



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:22 PM EDT

PDB ID : 6Z89 / pdb_00006z89
Title : human GTP cyclohydrolase I in complex with allosteric inhibitor
Authors : Ebenhoch, R.; Nar, H.
Deposited on : 2020-06-02
Resolution : 2.37 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

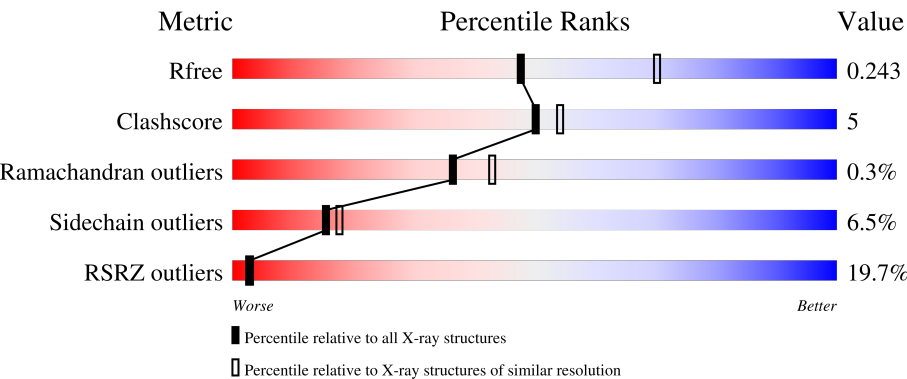
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	224	9% 74% 6% • 19%
1	B	224	13% 64% 13% 23%
1	C	224	13% 45% 8% 46%
1	D	224	19% 64% 14% • 20%
1	E	224	18% 58% 14% • 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6619 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 GTP cyclohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1427	903	246	271	7			
1	B	173	Total	C	N	O	S	0	1	0
			1372	870	238	254	10			
1	C	120	Total	C	N	O	S	0	0	0
			954	609	166	171	8			
1	D	180	Total	C	N	O	S	0	0	0
			1422	900	247	269	6			
1	E	167	Total	C	N	O	S	0	0	0
			1317	834	231	243	9			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP P30793
A	28	HIS	-	expression tag	UNP P30793
A	29	HIS	-	expression tag	UNP P30793
A	30	HIS	-	expression tag	UNP P30793
A	31	HIS	-	expression tag	UNP P30793
A	32	HIS	-	expression tag	UNP P30793
A	33	HIS	-	expression tag	UNP P30793
A	34	GLY	-	expression tag	UNP P30793
A	35	SER	-	expression tag	UNP P30793
A	36	ASP	-	expression tag	UNP P30793
A	37	ASP	-	expression tag	UNP P30793
A	38	ASP	-	expression tag	UNP P30793
A	39	ASP	-	expression tag	UNP P30793
A	40	LYS	-	expression tag	UNP P30793
B	27	MET	-	initiating methionine	UNP P30793
B	28	HIS	-	expression tag	UNP P30793
B	29	HIS	-	expression tag	UNP P30793
B	30	HIS	-	expression tag	UNP P30793
B	31	HIS	-	expression tag	UNP P30793

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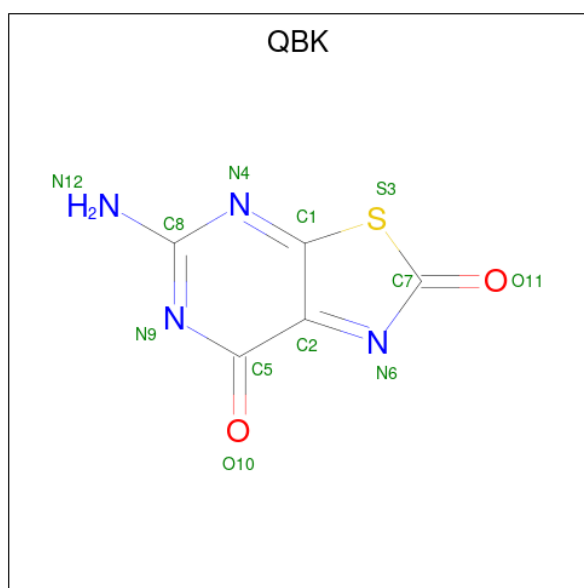
Chain	Residue	Modelled	Actual	Comment	Reference
B	32	HIS	-	expression tag	UNP P30793
B	33	HIS	-	expression tag	UNP P30793
B	34	GLY	-	expression tag	UNP P30793
B	35	SER	-	expression tag	UNP P30793
B	36	ASP	-	expression tag	UNP P30793
B	37	ASP	-	expression tag	UNP P30793
B	38	ASP	-	expression tag	UNP P30793
B	39	ASP	-	expression tag	UNP P30793
B	40	LYS	-	expression tag	UNP P30793
C	27	MET	-	initiating methionine	UNP P30793
C	28	HIS	-	expression tag	UNP P30793
C	29	HIS	-	expression tag	UNP P30793
C	30	HIS	-	expression tag	UNP P30793
C	31	HIS	-	expression tag	UNP P30793
C	32	HIS	-	expression tag	UNP P30793
C	33	HIS	-	expression tag	UNP P30793
C	34	GLY	-	expression tag	UNP P30793
C	35	SER	-	expression tag	UNP P30793
C	36	ASP	-	expression tag	UNP P30793
C	37	ASP	-	expression tag	UNP P30793
C	38	ASP	-	expression tag	UNP P30793
C	39	ASP	-	expression tag	UNP P30793
C	40	LYS	-	expression tag	UNP P30793
D	27	MET	-	initiating methionine	UNP P30793
D	28	HIS	-	expression tag	UNP P30793
D	29	HIS	-	expression tag	UNP P30793
D	30	HIS	-	expression tag	UNP P30793
D	31	HIS	-	expression tag	UNP P30793
D	32	HIS	-	expression tag	UNP P30793
D	33	HIS	-	expression tag	UNP P30793
D	34	GLY	-	expression tag	UNP P30793
D	35	SER	-	expression tag	UNP P30793
D	36	ASP	-	expression tag	UNP P30793
D	37	ASP	-	expression tag	UNP P30793
D	38	ASP	-	expression tag	UNP P30793
D	39	ASP	-	expression tag	UNP P30793
D	40	LYS	-	expression tag	UNP P30793
E	27	MET	-	initiating methionine	UNP P30793
E	28	HIS	-	expression tag	UNP P30793
E	29	HIS	-	expression tag	UNP P30793
E	30	HIS	-	expression tag	UNP P30793
E	31	HIS	-	expression tag	UNP P30793

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Chain	Residue	Modelled	Actual	Comment	Reference
E	32	HIS	-	expression tag	UNP P30793
E	33	HIS	-	expression tag	UNP P30793
E	34	GLY	-	expression tag	UNP P30793
E	35	SER	-	expression tag	UNP P30793
E	36	ASP	-	expression tag	UNP P30793
E	37	ASP	-	expression tag	UNP P30793
E	38	ASP	-	expression tag	UNP P30793
E	39	ASP	-	expression tag	UNP P30793
E	40	LYS	-	expression tag	UNP P30793

- Molecule 2 is 5-azanyl-[1,3]thiazolo[5,4-d]pyrimidine-2,7-dione (CCD ID: QBK) (formula: $C_5H_2N_4O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	5	4	2	1		
2	E	1	Total	C	N	O	S	0	0
			12	5	4	2	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0

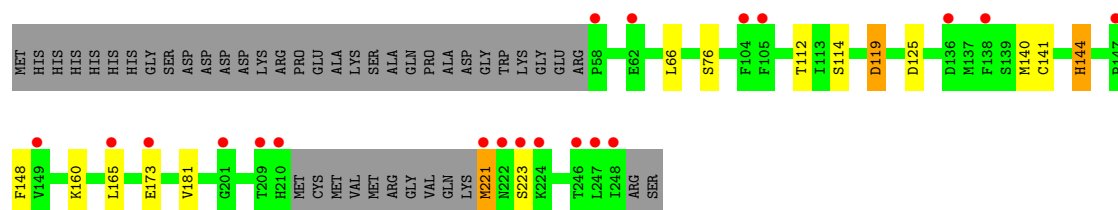
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	23	Total 23	O 23	0	0
4	C	6	Total 6	O 6	0	0
4	D	15	Total 15	O 15	0	0
4	E	18	Total 18	O 18	0	0

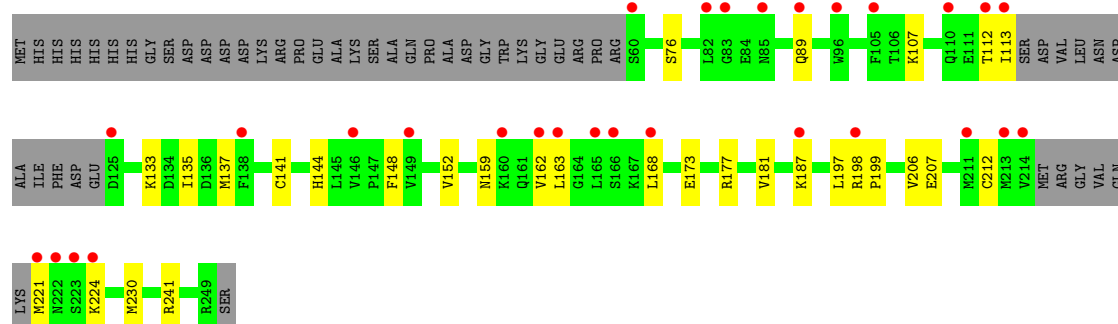
3 Residue-property plots [i](#)

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.

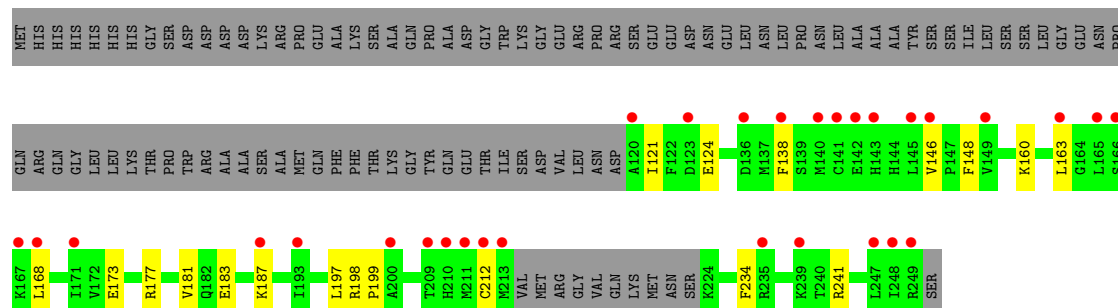
• Molecule 1: GTP cyclohydrolase 1



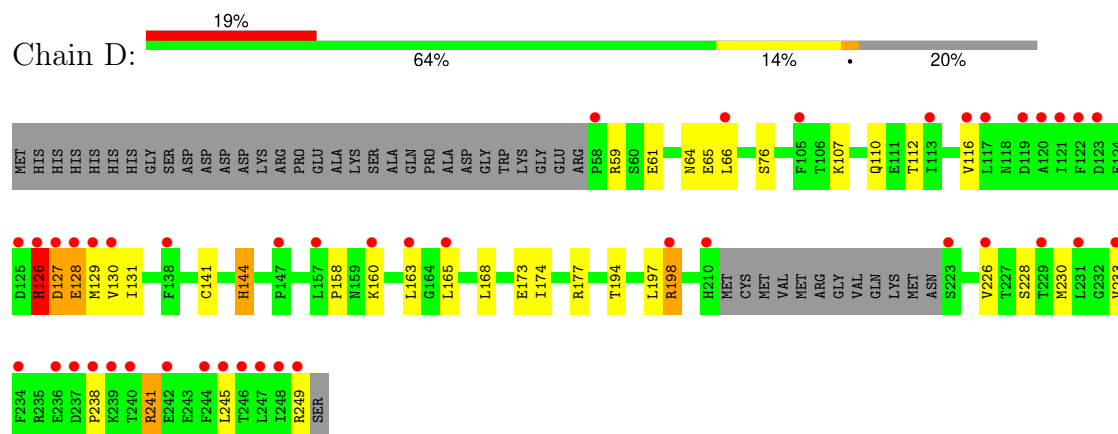
• Molecule 1: GTP cyclohydrolase 1



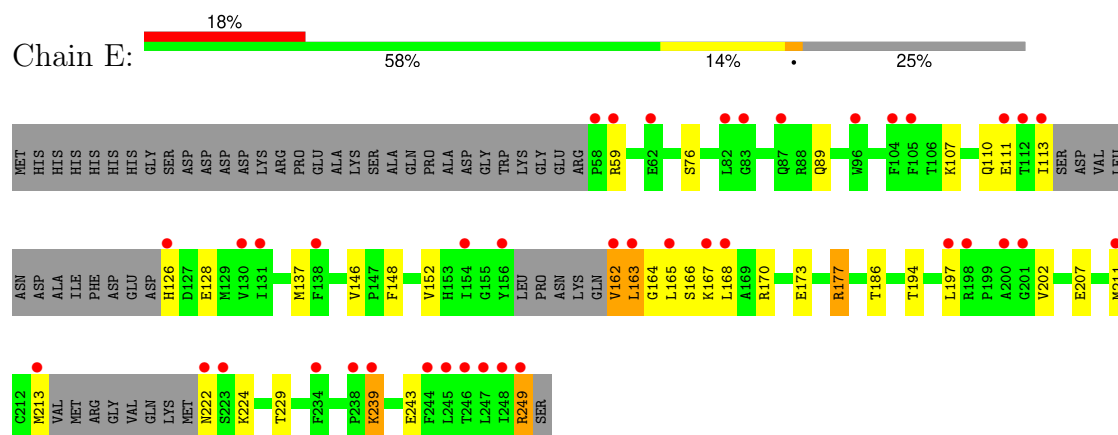
• Molecule 1: GTP cyclohydrolase 1



• Molecule 1: GTP cyclohydrolase 1



• Molecule 1: GTP cyclohydrolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.79Å 121.79Å 357.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	105.47 – 2.37 105.47 – 2.37	Depositor EDS
% Data completeness (in resolution range)	68.3 (105.47-2.37) 68.8 (105.47-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.234 , 0.238 0.236 , 0.243	Depositor DCC
R_{free} test set	2220 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6619	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: ZN, QBK

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	0.76	0/1451	1.09	2/1962 (0.1%)
1	B	0.75	0/1394	1.10	2/1880 (0.1%)
1	C	0.67	0/968	1.07	1/1304 (0.1%)
1	D	0.74	0/1446	1.11	1/1955 (0.1%)
1	E	0.71	0/1337	1.07	3/1801 (0.2%)
All	All	0.73	0/6596	1.09	9/8902 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	148	PHE	CA-CB-CG	7.59	121.39	113.80
1	B	148	PHE	CA-CB-CG	7.27	121.07	113.80
1	B	159	ASN	CA-CB-CG	6.47	119.07	112.60
1	C	148	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	119	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	127	ASP	N-CA-C	-5.62	98.11	107.99
1	A	148	PHE	CA-CB-CG	5.61	119.41	113.80
1	E	111	GLU	CA-C-N	5.27	130.51	121.87
1	E	111	GLU	C-N-CA	5.27	130.51	121.87

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	1427	0	1440	6	0
1	B	1372	0	1389	14	0
1	C	954	0	987	10	0
1	D	1422	0	1438	27	0
1	E	1317	0	1340	22	0
2	A	12	0	0	0	0
2	E	12	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	36	0	0	0	0
4	B	23	0	0	0	0
4	C	6	0	0	0	0
4	D	15	0	0	0	0
4	E	18	0	0	0	0
All	All	6619	0	6594	69	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 5.

All (69) 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:E:126:HIS:CE1	1:E:162:VAL:HG11	2.01	0.94
1:D:59:ARG:HD3	1:D:64:ASN:OD1	1.70	0.89
1:E:167:LYS:NZ	1:E:170:ARG:HD3	1.95	0.80
1:D:126:HIS:NE2	1:D:128:GLU:HA	1.98	0.79
1:E:186:THR:HG22	1:E:229:THR:HG22	1.65	0.79
1:A:223:SER:HB2	1:B:133:LYS:O	1.86	0.75
1:D:129:MET:HE3	1:D:131:ILE:HD11	1.68	0.75
1:A:165:LEU:HD23	1:E:213:MET:HE2	1.72	0.71
1:D:128:GLU:O	1:D:158:PRO:HD2	1.91	0.70
1:E:167:LYS:HZ2	1:E:170:ARG:HD3	1.55	0.69
1:E:167:LYS:HA	1:E:170:ARG:HB2	1.79	0.64
1:D:116:VAL:HG11	1:D:174:ILE:HD11	1.80	0.63
1:B:207:GLU:HG2	1:B:224:LYS:HD3	1.81	0.63
1:D:249:ARG:HE	1:E:249:ARG:HD3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HB2	1:B:197:LEU:HD21	1.82	0.62
1:C:121:ILE:HD12	1:C:197:LEU:HD23	1.83	0.60
1:A:125:ASP:HA	1:A:160:LYS:HD2	1.84	0.59
1:D:228:SER:O	1:E:128:GLU:HB2	2.03	0.58
1:C:124:GLU:O	1:C:160:LYS:O	2.23	0.56
1:C:138:PHE:HD1	1:C:177:ARG:NH1	2.04	0.56
1:D:59:ARG:HD2	1:D:110:GLN:HG2	1.88	0.56
1:D:116:VAL:CG1	1:D:174:ILE:HD11	2.35	0.55
1:D:141:CYS:HG	1:D:144:HIS:CD2	2.25	0.55
1:D:163:LEU:HB2	1:D:197:LEU:HD11	1.89	0.54
1:B:141:CYS:SG	1:B:212:CYS:SG	3.05	0.54
1:E:167:LYS:HZ3	1:E:170:ARG:HD3	1.71	0.54
1:D:126:HIS:HB3	1:D:160:LYS:HD3	1.91	0.53
1:B:135:ILE:CD1	1:B:168:LEU:HD21	2.39	0.52
1:D:249:ARG:NE	1:E:249:ARG:HD3	2.25	0.52
1:D:238:PRO:HB3	1:E:239:LYS:HG3	1.92	0.51
1:E:146:VAL:HG12	1:E:211:MET:HB2	1.93	0.51
1:E:207:GLU:HB3	1:E:224:LYS:CE	2.40	0.51
1:D:59:ARG:HD2	1:D:110:GLN:CG	2.41	0.51
1:D:238:PRO:HB3	1:E:239:LYS:CG	2.42	0.50
1:D:61:GLU:O	1:D:65:GLU:HG2	2.11	0.50
1:D:107:LYS:HE3	1:D:177:ARG:HD2	1.95	0.49
1:B:144:HIS:ND1	1:B:212:CYS:SG	2.84	0.49
1:C:146:VAL:HG21	1:C:212:CYS:HB3	1.95	0.49
1:D:127:ASP:O	1:D:128:GLU:O	2.32	0.48
1:B:163:LEU:HD23	1:B:168:LEU:HD12	1.95	0.48
1:D:126:HIS:CD2	1:D:128:GLU:HA	2.47	0.48
1:B:230:MET:HG3	1:B:241:ARG:NH2	2.29	0.48
1:D:245:LEU:HD11	1:E:243:GLU:HG3	1.95	0.47
1:E:163:LEU:HD21	1:E:168:LEU:HD12	1.97	0.46
1:B:135:ILE:HD11	1:B:168:LEU:HD21	1.98	0.46
1:E:194:THR:OG1	1:E:202:VAL:HG11	2.15	0.46
1:C:183:GLU:HB3	1:D:127:ASP:CB	2.46	0.45
1:E:163:LEU:HB3	1:E:197:LEU:HD21	1.97	0.45
1:B:137:MET:HB2	1:B:152:VAL:HG23	1.99	0.45
1:D:194:THR:HG22	1:D:198:ARG:HH21	1.82	0.45
1:D:141:CYS:SG	1:D:144:HIS:CD2	3.10	0.45
1:E:137:MET:HB2	1:E:152:VAL:HG23	1.99	0.45
1:A:141:CYS:HG	1:A:144:HIS:CD2	2.34	0.45
1:B:152:VAL:HG13	1:B:206:VAL:HG22	1.98	0.45
1:E:107:LYS:HE3	1:E:177:ARG:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HE3	1:B:177:ARG:HD2	1.99	0.44
1:C:138:PHE:CD1	1:C:177:ARG:NH1	2.85	0.44
1:D:163:LEU:HD23	1:D:168:LEU:HD12	2.02	0.42
1:C:234:PHE:O	1:C:241:ARG:HD2	2.19	0.42
1:E:224:LYS:HB3	1:E:224:LYS:HE2	1.80	0.41
1:A:221:MET:HE3	1:A:221:MET:HB3	1.87	0.41
1:B:135:ILE:HD13	1:B:168:LEU:HD21	2.02	0.41
1:A:141:CYS:SG	1:A:144:HIS:CD2	3.14	0.40
1:C:183:GLU:HB3	1:D:127:ASP:HB2	2.03	0.40
1:D:230:MET:HE3	1:D:241:ARG:HD2	2.02	0.40
1:E:164:GLY:O	1:E:166:SER:O	2.39	0.40
1:C:163:LEU:HD23	1:C:168:LEU:HD12	2.04	0.40
1:C:198:ARG:N	1:C:199:PRO:HD3	2.37	0.40
1:B:198:ARG:N	1:B:199:PRO:HD3	2.36	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	177/224 (79%)	174 (98%)	3 (2%)	0	100	100
1	B	168/224 (75%)	165 (98%)	3 (2%)	0	100	100
1	C	116/224 (52%)	113 (97%)	3 (3%)	0	100	100
1	D	176/224 (79%)	171 (97%)	3 (2%)	2 (1%)	11	11
1	E	159/224 (71%)	155 (98%)	4 (2%)	0	100	100
All	All	796/1120 (71%)	778 (98%)	16 (2%)	2 (0%)	36	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	GLU
1	D	126	HIS

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	159/195 (82%)	149 (94%)	10 (6%)	16	19
1	B	152/195 (78%)	143 (94%)	9 (6%)	18	22
1	C	107/195 (55%)	104 (97%)	3 (3%)	38	51
1	D	158/195 (81%)	146 (92%)	12 (8%)	12	13
1	E	146/195 (75%)	133 (91%)	13 (9%)	9	10
All	All	722/975 (74%)	675 (94%)	47 (6%)	15	18

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	76	SER
1	A	112	THR
1	A	114	SER
1	A	119	ASP
1	A	140	MET
1	A	144	HIS
1	A	173	GLU
1	A	181	VAL
1	A	221	MET
1	B	76	SER
1	B	89	GLN
1	B	112	THR
1	B	113	ILE
1	B	162	VAL
1	B	173	GLU
1	B	181	VAL
1	B	187	LYS

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Mol	Chain	Res	Type
1	B	221	MET
1	C	173	GLU
1	C	181	VAL
1	C	187	LYS
1	D	66	LEU
1	D	76	SER
1	D	112	THR
1	D	126	HIS
1	D	130	VAL
1	D	144	HIS
1	D	165	LEU
1	D	173	GLU
1	D	198	ARG
1	D	226	VAL
1	D	233	VAL
1	D	241	ARG
1	E	59	ARG
1	E	76	SER
1	E	89	GLN
1	E	110	GLN
1	E	113	ILE
1	E	162	VAL
1	E	163	LEU
1	E	165	LEU
1	E	173	GLU
1	E	177	ARG
1	E	222	ASN
1	E	239	LYS
1	E	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	89	GLN
1	A	180	GLN
1	A	188	GLN
1	B	64	ASN
1	B	70	ASN
1	B	110	GLN
1	B	180	GLN
1	B	188	GLN

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Mol	Chain	Res	Type
1	C	180	GLN
1	C	188	GLN
1	D	70	ASN
1	D	180	GLN
1	E	70	ASN
1	E	110	GLN
1	E	126	HIS
1	E	180	GLN

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](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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	QBK	E	302	-	11,13,13	0.62	0	8,19,19	2.12	2 (25%)
2	QBK	A	301	-	11,13,13	0.63	0	8,19,19	2.15	2 (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	QBK	E	302	-	-	-	0/2/2/2
2	QBK	A	301	-	-	-	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	QBK	C5-C2-C1	-4.78	118.43	122.09
2	E	302	QBK	C5-C2-C1	-4.65	118.53	122.09
2	A	301	QBK	N4-C8-N9	-2.59	122.33	126.44
2	E	302	QBK	N4-C8-N9	-2.55	122.40	126.44

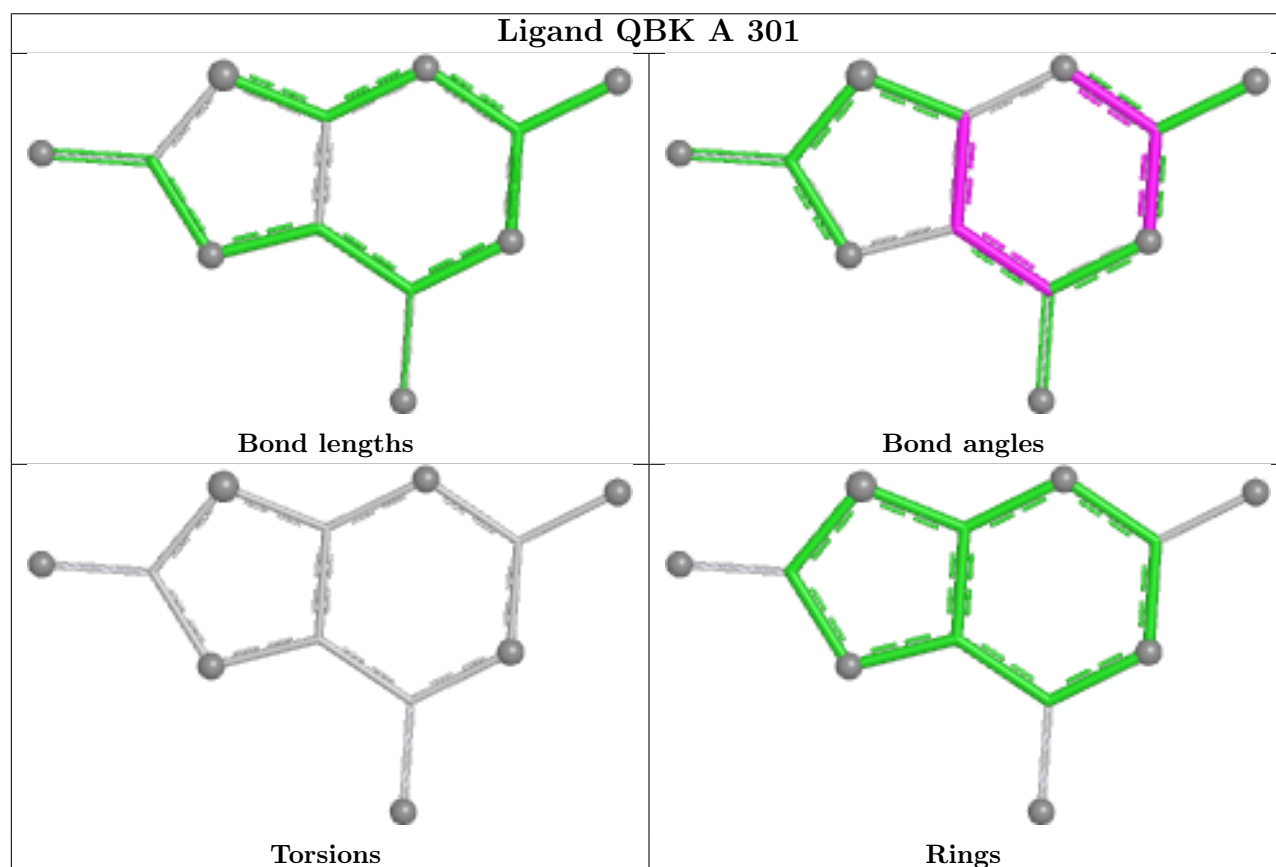
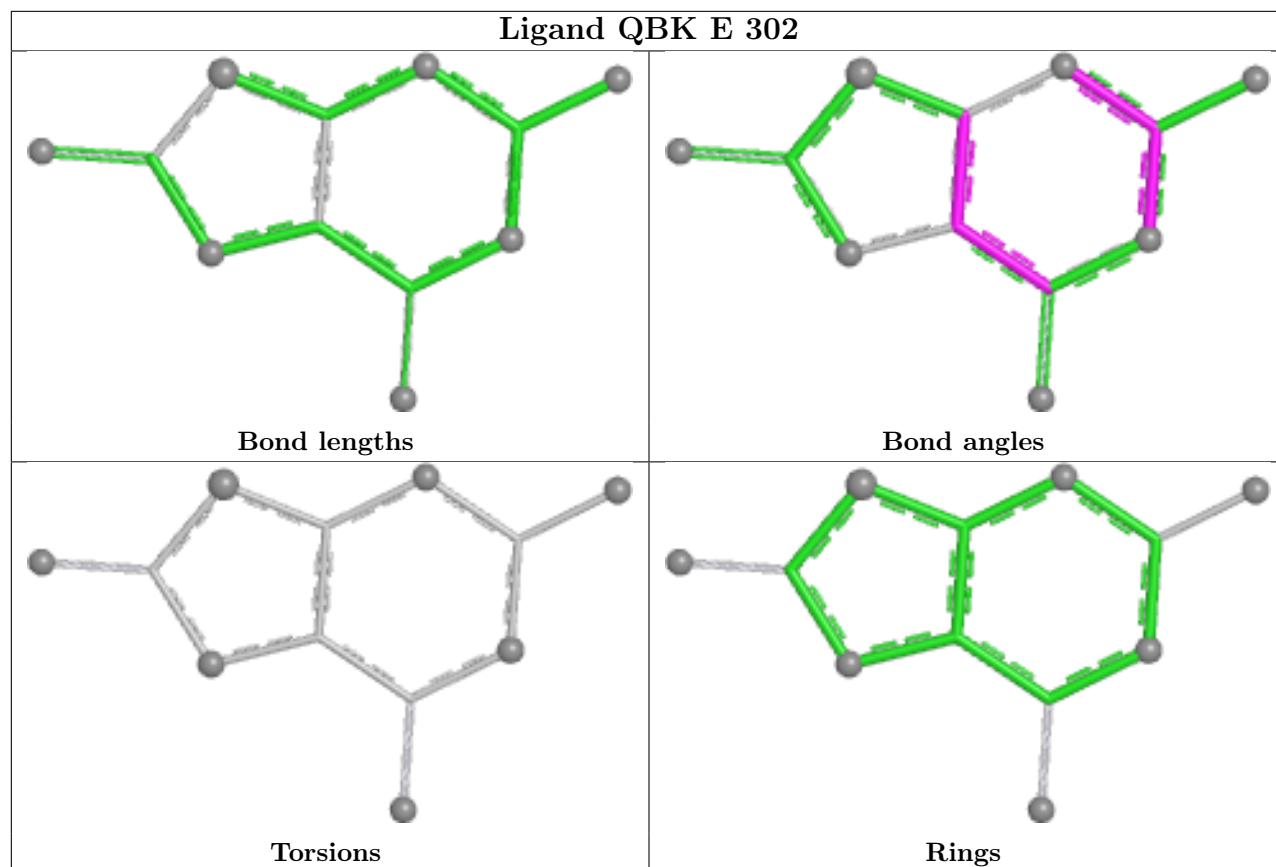
There are no chirality outliers.

There are no torsion outliers.

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	181/224 (80%)	0.80	20 (11%)	10 12	50, 63, 85, 109	0
1	B	173/224 (77%)	1.07	29 (16%)	4 4	30, 68, 101, 107	1 (0%)
1	C	120/224 (53%)	1.46	30 (25%)	2 1	59, 90, 120, 126	0
1	D	180/224 (80%)	1.27	43 (23%)	2 1	53, 79, 127, 138	0
1	E	167/224 (74%)	1.49	40 (23%)	2 1	53, 75, 109, 121	0
All	All	821/1120 (73%)	1.20	162 (19%)	3 3	30, 73, 110, 138	1 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	ILE	10.4
1	E	113	ILE	9.9
1	B	214	VAL	8.2
1	B	221	MET	6.7
1	D	127	ASP	6.5
1	A	138	PHE	6.4
1	E	165	LEU	6.2
1	E	58	PRO	6.0
1	C	138	PHE	5.4
1	E	105	PHE	5.3
1	E	104	PHE	5.1
1	E	162	VAL	5.1
1	D	138	PHE	5.0
1	E	138	PHE	5.0
1	D	121	ILE	4.9
1	D	113	ILE	4.9
1	E	248	ILE	4.7
1	C	136	ASP	4.7
1	A	149	VAL	4.6
1	E	222	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	223	SER	4.5
1	B	138[A]	PHE	4.5
1	C	149	VAL	4.5
1	D	229	THR	4.2
1	A	105	PHE	4.2
1	E	96	TRP	4.2
1	D	239	LYS	4.1
1	D	66	LEU	4.0
1	B	105	PHE	4.0
1	C	120	ALA	4.0
1	E	112	THR	4.0
1	D	245	LEU	3.9
1	E	167	LYS	3.9
1	D	244	PHE	3.8
1	A	209	THR	3.7
1	E	163	LEU	3.7
1	D	165	LEU	3.7
1	B	213	MET	3.6
1	E	59	ARG	3.6
1	E	211	MET	3.6
1	C	213	MET	3.5
1	B	60	SER	3.5
1	A	248	ILE	3.5
1	D	240	THR	3.4
1	D	126	HIS	3.4
1	E	246	THR	3.4
1	E	244	PHE	3.3
1	C	146	VAL	3.3
1	A	221	MET	3.3
1	C	165	LEU	3.3
1	D	248	ILE	3.3
1	A	104	PHE	3.2
1	A	223	SER	3.2
1	C	249	ARG	3.2
1	B	96	TRP	3.2
1	C	145	LEU	3.2
1	B	82	LEU	3.1
1	D	236	GLU	3.1
1	B	165	LEU	3.0
1	D	233	VAL	3.0
1	E	87	GLN	3.0
1	C	211	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	156	TYR	3.0
1	B	160	LYS	3.0
1	C	163	LEU	2.9
1	E	198	ARG	2.9
1	D	234	PHE	2.9
1	C	248	ILE	2.9
1	D	242	GLU	2.9
1	D	119	ASP	2.9
1	D	249	ARG	2.9
1	E	238	PRO	2.8
1	B	211	MET	2.8
1	B	83	GLY	2.8
1	C	235	ARG	2.8
1	D	223	SER	2.8
1	D	116	VAL	2.8
1	D	237	ASP	2.7
1	B	166	SER	2.7
1	B	222	ASN	2.7
1	C	166	SER	2.7
1	D	231	LEU	2.7
1	A	136	ASP	2.7
1	D	238	PRO	2.7
1	E	239	LYS	2.7
1	E	213	MET	2.7
1	A	247	LEU	2.7
1	D	117	LEU	2.7
1	D	210	HIS	2.6
1	D	226	VAL	2.6
1	E	83	GLY	2.6
1	B	223	SER	2.6
1	E	200	ALA	2.6
1	B	89	GLN	2.6
1	D	58	PRO	2.6
1	E	245	LEU	2.5
1	C	140	MET	2.5
1	B	146	VAL	2.5
1	D	163	LEU	2.5
1	D	123	ASP	2.5
1	C	210	HIS	2.5
1	E	247	LEU	2.5
1	B	125	ASP	2.5
1	A	210	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	141	CYS	2.4
1	E	131	ILE	2.4
1	B	168	LEU	2.4
1	D	160	LYS	2.4
1	E	126	HIS	2.4
1	B	110	GLN	2.4
1	A	246	THR	2.4
1	C	239	LYS	2.4
1	E	249	ARG	2.4
1	E	111	GLU	2.4
1	B	149	VAL	2.4
1	A	165	LEU	2.4
1	A	58	PRO	2.4
1	D	105	PHE	2.3
1	E	234	PHE	2.3
1	A	62	GLU	2.3
1	B	112	THR	2.3
1	C	209	THR	2.3
1	C	193	ILE	2.3
1	E	130	VAL	2.3
1	C	168	LEU	2.3
1	C	200	ALA	2.3
1	C	247	LEU	2.2
1	D	198	ARG	2.2
1	A	224	LYS	2.2
1	E	62	GLU	2.2
1	D	246	THR	2.2
1	E	197	LEU	2.2
1	D	128	GLU	2.2
1	C	167	LYS	2.2
1	A	222	ASN	2.2
1	D	129	MET	2.2
1	C	171	ILE	2.1
1	B	162	VAL	2.1
1	D	122	PHE	2.1
1	D	120	ALA	2.1
1	D	157	LEU	2.1
1	E	168	LEU	2.1
1	A	147	PRO	2.1
1	D	130	VAL	2.1
1	E	201	GLY	2.1
1	D	247	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	82	LEU	2.1
1	D	147	PRO	2.1
1	A	201	GLY	2.1
1	C	187	LYS	2.1
1	C	142	GLU	2.1
1	B	163	LEU	2.1
1	D	125	ASP	2.1
1	E	154	ILE	2.1
1	B	198	ARG	2.1
1	C	212	CYS	2.0
1	C	143	HIS	2.0
1	B	85	ASN	2.0
1	B	187	LYS	2.0
1	A	173	GLU	2.0
1	C	123	ASP	2.0
1	B	224	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](#)

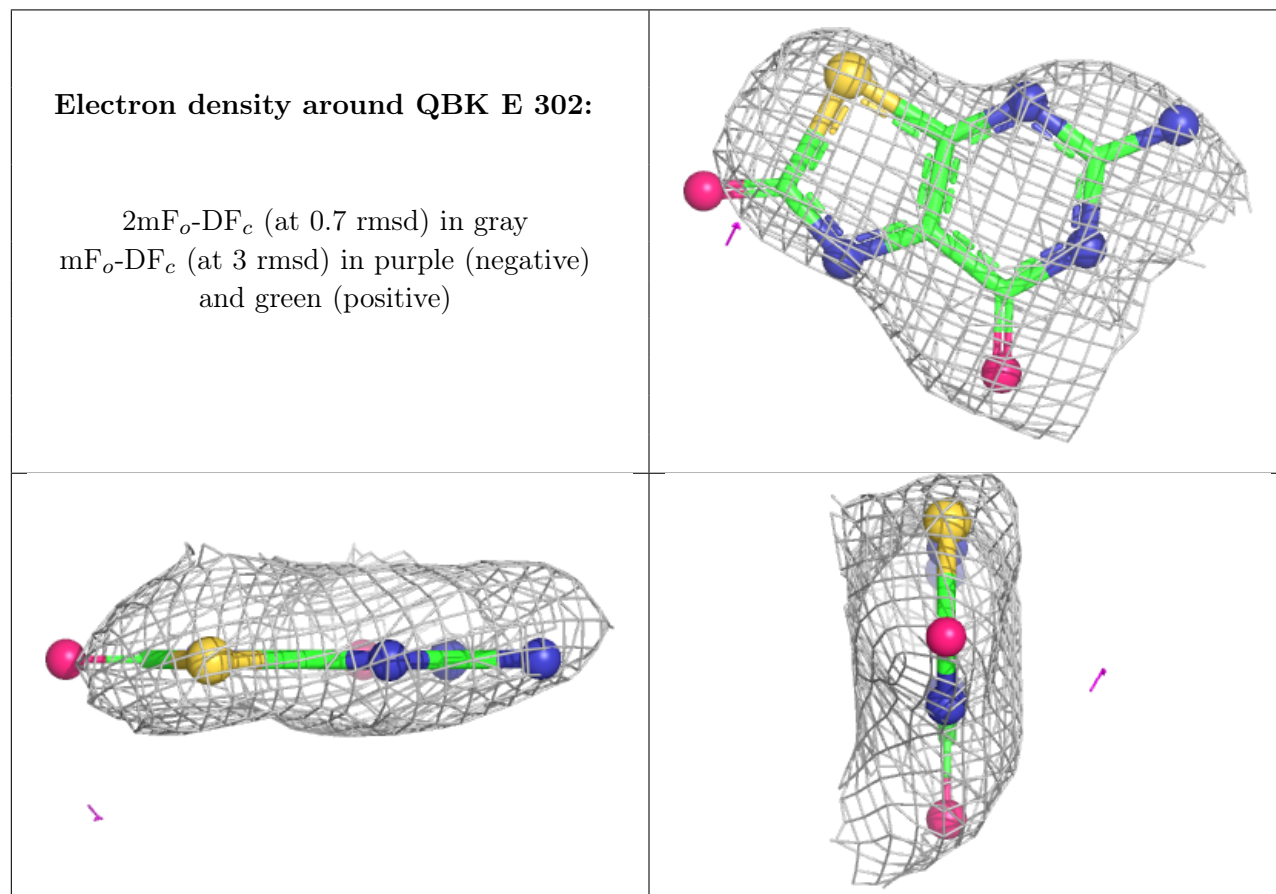
There are no oligosaccharides in this entry.

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.

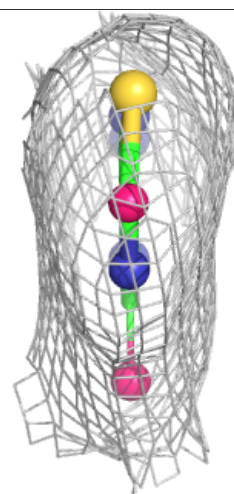
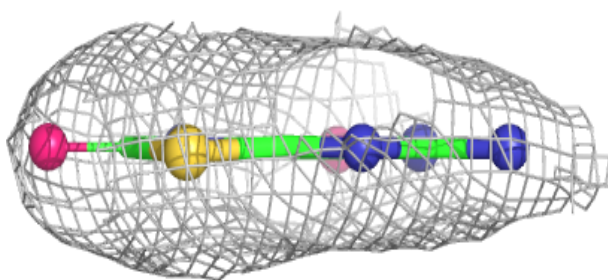
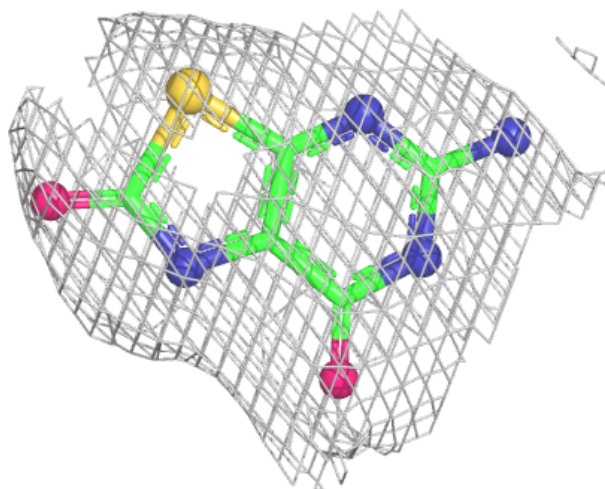
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	A	302	1/1	0.73	0.15	182,182,182,182	0
2	QBK	E	302	12/12	0.81	0.18	101,102,102,102	12
3	ZN	D	301	1/1	0.86	0.13	162,162,162,162	0
3	ZN	B	301	1/1	0.89	0.16	150,150,150,150	0
3	ZN	C	301	1/1	0.90	0.11	177,177,177,177	0
2	QBK	A	301	12/12	0.95	0.07	71,73,76,76	0
3	ZN	E	301	1/1	0.95	0.07	93,93,93,93	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around QBK A 301:

$2mF_o-DF_c$ (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.