



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2026 – 12:12 PM JST

PDB ID : 9WE5 / pdb_00009we5
Title : UDP-Glucose-bound UgtP with deletion of Pro48-Met91 and insertion of a Ser-Ser-Ser linker
Authors : Fujishiro, T.
Deposited on : 2025-08-19
Resolution : 3.70 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

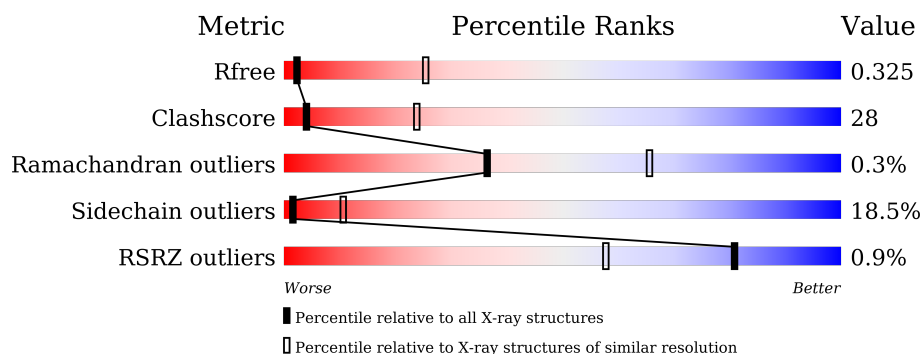
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	349	% 51% 34% 7% 7%
1	B	349	 42% 40% 10% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5201 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 Processive diacylglycerol beta-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2567	1632	441	480	14			
1	B	324	Total	C	N	O	S	0	0	0
			2562	1628	440	480	14			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P54166
A	?	-	ILE	deletion	UNP P54166
A	?	-	VAL	deletion	UNP P54166
A	?	-	SER	deletion	UNP P54166
A	?	-	GLU	deletion	UNP P54166
A	?	-	VAL	deletion	UNP P54166
A	?	-	THR	deletion	UNP P54166
A	?	-	GLN	deletion	UNP P54166
A	?	-	TYR	deletion	UNP P54166
A	?	-	LEU	deletion	UNP P54166
A	?	-	TYR	deletion	UNP P54166
A	?	-	LEU	deletion	UNP P54166
A	?	-	LYS	deletion	UNP P54166
A	?	-	SER	deletion	UNP P54166
A	?	-	PHE	deletion	UNP P54166
A	?	-	SER	deletion	UNP P54166
A	?	-	ILE	deletion	UNP P54166
A	?	-	GLY	deletion	UNP P54166
A	?	-	LYS	deletion	UNP P54166
A	?	-	GLN	deletion	UNP P54166
A	?	-	PHE	deletion	UNP P54166
A	?	-	TYR	deletion	UNP P54166
A	?	-	ARG	deletion	UNP P54166
A	?	-	LEU	deletion	UNP P54166
A	?	-	PHE	deletion	UNP P54166

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP P54166
A	?	-	TYR	deletion	UNP P54166
A	?	-	GLY	deletion	UNP P54166
A	?	-	VAL	deletion	UNP P54166
A	?	-	ASP	deletion	UNP P54166
A	?	-	LYS	deletion	UNP P54166
A	?	-	ILE	deletion	UNP P54166
A	?	-	TYR	deletion	UNP P54166
A	?	-	ASN	deletion	UNP P54166
A	?	-	LYS	deletion	UNP P54166
A	?	-	ARG	deletion	UNP P54166
A	?	-	LYS	deletion	UNP P54166
A	?	-	PHE	deletion	UNP P54166
A	?	-	ASN	deletion	UNP P54166
A	?	-	ILE	deletion	UNP P54166
A	?	-	TYR	deletion	UNP P54166
A	?	-	PHE	deletion	UNP P54166
A	?	-	LYS	deletion	UNP P54166
A	?	-	MET	deletion	UNP P54166
A	89	SER	-	linker	UNP P54166
A	90	SER	-	linker	UNP P54166
A	91	SER	-	linker	UNP P54166
A	383	LEU	-	expression tag	UNP P54166
A	384	GLU	-	expression tag	UNP P54166
A	385	HIS	-	expression tag	UNP P54166
A	386	HIS	-	expression tag	UNP P54166
A	387	HIS	-	expression tag	UNP P54166
A	388	HIS	-	expression tag	UNP P54166
A	389	HIS	-	expression tag	UNP P54166
A	390	HIS	-	expression tag	UNP P54166
B	?	-	PRO	deletion	UNP P54166
B	?	-	ILE	deletion	UNP P54166
B	?	-	VAL	deletion	UNP P54166
B	?	-	SER	deletion	UNP P54166
B	?	-	GLU	deletion	UNP P54166
B	?	-	VAL	deletion	UNP P54166
B	?	-	THR	deletion	UNP P54166
B	?	-	GLN	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	LEU	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	LEU	deletion	UNP P54166

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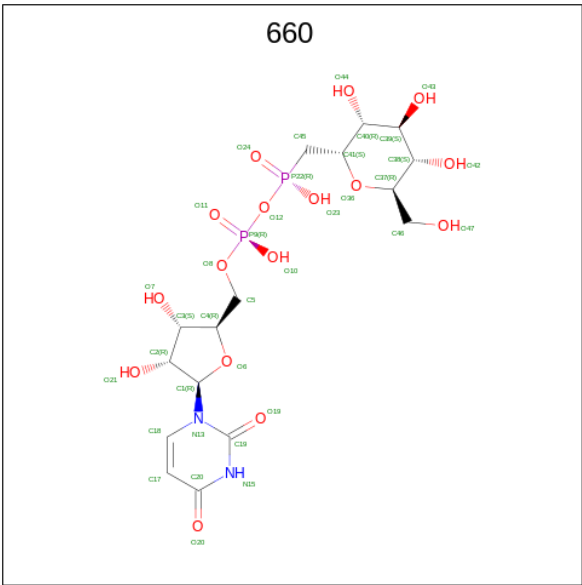
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP P54166
B	?	-	SER	deletion	UNP P54166
B	?	-	PHE	deletion	UNP P54166
B	?	-	SER	deletion	UNP P54166
B	?	-	ILE	deletion	UNP P54166
B	?	-	GLY	deletion	UNP P54166
B	?	-	LYS	deletion	UNP P54166
B	?	-	GLN	deletion	UNP P54166
B	?	-	PHE	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	ARG	deletion	UNP P54166
B	?	-	LEU	deletion	UNP P54166
B	?	-	PHE	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	GLY	deletion	UNP P54166
B	?	-	VAL	deletion	UNP P54166
B	?	-	ASP	deletion	UNP P54166
B	?	-	LYS	deletion	UNP P54166
B	?	-	ILE	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	ASN	deletion	UNP P54166
B	?	-	LYS	deletion	UNP P54166
B	?	-	ARG	deletion	UNP P54166
B	?	-	LYS	deletion	UNP P54166
B	?	-	PHE	deletion	UNP P54166
B	?	-	ASN	deletion	UNP P54166
B	?	-	ILE	deletion	UNP P54166
B	?	-	TYR	deletion	UNP P54166
B	?	-	PHE	deletion	UNP P54166
B	?	-	LYS	deletion	UNP P54166
B	?	-	MET	deletion	UNP P54166
B	89	SER	-	linker	UNP P54166
B	90	SER	-	linker	UNP P54166
B	91	SER	-	linker	UNP P54166
B	383	LEU	-	expression tag	UNP P54166
B	384	GLU	-	expression tag	UNP P54166
B	385	HIS	-	expression tag	UNP P54166
B	386	HIS	-	expression tag	UNP P54166
B	387	HIS	-	expression tag	UNP P54166
B	388	HIS	-	expression tag	UNP P54166
B	389	HIS	-	expression tag	UNP P54166

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Chain	Residue	Modelled	Actual	Comment	Reference
B	390	HIS	-	expression tag	UNP P54166

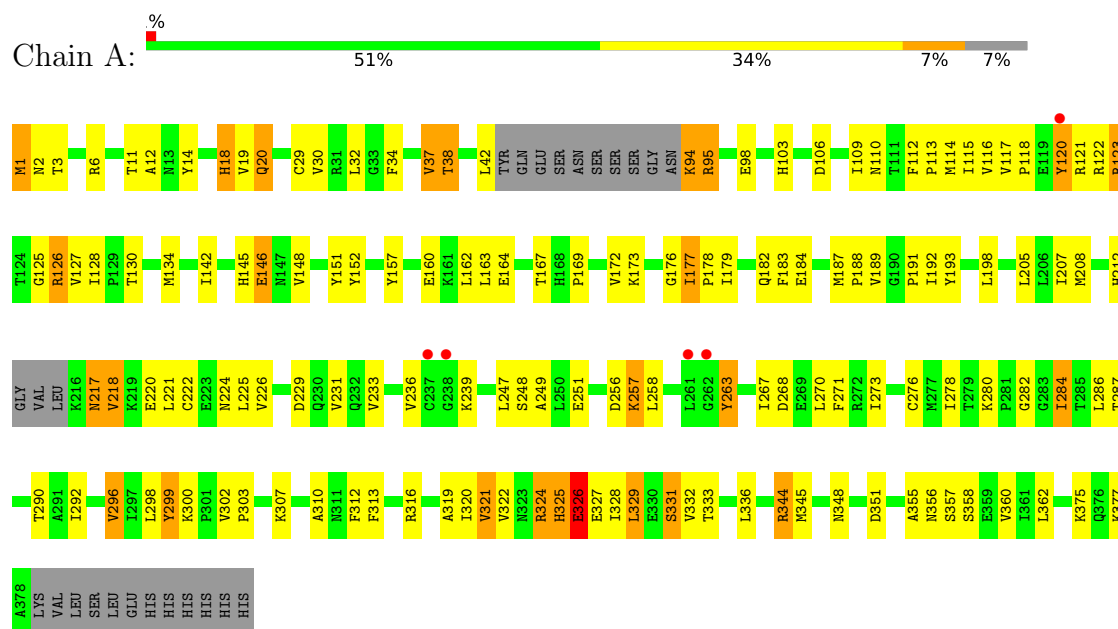
- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-[[[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]methyl]phosphinic acid (CCD ID: 660) (formula: C₁₆H₂₆N₂O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



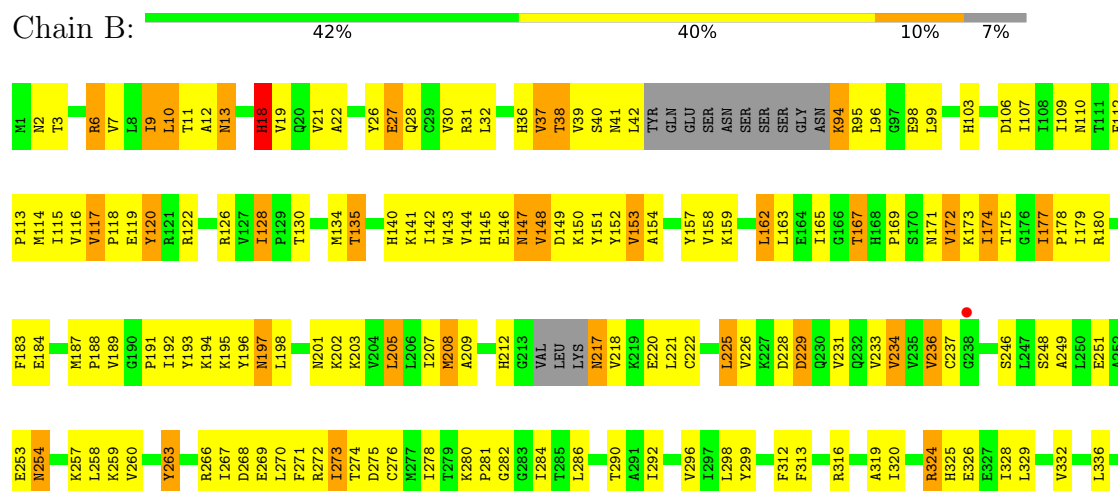
3 Residue-property plots

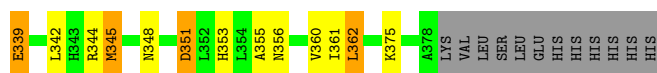
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Processive diacylglycerol beta-glucosyltransferase



• Molecule 1: Processive diacylglycerol beta-glucosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.12Å 64.08Å 110.66Å 90.00° 107.23° 90.00°	Depositor
Resolution (Å)	48.05 – 3.70 48.05 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.05-3.70) 99.5 (48.05-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.230 , 0.310 0.230 , 0.325	Depositor DCC
R_{free} test set	477 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 660

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	0.56	0/2608	1.27	3/3526 (0.1%)
1	B	0.56	0/2603	1.34	9/3520 (0.3%)
All	All	0.56	0/5211	1.30	12/7046 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	GLU	N-CA-C	-6.51	106.55	114.75
1	B	197	ASN	CA-CB-CG	6.33	118.92	112.60
1	A	18	HIS	CB-CA-C	5.93	118.64	109.03
1	B	41	ASN	CA-CB-CG	5.81	118.41	112.60
1	B	119	GLU	CB-CG-CD	5.75	122.37	112.60
1	B	135	THR	CA-CB-OG1	-5.40	101.50	109.60
1	B	41	ASN	CB-CA-C	-5.34	100.41	110.51
1	B	218	VAL	CA-C-N	5.26	128.71	120.82
1	B	218	VAL	C-N-CA	5.26	128.71	120.82
1	B	18	HIS	CA-CB-CG	5.25	119.05	113.80
1	B	13	ASN	CB-CA-C	5.20	119.05	110.88
1	A	146	GLU	CB-CA-C	5.04	117.98	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2641	125	0
1	B	2562	0	2631	165	0
2	A	36	0	0	4	0
2	B	36	0	0	0	0
All	All	5201	0	5272	291	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 28.

All (291) 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:229:ASP:HA	1:A:257:LYS:NZ	1.38	1.34
1:B:151:TYR:HD2	1:B:162:LEU:HD11	1.09	1.15
1:B:299:TYR:CD1	1:B:328:ILE:HD11	1.80	1.15
1:A:325:HIS:HA	1:A:328:ILE:HG23	1.26	1.14
1:A:224:ASN:HB3	1:A:329:LEU:CD2	1.87	1.04
1:A:113:PRO:HG2	1:A:114:MET:HE3	1.41	1.00
1:B:151:TYR:CD2	1:B:162:LEU:HD11	1.99	0.97
1:A:224:ASN:CB	1:A:329:LEU:HD23	1.95	0.96
1:A:229:ASP:CA	1:A:257:LYS:HZ1	1.80	0.95
1:A:224:ASN:HB3	1:A:329:LEU:HD23	1.50	0.93
1:A:229:ASP:HA	1:A:257:LYS:HZ3	1.33	0.92
1:B:113:PRO:HB2	1:B:140:HIS:CD2	2.06	0.91
1:B:117:VAL:HG12	1:B:144:VAL:HG23	1.53	0.89
1:B:205:LEU:HD11	1:B:278:ILE:HD11	1.52	0.88
1:B:217:ASN:N	1:B:220:GLU:HB2	1.87	0.87
1:B:153:VAL:HG12	1:B:158:VAL:HG12	1.56	0.85
1:A:151:TYR:HB2	1:A:172:VAL:HG22	1.59	0.85
1:A:267:ILE:HG21	2:A:401:660:O19	1.76	0.85
1:A:325:HIS:HA	1:A:328:ILE:CG2	2.05	0.85
1:A:239:LYS:HG2	1:A:263:TYR:CE2	2.13	0.82
1:A:251:GLU:HA	1:A:258:LEU:HD23	1.60	0.82
1:B:143:TRP:CZ3	1:B:145:HIS:HB3	2.13	0.82
1:A:224:ASN:CB	1:A:329:LEU:CD2	2.55	0.82
1:B:94:LYS:C	1:B:96:LEU:H	1.88	0.82
1:B:251:GLU:HA	1:B:258:LEU:HD23	1.60	0.82
1:B:205:LEU:HD11	1:B:278:ILE:CD1	2.09	0.81
1:B:151:TYR:HD2	1:B:162:LEU:CD1	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ALA:HB2	1:A:112:PHE:CD2	2.17	0.80
1:A:229:ASP:HA	1:A:257:LYS:HZ1	0.98	0.79
1:B:153:VAL:CG1	1:B:158:VAL:HG12	2.13	0.79
1:B:173:LYS:O	1:B:175:THR:HG23	1.82	0.78
1:B:7:VAL:HG12	1:B:107:ILE:HB	1.66	0.77
1:B:9:ILE:HG13	1:B:39:VAL:HG22	1.66	0.77
1:A:188:PRO:HG2	1:A:191:PRO:HG2	1.68	0.76
1:A:229:ASP:CA	1:A:257:LYS:NZ	2.34	0.76
1:B:299:TYR:HD1	1:B:328:ILE:HD11	1.47	0.75
1:B:263:TYR:HD1	1:B:263:TYR:H	1.34	0.75
1:B:203:LYS:HD3	1:B:336:LEU:HD22	1.67	0.75
1:B:324:ARG:HG2	1:B:326:GLU:OE1	1.88	0.74
1:A:12:ALA:HB2	1:A:112:PHE:CE2	2.22	0.74
1:B:196:TYR:CD1	1:B:270:LEU:HD21	2.23	0.74
1:B:228:ASP:HB3	1:B:231:VAL:HG12	1.71	0.73
1:A:205:LEU:HD11	1:A:278:ILE:HG13	1.70	0.72
1:A:224:ASN:HB2	1:A:329:LEU:HD23	1.70	0.72
1:B:229:ASP:HA	1:B:257:LYS:HE3	1.70	0.71
1:B:225:LEU:HD13	1:B:233:VAL:HG22	1.70	0.71
1:B:339:GLU:H	1:B:339:GLU:CD	1.96	0.71
1:B:6:ARG:HB3	1:B:36:HIS:HB2	1.74	0.70
1:A:332:VAL:HG12	1:A:336:LEU:HD12	1.75	0.69
1:B:114:MET:O	1:B:134:MET:HE1	1.91	0.69
1:B:117:VAL:HG22	1:B:118:PRO:HA	1.75	0.69
1:B:141:LYS:HE3	1:B:165:ILE:HG22	1.74	0.68
1:A:114:MET:O	1:A:134:MET:HE1	1.93	0.68
1:B:217:ASN:N	1:B:217:ASN:HD22	1.90	0.68
1:A:117:VAL:HG13	1:A:118:PRO:HA	1.75	0.68
1:B:203:LYS:HD2	1:B:336:LEU:HB3	1.76	0.68
1:B:299:TYR:CE1	1:B:328:ILE:HD11	2.26	0.68
1:A:178:PRO:HB3	1:A:358:SER:OG	1.94	0.68
1:B:94:LYS:O	1:B:96:LEU:N	2.27	0.67
1:B:313:PHE:HB3	1:B:319:ALA:HB2	1.76	0.66
1:B:205:LEU:HD21	1:B:207:ILE:HG13	1.76	0.66
1:B:153:VAL:HG12	1:B:158:VAL:CG1	2.24	0.66
1:B:234:VAL:HG22	1:B:259:LYS:HB2	1.77	0.65
1:B:188:PRO:HG2	1:B:191:PRO:HG2	1.76	0.65
1:B:163:LEU:HD22	1:B:169:PRO:HG3	1.76	0.65
1:B:209:ALA:HB2	1:B:237:CYS:HA	1.79	0.64
1:B:147:ASN:HD21	1:B:167:THR:HA	1.63	0.64
1:A:316:ARG:O	1:A:348:ASN:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:HG3	1:B:106:ASP:OD2	1.98	0.64
1:A:122:ARG:NH2	1:A:128:ILE:HG23	2.13	0.63
1:B:19:VAL:HG13	1:B:19:VAL:O	1.97	0.63
1:A:325:HIS:CD2	1:A:325:HIS:H	2.16	0.63
1:B:159:LYS:HE3	1:B:172:VAL:HG12	1.81	0.63
1:B:163:LEU:CD2	1:B:169:PRO:HG3	2.29	0.63
1:B:141:LYS:HE3	1:B:165:ILE:CG2	2.28	0.62
1:B:187:MET:HB2	1:B:188:PRO:HD2	1.79	0.62
1:A:189:VAL:HA	1:A:192:ILE:HD12	1.81	0.62
1:A:224:ASN:HB3	1:A:329:LEU:CG	2.30	0.62
1:B:147:ASN:OD1	1:B:147:ASN:N	2.29	0.61
1:B:316:ARG:O	1:B:348:ASN:HB3	1.99	0.61
1:A:110:ASN:HB3	1:A:112:PHE:CD1	2.35	0.61
1:B:151:TYR:HB2	1:B:172:VAL:HG22	1.81	0.61
1:A:192:ILE:HG21	1:A:273:ILE:HG23	1.81	0.61
1:A:110:ASN:HB3	1:A:112:PHE:HD1	1.66	0.60
1:B:26:TYR:HD1	1:B:37:VAL:HG22	1.65	0.60
1:B:152:TYR:CE2	1:B:361:ILE:HG23	2.37	0.60
1:B:179:ILE:HD12	1:B:183:PHE:HB2	1.83	0.60
1:B:313:PHE:HB3	1:B:319:ALA:CB	2.32	0.60
1:A:217:ASN:H	1:A:217:ASN:ND2	2.00	0.59
1:B:205:LEU:HD11	1:B:278:ILE:CG1	2.31	0.59
1:B:220:GLU:HG2	1:B:325:HIS:NE2	2.17	0.59
1:B:152:TYR:CD2	1:B:361:ILE:HG23	2.38	0.59
1:B:203:LYS:HD3	1:B:336:LEU:CD2	2.32	0.59
1:B:299:TYR:CD1	1:B:328:ILE:CD1	2.71	0.59
1:B:205:LEU:CD1	1:B:278:ILE:HD11	2.29	0.58
1:A:179:ILE:HD12	1:A:183:PHE:HB2	1.84	0.58
1:A:192:ILE:HG22	1:A:273:ILE:HG21	1.84	0.58
1:B:163:LEU:HD21	1:B:169:PRO:HB3	1.86	0.58
1:B:271:PHE:HB3	1:B:292:ILE:HG21	1.86	0.57
1:B:205:LEU:HD22	1:B:225:LEU:HD13	1.87	0.57
1:A:300:LYS:HD2	1:A:325:HIS:NE2	2.19	0.56
1:A:239:LYS:HG2	1:A:263:TYR:HE2	1.66	0.56
1:A:276:CYS:HB3	1:A:336:LEU:HD21	1.86	0.56
1:A:313:PHE:HB3	1:A:319:ALA:HB2	1.87	0.56
1:B:147:ASN:O	1:B:148:VAL:HG22	2.05	0.56
1:B:205:LEU:HD22	1:B:225:LEU:CD1	2.36	0.56
1:B:179:ILE:HD12	1:B:183:PHE:CB	2.36	0.56
1:A:151:TYR:CD2	1:A:162:LEU:HD11	2.42	0.55
1:B:344:ARG:O	1:B:348:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:HIS:CD2	1:A:325:HIS:N	2.74	0.54
1:A:187:MET:HB2	1:A:188:PRO:HD2	1.90	0.54
1:A:225:LEU:HD22	1:A:231:VAL:HG21	1.90	0.54
1:A:198:LEU:HD12	1:A:273:ILE:HD11	1.90	0.54
1:B:222:CYS:O	1:B:226:VAL:HG22	2.07	0.54
1:B:12:ALA:O	1:B:18:HIS:ND1	2.32	0.54
1:A:192:ILE:CG2	1:A:273:ILE:CG2	2.85	0.54
1:B:320:ILE:HD11	1:B:345:MET:SD	2.48	0.54
1:B:221:LEU:HD12	1:B:221:LEU:O	2.07	0.54
1:B:154:ALA:HB2	1:B:177:ILE:HD11	1.88	0.54
1:A:14:TYR:HD1	1:A:14:TYR:H	1.56	0.54
1:A:299:TYR:HD1	1:A:299:TYR:O	1.91	0.54
1:B:151:TYR:O	1:B:172:VAL:HA	2.08	0.54
1:A:19:VAL:C	1:A:20:GLN:HG2	2.33	0.53
2:A:401:660:O44	2:A:401:660:O12	2.27	0.53
1:A:12:ALA:HB2	1:A:112:PHE:HD2	1.67	0.53
1:A:303:PRO:HA	1:A:307:LYS:HB2	1.90	0.53
1:B:6:ARG:N	1:B:106:ASP:OD2	2.41	0.53
1:B:7:VAL:HG23	1:B:37:VAL:HG23	1.90	0.52
1:B:11:THR:O	1:B:112:PHE:CE2	2.62	0.52
1:B:193:TYR:O	1:B:197:ASN:N	2.42	0.52
1:A:271:PHE:HB3	1:A:292:ILE:HG21	1.90	0.52
1:B:147:ASN:ND2	1:B:167:THR:HA	2.22	0.52
1:B:217:ASN:N	1:B:217:ASN:ND2	2.58	0.52
1:A:179:ILE:HD12	1:A:183:PHE:CB	2.40	0.52
1:A:282:GLY:HA2	2:A:401:660:O42	2.09	0.52
1:B:205:LEU:HD13	1:B:332:VAL:HG11	1.91	0.52
1:A:176:GLY:O	1:A:357:SER:OG	2.28	0.52
1:B:162:LEU:HD22	1:B:167:THR:OG1	2.10	0.52
1:B:205:LEU:HD11	1:B:278:ILE:HG13	1.91	0.52
1:A:217:ASN:HB2	1:A:220:GLU:H	1.74	0.52
1:B:205:LEU:HD21	1:B:207:ILE:CG1	2.40	0.52
1:A:163:LEU:HD21	1:A:169:PRO:HA	1.92	0.51
1:B:114:MET:O	1:B:134:MET:CE	2.59	0.51
1:B:195:LYS:HD3	1:B:196:TYR:CE2	2.46	0.51
1:A:187:MET:HE2	1:A:192:ILE:HD11	1.93	0.51
1:B:6:ARG:CB	1:B:36:HIS:HB2	2.40	0.51
1:A:320:ILE:HD11	1:A:345:MET:SD	2.51	0.51
1:B:117:VAL:CG1	1:B:144:VAL:HG23	2.36	0.51
1:B:202:LYS:HD2	1:B:202:LYS:N	2.26	0.51
1:A:3:THR:HB	1:A:34:PHE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLN:O	1:B:32:LEU:HG	2.11	0.50
1:B:332:VAL:HG12	1:B:336:LEU:HD12	1.93	0.50
1:A:299:TYR:O	1:A:299:TYR:CD1	2.64	0.50
1:B:96:LEU:HD13	1:B:120:TYR:CD1	2.47	0.50
1:A:286:LEU:O	1:A:290:THR:HG23	2.11	0.50
1:B:96:LEU:HD21	1:B:120:TYR:HB3	1.94	0.49
1:B:163:LEU:HD21	1:B:169:PRO:CB	2.41	0.49
1:B:228:ASP:HB3	1:B:231:VAL:CG1	2.40	0.49
1:B:236:VAL:O	1:B:236:VAL:HG12	2.12	0.49
1:A:224:ASN:HB3	1:A:329:LEU:HG	1.95	0.49
1:A:121:ARG:HD3	1:A:125:GLY:O	2.13	0.49
1:A:184:GLU:OE2	1:A:355:ALA:HA	2.12	0.49
1:B:184:GLU:OE2	1:B:355:ALA:HA	2.13	0.49
1:A:117:VAL:CG1	1:A:118:PRO:HA	2.41	0.49
1:A:218:VAL:CG2	1:A:247:LEU:HD11	2.42	0.49
1:A:224:ASN:HB3	1:A:329:LEU:HD21	1.86	0.49
1:A:225:LEU:HD13	1:A:233:VAL:HG22	1.94	0.48
1:B:362:LEU:HD22	1:B:362:LEU:HA	1.73	0.48
1:B:6:ARG:HD2	1:B:106:ASP:OD2	2.13	0.48
1:A:312:PHE:O	1:A:316:ARG:HG2	2.13	0.48
1:A:177:ILE:HD12	1:A:287:THR:OG1	2.14	0.48
1:B:28:GLN:NE2	1:B:31:ARG:HD2	2.29	0.48
1:B:198:LEU:HD12	1:B:273:ILE:HD11	1.96	0.48
1:B:339:GLU:CD	1:B:339:GLU:N	2.70	0.48
1:B:9:ILE:H	1:B:9:ILE:HG12	1.51	0.48
1:B:117:VAL:HG12	1:B:144:VAL:CG2	2.34	0.48
1:B:157:TYR:CD2	1:B:312:PHE:CD1	3.01	0.48
1:B:225:LEU:HB3	1:B:233:VAL:HG21	1.96	0.48
1:A:192:ILE:CG2	1:A:273:ILE:HG23	2.44	0.48
1:B:12:ALA:O	1:B:18:HIS:HB3	2.14	0.47
1:B:10:LEU:HD21	1:B:42:LEU:HD13	1.95	0.47
1:B:11:THR:O	1:B:112:PHE:HE2	1.97	0.47
1:A:282:GLY:O	1:A:286:LEU:HG	2.15	0.47
1:B:122:ARG:HD3	1:B:128:ILE:HG23	1.95	0.47
1:B:254:ASN:N	1:B:254:ASN:HD22	2.13	0.47
1:B:348:ASN:O	1:B:351:ASP:HB2	2.15	0.47
1:B:94:LYS:HD2	1:B:94:LYS:HA	1.63	0.47
1:B:150:LYS:NZ	1:B:171:ASN:OD1	2.35	0.47
1:B:116:VAL:HG21	1:B:120:TYR:OH	2.14	0.47
1:B:196:TYR:CE1	1:B:270:LEU:HD21	2.49	0.47
1:B:203:LYS:HE3	1:B:336:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:HG21	1:A:19:VAL:HA	1.96	0.47
1:A:122:ARG:HH21	1:A:126:ARG:HH22	1.63	0.47
1:A:325:HIS:H	1:A:325:HIS:HD2	1.63	0.47
1:A:296:VAL:CG2	1:A:298:LEU:HD21	2.44	0.46
1:A:222:CYS:O	1:A:226:VAL:HG22	2.16	0.46
1:A:3:THR:HG21	1:A:32:LEU:O	2.16	0.46
1:A:205:LEU:HD23	1:A:225:LEU:HD13	1.98	0.46
1:B:290:THR:HB	1:B:353:HIS:HB2	1.98	0.46
1:A:29:CYS:HB2	1:A:37:VAL:HG11	1.97	0.46
1:B:110:ASN:HB3	1:B:112:PHE:CD1	2.50	0.46
1:B:282:GLY:O	1:B:286:LEU:HG	2.15	0.46
1:B:286:LEU:O	1:B:290:THR:HG23	2.15	0.46
1:A:324:ARG:HG2	1:A:326:GLU:CD	2.41	0.45
1:A:114:MET:O	1:A:134:MET:CE	2.61	0.45
1:A:296:VAL:HG23	1:A:298:LEU:HD21	1.97	0.45
1:B:345:MET:HA	1:B:348:ASN:HD22	1.82	0.45
1:A:38:THR:HG21	1:A:103:HIS:NE2	2.32	0.45
1:A:296:VAL:HG23	1:A:298:LEU:CD2	2.47	0.45
1:A:356:ASN:O	1:A:360:VAL:HG23	2.16	0.45
1:B:10:LEU:HD22	1:B:42:LEU:HD22	1.98	0.45
1:B:122:ARG:HB3	1:B:128:ILE:HD13	1.98	0.45
1:B:207:ILE:HD13	1:B:221:LEU:HD23	1.99	0.45
1:B:332:VAL:HG12	1:B:336:LEU:CD1	2.45	0.45
1:A:310:ALA:HB1	1:A:321:VAL:CG2	2.47	0.45
1:A:324:ARG:C	1:A:326:GLU:H	2.25	0.45
1:A:268:ASP:N	1:A:268:ASP:OD1	2.49	0.45
1:B:6:ARG:CG	1:B:6:ARG:HH11	2.30	0.45
1:A:116:VAL:HG21	1:A:120:TYR:OH	2.17	0.45
1:A:328:ILE:HG13	1:A:329:LEU:H	1.81	0.45
1:B:177:ILE:HG22	1:B:178:PRO:HD2	1.99	0.45
1:B:6:ARG:NH1	1:B:6:ARG:HG2	2.32	0.44
1:B:113:PRO:HD2	1:B:114:MET:SD	2.57	0.44
1:B:345:MET:HE2	1:B:345:MET:HB3	1.80	0.44
1:B:281:PRO:HB3	1:B:298:LEU:HD22	1.98	0.44
1:A:123:ARG:HD3	1:A:123:ARG:HA	1.65	0.44
1:B:145:HIS:C	1:B:146:GLU:HG3	2.43	0.44
1:A:192:ILE:CG2	1:A:273:ILE:HG21	2.47	0.44
1:A:345:MET:HE2	1:A:345:MET:HB3	1.72	0.44
1:B:38:THR:HG21	1:B:103:HIS:NE2	2.32	0.44
1:B:207:ILE:HD11	1:B:221:LEU:HG	1.99	0.44
1:A:12:ALA:HB2	1:A:112:PHE:HE2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:HG21	1:A:247:LEU:HD11	1.98	0.44
1:B:189:VAL:HA	1:B:192:ILE:HD12	2.00	0.44
1:B:192:ILE:HG21	1:B:273:ILE:HG23	2.00	0.44
1:B:203:LYS:CD	1:B:336:LEU:HD22	2.41	0.44
1:B:312:PHE:O	1:B:316:ARG:HG2	2.17	0.44
1:A:324:ARG:HG2	1:A:326:GLU:OE1	2.18	0.44
1:A:6:ARG:N	1:A:106:ASP:OD2	2.50	0.43
1:A:120:TYR:CD1	1:A:120:TYR:N	2.85	0.43
1:A:208:MET:HE3	1:A:208:MET:HB3	1.84	0.43
1:B:11:THR:HG22	1:B:22:ALA:CB	2.48	0.43
1:B:6:ARG:HH11	1:B:6:ARG:HG2	1.83	0.43
1:B:153:VAL:HG23	1:B:174:ILE:HA	2.00	0.43
1:A:313:PHE:HB3	1:A:319:ALA:CB	2.47	0.43
1:B:201:ASN:HB3	1:B:202:LYS:HD2	1.98	0.43
1:A:224:ASN:CB	1:A:329:LEU:HD21	2.45	0.43
1:B:180:ARG:HH21	1:B:267:ILE:CG2	2.31	0.43
1:B:27:GLU:HG3	1:B:31:ARG:HH12	1.83	0.43
1:A:145:HIS:O	1:A:146:GLU:HG2	2.18	0.43
1:A:217:ASN:H	1:A:217:ASN:HD22	1.64	0.43
1:B:268:ASP:OD1	1:B:269:GLU:N	2.52	0.43
1:B:221:LEU:O	1:B:225:LEU:HB2	2.19	0.43
1:B:94:LYS:C	1:B:96:LEU:N	2.57	0.43
1:A:193:TYR:CE1	1:A:273:ILE:HB	2.54	0.42
1:B:208:MET:HE3	1:B:208:MET:HB3	1.65	0.42
1:B:356:ASN:O	1:B:360:VAL:HG23	2.19	0.42
1:B:6:ARG:CG	1:B:106:ASP:OD2	2.65	0.42
1:A:348:ASN:O	1:A:351:ASP:HB2	2.19	0.42
1:B:157:TYR:HD2	1:B:312:PHE:CD1	2.38	0.42
1:A:94:LYS:HB3	1:A:95:ARG:H	1.64	0.42
1:A:248:SER:OG	1:A:249:ALA:N	2.53	0.42
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.69	0.42
1:B:320:ILE:CD1	1:B:345:MET:SD	3.07	0.42
1:A:94:LYS:HD2	1:A:94:LYS:HA	1.61	0.42
1:A:152:TYR:HA	1:A:173:LYS:O	2.19	0.42
1:B:162:LEU:CD2	1:B:167:THR:OG1	2.68	0.41
1:A:205:LEU:HD11	1:A:278:ILE:CG1	2.44	0.41
1:B:205:LEU:HD13	1:B:332:VAL:CG1	2.50	0.41
1:B:284:ILE:HD13	1:B:284:ILE:N	2.35	0.41
1:A:160:GLU:O	1:A:164:GLU:HG3	2.21	0.41
1:A:11:THR:O	1:A:42:LEU:HB2	2.21	0.41
1:A:284:ILE:N	1:A:284:ILE:HD13	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:O	1:B:39:VAL:HA	2.21	0.41
1:A:217:ASN:ND2	1:A:217:ASN:N	2.67	0.41
1:A:344:ARG:HD2	1:A:344:ARG:HA	1.56	0.41
1:A:282:GLY:HA3	2:A:401:660:O11	2.21	0.41
1:A:324:ARG:NH1	1:A:326:GLU:OE2	2.54	0.41
1:A:327:GLU:O	1:A:331:SER:OG	2.39	0.41
1:B:110:ASN:HB3	1:B:112:PHE:HD1	1.86	0.41
1:A:217:ASN:HD22	1:A:217:ASN:N	2.19	0.41
1:B:159:LYS:HE3	1:B:172:VAL:CG1	2.51	0.41
1:B:248:SER:OG	1:B:249:ALA:N	2.53	0.41
1:B:113:PRO:N	1:B:135:THR:HG22	2.35	0.41
1:A:1:MET:HB2	1:A:2:ASN:H	1.63	0.40
1:A:207:ILE:HD13	1:A:221:LEU:HD23	2.03	0.40
1:A:122:ARG:HE	1:A:126:ARG:NH2	2.19	0.40
1:B:187:MET:HE1	1:B:266:ARG:HH21	1.87	0.40
1:B:220:GLU:HB3	1:B:325:HIS:HE1	1.87	0.40
1:B:7:VAL:HA	1:B:107:ILE:O	2.21	0.40
1:B:174:ILE:H	1:B:174:ILE:HG12	1.57	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	318/349 (91%)	302 (95%)	16 (5%)	0	100	100
1	B	318/349 (91%)	296 (93%)	20 (6%)	2 (1%)	21	52
All	All	636/698 (91%)	598 (94%)	36 (6%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	ARG
1	B	148	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	290/313 (93%)	244 (84%)	46 (16%)	2	15
1	B	289/313 (92%)	228 (79%)	61 (21%)	1	7
All	All	579/626 (92%)	472 (82%)	107 (18%)	1	10

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	HIS
1	A	20	GLN
1	A	30	VAL
1	A	37	VAL
1	A	38	THR
1	A	94	LYS
1	A	95	ARG
1	A	98	GLU
1	A	109	ILE
1	A	115	ILE
1	A	120	TYR
1	A	123	ARG
1	A	126	ARG
1	A	127	VAL
1	A	130	THR
1	A	142	ILE
1	A	148	VAL
1	A	157	TYR
1	A	167	THR
1	A	177	ILE
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	212	HIS
1	A	217	ASN
1	A	218	VAL
1	A	236	VAL
1	A	256	ASP
1	A	257	LYS
1	A	263	TYR
1	A	280	LYS
1	A	284	ILE
1	A	296	VAL
1	A	299	TYR
1	A	302	VAL
1	A	321	VAL
1	A	322	VAL
1	A	324	ARG
1	A	325	HIS
1	A	326	GLU
1	A	329	LEU
1	A	331	SER
1	A	333	THR
1	A	344	ARG
1	A	362	LEU
1	A	375	LYS
1	A	377	LYS
1	B	2	ASN
1	B	3	THR
1	B	6	ARG
1	B	9	ILE
1	B	10	LEU
1	B	13	ASN
1	B	18	HIS
1	B	21	VAL
1	B	27	GLU
1	B	30	VAL
1	B	37	VAL
1	B	38	THR
1	B	40	SER
1	B	94	LYS
1	B	98	GLU
1	B	99	LEU
1	B	109	ILE
1	B	115	ILE

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Mol	Chain	Res	Type
1	B	117	VAL
1	B	120	TYR
1	B	126	ARG
1	B	128	ILE
1	B	130	THR
1	B	142	ILE
1	B	147	ASN
1	B	149	ASP
1	B	153	VAL
1	B	162	LEU
1	B	167	THR
1	B	172	VAL
1	B	174	ILE
1	B	177	ILE
1	B	194	LYS
1	B	205	LEU
1	B	208	MET
1	B	212	HIS
1	B	217	ASN
1	B	225	LEU
1	B	229	ASP
1	B	234	VAL
1	B	236	VAL
1	B	246	SER
1	B	253	GLU
1	B	254	ASN
1	B	260	VAL
1	B	263	TYR
1	B	272	ARG
1	B	273	ILE
1	B	274	THR
1	B	275	ASP
1	B	276	CYS
1	B	280	LYS
1	B	296	VAL
1	B	324	ARG
1	B	329	LEU
1	B	339	GLU
1	B	342	LEU
1	B	345	MET
1	B	351	ASP
1	B	362	LEU

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Mol	Chain	Res	Type
1	B	375	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	20	GLN
1	A	104	GLN
1	A	140	HIS
1	A	145	HIS
1	A	217	ASN
1	A	254	ASN
1	A	323	ASN
1	B	16	ASN
1	B	20	GLN
1	B	36	HIS
1	B	140	HIS
1	B	254	ASN
1	B	348	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	660	B	401	-	36,38,38	0.69	1 (2%)	49,58,58	0.88	2 (4%)
2	660	A	401	-	36,38,38	0.59	1 (2%)	49,58,58	0.61	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	660	B	401	-	-	14/20/59/59	0/3/3/3
2	660	A	401	-	-	2/20/59/59	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	660	P22-O23	-2.37	1.50	1.56
2	B	401	660	P22-O23	-2.35	1.50	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	660	C3-C2-C1	-2.53	96.61	101.43
2	B	401	660	O7-C3-C2	-2.31	104.34	111.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	660	O36-C41-C45-P22
2	B	401	660	C2-C1-N13-C18
2	B	401	660	C3-C4-C5-O8
2	B	401	660	C5-O8-P9-O10
2	B	401	660	C5-O8-P9-O12
2	B	401	660	P22-O12-P9-O8
2	B	401	660	C41-C45-P22-O12

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Mol	Chain	Res	Type	Atoms
2	B	401	660	C41-C45-P22-O23
2	B	401	660	C41-C45-P22-O24
2	B	401	660	C2-C1-N13-C19
2	B	401	660	O36-C37-C46-O47
2	B	401	660	O6-C4-C5-O8
2	B	401	660	O6-C1-N13-C19
2	B	401	660	O6-C1-N13-C18
2	B	401	660	C4-C5-O8-P9
2	A	401	660	O6-C4-C5-O8

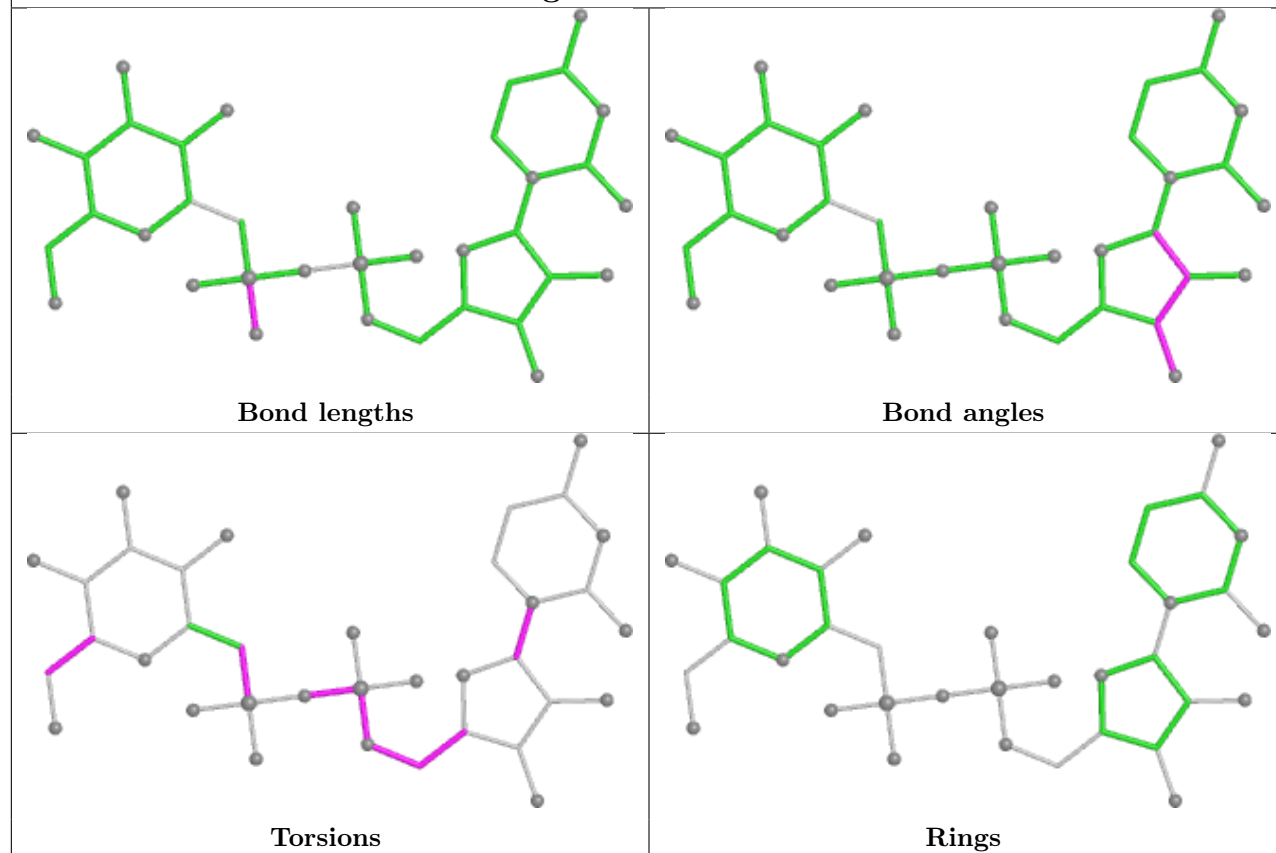
There are no ring outliers.

1 monomer is involved in 4 short contacts:

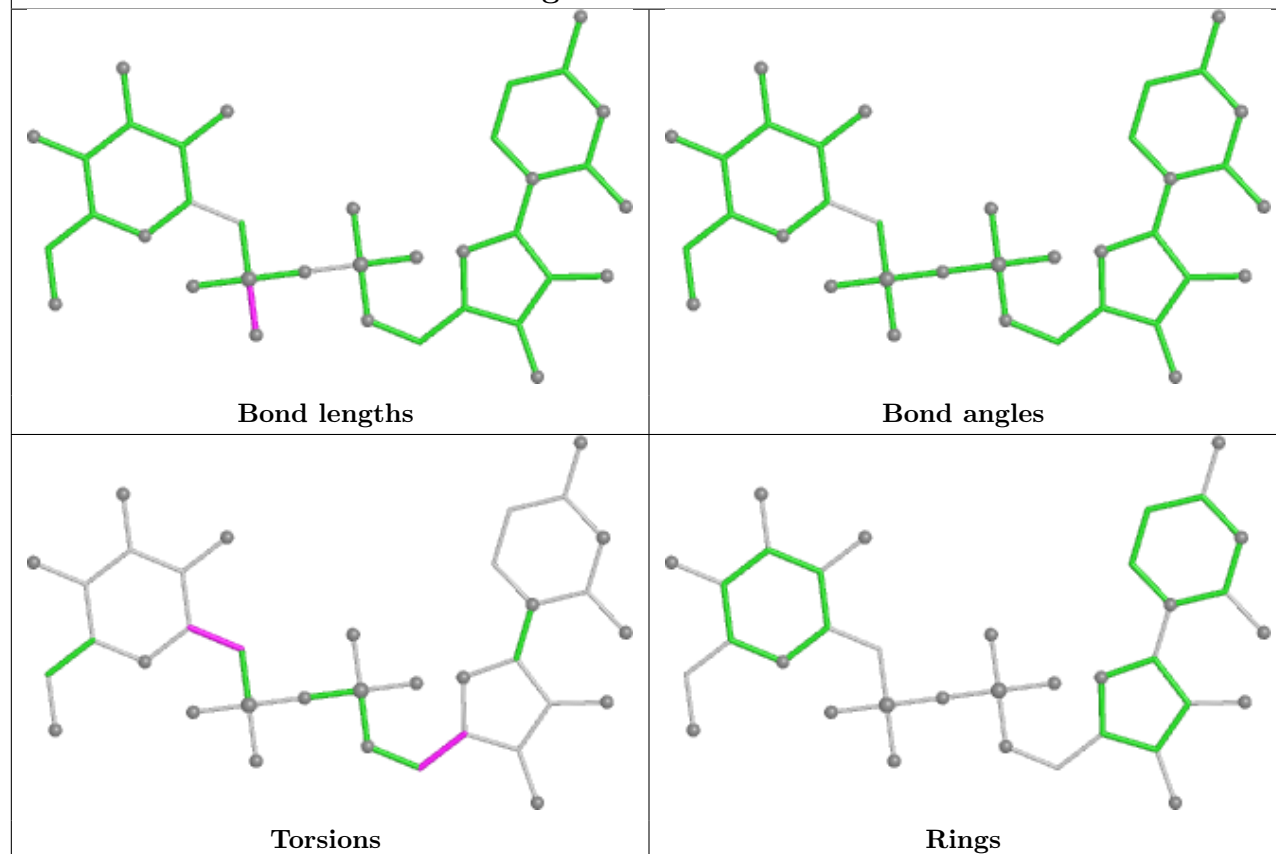
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	660	4	0

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.

Ligand 660 B 401



Ligand 660 A 401



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	324/349 (92%)	-0.42	5 (1%)	72 46	63, 120, 207, 271	0
1	B	324/349 (92%)	-0.42	1 (0%)	90 76	71, 120, 182, 220	0
All	All	648/698 (92%)	-0.42	6 (0%)	81 58	63, 120, 192, 271	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	GLY	4.1
1	A	261	LEU	2.4
1	A	237	CYS	2.2
1	B	238	GLY	2.2
1	A	120	TYR	2.2
1	A	238	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

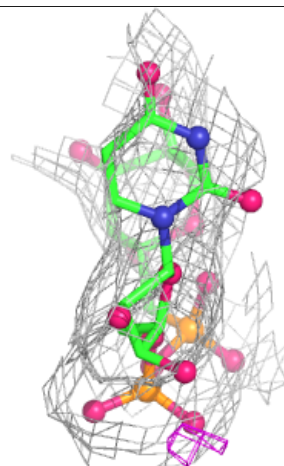
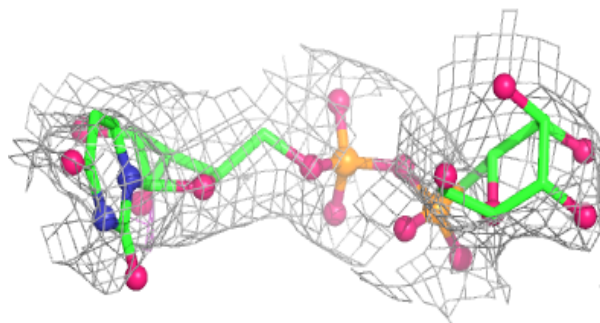
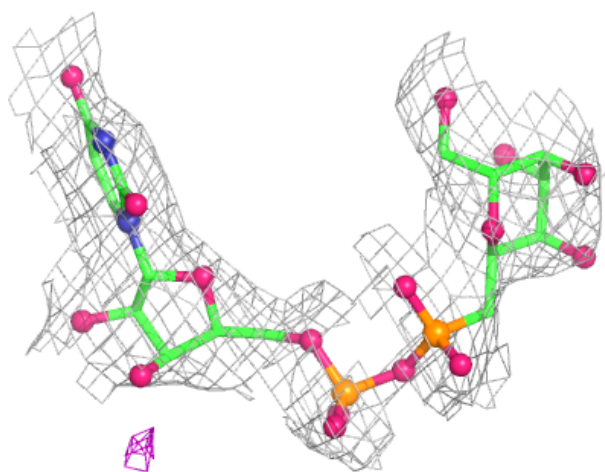
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	660	B	401	36/36	0.80	0.09	107,176,242,246	0
2	660	A	401	36/36	0.85	0.10	111,202,321,323	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.

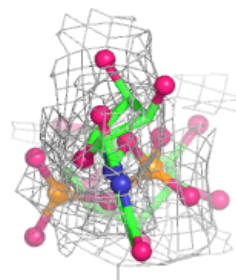
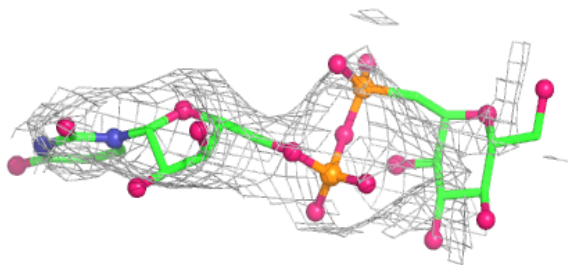
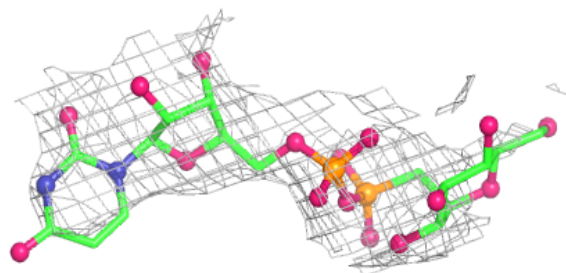
Electron density around 660 B 401:

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



Electron density around 660 A 401:

$2mF_o-DF_c$ (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.