WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 10:00 am GMT

PDB ID	:	2J91
Title	:	Crystal structure of Human Adenylosuccinate Lyase in complex with AMP
Authors	:	Stenmark, P.; Moche, M.; Arrowsmith, C.; Berglund, H.; Busam, R.; Collins, R.; Edwards, A.; Ericsson, U.B.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg Schiavone, L.; Hogbom, M.; Johansson, I.; Karlberg, T.; Kosinska, U.; Kotenyova, T.; Magnusdottir, A.; Nilsson, M.E.; Nilsson-Ehle, P.; Nyman, T.; Ogg, D.; Persson, C.; Sagemark, J.; Sundstrom, M.; Uppenberg, J.; Uppsten, M.; Thorsell, A.G.; van Den Berg, S.; Wallden, K.; Weigelt, J.; Nordlund, P.
Deposited on	:	2006-11-01
Resolution	:	1.80 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
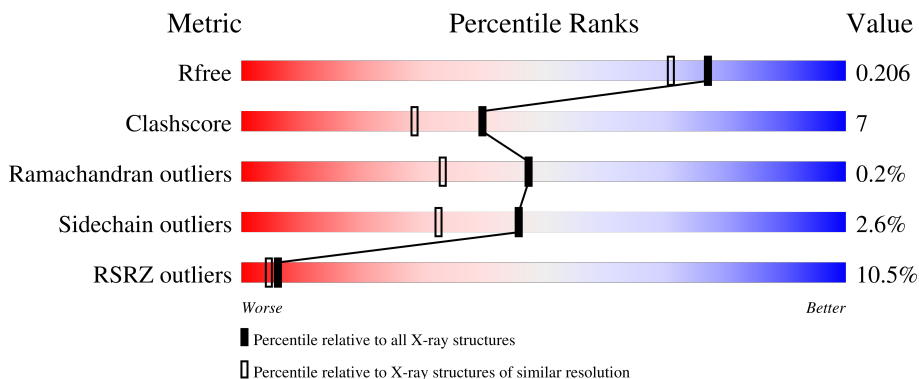http://www.wwpdb.org/validation/2017/FAQs#types.

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 1.80 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	Percentile Ranks	Value
Rfree		0.206
Clashscore		7
Ramachandran outliers		0.2%
Sidechain outliers		2.6%
RSRZ outliers		10.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

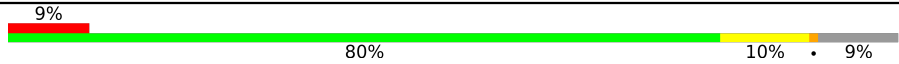| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	503	11% / 79% / 11% · 9%
1	B	503	8% / 80% / 11% · 8%

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CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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Mol	Chain	Length	Quality of chain
1	C	503	9% 80% 10% • 9%
1	D	503	10% 77% 13% • 9%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 16310 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 ADENYLOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	2	0
			3664	2308	652	679	25			
1	B	463	Total	C	N	O	S	0	1	0
			3702	2331	658	687	26			
1	C	456	Total	C	N	O	S	0	3	0
			3662	2306	655	675	26			
1	D	456	Total	C	N	O	S	0	4	0
			3667	2313	654	675	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ARG	GLN	engineered mutation	UNP P30566
B	63	ARG	GLN	engineered mutation	UNP P30566
C	63	ARG	GLN	engineered mutation	UNP P30566
D	63	ARG	GLN	engineered mutation	UNP P30566

• Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

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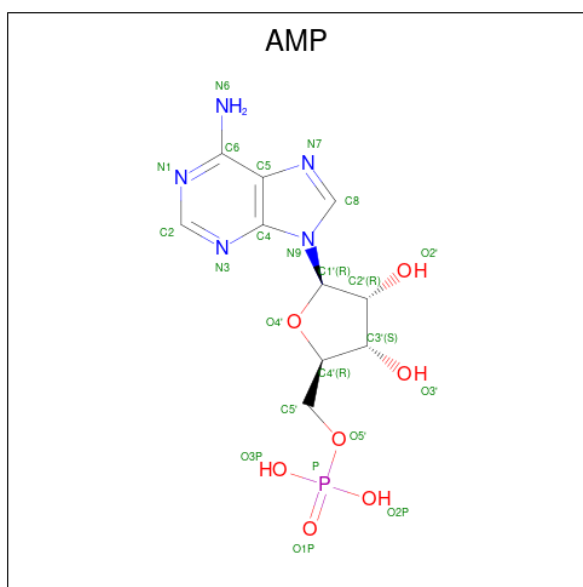
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	334	Total 334	O 334	0	0
5	B	377	Total 377	O 377	0	0
5	C	373	Total 373	O 373	0	0
5	D	411	Total 411	O 411	0	0

3 Residue-property plots (i)

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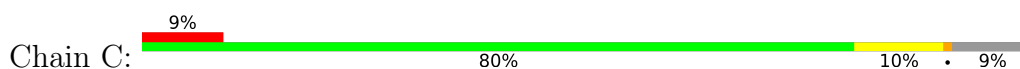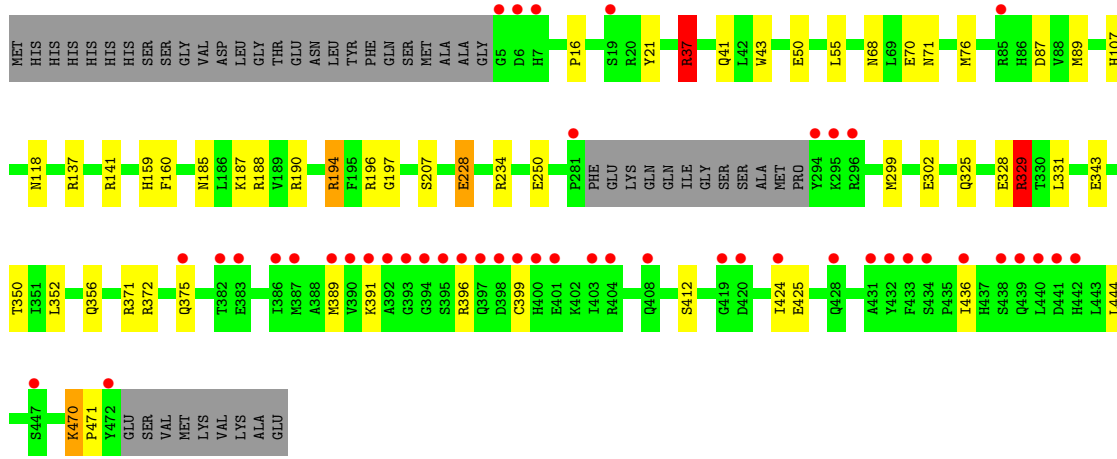
- Molecule 1: ADENYLOSUCCINATE LYASE
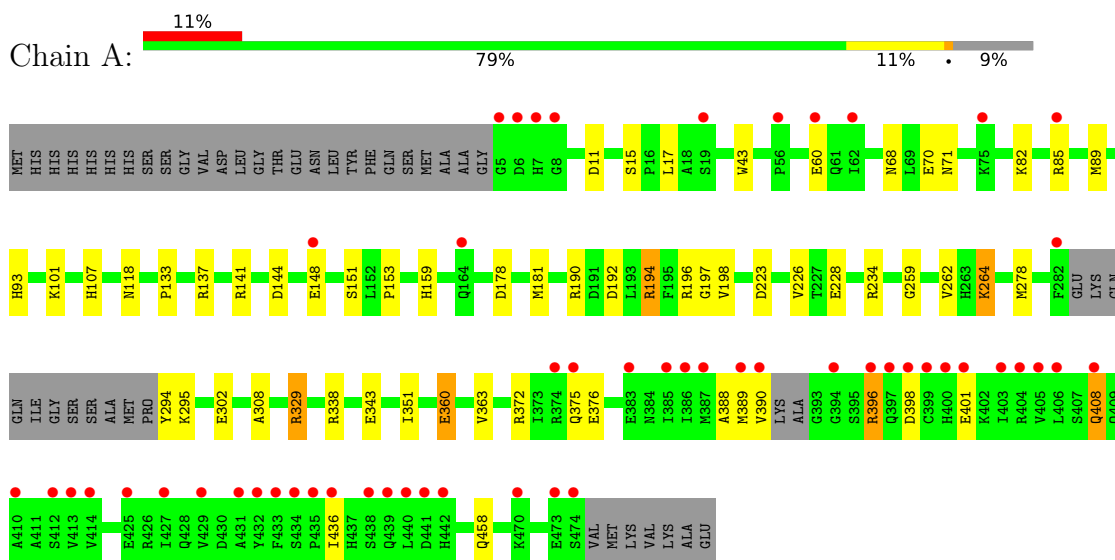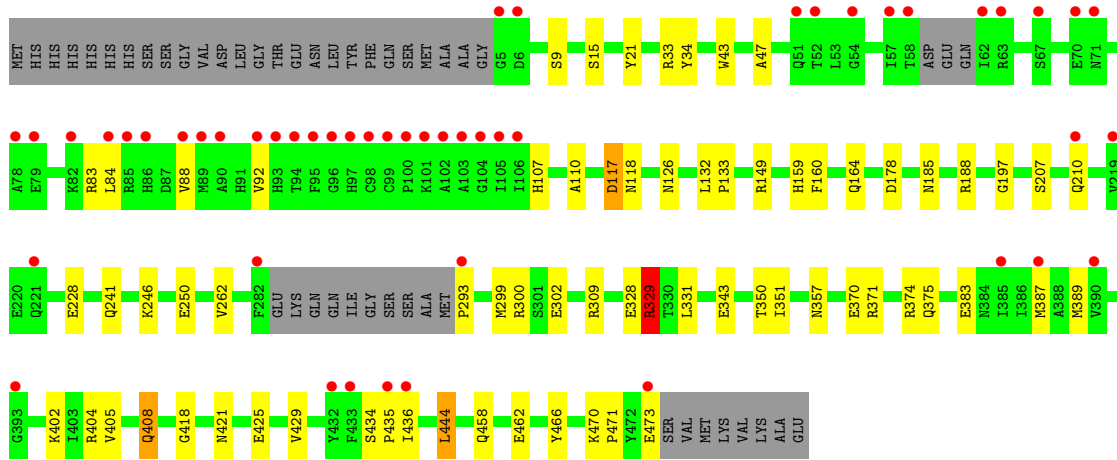
Chain A:

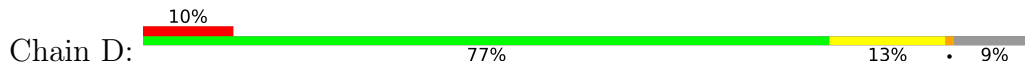

- Molecule 1: ADENYLOSUCCINATE LYASE

Chain B:

- Molecule 1: ADENYLOSUCCINATE LYASE

Chain C:
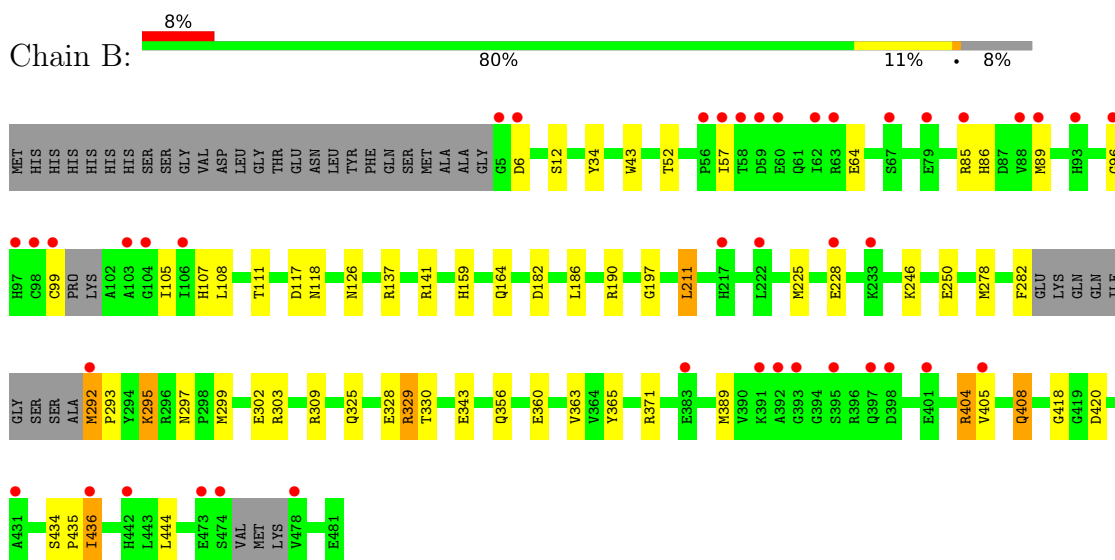
• Molecule 1: ADENYLOSUCCINATE LYASE

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.37Å 104.34Å 213.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.60 – 1.80 14.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (106.60-1.80) 100.0 (14.98-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.157 , 0.199 0.168 , 0.206	Depositor DCC
R_{free} test set	8809 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 65.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16310	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, CL

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	0.68	0/3737	0.76	6/5044 (0.1%)
1	B	0.70	1/3771 (0.0%)	0.74	2/5086 (0.0%)
1	C	0.71	0/3735	0.79	6/5041 (0.1%)
1	D	0.68	0/3744	0.76	5/5052 (0.1%)
All	All	0.69	1/14987 (0.0%)	0.76	19/20223 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	LYS	CE-NZ	6.33	1.64	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	A	194	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	194	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	309	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	137	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	194	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	137	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	149	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	D	444	LEU	CA-CB-CG	-5.84	101.86	115.30
1	C	87	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	87	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	37	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	D	178	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	338	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	309	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	37	ARG	CG-CD-NE	-5.40	100.47	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	178	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	295	LYS	CD-CE-NZ	5.10	123.43	111.70
1	B	295	LYS	CD-CE-NZ	5.08	123.39	111.70

There are no chirality outliers.

There are no planarity outliers.

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	3664	0	3674	47	0
1	B	3702	0	3712	64	0
1	C	3662	0	3686	47	0
1	D	3667	0	3692	72	0
2	A	23	0	12	1	0
2	B	23	0	12	1	0
2	C	23	0	12	2	0
2	D	23	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	334	0	0	11	1
5	B	377	0	0	17	1
5	C	373	0	0	12	0
5	D	411	0	0	17	0
All	All	16310	0	14844	217	1

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 7.

All (217) 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)
5:B:2094:HOH:O	1:C:331:LEU:HD23	1.29	1.29
5:A:2101:HOH:O	1:D:331:LEU:HD23	1.21	1.26
1:A:388:ALA:HB1	1:A:436:ILE:HD11	1.37	1.04
1:B:389:MET:HE3	1:B:436:ILE:HD13	1.38	1.02
1:D:331:LEU:HD13	5:D:2265:HOH:O	1.59	1.00
1:A:178:ASP:HA	1:A:181:MET:HE3	1.46	0.98
1:B:389:MET:CE	1:B:436:ILE:HD13	1.94	0.96
1:D:34:TYR:OH	1:D:126:ASN:ND2	1.99	0.95
1:D:389:MET:HE2	1:D:436:ILE:HG23	1.47	0.93
1:A:178:ASP:HA	1:A:181:MET:CE	1.99	0.92
1:A:389:MET:HE3	1:A:436:ILE:HD13	1.58	0.85
1:D:375:GLN:HE22	1:D:421:ASN:H	1.22	0.85
1:A:388:ALA:CB	1:A:436:ILE:HD11	2.06	0.85
1:D:389:MET:HE3	1:D:436:ILE:HG13	1.60	0.84
5:B:2094:HOH:O	1:C:331:LEU:CD2	1.97	0.82
1:D:293:PRO:N	5:D:2234:HOH:O	2.13	0.82
1:D:389:MET:CE	1:D:436:ILE:HG13	2.12	0.78
1:B:299:MET:HE1	5:C:2119:HOH:O	1.84	0.78
1:A:264:LYS:NZ	5:A:2222:HOH:O	2.07	0.77
1:A:294:TYR:N	5:A:2236:HOH:O	2.16	0.77
1:B:389:MET:HE3	1:B:436:ILE:CD1	2.14	0.77
1:D:299:MET:HE2	5:D:2253:HOH:O	1.86	0.76
1:D:299:MET:CE	5:D:2253:HOH:O	2.33	0.75
1:A:70:GLU:OE1	5:A:2062:HOH:O	2.05	0.74
1:D:458:GLN:HG3	5:D:2387:HOH:O	1.86	0.74
1:B:111:THR:HG22	3:B:1001:CL:CL	2.25	0.73
1:B:111:THR:CG2	5:B:2098:HOH:O	2.36	0.73
1:D:164:GLN:OE1	5:D:2142:HOH:O	2.05	0.72
1:B:137:ARG:HH11	1:B:356:GLN:HE22	1.36	0.72
1:B:299:MET:SD	5:C:2043:HOH:O	2.47	0.72
1:C:299[A]:MET:HE3	2:C:1000:AMP:C8	2.25	0.71
1:B:126:ASN:HB3	5:B:2107:HOH:O	1.89	0.71
1:B:282:PHE:C	5:B:2221:HOH:O	2.30	0.70
1:B:404:ARG:O	1:B:408:GLN:HG2	1.91	0.70
1:D:262:VAL:HG11	1:D:351:ILE:CG2	2.21	0.70
1:D:389:MET:HE2	1:D:436:ILE:CG2	2.20	0.70
1:C:228:GLU:HG2	5:C:2246:HOH:O	1.91	0.70
1:D:408:GLN:NE2	5:D:2337:HOH:O	2.25	0.69
1:D:370:GLU:OE1	5:D:2298:HOH:O	2.10	0.69
5:A:2222:HOH:O	1:B:325:GLN:O	2.10	0.68
1:D:375:GLN:NE2	1:D:421:ASN:H	1.91	0.68
1:B:389:MET:HE3	1:B:436:ILE:HB	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLN:OE1	5:B:2139:HOH:O	2.12	0.67
1:C:43:TRP:HE1	1:C:107:HIS:HD2	1.40	0.67
1:B:57:ILE:HG12	1:B:105:ILE:HD12	1.77	0.67
1:C:43:TRP:HE1	1:C:107:HIS:CD2	2.13	0.67
1:B:299:MET:CE	5:C:2119:HOH:O	2.42	0.66
1:D:389:MET:HE1	1:D:435:PRO:HD2	1.77	0.66
1:C:250:GLU:CD	5:C:2266:HOH:O	2.34	0.66
1:B:111:THR:HG23	5:B:2098:HOH:O	1.97	0.65
1:A:343:GLU:OE2	1:D:343:GLU:OE2	2.15	0.65
1:C:68:ASN:ND2	1:C:71:ASN:HD22	1.95	0.65
1:C:372:ARG:HA	1:C:375:GLN:CG	2.27	0.65
1:B:302:GLU:OE1	1:D:159:HIS:HD2	1.80	0.65
1:A:264:LYS:CE	5:A:2222:HOH:O	2.46	0.64
1:C:207:SER:OG	5:C:2220:HOH:O	1.88	0.64
1:A:198:VAL:HG13	1:A:226:VAL:HG21	1.79	0.63
1:D:408:GLN:HE21	1:D:408:GLN:HA	1.61	0.63
1:B:365:TYR:OH	5:B:2275:HOH:O	2.14	0.63
1:D:408:GLN:NE2	5:D:2336:HOH:O	2.30	0.63
1:B:141:ARG:CZ	1:B:360:GLU:OE2	2.48	0.62
1:A:302:GLU:OE1	1:C:159:HIS:HD2	1.82	0.62
1:C:89:MET:HG3	5:C:2016:HOH:O	1.99	0.62
1:A:144:ASP:O	1:A:148:GLU:HG3	1.99	0.62
1:B:389:MET:CE	1:B:436:ILE:HB	2.29	0.62
1:A:118:ASN:HD21	1:A:197:GLY:H	1.46	0.61
1:B:118:ASN:HD21	1:B:197:GLY:H	1.47	0.61
1:C:352:LEU:O	1:C:356:GLN:HG3	1.99	0.61
1:A:43:TRP:HE1	1:A:107:HIS:CD2	2.18	0.61
1:C:21:TYR:HB3	1:C:350:THR:HG21	1.81	0.61
1:C:118:ASN:HD21	1:C:197:GLY:H	1.48	0.61
1:A:82:LYS:HZ1	1:A:85:ARG:CZ	2.14	0.61
1:C:372:ARG:O	1:C:375:GLN:HG3	2.00	0.61
1:A:181:MET:CE	1:B:246:LYS:HD3	2.31	0.60
1:A:43:TRP:HE1	1:A:107:HIS:HD2	1.50	0.60
1:D:389:MET:CE	1:D:436:ILE:CG1	2.78	0.60
1:D:118:ASN:HD21	1:D:197:GLY:H	1.47	0.59
1:B:159:HIS:HD2	1:D:302:GLU:OE1	1.84	0.59
1:D:300:ARG:HH11	1:D:357:ASN:ND2	2.00	0.59
1:A:17:LEU:CD1	1:A:343:GLU:HG2	2.32	0.59
1:B:43:TRP:HE1	1:B:107:HIS:CD2	2.20	0.59
1:D:300:ARG:HH11	1:D:357:ASN:HD21	1.51	0.59
1:C:68:ASN:HD22	1:C:71:ASN:HD22	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASP:OD1	5:B:2101:HOH:O	2.18	0.57
1:C:37:ARG:HH12	1:C:41:GLN:HE21	1.52	0.56
1:D:246:LYS:O	1:D:250:GLU:HG2	2.05	0.56
1:D:389:MET:HE3	1:D:436:ILE:CG1	2.34	0.56
1:A:398:ASP:O	1:A:401:GLU:HG2	2.05	0.56
1:A:181:MET:HE1	1:B:246:LYS:HD3	1.87	0.56
1:D:470:LYS:HB3	1:D:471:PRO:HD3	1.88	0.55
1:A:372:ARG:HA	1:A:375:GLN:HG2	1.88	0.55
1:B:389:MET:HE2	1:B:436:ILE:HD13	1.81	0.55
1:C:185:ASN:HD22	1:C:188[A]:ARG:HH12	1.55	0.55
1:D:370:GLU:HG3	5:D:2293:HOH:O	2.07	0.54
1:B:328:GLU:O	1:B:329:ARG:HB2	2.07	0.54
1:D:389:MET:HE2	1:D:436:ILE:CG1	2.37	0.54
1:A:375:GLN:HG3	1:A:376:GLU:HG2	1.90	0.54
1:D:83:ARG:NH2	1:D:84:LEU:HD21	2.22	0.54
1:D:262:VAL:HG11	1:D:351:ILE:HG21	1.87	0.54
1:B:299:MET:HE3	2:B:1000:AMP:H2'	1.90	0.53
1:C:372:ARG:HA	1:C:375:GLN:HG2	1.91	0.53
1:C:16:PRO:HB2	1:C:21:TYR:CE2	2.44	0.53
1:C:137:ARG:HH11	1:C:356:GLN:HE22	1.55	0.52
1:B:420:ASP:OD1	1:D:371:ARG:NH2	2.40	0.52
5:A:2222:HOH:O	1:B:325:GLN:C	2.46	0.52
1:B:303:ARG:NH2	5:B:2240:HOH:O	2.42	0.52
1:B:96:GLY:O	1:B:99:CYS:O	2.28	0.51
1:C:389:MET:SD	1:C:436:ILE:HD13	2.50	0.51
1:B:43:TRP:HE1	1:B:107:HIS:HD2	1.59	0.51
1:A:194:ARG:HD3	1:A:234:ARG:CD	2.41	0.51
1:D:466:TYR:OH	5:D:2396:HOH:O	2.19	0.50
1:B:389:MET:HE3	1:B:436:ILE:CG1	2.42	0.50
1:C:375:GLN:HB3	5:C:2341:HOH:O	2.12	0.49
1:C:371:ARG:O	1:C:375:GLN:HG2	2.12	0.49
1:B:295:LYS:HE3	1:B:297:ASN:OD1	2.13	0.49
1:B:34:TYR:OH	1:B:126:ASN:ND2	2.29	0.49
1:C:187:LYS:HE2	5:C:2207:HOH:O	2.11	0.49
1:A:11:ASP:OD1	1:D:33:ARG:HD2	2.13	0.49
1:D:241:GLN:HB3	1:D:329:ARG:HG2	1.95	0.48
1:D:389:MET:HE2	1:D:436:ILE:HG13	1.94	0.48
1:A:178:ASP:HA	1:A:181:MET:HE2	1.93	0.48
1:B:137:ARG:HD2	1:B:356:GLN:HE21	1.79	0.48
1:B:292:MET:O	1:B:292:MET:HG2	2.12	0.48
1:A:262:VAL:HG11	1:A:351:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:LYS:HB3	1:C:471:PRO:HD3	1.95	0.48
1:B:52:THR:HB	1:B:225:MET:HE1	1.96	0.47
1:C:107:HIS:HE1	5:C:2146:HOH:O	1.97	0.47
1:C:141:ARG:NH2	1:C:356:GLN:HB3	2.30	0.47
1:A:159:HIS:HD2	1:C:302:GLU:OE1	1.98	0.47
1:B:137:ARG:HD2	1:B:356:GLN:NE2	2.30	0.47
1:B:389:MET:HE3	1:B:436:ILE:CB	2.43	0.47
1:C:194:ARG:HD3	1:C:234:ARG:CD	2.45	0.47
1:A:390:VAL:HG21	1:A:396:ARG:HH11	1.79	0.47
1:A:408:GLN:HE21	1:A:408:GLN:N	2.13	0.47
1:B:299:MET:HB3	5:B:2094:HOH:O	2.14	0.47
1:B:328:GLU:O	1:B:329:ARG:CB	2.61	0.47
1:A:141:ARG:CZ	1:A:360:GLU:OE2	2.62	0.47
1:D:331:LEU:CD1	5:D:2265:HOH:O	2.36	0.47
1:D:389:MET:HE1	1:D:435:PRO:CD	2.43	0.47
1:A:198:VAL:HG22	1:A:223:ASP:HA	1.97	0.47
1:A:262:VAL:HG11	1:A:351:ILE:CG2	2.45	0.47
1:A:264:LYS:HE3	5:A:2146:HOH:O	2.15	0.47
1:B:141:ARG:NH1	1:B:360:GLU:OE2	2.48	0.47
1:D:375:GLN:HE22	1:D:421:ASN:N	2.01	0.46
1:C:424:ILE:HG13	1:C:444:LEU:HD13	1.98	0.46
1:A:15:SER:HB2	1:D:15:SER:HB2	1.97	0.46
1:D:43:TRP:HE1	1:D:107:HIS:CD2	2.34	0.46
1:D:262:VAL:HG11	1:D:351:ILE:HG23	1.94	0.46
1:B:329:ARG:HG2	1:B:330:THR:N	2.30	0.46
5:B:2373:HOH:O	1:D:159:HIS:HE1	1.99	0.46
1:C:325:GLN:O	5:C:2299:HOH:O	2.20	0.45
1:B:371:ARG:HD2	1:D:418:GLY:O	2.17	0.45
1:B:64:GLU:OE2	1:B:99:CYS:C	2.55	0.45
1:D:132:LEU:HB2	1:D:133:PRO:HD3	1.98	0.45
1:B:389:MET:HE2	1:B:435:PRO:HB2	1.98	0.45
1:B:418:GLY:O	1:D:371:ARG:HD2	2.17	0.45
1:B:434:SER:N	1:B:435:PRO:CD	2.80	0.45
1:C:50:GLU:HB3	1:C:55:LEU:HD12	1.99	0.45
1:A:17:LEU:HD12	1:A:343:GLU:HG2	1.98	0.45
1:A:194:ARG:HD3	1:A:234:ARG:HD3	1.99	0.45
1:B:182:ASP:O	1:B:186:LEU:HD13	2.15	0.45
1:C:21:TYR:HB3	1:C:350:THR:CG2	2.47	0.45
1:A:141:ARG:CZ	5:A:2123:HOH:O	2.64	0.45
1:B:86:HIS:CE1	1:B:89:MET:HG2	2.52	0.45
1:D:299:MET:HE1	2:D:1000:AMP:H2'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:MET:N	1:B:293:PRO:CD	2.81	0.44
1:C:389:MET:HG2	1:C:399:CYS:SG	2.58	0.44
1:A:89:MET:O	1:A:93:HIS:HD2	2.00	0.44
1:D:88:VAL:O	1:D:92:VAL:HG23	2.18	0.44
1:D:185:ASN:HD22	1:D:188[A]:ARG:HH12	1.65	0.44
1:A:192:ASP:OD2	5:A:2160:HOH:O	2.21	0.44
1:B:246:LYS:O	1:B:250:GLU:HG2	2.18	0.44
1:C:389:MET:HA	1:C:436:ILE:HD11	2.00	0.44
1:A:151:SER:O	1:A:153:PRO:HD3	2.18	0.44
1:A:375:GLN:NE2	5:A:2288:HOH:O	2.51	0.44
1:B:108:LEU:HG	1:B:211:LEU:HD11	1.99	0.43
1:C:372:ARG:HA	1:C:375:GLN:CD	2.38	0.43
1:C:424:ILE:CD1	1:C:444:LEU:HD11	2.48	0.43
1:D:374:ARG:NH2	5:D:2305:HOH:O	2.44	0.43
5:B:2373:HOH:O	1:D:159:HIS:CE1	2.71	0.43
1:D:107:HIS:CD2	1:D:110:ALA:HB3	2.53	0.43
1:C:37:ARG:HH12	1:C:41:GLN:NE2	2.15	0.43
1:B:137:ARG:HH11	1:B:356:GLN:NE2	2.09	0.43
1:B:85:ARG:NH2	5:B:2076:HOH:O	2.51	0.42
2:A:1000:AMP:C8	1:D:331:LEU:HD22	2.54	0.42
1:A:68:ASN:ND2	1:A:71:ASN:HD22	2.17	0.42
1:B:343:GLU:OE1	1:C:343:GLU:OE2	2.38	0.42
1:C:76:MET:HE3	5:C:2096:HOH:O	2.19	0.42
1:D:207:SER:OG	5:D:2185:HOH:O	2.14	0.42
1:D:371:ARG:HG3	5:D:2308:HOH:O	2.18	0.42
1:D:434:SER:N	1:D:435:PRO:CD	2.82	0.42
1:A:278:MET:HA	1:A:363:VAL:O	2.19	0.42
1:D:425:GLU:O	1:D:429:VAL:HG13	2.20	0.42
1:B:107:HIS:HE1	5:B:2099:HOH:O	2.01	0.42
1:D:34:TYR:HH	1:D:126:ASN:ND2	2.12	0.42
1:D:458:GLN:O	1:D:462:GLU:HG3	2.20	0.42
1:A:118:ASN:ND2	1:A:196:ARG:HB3	2.34	0.42
1:D:299:MET:CE	2:D:1000:AMP:H2'	2.50	0.41
1:D:299:MET:HE1	2:D:1000:AMP:O2'	2.20	0.41
1:C:328:GLU:O	1:C:329:ARG:HB3	2.21	0.41
1:C:118:ASN:ND2	1:C:196:ARG:HB3	2.36	0.41
1:D:117:ASP:OD1	5:D:2084:HOH:O	2.20	0.41
1:D:118:ASN:HD21	1:D:197:GLY:N	2.16	0.41
1:B:12:SER:OG	5:B:2006:HOH:O	2.21	0.41
1:C:37:ARG:NE	1:C:70:GLU:OE2	2.53	0.41
1:D:383:GLU:OE2	1:D:387:MET:HE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLY:O	1:A:308:ALA:HB1	2.21	0.41
1:B:126:ASN:CB	5:B:2107:HOH:O	2.56	0.41
1:C:194:ARG:HD3	1:C:234:ARG:HD3	2.02	0.41
1:D:408:GLN:NE2	1:D:408:GLN:HA	2.30	0.41
1:D:328:GLU:O	1:D:329:ARG:HB3	2.21	0.41
1:D:383:GLU:HG3	1:D:387:MET:HE3	2.03	0.41
1:A:60:GLU:OE1	1:A:101:LYS:NZ	2.40	0.40
1:B:278:MET:HA	1:B:363:VAL:O	2.21	0.40
1:C:299[A]:MET:CE	2:C:1000:AMP:C8	3.02	0.40
1:D:47:ALA:HB2	5:D:2078:HOH:O	2.21	0.40
1:D:21:TYR:HB3	1:D:350:THR:HG21	2.04	0.40

All (1) 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)
5:A:2091:HOH:O	5:B:2124:HOH:O[3_555]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	453/503 (90%)	447 (99%)	5 (1%)	1 (0%)	47	33
1	B	456/503 (91%)	450 (99%)	5 (1%)	1 (0%)	47	33
1	C	455/503 (90%)	449 (99%)	5 (1%)	1 (0%)	47	33
1	D	454/503 (90%)	447 (98%)	6 (1%)	1 (0%)	47	33
All	All	1818/2012 (90%)	1793 (99%)	21 (1%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	B	329	ARG
1	C	329	ARG
1	D	329	ARG

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	403/438 (92%)	393 (98%)	10 (2%)	47	34
1	B	406/438 (93%)	396 (98%)	10 (2%)	47	34
1	C	402/438 (92%)	392 (98%)	10 (2%)	47	34
1	D	403/438 (92%)	390 (97%)	13 (3%)	39	25
All	All	1614/1752 (92%)	1571 (97%)	43 (3%)	46	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	190	ARG
1	A	228	GLU
1	A	264	LYS
1	A	329	ARG
1	A	360	GLU
1	A	396	ARG
1	A	408	GLN
1	A	458[A]	GLN
1	A	458[B]	GLN
1	B	6	ASP
1	B	190	ARG
1	B	211	LEU
1	B	228	GLU
1	B	292	MET
1	B	404	ARG
1	B	405	VAL
1	B	408	GLN

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Mol	Chain	Res	Type
1	B	436	ILE
1	B	444	LEU
1	C	37	ARG
1	C	160	PHE
1	C	190	ARG
1	C	228	GLU
1	C	329	ARG
1	C	391	LYS
1	C	396	ARG
1	C	412	SER
1	C	425	GLU
1	C	470	LYS
1	D	9	SER
1	D	117	ASP
1	D	160	PHE
1	D	210	GLN
1	D	228[A]	GLU
1	D	228[B]	GLU
1	D	329	ARG
1	D	402	LYS
1	D	404	ARG
1	D	405	VAL
1	D	408	GLN
1	D	444	LEU
1	D	473	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	93	HIS
1	A	107	HIS
1	A	118	ASN
1	A	126	ASN
1	A	159	HIS
1	A	177	GLN
1	A	185	ASN
1	A	408	GLN
1	A	439	GLN
1	B	68	ASN
1	B	107	HIS
1	B	118	ASN

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Mol	Chain	Res	Type
1	B	159	HIS
1	B	177	GLN
1	B	185	ASN
1	B	356	GLN
1	B	408	GLN
1	C	7	HIS
1	C	41	GLN
1	C	68	ASN
1	C	107	HIS
1	C	118	ASN
1	C	126	ASN
1	C	159	HIS
1	C	177	GLN
1	C	185	ASN
1	C	210	GLN
1	C	356	GLN
1	C	458	GLN
1	D	68	ASN
1	D	71	ASN
1	D	107	HIS
1	D	118	ASN
1	D	126	ASN
1	D	159	HIS
1	D	177	GLN
1	D	185	ASN
1	D	357	ASN
1	D	375	GLN
1	D	408	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	C	1000	-	22,25,25	1.30	3 (13%)	25,38,38	1.42	5 (20%)
2	AMP	B	1000	-	22,25,25	1.03	1 (4%)	25,38,38	1.49	4 (16%)
4	GOL	B	1482	-	5,5,5	0.43	0	5,5,5	0.64	0
2	AMP	D	1000	-	22,25,25	0.99	1 (4%)	25,38,38	1.63	6 (24%)
4	GOL	A	1475	-	5,5,5	0.40	0	5,5,5	0.58	0
4	GOL	D	1474	-	5,5,5	0.66	0	5,5,5	0.60	0
4	GOL	C	1473	-	5,5,5	0.48	0	5,5,5	0.32	0
2	AMP	A	1000	-	22,25,25	1.12	3 (13%)	25,38,38	1.41	3 (12%)

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	C	1000	-	-	1/6/26/26	0/3/3/3
2	AMP	B	1000	-	-	1/6/26/26	0/3/3/3
4	GOL	B	1482	-	-	1/4/4/4	-
2	AMP	D	1000	-	-	1/6/26/26	0/3/3/3
4	GOL	A	1475	-	-	0/4/4/4	-
4	GOL	D	1474	-	-	0/4/4/4	-
4	GOL	C	1473	-	-	0/4/4/4	-
2	AMP	A	1000	-	-	1/6/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	AMP	C2-N3	3.08	1.37	1.32
2	C	1000	AMP	O4'-C1'	2.92	1.45	1.41
2	C	1000	AMP	C5-C4	2.87	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	AMP	O4'-C1'	2.69	1.44	1.41
2	A	1000	AMP	C5-C4	2.48	1.47	1.40
2	A	1000	AMP	O4'-C1'	2.32	1.44	1.41
2	A	1000	AMP	C2-N3	2.32	1.35	1.32
2	C	1000	AMP	C2-N3	2.31	1.35	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1000	AMP	O3P-P-O5'	-3.63	97.07	106.73
2	D	1000	AMP	N6-C6-N1	3.49	125.83	118.57
2	C	1000	AMP	N3-C2-N1	-3.47	123.25	128.68
2	A	1000	AMP	N3-C2-N1	-3.41	123.35	128.68
2	D	1000	AMP	O4'-C1'-C2'	-3.36	102.02	106.93
2	B	1000	AMP	O4'-C1'-C2'	-2.98	102.56	106.93
2	D	1000	AMP	C5-C6-N6	-2.96	115.86	120.35
2	B	1000	AMP	N3-C2-N1	-2.92	124.11	128.68
2	D	1000	AMP	C1'-N9-C4	-2.77	121.77	126.64
2	C	1000	AMP	O3P-P-O5'	-2.65	99.69	106.73
2	B	1000	AMP	C1'-N9-C4	-2.36	122.49	126.64
2	A	1000	AMP	O2P-P-O1P	2.35	119.89	110.68
2	A	1000	AMP	C1'-N9-C4	-2.33	122.55	126.64
2	C	1000	AMP	C4-C5-N7	-2.30	107.00	109.40
2	C	1000	AMP	C2-N1-C6	2.17	122.47	118.75
2	D	1000	AMP	O3P-P-O2P	2.09	115.61	107.64
2	C	1000	AMP	C1'-N9-C4	-2.08	122.99	126.64
2	D	1000	AMP	N3-C2-N1	-2.03	125.50	128.68

There are no chirality outliers.
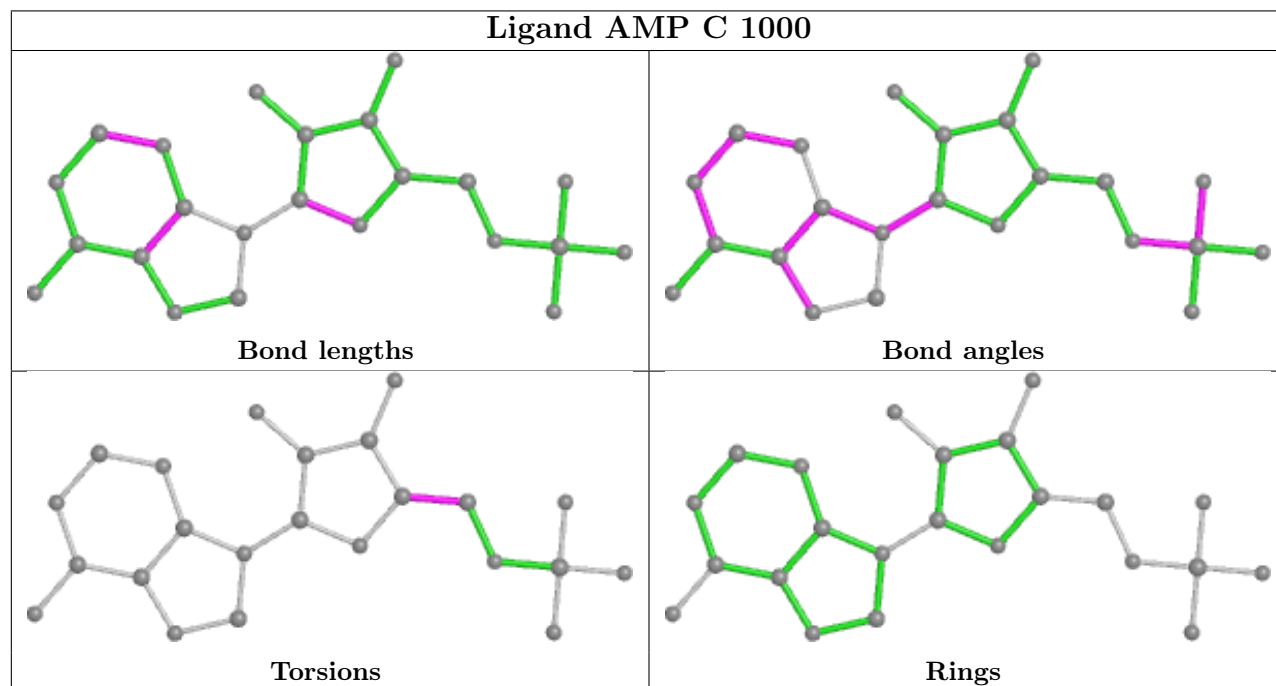
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1482	GOL	O1-C1-C2-C3
2	B	1000	AMP	O4'-C4'-C5'-O5'
2	C	1000	AMP	O4'-C4'-C5'-O5'
2	A	1000	AMP	O4'-C4'-C5'-O5'
2	D	1000	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	AMP	2	0
2	B	1000	AMP	1	0
2	D	1000	AMP	3	0
2	A	1000	AMP	1	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 then 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 C 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP B 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP D 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP A 1000

Bond lengths

Bond angles

Torsions

Rings
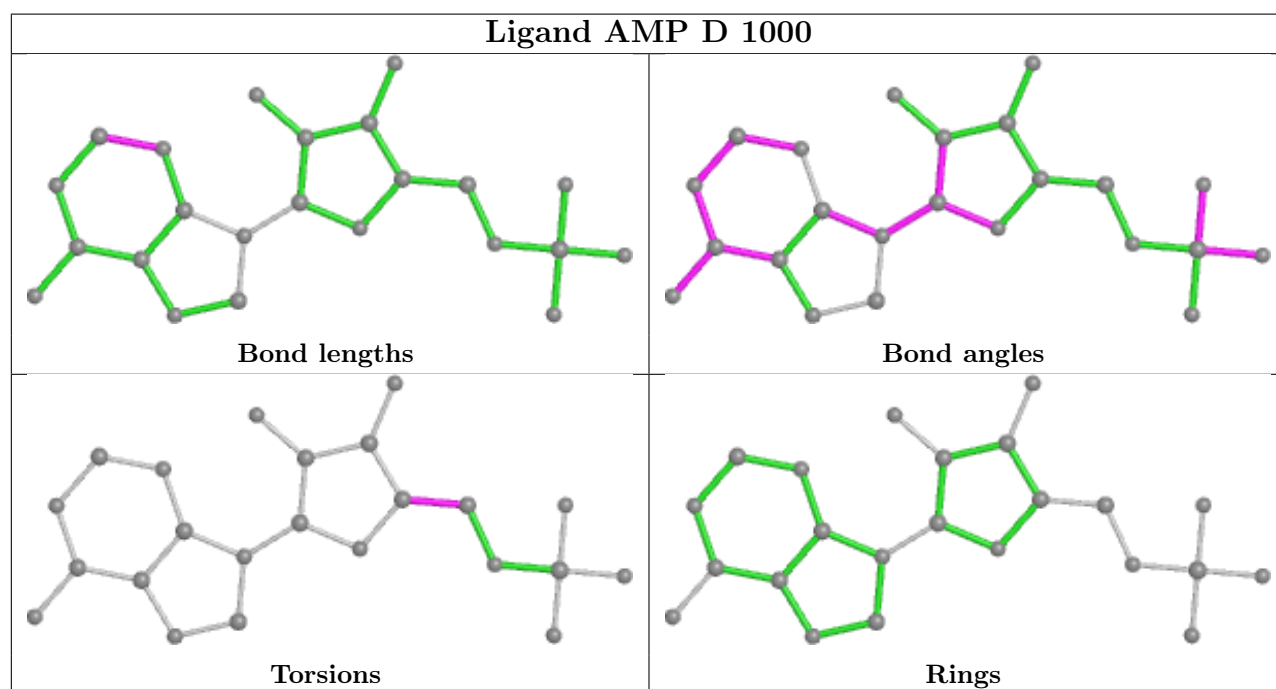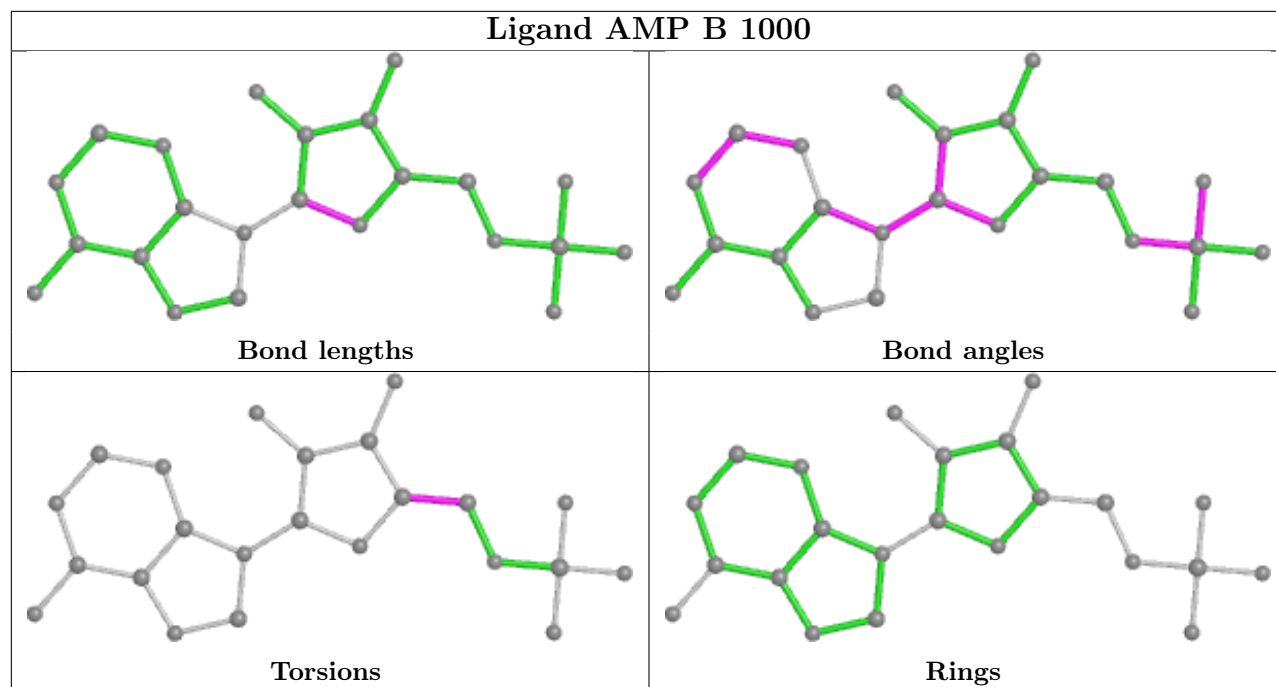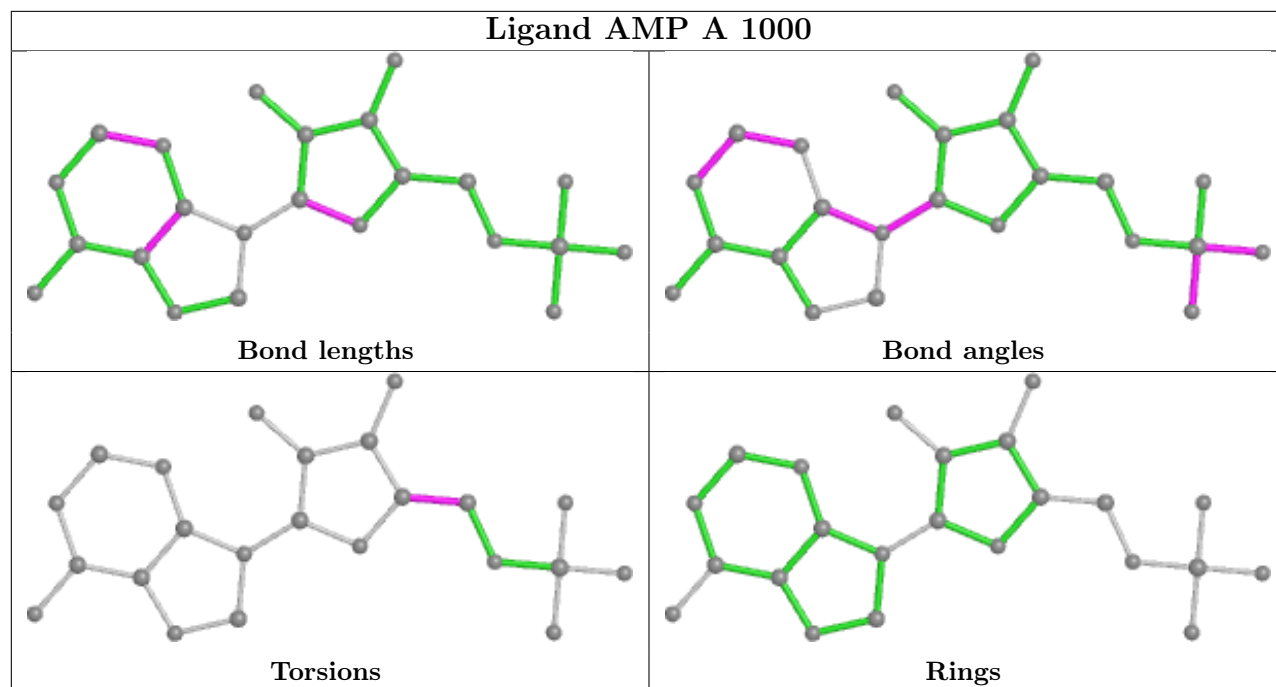
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	457/503 (90%)	0.65	54 (11%)	4	3	22, 28, 51, 72	0
1	B	463/503 (92%)	0.60	42 (9%)	9	7	23, 31, 49, 59	0
1	C	456/503 (90%)	0.59	46 (10%)	7	5	23, 28, 49, 62	0
1	D	456/503 (90%)	0.67	50 (10%)	5	4	23, 31, 53, 65	0
All	All	1832/2012 (91%)	0.63	192 (10%)	6	4	22, 29, 51, 72	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	TYR	8.4
1	A	19	SER	7.4
1	A	405	VAL	6.8
1	B	474	SER	6.6
1	C	438	SER	6.3
1	A	436	ILE	6.1
1	A	403	ILE	6.1
1	C	431	ALA	5.9
1	D	63	ARG	5.7
1	B	5	GLY	5.6
1	C	397	GLN	5.6
1	D	85	ARG	5.5
1	A	474	SER	5.5
1	A	404	ARG	5.4
1	C	391	LYS	5.4
1	D	100	PRO	5.4
1	D	93	HIS	5.4
1	D	62	ILE	5.2
1	D	5	GLY	5.1
1	A	397	GLN	5.1
1	A	406	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	97	HIS	5.0
1	D	104	GLY	5.0
1	B	401	GLU	5.0
1	A	5	GLY	4.9
1	C	393	GLY	4.9
1	D	82	LYS	4.8
1	A	401	GLU	4.8
1	C	441	ASP	4.7
1	A	399	CYS	4.6
1	D	99	CYS	4.6
1	B	67	SER	4.5
1	B	393	GLY	4.5
1	D	67	SER	4.4
1	B	391	LYS	4.4
1	D	89	MET	4.4
1	A	432	TYR	4.4
1	A	413	VAL	4.4
1	B	58	THR	4.4
1	B	292	MET	4.3
1	D	79	GLU	4.3
1	A	387	MET	4.3
1	A	442	HIS	4.3
1	C	6	ASP	4.2
1	C	392	ALA	4.2
1	B	99	CYS	4.2
1	D	101	LYS	4.1
1	D	102	ALA	4.1
1	C	399	CYS	4.0
1	A	398	ASP	4.0
1	A	408	GLN	4.0
1	C	19	SER	3.9
1	B	89	MET	3.9
1	D	94	THR	3.9
1	D	103	ALA	3.9
1	A	431	ALA	3.8
1	D	105	ILE	3.8
1	B	63	ARG	3.8
1	A	433	PHE	3.8
1	B	6	ASP	3.7
1	C	432	TYR	3.7
1	D	71	ASN	3.7
1	D	96	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	219	VAL	3.6
1	A	429	VAL	3.6
1	B	57	ILE	3.5
1	B	60	GLU	3.5
1	D	90	ALA	3.5
1	D	88	VAL	3.4
1	D	58	THR	3.4
1	B	397	GLN	3.4
1	A	438	SER	3.4
1	D	97	HIS	3.4
1	A	282	PHE	3.4
1	B	392	ALA	3.3
1	D	282	PHE	3.3
1	D	6	ASP	3.3
1	C	433	PHE	3.3
1	B	473	GLU	3.3
1	B	431	ALA	3.2
1	C	394	GLY	3.2
1	B	395	SER	3.1
1	C	396	ARG	3.1
1	B	56	PRO	3.1
1	A	427	ILE	3.1
1	A	6	ASP	3.1
1	A	473	GLU	3.1
1	A	439	GLN	3.1
1	C	375	GLN	3.1
1	A	412	SER	3.1
1	C	395	SER	3.1
1	A	385	ILE	3.0
1	C	408	GLN	3.0
1	D	57	ILE	3.0
1	D	387	MET	3.0
1	A	390	VAL	3.0
1	D	92	VAL	3.0
1	C	390	VAL	3.0
1	A	434	SER	3.0
1	D	293	PRO	3.0
1	D	435	PRO	2.9
1	B	96	GLY	2.9
1	B	104	GLY	2.9
1	C	442	HIS	2.9
1	C	281	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	383	GLU	2.9
1	D	390	VAL	2.9
1	D	385	ILE	2.9
1	C	386	ILE	2.8
1	C	295	LYS	2.8
1	A	414	VAL	2.8
1	C	382	THR	2.8
1	B	405	VAL	2.8
1	C	436	ILE	2.7
1	D	473	GLU	2.7
1	D	393	GLY	2.6
1	C	404	ARG	2.6
1	C	428	GLN	2.6
1	D	106	ILE	2.6
1	B	88	VAL	2.6
1	C	400	HIS	2.5
1	D	52	THR	2.5
1	A	60	GLU	2.5
1	C	387	MET	2.5
1	B	106	ILE	2.5
1	A	375	GLN	2.5
1	D	86	HIS	2.5
1	C	439	GLN	2.4
1	D	221	GLN	2.4
1	B	442	HIS	2.4
1	C	383	GLU	2.4
1	A	441	ASP	2.4
1	A	85	ARG	2.4
1	D	432	TYR	2.4
1	A	389	MET	2.4
1	A	396	ARG	2.4
1	C	5	GLY	2.3
1	C	424	ILE	2.3
1	C	472	TYR	2.3
1	C	398	ASP	2.3
1	B	79	GLU	2.3
1	C	434	SER	2.3
1	C	420	ASP	2.3
1	B	93	HIS	2.3
1	A	8	GLY	2.3
1	B	62	ILE	2.3
1	D	70	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	84	LEU	2.3
1	A	7	HIS	2.3
1	A	148	GLU	2.3
1	B	217	HIS	2.3
1	D	95	PHE	2.2
1	B	233	LYS	2.2
1	A	440	LEU	2.2
1	D	54	GLY	2.2
1	D	78	ALA	2.2
1	A	164	GLN	2.2
1	A	374	ARG	2.2
1	B	59	ASP	2.2
1	C	389	MET	2.2
1	A	470	LYS	2.2
1	D	98	CYS	2.2
1	C	296	ARG	2.2
1	B	398	ASP	2.2
1	C	401	GLU	2.2
1	D	436	ILE	2.2
1	B	222	LEU	2.2
1	B	85	ARG	2.2
1	B	103	ALA	2.2
1	C	7	HIS	2.1
1	B	383	GLU	2.1
1	A	75	LYS	2.1
1	C	447	SER	2.1
1	A	386	ILE	2.1
1	A	394	GLY	2.1
1	C	440	LEU	2.1
1	D	51	GLN	2.1
1	B	98	CYS	2.1
1	C	419	GLY	2.1
1	A	410	ALA	2.1
1	B	436	ILE	2.1
1	C	403	ILE	2.1
1	A	435	PRO	2.1
1	B	478	VAL	2.1
1	C	85	ARG	2.0
1	D	210	GLN	2.0
1	A	56	PRO	2.0
1	A	62	ILE	2.0
1	B	228	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	425	GLU	2.0
1	D	433	PHE	2.0
1	A	400	HIS	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 monosaccharides 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(Å^2)	Q<0.9
2	AMP	C	1000	23/23	0.77	0.31	35,46,47,49	0
4	GOL	B	1482	6/6	0.80	0.17	35,36,37,38	0
2	AMP	A	1000	23/23	0.88	0.19	26,35,38,40	0
4	GOL	A	1475	6/6	0.93	0.15	21,23,26,27	0
4	GOL	D	1474	6/6	0.95	0.15	21,25,28,28	0
2	AMP	D	1000	23/23	0.97	0.09	13,16,20,21	0
4	GOL	C	1473	6/6	0.97	0.14	17,23,24,25	0
2	AMP	B	1000	23/23	0.97	0.11	12,14,18,20	0
3	CL	B	1001	1/1	0.98	0.13	27,27,27,27	0
3	CL	D	1001	1/1	0.99	0.08	29,29,29,29	0
3	CL	C	1001	1/1	1.00	0.06	13,13,13,13	0
3	CL	A	1001	1/1	1.00	0.03	17,17,17,17	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 C 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
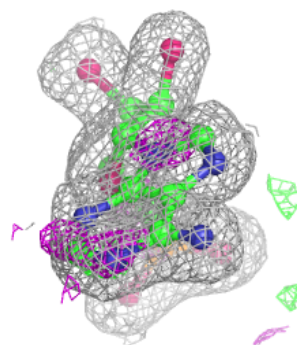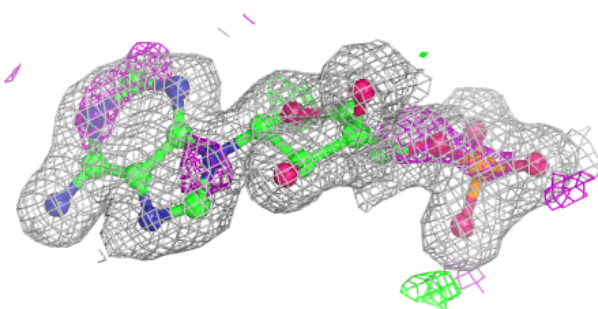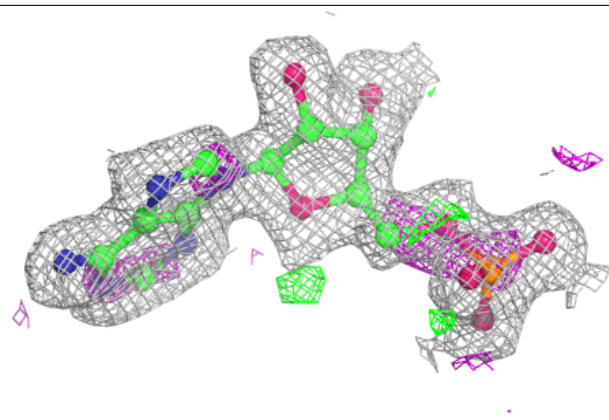and green (positive)
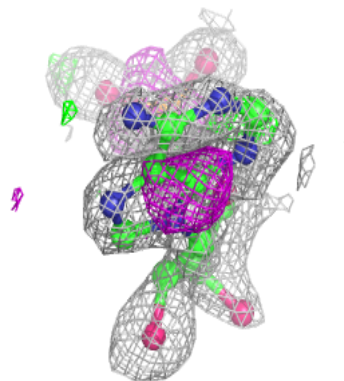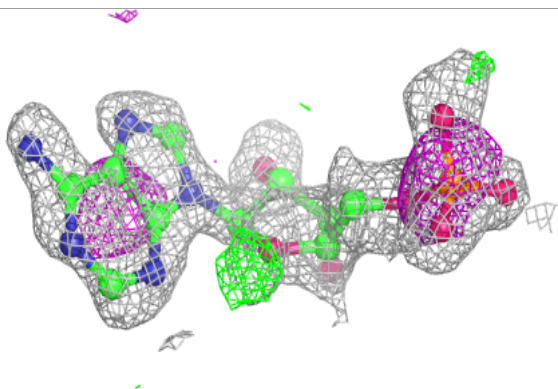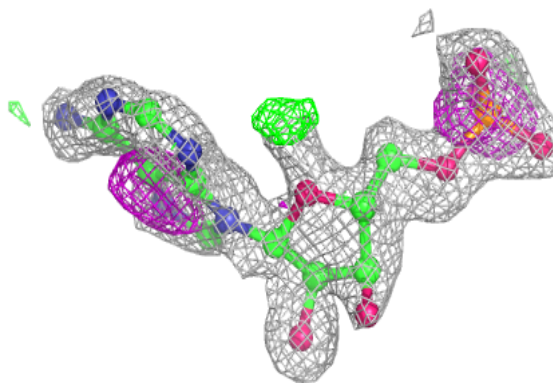
Electron density around AMP A 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
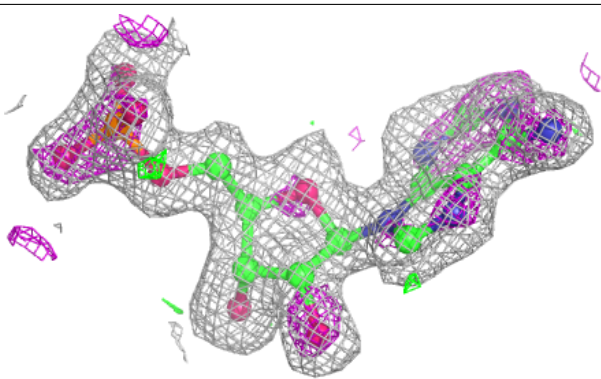mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
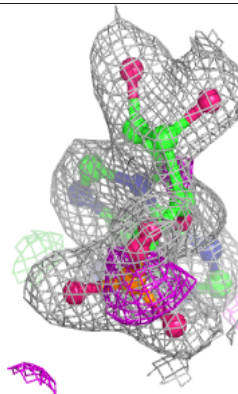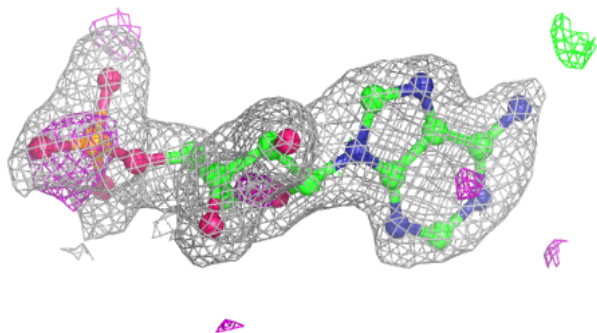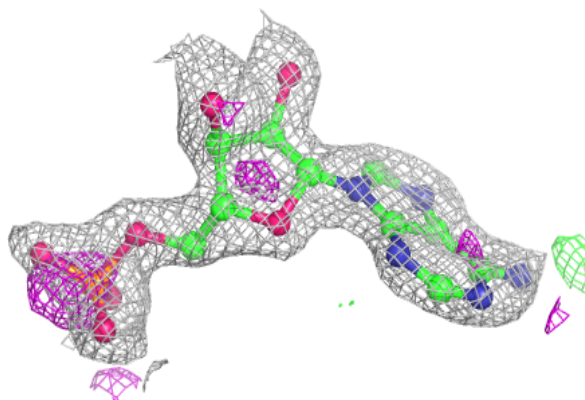
Electron density around AMP D 1000:

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

Electron density around AMP B 1000:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
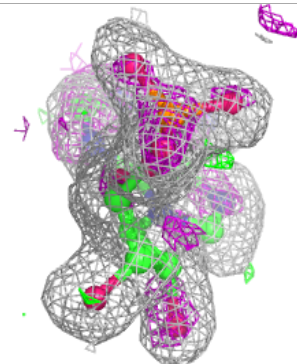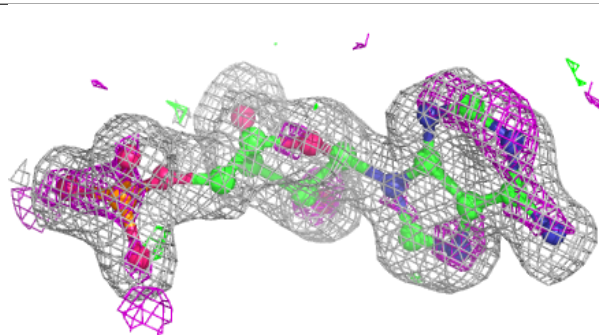
6.5 Other polymers (i)

There are no such residues in this entry.