



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:18 PM UTC

PDB ID : 8ZI6 / pdb_00008zi6
Title : Crystal structure of SrUGT76G4 in complex with UDP-glucose
Authors : Wang, Y.; Li, T.; Yin, H.
Deposited on : 2024-05-13
Resolution : 2.80 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

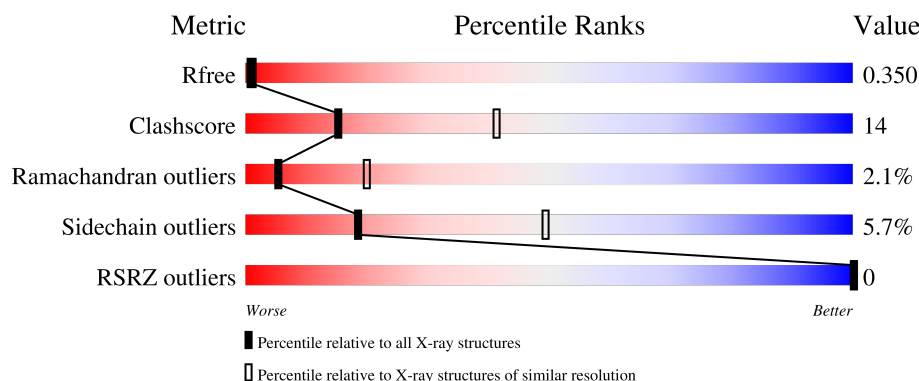
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	458	
1	B	458	
1	C	458	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	C	501	-	-	X	-

2 Entry composition [i](#)

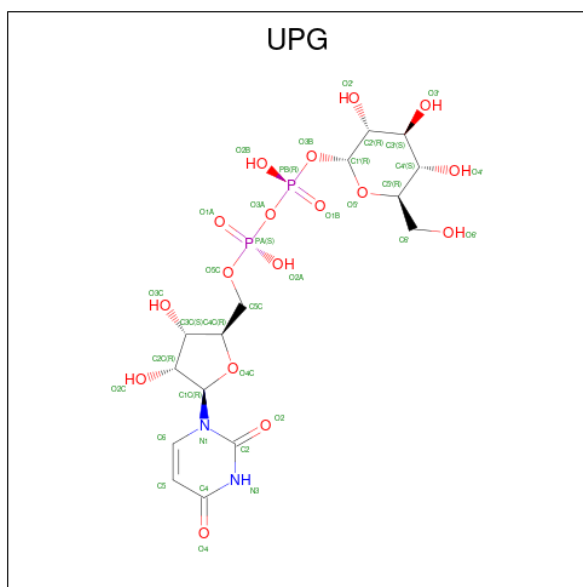
There are 5 unique types of molecules in this entry. The entry contains 9426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UGT-glycosyltransferase 76G4.

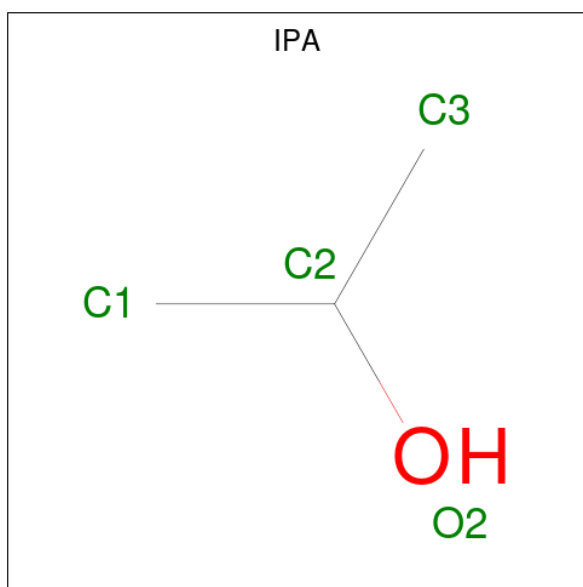
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3491	2241	587	652	11			
1	B	399	Total	C	N	O	S	0	0	0
			3190	2055	537	588	10			
1	C	338	Total	C	N	O	S	0	1	0
			2685	1729	445	503	8			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



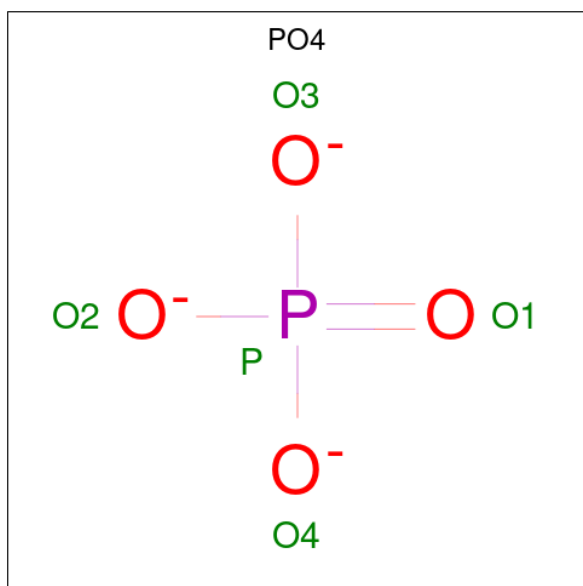
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

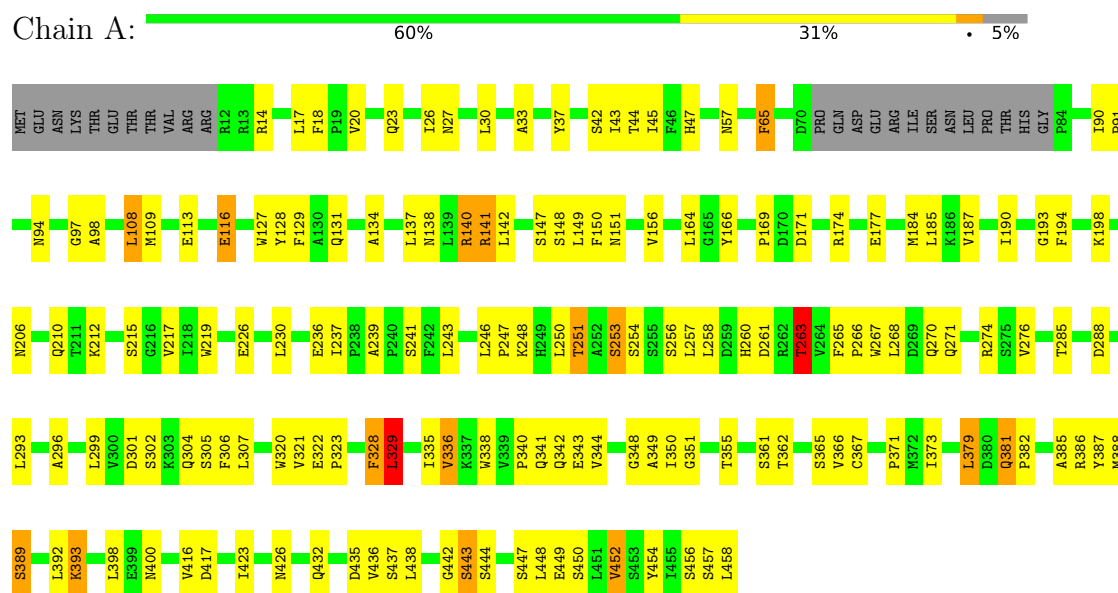
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

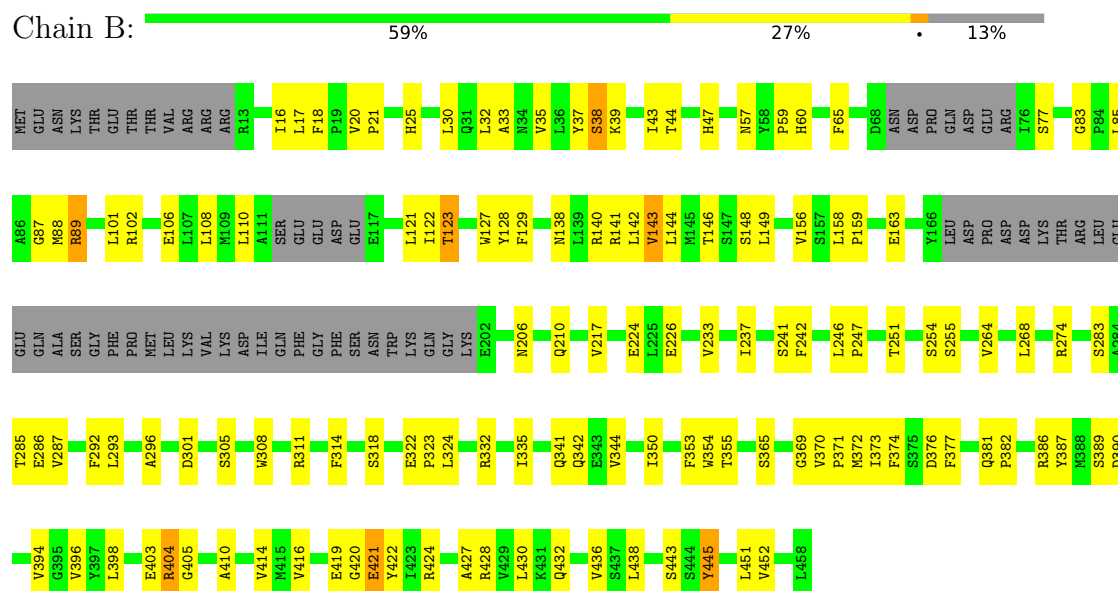
3 Residue-property plots

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.

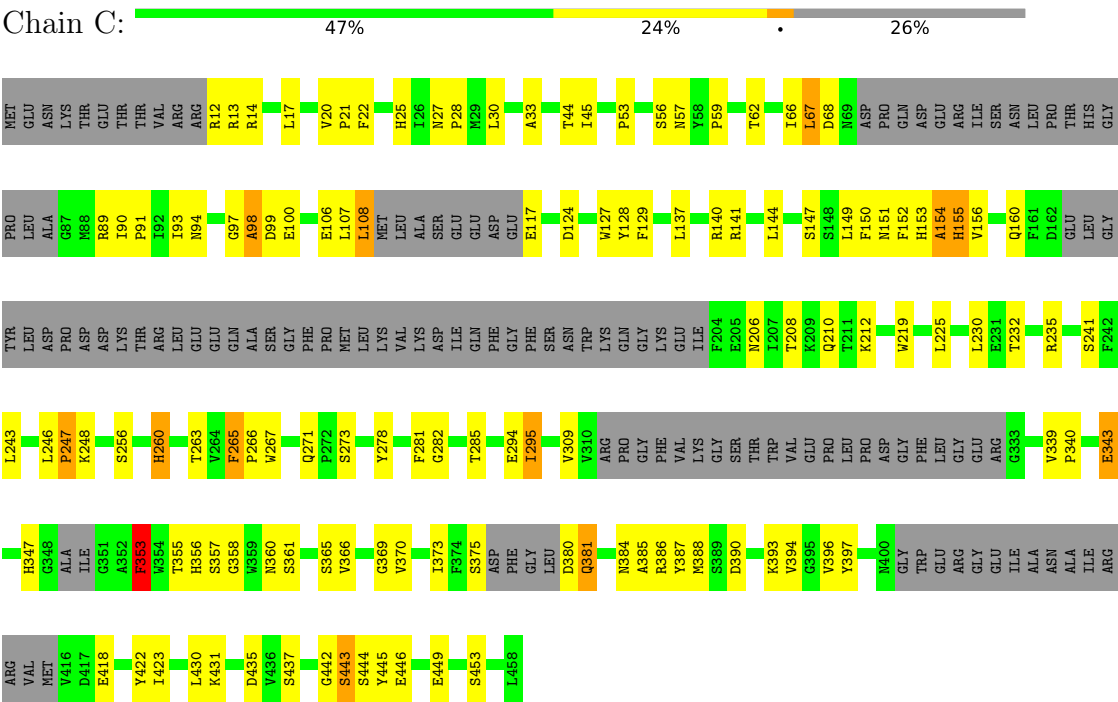
• Molecule 1: UGT-glycosyltransferase 76G4



• Molecule 1: UGT-glycosyltransferase 76G4



● Molecule 1: UGT-glycosyltransferase 76G4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	111.78Å 111.78Å 91.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.99 – 2.80 33.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (33.99-2.80) 96.0 (33.99-2.80)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.268 , 0.351 0.270 , 0.350	Depositor DCC
R_{free} test set	1561 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.097 for -h,-k,l 0.097 for h,-h-k,-l 0.418 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9426	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: PO4, UPG, IPA

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	0.51	0/3581	1.09	11/4851 (0.2%)
1	B	0.50	0/3270	1.06	5/4435 (0.1%)
1	C	0.52	0/2749	1.05	3/3727 (0.1%)
All	All	0.51	0/9600	1.07	19/13013 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	ARG	N-CA-CB	-6.36	102.13	110.59
1	A	263	THR	CA-CB-OG1	-6.33	100.10	109.60
1	A	381	GLN	CB-CA-C	6.14	122.27	110.17
1	C	265	PHE	N-CA-CB	6.09	118.87	110.11
1	A	452	VAL	N-CA-CB	5.93	117.49	110.55
1	C	353	PHE	N-CA-CB	-5.78	101.94	110.37
1	A	65	PHE	CB-CA-C	5.73	118.99	109.53
1	C	353	PHE	CB-CA-C	5.65	118.18	110.94
1	A	140	ARG	CB-CA-C	5.63	118.94	109.48
1	A	362	THR	CA-CB-OG1	-5.50	101.36	109.60
1	A	417	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	89	ARG	CB-CA-C	5.37	117.72	109.03
1	A	288	ASP	CA-CB-CG	5.33	117.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	TYR	N-CA-CB	5.29	117.68	110.01
1	A	301	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	21	PRO	N-CA-CB	-5.15	98.64	102.25
1	B	376	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	449	GLU	N-CA-CB	5.09	118.06	110.22
1	A	435	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain

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	3491	0	3436	90	0
1	B	3190	0	3152	76	0
1	C	2685	0	2618	88	0
2	A	25	0	11	2	0
2	B	25	0	11	1	0
3	A	4	0	8	0	0
4	C	5	0	0	2	0
5	A	1	0	0	0	0
All	All	9426	0	9236	253	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 14.

All (253) 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:C:445:TYR:O	1:C:449:GLU:HG2	1.59	1.02
1:C:384:ASN:O	1:C:388:MET:HG2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HD23	1:B:122:ILE:HB	1.65	0.77
1:C:386:ARG:HG3	1:C:386:ARG:HH11	1.55	0.71
1:B:102:ARG:HG2	1:B:106:GLU:OE2	1.92	0.69
1:C:248:LYS:NZ	1:C:435:ASP:OD1	2.24	0.69
1:C:235:ARG:HG2	1:C:235:ARG:HH11	1.58	0.68
1:B:106:GLU:O	1:B:110:LEU:HG	1.94	0.68
1:B:17:LEU:CD2	1:B:122:ILE:HB	2.24	0.66
1:A:389:SER:O	1:A:393:LYS:HA	1.98	0.64
1:C:28:PRO:HG3	1:C:360:ASN:OD1	1.98	0.63
1:B:16:ILE:HD11	1:B:108:LEU:HD22	1.79	0.63
1:C:94:ASN:OD1	1:C:129:PHE:HD1	1.81	0.63
1:A:20:VAL:HG22	1:A:127:TRP:CZ2	2.34	0.63
1:C:356:HIS:NE2	4:C:501:PO4:O2	2.31	0.63
1:C:97:GLY:O	1:C:98:ALA:C	2.43	0.62
1:B:44:THR:HG21	1:B:108:LEU:HD11	1.82	0.62
1:B:369:GLY:O	1:B:427:ALA:HB1	2.00	0.62
1:C:94:ASN:HA	1:C:129:PHE:CD1	2.35	0.61
1:C:97:GLY:O	1:C:99:ASP:N	2.33	0.61
1:A:276:VAL:HA	1:A:305:SER:O	2.01	0.61
1:A:320:TRP:CD1	1:A:321:VAL:HG13	2.36	0.61
1:A:448:LEU:O	1:A:452:VAL:HG23	2.01	0.61
1:C:17:LEU:CD1	1:C:33:ALA:HB2	2.32	0.60
1:A:109:MET:HE1	1:A:137:LEU:HD13	1.84	0.59
1:A:456:SER:O	1:A:458:LEU:N	2.35	0.59
1:C:445:TYR:O	1:C:449:GLU:CG	2.45	0.59
1:B:301:ASP:OD2	1:B:404:ARG:HD2	2.03	0.59
1:C:365:SER:O	1:C:369:GLY:N	2.35	0.59
1:A:17:LEU:CD1	1:A:33:ALA:HB2	2.31	0.59
1:B:381:GLN:N	1:B:382:PRO:CD	2.66	0.59
1:C:25:HIS:ND1	1:C:124:ASP:OD2	2.36	0.59
1:B:217:VAL:O	1:B:241:SER:HA	2.03	0.59
1:A:274:ARG:HD3	1:A:351:GLY:HA2	1.85	0.58
1:A:400:ASN:OD1	1:B:428:ARG:NH2	2.35	0.58
1:C:358:GLY:HA3	4:C:501:PO4:O2	2.04	0.58
1:A:94:ASN:HA	1:A:129:PHE:CD1	2.38	0.58
1:A:190:ILE:O	1:A:194:PHE:N	2.37	0.58
1:C:219:TRP:HB2	1:C:243:LEU:HD23	1.84	0.58
1:C:147:SER:HB3	1:C:151:ASN:HD22	1.67	0.58
1:C:265:PHE:HB2	1:C:266:PRO:HD3	1.86	0.58
1:B:87:GLY:C	1:B:89:ARG:H	2.12	0.57
1:B:432:GLN:O	1:B:436:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:GLY:O	1:C:443:SER:C	2.47	0.57
1:B:233:VAL:HG13	1:B:237:ILE:HD12	1.85	0.57
1:B:47:HIS:O	1:B:65:PHE:HA	2.03	0.57
1:B:353:PHE:CZ	1:B:355:THR:HB	2.39	0.57
1:A:149:LEU:N	1:A:226:GLU:OE1	2.35	0.56
1:C:90:ILE:HB	1:C:91:PRO:CD	2.35	0.56
1:C:267:TRP:O	1:C:271:GLN:NE2	2.35	0.56
1:A:257:LEU:O	1:A:258:LEU:HD12	2.06	0.56
1:A:248:LYS:HG2	1:A:367:CYS:HB3	1.88	0.56
1:C:235:ARG:HH11	1:C:235:ARG:CG	2.19	0.55
1:A:47:HIS:O	1:A:65:PHE:HA	2.06	0.55
1:A:256:SER:OG	1:A:338:TRP:NE1	2.34	0.55
1:A:131:GLN:HB2	1:A:141:ARG:HH21	1.71	0.55
1:B:35:VAL:O	1:B:38:SER:HB2	2.07	0.55
1:C:154:ALA:O	1:C:155:HIS:C	2.49	0.55
1:B:293:LEU:O	1:B:296:ALA:HB3	2.06	0.55
1:B:354:TRP:HA	1:B:373:ILE:O	2.06	0.55
1:A:149:LEU:HD23	1:A:219:TRP:CE3	2.43	0.54
1:B:365:SER:HB2	1:B:370:VAL:HB	1.90	0.54
1:A:355:THR:HG22	1:A:373:ILE:O	2.08	0.54
1:B:149:LEU:HD22	1:B:233:VAL:HG21	1.89	0.53
1:C:380:ASP:O	1:C:381:GLN:CB	2.55	0.53
1:A:267:TRP:O	1:A:270:GLN:N	2.32	0.53
1:C:366:VAL:HG11	1:C:430:LEU:HD23	1.91	0.53
1:B:251:THR:HG23	1:B:342:GLN:CD	2.34	0.53
1:C:151:ASN:HD21	1:C:384:ASN:HD21	1.56	0.53
1:B:322:GLU:N	1:B:323:PRO:CD	2.72	0.53
1:C:106:GLU:O	1:C:107:LEU:C	2.52	0.53
1:C:20:VAL:O	1:C:22:PHE:N	2.40	0.52
1:C:27:ASN:HB2	1:C:28:PRO:HD3	1.91	0.52
1:A:381:GLN:N	1:A:382:PRO:CD	2.73	0.52
1:B:332:ARG:HH11	1:B:332:ARG:HG3	1.75	0.52
1:C:14:ARG:HH21	1:C:108:LEU:HD21	1.74	0.52
1:A:212:LYS:NZ	1:A:236:GLU:OE1	2.33	0.51
1:B:128:TYR:CG	1:B:206:ASN:HB3	2.45	0.51
1:C:67:LEU:C	1:C:67:LEU:HD22	2.35	0.51
1:A:14:ARG:HG2	1:A:42:SER:OG	2.10	0.51
1:A:388:MET:SD	1:A:392:LEU:HD12	2.51	0.51
1:B:122:ILE:HG12	1:B:142:LEU:HB2	1.92	0.51
1:A:432:GLN:O	1:A:436:VAL:HG23	2.11	0.50
1:C:384:ASN:O	1:C:388:MET:CG	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ASN:OD1	1:B:140:ARG:NH2	2.39	0.50
1:A:299:LEU:O	1:A:302:SER:OG	2.29	0.50
1:A:442:GLY:O	1:A:443:SER:C	2.55	0.50
1:A:393:LYS:HB2	1:A:426:ASN:HD22	1.77	0.49
1:C:365:SER:OG	1:C:370:VAL:O	2.25	0.49
1:B:25:HIS:CE1	1:B:146:THR:HG21	2.47	0.49
1:A:23:GLN:NE2	1:A:338:TRP:CH2	2.80	0.49
1:A:322:GLU:N	1:A:323:PRO:CD	2.75	0.49
1:C:57:ASN:C	1:C:59:PRO:HD3	2.37	0.49
1:B:16:ILE:HA	1:B:44:THR:O	2.13	0.49
1:C:263:THR:O	1:C:263:THR:HG22	2.11	0.49
1:C:282:GLY:HA3	1:C:356:HIS:CD2	2.47	0.49
1:A:18:PHE:CE2	1:A:127:TRP:CD1	3.01	0.48
1:C:355:THR:OG1	1:C:356:HIS:N	2.45	0.48
1:A:373:ILE:N	1:A:373:ILE:HD12	2.27	0.48
1:C:149:LEU:O	1:C:152:PHE:N	2.42	0.48
1:A:361:SER:OG	2:A:501:UPG:O1A	2.22	0.48
1:C:153:HIS:O	1:C:153:HIS:ND1	2.46	0.48
1:C:235:ARG:CG	1:C:235:ARG:NH1	2.77	0.48
1:A:246:LEU:HB2	1:A:247:PRO:HD3	1.96	0.48
1:C:339:VAL:HB	1:C:340:PRO:CD	2.43	0.48
1:B:420:GLY:O	1:B:421:GLU:C	2.56	0.48
1:B:39:LYS:HE2	1:B:452:VAL:HG21	1.96	0.48
1:B:341:GLN:O	1:B:344:VAL:N	2.47	0.48
1:C:17:LEU:HD13	1:C:33:ALA:HB2	1.95	0.48
1:C:278:TYR:O	1:C:353:PHE:HA	2.14	0.48
1:B:59:PRO:HG2	1:B:60:HIS:CD2	2.49	0.47
1:A:134:ALA:O	1:A:138:ASN:N	2.44	0.47
1:A:265:PHE:N	1:A:266:PRO:CD	2.77	0.47
1:A:149:LEU:CD2	1:A:219:TRP:CD2	2.97	0.47
1:A:44:THR:HG21	1:A:108:LEU:HD11	1.97	0.47
1:A:217:VAL:O	1:A:241:SER:HA	2.14	0.47
1:C:375:SER:HA	1:C:397:TYR:HE1	1.79	0.47
1:A:90:ILE:HB	1:A:91:PRO:CD	2.44	0.47
1:B:287:VAL:HG22	1:B:314:PHE:CE2	2.50	0.47
1:C:67:LEU:HD13	1:C:68:ASP:N	2.28	0.47
1:C:246:LEU:HB2	1:C:247:PRO:HD3	1.97	0.47
1:C:256:SER:HB3	1:C:260:HIS:NE2	2.29	0.47
1:C:437:SER:HB3	1:C:444:SER:OG	2.15	0.47
1:B:311:ARG:HB2	1:B:314:PHE:HB2	1.97	0.47
1:A:131:GLN:HB2	1:A:141:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:SER:HB3	1:A:444:SER:OG	2.15	0.46
1:C:20:VAL:HG22	1:C:127:TRP:CE2	2.50	0.46
1:C:141:ARG:NH1	1:C:210:GLN:O	2.45	0.46
1:B:18:PHE:CZ	1:B:127:TRP:NE1	2.84	0.46
1:B:264:VAL:O	1:B:268:LEU:HG	2.14	0.46
1:C:153:HIS:O	1:C:156:VAL:HB	2.15	0.46
1:A:247:PRO:HB3	1:A:342[A]:GLN:HE21	1.80	0.46
1:B:403:GLU:O	1:B:404:ARG:C	2.58	0.46
1:A:237:ILE:HG22	1:A:239:ALA:O	2.16	0.46
1:A:37:TYR:HB2	1:A:43:ILE:HD12	1.97	0.46
1:C:30:LEU:HD21	1:C:45:ILE:HD13	1.96	0.46
1:A:248:LYS:HB3	1:A:438:LEU:HD11	1.97	0.46
1:A:251:THR:OG1	1:A:253:SER:OG	2.31	0.46
1:C:57:ASN:O	1:C:59:PRO:CD	2.64	0.46
1:C:339:VAL:HB	1:C:340:PRO:HD2	1.98	0.46
1:A:328:PHE:O	1:A:329:LEU:C	2.59	0.46
1:C:90:ILE:HB	1:C:91:PRO:HD3	1.97	0.45
1:A:174:ARG:HB2	1:A:177:GLU:HB3	1.98	0.45
1:B:421:GLU:O	1:B:422:TYR:C	2.59	0.45
1:A:57:ASN:ND2	1:A:254:SER:HB2	2.31	0.45
1:B:33:ALA:O	1:B:43:ILE:HD13	2.15	0.45
1:A:261:ASP:OD1	1:A:263:THR:HB	2.16	0.45
1:A:341:GLN:NE2	2:A:501:UPG:H2C	2.31	0.45
1:C:151:ASN:HD21	1:C:384:ASN:ND2	2.14	0.45
1:B:57:ASN:HB3	1:B:254:SER:HB2	1.97	0.45
1:B:83:GLY:C	1:B:85:LEU:H	2.25	0.45
1:B:353:PHE:CE2	1:B:355:THR:HB	2.52	0.45
1:A:212:LYS:HD3	1:A:236:GLU:O	2.17	0.45
1:A:304:GLN:HE22	1:A:416:VAL:HG11	1.82	0.45
1:B:32:LEU:O	1:B:33:ALA:C	2.60	0.45
1:A:307:LEU:HD11	1:A:336:VAL:HG21	2.00	0.44
1:A:343:GLU:OE2	1:A:343:GLU:HA	2.18	0.44
1:B:398:LEU:HD21	1:B:410:ALA:CB	2.47	0.44
1:A:17:LEU:HD13	1:A:33:ALA:HB2	1.98	0.44
1:B:102:ARG:CG	1:B:106:GLU:OE2	2.61	0.44
1:B:308:TRP:HB3	1:B:335:ILE:HD13	1.98	0.44
1:B:323:PRO:O	1:B:324:LEU:C	2.61	0.44
1:B:438:LEU:O	1:B:445:TYR:HB2	2.18	0.44
1:C:225:LEU:CD1	1:C:430:LEU:HD21	2.46	0.44
1:B:242:PHE:CD1	1:B:451:LEU:HB2	2.52	0.44
1:A:450:SER:O	1:A:454:TYR:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:HIS:HB3	1:A:340:PRO:HD3	1.99	0.44
1:B:285:THR:HG21	1:B:377:PHE:CZ	2.53	0.44
1:A:128:TYR:O	1:A:210:GLN:HG3	2.18	0.44
1:A:185:LEU:HA	1:A:386:ARG:HG2	2.00	0.44
1:B:287:VAL:CG2	1:B:314:PHE:CE2	3.01	0.44
1:B:354:TRP:CD1	1:B:373:ILE:HG22	2.53	0.44
1:A:150:PHE:HE2	1:A:185:LEU:HD21	1.83	0.43
1:C:390:ASP:O	1:C:393:LYS:HG3	2.18	0.43
1:A:193:GLY:O	1:A:379:LEU:O	2.36	0.43
1:C:355:THR:N	1:C:373:ILE:O	2.52	0.43
1:B:20:VAL:HG22	1:B:127:TRP:CE2	2.54	0.43
1:B:394:VAL:HG11	1:B:430:LEU:HD22	2.01	0.43
1:A:113:GLU:HB2	1:A:116:GLU:HG2	2.00	0.43
1:B:210:GLN:OE1	1:B:210:GLN:HA	2.19	0.43
1:B:292:PHE:CE2	1:B:324:LEU:HG	2.54	0.43
1:B:353:PHE:N	1:B:371:PRO:O	2.52	0.43
1:A:140:ARG:HB2	1:A:215:SER:OG	2.19	0.43
1:B:18:PHE:CE1	1:B:127:TRP:NE1	2.87	0.43
1:B:101:LEU:HD23	1:B:129:PHE:CE2	2.53	0.43
1:B:365:SER:O	1:B:370:VAL:N	2.45	0.43
1:C:93:ILE:HG22	1:C:129:PHE:CE1	2.53	0.43
1:C:149:LEU:O	1:C:150:PHE:C	2.61	0.43
1:C:14:ARG:NH2	1:C:108:LEU:HD21	2.34	0.43
1:B:141:ARG:NH2	1:B:143:VAL:HG12	2.34	0.43
1:B:420:GLY:O	1:B:422:TYR:N	2.51	0.43
1:C:30:LEU:CD2	1:C:45:ILE:HD13	2.49	0.43
1:C:67:LEU:HD23	1:C:100:GLU:OE2	2.19	0.43
1:C:386:ARG:HG3	1:C:386:ARG:NH1	2.29	0.43
1:C:357:SER:OG	1:C:385:ALA:HB2	2.18	0.42
1:A:20:VAL:HG22	1:A:127:TRP:CE2	2.53	0.42
1:A:257:LEU:C	1:A:258:LEU:HD12	2.44	0.42
1:B:148:SER:HB2	1:B:226:GLU:OE2	2.19	0.42
1:C:152:PHE:O	1:C:153:HIS:C	2.62	0.42
1:A:26:ILE:O	1:A:27:ASN:C	2.61	0.42
1:A:33:ALA:O	1:A:43:ILE:CD1	2.67	0.42
1:A:437:SER:HB3	1:A:444:SER:CB	2.50	0.42
1:C:366:VAL:O	1:C:431:LYS:HA	2.19	0.42
1:C:128:TYR:CD1	1:C:206:ASN:HB3	2.54	0.42
1:C:149:LEU:HD23	1:C:219:TRP:CE3	2.55	0.42
1:A:306:PHE:CE1	1:A:329:LEU:HD13	2.54	0.42
1:C:294:GLU:O	1:C:295:ILE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ALA:O	1:A:389:SER:OG	2.27	0.42
1:B:246:LEU:N	1:B:247:PRO:CD	2.82	0.42
1:B:386:ARG:NH1	1:B:390:ASP:OD2	2.40	0.42
1:B:403:GLU:O	1:B:405:GLY:N	2.53	0.42
1:B:274:ARG:CD	1:B:350:ILE:O	2.68	0.42
1:B:414:VAL:O	1:B:424:ARG:HD3	2.19	0.42
1:B:37:TYR:O	1:B:38:SER:C	2.61	0.42
1:C:44:THR:HA	1:C:62:THR:O	2.19	0.42
1:C:57:ASN:O	1:C:59:PRO:HD3	2.19	0.41
1:A:164:LEU:HD13	1:A:166:TYR:OH	2.20	0.41
1:C:265:PHE:HZ	1:C:343:GLU:HB3	1.85	0.41
1:B:283:SER:OG	2:B:501:UPG:O2B	2.30	0.41
1:C:140:ARG:HH11	1:C:140:ARG:HA	1.86	0.41
1:C:431:LYS:O	1:C:435:ASP:OD2	2.38	0.41
1:A:30:LEU:CD2	1:A:45:ILE:HD13	2.51	0.41
1:B:158:LEU:N	1:B:159:PRO:CD	2.84	0.41
1:C:93:ILE:O	1:C:97:GLY:N	2.54	0.41
1:C:265:PHE:CZ	1:C:343:GLU:HB3	2.56	0.41
1:A:57:ASN:HD22	1:A:254:SER:HB2	1.85	0.41
1:A:97:GLY:O	1:A:98:ALA:C	2.64	0.41
1:A:150:PHE:CD2	1:A:387:TYR:CD1	3.08	0.41
1:A:348:GLY:C	1:A:350:ILE:N	2.78	0.41
1:A:206:ASN:O	1:A:210:GLN:N	2.42	0.41
1:C:281:PHE:HA	1:C:356:HIS:HB3	2.03	0.41
1:C:281:PHE:O	1:C:285:THR:OG1	2.35	0.41
1:A:18:PHE:CD1	1:A:18:PHE:C	2.99	0.41
1:B:30:LEU:HD12	1:B:255:SER:CB	2.51	0.41
1:B:123:THR:OG1	1:B:141:ARG:NH2	2.54	0.41
1:B:353:PHE:O	1:B:372:MET:HA	2.20	0.41
1:C:21:PRO:O	1:C:22:PHE:CD1	2.74	0.41
1:C:91:PRO:HA	1:C:94:ASN:HB2	2.02	0.41
1:C:422:TYR:O	1:C:423:ILE:C	2.63	0.41
1:C:219:TRP:CD1	1:C:241:SER:HB2	2.56	0.41
1:A:166:TYR:CD1	1:A:187:VAL:HG13	2.56	0.40
1:A:365:SER:O	1:A:366:VAL:C	2.63	0.40
1:A:230:LEU:CD2	1:A:243:LEU:HD11	2.51	0.40
1:A:230:LEU:HD21	1:A:243:LEU:HD11	2.03	0.40
1:A:307:LEU:HD11	1:A:336:VAL:CG2	2.51	0.40
1:A:335:ILE:O	1:A:336:VAL:HG13	2.21	0.40
1:B:374:PHE:N	1:B:396:VAL:O	2.34	0.40
1:A:268:LEU:HA	1:A:271:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:CD2	1:C:219:TRP:CE3	3.04	0.40
1:A:371:PRO:HB3	1:A:423:ILE:HG22	2.03	0.40
1:A:293:LEU:O	1:A:296:ALA:HB3	2.21	0.40
1:C:154:ALA:O	1:C:156:VAL:N	2.54	0.40
1:C:208:THR:HG22	1:C:212:LYS:HE3	2.03	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	431/458 (94%)	372 (86%)	48 (11%)	11 (3%)	4	15
1	B	391/458 (85%)	341 (87%)	45 (12%)	5 (1%)	9	31
1	C	323/458 (70%)	269 (83%)	46 (14%)	8 (2%)	4	16
All	All	1145/1374 (83%)	982 (86%)	139 (12%)	24 (2%)	5	20

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	A	457	SER
1	B	419	GLU
1	C	98	ALA
1	C	381	GLN
1	A	398	LEU
1	A	116	GLU
1	A	250	LEU
1	A	329	LEU
1	A	349	ALA
1	A	379	LEU
1	A	393	LYS

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Mol	Chain	Res	Type
1	A	443	SER
1	B	77	SER
1	B	88	MET
1	B	404	ARG
1	B	421	GLU
1	C	154	ALA
1	C	155	HIS
1	C	273	SER
1	C	443	SER
1	C	295	ILE
1	A	344	VAL
1	C	394	VAL

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	386/408 (95%)	368 (95%)	18 (5%)	23	57
1	B	353/408 (86%)	338 (96%)	15 (4%)	26	61
1	C	299/408 (73%)	273 (91%)	26 (9%)	9	30
All	All	1038/1224 (85%)	979 (94%)	59 (6%)	18	49

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	142	LEU
1	A	147	SER
1	A	148	SER
1	A	151	ASN
1	A	156	VAL
1	A	169	PRO
1	A	184	MET
1	A	198	LYS
1	A	251	THR

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Mol	Chain	Res	Type
1	A	253	SER
1	A	263	THR
1	A	285	THR
1	A	328	PHE
1	A	329	LEU
1	A	336	VAL
1	A	389	SER
1	A	447	SER
1	B	38	SER
1	B	121	LEU
1	B	123	THR
1	B	143	VAL
1	B	144	LEU
1	B	156	VAL
1	B	163	GLU
1	B	224	GLU
1	B	286	GLU
1	B	305	SER
1	B	318	SER
1	B	387	TYR
1	B	389	SER
1	B	416	VAL
1	B	443	SER
1	C	12	ARG
1	C	13	ARG
1	C	53	PRO
1	C	56	SER
1	C	66	ILE
1	C	67	LEU
1	C	89	ARG
1	C	108	LEU
1	C	117	GLU
1	C	137	LEU
1	C	144	LEU
1	C	160	GLN
1	C	230	LEU
1	C	232	THR
1	C	247	PRO
1	C	260	HIS
1	C	309	VAL
1	C	343	GLU
1	C	347	HIS

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Mol	Chain	Res	Type
1	C	353	PHE
1	C	361	SER
1	C	387	TYR
1	C	396	VAL
1	C	418	GLU
1	C	446	GLU
1	C	453	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	153	HIS
1	A	199	GLN
1	A	270	GLN
1	A	304	GLN
1	A	341	GLN
1	A	360	ASN
1	A	426	ASN
1	B	34	ASN
1	B	60	HIS
1	B	82	HIS
1	B	155	HIS
1	B	342	GLN
1	B	432	GLN
1	C	23	GLN
1	C	34	ASN
1	C	151	ASN
1	C	160	GLN
1	C	341	GLN
1	C	384	ASN
1	C	425	GLN
1	C	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	IPA	A	502	-	3,3,3	0.25	0	3,3,3	0.26	0
4	PO4	C	501	-	4,4,4	0.69	0	6,6,6	0.59	0
2	UPG	B	501	-	25,26,38	0.65	0	38,40,58	0.68	0
2	UPG	A	501	-	25,26,38	0.76	1 (4%)	38,40,58	0.63	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	UPG	B	501	-	-	1/16/32/59	0/2/2/3
2	UPG	A	501	-	-	1/16/32/59	0/2/2/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UPG	PA-O3A	2.36	1.62	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

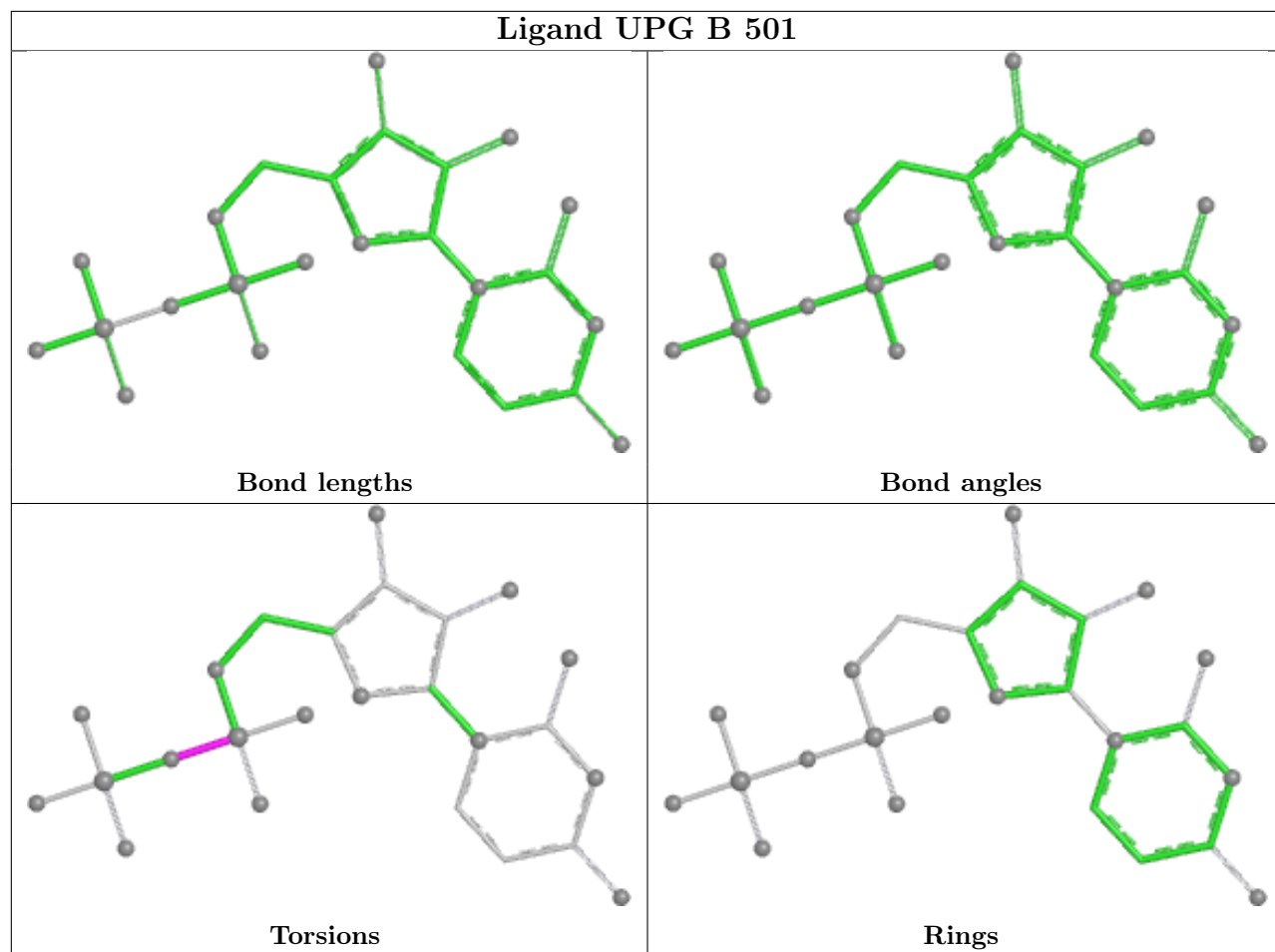
Mol	Chain	Res	Type	Atoms
2	A	501	UPG	PB-O3A-PA-O5C
2	B	501	UPG	PB-O3A-PA-O5C

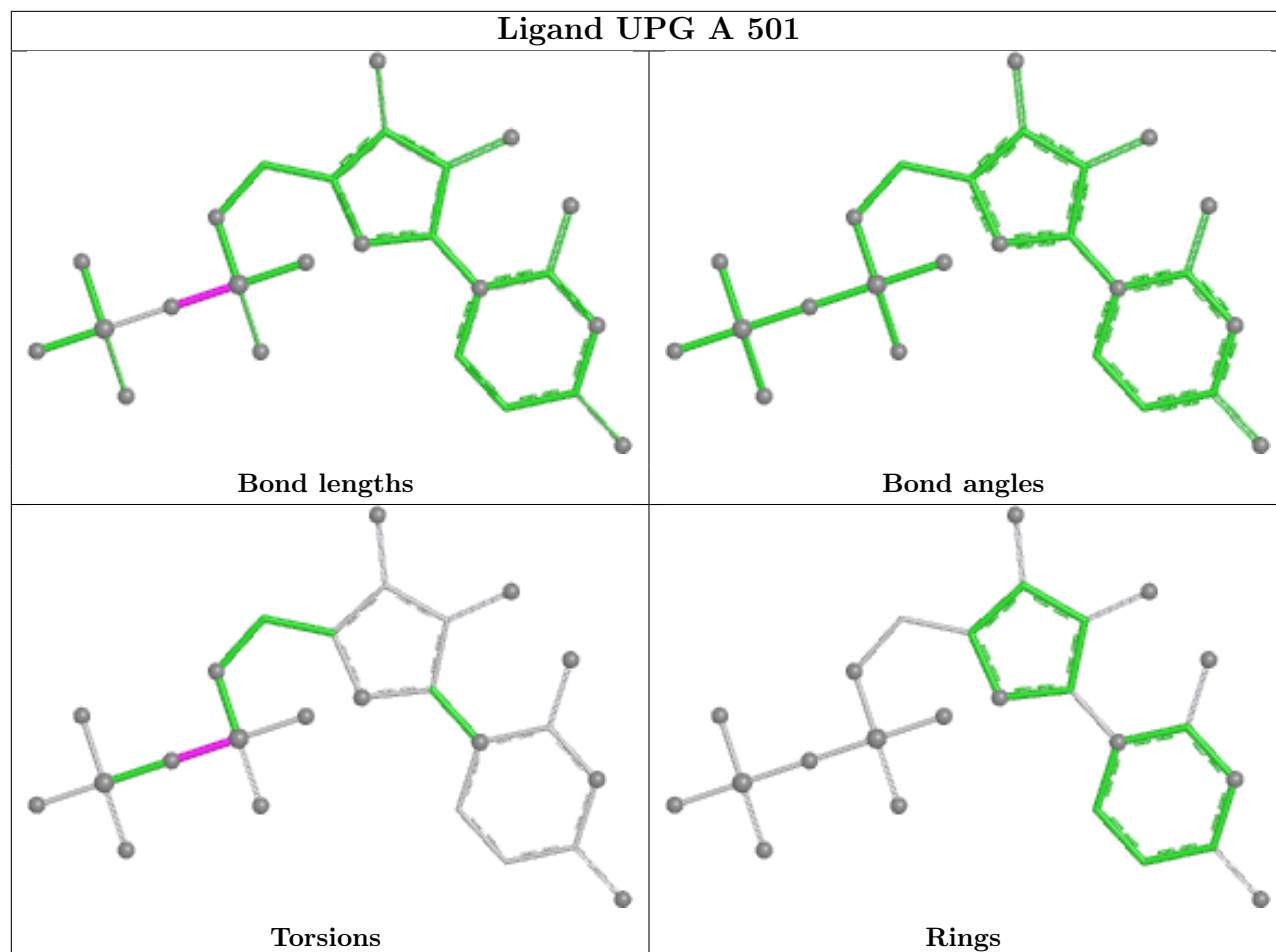
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	PO4	2	0
2	B	501	UPG	1	0
2	A	501	UPG	2	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 [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	434/458 (94%)	-1.59	0 100 100	16, 48, 96, 142	1 (0%)
1	B	399/458 (87%)	-1.61	0 100 100	26, 48, 88, 121	0
1	C	338/458 (73%)	-1.53	0 100 100	21, 65, 104, 129	1 (0%)
All	All	1171/1374 (85%)	-1.58	0 100 100	16, 52, 98, 142	2 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

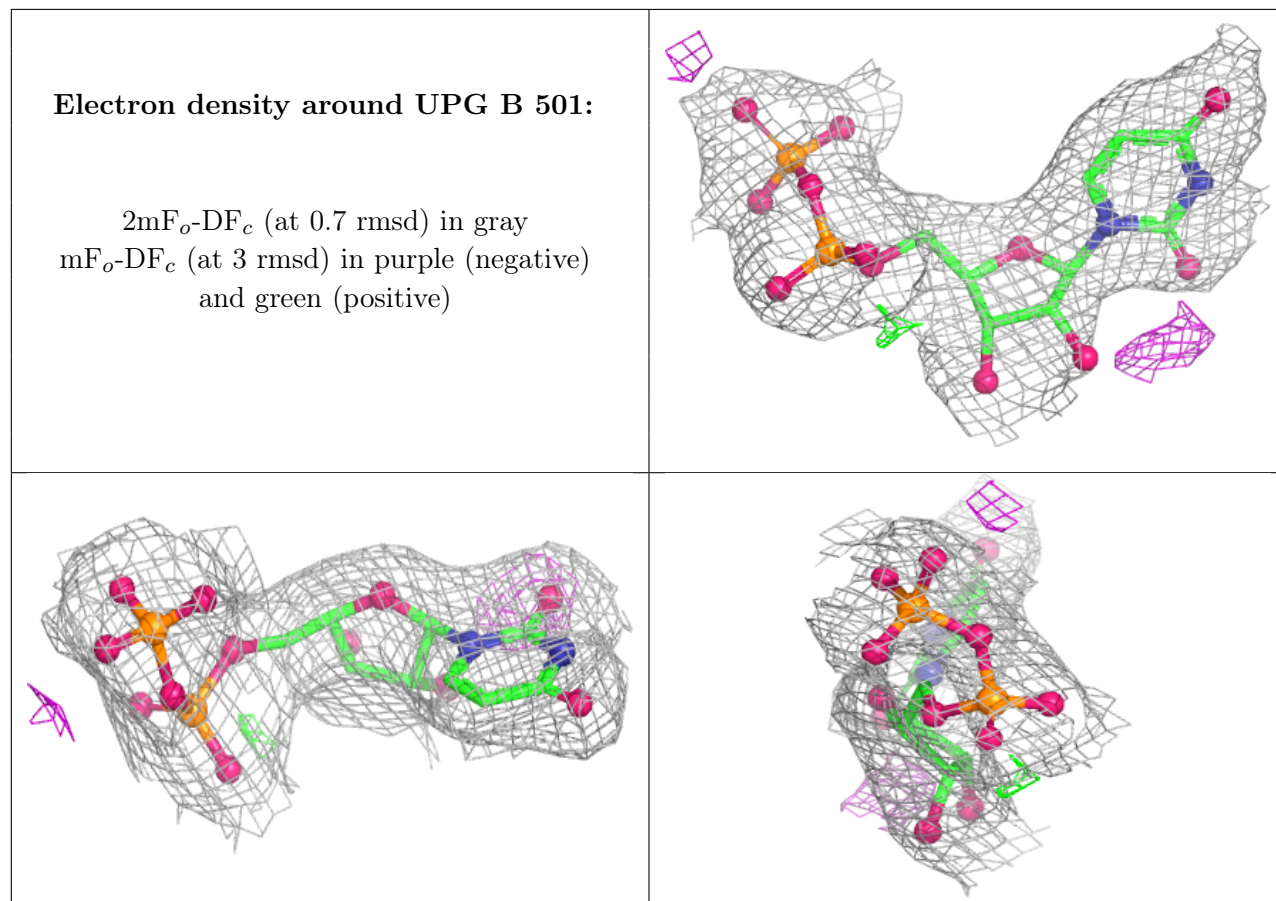
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	C	501	5/5	0.98	0.03	66,67,72,74	0
2	UPG	B	501	25/36	0.99	0.02	27,33,47,48	0
3	IPA	A	502	4/4	0.99	0.04	47,49,49,49	0
2	UPG	A	501	25/36	0.99	0.03	31,38,49,53	0

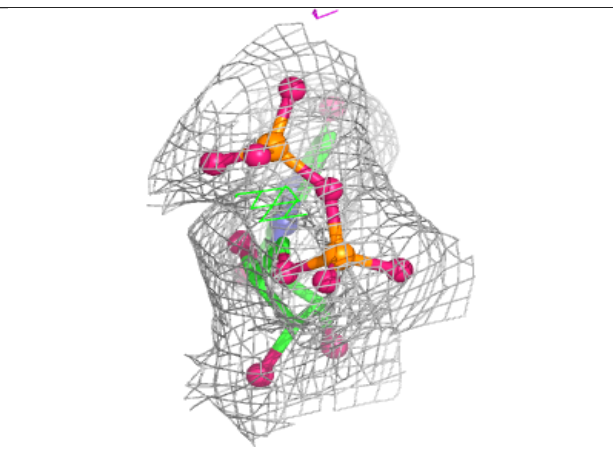
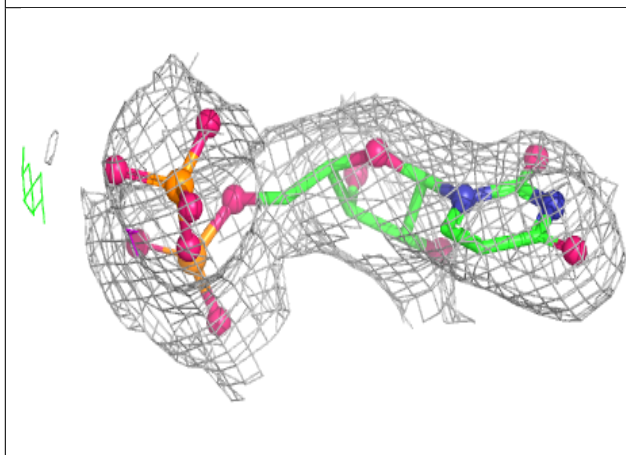
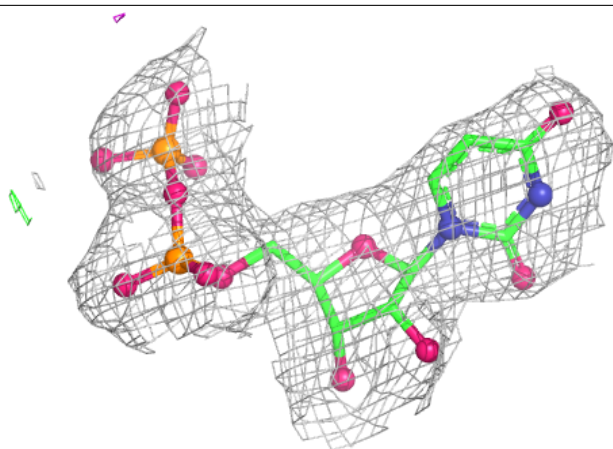
The following is a graphical depiction of the model fit to experimental electron density of all

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 UPG A 501:

$2mF_o-DF_c$ (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.