



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 PM UTC

PDB ID : 5KOD / pdb_00005kod
Title : Crystal Structure of GH3.5 Acyl Acid Amido Synthetase from Arabidopsis thaliana
Authors : Jez, J.M.; Westfall, C.S.; Zubieta, C.
Deposited on : 2016-06-30
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

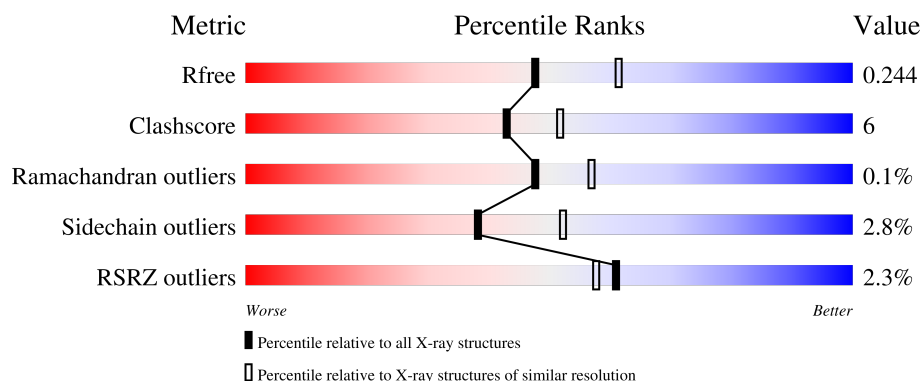
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	612	0% 81% 11% 6%
1	B	612	2% 81% 12% 6%
1	C	612	3% 75% 16% 8%
1	D	612	2% 80% 11% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IAC	A	702	-	X	-	-
3	IAC	B	702	-	X	-	-
3	IAC	C	702	-	X	-	-
3	IAC	D	702	-	X	-	-

2 Entry composition [i](#)

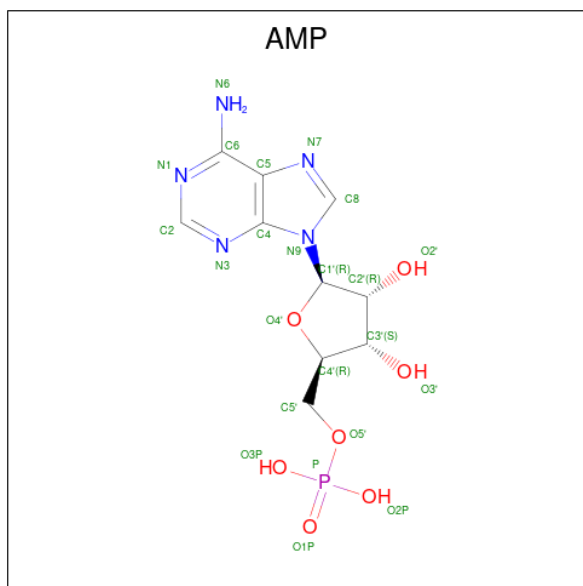
There are 5 unique types of molecules in this entry. The entry contains 19306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Indole-3-acetic acid-amido synthetase GH3.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	3	0
			4565	2920	750	870	25			
1	B	573	Total	C	N	O	S	0	0	0
			4570	2924	749	872	25			
1	C	566	Total	C	N	O	S	0	2	0
			4507	2882	740	860	25			
1	D	566	Total	C	N	O	S	0	1	0
			4509	2888	739	856	26			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



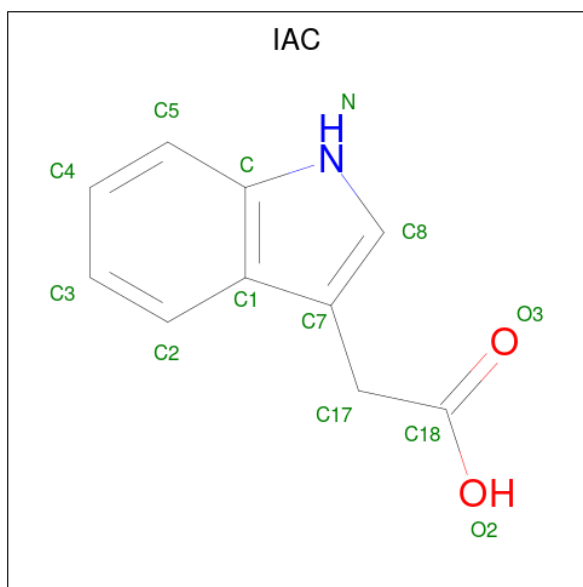
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is 1H-INDOL-3-YLACETIC ACID (CCD ID: IAC) (formula: $C_{10}H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	10	1	2		
3	B	1	Total	C	N	O	0	0
			13	10	1	2		
3	C	1	Total	C	N	O	0	0
			13	10	1	2		
3	D	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

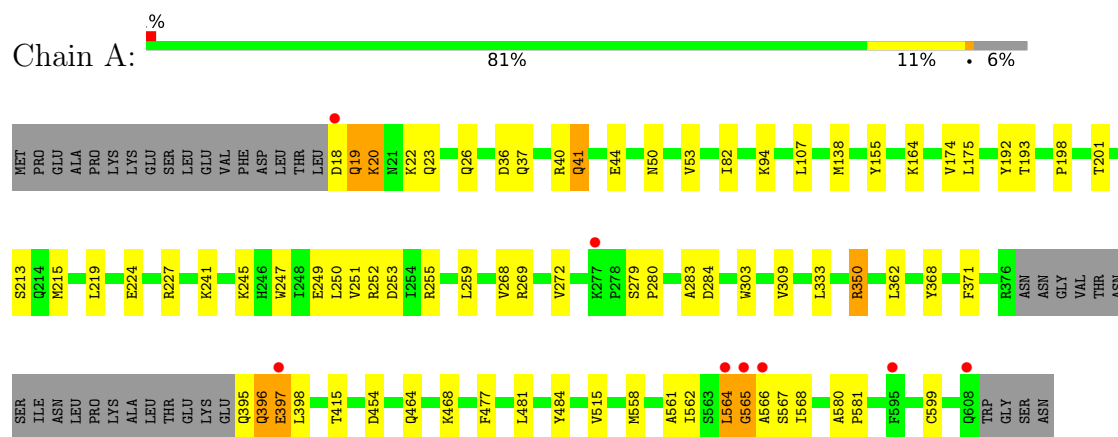
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	260	Total	O	0	0
			260	260		
5	C	215	Total	O	0	0
			215	215		
5	D	244	Total	O	0	0
			244	244		

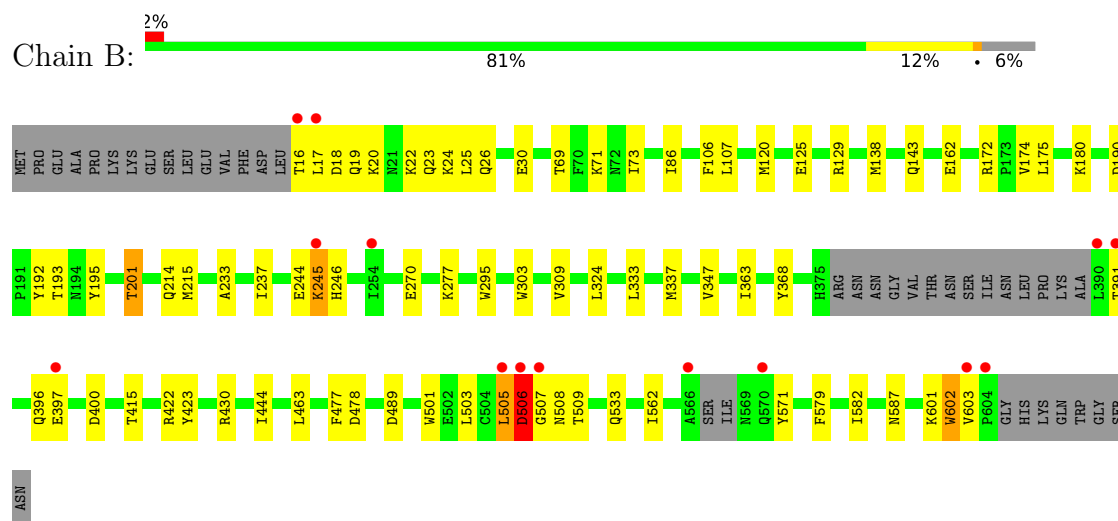
3 Residue-property plots

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.

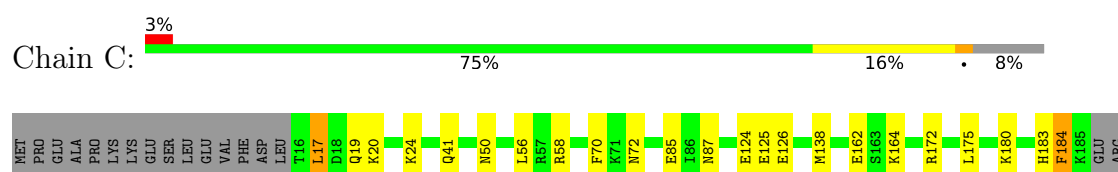
- Molecule 1: Indole-3-acetic acid-amido synthetase GH3.5

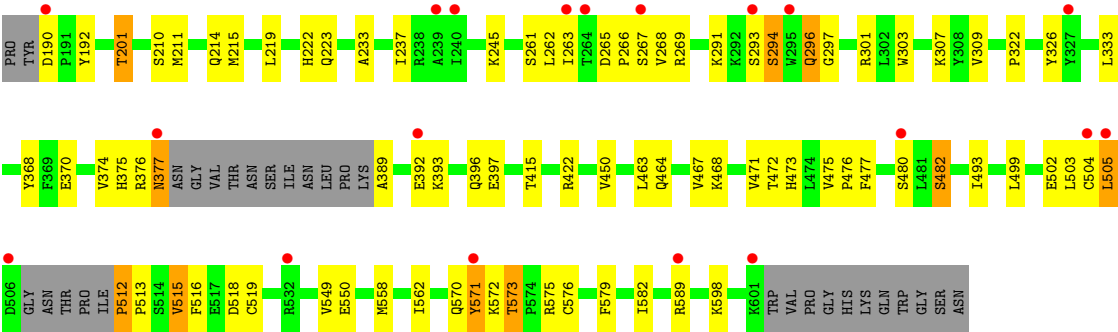


- Molecule 1: Indole-3-acetic acid-amido synthetase GH3.5

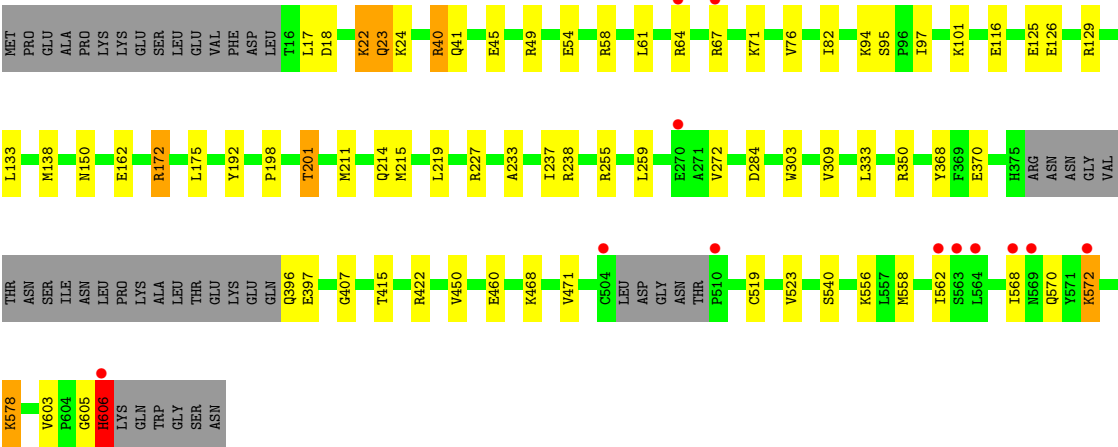
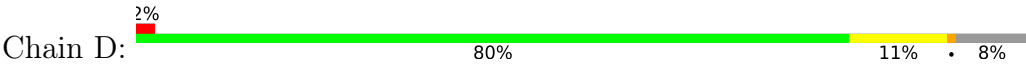


- Molecule 1: Indole-3-acetic acid-amido synthetase GH3.5





● Molecule 1: Indole-3-acetic acid-amido synthetase GH3.5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.61Å 143.52Å 102.32Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	42.16 – 2.20 42.16 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.5 (42.16-2.20) 89.5 (42.16-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.245 0.207 , 0.244	Depositor DCC
R_{free} test set	5422 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19306	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: IAC, SO4, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	5/4679 (0.1%)	0.85	5/6352 (0.1%)
1	B	0.71	8/4673 (0.2%)	0.90	8/6342 (0.1%)
1	C	0.77	16/4609 (0.3%)	1.00	18/6250 (0.3%)
1	D	0.61	3/4616 (0.1%)	0.85	4/6266 (0.1%)
All	All	0.68	32/18577 (0.2%)	0.91	35/25210 (0.1%)

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	C	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	571	TYR	C-N	11.04	1.48	1.33
1	C	571	TYR	CA-C	-7.66	1.42	1.52
1	C	183	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	501	TRP	NE1-CE2	-6.53	1.30	1.37
1	C	482	SER	C-O	-6.50	1.16	1.23
1	C	296	GLN	C-O	-6.38	1.16	1.24
1	A	398	LEU	C-O	-6.34	1.16	1.23
1	A	22	LYS	C-O	-6.24	1.16	1.24
1	C	293	SER	C-O	-6.18	1.16	1.24
1	B	562	ILE	C-O	-6.17	1.17	1.24
1	B	602	TRP	C-N	-6.01	1.26	1.33
1	C	17	LEU	C-O	-5.92	1.17	1.24
1	D	24	LYS	C-O	-5.86	1.17	1.24
1	D	22	LYS	C-O	-5.83	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	LYS	N-CA	-5.71	1.39	1.46
1	C	471	VAL	C-O	-5.69	1.17	1.24
1	C	573	THR	C-N	5.68	1.41	1.33
1	C	473	HIS	CG-ND1	-5.67	1.32	1.38
1	D	606	HIS	CG-ND1	-5.54	1.32	1.38
1	B	509	THR	C-N	5.46	1.40	1.33
1	C	513	PRO	N-CD	5.31	1.55	1.47
1	C	374	VAL	C-O	-5.29	1.18	1.24
1	C	476	PRO	N-CD	5.25	1.55	1.47
1	B	24	LYS	C-O	-5.24	1.18	1.24
1	A	396	GLN	CA-C	-5.23	1.46	1.52
1	C	19	GLN	C-N	-5.13	1.27	1.33
1	A	397	GLU	N-CA	-5.11	1.40	1.46
1	C	183	HIS	CG-ND1	-5.09	1.32	1.38
1	B	19	GLN	C-O	-5.08	1.18	1.24
1	B	25	LEU	C-O	-5.05	1.18	1.24
1	C	375	HIS	CD2-NE2	-5.04	1.32	1.37
1	C	19	GLN	C-O	-5.00	1.18	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	PHE	O-C-N	-17.22	96.49	122.67
1	C	184	PHE	CA-C-N	14.76	148.26	121.70
1	C	184	PHE	C-N-CA	14.76	148.26	121.70
1	B	601	LYS	CA-C-N	8.70	136.42	121.64
1	B	601	LYS	C-N-CA	8.70	136.42	121.64
1	D	605	GLY	N-CA-C	8.65	127.32	115.30
1	C	505	LEU	N-CA-C	8.57	120.70	111.36
1	C	296	GLN	N-CA-C	7.94	119.62	110.97
1	C	573	THR	CA-C-N	-7.68	112.09	119.85
1	C	573	THR	C-N-CA	-7.68	112.09	119.85
1	A	397	GLU	N-CA-C	7.20	119.20	111.36
1	B	601	LYS	O-C-N	-7.12	114.45	122.86
1	A	41	GLN	N-CA-C	-6.86	103.26	111.69
1	A	396	GLN	N-CA-C	-6.62	97.75	108.41
1	C	515	VAL	N-CA-C	6.52	117.31	110.72
1	B	509	THR	CA-C-N	-6.52	113.58	120.03
1	B	509	THR	C-N-CA	-6.52	113.58	120.03
1	A	371	PHE	CA-C-N	6.42	130.22	121.74
1	A	371	PHE	C-N-CA	6.42	130.22	121.74
1	C	268	VAL	N-CA-C	-5.79	105.08	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	GLN	N-CA-CB	-5.77	101.65	110.01
1	D	172	ARG	N-CA-C	5.64	113.29	108.22
1	C	512	PRO	CA-C-N	-5.62	112.81	119.05
1	C	512	PRO	C-N-CA	-5.62	112.81	119.05
1	D	572	LYS	CB-CG-CD	-5.60	98.41	111.30
1	C	172	ARG	N-CA-C	5.60	113.26	108.22
1	C	518	ASP	N-CA-C	-5.56	105.22	111.28
1	C	573	THR	N-CA-C	-5.51	102.83	109.83
1	C	475	VAL	O-C-N	5.48	123.96	120.07
1	C	293	SER	N-CA-C	5.34	117.10	111.28
1	B	571	TYR	O-C-N	-5.25	116.47	122.93
1	B	337	MET	N-CA-C	5.22	116.74	108.96
1	B	23	GLN	N-CA-C	5.03	116.45	111.07
1	C	475	VAL	CA-C-N	-5.00	113.49	119.05
1	C	475	VAL	C-N-CA	-5.00	113.49	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	PHE	Mainchain

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	4565	0	4547	60	0
1	B	4570	0	4563	40	0
1	C	4507	0	4510	72	3
1	D	4509	0	4495	54	3
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	13	0	8	2	0
3	B	13	0	8	3	0
3	C	13	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	13	0	8	2	0
4	B	10	0	0	0	0
5	A	282	0	0	9	1
5	B	260	0	0	5	0
5	C	215	0	0	5	1
5	D	244	0	0	6	0
All	All	19306	0	18195	226	4

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 (226) 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:C:480:SER:OG	1:C:504:CYS:CA	1.65	1.43
1:C:480:SER:OG	1:C:504:CYS:C	1.70	1.34
1:C:480:SER:OG	1:C:504:CYS:CB	1.77	1.31
1:A:19:GLN:HB2	5:A:1029:HOH:O	1.14	1.23
1:C:480:SER:OG	1:C:504:CYS:O	1.57	1.18
1:A:19:GLN:CG	5:A:1029:HOH:O	1.66	1.15
1:C:480:SER:OG	1:C:504:CYS:HB2	1.35	1.09
1:A:18:ASP:O	1:A:19:GLN:NE2	1.87	1.07
1:C:480:SER:CB	1:C:504:CYS:HB2	1.86	1.05
1:A:561:ALA:O	1:A:564:LEU:O	1.80	0.99
1:D:578:LYS:NZ	5:D:801:HOH:O	1.98	0.97
1:A:562:ILE:HG23	1:A:566:ALA:HB1	1.50	0.93
1:A:19:GLN:HG2	1:A:20:LYS:H	1.36	0.90
1:B:489:ASP:OD2	5:B:802:HOH:O	1.93	0.86
1:A:562:ILE:O	1:A:566:ALA:HB2	1.77	0.83
1:C:480:SER:N	1:C:504:CYS:O	2.14	0.80
1:C:480:SER:OG	1:C:504:CYS:N	2.16	0.78
1:A:562:ILE:HG23	1:A:566:ALA:CB	2.13	0.78
1:D:407:GLY:O	5:D:802:HOH:O	2.01	0.78
3:B:702:IAC:N	5:B:801:HOH:O	1.81	0.77
1:B:175:LEU:HG	3:B:702:IAC:H171	1.68	0.76
1:B:18:ASP:OD2	1:B:22:LYS:HE3	1.85	0.76
1:D:192:TYR:O	1:D:227:ARG:NH2	2.20	0.74
1:D:350:ARG:NH2	5:D:804:HOH:O	2.21	0.74
1:A:36:ASP:OD2	1:A:40:ARG:NH1	2.19	0.74
1:D:76:VAL:HG23	1:D:396:GLN:HB3	1.71	0.73
1:A:19:GLN:HG3	5:A:1029:HOH:O	1.51	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:GLU:HB2	5:C:883:HOH:O	1.89	0.72
1:B:162:GLU:OE1	1:B:180:LYS:NZ	2.22	0.71
1:C:263:ILE:HD11	1:C:269:ARG:HG2	1.71	0.71
1:C:570:GLN:N	1:C:570:GLN:OE1	2.25	0.70
1:D:175:LEU:HG	3:D:702:IAC:H171	1.74	0.69
1:C:482:SER:HB2	1:C:504:CYS:SG	2.33	0.69
1:C:17:LEU:HD11	1:C:192:TYR:CE2	2.29	0.68
1:C:296:GLN:OE1	1:C:297:GLY:N	2.28	0.67
1:A:198:PRO:O	1:A:201:THR:HG22	1.93	0.67
1:B:270:GLU:CD	1:D:23:GLN:HE21	2.02	0.67
1:C:322:PRO:HD2	5:C:830:HOH:O	1.94	0.66
1:C:20:LYS:HZ1	1:C:24:LYS:HG2	1.61	0.66
1:B:125:GLU:OE1	1:B:129:ARG:NH2	2.30	0.65
1:A:561:ALA:O	1:A:565:GLY:O	2.14	0.65
1:A:155:TYR:OH	1:A:227:ARG:NH1	2.29	0.65
1:D:54:GLU:OE2	1:D:58:ARG:NH2	2.30	0.65
1:C:558:MET:O	1:C:562:ILE:HG12	1.97	0.64
1:C:480:SER:CB	1:C:504:CYS:O	2.46	0.64
1:C:480:SER:O	1:C:503:LEU:HB3	1.98	0.64
1:A:193:THR:O	5:A:801:HOH:O	2.15	0.64
1:A:18:ASP:CG	1:A:19:GLN:H	2.06	0.63
1:A:19:GLN:CG	1:A:20:LYS:H	2.03	0.63
1:A:259:LEU:HD23	1:A:269:ARG:HB2	1.81	0.63
3:B:702:IAC:C8	5:B:801:HOH:O	2.37	0.62
1:A:19:GLN:CB	5:A:1029:HOH:O	1.64	0.62
1:A:175:LEU:HG	3:A:702:IAC:H171	1.80	0.62
1:C:138:MET:HG3	1:C:192:TYR:HB3	1.81	0.62
1:A:454:ASP:OD1	5:A:802:HOH:O	2.16	0.62
1:D:558:MET:O	1:D:562:ILE:HG12	2.00	0.60
1:C:263:ILE:HD11	1:C:269:ARG:HH11	1.66	0.60
1:A:252:ARG:NH1	1:A:253:ASP:OD1	2.35	0.60
1:C:175:LEU:HG	3:C:702:IAC:H171	1.84	0.60
1:C:201:THR:CG2	1:C:214:GLN:HG2	2.31	0.60
1:C:296:GLN:O	1:C:326:TYR:O	2.20	0.59
1:A:215:MET:HE1	1:A:303:TRP:CZ2	2.37	0.59
1:D:40:ARG:HG2	1:D:67:ARG:HH21	1.66	0.59
1:C:480:SER:O	1:C:503:LEU:CA	2.51	0.59
1:A:464:GLN:NE2	1:A:484:TYR:OH	2.35	0.58
1:D:162:GLU:HG3	1:D:172:ARG:HB3	1.85	0.58
1:A:255:ARG:NH2	1:A:284:ASP:OD1	2.36	0.58
1:B:245:LYS:HG3	1:B:246:HIS:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASN:ND2	5:D:803:HOH:O	2.19	0.58
1:C:392:GLU:O	1:C:396:GLN:HG3	2.04	0.57
1:D:396:GLN:O	1:D:422:ARG:NH2	2.37	0.57
1:D:40:ARG:HG3	1:D:40:ARG:HH11	1.70	0.57
1:A:268:VAL:O	1:A:269:ARG:HG2	2.05	0.57
1:B:396:GLN:O	1:B:422:ARG:NH2	2.38	0.57
1:D:255:ARG:NH2	1:D:284:ASP:OD1	2.38	0.56
1:A:224:GLU:OE2	5:A:803:HOH:O	2.18	0.56
1:A:350:ARG:HH11	1:A:350:ARG:HG2	1.69	0.56
1:D:61:LEU:O	1:D:64:ARG:HG3	2.06	0.56
1:C:480:SER:O	1:C:503:LEU:HA	2.06	0.56
1:B:26:GLN:O	1:B:30:GLU:HG3	2.05	0.56
1:C:512:PRO:HG2	1:C:515:VAL:HG23	1.87	0.56
1:C:477:PHE:N	1:C:477:PHE:CD1	2.73	0.56
1:C:20:LYS:NZ	1:C:24:LYS:HE2	2.21	0.56
1:B:270:GLU:CD	1:D:23:GLN:NE2	2.64	0.56
1:D:138:MET:HG3	1:D:192:TYR:HB3	1.87	0.56
1:C:20:LYS:NZ	1:C:24:LYS:HG2	2.20	0.55
1:D:450:VAL:HG21	1:D:460:GLU:HG3	1.89	0.55
1:B:120:MET:HE1	1:B:423:TYR:OH	2.07	0.55
1:A:395:GLN:O	1:A:395:GLN:HG3	2.06	0.54
1:A:37:GLN:O	1:A:41:GLN:HG3	2.08	0.54
1:B:245:LYS:HG3	1:B:246:HIS:NE2	2.22	0.54
1:C:464:GLN:HE21	1:C:575:ARG:HE	1.54	0.54
1:D:40:ARG:HG3	1:D:40:ARG:NH1	2.22	0.54
1:D:238:ARG:HD3	1:D:540:SER:HA	1.90	0.54
1:A:201:THR:OG1	1:A:213:SER:OG	2.17	0.54
1:C:516:PHE:O	1:C:519:CYS:HB2	2.07	0.53
1:C:370:GLU:OE1	1:C:422:ARG:HD2	2.09	0.53
1:B:190:ASP:HB3	1:B:193:THR:HG22	1.90	0.53
1:D:201:THR:HG23	1:D:214:GLN:HG2	1.91	0.53
1:C:389:ALA:N	5:C:809:HOH:O	2.41	0.53
1:D:116:GLU:HG3	1:D:606:HIS:HD2	1.73	0.53
1:A:18:ASP:C	1:A:19:GLN:HE21	2.16	0.52
1:A:19:GLN:CG	1:A:20:LYS:N	2.73	0.52
1:C:502:GLU:HG3	1:C:549:VAL:HG23	1.92	0.52
1:D:126:GLU:OE2	1:D:129:ARG:NH1	2.41	0.52
1:B:587:ASN:O	5:B:803:HOH:O	2.19	0.52
1:D:116:GLU:CD	1:D:606:HIS:CD2	2.88	0.52
1:A:215:MET:HE2	1:A:219:LEU:HG	1.93	0.51
1:C:162:GLU:OE2	1:C:180:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:SER:O	1:C:503:LEU:CB	2.58	0.51
1:A:241:LYS:HE3	1:A:245:LYS:HE3	1.93	0.51
1:B:233:ALA:O	1:B:237:ILE:HG12	2.10	0.51
1:D:18:ASP:O	1:D:22:LYS:HG2	2.11	0.50
1:C:368:TYR:HB3	1:C:415:THR:HB	1.93	0.50
1:C:58:ARG:NH1	1:C:85:GLU:OE2	2.45	0.50
1:A:245:LYS:HD2	5:A:1030:HOH:O	2.13	0.49
1:B:138:MET:HG3	1:B:192:TYR:HB3	1.94	0.49
1:C:233:ALA:O	1:C:237:ILE:HG12	2.11	0.49
3:C:702:IAC:H8	5:C:817:HOH:O	2.12	0.49
1:C:20:LYS:HZ3	1:C:24:LYS:HE2	1.77	0.49
1:D:45:GLU:HG2	1:D:49:ARG:HE	1.77	0.49
1:D:211:MET:HE3	1:D:211:MET:O	2.12	0.49
1:D:519:CYS:O	1:D:523:VAL:HG23	2.13	0.49
1:C:377:ASN:C	1:C:377:ASN:ND2	2.71	0.48
1:D:259:LEU:HD13	1:D:272:VAL:HG11	1.94	0.48
1:A:558:MET:O	1:A:562:ILE:HD12	2.14	0.48
1:B:162:GLU:HG3	1:B:172:ARG:HB3	1.95	0.48
1:B:215:MET:HE1	1:B:303:TRP:CZ2	2.48	0.48
1:C:570:GLN:N	1:C:570:GLN:CD	2.72	0.47
1:D:309:VAL:HB	1:D:333:LEU:HD23	1.96	0.47
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.80	0.47
1:B:478:ASP:O	1:B:506:ASP:HA	2.14	0.47
1:C:20:LYS:HZ1	1:C:24:LYS:CG	2.27	0.47
1:C:215:MET:HE2	1:C:219:LEU:HG	1.95	0.47
1:A:18:ASP:CG	1:A:19:GLN:N	2.72	0.47
1:A:269:ARG:HA	1:A:272:VAL:HB	1.96	0.47
1:B:507:GLY:O	1:B:508:ASN:HB2	2.14	0.47
1:B:533:GLN:HB2	1:B:602:TRP:NE1	2.30	0.47
1:B:201:THR:CG2	1:B:214:GLN:HG2	2.45	0.47
1:D:215[A]:MET:HE1	1:D:303:TRP:CZ2	2.50	0.47
1:B:215:MET:HE1	1:B:303:TRP:CH2	2.50	0.47
1:C:70:PHE:CE2	1:C:422:ARG:HD3	2.50	0.46
1:A:107:LEU:HD22	1:A:174:VAL:HA	1.97	0.46
1:A:309:VAL:HB	1:A:333:LEU:HD23	1.98	0.46
1:D:201:THR:CG2	1:D:214:GLN:HG2	2.46	0.46
1:B:309:VAL:HB	1:B:333:LEU:HD23	1.96	0.46
1:C:211:MET:HE3	1:C:211:MET:O	2.16	0.46
1:C:464:GLN:HE21	1:C:575:ARG:NE	2.14	0.46
1:D:233:ALA:O	1:D:237:ILE:HG12	2.16	0.46
1:A:138:MET:HG3	1:A:192:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HD23	1:A:269:ARG:CB	2.44	0.46
1:C:294:SER:HB2	1:C:296:GLN:H	1.81	0.46
1:C:265:ASP:HA	1:C:266:PRO:HD3	1.83	0.46
1:A:175:LEU:HG	3:A:702:IAC:H2	1.98	0.45
1:A:558:MET:O	1:A:562:ILE:CD1	2.64	0.45
1:A:215:MET:HE3	1:A:215:MET:O	2.16	0.45
1:B:347:VAL:HG22	1:B:363:ILE:HD11	1.96	0.45
1:B:477:PHE:O	1:B:506:ASP:HB2	2.16	0.45
1:D:370:GLU:OE2	1:D:422:ARG:NH1	2.49	0.45
1:D:606:HIS:HB3	5:D:1012:HOH:O	2.17	0.45
1:C:480:SER:O	1:C:504:CYS:N	2.50	0.45
1:D:76:VAL:CG2	1:D:396:GLN:HB3	2.45	0.45
1:D:468:LYS:HD2	1:D:468:LYS:HA	1.73	0.45
1:B:579:PHE:HB3	1:B:582:ILE:HD12	1.97	0.45
1:C:480:SER:CB	1:C:504:CYS:CB	2.68	0.45
1:C:512:PRO:HG2	1:C:515:VAL:CG2	2.47	0.45
1:B:195:TYR:HB3	5:B:953:HOH:O	2.17	0.45
1:D:368:TYR:HB3	1:D:415:THR:HB	1.99	0.45
1:D:95:SER:O	1:D:97:ILE:HG13	2.17	0.45
1:D:101:LYS:NZ	1:D:125:GLU:OE2	2.50	0.45
1:A:215:MET:HE1	1:A:303:TRP:HZ2	1.80	0.44
1:B:190:ASP:HB3	1:B:193:THR:CG2	2.47	0.44
1:C:210:SER:O	1:C:214:GLN:HG3	2.17	0.44
1:C:579:PHE:HB3	1:C:582:ILE:HD12	1.99	0.44
1:B:143:GLN:O	1:C:307:LYS:NZ	2.47	0.44
1:C:309:VAL:HB	1:C:333:LEU:HD23	2.00	0.44
1:D:94:LYS:HE3	1:D:94:LYS:HB2	1.86	0.44
1:D:468:LYS:O	1:D:471:VAL:HG22	2.18	0.44
1:A:477:PHE:CE2	1:A:515:VAL:HG21	2.52	0.43
1:D:198:PRO:O	1:D:201:THR:HG22	2.18	0.43
1:C:237:ILE:CG2	1:C:493:ILE:HD13	2.47	0.43
1:A:368:TYR:HB3	1:A:415:THR:HB	2.00	0.43
1:B:368:TYR:HB3	1:B:415:THR:HB	2.00	0.43
1:C:50:ASN:O	1:C:56:LEU:HD22	2.17	0.43
1:C:222:HIS:CE1	1:C:223:GLN:HG3	2.53	0.43
1:D:578:LYS:HD2	1:D:578:LYS:HA	1.69	0.43
1:B:244:GLU:HA	1:B:295:TRP:CH2	2.53	0.43
1:C:215:MET:HE1	1:C:303:TRP:CH2	2.54	0.43
1:C:393:LYS:NZ	1:C:397:GLU:OE2	2.44	0.43
1:D:41:GLN:O	1:D:45:GLU:HB2	2.18	0.43
1:D:397:GLU:OE1	1:D:397:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:HG3	5:A:807:HOH:O	2.17	0.42
1:A:50:ASN:O	1:A:53:VAL:HG22	2.20	0.42
1:B:107:LEU:HD22	1:B:174:VAL:HA	2.00	0.42
1:D:215[A]:MET:HE2	1:D:219:LEU:HG	2.01	0.42
1:C:237:ILE:HG22	1:C:493:ILE:HD13	2.01	0.42
1:C:190:ASP:OD2	1:C:192:TYR:HB2	2.20	0.42
1:D:556:LYS:HE2	1:D:556:LYS:HB3	1.84	0.42
1:A:193:THR:O	1:A:193:THR:HG22	2.20	0.42
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.82	0.42
1:A:247:TRP:HA	1:A:250:LEU:HD12	2.01	0.42
1:B:233:ALA:HB1	1:B:324:LEU:HD11	2.02	0.42
1:C:450:VAL:HG13	1:C:576:CYS:HB2	2.02	0.42
1:C:550:GLU:HB2	1:C:589:ARG:HG3	2.01	0.42
1:D:162:GLU:HG2	5:D:822:HOH:O	2.19	0.42
1:D:201:THR:HG23	1:D:214:GLN:CG	2.49	0.42
1:B:71:LYS:HE3	1:B:400:ASP:OD2	2.19	0.41
1:D:71:LYS:HB3	1:D:397:GLU:OE2	2.21	0.41
1:A:215:MET:HE1	1:A:303:TRP:CH2	2.55	0.41
1:B:16:THR:O	1:B:17:LEU:HB3	2.20	0.41
1:D:116:GLU:HG3	1:D:606:HIS:CD2	2.54	0.41
1:B:190:ASP:O	1:B:193:THR:HG22	2.20	0.41
1:C:512:PRO:HD2	1:C:515:VAL:HG21	2.01	0.41
1:D:175:LEU:CG	3:D:702:IAC:H171	2.45	0.41
1:B:69:THR:HG23	1:B:73:ILE:HD12	2.03	0.41
1:A:397:GLU:OE2	1:A:397:GLU:HA	2.21	0.41
1:B:86:ILE:HG23	1:B:106:PHE:CE1	2.56	0.41
1:B:430:ARG:HB2	1:B:444:ILE:HD11	2.03	0.41
1:A:580:ALA:HB3	1:A:581:PRO:HD3	2.04	0.40
1:C:215:MET:HE1	1:C:303:TRP:CZ2	2.56	0.40
1:A:251:VAL:HG13	1:A:283:ALA:HB1	2.02	0.40
1:A:481:LEU:HD21	1:A:484:TYR:HB3	2.03	0.40
1:A:350:ARG:HG2	1:A:350:ARG:NH1	2.36	0.40
1:A:279:SER:HA	1:A:280:PRO:HD2	1.94	0.40
1:C:126:GLU:OE1	5:C:801:HOH:O	2.22	0.40
1:C:463:LEU:O	1:C:467:VAL:HG23	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ASN:CB	1:D:572:LYS:CE[1_556]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ASN:CB	1:D:572:LYS:CD[1_556]	2.10	0.10
1:C:377:ASN:CB	1:D:572:LYS:NZ[1_556]	2.11	0.09
5:A:901:HOH:O	5:C:861:HOH:O[1_655]	2.16	0.04

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	572/612 (94%)	561 (98%)	10 (2%)	1 (0%)	43	51
1	B	567/612 (93%)	554 (98%)	11 (2%)	2 (0%)	30	34
1	C	560/612 (92%)	547 (98%)	13 (2%)	0	100	100
1	D	561/612 (92%)	551 (98%)	10 (2%)	0	100	100
All	All	2260/2448 (92%)	2213 (98%)	44 (2%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	505	LEU
1	A	565	GLY
1	B	506	ASP

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	522/557 (94%)	507 (97%)	15 (3%)	37	51
1	B	523/557 (94%)	512 (98%)	11 (2%)	47	63
1	C	516/557 (93%)	494 (96%)	22 (4%)	26	35
1	D	515/557 (92%)	505 (98%)	10 (2%)	50	66
All	All	2076/2228 (93%)	2018 (97%)	58 (3%)	38	52

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	23	GLN
1	A	26	GLN
1	A	44	GLU
1	A	82	ILE
1	A	94	LYS
1	A	164	LYS
1	A	350	ARG
1	A	362	LEU
1	A	396	GLN
1	A	468	LYS
1	A	564	LEU
1	A	567	SER
1	A	568	ILE
1	A	599	CYS
1	B	20	LYS
1	B	201	THR
1	B	245	LYS
1	B	277	LYS
1	B	391	THR
1	B	397	GLU
1	B	463	LEU
1	B	503	LEU
1	B	505	LEU
1	B	506	ASP
1	B	603	VAL
1	C	41	GLN
1	C	72	ASN
1	C	87	ASN
1	C	124	GLU
1	C	164	LYS
1	C	201	THR
1	C	245	LYS

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Mol	Chain	Res	Type
1	C	261	SER
1	C	267	SER
1	C	291	LYS
1	C	294	SER
1	C	301	ARG
1	C	376	ARG
1	C	377	ASN
1	C	468	LYS
1	C	472	THR
1	C	499	LEU
1	C	505	LEU
1	C	571	TYR
1	C	572	LYS
1	C	573	THR
1	C	598	LYS
1	D	17	LEU
1	D	40	ARG
1	D	82	ILE
1	D	133	LEU
1	D	201	THR
1	D	568	ILE
1	D	570	GLN
1	D	578	LYS
1	D	603	VAL
1	D	606	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	26	GLN
1	A	41	GLN
1	A	72	ASN
1	A	194	ASN
1	A	246	HIS
1	A	440	GLN
1	A	464	GLN
1	A	473	HIS
1	B	23	GLN
1	B	34	ASN
1	B	37	GLN
1	B	143	GLN

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Mol	Chain	Res	Type
1	C	72	ASN
1	C	87	ASN
1	C	143	GLN
1	C	246	HIS
1	C	377	ASN
1	C	464	GLN
1	D	21	ASN
1	D	23	GLN
1	D	150	ASN
1	D	296	GLN
1	D	319	GLN
1	D	606	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](#)

10 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	$\# Z > 2$
3	IAC	B	702	-	14,14,14	3.64	8 (57%)	19,19,19	4.08	12 (63%)
4	SO4	B	703	-	4,4,4	0.21	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AMP	A	701	-	25,25,25	1.41	4 (16%)	37,38,38	1.65	8 (21%)
3	IAC	C	702	-	14,14,14	3.55	7 (50%)	19,19,19	3.62	12 (63%)
3	IAC	A	702	-	14,14,14	3.55	8 (57%)	19,19,19	3.92	11 (57%)
2	AMP	C	701	-	25,25,25	1.35	3 (12%)	37,38,38	1.94	9 (24%)
2	AMP	D	701	-	25,25,25	1.31	4 (16%)	37,38,38	1.98	11 (29%)
4	SO4	B	704	-	4,4,4	0.24	0	6,6,6	0.20	0
3	IAC	D	702	-	14,14,14	3.62	7 (50%)	19,19,19	3.98	12 (63%)
2	AMP	B	701	-	25,25,25	1.40	2 (8%)	37,38,38	2.00	10 (27%)

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
3	IAC	B	702	-	-	4/4/4/4	0/2/2/2
2	AMP	A	701	-	-	0/10/26/26	0/3/3/3
3	IAC	C	702	-	-	2/4/4/4	0/2/2/2
3	IAC	A	702	-	-	4/4/4/4	0/2/2/2
2	AMP	C	701	-	-	3/10/26/26	0/3/3/3
2	AMP	D	701	-	-	0/10/26/26	0/3/3/3
3	IAC	D	702	-	-	4/4/4/4	0/2/2/2
2	AMP	B	701	-	-	0/10/26/26	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	IAC	C-N	7.75	1.50	1.37
3	B	702	IAC	C-N	7.50	1.49	1.37
3	C	702	IAC	C-N	7.43	1.49	1.37
3	D	702	IAC	C-N	7.34	1.49	1.37
3	C	702	IAC	C1-C	6.52	1.49	1.41
3	D	702	IAC	C1-C	6.42	1.49	1.41
3	B	702	IAC	C1-C	5.94	1.48	1.41
3	A	702	IAC	C1-C	5.79	1.48	1.41
3	B	702	IAC	C8-C7	-5.42	1.28	1.36
3	D	702	IAC	C8-C7	-5.20	1.29	1.36
3	A	702	IAC	C8-C7	-4.97	1.29	1.36
3	C	702	IAC	C8-C7	-4.73	1.29	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	AMP	C5-C4	4.72	1.47	1.39
2	B	701	AMP	C5-C4	4.65	1.47	1.39
2	C	701	AMP	C5-C4	4.46	1.47	1.39
3	B	702	IAC	C3-C2	4.46	1.46	1.38
3	D	702	IAC	C3-C2	4.43	1.46	1.38
3	A	702	IAC	C3-C2	4.41	1.46	1.38
3	C	702	IAC	C3-C2	4.26	1.46	1.38
2	D	701	AMP	C5-C4	4.20	1.46	1.39
3	D	702	IAC	C17-C7	4.16	1.55	1.50
3	B	702	IAC	C17-C7	4.01	1.55	1.50
3	C	702	IAC	C4-C3	3.75	1.46	1.38
3	B	702	IAC	C4-C3	3.68	1.46	1.38
3	C	702	IAC	C17-C7	3.60	1.54	1.50
3	D	702	IAC	C4-C3	3.54	1.46	1.38
3	A	702	IAC	C17-C7	3.53	1.54	1.50
3	A	702	IAC	C4-C3	3.44	1.45	1.38
2	B	701	AMP	C5-C6	2.95	1.49	1.41
2	A	701	AMP	C4-N9	-2.81	1.31	1.37
2	C	701	AMP	C5-C6	2.64	1.48	1.41
2	D	701	AMP	C5-C6	2.62	1.48	1.41
3	B	702	IAC	O2-C18	-2.40	1.22	1.30
3	A	702	IAC	O2-C18	-2.33	1.23	1.30
2	D	701	AMP	C8-N7	2.32	1.36	1.31
2	A	701	AMP	C8-N7	2.31	1.36	1.31
3	A	702	IAC	C5-C	-2.26	1.36	1.39
3	C	702	IAC	C5-C	-2.26	1.36	1.39
3	D	702	IAC	O2-C18	-2.20	1.23	1.30
3	B	702	IAC	C5-C	-2.20	1.36	1.39
2	A	701	AMP	C5-C6	2.17	1.47	1.41
2	C	701	AMP	C8-N7	2.16	1.35	1.31
2	D	701	AMP	C4-N9	-2.04	1.33	1.37

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	IAC	C1-C-N	-9.56	99.55	107.52
3	D	702	IAC	C1-C-N	-9.55	99.56	107.52
3	A	702	IAC	C1-C-N	-9.28	99.79	107.52
3	C	702	IAC	C1-C-N	-9.06	99.97	107.52
3	A	702	IAC	C1-C7-C8	7.88	114.22	106.16
3	C	702	IAC	C1-C7-C8	7.65	113.99	106.16
3	B	702	IAC	C1-C7-C8	7.50	113.83	106.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	IAC	C1-C7-C8	7.03	113.35	106.16
3	D	702	IAC	C2-C1-C	-5.98	112.64	118.84
2	C	701	AMP	C5-C4-N3	-5.65	118.94	126.72
3	B	702	IAC	C17-C7-C8	-5.63	119.14	126.84
3	B	702	IAC	C2-C1-C	-5.54	113.10	118.84
2	B	701	AMP	C5-C4-N3	-5.49	119.15	126.72
3	A	702	IAC	C2-C1-C	-5.35	113.30	118.84
2	D	701	AMP	C5-C4-N3	-5.17	119.59	126.72
3	D	702	IAC	C2-C1-C7	4.96	141.24	133.85
3	B	702	IAC	C2-C1-C7	4.89	141.14	133.85
3	A	702	IAC	C2-C1-C7	4.83	141.05	133.85
2	B	701	AMP	N3-C4-N9	4.80	135.33	127.17
3	D	702	IAC	C17-C7-C8	-4.71	120.40	126.84
2	C	701	AMP	N3-C4-N9	4.67	135.12	127.17
3	B	702	IAC	C-N-C8	4.52	113.10	109.08
3	A	702	IAC	C17-C7-C8	-4.38	120.86	126.84
3	A	702	IAC	C-N-C8	4.37	112.97	109.08
3	D	702	IAC	C-N-C8	4.29	112.89	109.08
2	D	701	AMP	N3-C4-N9	4.13	134.20	127.17
3	C	702	IAC	C2-C1-C	-4.11	114.58	118.84
3	C	702	IAC	C2-C1-C7	3.99	139.81	133.85
2	A	701	AMP	N3-C2-N1	-3.96	122.59	128.58
3	C	702	IAC	C-N-C8	3.86	112.51	109.08
3	C	702	IAC	C17-C7-C8	-3.84	121.58	126.84
2	D	701	AMP	N3-C2-N1	-3.82	122.79	128.58
2	C	701	AMP	C2-N3-C4	3.74	120.96	111.83
2	B	701	AMP	C2-N3-C4	3.73	120.94	111.83
2	B	701	AMP	N3-C2-N1	-3.71	122.97	128.58
2	A	701	AMP	C5-C4-N3	-3.66	121.68	126.72
2	D	701	AMP	C2-N3-C4	3.64	120.72	111.83
2	D	701	AMP	C4-C5-N7	-3.60	106.47	110.58
3	D	702	IAC	C3-C4-C5	-3.57	115.83	120.24
2	B	701	AMP	C4-N9-C8	3.55	109.46	105.74
2	D	701	AMP	C4-N9-C8	3.54	109.45	105.74
3	B	702	IAC	C5-C-N	3.49	136.33	130.74
2	B	701	AMP	C4-C5-N7	-3.49	106.59	110.58
3	B	702	IAC	O2-C18-O3	-3.49	114.36	123.33
2	C	701	AMP	C4-C5-N7	-3.42	106.67	110.58
3	A	702	IAC	C5-C-N	3.42	136.22	130.74
2	C	701	AMP	N3-C2-N1	-3.38	123.47	128.58
3	A	702	IAC	C3-C4-C5	-3.24	116.24	120.24
3	D	702	IAC	C5-C-N	3.21	135.88	130.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	AMP	C2-N1-C6	3.21	124.00	118.73
3	D	702	IAC	O2-C18-O3	-3.05	115.48	123.33
2	A	701	AMP	N3-C4-N9	3.02	132.31	127.17
2	A	701	AMP	C2-N3-C4	3.02	119.20	111.83
3	C	702	IAC	C5-C-N	2.96	135.49	130.74
2	C	701	AMP	C4-N9-C8	2.89	108.78	105.74
2	A	701	AMP	C4-N9-C8	2.88	108.76	105.74
2	D	701	AMP	C5-N7-C8	2.78	107.82	103.45
3	B	702	IAC	O2-C18-C17	2.77	123.11	114.51
2	B	701	AMP	C5-N7-C8	2.76	107.79	103.45
2	D	701	AMP	N9-C8-N7	-2.76	110.02	113.94
3	A	702	IAC	C7-C8-N	-2.68	107.37	110.31
2	C	701	AMP	C5-N7-C8	2.63	107.59	103.45
3	C	702	IAC	O2-C18-O3	-2.46	117.00	123.33
2	A	701	AMP	C4-C5-N7	-2.46	107.78	110.58
3	D	702	IAC	C5-C-C1	2.45	124.56	122.19
3	B	702	IAC	C18-C17-C7	-2.45	111.17	114.93
3	C	702	IAC	C5-C-C1	2.43	124.54	122.19
2	D	701	AMP	C6-C5-N7	2.39	136.71	132.09
3	B	702	IAC	C3-C4-C5	-2.36	117.33	120.24
3	C	702	IAC	O2-C18-C17	2.36	121.83	114.51
3	D	702	IAC	O2-C18-C17	2.36	121.82	114.51
2	A	701	AMP	C6-C5-N7	2.34	136.61	132.09
2	D	701	AMP	C2-N1-C6	2.34	122.58	118.73
2	B	701	AMP	N9-C8-N7	-2.33	110.63	113.94
3	B	702	IAC	C7-C8-N	-2.32	107.76	110.31
2	B	701	AMP	C2-N1-C6	2.29	122.50	118.73
2	B	701	AMP	C6-C5-N7	2.22	136.38	132.09
3	C	702	IAC	C7-C8-N	-2.18	107.92	110.31
3	A	702	IAC	O2-C18-O3	-2.12	117.87	123.33
3	A	702	IAC	O2-C18-C17	2.10	121.02	114.51
2	C	701	AMP	O3P-P-O2P	2.09	115.65	107.80
3	C	702	IAC	C18-C17-C7	-2.09	111.72	114.93
2	C	701	AMP	N9-C8-N7	-2.06	111.01	113.94
3	D	702	IAC	C7-C8-N	-2.03	108.08	110.31
2	D	701	AMP	O3P-P-O5'	-2.02	101.39	106.67

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	AMP	C5'-O5'-P-O2P

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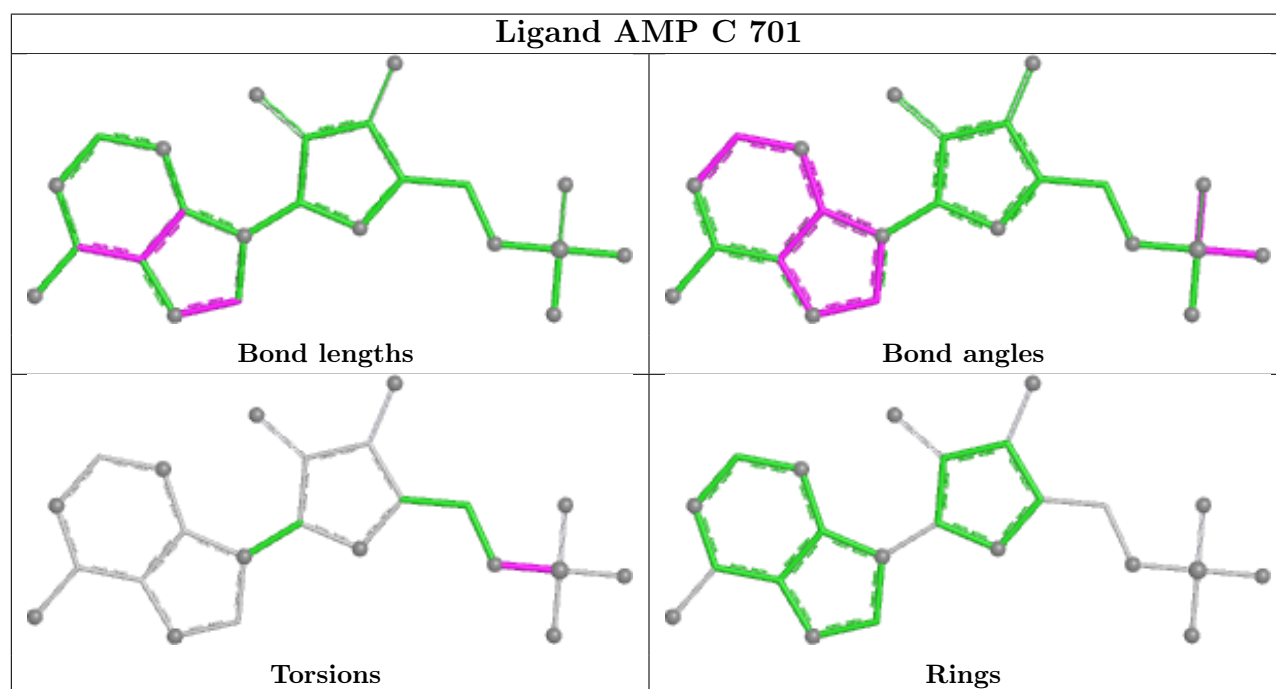
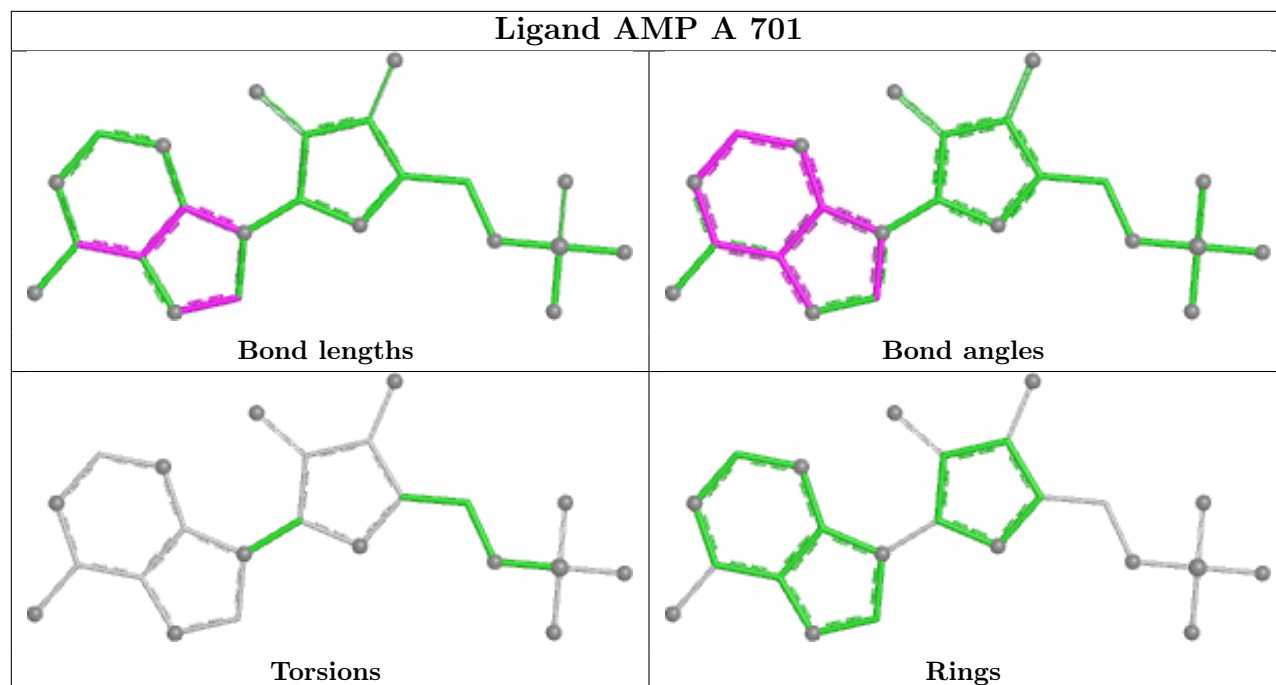
Mol	Chain	Res	Type	Atoms
2	C	701	AMP	C5'-O5'-P-O3P
3	B	702	IAC	C18-C17-C7-C1
3	B	702	IAC	C18-C17-C7-C8
3	D	702	IAC	C18-C17-C7-C1
3	D	702	IAC	C18-C17-C7-C8
3	A	702	IAC	C18-C17-C7-C1
3	A	702	IAC	C18-C17-C7-C8
3	A	702	IAC	C7-C17-C18-O2
3	A	702	IAC	C7-C17-C18-O3
3	D	702	IAC	C7-C17-C18-O2
3	D	702	IAC	C7-C17-C18-O3
3	B	702	IAC	C7-C17-C18-O2
3	C	702	IAC	C18-C17-C7-C1
3	B	702	IAC	C7-C17-C18-O3
2	C	701	AMP	C5'-O5'-P-O1P
3	C	702	IAC	C18-C17-C7-C8

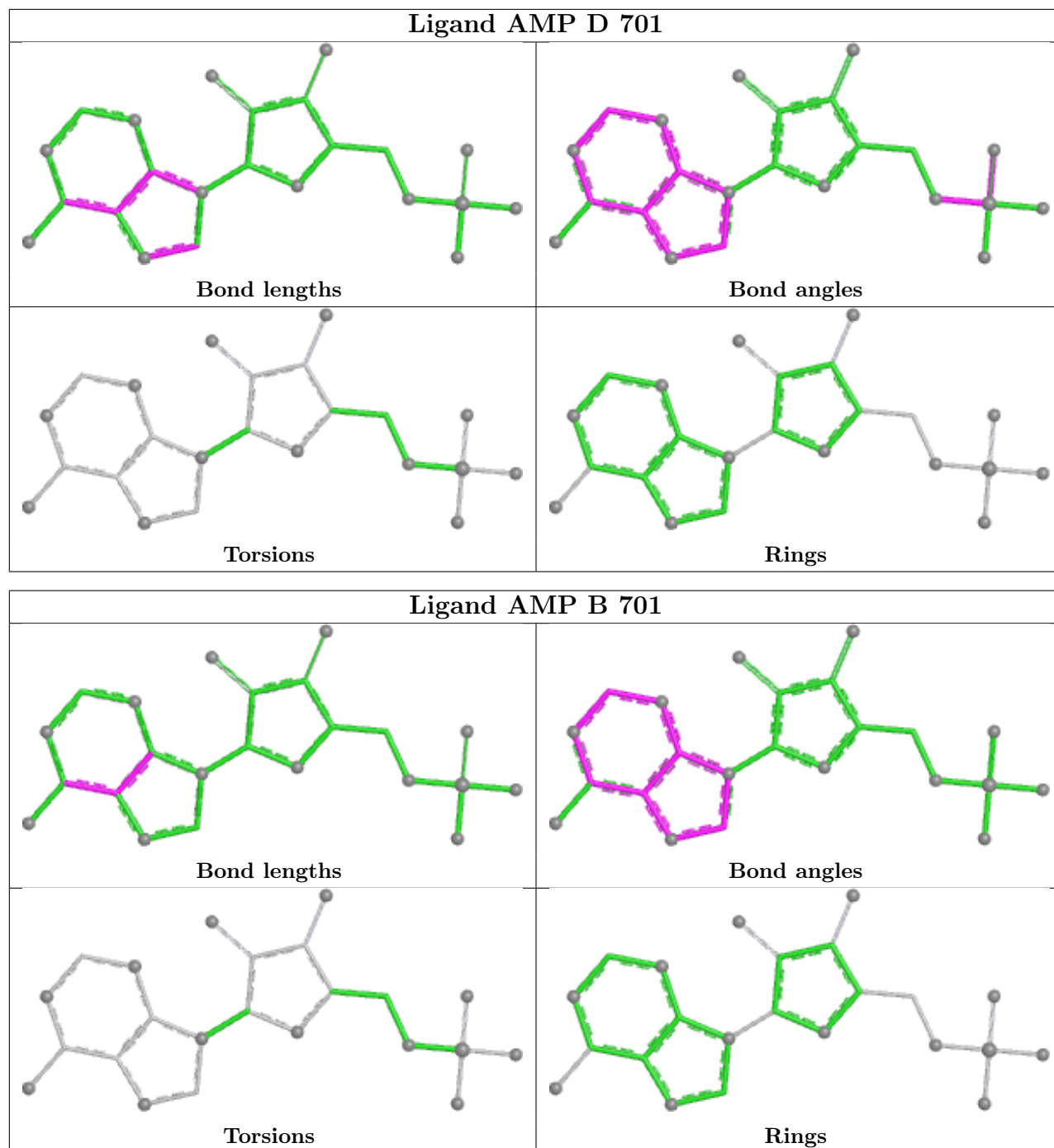
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	IAC	3	0
3	C	702	IAC	2	0
3	A	702	IAC	2	0
3	D	702	IAC	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 [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	573/612 (93%)	-0.01	8 (1%) 73 71	15, 27, 48, 70	3 (0%)
1	B	573/612 (93%)	0.02	14 (2%) 59 56	13, 27, 48, 68	0
1	C	566/612 (92%)	0.26	19 (3%) 48 45	12, 31, 59, 79	2 (0%)
1	D	566/612 (92%)	0.04	12 (2%) 63 60	11, 27, 50, 68	1 (0%)
All	All	2278/2448 (93%)	0.08	53 (2%) 61 58	11, 28, 51, 79	6 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	571	TYR	5.8
1	B	505	LEU	4.8
1	B	390	LEU	4.4
1	C	480	SER	4.4
1	C	263	ILE	4.2
1	C	377	ASN	4.2
1	C	239	ALA	3.9
1	D	569	ASN	3.8
1	B	506	ASP	3.6
1	B	391	THR	3.5
1	D	510	PRO	3.4
1	C	295	TRP	3.4
1	C	267	SER	3.3
1	C	504	CYS	3.3
1	B	397	GLU	3.2
1	D	504	CYS	3.2
1	A	18	ASP	3.0
1	A	564	LEU	2.8
1	C	240	ILE	2.8
1	C	190	ASP	2.8
1	C	293	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	603	VAL	2.7
1	B	16	THR	2.7
1	B	604	PRO	2.7
1	D	563	SER	2.7
1	C	327	TYR	2.7
1	C	589	ARG	2.6
1	D	562	ILE	2.6
1	B	245	LYS	2.6
1	A	608	GLN	2.6
1	D	564	LEU	2.6
1	A	595	PHE	2.5
1	D	606	HIS	2.5
1	C	505	LEU	2.5
1	D	270	GLU	2.4
1	C	264	THR	2.4
1	B	507	GLY	2.3
1	D	64	ARG	2.3
1	A	566	ALA	2.3
1	C	532	ARG	2.3
1	B	17	LEU	2.2
1	C	392	GLU	2.2
1	B	570	GLN	2.2
1	A	397	GLU	2.2
1	C	601	LYS	2.2
1	D	572	LYS	2.2
1	A	565	GLY	2.1
1	B	566	ALA	2.1
1	A	277	LYS	2.1
1	D	568	ILE	2.1
1	C	506	ASP	2.0
1	B	254	ILE	2.0
1	D	67	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

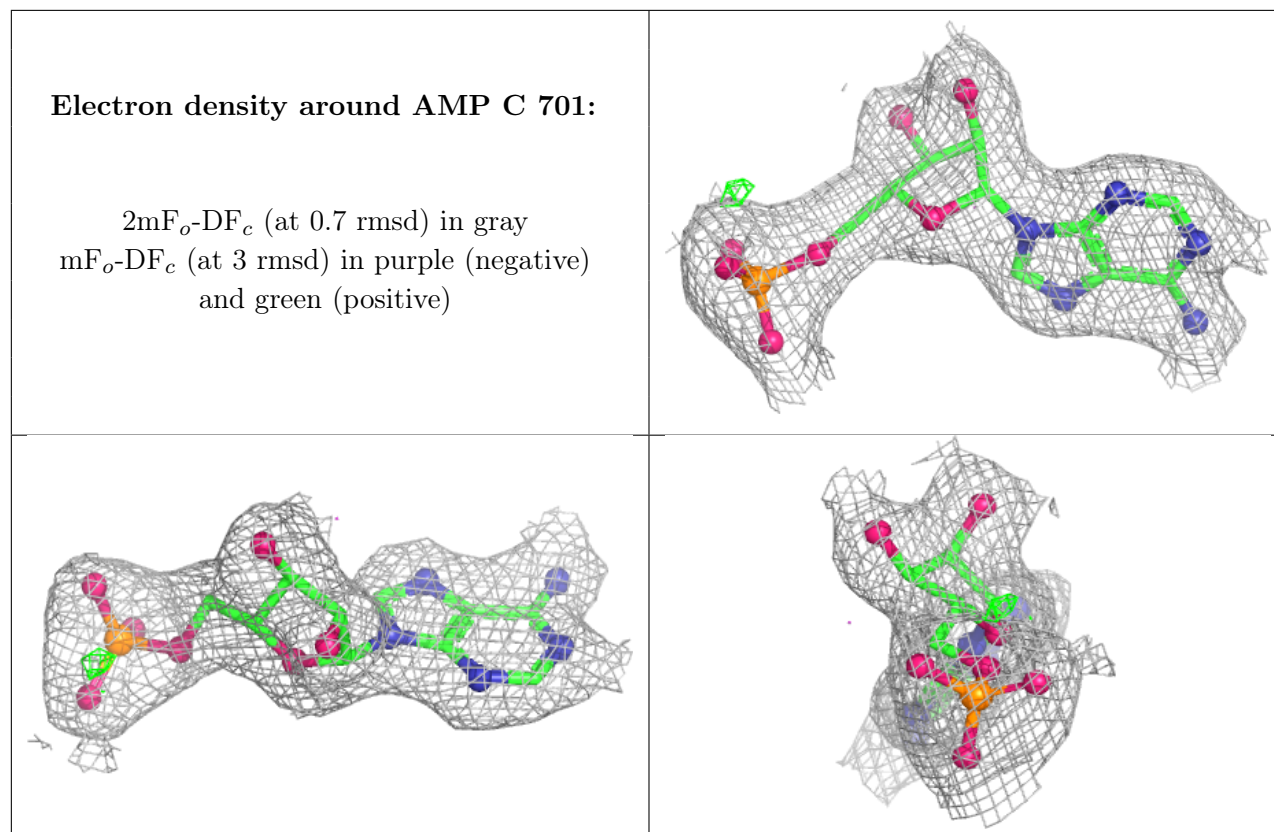
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

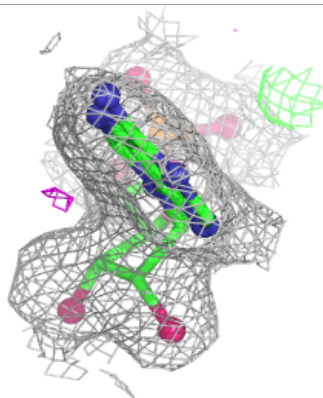
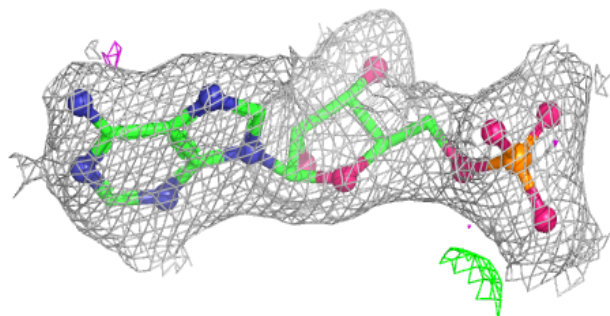
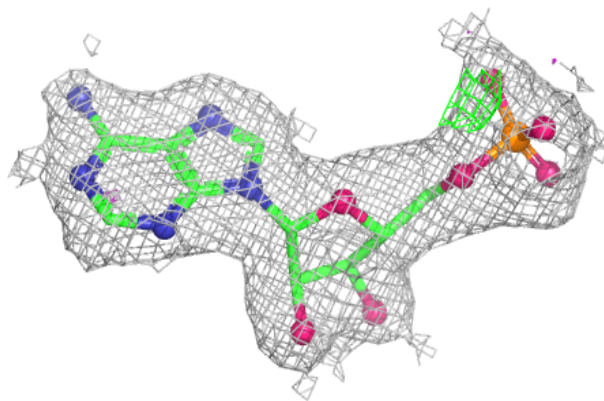
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	703	5/5	0.69	0.23	47,48,57,62	0
4	SO4	B	704	5/5	0.70	0.21	72,76,77,78	0
3	IAC	C	702	13/13	0.80	0.18	34,44,52,53	0
3	IAC	A	702	13/13	0.87	0.21	9,35,41,42	0
3	IAC	D	702	13/13	0.88	0.18	10,33,41,43	0
3	IAC	B	702	13/13	0.91	0.14	5,29,35,38	0
2	AMP	C	701	23/23	0.96	0.06	12,17,25,29	0
2	AMP	D	701	23/23	0.96	0.05	10,16,22,25	0
2	AMP	A	701	23/23	0.96	0.06	12,18,23,27	0
2	AMP	B	701	23/23	0.96	0.06	12,16,19,27	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.

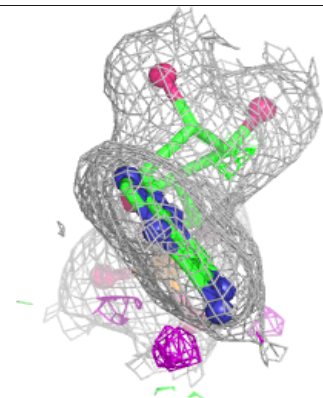
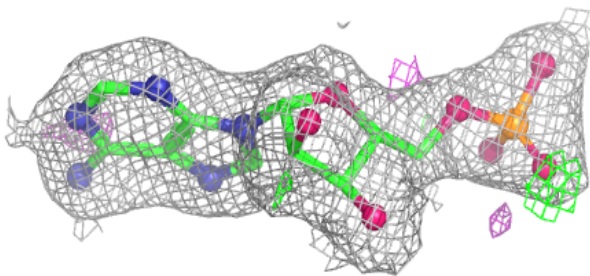
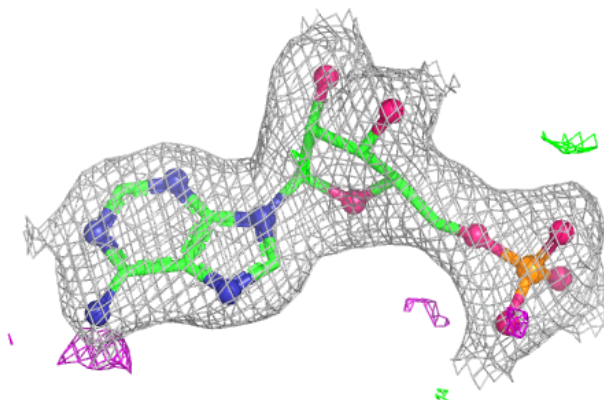


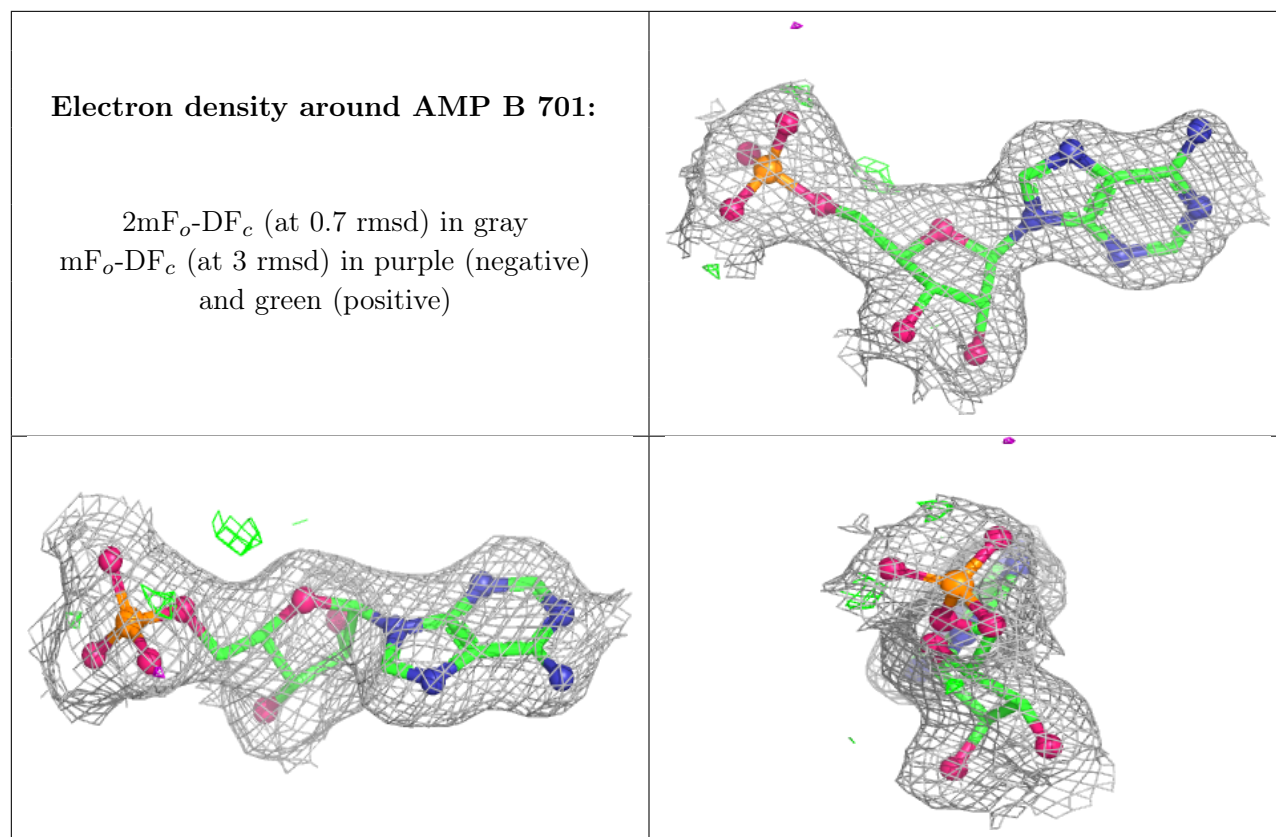
Electron density around AMP D 701:

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

**Electron density around AMP A 701:**

$2mF_o-DF_c$ (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.