



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:06 PM UTC

PDB ID : 8TLC / pdb_00008tlc
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	:	4-5-2 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

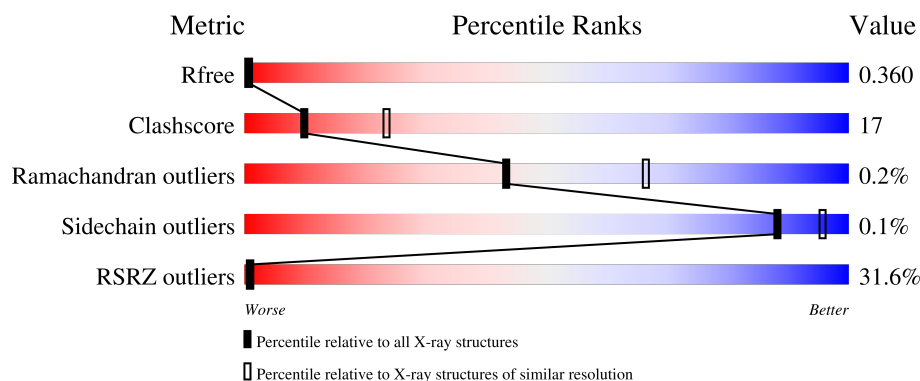
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 $\leq 5\%$. 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	493	12% 65% 27% 8%
1	B	493	45% 58% 32% 9%

2 Entry composition

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:

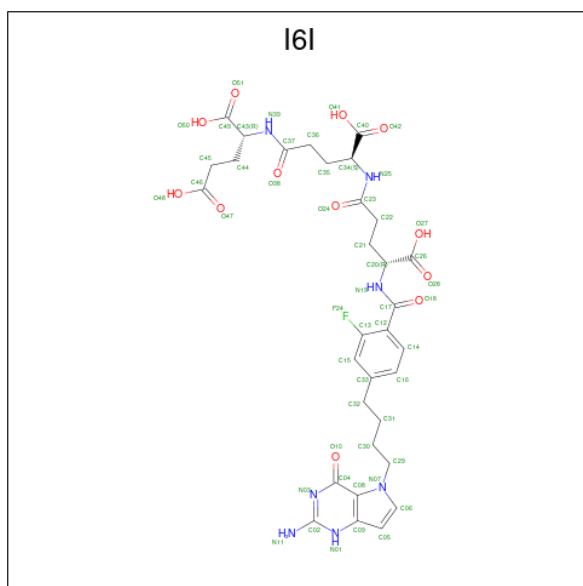
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P34897
A	13	GLY	-	expression tag	UNP P34897
A	14	SER	-	expression tag	UNP P34897
A	15	SER	-	expression tag	UNP P34897
A	16	HIS	-	expression tag	UNP P34897
A	17	HIS	-	expression tag	UNP P34897
A	18	HIS	-	expression tag	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 (CCD ID: I6I) (formula: C₃₂H₃₈FN₇O₁₂) (labeled as "Ligand of Interest" by depositor).



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

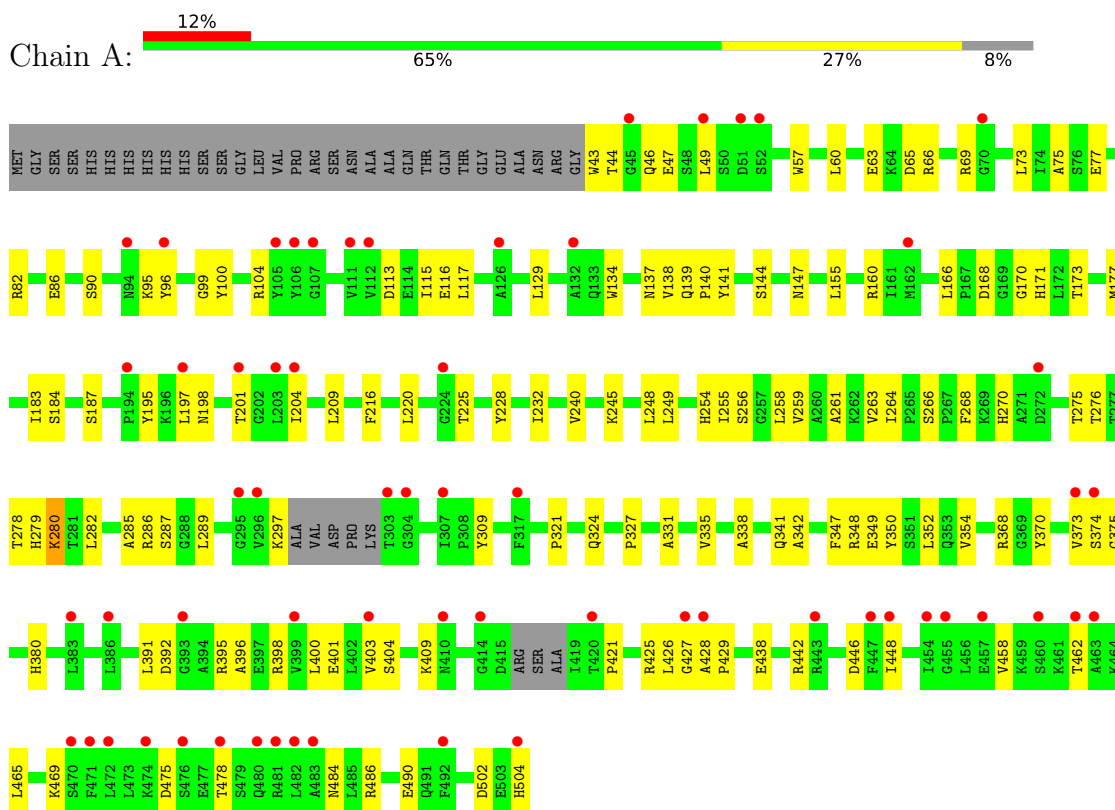
- Molecule 3 is water.

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

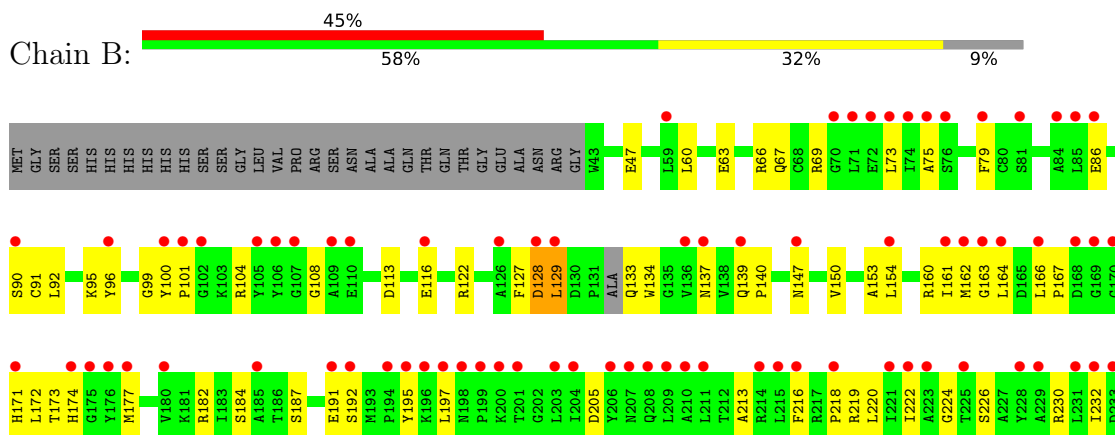
3 Residue-property plots

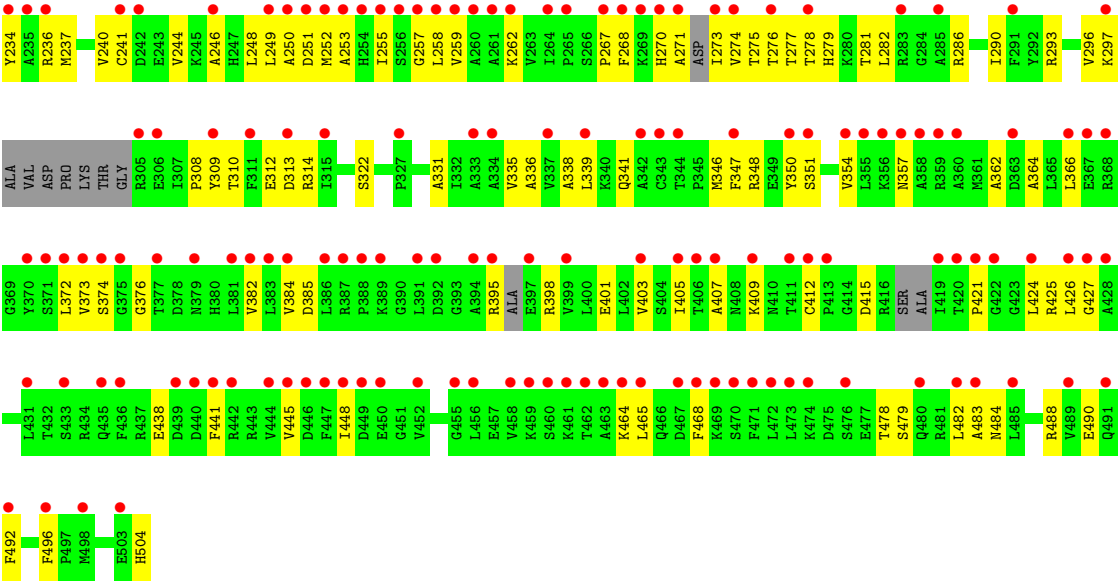
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Serine hydroxymethyltransferase, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.306 , 0.359 0.307 , 0.360	Depositor DCC
R_{free} test set	2050 reflections (4.89%)	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)	0.32 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	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.*

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: I6I, LLP

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	0.18	0/3585	0.41	0/4850
1	B	0.20	0/3441	0.48	0/4665
All	All	0.19	0/7026	0.44	0/9515

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	3540	0	3484	106	0
1	B	3401	0	3205	152	0
2	A	52	0	0	1	0
3	A	10	0	0	0	0
All	All	7003	0	6689	239	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 (239) 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: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:484:ASN:CG	1:B:488:ARG:HH12	2.03	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:A:171:HIS:HB2	1:A:280:LLP:H2'2	1.79	0.65
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: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:B:162:MET:HE3	1:B:218:PRO:HG3	1.82	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
1:B:174:HIS:CD2	1:B:222:ILE:HD13	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:183:ILE:HG13	1:A:184:SER:N	2.19	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: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:162:MET:HE1	1:B:213:ALA:HA	1.89	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
1:B:127:PHE:HB3	1:B:268:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:280:LLP:OP1	1:B:96:TYR:OH	2.27	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
1:B:252:MET:HB2	1:B:276:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:278:THR:OG1	1:A:285:ALA:O	2.23	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: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:A:403:VAL:O	1:A:404:SER:HB2	2.17	0.44
1:B:251:ASP:C	1:B:253:ALA:H	2.26	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:B:464:LYS:C	1:B:465:LEU:HD23	2.43	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:43:TRP:CG	1:B:346:MET:HE3	2.53	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:177:MET:HE3	1:B:182:ARG:HG2	2.01	0.42
1:A:484:ASN:C	1:A:484:ASN:OD1	2.63	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:A:166:LEU:C	1:A:168:ASP:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:C	1:A:375:GLY:H	2.29	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
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: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:A:373:VAL:O	1:A:374:SER:OG	2.32	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

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	447/493 (91%)	405 (91%)	42 (9%)	0	100	100
1	B	437/493 (89%)	394 (90%)	41 (9%)	2 (0%)	24	46
All	All	884/986 (90%)	799 (90%)	83 (9%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

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

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	367/404 (91%)	366 (100%)	1 (0%)	86	93
1	B	335/404 (83%)	335 (100%)	0	100	100
All	All	702/808 (87%)	701 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	324	GLN
1	B	137	ASN
1	B	174	HIS

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Mol	Chain	Res	Type
1	B	435	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	2.48	6 (26%)	25,32,34	1.44	4 (16%)

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'	7.11	1.61	1.46
1	A	280	LLP	C4'-NZ	4.97	1.43	1.27
1	A	280	LLP	C2'-C2	3.78	1.56	1.50
1	A	280	LLP	C4-C5	-3.69	1.36	1.42
1	A	280	LLP	C6-N1	3.05	1.40	1.34
1	A	280	LLP	C5'-C5	2.21	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LLP	OP4-C5'-C5	3.49	115.89	109.36
1	A	280	LLP	C4-C4'-NZ	-3.16	109.44	124.04
1	A	280	LLP	CE-NZ-C4'	-2.79	109.79	118.72
1	A	280	LLP	C5-C6-N1	-2.01	120.56	123.83

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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	53,54,54	2.40	15 (28%)	66,74,74	1.24	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	-	-	17/50/50/50	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	I6I	C23-N25	6.86	1.48	1.34
2	A	601	I6I	C37-N39	6.36	1.47	1.34
2	A	601	I6I	C17-N19	6.02	1.48	1.34
2	A	601	I6I	C02-N03	5.05	1.45	1.33
2	A	601	I6I	C09-N01	5.04	1.49	1.38
2	A	601	I6I	C02-N11	4.92	1.45	1.34
2	A	601	I6I	C02-N01	3.93	1.47	1.37
2	A	601	I6I	C04-N03	3.36	1.43	1.38
2	A	601	I6I	C12-C17	2.89	1.56	1.50
2	A	601	I6I	O10-C04	-2.81	1.18	1.23
2	A	601	I6I	C08-N07	-2.62	1.34	1.39
2	A	601	I6I	C06-N07	-2.28	1.33	1.38
2	A	601	I6I	C36-C37	2.22	1.55	1.51
2	A	601	I6I	O38-C37	-2.06	1.19	1.23
2	A	601	I6I	O24-C23	-2.03	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	I6I	C15-C13-C12	-3.13	120.02	123.48
2	A	601	I6I	C14-C12-C13	2.89	119.91	116.70
2	A	601	I6I	C36-C37-N39	2.78	120.76	115.86
2	A	601	I6I	C29-N07-C08	-2.20	125.24	128.85
2	A	601	I6I	C22-C23-N25	2.07	119.52	115.86

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	I6I	C36-C37-N39-C43
2	A	601	I6I	N25-C34-C35-C36
2	A	601	I6I	O38-C37-N39-C43

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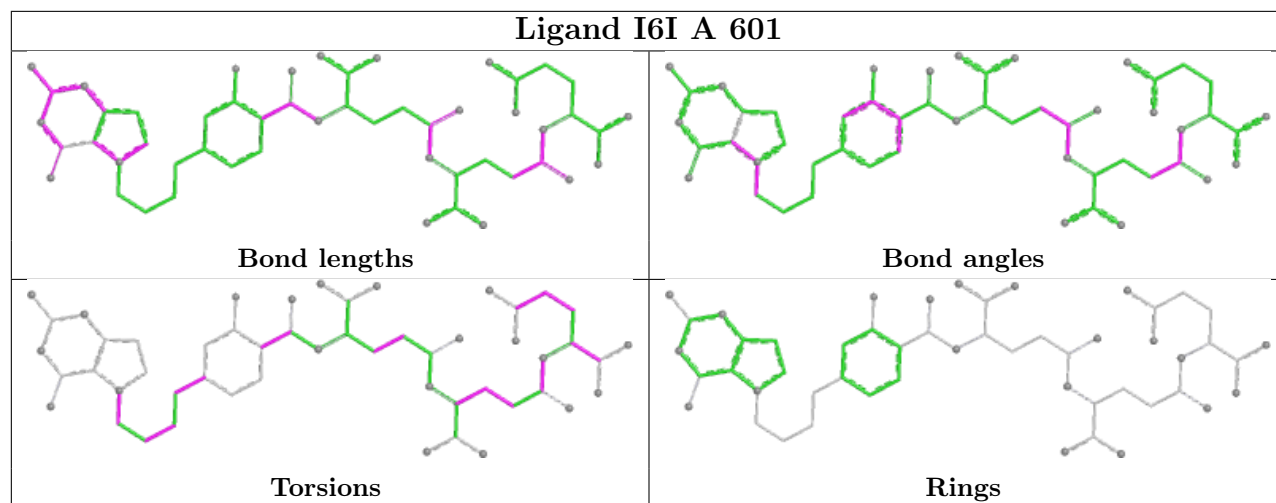
Mol	Chain	Res	Type	Atoms
2	A	601	I6I	C20-C21-C22-C23
2	A	601	I6I	C13-C12-C17-N19
2	A	601	I6I	N39-C43-C49-O50
2	A	601	I6I	N39-C43-C49-O51
2	A	601	I6I	C40-C34-C35-C36
2	A	601	I6I	C13-C12-C17-O18
2	A	601	I6I	C29-C30-C31-C32
2	A	601	I6I	C34-C35-C36-C37
2	A	601	I6I	C44-C45-C46-O47
2	A	601	I6I	C44-C45-C46-O48
2	A	601	I6I	C31-C32-C33-C16
2	A	601	I6I	C30-C29-N07-C08
2	A	601	I6I	C31-C32-C33-C15
2	A	601	I6I	C43-C44-C45-C46

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 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	453/493 (91%)	1.09	61 (13%) 7 6	15, 48, 80, 102	0
1	B	449/493 (91%)	2.10	224 (49%) 0 0	35, 78, 108, 127	0
All	All	902/986 (91%)	1.59	285 (31%) 1 1	15, 61, 102, 127	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	LEU	6.1
1	B	441	PHE	6.0
1	B	445	VAL	5.7
1	B	413	PRO	5.6
1	B	195	TYR	5.4
1	B	180	VAL	5.2
1	B	388	PRO	5.1
1	B	273	ILE	5.0
1	B	422	GLY	5.0
1	B	171	HIS	4.8
1	B	460	SER	4.8
1	B	70	GLY	4.8
1	B	229	ALA	4.7
1	B	253	ALA	4.7
1	B	106	TYR	4.7
1	B	412	CYS	4.6
1	B	211	LEU	4.5
1	B	399	VAL	4.5
1	B	264	ILE	4.5
1	B	262	LYS	4.4
1	B	366	LEU	4.4
1	B	427	GLY	4.4
1	B	426	LEU	4.3
1	B	428	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	168	ASP	4.2
1	B	351	SER	4.2
1	B	394	ALA	4.2
1	A	393	GLY	4.2
1	A	106	TYR	4.1
1	B	463	ALA	4.1
1	B	96	TYR	4.1
1	B	367	GLU	4.1
1	A	482	LEU	4.1
1	B	374	SER	4.1
1	B	232	ILE	4.0
1	B	343	CYS	4.0
1	B	462	THR	3.9
1	B	383	LEU	3.9
1	B	206	TYR	3.9
1	B	471	PHE	3.9
1	B	207	ASN	3.8
1	B	371	SER	3.8
1	A	504	HIS	3.7
1	B	377	THR	3.7
1	A	420	THR	3.6
1	B	107	GLY	3.6
1	B	175	GLY	3.6
1	B	360	ALA	3.6
1	A	296	VAL	3.6
1	B	467	ASP	3.6
1	B	464	LYS	3.6
1	B	375	GLY	3.6
1	B	455	GLY	3.5
1	B	222	ILE	3.5
1	B	405	ILE	3.5
1	A	132	ALA	3.5
1	B	170	GLY	3.4
1	B	209	LEU	3.4
1	B	472	LEU	3.4
1	B	204	ILE	3.4
1	B	448	ILE	3.4
1	A	49	LEU	3.4
1	B	250	ALA	3.4
1	A	386	LEU	3.4
1	B	333	ALA	3.3
1	B	435	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	468	PHE	3.3
1	A	201	THR	3.3
1	A	107	GLY	3.3
1	B	261	ALA	3.3
1	B	75	ALA	3.3
1	B	311	PHE	3.3
1	B	492	PHE	3.3
1	B	392	ASP	3.3
1	B	101	PRO	3.3
1	B	267	PRO	3.3
1	B	447	PHE	3.3
1	B	236	ARG	3.2
1	B	278	THR	3.2
1	B	249	LEU	3.2
1	B	456	LEU	3.2
1	B	355	LEU	3.2
1	B	433	SER	3.2
1	A	105	TYR	3.2
1	A	471	PHE	3.2
1	A	443	ARG	3.1
1	B	297	LYS	3.1
1	B	439	ASP	3.1
1	A	111	VAL	3.1
1	B	382	VAL	3.1
1	B	201	THR	3.1
1	B	79	PHE	3.1
1	A	374	SER	3.1
1	B	228	TYR	3.0
1	A	462	THR	3.0
1	B	407	ALA	3.0
1	B	268	PHE	3.0
1	B	271	ALA	3.0
1	A	51	ASP	3.0
1	B	255	ILE	3.0
1	B	136	VAL	3.0
1	B	251	ASP	2.9
1	B	276	THR	2.9
1	B	210	ALA	2.9
1	B	274	VAL	2.9
1	B	154	LEU	2.9
1	A	478	THR	2.9
1	B	334	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	73	LEU	2.9
1	B	166	LEU	2.9
1	B	305	ARG	2.9
1	B	370	TYR	2.9
1	B	411	THR	2.9
1	B	71	LEU	2.9
1	B	242	ASP	2.9
1	B	363	ASP	2.9
1	B	258	LEU	2.9
1	B	373	VAL	2.9
1	B	465	LEU	2.9
1	A	480	GLN	2.8
1	B	313	ASP	2.8
1	A	197	LEU	2.8
1	B	265	PRO	2.8
1	B	221	ILE	2.8
1	B	419	ILE	2.8
1	B	223	ALA	2.8
1	B	285	ALA	2.8
1	B	503	GLU	2.8
1	A	476	SER	2.8
1	B	389	LYS	2.8
1	B	379	ASN	2.8
1	B	215	LEU	2.8
1	B	162	MET	2.8
1	B	347	PHE	2.8
1	B	476	SER	2.8
1	B	235	ALA	2.8
1	B	291	PHE	2.8
1	B	283	ARG	2.8
1	A	470	SER	2.7
1	B	252	MET	2.7
1	A	399	VAL	2.7
1	A	428	ALA	2.7
1	B	395	ARG	2.7
1	B	491	GLN	2.7
1	B	270	HIS	2.7
1	B	110	GLU	2.7
1	B	192	SER	2.7
1	B	257	GLY	2.7
1	A	307	ILE	2.7
1	B	161	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	256	SER	2.7
1	B	421	PRO	2.7
1	B	449	ASP	2.7
1	A	295	GLY	2.6
1	B	459	LYS	2.6
1	B	403	VAL	2.6
1	B	129	LEU	2.6
1	B	461	LYS	2.6
1	B	234	TYR	2.6
1	B	372	LEU	2.6
1	B	381	LEU	2.6
1	B	254	HIS	2.6
1	B	368	ARG	2.6
1	B	191	GLU	2.6
1	A	224	GLY	2.6
1	B	442	ARG	2.6
1	B	194	PRO	2.6
1	B	452	VAL	2.6
1	A	94	ASN	2.6
1	A	483	ALA	2.5
1	B	431	LEU	2.5
1	A	112	VAL	2.5
1	B	384	VAL	2.5
1	B	137	ASN	2.5
1	B	420	THR	2.5
1	B	356	LYS	2.5
1	B	359	ARG	2.5
1	B	391	LEU	2.5
1	B	483	ALA	2.5
1	B	306	GLU	2.5
1	B	169	GLY	2.5
1	B	480	GLN	2.5
1	A	447	PHE	2.5
1	B	496	PHE	2.5
1	B	350	TYR	2.4
1	B	214	ARG	2.4
1	B	174	HIS	2.4
1	A	304	GLY	2.4
1	A	448	ILE	2.4
1	B	397	GLU	2.4
1	B	163	GLY	2.4
1	B	199	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	269	LYS	2.4
1	B	81	SER	2.4
1	A	474	LYS	2.4
1	B	200	LYS	2.4
1	B	185	ALA	2.4
1	B	339	LEU	2.3
1	B	86	GLU	2.3
1	A	317	PHE	2.3
1	B	342	ALA	2.3
1	B	176	TYR	2.3
1	A	410	ASN	2.3
1	B	208	GLN	2.3
1	B	489	VAL	2.3
1	B	231	LEU	2.3
1	B	74	ILE	2.3
1	B	469	LYS	2.3
1	B	233	ASP	2.3
1	B	327	PRO	2.3
1	A	383	LEU	2.3
1	B	241	CYS	2.3
1	B	458	VAL	2.3
1	B	409	LYS	2.3
1	B	105	TYR	2.3
1	B	386	LEU	2.3
1	B	424	LEU	2.3
1	B	246	ALA	2.2
1	A	303	THR	2.2
1	B	218	PRO	2.2
1	B	470	SER	2.2
1	A	126	ALA	2.2
1	B	357	ASN	2.2
1	B	128	ASP	2.2
1	B	197	LEU	2.2
1	A	373	VAL	2.2
1	B	196	LYS	2.2
1	B	444	VAL	2.2
1	A	204	ILE	2.2
1	B	126	ALA	2.2
1	B	102	GLY	2.2
1	B	446	ASP	2.2
1	A	162	MET	2.2
1	B	358	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	344	THR	2.2
1	A	455	GLY	2.2
1	B	473	LEU	2.2
1	B	482	LEU	2.2
1	B	485	LEU	2.2
1	A	460	SER	2.2
1	B	259	VAL	2.2
1	B	260	ALA	2.1
1	B	72	GLU	2.1
1	B	387	ARG	2.1
1	B	139	GLN	2.1
1	B	198	ASN	2.1
1	B	354	VAL	2.1
1	B	406	THR	2.1
1	A	194	PRO	2.1
1	B	59	LEU	2.1
1	B	164	LEU	2.1
1	A	272	ASP	2.1
1	A	403	VAL	2.1
1	A	52	SER	2.1
1	A	463	ALA	2.1
1	A	481	ARG	2.1
1	B	225	THR	2.1
1	B	474	LYS	2.1
1	B	177	MET	2.1
1	A	70	GLY	2.1
1	B	309	TYR	2.1
1	A	457	GLU	2.1
1	A	472	LEU	2.1
1	B	85	LEU	2.1
1	A	96	TYR	2.1
1	A	454	ILE	2.1
1	B	216	PHE	2.1
1	B	436	PHE	2.1
1	B	440	ASP	2.0
1	B	116	GLU	2.0
1	B	90	SER	2.0
1	B	109	ALA	2.0
1	B	450	GLU	2.0
1	A	203	LEU	2.0
1	B	147	ASN	2.0
1	B	315	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	337	VAL	2.0
1	A	492	PHE	2.0
1	B	84	ALA	2.0
1	B	76	SER	2.0
1	B	498	MET	2.0
1	A	45	GLY	2.0
1	A	414	GLY	2.0
1	A	427	GLY	2.0
1	B	100	TYR	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, 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
1	LLP	B	280[A]	24/25	0.90	0.15	39,58,73,80	0
1	LLP	A	280	24/25	0.91	0.14	21,47,59,66	0

6.3 Carbohydrates [i](#)

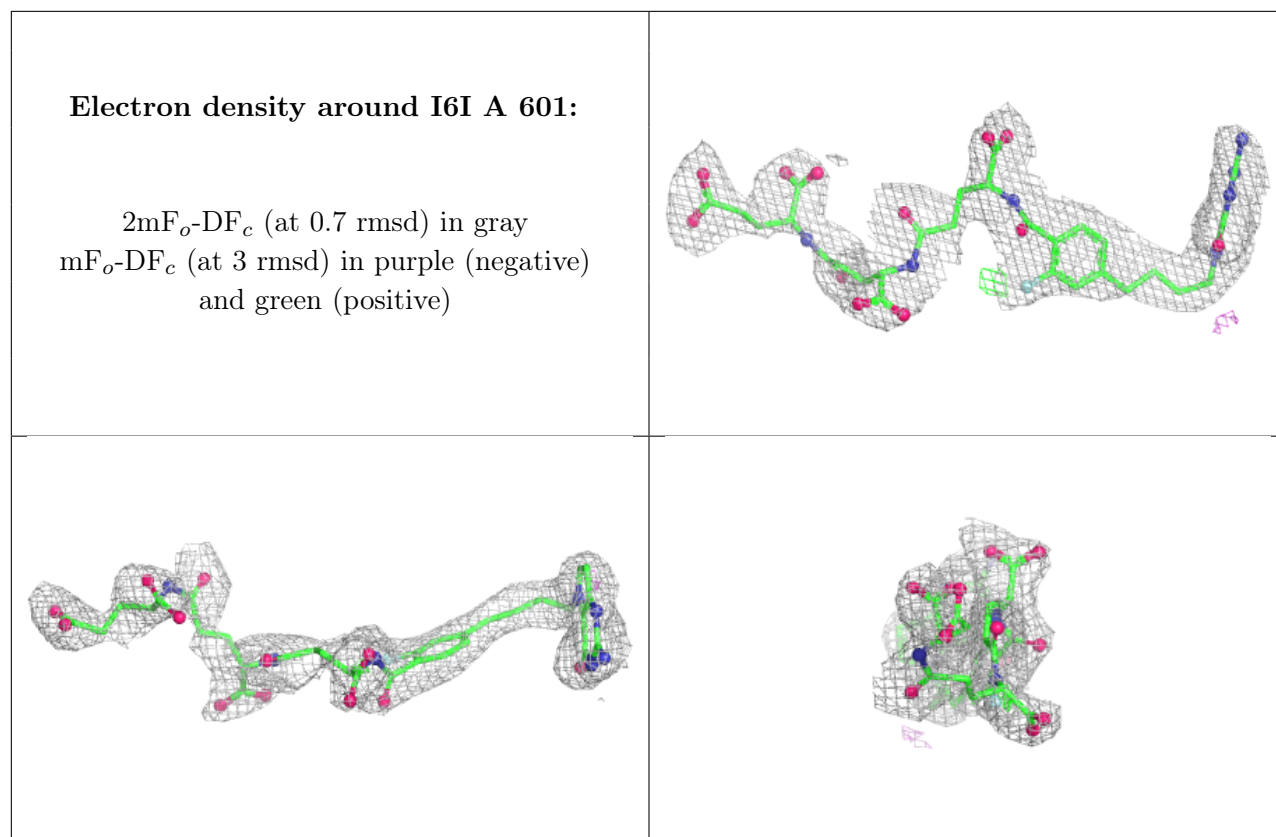
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	I6I	A	601	52/52	0.82	0.15	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.