



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 10:14 AM JST

PDB ID : 6LD9
Title : Crystal structure of cystathionine gamma synthase from *Xanthomonas oryzae* pv. *oryzae* in complex with cystathionine
Authors : Ngo, H.P.T.; Nguyen, T.D.Q.; Kang, L.W.
Deposited on : 2019-11-20
Resolution : 2.50 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 : 2.14.6
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) : 2.14.6

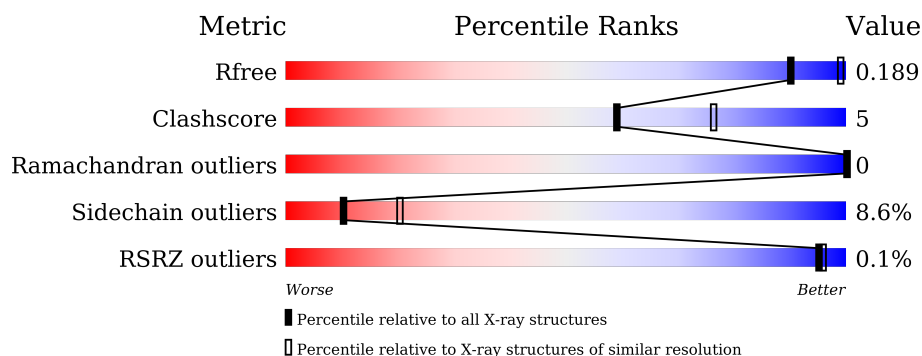
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	408	
1	B	408	
1	C	408	
1	D	408	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12052 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.

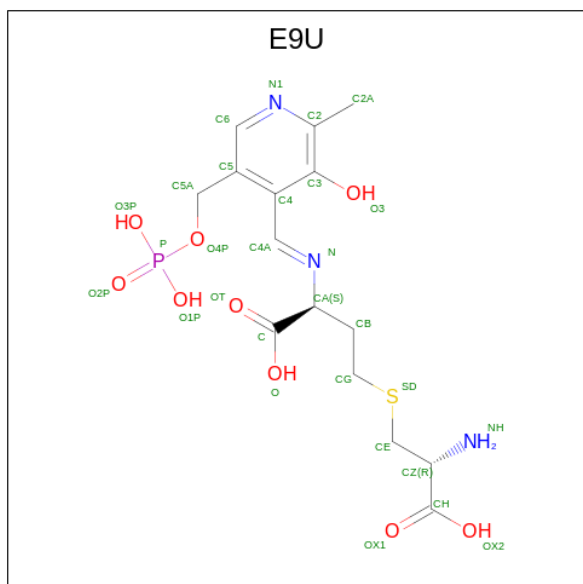
- Molecule 1 is a protein called Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2871	1813	506	545	7			
1	B	387	Total	C	N	O	S	0	0	0
			2871	1813	506	545	7			
1	C	388	Total	C	N	O	S	0	0	0
			2876	1816	507	546	7			
1	D	387	Total	C	N	O	S	0	0	0
			2871	1813	506	545	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5H1U9
A	-1	SER	-	expression tag	UNP Q5H1U9
A	0	HIS	-	expression tag	UNP Q5H1U9
A	5	TYR	ASP	engineered mutation	UNP Q5H1U9
A	8	ASP	HIS	engineered mutation	UNP Q5H1U9
B	-2	GLY	-	expression tag	UNP Q5H1U9
B	-1	SER	-	expression tag	UNP Q5H1U9
B	0	HIS	-	expression tag	UNP Q5H1U9
B	5	TYR	ASP	engineered mutation	UNP Q5H1U9
B	8	ASP	HIS	engineered mutation	UNP Q5H1U9
C	-2	GLY	-	expression tag	UNP Q5H1U9
C	-1	SER	-	expression tag	UNP Q5H1U9
C	0	HIS	-	expression tag	UNP Q5H1U9
C	5	TYR	ASP	engineered mutation	UNP Q5H1U9
C	8	ASP	HIS	engineered mutation	UNP Q5H1U9
D	-2	GLY	-	expression tag	UNP Q5H1U9
D	-1	SER	-	expression tag	UNP Q5H1U9
D	0	HIS	-	expression tag	UNP Q5H1U9
D	5	TYR	ASP	engineered mutation	UNP Q5H1U9
D	8	ASP	HIS	engineered mutation	UNP Q5H1U9

- Molecule 2 is (2 {S})-4-[(2 {R})-2-azanyl-3-oxidanyl-3-oxidanylidene-propyl]sulfanyl-2-[({E})-2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]methylenediamino]butanoic acid (three-letter code: E9U) (formula: C₁₅H₂₂N₃O₉PS) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 29	C 15	N 3	O 9	P 1	S 1	0	0
2	B	1	Total 29	C 15	N 3	O 9	P 1	S 1	0	0
2	C	1	Total 29	C 15	N 3	O 9	P 1	S 1	0	0
2	D	1	Total 29	C 15	N 3	O 9	P 1	S 1	0	0


- Molecule 3 is water.

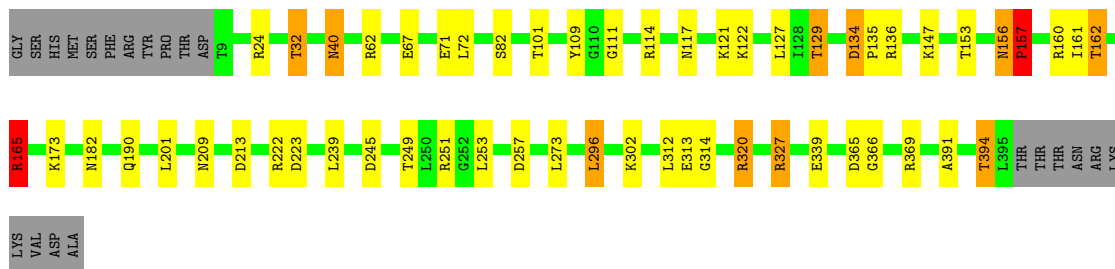
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	104	Total	O	0	0
			104	104		
3	C	119	Total	O	0	0
			119	119		
3	D	117	Total	O	0	0
			117	117		

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.

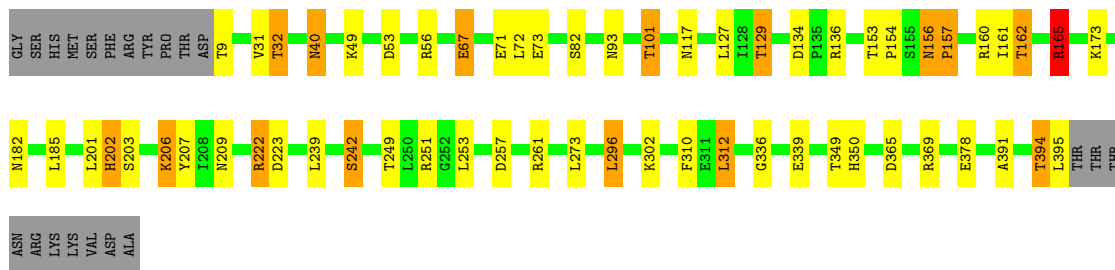
• Molecule 1: Cystathionine gamma-synthase

Chain A: 




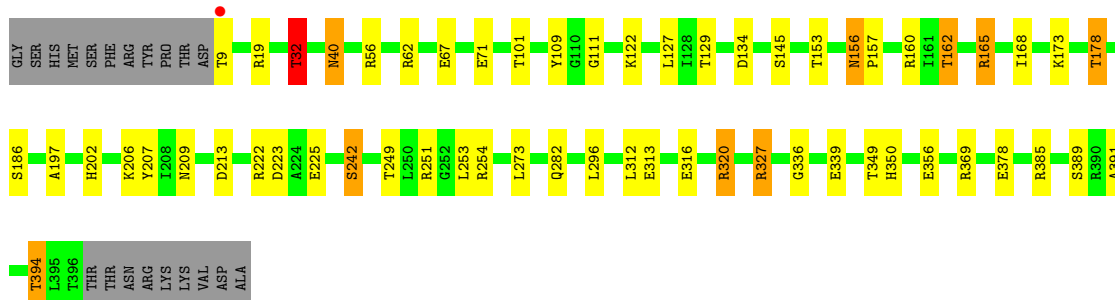
• Molecule 1: Cystathionine gamma-synthase

Chain B: 



• Molecule 1: Cystathionine gamma-synthase

Chain C: 



● Molecule 1: Cystathionine gamma-synthase

Chain D:

80%

12%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	161.15Å 161.15Å 245.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.06 – 2.50 47.06 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.06-2.50) 99.8 (47.06-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.50 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.153 , 0.186 0.157 , 0.189	Depositor DCC
R_{free} test set	5331 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 9.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12052	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: E9U

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	1.00	6/2925 (0.2%)	1.18	15/3981 (0.4%)
1	B	0.97	3/2925 (0.1%)	1.13	12/3981 (0.3%)
1	C	0.99	6/2930 (0.2%)	1.17	15/3988 (0.4%)
1	D	0.99	4/2925 (0.1%)	1.12	8/3981 (0.2%)
All	All	0.99	19/11705 (0.2%)	1.15	50/15931 (0.3%)

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	0	1
1	C	0	2
1	D	0	2
All	All	0	5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	GLU	CD-OE1	7.40	1.33	1.25
1	C	339	GLU	CD-OE1	7.14	1.33	1.25
1	B	203	SER	CA-CB	-6.40	1.43	1.52
1	B	339	GLU	CD-OE1	6.40	1.32	1.25
1	C	356	GLU	CD-OE2	6.40	1.32	1.25
1	A	67	GLU	CD-OE2	6.27	1.32	1.25
1	A	339	GLU	CD-OE2	6.21	1.32	1.25
1	A	257	ASP	CG-OD2	5.89	1.39	1.25
1	B	257	ASP	CG-OD2	5.86	1.38	1.25
1	D	339	GLU	CD-OE2	5.68	1.31	1.25
1	A	366	GLY	C-O	5.67	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	SER	CB-OG	-5.62	1.34	1.42
1	D	339	GLU	CD-OE1	5.58	1.31	1.25
1	D	67	GLU	CD-OE2	5.51	1.31	1.25
1	C	225	GLU	CD-OE2	5.43	1.31	1.25
1	A	314	GLY	C-O	5.35	1.32	1.23
1	D	45	GLY	C-O	5.32	1.32	1.23
1	C	378	GLU	CD-OE2	5.29	1.31	1.25
1	C	67	GLU	CD-OE1	5.15	1.31	1.25

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ARG	NE-CZ-NH2	-11.65	114.47	120.30
1	D	385	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	A	114	ARG	CG-CD-NE	10.23	133.28	111.80
1	C	385	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	C	62	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	D	62	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	C	62	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	254	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	165	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	D	134	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	165	ARG	CG-CD-NE	-7.18	96.72	111.80
1	C	160	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	254	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	261	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	160	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	32	THR	CA-CB-OG1	-6.86	94.60	109.00
1	A	32	THR	CA-CB-OG1	-6.84	94.64	109.00
1	D	160	ARG	CG-CD-NE	-6.75	97.63	111.80
1	A	114	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	160	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	117	ASN	CB-CA-C	6.57	123.54	110.40
1	B	365	ASP	CB-CG-OD1	6.35	124.01	118.30
1	C	134	ASP	N-CA-CB	-6.28	99.30	110.60
1	A	327	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	129	THR	CB-CA-C	6.10	128.07	111.60
1	C	160	ARG	CG-CD-NE	-6.06	99.08	111.80
1	D	32	THR	CA-CB-OG1	-6.02	96.35	109.00
1	C	165	ARG	CB-CG-CD	5.97	127.12	111.60
1	C	134	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	206	LYS	CB-CA-C	5.88	122.16	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	385	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	365	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	160	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	117	ASN	CB-CA-C	5.74	121.87	110.40
1	A	160	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	56	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	134	ASP	CB-CA-C	5.44	121.28	110.40
1	B	165	ARG	CG-CD-NE	-5.39	100.48	111.80
1	B	206	LYS	CB-CA-C	5.35	121.11	110.40
1	A	320	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	365	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	157	PRO	N-CA-CB	-5.21	96.87	102.60
1	A	62	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	67	GLU	CB-CA-C	5.17	120.75	110.40
1	C	327	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	223	ASP	CB-CA-C	5.16	120.72	110.40
1	C	32	THR	CA-CB-OG1	-5.15	98.19	109.00
1	C	160	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	222	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	129	THR	CB-CA-C	5.07	125.30	111.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	202	HIS	Peptide
1	C	202	HIS	Peptide
1	C	9	THR	Peptide
1	D	202	HIS	Peptide
1	D	9	THR	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	2871	0	2868	29	0
1	B	2871	0	2868	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2876	0	2870	27	0
1	D	2871	0	2868	30	0
2	A	29	0	0	0	0
2	B	29	0	0	2	0
2	C	29	0	0	1	0
2	D	29	0	0	3	0
3	A	107	0	0	1	0
3	B	104	0	0	7	0
3	C	119	0	0	5	0
3	D	117	0	0	3	0
All	All	12052	0	11474	109	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 (109) 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:251:ARG:HH22	1:C:209:ASN:HD21	1.32	0.77
1:A:165:ARG:HH21	1:A:165:ARG:HG2	1.52	0.72
1:B:40:ASN:H	1:B:40:ASN:HD22	1.39	0.71
1:D:316:GLU:OE2	1:D:320:ARG:NH2	2.25	0.69
1:B:209:ASN:HD21	1:D:251:ARG:HH22	1.41	0.69
1:B:391:ALA:O	1:B:394:THR:HB	1.92	0.69
1:A:209:ASN:HD21	1:C:251:ARG:HH22	1.41	0.69
1:C:156:ASN:HD21	1:C:369:ARG:HH11	1.40	0.68
1:A:40:ASN:HD22	1:A:40:ASN:H	1.41	0.68
1:B:162:THR:HG22	3:B:948:HOH:O	1.94	0.67
1:B:251:ARG:HH22	1:D:209:ASN:HD21	1.43	0.67
1:B:209:ASN:HD21	1:D:251:ARG:NH2	1.94	0.66
1:A:134:ASP:OD1	1:A:134:ASP:C	2.34	0.65
1:A:201:LEU:C	1:A:201:LEU:HD12	2.17	0.65
1:A:209:ASN:HD22	1:A:249:THR:HA	1.62	0.65
1:C:153:THR:HB	1:C:162:THR:HG23	1.81	0.63
1:A:251:ARG:NH2	1:C:209:ASN:HD21	1.96	0.63
1:B:134:ASP:C	1:B:134:ASP:OD1	2.37	0.62
1:C:209:ASN:HD22	1:C:249:THR:HA	1.64	0.62
1:B:101:THR:HG23	3:B:902:HOH:O	1.99	0.62
1:B:40:ASN:N	1:B:40:ASN:HD22	1.96	0.61
1:D:349:THR:OG1	1:D:350:HIS:HD2	1.84	0.61
1:A:153:THR:HB	1:A:162:THR:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:THR:HB	1:D:162:THR:HG23	1.81	0.61
1:D:156:ASN:HD21	1:D:369:ARG:HH11	1.50	0.60
1:A:209:ASN:HD21	1:C:251:ARG:NH2	1.99	0.59
1:B:209:ASN:HD22	1:B:249:THR:HA	1.67	0.59
1:D:391:ALA:O	1:D:394:THR:HB	2.03	0.59
1:A:40:ASN:N	1:A:40:ASN:HD22	1.98	0.58
1:B:156:ASN:HD21	1:B:369:ARG:HH11	1.51	0.58
1:B:201:LEU:HD12	1:B:201:LEU:C	2.22	0.58
1:B:251:ARG:NH2	1:D:209:ASN:HD21	2.02	0.57
1:D:162:THR:HG22	3:D:943:HOH:O	2.05	0.57
1:D:162:THR:CG2	3:D:943:HOH:O	2.51	0.56
1:A:156:ASN:HD21	1:A:369:ARG:HH11	1.52	0.56
1:B:162:THR:CG2	3:B:948:HOH:O	2.53	0.56
1:C:197:ALA:O	1:C:222:ARG:NH2	2.39	0.56
1:C:349:THR:OG1	1:C:350:HIS:HD2	1.88	0.56
1:A:391:ALA:O	1:A:394:THR:HB	2.05	0.55
1:A:32:THR:HG21	1:C:213:ASP:HB3	1.89	0.55
1:B:223:ASP:HB3	3:B:975:HOH:O	2.06	0.54
1:D:40:ASN:H	1:D:40:ASN:HD22	1.54	0.54
1:A:162:THR:HG21	3:A:966:HOH:O	2.08	0.53
1:C:109:TYR:CE2	1:C:111:GLY:HA3	2.44	0.53
1:D:209:ASN:HD22	1:D:249:THR:HA	1.73	0.53
1:C:162:THR:HG22	3:C:948:HOH:O	2.08	0.53
1:C:391:ALA:O	1:C:394:THR:HB	2.07	0.53
1:B:153:THR:HB	1:B:162:THR:HG23	1.91	0.52
1:D:201:LEU:C	1:D:201:LEU:HD12	2.30	0.52
1:A:122:LYS:NZ	1:B:93:ASN:O	2.42	0.52
1:C:19:ARG:HD3	3:C:943:HOH:O	2.09	0.52
1:A:109:TYR:CE2	1:A:111:GLY:HA3	2.45	0.51
1:B:32:THR:HG21	1:D:213:ASP:HB3	1.92	0.51
1:C:282:GLN:NE2	3:C:904:HOH:O	2.44	0.51
1:B:161:ILE:HG22	1:B:296:LEU:HD13	1.93	0.50
1:C:162:THR:HG21	3:C:1006:HOH:O	2.10	0.50
1:B:310:PHE:HE2	1:B:312:LEU:HD13	1.75	0.50
1:C:40:ASN:HD22	1:C:40:ASN:H	1.58	0.50
1:D:73:GLU:OE2	1:D:202:HIS:NE2	2.37	0.49
1:B:310:PHE:CE2	1:B:312:LEU:HD13	2.46	0.49
1:B:206:LYS:HZ1	2:B:801:E9U:C4A	2.26	0.48
1:B:162:THR:HG21	3:B:967:HOH:O	2.13	0.47
1:A:156:ASN:HD22	1:A:157:PRO:CA	2.27	0.47
1:C:168:ILE:HG12	1:C:178:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:HD2	3:B:977:HOH:O	2.13	0.47
1:B:49:LYS:HD2	1:B:53:ASP:OD2	2.15	0.47
1:C:162:THR:CG2	3:C:948:HOH:O	2.62	0.46
1:B:156:ASN:HA	1:B:157:PRO:HA	1.75	0.46
1:B:349:THR:OG1	1:B:350:HIS:HD2	1.98	0.46
1:C:122:LYS:O	1:D:98:PRO:HD2	2.14	0.46
1:B:207:TYR:CE1	1:B:336:GLY:HA2	2.51	0.46
1:D:11:CYS:HB2	1:D:15:THR:HB	1.98	0.46
1:D:161:ILE:HG22	1:D:296:LEU:HD13	1.97	0.46
1:B:40:ASN:ND2	1:B:40:ASN:N	2.64	0.45
1:D:114:ARG:HH22	2:D:801:E9U:CH	2.29	0.45
1:D:40:ASN:N	1:D:40:ASN:HD22	2.13	0.44
2:B:801:E9U:N	2:B:801:E9U:O3	2.50	0.44
1:B:101:THR:CG2	3:B:902:HOH:O	2.61	0.44
1:A:251:ARG:HH22	1:C:209:ASN:ND2	2.08	0.44
1:C:316:GLU:OE2	1:C:320:ARG:NH2	2.51	0.43
1:A:182:ASN:HD21	1:A:190:GLN:HB3	1.83	0.43
1:C:207:TYR:CE1	1:C:336:GLY:HA2	2.53	0.43
1:D:19:ARG:HD3	3:D:981:HOH:O	2.17	0.43
1:D:281:ASN:HB2	1:D:313:GLU:OE1	2.18	0.43
1:B:154:PRO:HD3	1:B:185:LEU:CD1	2.48	0.43
1:D:181:ASP:OD2	2:D:801:E9U:N1	2.51	0.43
1:B:156:ASN:HD22	1:B:157:PRO:CA	2.32	0.43
2:C:801:E9U:O3	2:C:801:E9U:N	2.52	0.43
1:C:242:SER:HB2	1:D:245:ASP:OD2	2.18	0.42
1:B:209:ASN:ND2	1:D:251:ARG:HH22	2.11	0.42
1:A:82:SER:HB3	1:B:82:SER:HB3	2.00	0.42
1:C:40:ASN:HD22	1:C:40:ASN:N	2.15	0.42
1:D:207:TYR:CE1	1:D:336:GLY:HA2	2.55	0.42
1:A:245:ASP:OD2	1:B:242:SER:HB2	2.19	0.42
1:B:31:VAL:HB	1:C:40:ASN:ND2	2.35	0.42
2:D:801:E9U:O3	2:D:801:E9U:N	2.53	0.41
1:A:40:ASN:N	1:A:40:ASN:ND2	2.65	0.41
1:B:73:GLU:OE2	1:B:202:HIS:NE2	2.48	0.41
1:A:134:ASP:HA	1:A:135:PRO:HD3	1.99	0.41
1:D:165:ARG:NH1	1:D:165:ARG:HG2	2.36	0.41
1:A:121:LYS:HE2	1:A:121:LYS:HB3	1.85	0.41
1:D:299:ARG:NH1	1:D:299:ARG:HB2	2.36	0.41
1:A:213:ASP:HB3	1:C:32:THR:HG21	2.03	0.41
1:D:105:PRO:HD3	1:D:150:LEU:O	2.21	0.40
1:B:56:ARG:HH11	1:B:56:ARG:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:HA	1:A:182:ASN:HD22	1.74	0.40
1:A:161:ILE:HG22	1:A:296:LEU:HD13	2.02	0.40
1:B:182:ASN:HA	1:B:182:ASN:HD22	1.72	0.40
1:A:239:LEU:HD23	1:B:239:LEU:HD23	2.02	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	385/408 (94%)	372 (97%)	13 (3%)	0	100	100
1	B	385/408 (94%)	371 (96%)	14 (4%)	0	100	100
1	C	386/408 (95%)	376 (97%)	10 (3%)	0	100	100
1	D	385/408 (94%)	375 (97%)	10 (3%)	0	100	100
All	All	1541/1632 (94%)	1494 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	291/310 (94%)	266 (91%)	25 (9%)	10	20
1	B	291/310 (94%)	267 (92%)	24 (8%)	11	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	291/310 (94%)	267 (92%)	24 (8%)	11	22
1	D	291/310 (94%)	264 (91%)	27 (9%)	9	17
All	All	1164/1240 (94%)	1064 (91%)	100 (9%)	10	20

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	40	ASN
1	A	71	GLU
1	A	72	LEU
1	A	101	THR
1	A	127	LEU
1	A	129	THR
1	A	136	ARG
1	A	147	LYS
1	A	156	ASN
1	A	157	PRO
1	A	162	THR
1	A	165	ARG
1	A	173	LYS
1	A	222	ARG
1	A	223	ASP
1	A	253	LEU
1	A	273	LEU
1	A	296	LEU
1	A	302	LYS
1	A	312	LEU
1	A	313	GLU
1	A	320	ARG
1	A	327	ARG
1	A	394	THR
1	B	9	THR
1	B	40	ASN
1	B	67	GLU
1	B	71	GLU
1	B	72	LEU
1	B	101	THR
1	B	127	LEU
1	B	129	THR
1	B	136	ARG

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Mol	Chain	Res	Type
1	B	156	ASN
1	B	157	PRO
1	B	162	THR
1	B	165	ARG
1	B	173	LYS
1	B	222	ARG
1	B	242	SER
1	B	253	LEU
1	B	273	LEU
1	B	296	LEU
1	B	302	LYS
1	B	312	LEU
1	B	378	GLU
1	B	394	THR
1	B	395	LEU
1	C	32	THR
1	C	40	ASN
1	C	71	GLU
1	C	101	THR
1	C	127	LEU
1	C	129	THR
1	C	145	SER
1	C	156	ASN
1	C	157	PRO
1	C	162	THR
1	C	165	ARG
1	C	173	LYS
1	C	178	THR
1	C	186	SER
1	C	223	ASP
1	C	242	SER
1	C	253	LEU
1	C	273	LEU
1	C	296	LEU
1	C	312	LEU
1	C	313	GLU
1	C	320	ARG
1	C	327	ARG
1	C	394	THR
1	D	9	THR
1	D	32	THR
1	D	40	ASN

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Mol	Chain	Res	Type
1	D	49	LYS
1	D	71	GLU
1	D	72	LEU
1	D	101	THR
1	D	127	LEU
1	D	129	THR
1	D	136	ARG
1	D	144	GLN
1	D	147	LYS
1	D	156	ASN
1	D	157	PRO
1	D	162	THR
1	D	178	THR
1	D	184	PHE
1	D	223	ASP
1	D	253	LEU
1	D	273	LEU
1	D	282	GLN
1	D	296	LEU
1	D	299	ARG
1	D	312	LEU
1	D	313	GLU
1	D	316	GLU
1	D	394	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	48	ASN
1	A	97	GLN
1	A	156	ASN
1	A	182	ASN
1	A	190	GLN
1	A	209	ASN
1	A	282	GLN
1	A	350	HIS
1	B	40	ASN
1	B	48	ASN
1	B	97	GLN
1	B	156	ASN
1	B	182	ASN

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Mol	Chain	Res	Type
1	B	190	GLN
1	B	209	ASN
1	B	282	GLN
1	B	350	HIS
1	C	40	ASN
1	C	97	GLN
1	C	156	ASN
1	C	182	ASN
1	C	190	GLN
1	C	209	ASN
1	C	350	HIS
1	D	40	ASN
1	D	97	GLN
1	D	156	ASN
1	D	182	ASN
1	D	190	GLN
1	D	209	ASN
1	D	301	GLN
1	D	350	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	E9U	D	801	-	23,29,29	2.09	3 (13%)	26,40,40	2.31	8 (30%)
2	E9U	A	801	-	23,29,29	1.71	5 (21%)	26,40,40	3.01	9 (34%)
2	E9U	C	801	-	23,29,29	2.07	5 (21%)	26,40,40	2.18	9 (34%)
2	E9U	B	801	-	23,29,29	2.12	6 (26%)	26,40,40	2.82	8 (30%)

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	E9U	D	801	-	-	6/18/26/26	0/1/1/1
2	E9U	A	801	-	-	6/18/26/26	0/1/1/1
2	E9U	C	801	-	-	8/18/26/26	0/1/1/1
2	E9U	B	801	-	-	6/18/26/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	E9U	C3-C2	7.15	1.48	1.40
2	C	801	E9U	C3-C2	5.71	1.46	1.40
2	B	801	E9U	C3-C2	5.56	1.46	1.40
2	A	801	E9U	C3-C2	5.02	1.45	1.40
2	C	801	E9U	C4-C5	4.91	1.48	1.42
2	B	801	E9U	CB-CA	4.24	1.58	1.53
2	B	801	E9U	CA-N	4.02	1.50	1.46
2	D	801	E9U	C4-C5	3.97	1.47	1.42
2	B	801	E9U	C4-C3	3.84	1.46	1.40
2	D	801	E9U	C4-C3	3.71	1.46	1.40
2	A	801	E9U	C4-C3	3.39	1.45	1.40
2	B	801	E9U	C4-C5	3.16	1.45	1.42
2	A	801	E9U	C4-C5	2.88	1.45	1.42
2	C	801	E9U	C4-C3	2.87	1.45	1.40
2	A	801	E9U	CA-N	2.53	1.49	1.46
2	A	801	E9U	CB-CA	2.51	1.56	1.53
2	C	801	E9U	C2-N1	2.51	1.38	1.33
2	B	801	E9U	C6-C5	2.14	1.42	1.37
2	C	801	E9U	P-O4P	2.02	1.66	1.60

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	E9U	CA-N-C4A	7.19	127.15	117.40
2	A	801	E9U	CE-SD-CG	6.57	121.97	102.27
2	B	801	E9U	C2A-C2-C3	-6.37	113.02	120.89
2	A	801	E9U	C2A-C2-C3	-6.29	113.12	120.89
2	B	801	E9U	CE-SD-CG	6.20	120.87	102.27
2	A	801	E9U	C3-C4-C5	-6.16	113.54	118.26
2	B	801	E9U	CA-N-C4A	5.47	124.82	117.40
2	C	801	E9U	CZ-CE-SD	5.22	132.84	113.74
2	B	801	E9U	C3-C4-C5	-5.18	114.29	118.26
2	D	801	E9U	CZ-CE-SD	5.04	132.22	113.74
2	D	801	E9U	C3-C4-C5	-4.63	114.71	118.26
2	D	801	E9U	C4-C3-C2	-4.47	117.42	120.19
2	D	801	E9U	CA-N-C4A	4.19	123.09	117.40
2	B	801	E9U	C5-C4-C4A	4.02	128.18	121.56
2	C	801	E9U	CA-N-C4A	4.01	122.84	117.40
2	C	801	E9U	C4-C3-C2	-3.99	117.72	120.19
2	A	801	E9U	CB-CG-SD	-3.90	104.55	113.31
2	B	801	E9U	CB-CG-SD	-3.70	105.00	113.31
2	D	801	E9U	CE-SD-CG	3.47	112.67	102.27
2	B	801	E9U	C2A-C2-N1	3.36	124.22	117.67
2	C	801	E9U	CE-SD-CG	3.30	112.16	102.27
2	C	801	E9U	C3-C4-C5	-3.27	115.75	118.26
2	A	801	E9U	C5-C4-C4A	3.23	126.86	121.56
2	A	801	E9U	C2A-C2-N1	3.07	123.66	117.67
2	D	801	E9U	O3-C3-C2	2.68	123.34	117.49
2	C	801	E9U	O4P-P-O2P	-2.62	99.13	106.47
2	D	801	E9U	C5-C4-C4A	2.61	125.86	121.56
2	B	801	E9U	O3P-P-O4P	2.55	113.51	106.73
2	C	801	E9U	C2A-C2-C3	-2.43	117.89	120.89
2	C	801	E9U	C5-C4-C4A	2.39	125.48	121.56
2	A	801	E9U	CG-CB-CA	2.38	120.28	113.97
2	A	801	E9U	O1P-P-O4P	2.31	112.87	106.73
2	D	801	E9U	C3-C2-N1	2.17	123.56	120.77
2	C	801	E9U	O3-C3-C2	2.10	122.07	117.49

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	E9U	C-CA-N-C4A
2	D	801	E9U	CB-CA-N-C4A

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Mol	Chain	Res	Type	Atoms
2	D	801	E9U	SD-CE-CZ-CH
2	D	801	E9U	SD-CE-CZ-NH
2	A	801	E9U	C-CA-N-C4A
2	A	801	E9U	CB-CA-N-C4A
2	A	801	E9U	N-CA-CB-CG
2	A	801	E9U	C-CA-CB-CG
2	A	801	E9U	SD-CE-CZ-CH
2	A	801	E9U	SD-CE-CZ-NH
2	C	801	E9U	C-CA-N-C4A
2	C	801	E9U	CB-CA-N-C4A
2	C	801	E9U	N-CA-CB-CG
2	C	801	E9U	SD-CE-CZ-CH
2	C	801	E9U	SD-CE-CZ-NH
2	B	801	E9U	C-CA-N-C4A
2	B	801	E9U	CB-CA-N-C4A
2	B	801	E9U	N-CA-CB-CG
2	B	801	E9U	C-CA-CB-CG
2	B	801	E9U	SD-CE-CZ-CH
2	B	801	E9U	SD-CE-CZ-NH
2	D	801	E9U	CA-CB-CG-SD
2	C	801	E9U	CZ-CE-SD-CG
2	C	801	E9U	CA-CB-CG-SD
2	C	801	E9U	C-CA-CB-CG
2	D	801	E9U	CZ-CE-SD-CG

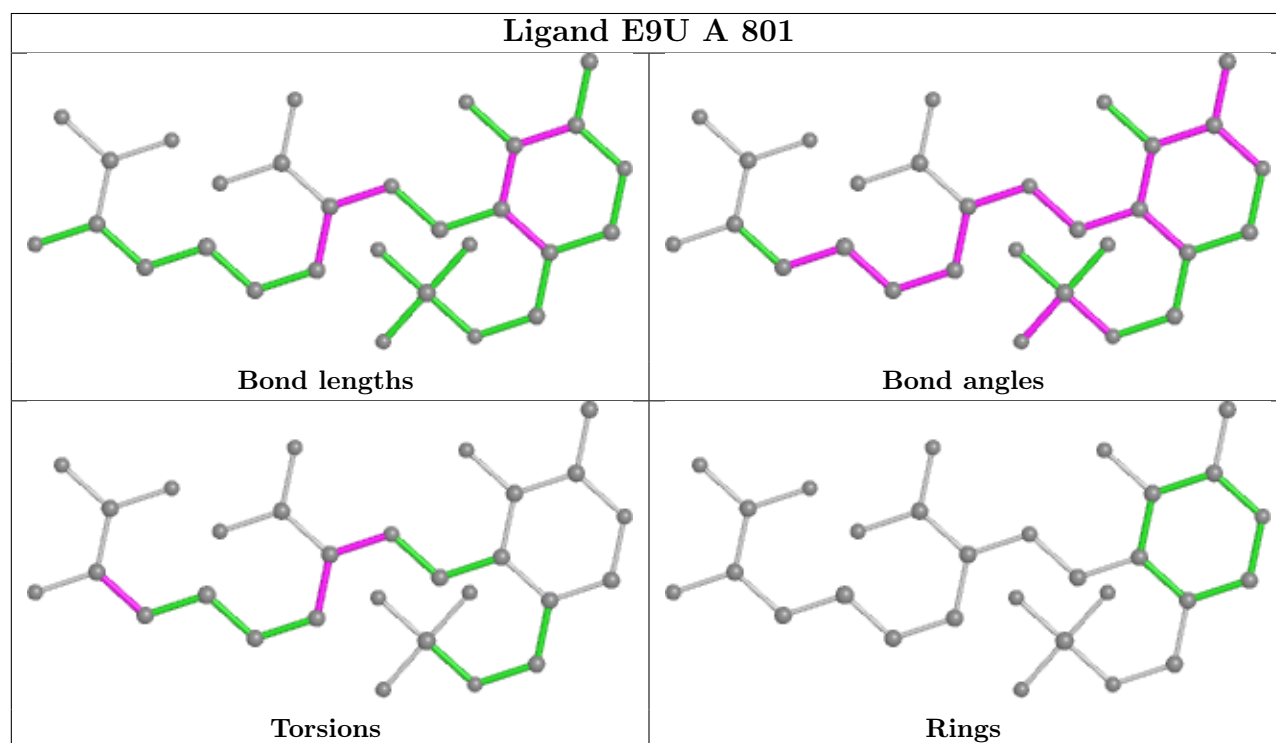
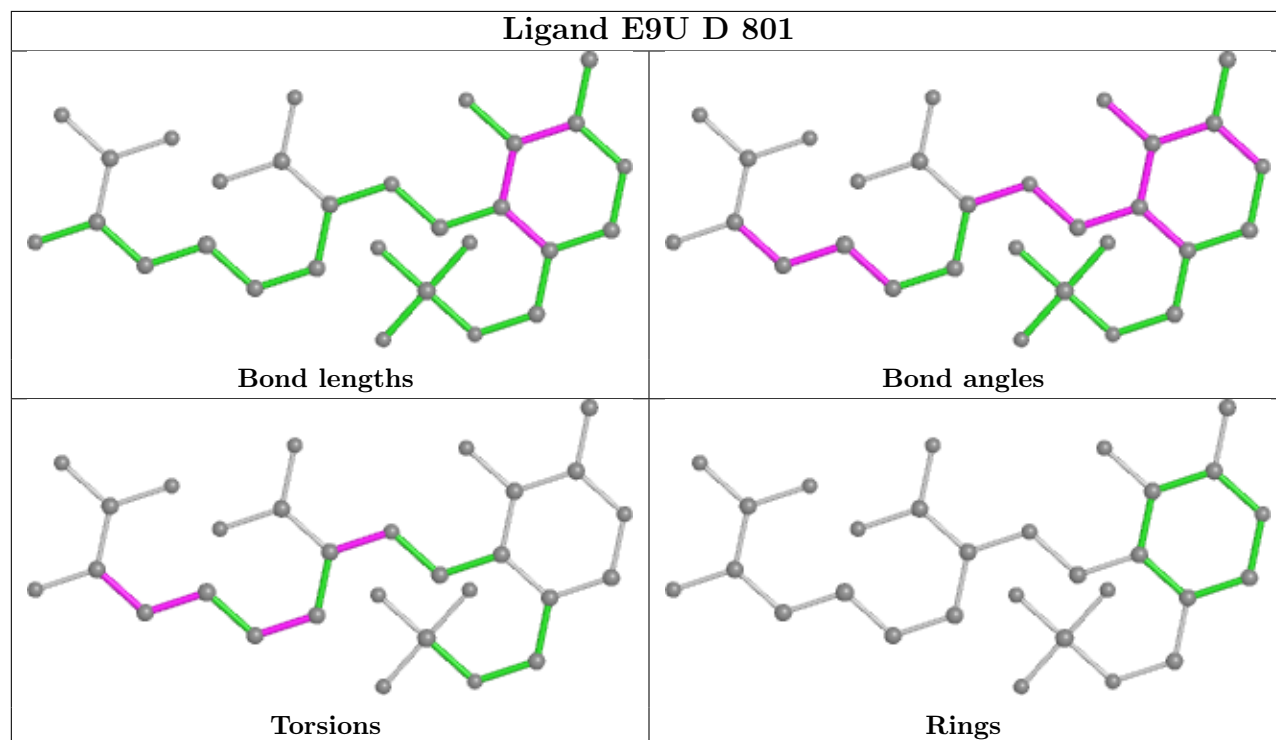
There are no ring outliers.

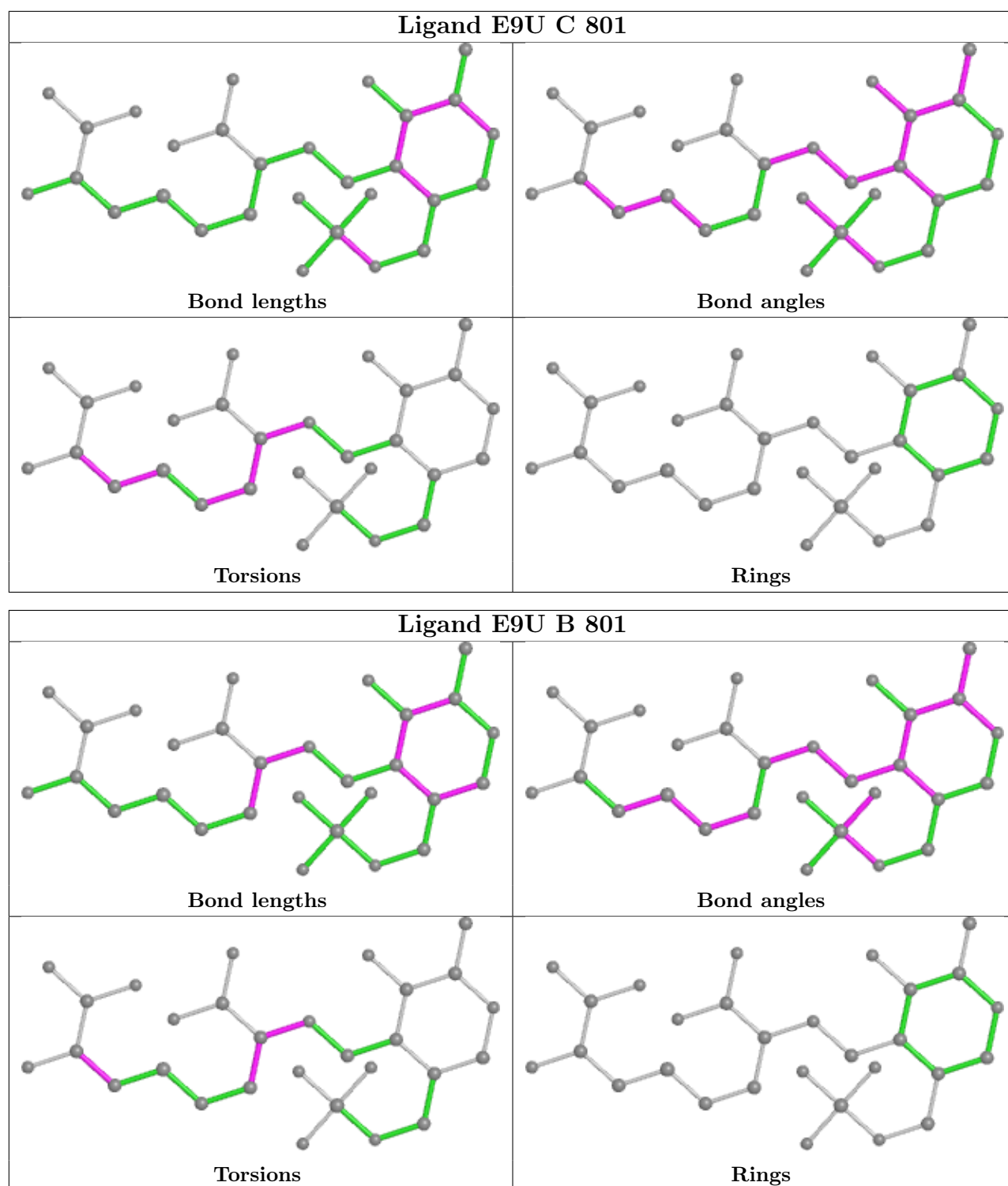
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	E9U	3	0
2	C	801	E9U	1	0
2	B	801	E9U	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

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 [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	387/408 (94%)	-0.48	0	100 100	18, 30, 52, 80	0
1	B	387/408 (94%)	-0.47	0	100 100	19, 30, 51, 85	0
1	C	388/408 (95%)	-0.46	1 (0%)	94 94	20, 31, 53, 102	0
1	D	387/408 (94%)	-0.46	1 (0%)	94 94	19, 31, 54, 94	0
All	All	1549/1632 (94%)	-0.47	2 (0%)	95 96	18, 31, 54, 102	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	9	THR	3.0
1	C	9	THR	2.9

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 monosaccharides in this entry.

6.4 Ligands [i](#)

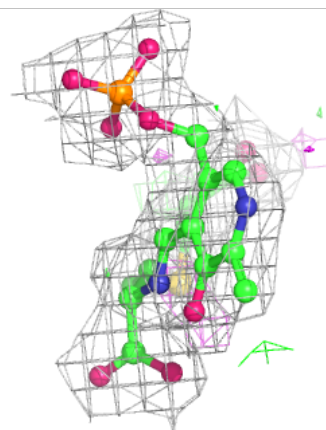
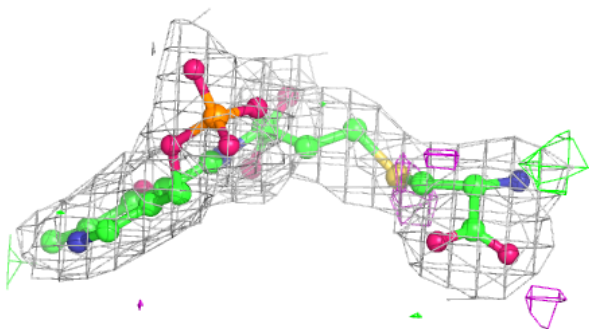
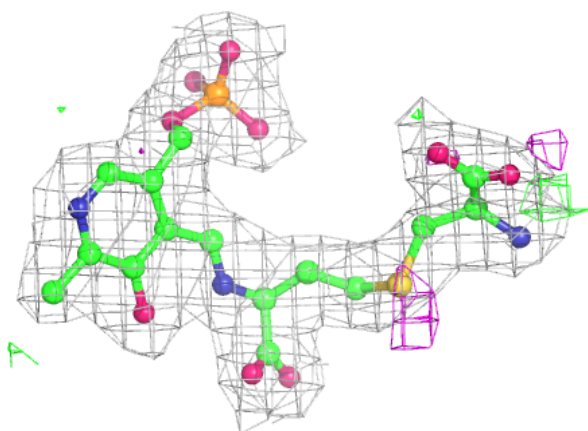
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	E9U	D	801	29/29	0.98	0.12	22,28,42,64	0
2	E9U	A	801	29/29	0.98	0.12	22,29,43,56	0
2	E9U	C	801	29/29	0.98	0.11	21,27,44,63	0
2	E9U	B	801	29/29	0.98	0.11	23,28,43,57	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.

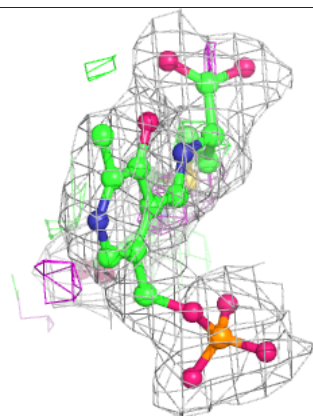
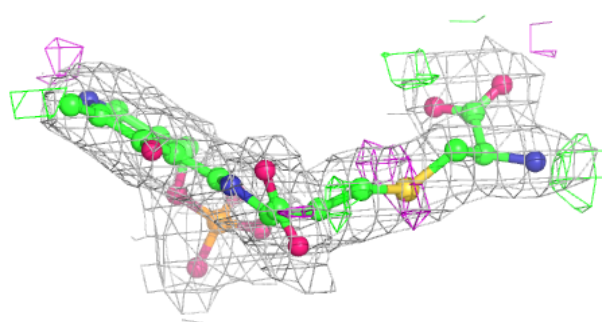
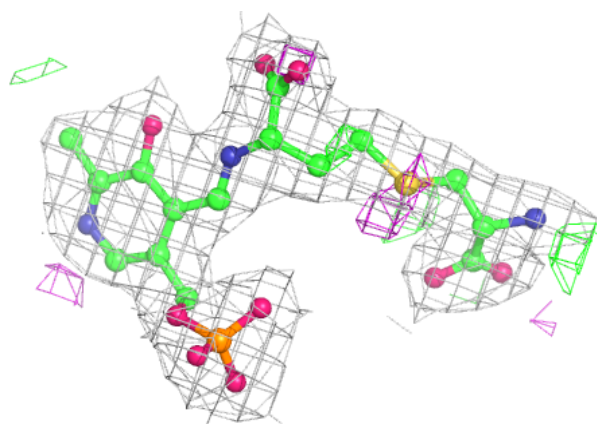
Electron density around E9U D 801:

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



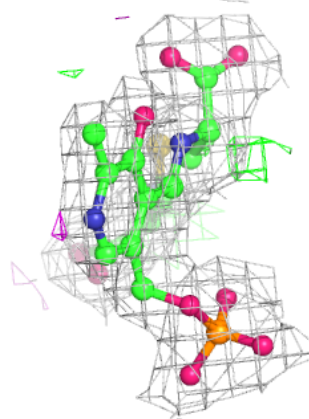
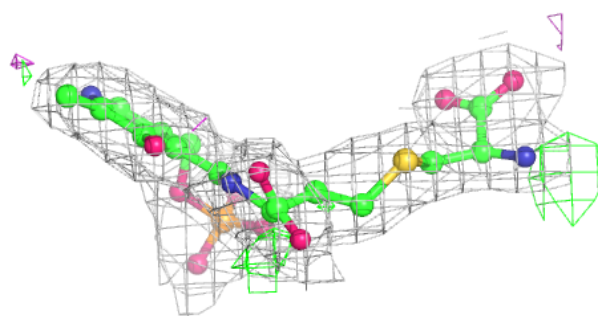
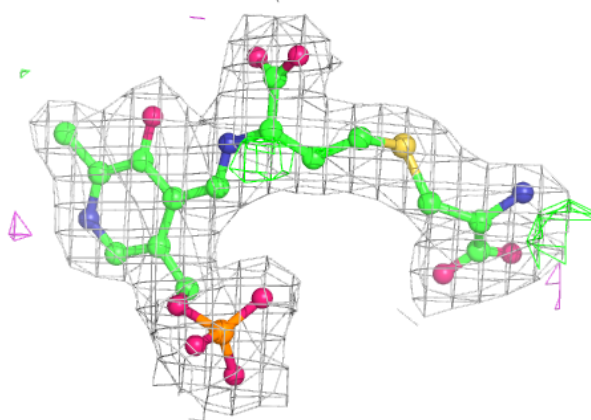
Electron density around E9U A 801:

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



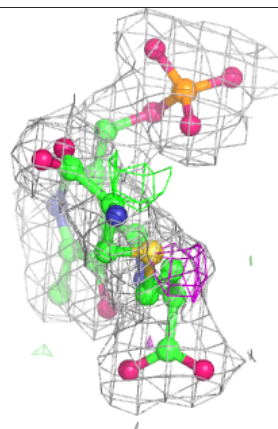
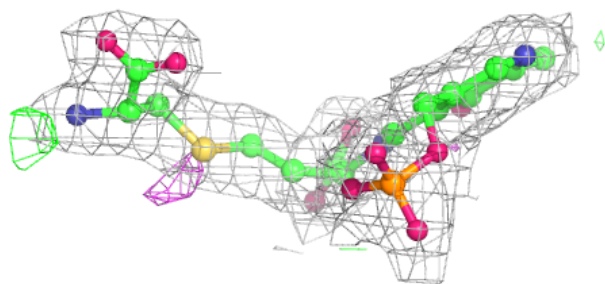
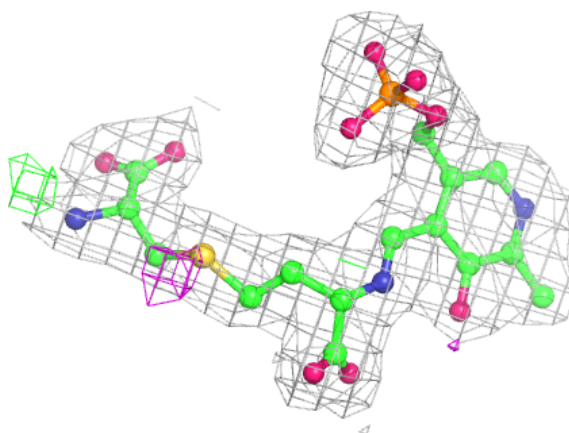
Electron density around E9U C 801:

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



Electron density around E9U B 801:

$2mF_o - DF_c$ (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.