



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:55 PM UTC

PDB ID : 1UQU / pdb_00001uqu
Title : Trehalose-6-phosphate from E. coli bound with UDP-glucose.
Authors : Gibson, R.P.; Tarling, C.A.; Roberts, S.; Withers, S.G.; Davies, G.J.
Deposited on : 2003-10-20
Resolution : 2.00 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

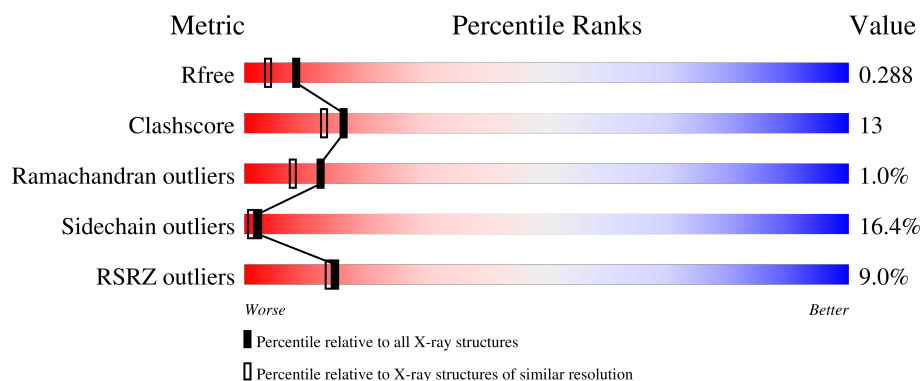
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	482	
1	B	482	

2 Entry composition [i](#)

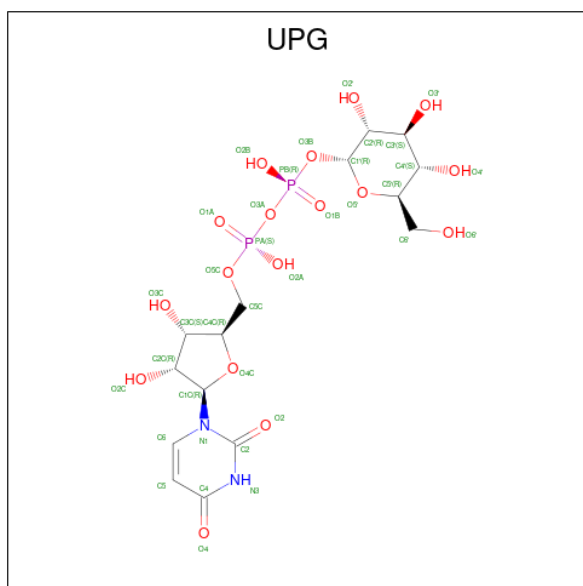
There are 3 unique types of molecules in this entry. The entry contains 7360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3625	2329	631	658	7			
1	B	449	Total	C	N	O	S	0	0	0
			3604	2317	628	652	7			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		

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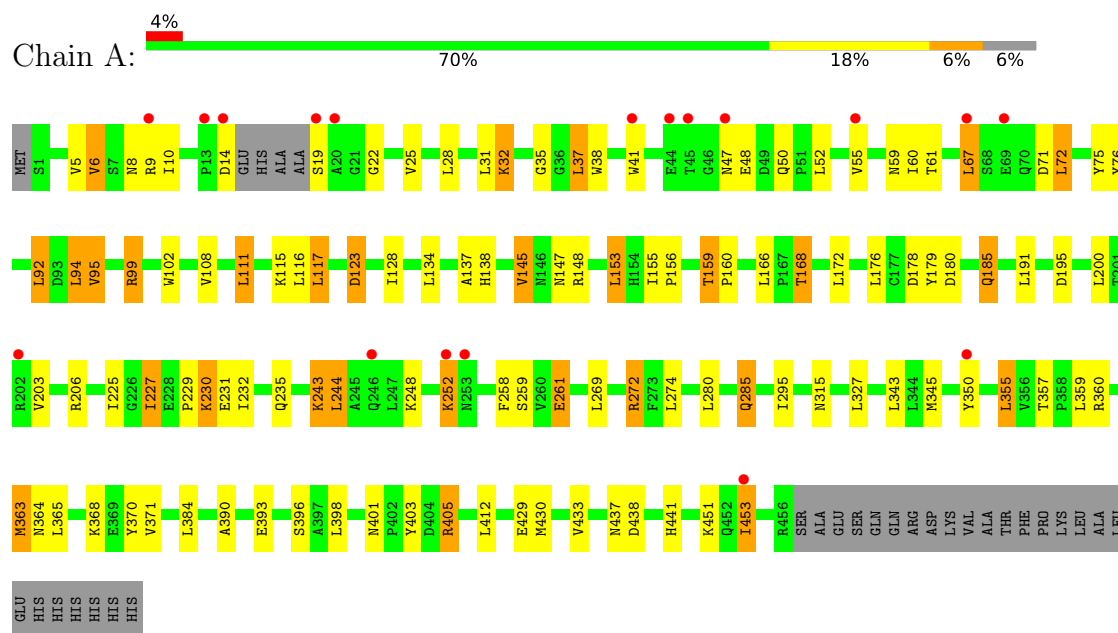
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	21	Total	O	0	0
			21	21		

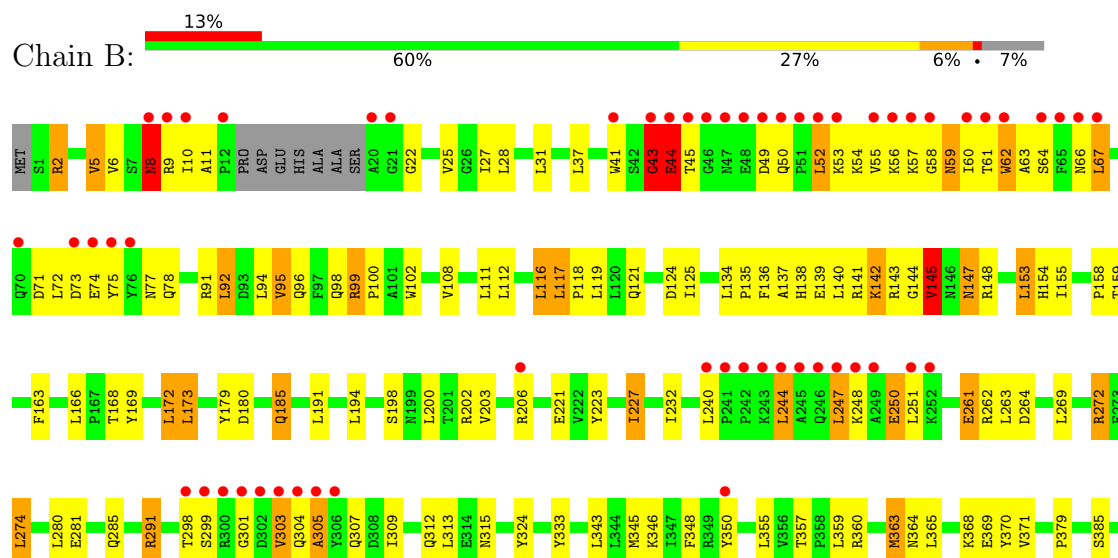
3 Residue-property plots

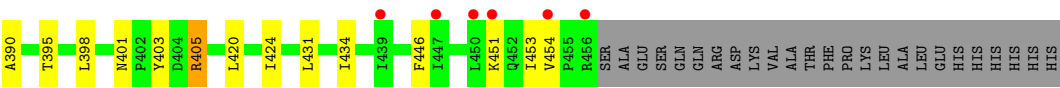
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.91Å 102.31Å 118.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.96-2.00) 94.0 (19.96-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.269 0.259 , 0.288	Depositor DCC
R_{free} test set	6389 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7360	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: UPG

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	0.80	2/3716 (0.1%)	1.00	7/5051 (0.1%)
1	B	0.80	4/3694 (0.1%)	1.07	14/5020 (0.3%)
All	All	0.80	6/7410 (0.1%)	1.04	21/10071 (0.2%)

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	B	1	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	MET	SD-CE	-16.64	1.38	1.79
1	B	44	GLU	CA-C	14.02	1.71	1.52
1	B	363	MET	SD-CE	-13.65	1.45	1.79
1	B	44	GLU	N-CA	-12.53	1.30	1.46
1	A	430	MET	SD-CE	-6.63	1.62	1.79
1	B	43	GLY	CA-C	5.45	1.59	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASN	N-CA-C	12.99	132.80	111.37
1	B	9	ARG	N-CA-C	-10.52	93.36	109.24
1	B	5	VAL	CA-C-N	-7.79	112.12	122.94
1	B	5	VAL	C-N-CA	-7.79	112.12	122.94
1	B	44	GLU	CB-CG-CD	7.71	125.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	VAL	CA-C-N	-7.04	113.15	122.94
1	A	5	VAL	C-N-CA	-7.04	113.15	122.94
1	A	94	LEU	CA-C-N	-6.90	110.58	121.62
1	A	94	LEU	C-N-CA	-6.90	110.58	121.62
1	B	370	TYR	CA-C-N	-6.61	109.80	120.64
1	B	370	TYR	C-N-CA	-6.61	109.80	120.64
1	A	370	TYR	CA-C-N	-6.42	110.12	120.64
1	A	370	TYR	C-N-CA	-6.42	110.12	120.64
1	B	144	GLY	CA-C-N	-6.21	113.10	121.80
1	B	144	GLY	C-N-CA	-6.21	113.10	121.80
1	B	44	GLU	CA-CB-CG	-6.11	101.89	114.10
1	B	250	GLU	N-CA-C	-5.94	106.19	113.50
1	A	227	ILE	N-CA-CB	-5.91	104.24	112.52
1	B	44	GLU	N-CA-CB	5.85	120.38	110.49
1	B	45	THR	N-CA-C	5.57	126.61	111.00
1	B	145	VAL	O-C-N	5.14	128.59	122.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	8	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	GLY	Peptide

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	3625	0	3600	87	0
1	B	3604	0	3584	104	0
2	A	36	0	22	0	0
3	A	74	0	0	6	0
3	B	21	0	0	1	0
All	All	7360	0	7206	188	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 13.

All (188) 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:272:ARG:HD2	1:A:357:THR:OG1	1.53	1.07
1:B:232:ILE:HG23	1:B:345:MET:HE2	1.40	1.01
1:B:363:MET:HE2	1:B:368:LYS:HE3	1.41	0.99
1:A:230:LYS:H	1:A:230:LYS:HD2	1.26	0.98
1:A:75:TYR:CD2	1:A:108:VAL:HG21	1.99	0.97
1:A:75:TYR:CG	1:A:108:VAL:HG21	2.00	0.96
1:A:230:LYS:H	1:A:230:LYS:CD	1.85	0.89
1:B:363:MET:HE2	1:B:368:LYS:CE	2.04	0.87
1:A:363:MET:HE2	1:A:368:LYS:HE3	1.58	0.86
1:B:140:LEU:O	1:B:145:VAL:HG13	1.79	0.83
1:B:363:MET:HE3	1:B:390:ALA:HB2	1.60	0.82
1:A:363:MET:CE	1:A:390:ALA:HA	2.09	0.82
1:B:41:TRP:CZ3	1:B:67:LEU:HB2	2.15	0.81
1:B:75:TYR:CG	1:B:108:VAL:HG11	2.18	0.79
1:A:363:MET:HE1	1:A:390:ALA:HA	1.66	0.77
1:B:363:MET:HE1	1:B:390:ALA:HA	1.63	0.77
1:B:73:ASP:HA	1:B:77:ASN:HB2	1.69	0.74
1:A:148:ARG:HG2	1:A:453:ILE:HG13	1.70	0.74
1:B:41:TRP:CH2	1:B:43:GLY:HA2	2.23	0.73
1:B:41:TRP:CZ2	1:B:43:GLY:HA2	2.24	0.73
1:B:77:ASN:O	1:B:303:VAL:HG21	1.90	0.71
1:A:159:THR:HG22	1:A:160:PRO:HD2	1.72	0.70
1:A:235:GLN:HG2	3:A:2053:HOH:O	1.92	0.70
1:A:272:ARG:CD	1:A:357:THR:OG1	2.35	0.70
1:A:315:ASN:HB2	3:A:2051:HOH:O	1.90	0.70
1:B:291:ARG:HD2	1:B:333:TYR:CD1	2.26	0.69
1:A:261:GLU:CD	1:A:272:ARG:HH22	2.02	0.68
1:B:363:MET:CE	1:B:368:LYS:HE3	2.19	0.68
1:B:75:TYR:CD2	1:B:108:VAL:HG11	2.30	0.67
1:A:363:MET:HE3	1:A:390:ALA:CA	2.24	0.67
1:A:8:ASN:ND2	1:A:75:TYR:OH	2.27	0.66
3:A:2051:HOH:O	1:B:315:ASN:HB2	1.94	0.66
1:A:327:LEU:CD1	1:B:244:LEU:HD11	2.25	0.66
1:B:363:MET:CE	1:B:390:ALA:HA	2.25	0.66
1:A:258:PHE:CZ	1:A:295:ILE:HD12	2.32	0.64
1:A:252:LYS:NZ	1:A:252:LYS:HB3	2.13	0.64
1:A:258:PHE:HZ	1:A:295:ILE:HD12	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:MET:HE3	1:B:390:ALA:CB	2.28	0.64
1:A:327:LEU:HD13	1:B:244:LEU:HD11	1.80	0.64
1:B:31:LEU:HB3	1:B:60:ILE:HG12	1.79	0.63
1:B:53:LYS:O	1:B:63:ALA:HA	1.98	0.63
1:B:137:ALA:O	1:B:141:ARG:HG2	1.98	0.63
1:B:345:MET:HE1	1:B:369:GLU:HB3	1.81	0.62
1:B:52:LEU:HD11	1:B:119:LEU:HD11	1.82	0.62
1:B:57:LYS:HB2	1:B:62:TRP:HZ3	1.65	0.61
1:B:125:ILE:HD11	1:B:148:ARG:CZ	2.30	0.61
1:A:252:LYS:HB3	1:A:252:LYS:HZ2	1.66	0.61
1:A:363:MET:HE2	1:A:368:LYS:CE	2.28	0.61
1:A:75:TYR:CD2	1:A:108:VAL:CG2	2.81	0.61
1:A:92:LEU:O	1:A:95:VAL:HG13	2.01	0.61
1:A:31:LEU:HB3	1:A:60:ILE:HG12	1.83	0.60
1:B:345:MET:HA	1:B:345:MET:HE3	1.83	0.60
1:A:363:MET:HE3	1:A:390:ALA:HA	1.80	0.59
1:A:393:GLU:HB2	1:A:433:VAL:HG11	1.83	0.59
1:B:232:ILE:CG2	1:B:345:MET:HE2	2.22	0.59
1:B:57:LYS:CB	1:B:62:TRP:HZ3	2.16	0.59
1:B:8:ASN:O	1:B:41:TRP:HB3	2.03	0.59
1:A:75:TYR:CB	1:A:108:VAL:HG21	2.33	0.58
1:A:261:GLU:OE2	1:A:272:ARG:NH2	2.35	0.58
1:B:401:ASN:HD22	1:B:401:ASN:C	2.11	0.58
1:A:48:GLU:H	1:A:48:GLU:CD	2.10	0.58
1:A:75:TYR:HB2	1:A:108:VAL:HG21	1.87	0.57
1:B:247:LEU:HA	1:B:250:GLU:HB2	1.87	0.57
1:B:247:LEU:O	1:B:247:LEU:HG	2.04	0.57
1:A:147:ASN:HD22	1:A:147:ASN:H	1.53	0.57
1:B:420:LEU:O	1:B:424:ILE:HG12	2.06	0.56
1:B:303:VAL:C	1:B:305:ALA:H	2.13	0.56
1:A:396:SER:OG	1:A:429:GLU:CD	2.50	0.55
1:B:147:ASN:HD22	1:B:147:ASN:H	1.54	0.55
1:A:71:ASP:O	1:A:75:TYR:HB3	2.06	0.55
1:B:363:MET:HE2	1:B:368:LYS:NZ	2.22	0.55
1:A:231:GLU:HG3	1:A:235:GLN:NE2	2.22	0.55
1:A:8:ASN:O	1:A:41:TRP:HB3	2.07	0.55
1:B:99:ARG:N	1:B:100:PRO:HD2	2.23	0.54
1:B:227:ILE:HD12	1:B:365:LEU:HD22	1.90	0.54
1:B:57:LYS:HB2	1:B:62:TRP:CZ3	2.43	0.54
1:B:168:THR:HG23	1:B:172:LEU:HD22	1.90	0.54
1:B:363:MET:HE2	1:B:368:LYS:HZ1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD23	1:A:61:THR:HB	1.91	0.53
1:A:363:MET:HE3	1:A:390:ALA:HB2	1.89	0.53
1:A:401:ASN:C	1:A:401:ASN:HD22	2.17	0.52
1:B:71:ASP:O	1:B:75:TYR:HB3	2.09	0.52
1:A:67:LEU:HD23	1:A:72:LEU:HD23	1.92	0.52
1:B:52:LEU:CD1	1:B:119:LEU:HD11	2.39	0.52
1:B:247:LEU:HD21	1:B:291:ARG:NH2	2.25	0.52
1:B:92:LEU:HA	1:B:95:VAL:HG13	1.92	0.52
1:A:248:LYS:HE3	1:A:350:TYR:CD2	2.45	0.52
1:A:405:ARG:HD2	3:A:2064:HOH:O	2.09	0.52
1:A:185:GLN:HE22	1:A:225:ILE:H	1.58	0.52
1:A:102:TRP:CZ3	1:A:168:THR:HG21	2.45	0.52
1:A:363:MET:HE3	1:A:390:ALA:CB	2.41	0.51
1:B:274:LEU:HG	1:B:405:ARG:NH2	2.25	0.51
1:A:355:LEU:HG	1:A:412:LEU:HD21	1.92	0.51
1:A:102:TRP:CE3	1:A:168:THR:HG21	2.45	0.51
1:B:2:ARG:HD3	1:B:121:GLN:NE2	2.25	0.51
1:B:75:TYR:HB2	1:B:108:VAL:HG11	1.93	0.51
1:A:72:LEU:HD22	1:A:76:TYR:HB3	1.92	0.50
1:B:2:ARG:HB3	1:B:124:ASP:OD1	2.12	0.50
1:B:102:TRP:CE3	1:B:168:THR:HG21	2.46	0.50
1:A:327:LEU:HD12	1:B:244:LEU:HD11	1.93	0.50
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.25	0.50
1:A:153:LEU:HD13	1:A:155:ILE:O	2.11	0.50
1:B:431:LEU:HA	1:B:434:ILE:HG12	1.92	0.50
1:A:155:ILE:HB	1:A:156:PRO:CD	2.42	0.49
1:B:221:GLU:HB3	1:B:223:TYR:CE2	2.47	0.49
1:B:401:ASN:ND2	1:B:403:TYR:H	2.10	0.49
1:A:225:ILE:HG23	1:A:365:LEU:HD21	1.95	0.49
1:A:117:LEU:HD21	1:A:145:VAL:HG12	1.95	0.49
1:B:153:LEU:HD13	1:B:155:ILE:O	2.13	0.48
1:B:363:MET:CE	1:B:390:ALA:CA	2.90	0.48
1:B:345:MET:HE3	1:B:348:PHE:HD2	1.78	0.48
1:B:52:LEU:CD2	1:B:52:LEU:H	2.26	0.48
1:B:261:GLU:OE1	1:B:272:ARG:NH2	2.48	0.47
1:B:261:GLU:OE2	1:B:272:ARG:NH2	2.48	0.47
1:A:138:HIS:HD2	1:A:178:ASP:OD2	1.98	0.47
1:A:259:SER:HB3	1:A:272:ARG:HH21	1.79	0.47
1:B:244:LEU:HG	1:B:343:LEU:HD11	1.97	0.47
1:B:10:ILE:HG23	1:B:11:ALA:N	2.29	0.47
1:A:31:LEU:O	1:A:35:GLY:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:HA	1:B:78:GLN:HB2	1.97	0.46
1:A:111:LEU:O	1:A:115:LYS:HG3	2.16	0.46
1:B:75:TYR:CB	1:B:108:VAL:HG11	2.46	0.46
1:B:10:ILE:HG12	1:B:11:ALA:H	1.79	0.46
1:B:55:VAL:O	1:B:61:THR:O	2.34	0.46
1:B:139:GLU:O	1:B:143:ARG:HD2	2.16	0.46
1:B:137:ALA:HB2	1:B:179:TYR:CE1	2.50	0.45
1:B:145:VAL:HG22	1:B:145:VAL:O	2.15	0.45
1:B:158:PRO:HG2	1:B:163:PHE:HB2	1.98	0.45
1:A:244:LEU:HD23	1:A:343:LEU:HD11	1.98	0.45
1:B:75:TYR:CD2	1:B:108:VAL:CG1	2.99	0.45
1:B:291:ARG:HG2	3:B:2010:HOH:O	2.15	0.45
1:A:59:ASN:CB	3:A:2005:HOH:O	2.64	0.45
1:A:28:LEU:HB3	1:A:32:LYS:HE3	1.99	0.45
1:A:75:TYR:HB2	1:A:108:VAL:CG2	2.47	0.45
1:A:180:ASP:HB3	1:A:453:ILE:HD13	1.99	0.45
1:A:401:ASN:HD21	1:A:403:TYR:HD1	1.65	0.45
1:A:243:LYS:HB2	1:A:243:LYS:HE3	1.67	0.45
1:A:59:ASN:HB2	3:A:2005:HOH:O	2.16	0.44
1:A:123:ASP:OD2	1:A:123:ASP:N	2.49	0.44
1:A:229:PRO:HD2	1:A:230:LYS:HD2	1.99	0.44
1:A:437:ASN:HD22	1:A:441:HIS:HD2	1.66	0.44
1:B:8:ASN:O	1:B:41:TRP:CD1	2.70	0.44
1:B:66:ASN:HB3	1:B:67:LEU:H	1.60	0.44
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.83	0.44
1:A:232:ILE:HD12	1:A:345:MET:SD	2.57	0.44
1:A:396:SER:HG	1:A:429:GLU:CD	2.26	0.44
1:A:10:ILE:HG22	1:A:38:TRP:NE1	2.33	0.43
1:B:163:PHE:CE2	1:B:173:LEU:HD13	2.53	0.43
1:A:137:ALA:HB2	1:A:179:TYR:CE1	2.54	0.43
1:B:59:ASN:HD22	1:B:59:ASN:HA	1.56	0.43
1:A:229:PRO:HD2	1:A:230:LYS:CD	2.48	0.43
1:B:134:LEU:N	1:B:135:PRO:CD	2.80	0.43
1:A:134:LEU:HD22	1:A:176:LEU:HD21	2.01	0.43
1:B:261:GLU:CD	1:B:272:ARG:NH2	2.76	0.43
1:B:138:HIS:CE1	1:B:142:LYS:HD2	2.54	0.43
1:B:379:PRO:CD	1:B:424:ILE:HD13	2.49	0.43
1:B:56:LYS:HG3	1:B:61:THR:HG23	2.01	0.43
1:A:285:GLN:HE21	1:A:285:GLN:HB2	1.44	0.43
1:A:230:LYS:CD	1:A:230:LYS:N	2.66	0.42
1:B:5:VAL:HG21	1:B:27:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:CD1	1:B:365:LEU:HD22	2.49	0.42
1:A:22:GLY:O	1:A:25:VAL:HG22	2.20	0.42
1:B:180:ASP:HB3	1:B:453:ILE:HD13	2.01	0.42
1:B:185:GLN:HE21	1:B:185:GLN:HB2	1.47	0.42
1:B:240:LEU:HD12	1:B:240:LEU:H	1.85	0.42
1:A:285:GLN:H	1:A:285:GLN:HG3	1.02	0.42
1:A:138:HIS:CD2	1:A:178:ASP:OD2	2.72	0.42
1:B:2:ARG:NH1	1:B:124:ASP:OD1	2.53	0.42
1:B:117:LEU:HB3	1:B:118:PRO:HD3	2.01	0.42
1:B:154:HIS:C	1:B:185:GLN:HE22	2.27	0.42
1:B:281:GLU:OE1	1:B:324:TYR:OH	2.37	0.42
1:B:301:GLY:HA2	1:B:305:ALA:HA	2.02	0.42
1:A:261:GLU:CD	1:A:272:ARG:NH2	2.76	0.42
1:B:116:LEU:HD12	1:B:136:PHE:CZ	2.54	0.42
1:B:56:LYS:CG	1:B:61:THR:HG23	2.49	0.42
1:B:163:PHE:CE2	1:B:169:TYR:HB2	2.54	0.42
1:B:346:LYS:O	1:B:350:TYR:HD1	2.03	0.42
1:B:363:MET:CE	1:B:368:LYS:CE	2.86	0.42
1:B:145:VAL:O	1:B:145:VAL:CG2	2.66	0.41
1:B:73:ASP:O	1:B:78:GLN:HB2	2.19	0.41
1:B:363:MET:HE3	1:B:390:ALA:CA	2.50	0.41
1:B:357:THR:HA	1:B:385:SER:HB2	2.02	0.41
1:A:185:GLN:NE2	1:A:225:ILE:H	2.19	0.41
1:A:363:MET:CE	1:A:390:ALA:CA	2.83	0.41
1:A:6:VAL:HG13	1:A:128:ILE:CD1	2.51	0.40
1:A:272:ARG:NH1	1:A:357:THR:H	2.18	0.40
1:B:431:LEU:HD12	1:B:434:ILE:HD11	2.03	0.40
1:B:223:TYR:CE1	1:B:446:PHE:HA	2.57	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	448/482 (93%)	433 (97%)	14 (3%)	1 (0%)	43	42
1	B	445/482 (92%)	415 (93%)	22 (5%)	8 (2%)	6	3
All	All	893/964 (93%)	848 (95%)	36 (4%)	9 (1%)	12	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	GLU
1	B	62	TRP
1	B	58	GLY
1	B	304	GLN
1	B	305	ALA
1	B	307	GLN
1	A	364	ASN
1	B	364	ASN
1	B	22	GLY

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	382/407 (94%)	329 (86%)	53 (14%)	3	2
1	B	379/407 (93%)	307 (81%)	72 (19%)	1	1
All	All	761/814 (94%)	636 (84%)	125 (16%)	2	1

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	9	ARG
1	A	14	ASP
1	A	19	SER
1	A	32	LYS
1	A	37	LEU
1	A	47	ASN

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Mol	Chain	Res	Type
1	A	50	GLN
1	A	52	LEU
1	A	55	VAL
1	A	67	LEU
1	A	72	LEU
1	A	92	LEU
1	A	94	LEU
1	A	95	VAL
1	A	99	ARG
1	A	111	LEU
1	A	116	LEU
1	A	117	LEU
1	A	123	ASP
1	A	145	VAL
1	A	153	LEU
1	A	159	THR
1	A	166	LEU
1	A	168	THR
1	A	172	LEU
1	A	185	GLN
1	A	191	LEU
1	A	195	ASP
1	A	200	LEU
1	A	203	VAL
1	A	206	ARG
1	A	227	ILE
1	A	230	LYS
1	A	243	LYS
1	A	244	LEU
1	A	252	LYS
1	A	261	GLU
1	A	269	LEU
1	A	272	ARG
1	A	274	LEU
1	A	280	LEU
1	A	285	GLN
1	A	355	LEU
1	A	359	LEU
1	A	360	ARG
1	A	371	VAL
1	A	384	LEU
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	405	ARG
1	A	438	ASP
1	A	451	LYS
1	A	453	ILE
1	B	2	ARG
1	B	6	VAL
1	B	8	ASN
1	B	25	VAL
1	B	28	LEU
1	B	37	LEU
1	B	44	GLU
1	B	49	ASP
1	B	50	GLN
1	B	52	LEU
1	B	54	LYS
1	B	59	ASN
1	B	64	SER
1	B	67	LEU
1	B	72	LEU
1	B	91	ARG
1	B	92	LEU
1	B	94	LEU
1	B	95	VAL
1	B	96	GLN
1	B	98	GLN
1	B	99	ARG
1	B	111	LEU
1	B	112	LEU
1	B	116	LEU
1	B	117	LEU
1	B	142	LYS
1	B	145	VAL
1	B	147	ASN
1	B	153	LEU
1	B	159	THR
1	B	166	LEU
1	B	172	LEU
1	B	173	LEU
1	B	185	GLN
1	B	191	LEU
1	B	194	LEU
1	B	198	SER

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Mol	Chain	Res	Type
1	B	200	LEU
1	B	202	ARG
1	B	203	VAL
1	B	206	ARG
1	B	227	ILE
1	B	244	LEU
1	B	247	LEU
1	B	248	LYS
1	B	251	LEU
1	B	261	GLU
1	B	262	ARG
1	B	263	LEU
1	B	264	ASP
1	B	269	LEU
1	B	272	ARG
1	B	274	LEU
1	B	280	LEU
1	B	285	GLN
1	B	291	ARG
1	B	298	THR
1	B	299	SER
1	B	303	VAL
1	B	309	ILE
1	B	312	GLN
1	B	313	LEU
1	B	355	LEU
1	B	359	LEU
1	B	360	ARG
1	B	371	VAL
1	B	395	THR
1	B	398	LEU
1	B	405	ARG
1	B	451	LYS
1	B	454	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	77	ASN
1	A	78	GLN
1	A	121	GLN

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Mol	Chain	Res	Type
1	A	138	HIS
1	A	147	ASN
1	A	175	GLN
1	A	185	GLN
1	A	235	GLN
1	A	255	GLN
1	A	285	GLN
1	A	386	GLN
1	A	401	ASN
1	A	437	ASN
1	B	59	ASN
1	B	77	ASN
1	B	78	GLN
1	B	121	GLN
1	B	147	ASN
1	B	175	GLN
1	B	185	GLN
1	B	255	GLN
1	B	256	ASN
1	B	401	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](#)

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	UPG	A	1457	-	37,38,38	2.29	8 (21%)	55,58,58	3.05	14 (25%)

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	A	1457	-	-	8/23/59/59	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1457	UPG	C4'-C5'	7.78	1.69	1.53
2	A	1457	UPG	O3'-C3'	5.30	1.56	1.43
2	A	1457	UPG	O4'-C4'	4.85	1.55	1.43
2	A	1457	UPG	O5'-C1'	4.20	1.52	1.41
2	A	1457	UPG	C3'-C2'	4.17	1.63	1.52
2	A	1457	UPG	C6-C5	2.54	1.41	1.35
2	A	1457	UPG	C6'-C5'	2.21	1.59	1.51
2	A	1457	UPG	PA-O1A	-2.10	1.43	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1457	UPG	O3B-C1'-C2'	12.05	130.45	108.38
2	A	1457	UPG	O5'-C1'-O3B	-11.07	96.89	111.36
2	A	1457	UPG	O5'-C1'-C2'	-6.21	97.62	110.37
2	A	1457	UPG	C4-N3-C2	-5.98	119.19	126.61
2	A	1457	UPG	C1'-O5'-C5'	5.12	123.71	113.72
2	A	1457	UPG	O3'-C3'-C2'	4.93	121.99	110.38
2	A	1457	UPG	N3-C2-N1	4.82	121.17	114.89
2	A	1457	UPG	C5-C4-N3	3.66	119.92	114.80
2	A	1457	UPG	O3B-PB-O1B	-3.25	99.41	109.81
2	A	1457	UPG	O2-C2-N1	-2.92	118.99	122.80
2	A	1457	UPG	O5'-C5'-C4'	-2.55	105.10	109.70
2	A	1457	UPG	C6'-C5'-C4'	-2.49	106.91	113.02
2	A	1457	UPG	O2B-PB-O1B	-2.48	100.90	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1457	UPG	C1'-C2'-C3'	2.05	114.33	110.01

There are no chirality outliers.

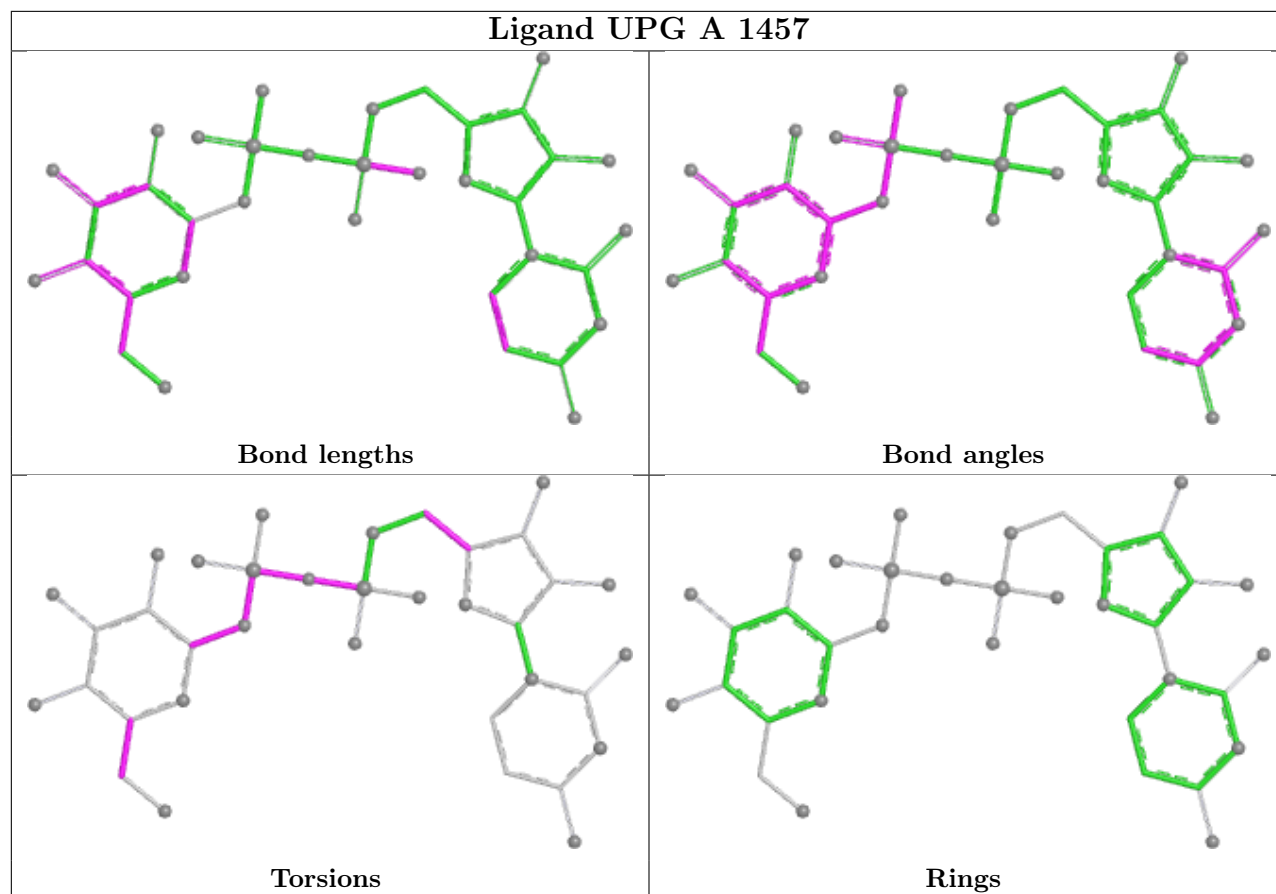
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1457	UPG	PB-O3A-PA-O5C
2	A	1457	UPG	C2'-C1'-O3B-PB
2	A	1457	UPG	O5'-C1'-O3B-PB
2	A	1457	UPG	C3C-C4C-C5C-O5C
2	A	1457	UPG	O4C-C4C-C5C-O5C
2	A	1457	UPG	PA-O3A-PB-O3B
2	A	1457	UPG	C1'-O3B-PB-O1B
2	A	1457	UPG	C4'-C5'-C6'-O6'

There are no ring outliers.

No monomer is involved in short contacts.

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	452/482 (93%)	0.31	18 (3%) 42 41	13, 19, 27, 34	0
1	B	449/482 (93%)	0.82	63 (14%) 6 5	13, 20, 39, 52	0
All	All	901/964 (93%)	0.57	81 (8%) 15 14	13, 20, 34, 52	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	9.3
1	B	249	ALA	7.4
1	B	41	TRP	6.1
1	B	46	GLY	6.0
1	B	299	SER	5.9
1	B	302	ASP	5.5
1	B	306	TYR	5.2
1	B	55	VAL	5.2
1	B	43	GLY	4.7
1	B	67	LEU	4.7
1	B	304	GLN	4.3
1	B	245	ALA	4.3
1	A	20	ALA	4.0
1	B	44	GLU	4.0
1	B	247	LEU	3.8
1	A	44	GLU	3.7
1	B	301	GLY	3.6
1	B	45	THR	3.6
1	B	20	ALA	3.6
1	B	49	ASP	3.6
1	A	14	ASP	3.5
1	B	47	ASN	3.5
1	B	50	GLN	3.4
1	A	41	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	241	PRO	3.2
1	B	60	ILE	3.1
1	B	61	THR	3.1
1	B	298	THR	3.1
1	A	350	TYR	3.0
1	B	305	ALA	3.0
1	B	73	ASP	3.0
1	B	10	ILE	2.9
1	B	251	LEU	2.9
1	B	350	TYR	2.9
1	B	248	LYS	2.9
1	B	58	GLY	2.9
1	B	53	LYS	2.8
1	B	454	VAL	2.8
1	A	252	LYS	2.7
1	B	300	ARG	2.7
1	B	76	TYR	2.7
1	B	246	GLN	2.7
1	B	12	PRO	2.6
1	B	62	TRP	2.6
1	B	56	LYS	2.6
1	A	47	ASN	2.6
1	B	243	LYS	2.6
1	B	70	GLN	2.6
1	A	69	GLU	2.6
1	B	8	ASN	2.6
1	B	240	LEU	2.6
1	A	45	THR	2.5
1	B	52	LEU	2.5
1	B	51	PRO	2.5
1	B	65	PHE	2.5
1	B	447	ILE	2.5
1	B	242	PRO	2.4
1	B	439	ILE	2.4
1	A	9	ARG	2.4
1	B	206	ARG	2.4
1	A	253	ASN	2.4
1	A	55	VAL	2.4
1	A	202	ARG	2.4
1	B	450	LEU	2.3
1	A	67	LEU	2.3
1	A	19	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	9	ARG	2.2
1	B	252	LYS	2.2
1	B	21	GLY	2.2
1	B	456	ARG	2.2
1	B	66	ASN	2.2
1	B	74	GLU	2.2
1	A	246	GLN	2.1
1	B	75	TYR	2.1
1	A	453	ILE	2.1
1	B	451	LYS	2.1
1	B	64	SER	2.1
1	B	48	GLU	2.1
1	A	13	PRO	2.1
1	B	244	LEU	2.0
1	B	57	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

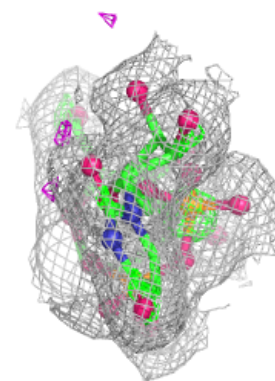
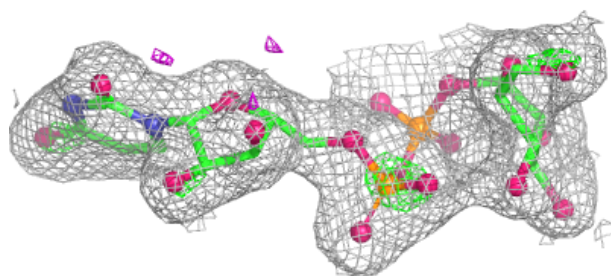
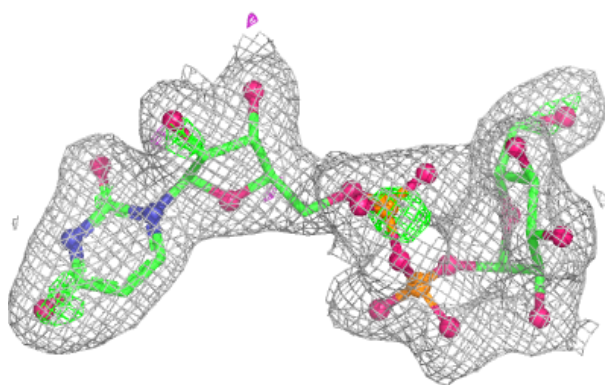
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UPG	A	1457	36/36	0.94	0.09	22,27,30,30	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 1457:

$2mF_o-DF_c$ (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.