B	206	TYR	2.3
1	B	297	LYS	2.3
1	B	268	PHE	2.3
1	B	171	HIS	2.3
1	A	471	PHE	2.3
1	B	70	GLY	2.2
1	B	445	VAL	2.2
1	B	426	LEU	2.2
1	B	168	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	473	LEU	2.2
1	B	397	GLU	2.2
1	A	369	GLY	2.2
1	B	162	MET	2.2
1	B	269	LYS	2.1
1	B	79	PHE	2.1
1	A	305	ARG	2.1
1	B	394	ALA	2.1
1	B	489	VAL	2.1
1	B	311	PHE	2.1
1	B	166	LEU	2.1
1	A	45	GLY	2.1
1	B	154	LEU	2.1
1	A	308	PRO	2.1
1	B	477	GLU	2.1
1	B	310	THR	2.1
1	B	465	LEU	2.0
1	B	236	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	LLP	B	280[A]	24/25	0.93	0.20	39,58,73,80	0
1	LLP	A	280	24/25	0.94	0.23	21,47,59,66	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

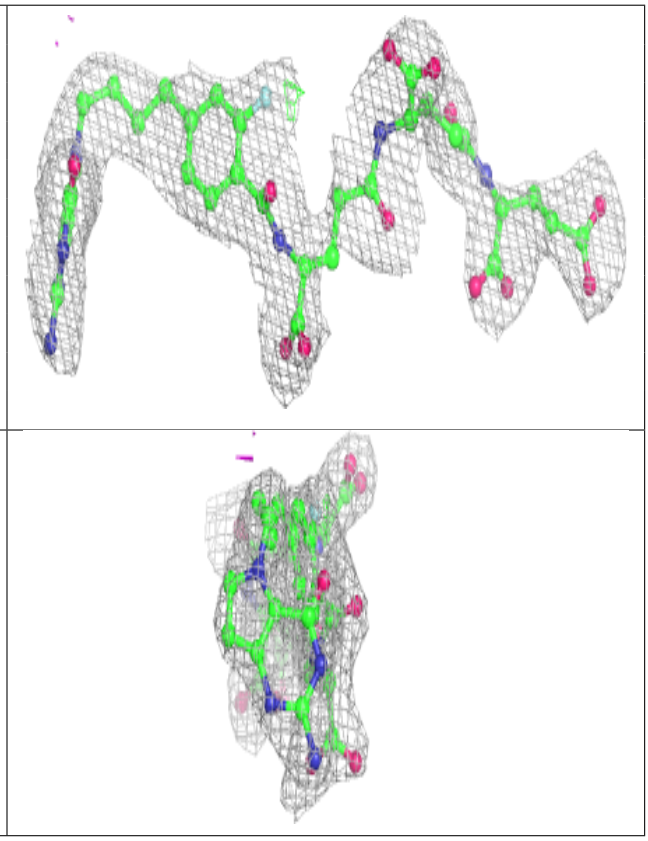
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	I6I	A	601	52/52	0.81	0.29	25,66,93,93	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 I6I A 601:

$2mF_o$-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.