



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:30 PM UTC

PDB ID : 4Q86 / pdb_00004q86
Title : YcaO with AMP Bound
Authors : Chekan, J.R.; Nair, S.K.
Deposited on : 2014-04-25
Resolution : 2.25 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

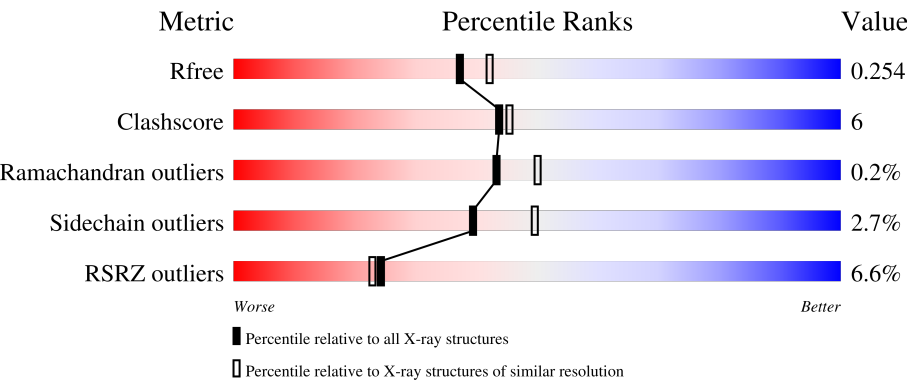
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	586	91%7% ..
1	B	586	% 90%8% ...
1	C	586	2% 87%9% ..
1	D	586	2% 90%8% ..
1	E	586	3% 88%10% ..

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Mol	Chain	Length	Quality of chain
1	F	586	40% 82% 13% ..
1	G	586	4% 85% 11% ..
1	H	586	87% 10% ...

2 Entry composition

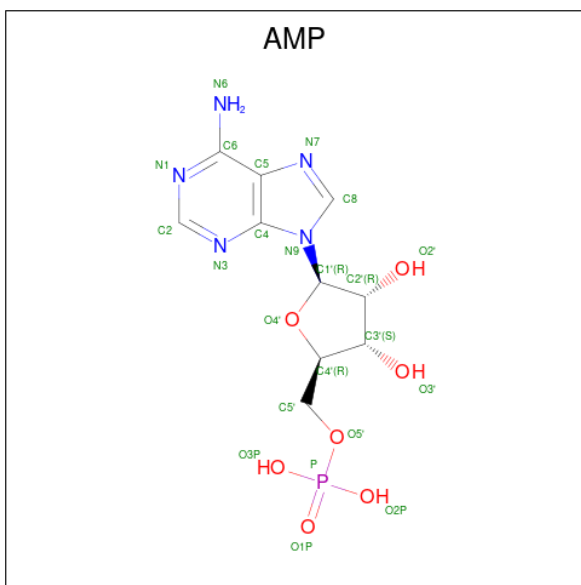
There are 4 unique types of molecules in this entry. The entry contains 38743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosomal protein S12 methylthiotransferase accessory factor YcaO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4599	2935	748	899	17			
1	B	583	Total	C	N	O	S	0	0	0
			4613	2946	750	900	17			
1	C	570	Total	C	N	O	S	0	0	0
			4508	2875	734	882	17			
1	D	582	Total	C	N	O	S	0	0	0
			4599	2935	748	899	17			
1	E	578	Total	C	N	O	S	0	0	0
			4567	2914	743	893	17			
1	F	574	Total	C	N	O	S	0	0	0
			4534	2890	739	888	17			
1	G	575	Total	C	N	O	S	0	0	0
			4541	2895	740	889	17			
1	H	583	Total	C	N	O	S	0	0	0
			4613	2946	750	900	17			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	E	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Mg 3	0	0
3	H	3	Total 3	Mg 3	0	0

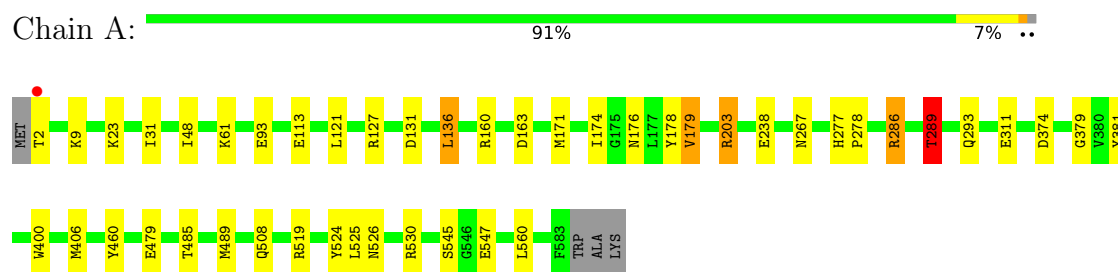
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	334	Total 334	O 334	0	0
4	B	336	Total 336	O 336	0	0
4	C	231	Total 231	O 231	0	0
4	D	255	Total 255	O 255	0	0
4	E	215	Total 215	O 215	0	0
4	F	111	Total 111	O 111	0	0
4	G	197	Total 197	O 197	0	0
4	H	308	Total 308	O 308	0	0

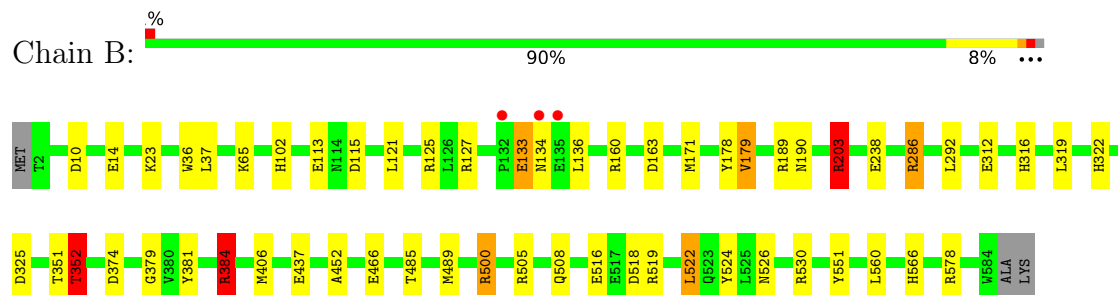
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

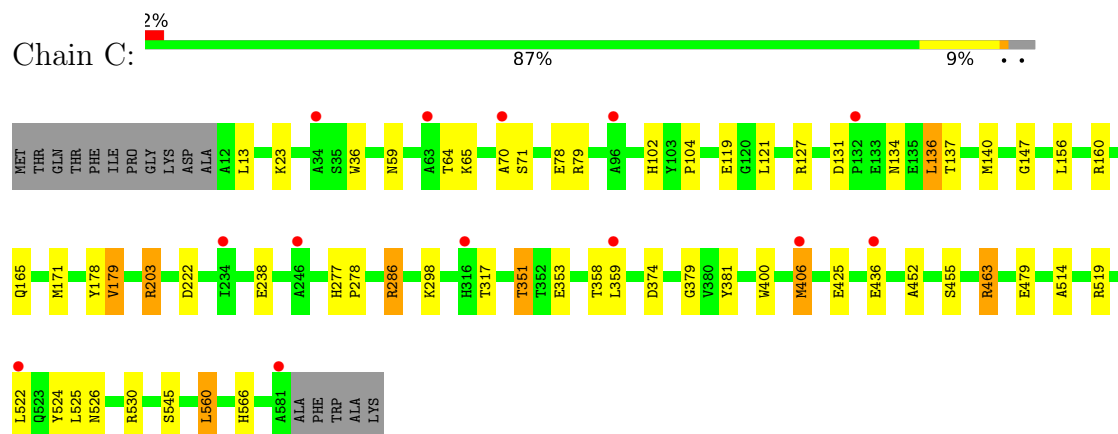
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



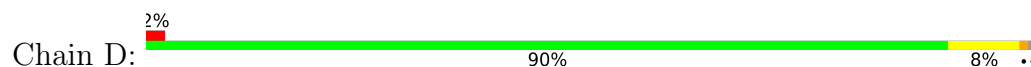
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

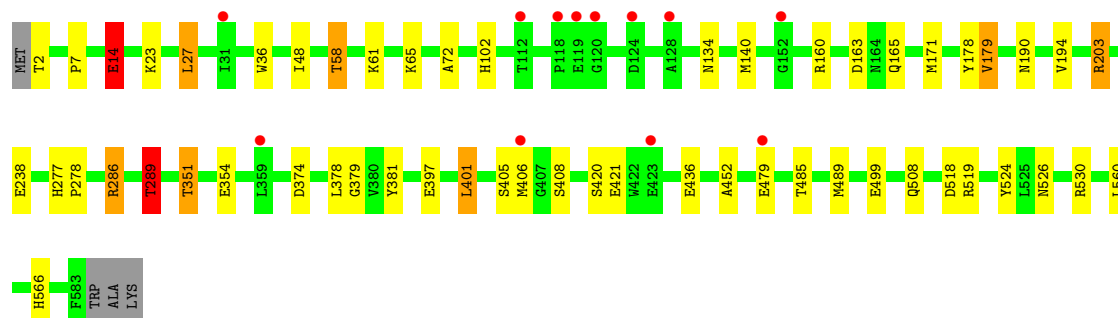


- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



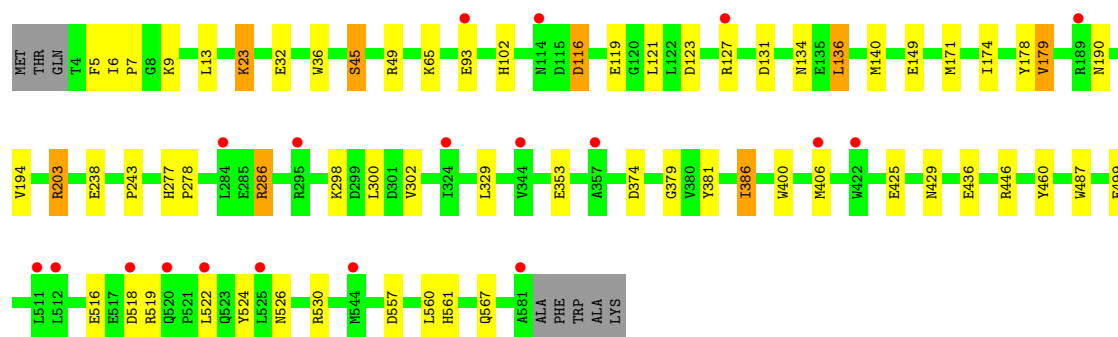
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO





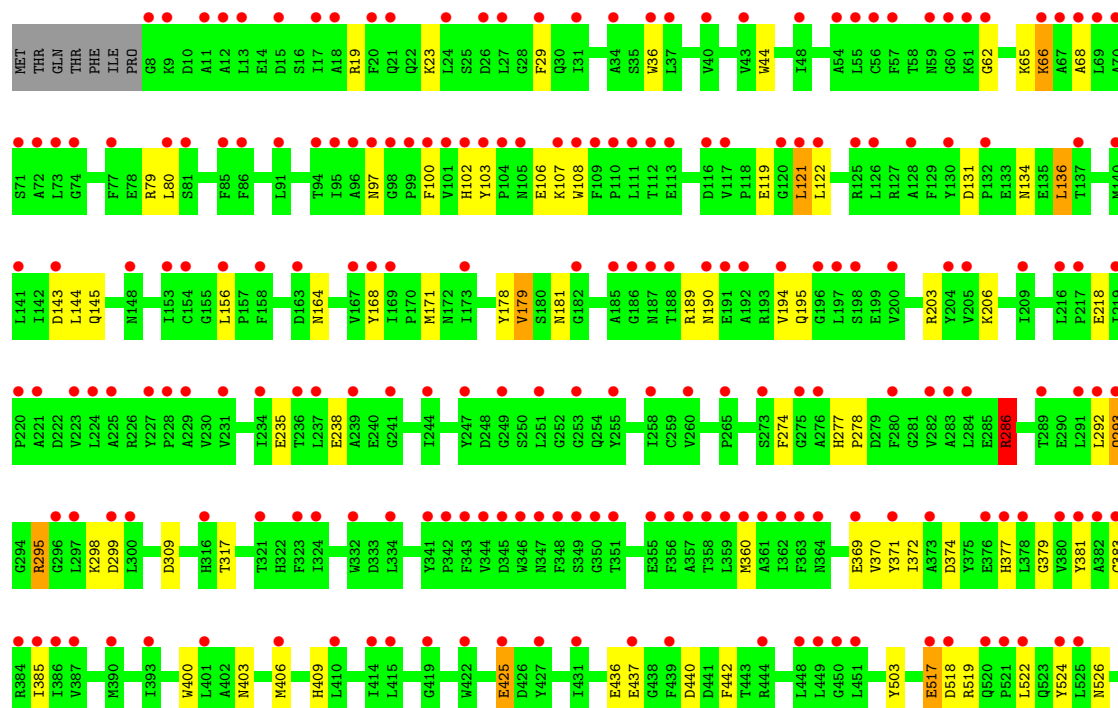
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain E: 3% 88% 10% ..



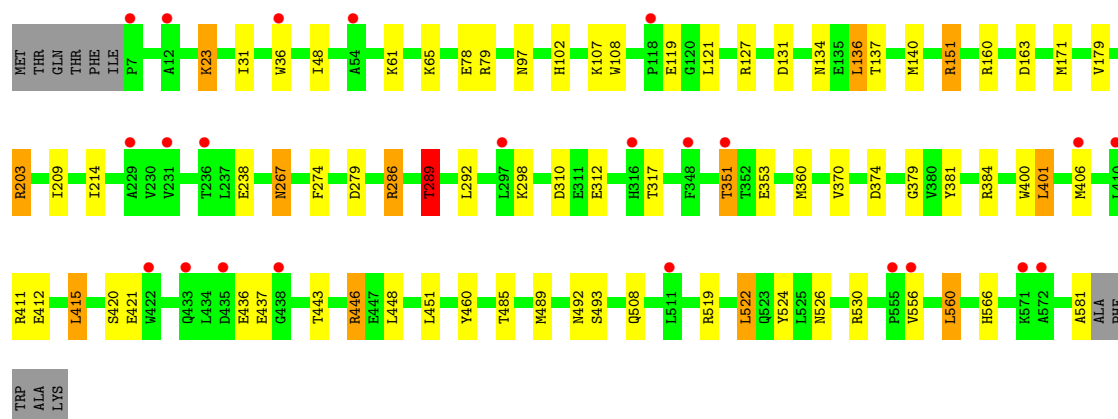
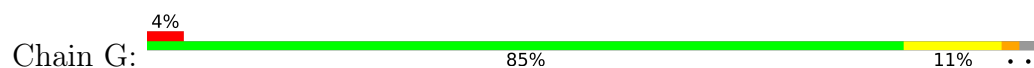
• Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain F: 40% 82% 13% ..

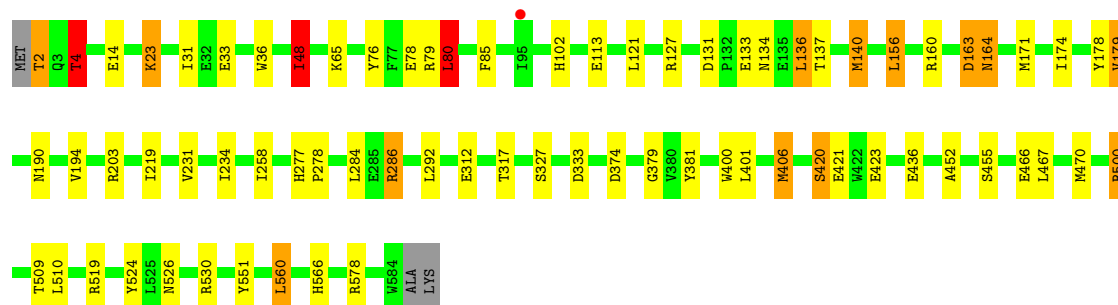
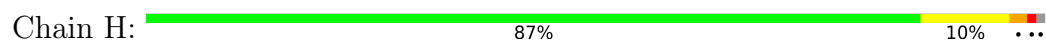




- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	111.25Å 112.95Å 132.89Å 89.94° 73.51° 77.23°	Depositor
Resolution (Å)	127.14 – 2.25 127.14 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.1 (127.14-2.25) 93.1 (127.14-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.218 , 0.250 0.221 , 0.254	Depositor DCC
R_{free} test set	13386 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	38743	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: AMP, MG

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	0.86	0/4713	0.86	6/6411 (0.1%)
1	B	0.90	0/4729	0.91	9/6434 (0.1%)
1	C	0.74	0/4619	0.87	7/6283 (0.1%)
1	D	0.81	0/4713	0.87	10/6411 (0.2%)
1	E	0.77	0/4680	0.86	8/6366 (0.1%)
1	F	0.68	0/4645	0.92	13/6317 (0.2%)
1	G	0.77	0/4653	0.89	12/6328 (0.2%)
1	H	0.90	2/4729 (0.0%)	0.95	14/6434 (0.2%)
All	All	0.81	2/37481 (0.0%)	0.89	79/50984 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	164	ASN	N-CA	5.51	1.54	1.46
1	H	164	ASN	CA-C	-5.05	1.44	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	ARG	NE-CZ-NH2	16.54	134.09	119.20
1	H	203	ARG	NE-CZ-NH1	-11.88	109.62	121.50
1	F	119	GLU	N-CA-C	-10.11	94.24	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	384	ARG	CG-CD-NE	10.10	134.21	112.00
1	F	122	LEU	N-CA-C	-9.64	100.88	108.78
1	E	386	ILE	CB-CG1-CD1	9.52	133.79	113.80
1	A	267	ASN	N-CA-CB	-9.13	98.86	111.00
1	C	406	MET	N-CA-C	-9.00	96.55	109.96
1	H	163	ASP	CA-C-N	-8.79	106.51	123.13
1	H	163	ASP	C-N-CA	-8.79	106.51	123.13
1	G	267	ASN	N-CA-CB	-8.70	99.33	110.90
1	A	267	ASN	CB-CA-C	-8.59	95.73	109.13
1	C	104	PRO	CA-C-N	8.54	134.99	120.72
1	C	104	PRO	C-N-CA	8.54	134.99	120.72
1	G	406	MET	N-CA-C	-7.92	97.95	109.59
1	E	406	MET	N-CA-C	-7.33	98.81	109.59
1	F	554	GLN	CA-CB-CG	7.26	128.62	114.10
1	F	122	LEU	N-CA-CB	-7.14	98.42	110.49
1	F	406	MET	N-CA-C	7.13	120.88	111.75
1	F	235	GLU	CB-CA-C	-7.06	99.51	110.81
1	G	267	ASN	CB-CA-C	-6.96	97.33	109.02
1	G	446	ARG	CA-CB-CG	6.94	127.99	114.10
1	B	286	ARG	CB-CA-C	-6.84	99.05	110.68
1	F	121	LEU	N-CA-C	6.83	125.35	110.80
1	E	386	ILE	CA-CB-CG1	-6.82	98.80	110.40
1	G	286	ARG	CB-CA-C	-6.75	99.20	110.68
1	E	286	ARG	CB-CA-C	-6.72	99.25	110.68
1	G	151	ARG	NE-CZ-NH2	-6.67	113.19	119.20
1	D	289	THR	N-CA-CB	-6.67	99.94	110.28
1	G	289	THR	N-CA-CB	-6.65	99.97	110.28
1	A	286	ARG	CB-CA-C	-6.65	99.38	110.68
1	H	286	ARG	CB-CA-C	-6.62	99.42	110.68
1	D	286	ARG	CB-CA-C	-6.57	99.50	110.68
1	B	352	THR	CB-CA-C	6.50	121.59	110.79
1	A	289	THR	N-CA-CB	-6.50	100.20	110.28
1	H	578	ARG	CG-CD-NE	6.45	126.18	112.00
1	G	151	ARG	NE-CZ-NH1	6.43	127.93	121.50
1	C	286	ARG	CB-CA-C	-6.37	99.86	110.68
1	H	4	THR	CB-CA-C	6.33	120.67	110.16
1	H	420	SER	N-CA-C	6.23	124.06	110.80
1	G	351	THR	N-CA-CB	-6.19	101.50	110.36
1	D	406	MET	N-CA-C	6.18	119.66	111.75
1	B	406	MET	N-CA-C	6.18	119.66	111.75
1	F	576	LEU	CA-CB-CG	6.17	137.89	116.30
1	F	134	ASN	CB-CA-C	-6.15	102.99	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	GLU	N-CA-CB	6.10	119.73	110.28
1	A	406	MET	N-CA-C	6.05	119.50	111.75
1	B	203	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	H	406	MET	N-CA-C	6.00	119.43	111.75
1	C	351	THR	N-CA-CB	-5.93	101.89	110.36
1	B	578	ARG	CG-CD-NE	5.87	124.91	112.00
1	C	463	ARG	CD-NE-CZ	5.79	132.51	124.40
1	F	295	ARG	CG-CD-NE	-5.74	99.36	112.00
1	E	45	SER	N-CA-CB	-5.68	100.96	111.52
1	D	7	PRO	N-CA-C	5.67	124.15	112.47
1	F	286	ARG	CB-CA-C	5.64	121.06	110.63
1	B	352	THR	N-CA-CB	-5.63	101.84	110.12
1	A	203	ARG	NE-CZ-NH2	-5.63	114.14	119.20
1	F	66	LYS	CG-CD-CE	5.60	124.19	111.30
1	E	203	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	H	163	ASP	N-CA-C	-5.53	99.03	110.80
1	D	203	ARG	NE-CZ-NH2	-5.45	114.30	119.20
1	H	80	LEU	CA-CB-CG	5.43	135.31	116.30
1	B	384	ARG	CG-CD-NE	5.38	123.83	112.00
1	H	500	ARG	CG-CD-NE	-5.31	100.31	112.00
1	G	203	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	F	293	GLN	O-C-N	-5.28	116.99	122.96
1	G	151	ARG	CB-CG-CD	5.26	123.41	111.30
1	H	48	ILE	CB-CA-C	5.25	119.08	110.69
1	B	500	ARG	CG-CD-NE	-5.20	100.56	112.00
1	H	140	MET	CB-CA-C	-5.17	99.66	109.95
1	E	140	MET	CA-CB-CG	5.16	124.42	114.10
1	D	140	MET	CA-CB-CG	5.14	124.39	114.10
1	B	351	THR	N-CA-C	-5.13	103.91	110.53
1	E	386	ILE	CG1-CB-CG2	-5.09	95.42	110.70
1	D	27	LEU	CB-CG-CD2	-5.07	95.48	110.70
1	D	14	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	203	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	D	14	GLU	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	293	GLN	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	4599	0	4372	36	0
1	B	4613	0	4382	51	0
1	C	4508	0	4284	49	0
1	D	4599	0	4372	46	0
1	E	4567	0	4343	51	0
1	F	4534	0	4309	69	0
1	G	4541	0	4317	66	0
1	H	4613	0	4382	77	0
2	A	23	0	12	1	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	2	0
2	E	23	0	12	2	0
2	G	23	0	12	0	0
2	H	23	0	12	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	334	0	0	7	0
4	B	336	0	0	18	0
4	C	231	0	0	16	0
4	D	255	0	0	16	0
4	E	215	0	0	19	0
4	F	111	0	0	24	0
4	G	197	0	0	16	0
4	H	308	0	0	25	0
All	All	38743	0	34845	434	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 6.

All (434) 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:F:68:ALA:HB2	4:F:633:HOH:O	1.36	1.26
1:E:171:MET:SD	4:E:738:HOH:O	2.04	1.15
1:B:171:MET:SD	4:B:1021:HOH:O	2.02	1.15
1:G:78:GLU:OE2	1:G:79:ARG:NH1	1.86	1.08
1:F:550:PHE:HB3	1:F:553:LEU:HD12	1.33	1.06
1:C:78:GLU:OE2	1:C:79:ARG:NH1	1.88	1.06
1:F:576:LEU:O	1:F:580:LYS:HG2	1.54	1.05
1:H:78:GLU:OE2	1:H:79:ARG:NH1	1.88	1.05
1:H:136:LEU:HD12	1:H:140:MET:HE1	1.03	1.00
1:C:358:THR:HG22	4:C:878:HOH:O	1.61	0.98
1:H:231:VAL:HA	4:H:822:HOH:O	1.63	0.98
1:H:136:LEU:CD1	1:H:140:MET:HE1	1.93	0.98
1:F:106:GLU:HG3	4:F:624:HOH:O	1.65	0.97
1:F:121:LEU:O	1:F:168:TYR:O	1.81	0.97
1:F:103:TYR:HD1	1:F:580:LYS:HZ1	1.14	0.96
1:H:171:MET:SD	4:H:972:HOH:O	2.22	0.95
1:E:561:HIS:HA	1:E:567:GLN:OE1	1.67	0.93
1:H:171:MET:HE1	4:H:715:HOH:O	1.66	0.93
1:H:234:ILE:HB	4:H:822:HOH:O	1.71	0.90
1:B:312:GLU:HG2	4:B:948:HOH:O	1.70	0.90
1:H:423:GLU:HB2	4:H:813:HOH:O	1.71	0.88
1:B:171:MET:HE1	4:B:784:HOH:O	1.73	0.88
1:H:467:LEU:HA	1:H:470:MET:HE2	1.56	0.88
1:E:487:TRP:HB2	4:E:753:HOH:O	1.72	0.88
1:G:581:ALA:HA	4:G:857:HOH:O	1.72	0.88
1:H:467:LEU:HA	1:H:470:MET:CE	2.04	0.87
1:B:500:ARG:NH1	4:B:705:HOH:O	2.05	0.87
1:B:10:ASP:OD2	1:B:352:THR:HG21	1.76	0.85
1:C:560:LEU:HD13	1:C:566:HIS:CE1	2.12	0.85
1:C:70:ALA:HB2	4:C:893:HOH:O	1.76	0.84
1:H:4:THR:CG2	1:H:14:GLU:OE2	2.26	0.84
1:E:171:MET:CE	4:E:857:HOH:O	2.27	0.83
1:E:557:ASP:CB	1:H:113:GLU:OE2	2.27	0.83
1:D:171:MET:HE1	4:D:735:HOH:O	1.80	0.82
1:D:408:SER:HB2	4:D:937:HOH:O	1.79	0.82
1:D:58:THR:HG21	1:D:72:ALA:O	1.79	0.82
1:G:560:LEU:HD13	1:G:566:HIS:CE1	2.15	0.82
1:H:560:LEU:HD13	1:H:566:HIS:CE1	2.14	0.82
2:D:601:AMP:N1	4:D:737:HOH:O	2.14	0.81
1:G:560:LEU:HD13	1:G:566:HIS:NE2	1.96	0.81
1:B:516:GLU:OE1	1:B:519:ARG:NH1	2.15	0.80
1:C:463:ARG:NH1	4:C:885:HOH:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:ILE:CG2	4:H:950:HOH:O	2.30	0.79
1:H:258:ILE:HG23	4:H:950:HOH:O	1.81	0.79
1:E:171:MET:HE3	4:E:857:HOH:O	1.83	0.78
1:H:171:MET:SD	4:H:913:HOH:O	2.42	0.77
1:E:516:GLU:OE1	1:E:519:ARG:NH1	2.18	0.77
1:D:72:ALA:HB1	4:D:939:HOH:O	1.83	0.77
1:F:517:GLU:N	1:F:517:GLU:OE1	2.18	0.77
1:F:554:GLN:HG2	4:F:636:HOH:O	1.86	0.76
1:H:4:THR:HG23	1:H:14:GLU:OE2	1.86	0.76
1:D:163:ASP:OD2	4:D:909:HOH:O	2.02	0.76
1:A:311:GLU:OE1	4:A:790:HOH:O	2.04	0.76
1:E:557:ASP:HB3	1:H:113:GLU:OE2	1.86	0.76
1:F:383:CYS:HB2	4:F:629:HOH:O	1.85	0.76
2:D:601:AMP:C2	4:D:737:HOH:O	2.38	0.75
1:F:385:ILE:HG13	4:F:629:HOH:O	1.84	0.75
1:A:61:LYS:HD2	1:A:289:THR:HG22	1.69	0.75
1:C:171:MET:HE1	4:C:806:HOH:O	1.87	0.75
1:D:61:LYS:HD2	1:D:289:THR:HG22	1.69	0.74
1:G:61:LYS:HD2	1:G:289:THR:HG22	1.69	0.74
1:C:317:THR:HG23	4:C:782:HOH:O	1.87	0.74
1:C:13:LEU:HD22	4:C:893:HOH:O	1.87	0.73
1:F:108:TRP:CD1	4:F:624:HOH:O	2.40	0.73
1:H:500:ARG:NH1	4:H:781:HOH:O	2.21	0.73
1:G:108:TRP:CE2	1:G:151:ARG:HD2	2.24	0.72
1:F:44:TRP:HB2	4:F:633:HOH:O	1.90	0.72
1:E:32:GLU:OE2	1:E:49:ARG:CZ	2.37	0.72
1:C:70:ALA:CB	4:C:893:HOH:O	2.33	0.71
1:E:243:PRO:O	4:E:897:HOH:O	2.08	0.70
1:H:219:ILE:CD1	4:H:950:HOH:O	2.38	0.70
1:G:171:MET:HE1	4:G:793:HOH:O	1.91	0.70
1:H:102:HIS:CE1	1:H:171:MET:HE3	2.26	0.70
1:B:322:HIS:O	4:B:1036:HOH:O	2.09	0.70
1:D:48:ILE:HG12	4:D:939:HOH:O	1.91	0.70
1:G:522:LEU:HD23	1:G:522:LEU:H	1.57	0.70
1:D:401:LEU:HD23	4:D:945:HOH:O	1.90	0.70
1:C:222:ASP:HB3	4:C:856:HOH:O	1.91	0.69
1:G:31:ILE:CG2	1:G:48:ILE:HG22	2.21	0.69
1:B:522:LEU:HG	4:B:856:HOH:O	1.92	0.69
1:A:31:ILE:CG2	1:A:48:ILE:HG22	2.23	0.69
1:A:547:GLU:O	4:A:808:HOH:O	2.10	0.69
1:C:238:GLU:OE2	1:D:530:ARG:NH2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:LEU:HD22	4:G:756:HOH:O	1.93	0.68
1:A:93:GLU:HG3	4:A:915:HOH:O	1.92	0.68
1:A:176:ASN:ND2	4:A:982:HOH:O	2.26	0.68
1:B:102:HIS:ND1	1:B:171:MET:CE	2.57	0.67
1:F:100:PHE:CE1	1:F:577:GLN:HG3	2.30	0.67
1:H:102:HIS:ND1	1:H:171:MET:CE	2.57	0.67
1:H:219:ILE:HD11	4:H:950:HOH:O	1.92	0.67
1:E:557:ASP:HB2	1:H:113:GLU:OE2	1.94	0.67
1:C:102:HIS:CE1	1:C:171:MET:HE3	2.31	0.66
1:F:103:TYR:HD1	1:F:580:LYS:NZ	1.89	0.66
1:G:310:ASP:OD2	4:G:890:HOH:O	2.12	0.66
1:B:102:HIS:CE1	1:B:171:MET:HE3	2.31	0.66
1:F:195:GLN:HG3	4:F:652:HOH:O	1.95	0.66
1:G:31:ILE:CG2	1:G:48:ILE:CG2	2.74	0.65
1:D:102:HIS:CD2	1:D:171:MET:CE	2.79	0.65
1:E:6:ILE:HG23	1:E:7:PRO:HD2	1.79	0.65
1:G:279:ASP:HA	4:G:832:HOH:O	1.97	0.65
1:C:560:LEU:HD13	1:C:566:HIS:NE2	2.11	0.65
1:E:174:ILE:CD1	1:E:386:ILE:HD13	2.27	0.64
1:H:466:GLU:OE2	1:H:500:ARG:NH1	2.29	0.64
1:B:384:ARG:NH1	4:B:1020:HOH:O	2.23	0.64
1:F:181:ASN:O	4:F:711:HOH:O	2.15	0.64
1:B:466:GLU:OE2	1:B:500:ARG:NH1	2.30	0.64
1:E:6:ILE:CG2	4:E:821:HOH:O	2.46	0.64
1:E:93:GLU:HG3	4:E:748:HOH:O	1.96	0.64
1:G:31:ILE:HG22	1:G:48:ILE:CG2	2.27	0.64
1:A:31:ILE:HG22	1:A:48:ILE:CG2	2.28	0.64
1:F:377:HIS:CD2	1:F:580:LYS:HD2	2.33	0.64
1:B:452:ALA:H	1:B:566:HIS:HD2	1.46	0.64
1:C:560:LEU:CD1	1:C:566:HIS:CE1	2.81	0.63
1:A:31:ILE:CG2	1:A:48:ILE:CG2	2.76	0.63
1:C:530:ARG:NH2	1:D:238:GLU:OE2	2.31	0.63
1:E:121:LEU:O	1:E:127:ARG:NH2	2.32	0.63
1:E:353:GLU:HB2	4:E:828:HOH:O	1.99	0.63
1:E:519:ARG:HD3	1:E:524:TYR:OH	2.00	0.62
1:D:102:HIS:CD2	1:D:171:MET:HE3	2.35	0.62
1:C:121:LEU:O	1:C:127:ARG:NH2	2.33	0.61
1:H:452:ALA:H	1:H:566:HIS:HD2	1.48	0.61
1:B:519:ARG:HD3	1:B:524:TYR:OH	2.00	0.61
1:G:448:LEU:HB2	4:G:756:HOH:O	1.99	0.61
1:C:102:HIS:ND1	1:C:171:MET:CE	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:GLU:HB2	4:D:945:HOH:O	1.99	0.61
1:G:121:LEU:O	1:G:127:ARG:NH2	2.34	0.61
1:H:102:HIS:ND1	1:H:171:MET:HE3	2.15	0.61
1:E:136:LEU:HD13	1:E:400:TRP:CZ2	2.36	0.61
1:F:102:HIS:CD2	1:F:171:MET:CE	2.83	0.61
1:G:489:MET:HE1	1:G:508:GLN:HB2	1.83	0.61
1:H:560:LEU:CD1	1:H:566:HIS:CE1	2.83	0.60
1:A:171:MET:HE3	1:A:174:ILE:HB	1.82	0.60
1:E:45:SER:HB2	4:E:710:HOH:O	1.99	0.60
1:G:108:TRP:CD2	1:G:151:ARG:HD2	2.36	0.60
1:G:136:LEU:HD13	1:G:400:TRP:CZ2	2.36	0.60
1:G:401:LEU:HD12	4:G:759:HOH:O	2.01	0.60
1:F:218:GLU:HG3	4:F:688:HOH:O	2.01	0.60
1:H:171:MET:CE	4:H:715:HOH:O	2.37	0.60
1:A:121:LEU:O	1:A:127:ARG:NH2	2.34	0.60
1:F:102:HIS:CD2	1:F:171:MET:HE3	2.37	0.60
1:A:289:THR:HG21	4:A:862:HOH:O	2.02	0.60
1:F:189:ARG:HD3	4:F:694:HOH:O	2.02	0.60
1:G:108:TRP:CZ2	1:G:151:ARG:HD2	2.37	0.60
1:H:121:LEU:O	1:H:127:ARG:NH2	2.34	0.60
1:H:33:GLU:HG2	1:H:48:ILE:HD11	1.84	0.59
1:G:267:ASN:ND2	4:G:703:HOH:O	2.36	0.59
1:G:560:LEU:HD13	1:G:566:HIS:CD2	2.36	0.59
1:B:489:MET:HE1	1:B:508:GLN:HB2	1.84	0.59
1:E:499:GLU:HB2	4:E:850:HOH:O	2.03	0.59
1:B:102:HIS:ND1	1:B:171:MET:HE3	2.18	0.59
1:D:289:THR:HG21	4:D:828:HOH:O	2.03	0.59
1:H:560:LEU:HD13	1:H:566:HIS:NE2	2.18	0.59
1:H:136:LEU:HD13	1:H:400:TRP:CZ2	2.38	0.58
1:H:234:ILE:HD12	4:H:822:HOH:O	2.02	0.58
1:B:121:LEU:O	1:B:127:ARG:NH2	2.36	0.58
1:F:136:LEU:HD13	1:F:400:TRP:CZ2	2.38	0.58
1:H:467:LEU:HD12	1:H:470:MET:HE3	1.86	0.58
1:G:107:LYS:HD2	4:G:749:HOH:O	2.02	0.58
1:D:489:MET:HE1	1:D:508:GLN:HB2	1.85	0.58
1:F:103:TYR:CD1	1:F:580:LYS:NZ	2.55	0.58
1:C:136:LEU:HD13	1:C:400:TRP:CZ2	2.39	0.58
1:D:351:THR:HG22	1:D:354:GLU:H	1.69	0.57
1:F:372:ILE:HG23	4:F:629:HOH:O	2.02	0.57
1:F:369:GLU:HG3	1:F:371:TYR:HE1	1.68	0.57
1:B:190:ASN:CB	1:B:352:THR:HG23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:HIS:ND1	1:C:171:MET:HE3	2.20	0.57
1:D:452:ALA:H	1:D:566:HIS:HD2	1.51	0.57
1:A:136:LEU:HD13	1:A:400:TRP:CZ2	2.39	0.57
1:D:58:THR:CG2	1:D:72:ALA:O	2.52	0.57
1:D:61:LYS:HB2	1:D:289:THR:HG23	1.87	0.57
1:A:530:ARG:NH2	1:B:238:GLU:OE1	2.38	0.57
1:E:171:MET:HE1	4:E:857:HOH:O	1.99	0.57
1:G:97:ASN:HA	1:G:151:ARG:HH21	1.69	0.57
1:F:295:ARG:NH2	1:F:299:ASP:O	2.37	0.56
1:A:489:MET:HE1	1:A:508:GLN:HB2	1.86	0.56
1:D:48:ILE:HG12	1:D:58:THR:HG22	1.87	0.56
1:H:33:GLU:HA	1:H:48:ILE:HG12	1.86	0.56
1:B:102:HIS:ND1	1:B:171:MET:HE2	2.20	0.56
1:H:286:ARG:HH11	1:H:286:ARG:HG2	1.69	0.56
1:C:452:ALA:H	1:C:566:HIS:HD2	1.52	0.56
1:H:156:LEU:CD2	4:H:913:HOH:O	2.54	0.56
1:F:374:ASP:OD1	1:F:381:TYR:OH	2.20	0.55
1:D:48:ILE:CG1	1:D:58:THR:HG22	2.36	0.55
1:E:6:ILE:HD12	1:E:13:LEU:HD11	1.88	0.55
1:G:560:LEU:CD1	1:G:566:HIS:NE2	2.68	0.55
1:G:108:TRP:CE2	1:G:151:ARG:CD	2.89	0.55
1:C:374:ASP:OD1	1:C:381:TYR:OH	2.20	0.55
1:H:80:LEU:HD13	1:H:85:PHE:HE2	1.71	0.55
1:H:374:ASP:OD1	1:H:381:TYR:OH	2.20	0.55
1:E:32:GLU:OE2	1:E:49:ARG:NH2	2.39	0.55
1:H:4:THR:HG21	4:H:814:HOH:O	2.06	0.55
1:D:2:THR:O	1:D:14:GLU:HG2	2.07	0.54
1:F:295:ARG:NH2	1:F:295:ARG:HG2	2.22	0.54
1:G:108:TRP:CD2	1:G:151:ARG:CD	2.90	0.54
1:E:302:VAL:HB	4:E:824:HOH:O	2.07	0.54
1:C:286:ARG:HH11	1:C:286:ARG:HG2	1.73	0.54
1:H:500:ARG:NH2	1:H:551:TYR:O	2.40	0.54
1:D:27:LEU:HD21	1:D:378:LEU:HD22	1.88	0.54
1:E:425:GLU:O	1:E:429:ASN:HB2	2.07	0.54
1:F:19:ARG:HG2	4:F:666:HOH:O	2.07	0.54
1:F:518:ASP:HB2	4:F:680:HOH:O	2.08	0.54
1:H:102:HIS:CE1	1:H:171:MET:CE	2.90	0.54
1:F:440:ASP:OD2	1:F:442:PHE:HB2	2.08	0.53
1:G:374:ASP:OD1	1:G:381:TYR:OH	2.21	0.53
1:H:31:ILE:CG2	1:H:48:ILE:HG23	2.38	0.53
1:B:37:LEU:HB3	4:B:909:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ILE:HD13	1:E:386:ILE:HD13	1.90	0.53
1:G:61:LYS:HB2	1:G:289:THR:HG23	1.88	0.53
1:B:374:ASP:OD1	1:B:381:TYR:OH	2.19	0.53
1:G:360:MET:HE1	1:G:370:VAL:HG11	1.90	0.53
1:F:576:LEU:O	1:F:580:LYS:CG	2.43	0.53
1:A:489:MET:HE1	1:A:508:GLN:OE1	2.09	0.53
1:F:206:LYS:HG3	1:F:274:PHE:CE2	2.44	0.53
1:F:561:HIS:HB2	4:F:619:HOH:O	2.07	0.53
1:A:238:GLU:OE2	1:B:530:ARG:NH2	2.41	0.53
1:A:61:LYS:HB2	1:A:289:THR:HG23	1.91	0.52
1:D:2:THR:N	4:D:815:HOH:O	2.41	0.52
1:F:360:MET:HE1	1:F:370:VAL:HG11	1.90	0.52
1:B:286:ARG:HG2	1:B:286:ARG:HH11	1.74	0.52
1:F:554:GLN:CG	4:F:636:HOH:O	2.53	0.52
1:G:286:ARG:HG2	1:G:286:ARG:HH11	1.74	0.52
1:G:446:ARG:NH1	4:G:876:HOH:O	2.33	0.52
1:B:102:HIS:CE1	1:B:171:MET:CE	2.93	0.52
1:B:500:ARG:NH2	1:B:551:TYR:O	2.43	0.52
1:F:369:GLU:OE1	1:F:371:TYR:OH	2.20	0.52
1:G:351:THR:HG22	1:G:353:GLU:H	1.75	0.52
1:H:102:HIS:ND1	1:H:171:MET:HE2	2.24	0.52
1:B:125:ARG:HG3	4:B:982:HOH:O	2.09	0.52
1:D:286:ARG:HG2	1:D:286:ARG:HH11	1.75	0.52
1:F:385:ILE:CG1	4:F:629:HOH:O	2.48	0.52
1:H:327:SER:N	4:H:755:HOH:O	2.42	0.52
1:F:143:ASP:OD1	1:F:144:LEU:N	2.43	0.52
1:E:238:GLU:OE2	1:F:530:ARG:NH2	2.43	0.52
1:G:581:ALA:CA	4:G:857:HOH:O	2.41	0.52
1:A:545:SER:HB3	1:C:525:LEU:HD21	1.92	0.51
1:B:190:ASN:HB2	1:B:352:THR:HG23	1.92	0.51
1:D:102:HIS:CD2	1:D:171:MET:HE2	2.45	0.51
1:G:411:ARG:HG2	1:G:415:LEU:HD22	1.92	0.51
1:H:76:TYR:HD1	1:H:80:LEU:HD22	1.75	0.51
1:D:374:ASP:OD1	1:D:381:TYR:OH	2.20	0.51
1:D:499:GLU:HB2	4:D:762:HOH:O	2.11	0.51
1:D:485:THR:HG22	1:D:489:MET:HE2	1.92	0.51
1:A:286:ARG:HG2	1:A:286:ARG:HH11	1.75	0.51
1:C:147:GLY:HA2	4:C:771:HOH:O	2.11	0.50
2:E:601:AMP:N1	4:E:795:HOH:O	2.33	0.50
1:D:519:ARG:HD3	1:D:524:TYR:OH	2.11	0.50
1:E:9:LYS:HE3	2:E:601:AMP:N1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ASP:HA	4:F:610:HOH:O	2.11	0.50
1:G:519:ARG:HD3	1:G:524:TYR:OH	2.12	0.50
1:E:102:HIS:CE1	1:E:171:MET:HE2	2.47	0.50
1:F:143:ASP:OD1	1:F:143:ASP:C	2.53	0.50
1:H:178:TYR:O	1:H:179:VAL:C	2.54	0.50
1:D:102:HIS:CG	1:D:171:MET:HE2	2.47	0.49
1:C:102:HIS:CE1	1:C:171:MET:CE	2.95	0.49
1:E:171:MET:HE1	4:E:745:HOH:O	2.11	0.49
1:G:131:ASP:HB2	1:G:136:LEU:HD22	1.94	0.49
1:A:374:ASP:OD1	1:A:381:TYR:OH	2.20	0.49
1:E:116:ASP:C	1:E:116:ASP:OD1	2.55	0.49
1:C:317:THR:CG2	4:C:782:HOH:O	2.54	0.49
1:H:519:ARG:HD3	1:H:524:TYR:OH	2.13	0.49
1:A:525:LEU:HD21	1:C:545:SER:HB3	1.95	0.49
1:C:351:THR:HG22	1:C:353:GLU:H	1.78	0.49
1:E:286:ARG:HG2	1:E:286:ARG:HH11	1.78	0.49
1:G:581:ALA:C	4:G:857:HOH:O	2.55	0.49
1:A:131:ASP:HB2	1:A:136:LEU:HD22	1.95	0.49
1:H:2:THR:HG21	4:H:855:HOH:O	2.13	0.49
1:B:171:MET:CE	4:B:784:HOH:O	2.46	0.49
1:C:64:THR:HB	4:C:811:HOH:O	2.13	0.49
1:D:238:GLU:OE1	4:D:868:HOH:O	2.20	0.49
1:F:517:GLU:OE2	1:F:518:ASP:OD2	2.31	0.49
1:G:485:THR:HG22	1:G:489:MET:HE2	1.95	0.49
1:B:316:HIS:HB3	4:B:934:HOH:O	2.13	0.48
1:F:519:ARG:HD3	1:F:524:TYR:OH	2.13	0.48
1:B:485:THR:HG22	1:B:489:MET:HE2	1.95	0.48
1:F:425:GLU:N	1:F:425:GLU:OE1	2.47	0.48
1:G:274:PHE:HB2	4:G:768:HOH:O	2.12	0.48
1:H:284:LEU:HD13	4:H:950:HOH:O	2.13	0.48
1:B:102:HIS:CG	1:B:171:MET:HE2	2.49	0.48
1:D:165:GLN:CD	4:D:941:HOH:O	2.55	0.48
1:E:5:PHE:HA	4:E:890:HOH:O	2.13	0.48
1:C:519:ARG:HD3	1:C:524:TYR:OH	2.14	0.48
1:F:143:ASP:OD1	1:F:145:GLN:N	2.36	0.48
1:H:510:LEU:HD23	4:H:960:HOH:O	2.13	0.48
1:A:171:MET:HE3	1:A:171:MET:O	2.14	0.48
1:A:519:ARG:HD3	1:A:524:TYR:OH	2.13	0.48
1:B:325:ASP:OD2	4:B:785:HOH:O	2.20	0.48
1:G:415:LEU:HG	1:G:556:VAL:HB	1.96	0.48
1:H:36:TRP:CZ3	1:H:65:LYS:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:317:THR:HB	4:H:894:HOH:O	2.15	0.47
1:F:567:GLN:HB2	4:F:639:HOH:O	2.14	0.47
1:G:238:GLU:OE2	1:H:530:ARG:NH2	2.47	0.47
1:B:452:ALA:H	1:B:566:HIS:CD2	2.29	0.47
1:C:526:ASN:O	1:C:530:ARG:HG3	2.14	0.47
1:H:4:THR:HG22	1:H:14:GLU:OE2	2.10	0.47
1:C:102:HIS:ND1	1:C:171:MET:HE2	2.29	0.47
1:E:526:ASN:O	1:E:530:ARG:HG3	2.15	0.47
1:G:522:LEU:H	1:G:522:LEU:CD2	2.10	0.47
1:E:131:ASP:HB2	1:E:136:LEU:HD22	1.95	0.47
1:F:298:LYS:O	1:F:298:LYS:HG2	2.15	0.47
1:E:6:ILE:CD1	1:E:13:LEU:HD11	2.45	0.46
1:B:133:GLU:N	1:B:133:GLU:OE1	2.49	0.46
1:E:446:ARG:NH1	1:E:460:TYR:O	2.48	0.46
1:H:406:MET:HB2	4:H:857:HOH:O	2.14	0.46
1:B:134:ASN:ND2	4:B:1005:HOH:O	2.26	0.46
1:F:503:TYR:OH	4:F:606:HOH:O	2.20	0.46
1:B:526:ASN:O	1:B:530:ARG:HG3	2.15	0.46
1:C:131:ASP:HB2	1:C:136:LEU:HD22	1.97	0.46
1:C:425:GLU:HG2	4:C:796:HOH:O	2.15	0.46
1:D:526:ASN:O	1:D:530:ARG:HG3	2.16	0.46
1:F:80:LEU:HD22	1:F:576:LEU:HD11	1.98	0.46
1:F:131:ASP:HB2	1:F:136:LEU:HD22	1.96	0.46
1:E:374:ASP:OD1	1:E:381:TYR:OH	2.19	0.46
1:A:485:THR:HG22	1:A:489:MET:HE2	1.98	0.46
1:B:134:ASN:HB2	1:H:133:GLU:HG3	1.96	0.46
1:F:526:ASN:O	1:F:530:ARG:HG3	2.16	0.46
1:F:102:HIS:CD2	1:F:171:MET:HE2	2.51	0.46
1:G:443:THR:CG2	4:G:756:HOH:O	2.64	0.46
1:F:286:ARG:HE	1:F:286:ARG:HB2	1.53	0.46
1:G:97:ASN:HA	1:G:151:ARG:NH2	2.31	0.46
1:G:446:ARG:HG3	1:G:451:LEU:O	2.17	0.45
1:G:526:ASN:O	1:G:530:ARG:HG3	2.15	0.45
1:F:62:GLY:N	4:F:633:HOH:O	2.49	0.45
1:D:171:MET:CE	4:D:735:HOH:O	2.51	0.45
1:E:119:GLU:HA	4:E:840:HOH:O	2.16	0.45
1:G:160:ARG:HD2	1:G:163:ASP:OD1	2.16	0.45
1:H:131:ASP:HB2	1:H:136:LEU:HD22	1.97	0.45
1:D:36:TRP:CZ3	1:D:65:LYS:HG3	2.52	0.45
1:D:165:GLN:HG2	4:D:941:HOH:O	2.17	0.45
1:F:102:HIS:CG	1:F:171:MET:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:526:ASN:O	1:H:530:ARG:HG3	2.17	0.45
1:A:293:GLN:NE2	4:A:717:HOH:O	2.34	0.45
1:G:137:THR:HG1	1:G:140:MET:HG2	1.81	0.45
1:H:102:HIS:CG	1:H:171:MET:HE2	2.51	0.45
1:F:403:ASN:CG	4:F:634:HOH:O	2.60	0.45
1:H:509:THR:HG22	4:H:960:HOH:O	2.17	0.45
1:G:420:SER:C	1:G:421:GLU:HG2	2.41	0.44
1:C:13:LEU:CD2	4:C:893:HOH:O	2.54	0.44
1:F:36:TRP:CZ3	1:F:65:LYS:HG3	2.51	0.44
1:H:327:SER:CA	4:H:755:HOH:O	2.65	0.44
1:A:489:MET:CE	1:A:508:GLN:OE1	2.65	0.44
1:H:4:THR:HG23	1:H:14:GLU:CD	2.42	0.44
1:H:277:HIS:CG	1:H:278:PRO:HD2	2.52	0.44
1:H:286:ARG:HG2	1:H:286:ARG:NH1	2.31	0.44
1:A:277:HIS:CG	1:A:278:PRO:HD2	2.52	0.44
1:H:160:ARG:HD2	1:H:163:ASP:OD1	2.17	0.44
1:H:510:LEU:N	4:H:960:HOH:O	2.50	0.44
1:A:178:TYR:O	1:A:179:VAL:C	2.59	0.44
1:D:23:LYS:HE3	1:D:379:GLY:HA3	2.00	0.44
1:A:526:ASN:O	1:A:530:ARG:HG3	2.17	0.44
1:H:420:SER:O	1:H:421:GLU:HB2	2.17	0.44
1:G:36:TRP:CZ3	1:G:65:LYS:HG3	2.53	0.44
1:A:31:ILE:HG22	1:A:48:ILE:HG22	1.94	0.43
1:D:420:SER:C	1:D:421:GLU:HG2	2.43	0.43
1:C:277:HIS:CG	1:C:278:PRO:HD2	2.53	0.43
1:C:560:LEU:HD13	1:C:566:HIS:CD2	2.54	0.43
1:D:286:ARG:HG2	1:D:286:ARG:NH1	2.33	0.43
1:F:23:LYS:HE3	1:F:379:GLY:HA3	2.00	0.43
1:B:23:LYS:HE3	1:B:379:GLY:HA3	2.00	0.43
1:B:160:ARG:HD2	1:B:163:ASP:OD1	2.19	0.43
1:B:178:TYR:O	1:B:179:VAL:C	2.60	0.43
1:C:23:LYS:HE3	1:C:379:GLY:HA3	1.99	0.43
1:C:36:TRP:CZ3	1:C:65:LYS:HG3	2.53	0.43
1:C:160:ARG:HH21	1:C:165:GLN:HB2	1.84	0.43
1:E:23:LYS:HE3	1:E:379:GLY:HA3	2.01	0.43
1:F:178:TYR:HB3	4:F:693:HOH:O	2.17	0.43
1:G:519:ARG:NH1	1:H:333:ASP:OD2	2.52	0.43
1:B:286:ARG:HG2	1:B:286:ARG:NH1	2.33	0.43
1:D:160:ARG:HD2	1:D:163:ASP:OD1	2.18	0.43
1:E:36:TRP:CZ3	1:E:65:LYS:HG3	2.53	0.43
1:E:149:GLU:HB3	4:E:867:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:PHE:N	1:F:29:PHE:HD1	2.17	0.43
1:H:23:LYS:HE3	1:H:379:GLY:HA3	1.99	0.43
1:D:178:TYR:O	1:D:179:VAL:C	2.61	0.43
1:A:286:ARG:HG2	1:A:286:ARG:NH1	2.33	0.42
1:C:71:SER:OG	2:C:601:AMP:O1P	2.32	0.42
1:G:286:ARG:HG2	1:G:286:ARG:NH1	2.34	0.42
1:E:286:ARG:HG2	1:E:286:ARG:NH1	2.35	0.42
1:F:29:PHE:N	1:F:29:PHE:CD1	2.87	0.42
1:F:178:TYR:O	1:F:179:VAL:C	2.62	0.42
1:G:102:HIS:CE1	1:G:171:MET:HG2	2.54	0.42
1:C:178:TYR:O	1:C:179:VAL:C	2.62	0.42
1:G:522:LEU:HD23	1:G:522:LEU:N	2.29	0.42
1:H:174:ILE:HB	4:H:913:HOH:O	2.18	0.42
1:C:452:ALA:H	1:C:566:HIS:CD2	2.36	0.42
1:H:23:LYS:HD3	1:H:23:LYS:HA	1.97	0.42
1:A:160:ARG:HD2	1:A:163:ASP:OD1	2.19	0.42
1:C:351:THR:HG22	1:C:353:GLU:N	2.34	0.42
1:E:123:ASP:OD1	1:E:123:ASP:C	2.63	0.42
1:E:190:ASN:O	1:E:194:VAL:HG23	2.20	0.42
1:E:530:ARG:NH2	1:F:238:GLU:OE2	2.53	0.42
1:B:190:ASN:HB3	1:B:352:THR:HG23	2.00	0.42
1:B:14:GLU:HG2	4:B:702:HOH:O	2.19	0.42
1:D:277:HIS:CG	1:D:278:PRO:HD2	2.55	0.42
1:E:329:LEU:HA	4:E:907:HOH:O	2.19	0.42
1:D:452:ALA:H	1:D:566:HIS:CD2	2.34	0.42
1:B:136:LEU:HA	1:B:136:LEU:HD23	1.85	0.41
1:F:79:ARG:NH1	4:F:695:HOH:O	2.35	0.41
1:F:369:GLU:CD	1:F:371:TYR:OH	2.63	0.41
1:E:178:TYR:O	1:E:179:VAL:C	2.62	0.41
1:G:446:ARG:NH1	1:G:460:TYR:O	2.51	0.41
1:B:518:ASP:HA	4:B:905:HOH:O	2.19	0.41
1:H:470:MET:HE3	1:H:470:MET:HB2	1.68	0.41
1:B:203:ARG:NH2	4:B:757:HOH:O	2.46	0.41
1:E:277:HIS:CG	1:E:278:PRO:HD2	2.55	0.41
1:F:277:HIS:CG	1:F:278:PRO:HD2	2.55	0.41
1:B:115:ASP:HA	4:B:737:HOH:O	2.20	0.41
1:C:359:LEU:HD23	4:C:878:HOH:O	2.21	0.41
1:G:97:ASN:C	1:G:151:ARG:HH22	2.29	0.41
1:F:29:PHE:HE2	1:F:80:LEU:HD21	1.85	0.41
1:G:127:ARG:NE	4:G:839:HOH:O	2.04	0.41
1:G:137:THR:OG1	1:G:140:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HE3	2:A:601:AMP:N1	2.36	0.41
1:B:189:ARG:HA	1:B:381:TYR:CD2	2.55	0.41
1:G:209:ILE:HA	1:G:214:ILE:HD12	2.03	0.41
1:C:286:ARG:HG2	1:C:286:ARG:NH1	2.34	0.41
1:D:190:ASN:O	1:D:194:VAL:HG23	2.21	0.41
1:G:97:ASN:HB3	4:G:853:HOH:O	2.21	0.41
1:C:137:THR:HG1	1:C:140:MET:HG2	1.86	0.40
1:D:2:THR:O	1:D:14:GLU:CG	2.69	0.40
1:A:460:TYR:OH	4:A:1025:HOH:O	2.17	0.40
1:B:36:TRP:CZ3	1:B:65:LYS:HG3	2.56	0.40
1:C:59:ASN:ND2	4:C:880:HOH:O	2.54	0.40
1:C:514:ALA:HA	4:C:874:HOH:O	2.22	0.40
1:H:80:LEU:HD13	1:H:85:PHE:CE2	2.55	0.40
1:H:137:THR:HG1	1:H:140:MET:HG3	1.86	0.40
1:A:23:LYS:HE3	1:A:379:GLY:HA3	2.03	0.40
1:E:127:ARG:NH2	4:E:840:HOH:O	2.54	0.40
1:F:190:ASN:O	1:F:194:VAL:HG23	2.21	0.40
1:G:23:LYS:HE3	1:G:379:GLY:HA3	2.02	0.40
1:G:108:TRP:CE3	1:G:151:ARG:HD2	2.57	0.40
1:G:351:THR:HG22	1:G:353:GLU:N	2.34	0.40
1:H:190:ASN:O	1:H:194:VAL:HG23	2.20	0.40
1:B:505:ARG:NH2	4:B:1003:HOH:O	2.54	0.40
1:G:492:ASN:O	1:G:493:SER:C	2.64	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	580/586 (99%)	569 (98%)	10 (2%)	1 (0%)	43 50
1	B	581/586 (99%)	567 (98%)	13 (2%)	1 (0%)	43 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	568/586 (97%)	555 (98%)	12 (2%)	1 (0%)	43	50
1	D	580/586 (99%)	566 (98%)	13 (2%)	1 (0%)	43	50
1	E	576/586 (98%)	564 (98%)	11 (2%)	1 (0%)	43	50
1	F	572/586 (98%)	557 (97%)	14 (2%)	1 (0%)	43	50
1	G	573/586 (98%)	560 (98%)	12 (2%)	1 (0%)	43	50
1	H	581/586 (99%)	566 (97%)	14 (2%)	1 (0%)	43	50
All	All	4611/4688 (98%)	4504 (98%)	99 (2%)	8 (0%)	43	50

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	B	179	VAL
1	C	179	VAL
1	D	179	VAL
1	E	179	VAL
1	F	179	VAL
1	G	179	VAL
1	H	179	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/487 (99%)	477 (99%)	7 (1%)	59	70
1	B	485/487 (100%)	475 (98%)	10 (2%)	47	58
1	C	475/487 (98%)	463 (98%)	12 (2%)	42	52
1	D	484/487 (99%)	472 (98%)	12 (2%)	42	52
1	E	481/487 (99%)	470 (98%)	11 (2%)	44	55
1	F	477/487 (98%)	456 (96%)	21 (4%)	25	29
1	G	478/487 (98%)	461 (96%)	17 (4%)	31	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	485/487 (100%)	470 (97%)	15 (3%)	35	44
All	All	3849/3896 (99%)	3744 (97%)	105 (3%)	39	49

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	113	GLU
1	A	136	LEU
1	A	203	ARG
1	A	289	THR
1	A	479	GLU
1	A	560	LEU
1	B	113	GLU
1	B	133	GLU
1	B	203	ARG
1	B	292	LEU
1	B	319	LEU
1	B	352	THR
1	B	384	ARG
1	B	437	GLU
1	B	522	LEU
1	B	560	LEU
1	C	119	GLU
1	C	134	ASN
1	C	136	LEU
1	C	156	LEU
1	C	203	ARG
1	C	298	LYS
1	C	406	MET
1	C	436	GLU
1	C	455	SER
1	C	479	GLU
1	C	522	LEU
1	C	560	LEU
1	D	14	GLU
1	D	58	THR
1	D	134	ASN
1	D	203	ARG
1	D	289	THR
1	D	351	THR
1	D	401	LEU

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Mol	Chain	Res	Type
1	D	405	SER
1	D	436	GLU
1	D	479	GLU
1	D	518	ASP
1	D	560	LEU
1	E	23	LYS
1	E	116	ASP
1	E	134	ASN
1	E	136	LEU
1	E	203	ARG
1	E	298	LYS
1	E	300	LEU
1	E	436	GLU
1	E	518	ASP
1	E	522	LEU
1	E	560	LEU
1	F	66	LYS
1	F	97	ASN
1	F	107	LYS
1	F	136	LEU
1	F	156	LEU
1	F	164	ASN
1	F	203	ARG
1	F	286	ARG
1	F	292	LEU
1	F	317	THR
1	F	409	HIS
1	F	425	GLU
1	F	436	GLU
1	F	437	GLU
1	F	517	GLU
1	F	522	LEU
1	F	547	GLU
1	F	560	LEU
1	F	576	LEU
1	F	577	GLN
1	F	580	LYS
1	G	23	LYS
1	G	119	GLU
1	G	134	ASN
1	G	136	LEU
1	G	203	ARG

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Mol	Chain	Res	Type
1	G	289	THR
1	G	292	LEU
1	G	298	LYS
1	G	312	GLU
1	G	317	THR
1	G	401	LEU
1	G	412	GLU
1	G	415	LEU
1	G	436	GLU
1	G	437	GLU
1	G	522	LEU
1	G	560	LEU
1	H	2	THR
1	H	4	THR
1	H	23	LYS
1	H	48	ILE
1	H	80	LEU
1	H	134	ASN
1	H	136	LEU
1	H	156	LEU
1	H	164	ASN
1	H	292	LEU
1	H	312	GLU
1	H	401	LEU
1	H	436	GLU
1	H	455	SER
1	H	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	A	520	GLN
1	B	30	GLN
1	B	42	ASN
1	B	134	ASN
1	B	161	GLN
1	B	195	GLN
1	B	480	GLN
1	B	566	HIS
1	B	567	GLN
1	C	42	ASN

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Mol	Chain	Res	Type
1	C	59	ASN
1	C	364	ASN
1	C	566	HIS
1	C	567	GLN
1	D	102	HIS
1	D	145	GLN
1	D	515	GLN
1	D	566	HIS
1	F	97	ASN
1	F	102	HIS
1	F	195	GLN
1	F	293	GLN
1	F	567	GLN
1	G	42	ASN
1	G	102	HIS
1	G	145	GLN
1	G	195	GLN
1	G	561	HIS
1	G	567	GLN
1	H	195	GLN
1	H	566	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 21 are monoatomic - leaving 7 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	AMP	A	601	-	25,25,25	2.04	6 (24%)	37,38,38	2.48	13 (35%)
2	AMP	B	601	-	25,25,25	1.74	4 (16%)	37,38,38	1.94	8 (21%)
2	AMP	H	601	-	25,25,25	1.42	5 (20%)	37,38,38	2.31	9 (24%)
2	AMP	E	601	-	25,25,25	1.85	4 (16%)	37,38,38	2.03	10 (27%)
2	AMP	G	601	-	25,25,25	1.56	4 (16%)	37,38,38	2.20	15 (40%)
2	AMP	C	601	-	25,25,25	1.54	5 (20%)	37,38,38	2.16	13 (35%)
2	AMP	D	601	-	25,25,25	2.02	6 (24%)	37,38,38	2.12	12 (32%)

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	AMP	A	601	-	-	0/10/26/26	0/3/3/3
2	AMP	B	601	-	-	0/10/26/26	0/3/3/3
2	AMP	H	601	-	-	0/10/26/26	0/3/3/3
2	AMP	E	601	-	-	0/10/26/26	0/3/3/3
2	AMP	G	601	-	-	0/10/26/26	0/3/3/3
2	AMP	C	601	-	-	2/10/26/26	0/3/3/3
2	AMP	D	601	-	-	0/10/26/26	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	AMP	C5-C4	6.24	1.50	1.39
2	B	601	AMP	C5-C4	5.76	1.49	1.39
2	A	601	AMP	C4-N9	-5.61	1.26	1.37
2	E	601	AMP	C4-N9	-5.17	1.26	1.37
2	A	601	AMP	C5-C4	5.04	1.48	1.39
2	E	601	AMP	C5-C4	4.98	1.48	1.39
2	C	601	AMP	C5-C4	4.73	1.47	1.39
2	G	601	AMP	C5-C4	4.47	1.47	1.39
2	D	601	AMP	C4-N9	-4.27	1.28	1.37
2	B	601	AMP	C5-N7	-4.19	1.31	1.39
2	A	601	AMP	C2-N3	-3.71	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	AMP	C5-C6	3.42	1.50	1.41
2	D	601	AMP	C8-N7	3.12	1.37	1.31
2	E	601	AMP	C8-N7	3.02	1.37	1.31
2	G	601	AMP	C5-N7	-3.01	1.33	1.39
2	H	601	AMP	C5-C6	2.92	1.49	1.41
2	A	601	AMP	C8-N7	2.90	1.37	1.31
2	H	601	AMP	C8-N9	-2.76	1.32	1.37
2	D	601	AMP	C1'-N9	2.67	1.53	1.46
2	A	601	AMP	C5-N7	-2.62	1.34	1.39
2	D	601	AMP	C5-N7	-2.61	1.34	1.39
2	B	601	AMP	C5-C6	2.61	1.48	1.41
2	H	601	AMP	C5-C4	2.60	1.43	1.39
2	E	601	AMP	C2-N3	-2.60	1.29	1.33
2	A	601	AMP	C1'-N9	2.53	1.53	1.46
2	H	601	AMP	O4'-C1'	2.48	1.47	1.42
2	C	601	AMP	C4-N9	-2.41	1.32	1.37
2	G	601	AMP	C8-N7	2.40	1.36	1.31
2	D	601	AMP	C3'-C4'	-2.38	1.47	1.53
2	B	601	AMP	C4-N9	-2.26	1.33	1.37
2	C	601	AMP	C5-N7	-2.20	1.35	1.39
2	H	601	AMP	C8-N7	2.16	1.35	1.31
2	G	601	AMP	C4-N3	2.04	1.38	1.34
2	C	601	AMP	C8-N7	2.01	1.35	1.31

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	C2-N1-C6	7.32	130.75	118.73
2	H	601	AMP	C5-C4-N3	-6.81	117.34	126.72
2	E	601	AMP	C2-N1-C6	6.67	129.68	118.73
2	B	601	AMP	C5-C4-N3	-6.03	118.41	126.72
2	A	601	AMP	N3-C2-N1	-5.32	120.53	128.58
2	H	601	AMP	N3-C4-N9	5.20	136.01	127.17
2	A	601	AMP	C2'-C1'-N9	5.17	126.15	113.30
2	C	601	AMP	C5-C4-N3	-5.08	119.72	126.72
2	D	601	AMP	C2-N1-C6	4.74	126.52	118.73
2	H	601	AMP	C2-N3-C4	4.74	123.40	111.83
2	G	601	AMP	C5-C4-N3	-4.48	120.54	126.72
2	G	601	AMP	N3-C4-N9	4.47	134.77	127.17
2	A	601	AMP	O4'-C1'-C2'	-4.45	97.10	106.62
2	B	601	AMP	N3-C4-N9	4.44	134.71	127.17
2	C	601	AMP	C4-C5-N7	-4.39	105.56	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	AMP	N3-C2-N1	-4.20	122.22	128.58
2	H	601	AMP	N3-C2-N1	-4.03	122.49	128.58
2	C	601	AMP	C2-N3-C4	3.99	121.57	111.83
2	H	601	AMP	C4-C5-N7	-3.95	106.06	110.58
2	D	601	AMP	N3-C2-N1	-3.94	122.62	128.58
2	C	601	AMP	N3-C2-N1	-3.93	122.63	128.58
2	G	601	AMP	N3-C2-N1	-3.84	122.77	128.58
2	B	601	AMP	O2P-P-O5'	-3.81	96.72	106.67
2	A	601	AMP	C6-C5-C4	-3.63	112.22	117.18
2	C	601	AMP	N3-C4-N9	3.62	133.32	127.17
2	D	601	AMP	O4'-C1'-C2'	-3.61	98.89	106.62
2	H	601	AMP	C4-N9-C8	3.55	109.46	105.74
2	A	601	AMP	C4-N9-C1'	-3.47	118.52	126.63
2	D	601	AMP	O2'-C2'-C1'	3.43	121.91	110.10
2	A	601	AMP	C5-C4-N3	3.40	131.40	126.72
2	G	601	AMP	C4-N9-C8	3.40	109.31	105.74
2	C	601	AMP	C6-C5-N7	3.36	138.57	132.09
2	D	601	AMP	O4'-C1'-N9	3.33	114.49	108.09
2	D	601	AMP	O4'-C4'-C5'	3.33	120.01	109.33
2	C	601	AMP	C5-N7-C8	3.22	108.51	103.45
2	B	601	AMP	C2-N3-C4	3.19	119.62	111.83
2	A	601	AMP	N6-C6-N1	3.14	125.36	118.38
2	E	601	AMP	O2P-P-O5'	-3.11	98.56	106.67
2	D	601	AMP	O2'-C2'-C3'	-3.09	101.90	111.82
2	G	601	AMP	O5'-P-O1P	3.05	114.67	106.44
2	B	601	AMP	C4-C5-N7	-3.03	107.11	110.58
2	D	601	AMP	O3'-C3'-C4'	-2.99	102.51	111.08
2	G	601	AMP	C2-N3-C4	2.97	119.09	111.83
2	B	601	AMP	O2'-C2'-C1'	2.90	120.10	110.10
2	H	601	AMP	N9-C8-N7	-2.87	109.86	113.94
2	C	601	AMP	C4-N9-C8	2.86	108.74	105.74
2	E	601	AMP	O5'-P-O1P	2.84	114.11	106.44
2	H	601	AMP	C5-N7-C8	2.83	107.89	103.45
2	H	601	AMP	O3P-P-O2P	2.80	118.32	107.80
2	A	601	AMP	O2'-C2'-C1'	2.79	119.70	110.10
2	A	601	AMP	C1'-N9-C8	2.78	133.26	127.09
2	G	601	AMP	O2P-P-O5'	-2.70	99.63	106.67
2	D	601	AMP	C2'-C1'-N9	2.68	119.96	113.30
2	G	601	AMP	C5-N7-C8	2.62	107.57	103.45
2	C	601	AMP	N9-C8-N7	-2.61	110.24	113.94
2	G	601	AMP	N9-C8-N7	-2.59	110.26	113.94
2	G	601	AMP	O4'-C1'-N9	2.57	113.03	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	AMP	C4-N9-C1'	-2.56	120.65	126.63
2	B	601	AMP	C5-N7-C8	2.55	107.46	103.45
2	G	601	AMP	C2-N1-C6	2.49	122.83	118.73
2	D	601	AMP	C5'-C4'-C3'	-2.49	106.25	115.21
2	D	601	AMP	N6-C6-N1	2.47	123.89	118.38
2	D	601	AMP	O3P-P-O5'	-2.45	100.27	106.67
2	G	601	AMP	C3'-C2'-C1'	-2.45	96.82	101.46
2	C	601	AMP	C2-N1-C6	2.44	122.73	118.73
2	E	601	AMP	C2'-C1'-N9	2.42	119.31	113.30
2	C	601	AMP	O2'-C2'-C1'	2.40	118.37	110.10
2	E	601	AMP	C6-C5-C4	-2.37	113.94	117.18
2	A	601	AMP	C5-N7-C8	-2.33	99.79	103.45
2	A	601	AMP	N3-C4-N9	-2.30	123.25	127.17
2	G	601	AMP	C4-N9-C1'	-2.28	121.31	126.63
2	C	601	AMP	C4-N9-C1'	-2.25	121.37	126.63
2	C	601	AMP	O4'-C1'-N9	-2.25	103.77	108.09
2	B	601	AMP	O3P-P-O5'	2.16	112.30	106.67
2	G	601	AMP	N6-C6-N1	2.16	123.19	118.38
2	A	601	AMP	C5-C6-N1	-2.14	112.08	117.51
2	G	601	AMP	C4-C5-N7	-2.11	108.17	110.58
2	E	601	AMP	C5-C6-N1	-2.07	112.26	117.51
2	E	601	AMP	C3'-C2'-C1'	-2.04	97.61	101.46
2	E	601	AMP	C1'-N9-C8	2.02	131.57	127.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	AMP	C5'-O5'-P-O2P
2	C	601	AMP	C5'-O5'-P-O3P

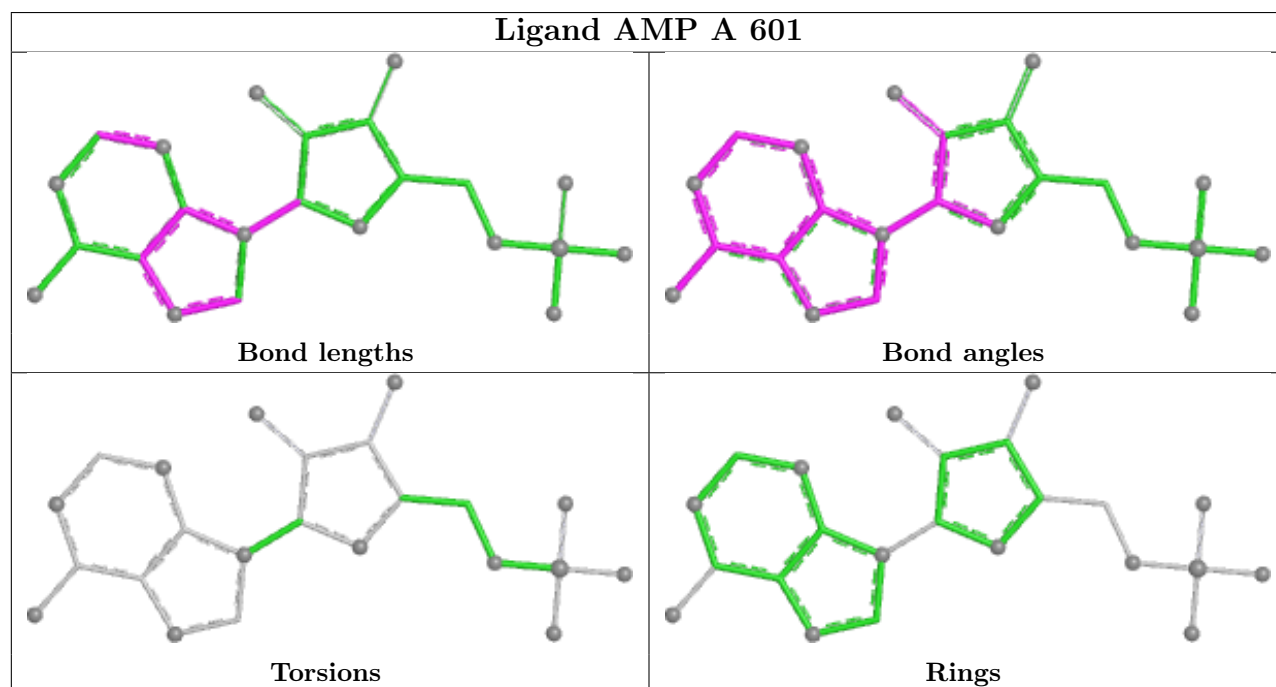
There are no ring outliers.

4 monomers are involved in 6 short contacts:

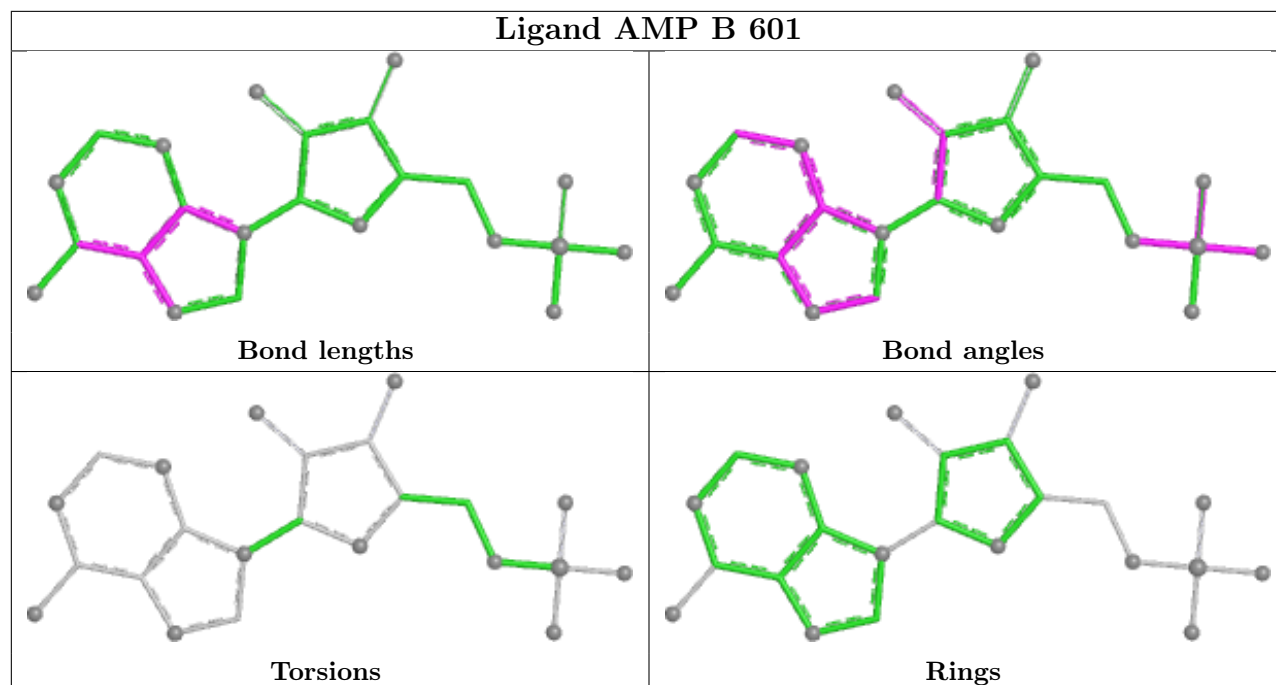
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AMP	1	0
2	E	601	AMP	2	0
2	C	601	AMP	1	0
2	D	601	AMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

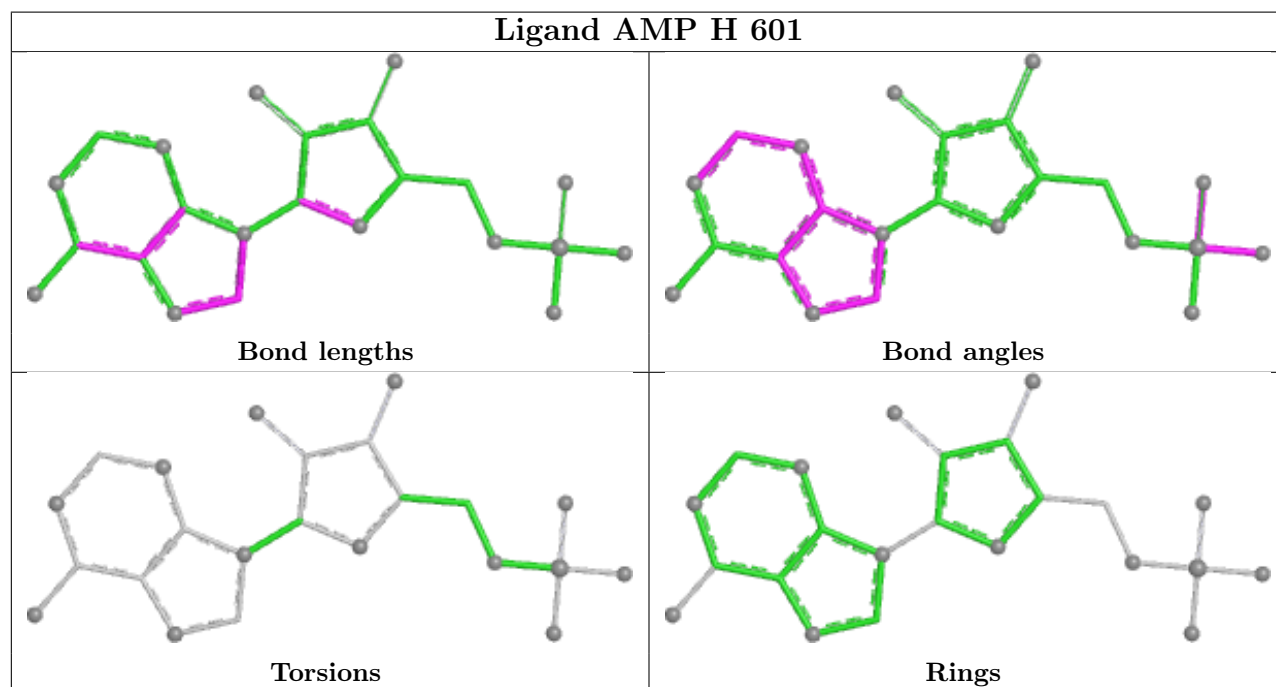
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

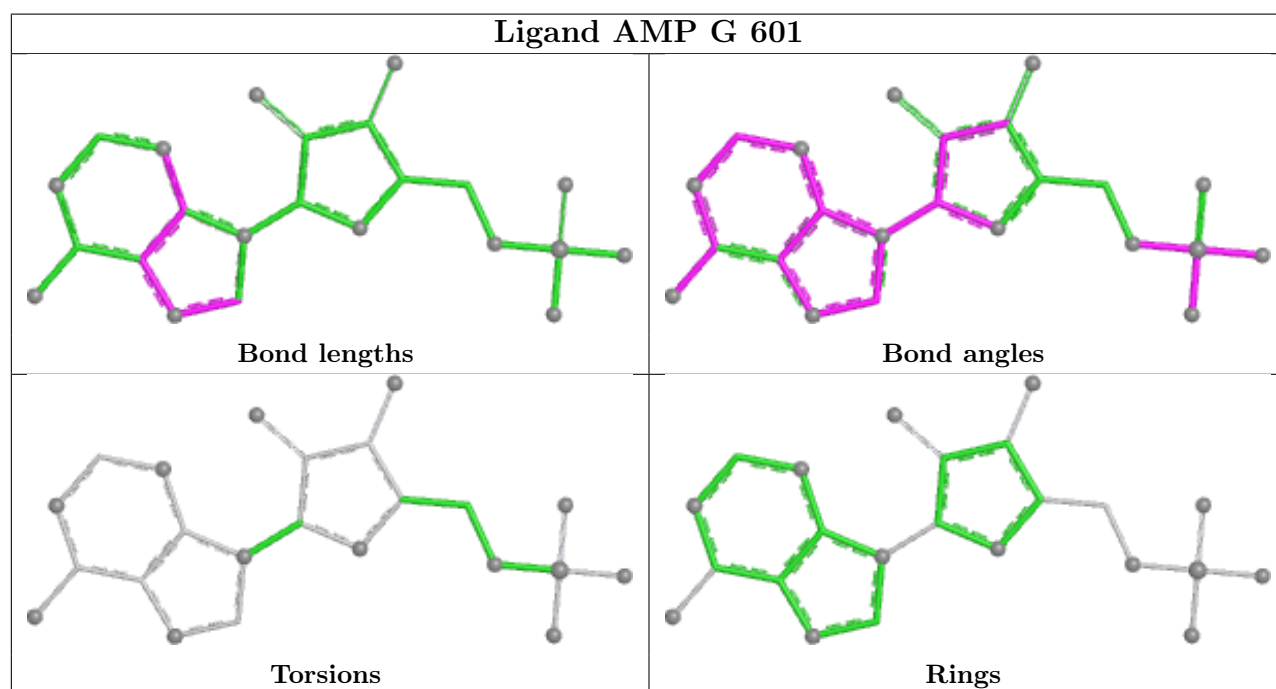
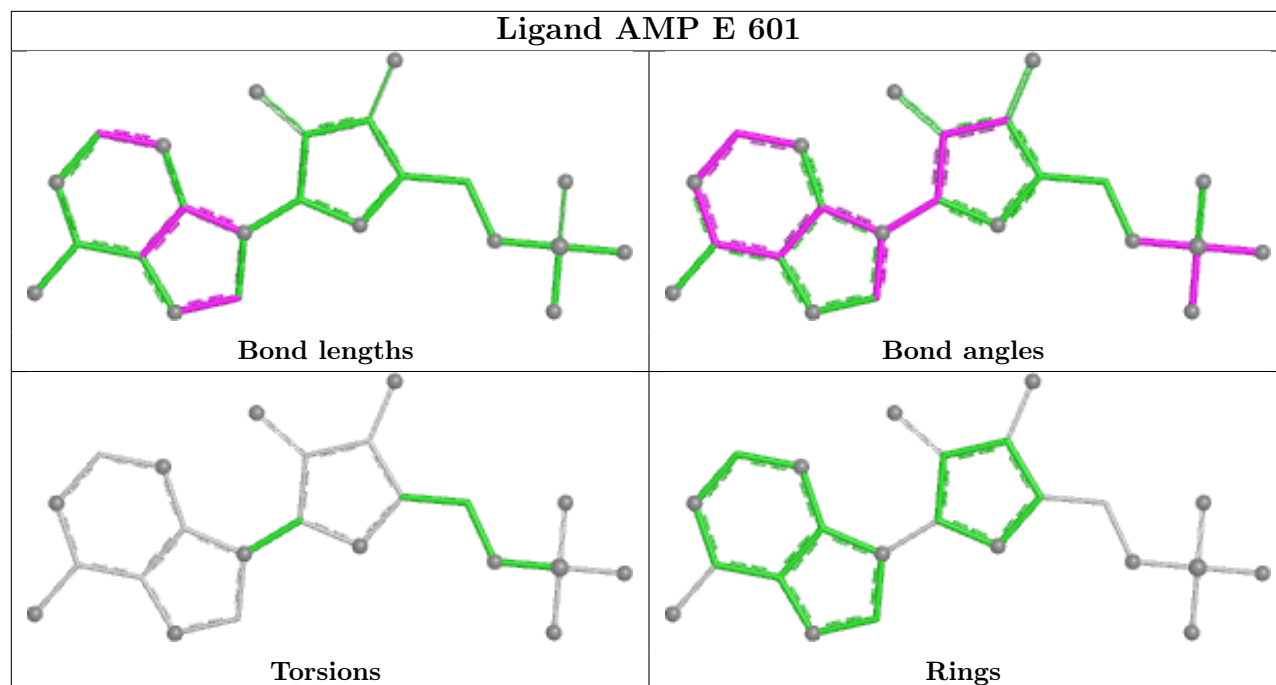


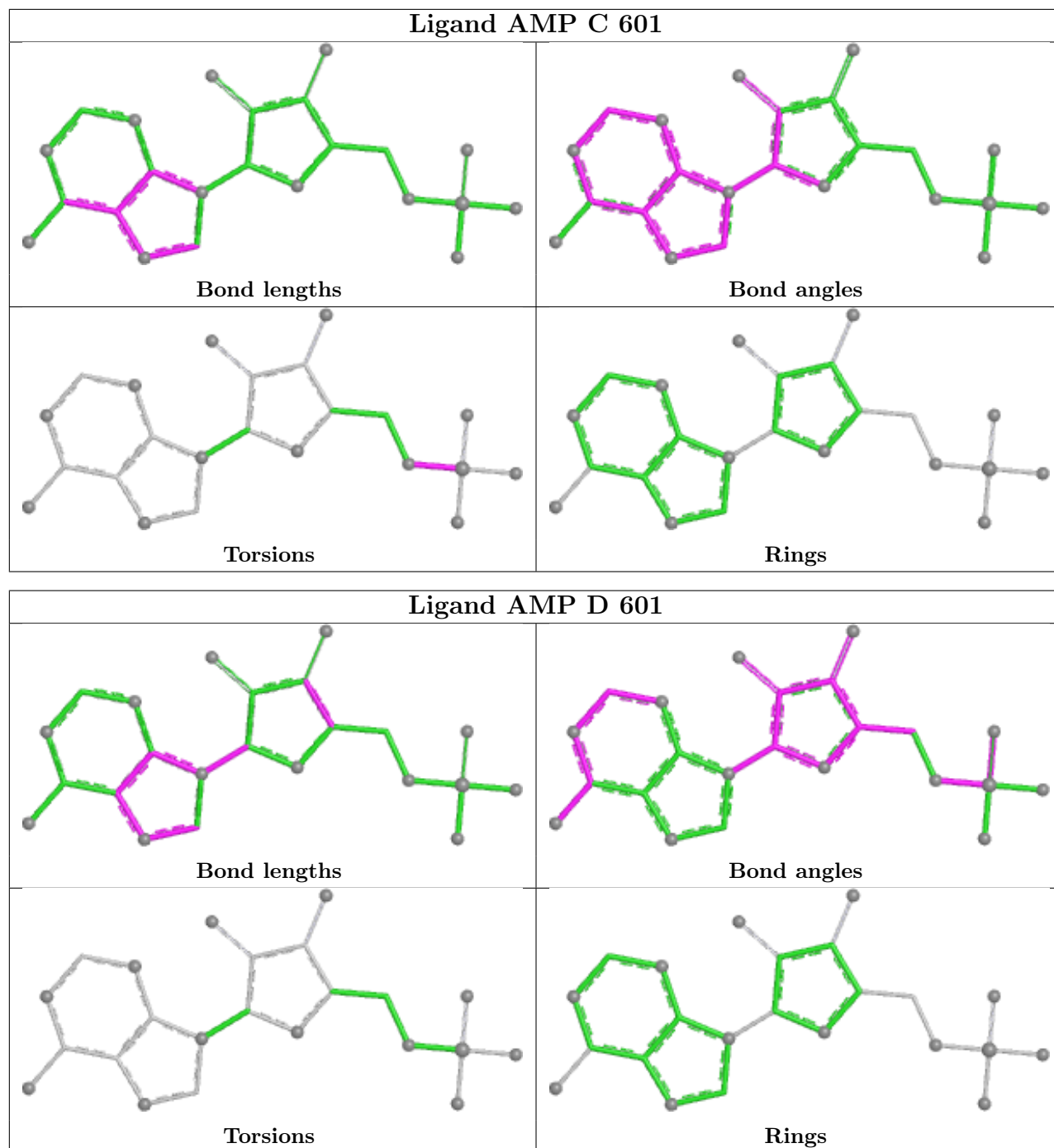
Ligand AMP B 601



Ligand AMP H 601







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	582/586 (99%)	-0.11	1 (0%) 91 92	17, 28, 45, 64	0
1	B	583/586 (99%)	-0.09	3 (0%) 87 88	15, 26, 47, 82	0
1	C	570/586 (97%)	0.43	13 (2%) 61 61	22, 39, 57, 93	0
1	D	582/586 (99%)	0.32	12 (2%) 63 64	21, 36, 57, 86	0
1	E	578/586 (98%)	0.59	19 (3%) 49 49	24, 40, 63, 87	0
1	F	574/586 (97%)	1.83	233 (40%) 0 0	35, 66, 93, 111	0
1	G	575/586 (98%)	0.56	23 (4%) 42 42	23, 40, 60, 92	0
1	H	583/586 (99%)	0.01	1 (0%) 91 92	14, 30, 49, 74	0
All	All	4627/4688 (98%)	0.44	305 (6%) 24 23	14, 36, 71, 111	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	185	ALA	5.0
1	F	297	LEU	4.8
1	F	186	GLY	4.5
1	F	341	TYR	4.5
1	F	359	LEU	4.3
1	F	351	THR	4.3
1	F	101	VAL	4.2
1	F	378	LEU	4.1
1	F	227	TYR	4.1
1	F	224	LEU	4.0
1	E	522	LEU	4.0
1	F	553	LEU	3.9
1	F	77	PHE	3.9
1	F	557	ASP	3.8
1	F	280	PHE	3.8
1	F	228	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	74	GLY	3.8
1	C	581	ALA	3.8
1	F	70	ALA	3.8
1	F	192	ALA	3.8
1	F	169	ILE	3.8
1	F	363	PHE	3.8
1	F	572	ALA	3.7
1	C	406	MET	3.7
1	F	225	ALA	3.7
1	F	27	LEU	3.7
1	F	221	ALA	3.7
1	F	197	LEU	3.7
1	F	448	LEU	3.7
1	F	100	PHE	3.6
1	F	121	LEU	3.6
1	F	237	LEU	3.6
1	F	380	VAL	3.6
1	F	283	ALA	3.6
1	F	209	ILE	3.5
1	F	518	ASP	3.5
1	F	581	ALA	3.5
1	F	219	ILE	3.5
1	F	284	LEU	3.5
1	F	345	ASP	3.5
1	F	522	LEU	3.4
1	F	158	PHE	3.4
1	F	419	GLY	3.4
1	F	80	LEU	3.4
1	F	85	PHE	3.4
1	F	182	GLY	3.4
1	F	37	LEU	3.4
1	F	18	ALA	3.4
1	F	117	VAL	3.3
1	F	72	ALA	3.3
1	G	410	LEU	3.3
1	E	357	ALA	3.2
1	F	13	LEU	3.2
1	F	344	VAL	3.2
1	F	126	LEU	3.2
1	F	95	ILE	3.2
1	F	348	PHE	3.2
1	F	406	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	346	TRP	3.2
1	F	31	ILE	3.2
1	F	347	ASN	3.1
1	F	362	ILE	3.1
1	F	377	HIS	3.1
1	F	153	ILE	3.1
1	F	8	GLY	3.1
1	F	253	GLY	3.1
1	F	12	ALA	3.1
1	F	109	PHE	3.1
1	F	104	PRO	3.1
1	F	205	VAL	3.1
1	F	282	VAL	3.1
1	F	191	GLU	3.0
1	F	265	PRO	3.0
1	F	381	TYR	3.0
1	E	114	ASN	3.0
1	F	529	VAL	3.0
1	F	48	ILE	3.0
1	F	247	TYR	3.0
1	F	11	ALA	3.0
1	F	216	LEU	3.0
1	F	103	TYR	3.0
1	F	573	TYR	3.0
1	B	132	PRO	3.0
1	E	525	LEU	2.9
1	F	576	LEU	2.9
1	F	66	LYS	2.9
1	F	198	SER	2.9
1	F	20	PHE	2.9
1	F	73	LEU	2.9
1	F	229	ALA	2.9
1	F	321	THR	2.9
1	C	70	ALA	2.9
1	G	297	LEU	2.9
1	F	234	ILE	2.9
1	F	167	VAL	2.9
1	F	102	HIS	2.8
1	F	255	TYR	2.8
1	F	357	ALA	2.8
1	F	36	TRP	2.8
1	F	369	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	61	LYS	2.8
1	F	220	PRO	2.8
1	F	356	PHE	2.8
1	F	548	ALA	2.8
1	F	194	VAL	2.8
1	F	414	ILE	2.8
1	F	62	GLY	2.8
1	F	296	GLY	2.8
1	F	91	LEU	2.8
1	F	556	VAL	2.8
1	D	124	ASP	2.8
1	F	110	PRO	2.8
1	F	342	PRO	2.8
1	E	512	LEU	2.8
1	E	581	ALA	2.8
1	G	433	GLN	2.7
1	F	156	LEU	2.7
1	F	15	ASP	2.7
1	F	143	ASP	2.7
1	F	130	TYR	2.7
1	F	57	PHE	2.7
1	F	223	VAL	2.7
1	F	293	GLN	2.7
1	F	132	PRO	2.7
1	F	56	CYS	2.7
1	F	140	MET	2.7
1	E	511	LEU	2.7
1	F	382	ALA	2.7
1	G	12	ALA	2.7
1	F	187	ASN	2.7
1	F	258	ILE	2.7
1	F	154	CYS	2.7
1	F	108	TRP	2.7
1	F	122	LEU	2.7
1	F	449	LEU	2.7
1	F	163	ASP	2.6
1	F	525	LEU	2.6
1	F	128	ALA	2.6
1	F	373	ALA	2.6
1	F	29	PHE	2.6
1	F	59	ASN	2.6
1	F	112	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	231	VAL	2.6
1	F	358	THR	2.6
1	G	406	MET	2.6
1	F	566	HIS	2.6
1	F	410	LEU	2.6
1	C	96	ALA	2.6
1	F	275	GLY	2.6
1	F	350	GLY	2.6
1	F	371	TYR	2.6
1	C	234	ILE	2.6
1	F	107	LYS	2.6
1	F	422	TRP	2.6
1	G	422	TRP	2.6
1	F	364	ASN	2.6
1	F	544	MET	2.6
1	A	2	THR	2.6
1	F	60	GLY	2.6
1	F	98	GLY	2.6
1	F	292	LEU	2.5
1	F	148	ASN	2.5
1	F	86	PHE	2.5
1	F	437	GLU	2.5
1	D	120	GLY	2.5
1	F	439	PHE	2.5
1	F	40	VAL	2.5
1	B	134	ASN	2.5
1	F	239	ALA	2.5
1	F	520	GLN	2.5
1	F	561	HIS	2.5
1	F	120	GLY	2.5
1	F	217	PRO	2.5
1	F	384	ARG	2.4
1	F	387	VAL	2.4
1	F	97	ASN	2.4
1	F	116	ASP	2.4
1	F	21	GLN	2.4
1	F	99	PRO	2.4
1	F	560	LEU	2.4
1	F	113	GLU	2.4
1	C	132	PRO	2.4
1	F	96	ALA	2.4
1	F	196	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	450	GLY	2.4
1	G	236	THR	2.4
1	F	81	SER	2.4
1	F	9	LYS	2.4
1	F	111	LEU	2.4
1	F	291	LEU	2.4
1	F	401	LEU	2.4
1	F	415	LEU	2.4
1	F	570	LEU	2.4
1	F	241	GLY	2.4
1	F	549	ALA	2.4
1	F	94	THR	2.4
1	F	343	PHE	2.4
1	F	521	PRO	2.3
1	G	118	PRO	2.3
1	F	276	ALA	2.3
1	F	349	SER	2.3
1	H	95	ILE	2.3
1	G	435	ASP	2.3
1	G	36	TRP	2.3
1	F	361	ALA	2.3
1	E	544	MET	2.3
1	F	137	THR	2.3
1	F	236	THR	2.3
1	F	289	THR	2.3
1	F	273	SER	2.3
1	G	231	VAL	2.3
1	F	334	LEU	2.3
1	D	118	PRO	2.3
1	F	390	MET	2.3
1	F	71	SER	2.3
1	C	316	HIS	2.3
1	F	554	GLN	2.3
1	F	141	LEU	2.3
1	F	300	LEU	2.3
1	F	299	ASP	2.3
1	E	422	TRP	2.3
1	F	67	ALA	2.3
1	F	568	SER	2.3
1	D	423	GLU	2.3
1	F	385	ILE	2.3
1	F	69	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	251	LEU	2.2
1	G	511	LEU	2.2
1	F	190	ASN	2.2
1	D	128	ALA	2.2
1	F	173	ILE	2.2
1	F	569	LEU	2.2
1	G	348	PHE	2.2
1	G	438	GLY	2.2
1	F	355	GLU	2.2
1	G	229	ALA	2.2
1	F	17	ILE	2.2
1	F	393	ILE	2.2
1	E	284	LEU	2.2
1	F	200	VAL	2.2
1	F	260	VAL	2.2
1	F	26	ASP	2.2
1	F	360	MET	2.2
1	F	383	CYS	2.2
1	F	425	GLU	2.2
1	D	112	THR	2.2
1	D	359	LEU	2.2
1	F	244	ILE	2.2
1	F	451	LEU	2.2
1	F	323	PHE	2.2
1	G	7	PRO	2.2
1	B	135	GLU	2.2
1	E	93	GLU	2.2
1	F	376	GLU	2.2
1	E	520	GLN	2.2
1	F	68	ALA	2.2
1	E	127	ARG	2.1
1	E	189	ARG	2.1
1	F	204	TYR	2.1
1	F	427	TYR	2.1
1	F	55	LEU	2.1
1	F	332	TRP	2.1
1	C	436	GLU	2.1
1	D	119	GLU	2.1
1	G	555	PRO	2.1
1	D	152	GLY	2.1
1	F	34	ALA	2.1
1	F	54	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	188	THR	2.1
1	G	54	ALA	2.1
1	E	295	ARG	2.1
1	F	125	ARG	2.1
1	F	168	TYR	2.1
1	F	524	TYR	2.1
1	F	517	GLU	2.1
1	F	537	VAL	2.1
1	G	556	VAL	2.1
1	E	406	MET	2.1
1	F	580	LYS	2.1
1	C	359	LEU	2.1
1	E	324	ILE	2.1
1	F	431	ILE	2.1
1	F	43	VAL	2.1
1	C	246	ALA	2.1
1	G	572	ALA	2.1
1	D	31	ILE	2.1
1	F	324	ILE	2.1
1	F	249	GLY	2.1
1	G	571	LYS	2.0
1	G	351	THR	2.0
1	D	406	MET	2.0
1	D	479	GLU	2.0
1	C	522	LEU	2.0
1	F	386	ILE	2.0
1	E	344	VAL	2.0
1	F	558	SER	2.0
1	C	34	ALA	2.0
1	C	63	ALA	2.0
1	F	316	HIS	2.0
1	G	316	HIS	2.0
1	E	518	ASP	2.0
1	F	24	LEU	2.0
1	F	105	ASN	2.0
1	F	559	ASP	2.0
1	F	444	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

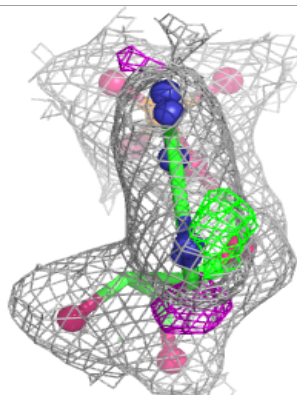
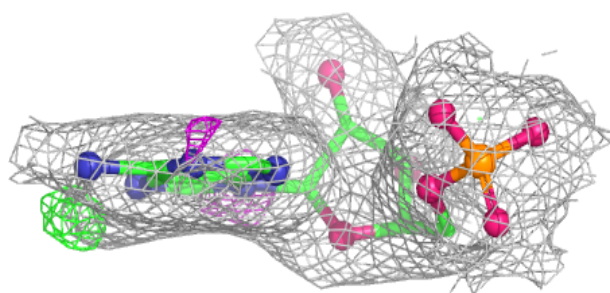
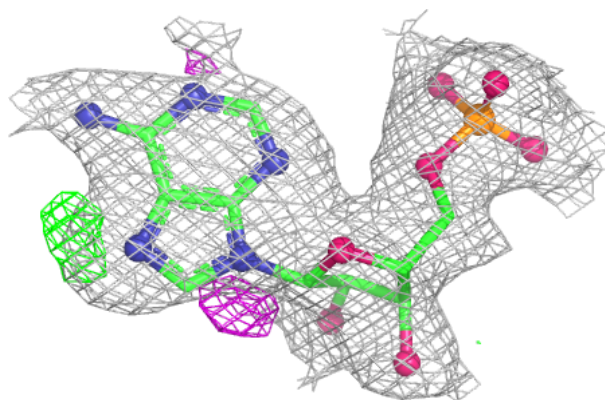
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	E	601	23/23	0.94	0.09	23,31,35,40	0
3	MG	E	602	1/1	0.94	0.05	27,27,27,27	0
3	MG	G	604	1/1	0.94	0.13	49,49,49,49	0
2	AMP	D	601	23/23	0.95	0.10	18,25,44,57	0
2	AMP	C	601	23/23	0.95	0.09	30,38,56,61	0
2	AMP	A	601	23/23	0.96	0.08	19,24,30,37	0
2	AMP	G	601	23/23	0.96	0.07	28,36,42,45	0
3	MG	H	604	1/1	0.96	0.04	29,29,29,29	0
3	MG	D	602	1/1	0.97	0.06	15,15,15,15	0
2	AMP	B	601	23/23	0.98	0.05	16,19,21,23	0
3	MG	D	603	1/1	0.98	0.07	28,28,28,28	0
3	MG	D	604	1/1	0.98	0.04	34,34,34,34	0
2	AMP	H	601	23/23	0.98	0.05	16,19,23,25	0
3	MG	C	603	1/1	0.98	0.03	26,26,26,26	0
3	MG	C	604	1/1	0.98	0.05	36,36,36,36	0
3	MG	A	602	1/1	0.99	0.03	14,14,14,14	0
3	MG	A	603	1/1	0.99	0.01	18,18,18,18	0
3	MG	E	604	1/1	0.99	0.03	39,39,39,39	0
3	MG	G	602	1/1	0.99	0.05	19,19,19,19	0
3	MG	G	603	1/1	0.99	0.03	34,34,34,34	0
3	MG	A	604	1/1	0.99	0.03	31,31,31,31	0
3	MG	H	602	1/1	0.99	0.02	15,15,15,15	0
3	MG	H	603	1/1	0.99	0.04	20,20,20,20	0
3	MG	C	602	1/1	0.99	0.05	17,17,17,17	0
3	MG	E	603	1/1	1.00	0.02	34,34,34,34	0
3	MG	B	603	1/1	1.00	0.03	17,17,17,17	0
3	MG	B	604	1/1	1.00	0.04	24,24,24,24	0
3	MG	B	602	1/1	1.00	0.06	7,7,7,7	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.

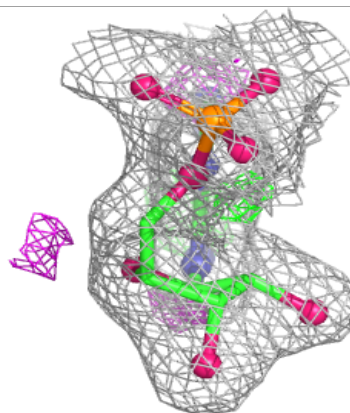
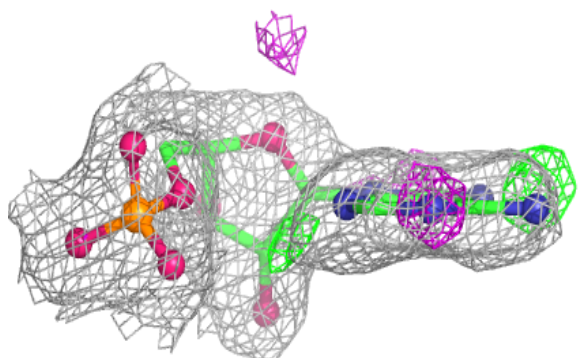
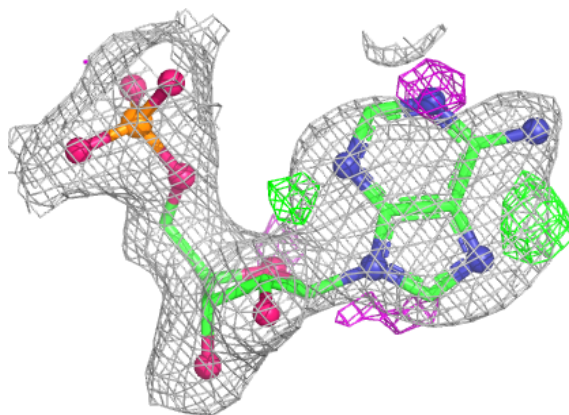
Electron density around AMP E 601:

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



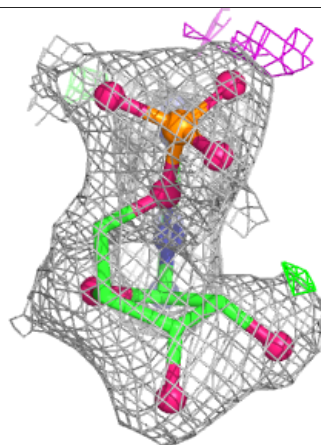
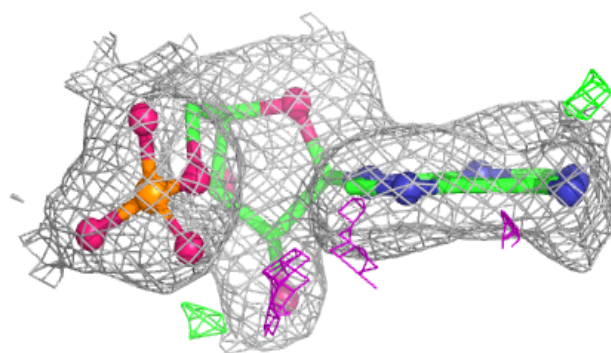
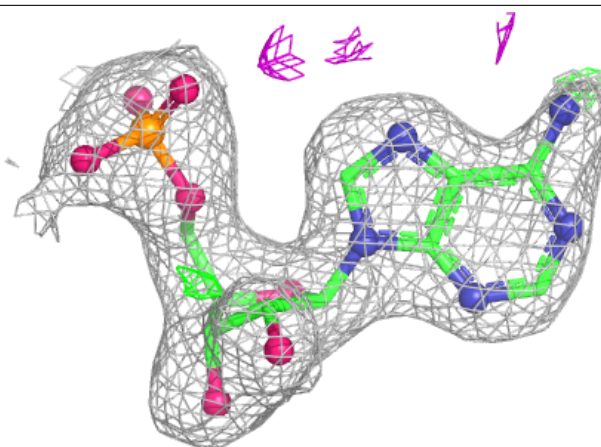
Electron density around AMP D 601:

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



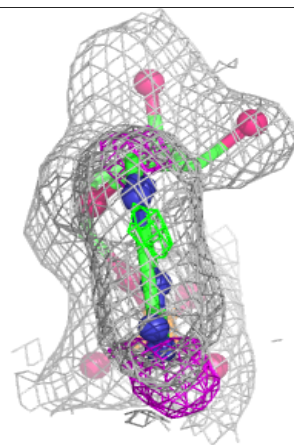
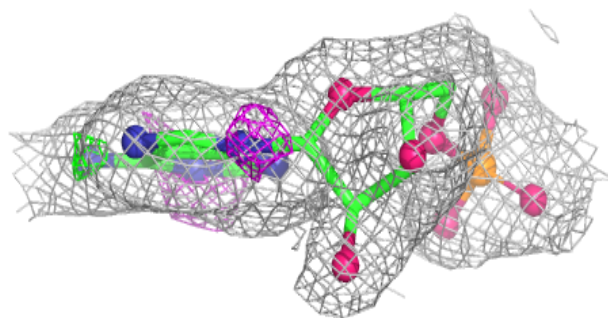
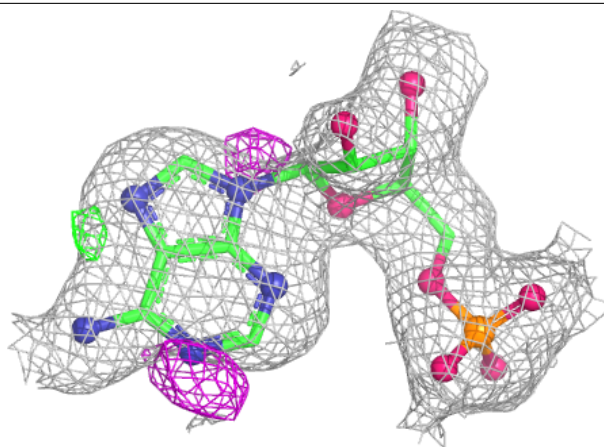
Electron density around AMP C 601:

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



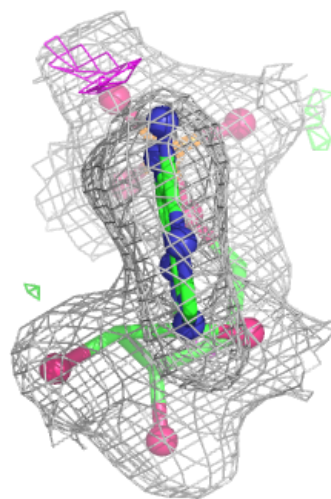
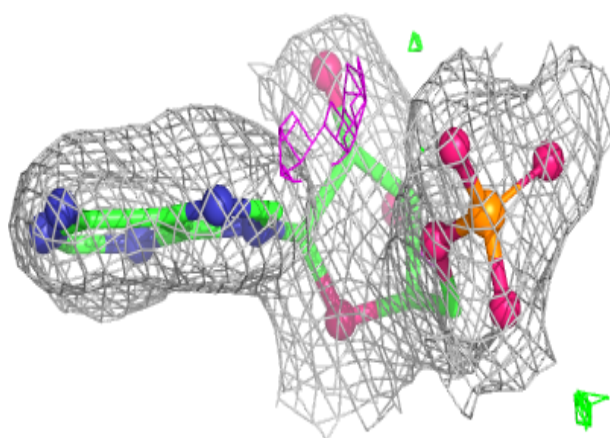
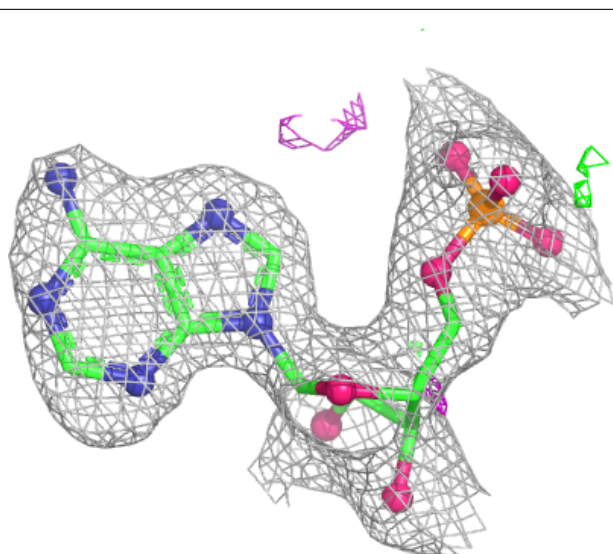
Electron density around AMP A 601:

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



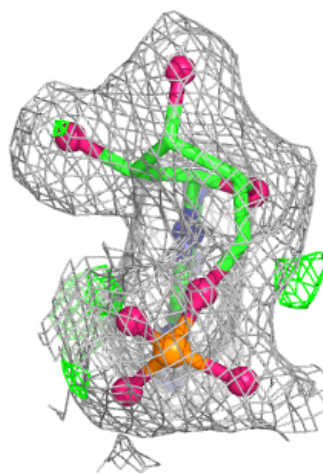
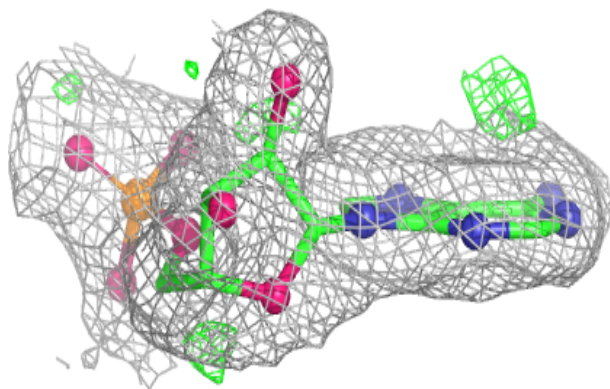
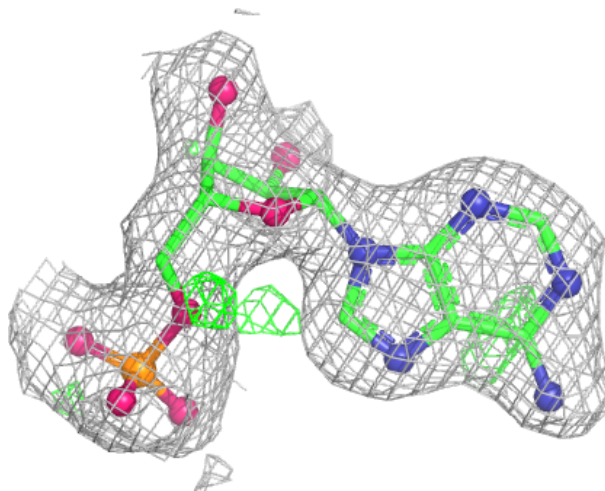
Electron density around AMP G 601:

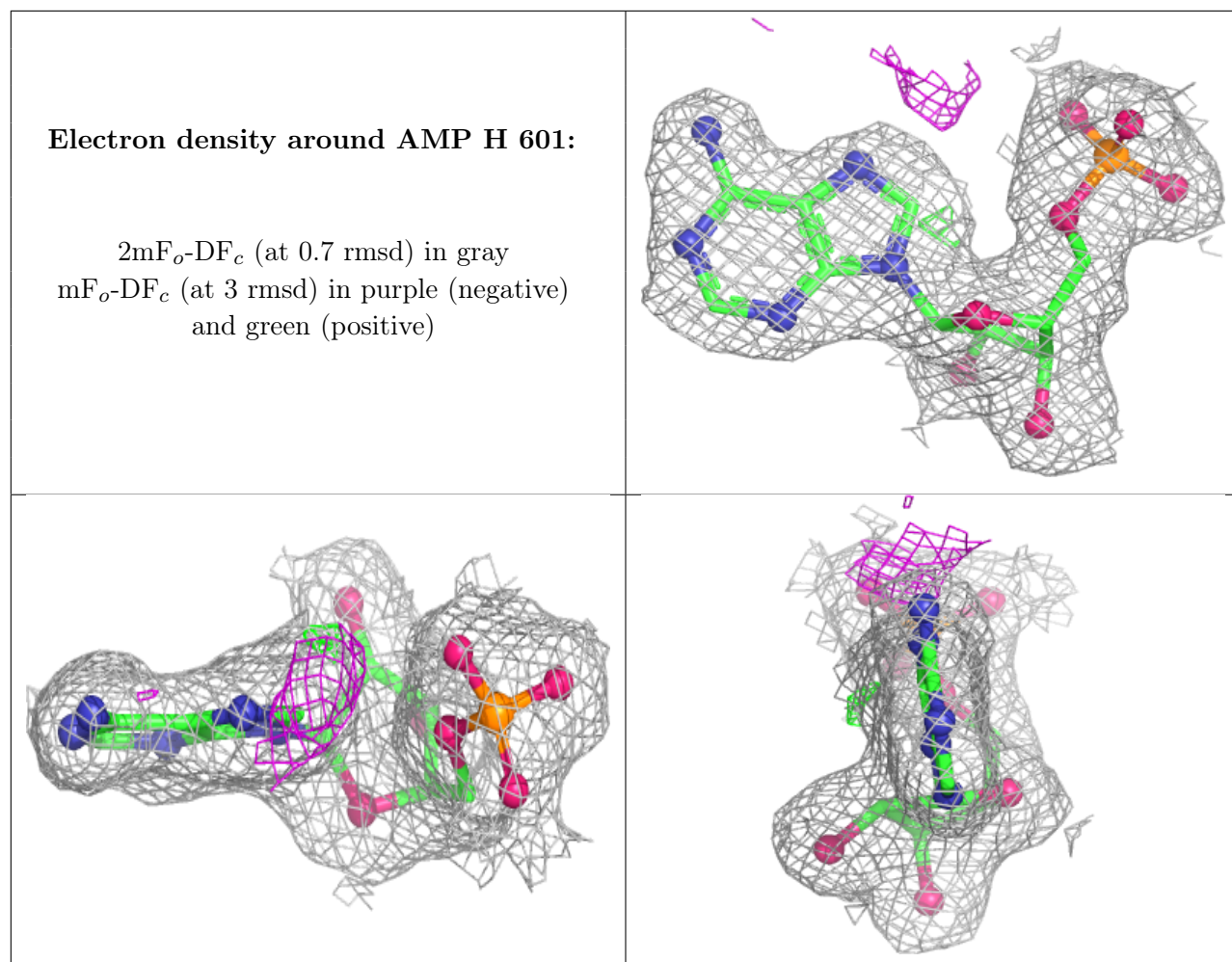
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP B 601:

$2mF_o-DF_c$ (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.