



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:05 am BST

PDB ID : 1UQU
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

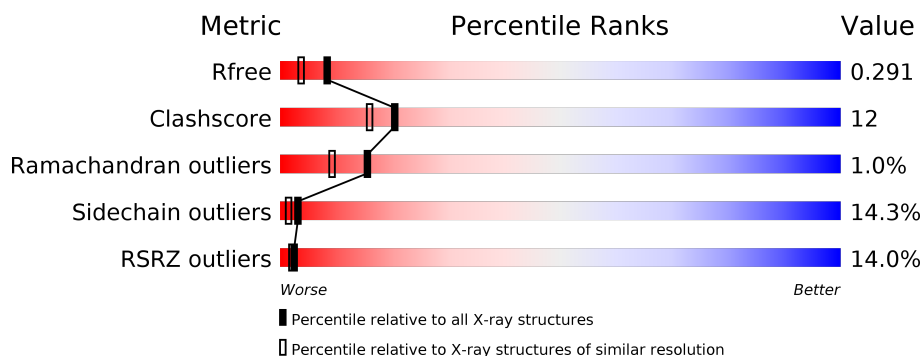
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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](#)

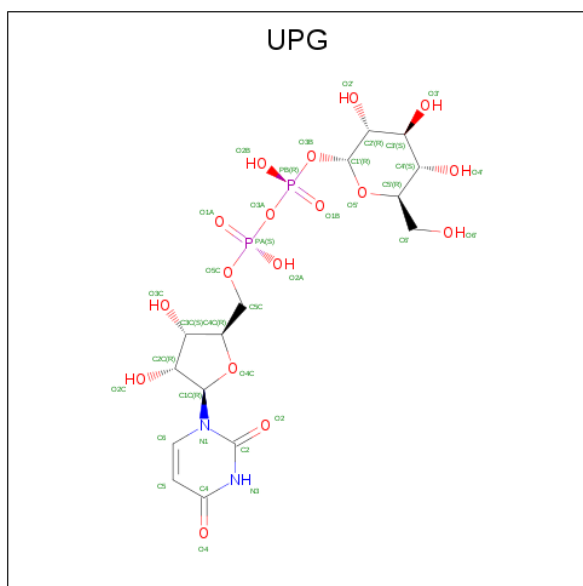
There are 3 unique types of molecules in this entry. The entry contains 7360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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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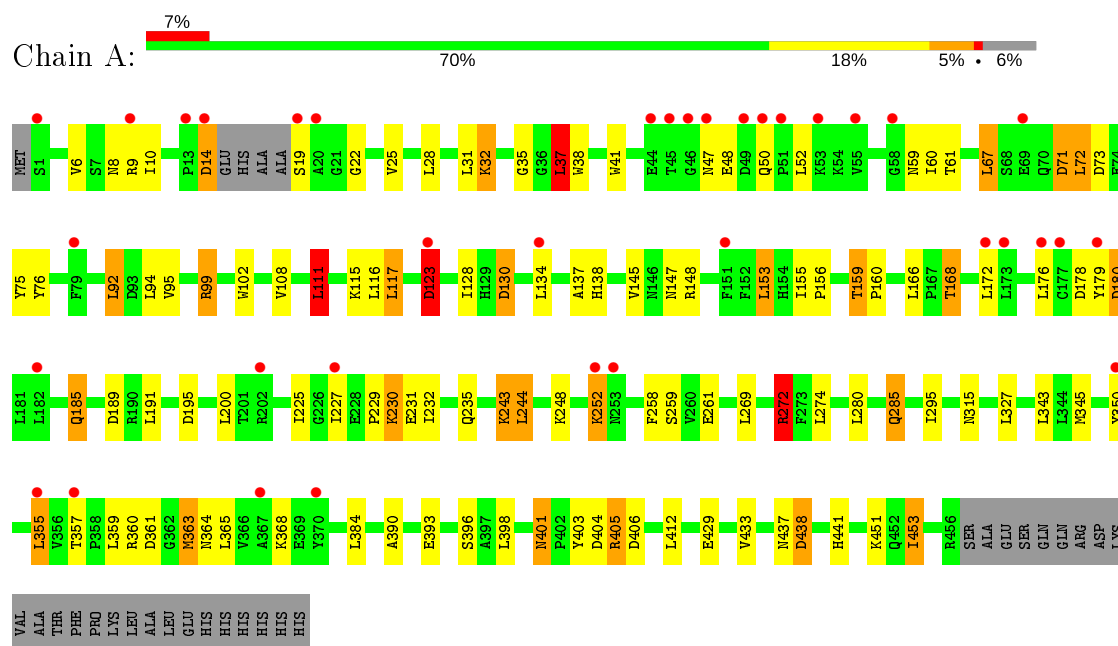
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	21	Total	O	0	0
			21	21		

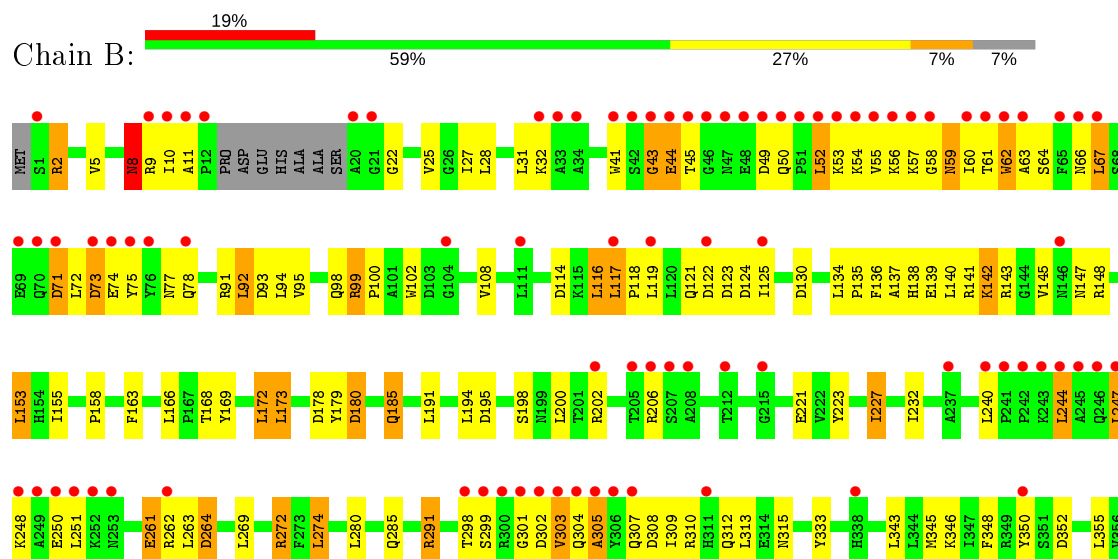
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 19.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.96-2.00) 94.1 (19.94-2.00)	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 0.263 , 0.291	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)	0.37 , 39.6	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	0.64	1/3716 (0.0%)	0.87	15/5051 (0.3%)
1	B	0.61	3/3694 (0.1%)	0.91	25/5020 (0.5%)
All	All	0.62	4/7410 (0.1%)	0.89	40/10071 (0.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	44	GLU	N-CA	-8.16	1.30	1.46
1	B	44	GLU	CA-C	7.16	1.71	1.52
1	A	363	MET	SD-CE	-7.12	1.38	1.77
1	B	363	MET	SD-CE	-5.79	1.45	1.77

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ASN	N-CA-C	8.07	132.80	111.00
1	A	438	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	14	ASP	CB-CG-OD2	7.24	124.82	118.30
1	B	195	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	406	ASP	CB-CG-OD2	7.11	124.69	118.30
1	A	272	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	123	ASP	CB-CG-OD2	6.84	124.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	ASP	CB-CG-OD2	6.79	124.42	118.30
1	B	404	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	9	ARG	N-CA-C	-6.53	93.36	111.00
1	B	264	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	91	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	71	ASP	CB-CG-OD2	6.42	124.07	118.30
1	A	406	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	93	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	404	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	180	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	130	ASP	CB-CG-OD2	6.05	123.74	118.30
1	B	122	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	111	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	45	THR	N-CA-C	5.78	126.61	111.00
1	A	438	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	B	449	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	432	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	71	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	361	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	37	LEU	CA-CB-CG	5.63	128.26	115.30
1	B	302	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	352	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	44	GLU	N-CA-CB	5.43	120.38	110.60
1	A	73	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	308	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	180	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	413	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	44	GLU	CA-CB-CG	-5.23	101.89	113.40
1	B	114	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	123	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	178	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	73	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	189	ASP	CB-CG-OD2	5.09	122.89	118.30

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 ⓘ

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	84	0
1	B	3604	0	3584	98	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	179	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 12.

All (179) 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:363:MET:HE3	1:A:390:ALA:HA	1.30	1.12
1:A:272:ARG:HD2	1:A:357:THR:OG1	1.53	1.07
1:B:363:MET:HE2	1:B:368:LYS:HE3	1.39	1.02
1:A:363:MET:HE3	1:A:390:ALA:CA	1.92	0.99
1:A:230:LYS:HD2	1:A:230:LYS:H	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:CD	1:A:230:LYS:H	1.85	0.89
1:B:363:MET:HE3	1:B:390:ALA:HB2	1.58	0.84
1:B:140:LEU:O	1:B:145:VAL:HG13	1.79	0.83
1:A:363:MET:CE	1:A:390:ALA:HA	2.09	0.81
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:B:345:MET:HE3	1:B:348:PHE:HD2	1.48	0.77
1:B:363:MET:HE3	1:B:390:ALA:CB	2.15	0.75
1:B:73:ASP:HA	1:B:77:ASN:HB2	1.69	0.74
1:B:363:MET:HE2	1:B:368:LYS:CE	2.15	0.74
1:A:148:ARG:HG2	1:A:453:ILE:HG13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:345:MET:HE3	1:B:348:PHE:CD2	2.25	0.71
1:A:159:THR:HG22	1:A:160:PRO:HD2	1.72	0.70
1:B:363:MET:CE	1:B:368:LYS:HE3	2.19	0.70
1:B:363:MET:HE3	1:B:390:ALA:CA	2.22	0.70
1:A:235:GLN:HG2	3:A:2053:HOH:O	1.92	0.70
1:A:315:ASN:HB2	3:A:2051:HOH:O	1.90	0.70
1:A:272:ARG:CD	1:A:357:THR:OG1	2.35	0.70
1:B:291:ARG:HD2	1:B:333:TYR:CD1	2.26	0.69
1:B:75:TYR:CD2	1:B:108:VAL:HG11	2.30	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:HB3	1:A:252:LYS:NZ	2.13	0.64
1:A:258:PHE:HZ	1:A:295:ILE:HD12	1.61	0.64
1:A:327:LEU:HD13	1:B:244:LEU:HD11	1.80	0.64
1:A:261:GLU:CD	1:A:272:ARG:HH22	2.02	0.63
1:B:31:LEU:HB3	1:B:60:ILE:HG12	1.79	0.63
1:B:137:ALA:O	1:B:141:ARG:HG2	1.98	0.63
1:B:53:LYS:O	1:B:63:ALA:HA	1.98	0.63
1:B:52:LEU:HD11	1:B:119:LEU:HD11	1.82	0.62
1:B:125:ILE:HD11	1:B:148:ARG:CZ	2.30	0.61
1:B:57:LYS:HB2	1:B:62:TRP:HZ3	1.65	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:A:393:GLU:HB2	1:A:433:VAL:HG11	1.83	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:232:ILE:HG23	1:B:345:MET:HE1	1.85	0.58
1:A:363:MET:HE2	1:A:368:LYS:HE3	1.85	0.58
1:A:75:TYR:HB2	1:A:108:VAL:HG21	1.87	0.57
1:B:232:ILE:HG23	1:B:345:MET:CE	2.35	0.57
1:B:247:LEU:HA	1:B:250:GLU:HB2	1.87	0.57
1:B:247:LEU:HG	1:B:247:LEU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:HD22	1:A:147:ASN:H	1.53	0.57
1:A:363:MET:HE3	1:A:390:ALA:N	2.21	0.56
1:B:420:LEU:O	1:B:424:ILE:HG12	2.06	0.56
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: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:401:ASN:C	1:B:401:ASN:HD22	2.11	0.54
1:B:168:THR:HG23	1:B:172:LEU:HD22	1.90	0.54
1:B:57:LYS:HB2	1:B:62:TRP:CZ3	2.43	0.54
1:A:37:LEU:HD23	1:A:61:THR:HB	1.91	0.53
1:B:363:MET:HE3	1:B:390:ALA:HA	1.85	0.53
1:A:48:GLU:CD	1:A:48:GLU:H	2.10	0.53
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:303:VAL:C	1:B:305:ALA:H	2.13	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: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:363:MET:CE	1:B:368:LYS:CE	2.86	0.51
1:B:75:TYR:HB2	1:B:108:VAL:HG11	1.93	0.51
1:A:396:SER:OG	1:A:429:GLU:CD	2.50	0.50
1:A:72:LEU:HD22	1:A:76:TYR:HB3	1.92	0.50
1:A:363:MET:CE	1:A:368:LYS:HE3	2.40	0.50
1:B:102:TRP:CE3	1:B:168:THR:HG21	2.46	0.50
1:B:2:ARG:HB3	1:B:124:ASP:OD1	2.12	0.50
1:A:327:LEU:HD12	1:B:244:LEU:HD11	1.93	0.50
1:A:153:LEU:HD13	1:A:155:ILE:O	2.11	0.50
1:A:99:ARG:HH11	1:A:99:ARG:CG	2.25	0.50
1:B:363:MET:HE1	1:B:390:ALA:HA	1.93	0.50
1:B:431:LEU:HA	1:B:434:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:252:LYS:HZ3	1:A:252:LYS:HB3	1.79	0.48
1:B:153:LEU:HD13	1:B:155:ILE:O	2.13	0.48
1:A:401:ASN:HD22	1:A:401:ASN:C	2.17	0.48
1:B:52:LEU:H	1:B:52:LEU:CD2	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
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:O	1:B:145:VAL:HG22	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:291:ARG:HG2	3:B:2010:HOH:O	2.15	0.45
1:B:75:TYR:CD2	1:B:108:VAL:CG1	2.99	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:401:ASN:HD21	1:A:403:TYR:HD1	1.65	0.45
1:A:180:ASP:HB3	1:A:453:ILE:HD13	1.99	0.45
1:A:243:LYS:HB2	1:A:243:LYS:HE3	1.67	0.45
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:272:ARG:HD2	1:A:357:THR:HG1	1.76	0.44
1:A:59:ASN:HB2	3:A:2005:HOH:O	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HD12	1:A:345:MET:SD	2.57	0.44
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.83	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:HA	1:B:59:ASN:HD22	1.56	0.43
1:A:229:PRO:HD2	1:A:230:LYS:CD	2.48	0.43
1:A:259:SER:HG	1:A:355:LEU:HB3	1.83	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: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
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:HB2	1:B:185:GLN:HE21	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:117:LEU:HB3	1:B:118:PRO:HD3	2.01	0.42
1:B:2:ARG:NH1	1:B:124:ASP:OD1	2.53	0.42
1:B:301:GLY:HA2	1:B:305:ALA:HA	2.02	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: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: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:272:ARG:NH1	1:A:357:THR:H	2.18	0.40
1:A:6:VAL:HG13	1:A:128:ILE:CD1	2.51	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%)	47	44
1	B	445/482 (92%)	415 (93%)	22 (5%)	8 (2%)	8	3
All	All	893/964 (93%)	848 (95%)	36 (4%)	9 (1%)	15	9

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/407 (94%)	335 (88%)	47 (12%)	4	2
1	B	379/407 (93%)	317 (84%)	62 (16%)	2	1
All	All	761/814 (94%)	652 (86%)	109 (14%)	3	1

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	14	ASP
1	A	19	SER
1	A	32	LYS
1	A	37	LEU
1	A	47	ASN
1	A	50	GLN
1	A	52	LEU
1	A	67	LEU
1	A	72	LEU
1	A	92	LEU
1	A	94	LEU
1	A	99	ARG
1	A	111	LEU
1	A	116	LEU
1	A	117	LEU
1	A	123	ASP
1	A	130	ASP
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	227	ILE
1	A	230	LYS
1	A	243	LYS
1	A	244	LEU
1	A	252	LYS
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	384	LEU
1	A	398	LEU

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Mol	Chain	Res	Type
1	A	401	ASN
1	A	405	ARG
1	A	438	ASP
1	A	451	LYS
1	A	453	ILE
1	B	2	ARG
1	B	8	ASN
1	B	25	VAL
1	B	28	LEU
1	B	32	LYS
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	92	LEU
1	B	94	LEU
1	B	98	GLN
1	B	99	ARG
1	B	116	LEU
1	B	117	LEU
1	B	130	ASP
1	B	142	LYS
1	B	153	LEU
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
1	B	200	LEU
1	B	202	ARG
1	B	206	ARG
1	B	227	ILE
1	B	244	LEU
1	B	247	LEU
1	B	248	LYS
1	B	251	LEU

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Mol	Chain	Res	Type
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	310	ARG
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	398	LEU
1	B	401	ASN
1	B	405	ARG
1	B	451	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	77	ASN
1	A	121	GLN
1	A	138	HIS
1	A	147	ASN
1	A	175	GLN
1	A	185	GLN
1	A	235	GLN
1	A	285	GLN
1	A	401	ASN
1	A	437	ASN
1	B	59	ASN
1	B	77	ASN

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Mol	Chain	Res	Type
1	B	78	GLN
1	B	121	GLN
1	B	147	ASN
1	B	185	GLN
1	B	256	ASN
1	B	307	GLN
1	B	401	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	31,38,38	2.66	11 (35%)	41,58,58	3.96	11 (26%)

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	-	-	8/21/59/59	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1457	UPG	C4'-C5'	7.88	1.69	1.53
2	A	1457	UPG	O3'-C3'	5.56	1.56	1.43
2	A	1457	UPG	O4'-C4'	5.09	1.55	1.43
2	A	1457	UPG	C3'-C2'	4.26	1.63	1.52
2	A	1457	UPG	O5'-C1'	4.24	1.52	1.41
2	A	1457	UPG	C4-N3	3.88	1.39	1.33
2	A	1457	UPG	C6-N1	3.22	1.39	1.35
2	A	1457	UPG	C2C-C1C	-3.21	1.48	1.53
2	A	1457	UPG	C6'-C5'	2.20	1.59	1.51
2	A	1457	UPG	PA-O1A	-2.08	1.43	1.50
2	A	1457	UPG	C4'-C3'	2.00	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1457	UPG	O3A-PB-O3B	14.99	132.72	102.48
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'	-6.01	97.62	110.35
2	A	1457	UPG	C1'-O5'-C5'	5.11	123.71	113.69
2	A	1457	UPG	O3'-C3'-C2'	5.04	121.99	110.35
2	A	1457	UPG	O3B-PB-O1B	-2.68	99.41	109.47
2	A	1457	UPG	C6'-C5'-C4'	-2.60	106.91	113.00
2	A	1457	UPG	O5'-C5'-C4'	-2.53	105.10	109.69
2	A	1457	UPG	O2B-PB-O1B	-2.29	100.90	112.24
2	A	1457	UPG	C1'-C2'-C3'	2.08	114.33	110.00

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

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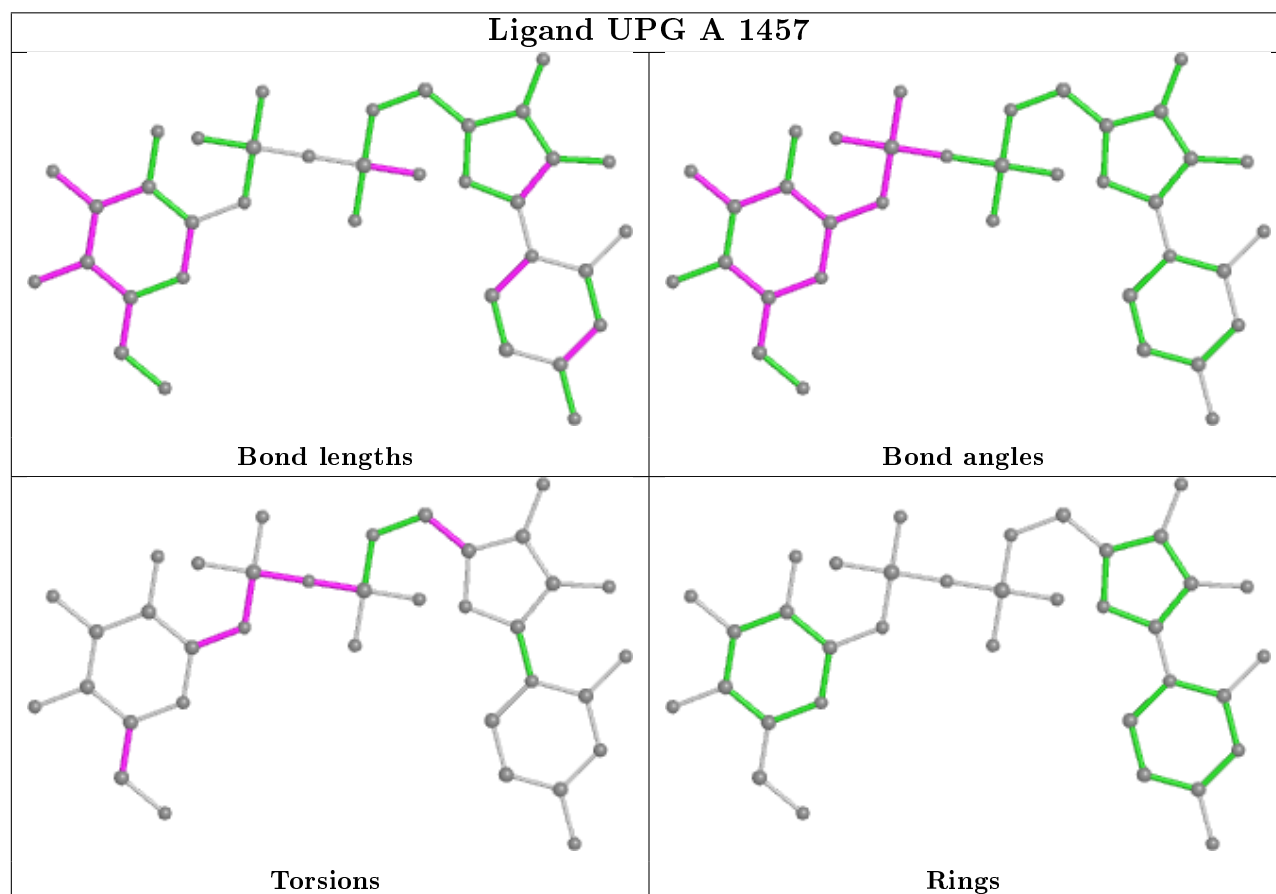
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Mol	Chain	Res	Type	Atoms
2	A	1457	UPG	C4'-C5'-C6'-O6'
2	A	1457	UPG	C1'-O3B-PB-O3A

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.60	36 (7%) 12 11	13, 19, 27, 34	0
1	B	449/482 (93%)	1.24	90 (20%) 1 0	13, 20, 39, 52	0
All	All	901/964 (93%)	0.91	126 (13%) 2 2	13, 20, 34, 52	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	VAL	18.5
1	B	249	ALA	12.9
1	B	299	SER	11.9
1	B	302	ASP	11.0
1	B	304	GLN	9.4
1	B	55	VAL	9.0
1	B	67	LEU	8.2
1	B	46	GLY	8.0
1	B	41	TRP	7.7
1	B	300	ARG	6.7
1	B	44	GLU	6.5
1	B	306	TYR	6.3
1	B	43	GLY	5.8
1	B	246	GLN	5.8
1	B	52	LEU	5.7
1	B	49	ASP	5.4
1	B	253	ASN	5.4
1	B	245	ALA	5.4
1	B	243	LYS	5.3
1	A	14	ASP	5.3
1	B	252	LYS	5.3
1	B	57	LYS	5.3
1	B	10	ILE	5.2
1	B	50	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	THR	5.0
1	B	12	PRO	5.0
1	B	47	ASN	4.9
1	B	60	ILE	4.8
1	B	11	ALA	4.7
1	B	301	GLY	4.7
1	B	53	LYS	4.6
1	B	206	ARG	4.6
1	A	19	SER	4.6
1	B	241	PRO	4.5
1	B	76	TYR	4.4
1	B	9	ARG	4.4
1	B	251	LEU	4.3
1	B	51	PRO	4.3
1	B	240	LEU	4.3
1	B	298	THR	4.2
1	B	250	GLU	4.2
1	B	305	ALA	4.1
1	B	70	GLN	4.1
1	B	56	LYS	4.0
1	B	350	TYR	4.0
1	A	13	PRO	3.9
1	A	176	LEU	3.9
1	B	242	PRO	3.6
1	B	208	ALA	3.5
1	B	1	SER	3.5
1	A	47	ASN	3.4
1	B	244	LEU	3.4
1	B	62	TRP	3.3
1	B	247	LEU	3.3
1	B	32	LYS	3.2
1	B	73	ASP	3.2
1	B	20	ALA	3.2
1	B	202	ARG	3.2
1	B	48	GLU	3.1
1	A	45	THR	3.1
1	A	177	CYS	3.1
1	B	42	SER	3.1
1	A	46	GLY	3.0
1	A	51	PRO	3.0
1	A	134	LEU	3.0
1	B	74	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	2.9
1	B	237	ALA	2.9
1	B	338	HIS	2.9
1	B	61	THR	2.8
1	B	54	LYS	2.8
1	A	44	GLU	2.8
1	B	248	LYS	2.8
1	A	69	GLU	2.7
1	B	207	SER	2.7
1	B	215	GLY	2.7
1	B	307	GLN	2.7
1	B	21	GLY	2.6
1	A	202	ARG	2.6
1	A	182	LEU	2.6
1	A	55	VAL	2.6
1	B	146	ASN	2.6
1	B	447	ILE	2.6
1	A	173	LEU	2.6
1	B	66	ASN	2.6
1	A	367	ALA	2.6
1	B	446	PHE	2.6
1	B	34	ALA	2.5
1	B	58	GLY	2.5
1	A	252	LYS	2.5
1	B	104	GLY	2.5
1	B	78	GLN	2.5
1	A	49	ASP	2.5
1	B	71	ASP	2.5
1	B	262	ARG	2.4
1	A	151	PHE	2.4
1	B	111	LEU	2.4
1	B	122	ASP	2.4
1	A	179	TYR	2.4
1	A	58	GLY	2.4
1	A	350	TYR	2.4
1	A	370	TYR	2.4
1	B	63	ALA	2.4
1	A	50	GLN	2.3
1	B	450	LEU	2.3
1	A	123	ASP	2.3
1	B	69	GLU	2.2
1	A	1	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	65	PHE	2.2
1	B	75	TYR	2.2
1	B	311	HIS	2.2
1	A	355	LEU	2.2
1	B	33	ALA	2.1
1	B	212	THR	2.1
1	B	117	LEU	2.1
1	B	371	VAL	2.1
1	A	9	ARG	2.1
1	B	119	LEU	2.1
1	A	357	THR	2.1
1	A	79	PHE	2.1
1	A	53	LYS	2.1
1	B	205	THR	2.0
1	A	253	ASN	2.0
1	A	227	ILE	2.0
1	A	172	LEU	2.0
1	B	125	ILE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

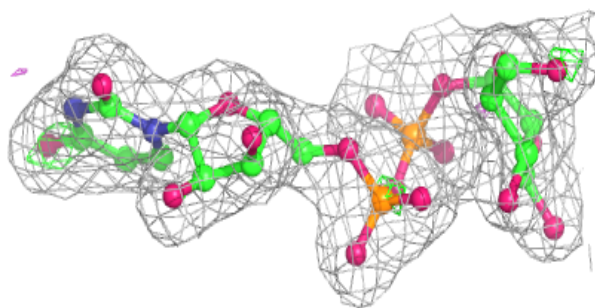
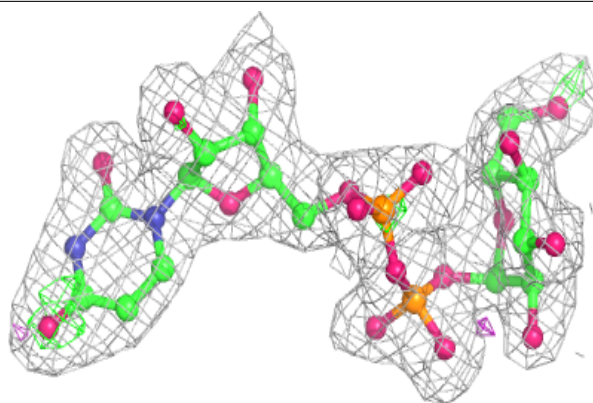
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UPG	A	1457	36/36	0.95	0.15	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.