



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:53 AM UTC

PDB ID : 2FSH / pdb_00002fsh
Title : Complex SecA:AMP-PNP from Escherichia coli
Authors : Papanikolaou, Y.; Petratos, K.; Economou, A.
Deposited on : 2006-01-23
Resolution : 2.00 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

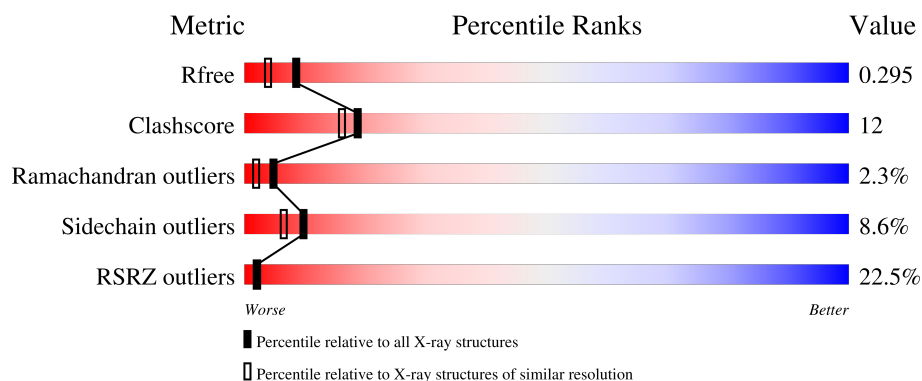
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	853	
1	B	853	

2 Entry composition [i](#)

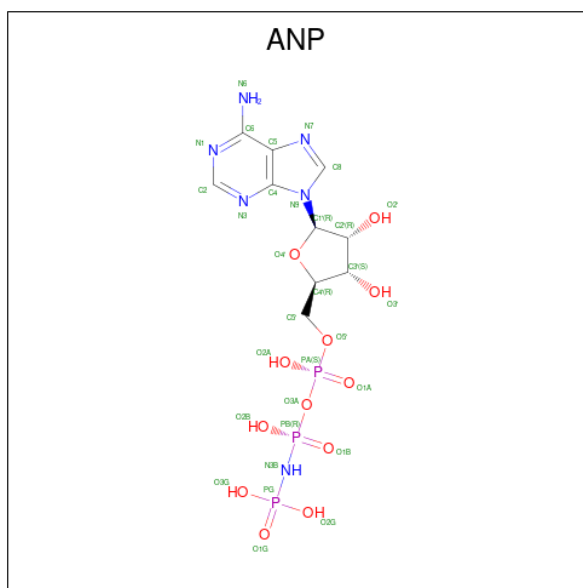
There are 3 unique types of molecules in this entry. The entry contains 11728 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Preprotein translocase secA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5500	3445	971	1058	26			
1	B	722	Total	C	N	O	S	0	0	0
			5735	3596	1008	1102	29			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	189	Total 189	O 189	0	0
3	B	242	Total 242	O 242	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.02Å 90.01Å 163.02Å 90.00° 100.52° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.5 (19.97-2.00) 90.4 (19.97-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.204 , 0.255 0.255 , 0.295	Depositor DCC
R_{free} test set	6538 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11728	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: ANP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.47	29/5590 (0.5%)	1.26	24/7542 (0.3%)
1	B	1.61	58/5827 (1.0%)	1.33	32/7861 (0.4%)
All	All	1.54	87/11417 (0.8%)	1.29	56/15403 (0.4%)

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	A	0	3
1	B	0	4
All	All	0	7

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	GLU	C-O	27.57	1.56	1.24
1	B	64	ILE	CA-CB	14.56	1.62	1.54
1	A	697	LEU	C-N	12.22	1.50	1.33
1	B	32	GLU	C-O	-9.98	1.14	1.24
1	A	693	PRO	C-O	9.65	1.35	1.24
1	B	393	THR	CA-CB	9.63	1.71	1.53
1	B	394	ALA	CA-C	9.07	1.65	1.52
1	B	672	VAL	CA-CB	8.89	1.64	1.54
1	B	393	THR	N-CA	8.82	1.58	1.46
1	B	23	LYS	CE-NZ	8.70	1.75	1.49
1	B	156	ILE	C-O	-8.63	1.14	1.24
1	B	405	TYR	CA-C	-8.46	1.41	1.52
1	A	699	GLU	CD-OE2	8.39	1.41	1.25
1	B	402	SER	N-CA	-7.82	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	789	ILE	CA-CB	7.61	1.64	1.54
1	B	114	LEU	N-CA	-7.56	1.41	1.46
1	B	394	ALA	CA-CB	7.52	1.66	1.53
1	A	393	THR	CA-CB	7.34	1.65	1.53
1	B	626	ALA	CA-CB	-7.23	1.42	1.53
1	A	393	THR	CA-C	7.13	1.62	1.52
1	B	163	ALA	CA-CB	6.98	1.63	1.53
1	A	697	LEU	C-O	6.95	1.33	1.23
1	A	696	SER	CB-OG	6.83	1.55	1.42
1	B	503	ALA	CA-CB	-6.79	1.38	1.53
1	A	696	SER	CA-C	6.76	1.62	1.53
1	B	88	LEU	N-CA	6.72	1.54	1.46
1	B	806	GLU	C-O	-6.72	1.16	1.24
1	A	378	GLN	N-CA	-6.71	1.38	1.46
1	A	789	ILE	CA-CB	6.69	1.61	1.53
1	B	140	ALA	N-CA	-6.54	1.38	1.46
1	A	163	ALA	C-O	-6.49	1.18	1.24
1	B	199	VAL	N-CA	6.46	1.53	1.45
1	B	393	THR	CA-C	6.39	1.61	1.52
1	B	217	ASP	C-O	-6.32	1.16	1.24
1	B	379	ASN	C-O	-6.24	1.16	1.24
1	B	204	HIS	N-CA	6.23	1.54	1.46
1	B	23	LYS	CG-CD	6.22	1.71	1.52
1	A	686	ALA	C-O	-6.16	1.17	1.24
1	A	394	ALA	N-CA	6.13	1.54	1.46
1	B	404	ILE	CA-C	6.09	1.61	1.52
1	B	404	ILE	CA-CB	-6.01	1.46	1.54
1	A	574	ARG	N-CA	-6.00	1.38	1.46
1	B	636	SER	N-CA	-5.91	1.38	1.46
1	B	392	GLY	N-CA	5.88	1.53	1.45
1	B	448	LYS	CE-NZ	5.88	1.67	1.49
1	A	437	ALA	C-O	-5.86	1.17	1.24
1	B	512	ASP	CA-C	5.86	1.60	1.52
1	B	66	GLU	CA-C	-5.80	1.45	1.52
1	B	651	VAL	CA-CB	-5.80	1.47	1.54
1	B	393	THR	C-O	5.79	1.31	1.24
1	A	98	CYS	CB-SG	-5.78	1.62	1.81
1	B	200	GLN	N-CA	-5.75	1.38	1.45
1	B	767	MET	N-CA	-5.73	1.39	1.46
1	A	225	ILE	CA-C	-5.66	1.46	1.52
1	B	472	ALA	CA-CB	-5.66	1.44	1.53
1	B	512	ASP	CB-CG	5.65	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	800	LYS	C-O	-5.57	1.17	1.24
1	A	135	LEU	C-O	-5.56	1.17	1.24
1	A	439	ILE	CA-CB	5.55	1.60	1.54
1	B	395	ASP	N-CA	5.46	1.53	1.46
1	B	86	VAL	N-CA	5.46	1.53	1.46
1	A	180	ASN	N-CA	-5.42	1.39	1.46
1	A	495	GLY	C-O	-5.40	1.19	1.24
1	B	658	ALA	CA-CB	-5.38	1.44	1.53
1	B	170	TYR	N-CA	-5.37	1.39	1.46
1	B	571	LEU	CA-C	5.31	1.59	1.52
1	B	652	ALA	CA-CB	5.31	1.61	1.53
1	B	112	ALA	C-O	5.29	1.30	1.24
1	A	554	LEU	C-O	-5.29	1.17	1.23
1	A	177	GLY	C-O	-5.22	1.17	1.24
1	A	476	HIS	N-CA	-5.20	1.40	1.46
1	B	103	ARG	CG-CD	5.20	1.68	1.52
1	B	114	LEU	C-O	-5.15	1.20	1.24
1	B	831	VAL	CA-CB	5.13	1.61	1.54
1	B	572	ARG	CB-CG	-5.12	1.37	1.52
1	B	110	LEU	C-O	5.10	1.30	1.24
1	A	752	GLU	CG-CD	5.09	1.64	1.52
1	B	64	ILE	C-O	-5.05	1.20	1.24
1	B	551	ALA	CA-CB	-5.04	1.44	1.53
1	A	466	SER	C-O	5.04	1.29	1.24
1	B	630	ALA	CA-CB	-5.03	1.45	1.53
1	B	404	ILE	C-O	5.03	1.30	1.24
1	A	120	ALA	CA-CB	-5.02	1.45	1.53
1	B	108	LYS	CG-CD	5.02	1.67	1.52
1	B	136	ALA	CA-CB	5.01	1.61	1.53
1	B	117	TYR	CA-C	-5.00	1.46	1.52
1	B	128	VAL	N-CA	-5.00	1.40	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	723	TRP	N-CA-C	-10.36	99.54	111.03
1	A	672	VAL	N-CA-CB	-8.26	101.60	112.26
1	A	367	ASN	N-CA-C	8.24	121.33	109.71
1	B	228	PRO	N-CA-C	-7.53	103.06	113.53
1	B	657	ARG	NE-CZ-NH2	7.41	125.87	119.20
1	A	697	LEU	N-CA-C	-7.23	101.21	110.53
1	A	697	LEU	O-C-N	7.08	131.36	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	568	ASP	N-CA-C	-6.80	103.95	111.36
1	B	801	GLN	N-CA-CB	6.62	121.68	110.49
1	A	672	VAL	CB-CA-C	6.58	119.36	111.20
1	A	664	ASN	N-CA-C	6.51	118.45	111.36
1	B	800	LYS	N-CA-C	-6.45	100.28	109.96
1	B	14	ASN	N-CA-C	-6.41	104.37	111.36
1	B	36	GLU	N-CA-C	6.39	119.06	111.71
1	A	697	LEU	CA-C-N	-6.36	111.26	120.29
1	A	697	LEU	C-N-CA	-6.36	111.26	120.29
1	B	519	TRP	N-CA-C	-6.30	104.15	112.72
1	A	530	THR	N-CA-C	6.14	117.49	107.23
1	A	72	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	A	669	VAL	N-CA-C	6.10	118.25	108.85
1	B	209	ASP	N-CA-C	6.03	118.81	111.82
1	A	180	ASN	N-CA-C	5.98	118.29	111.11
1	B	217	ASP	N-CA-C	-5.98	104.76	111.28
1	A	158	LEU	CA-C-N	5.97	126.27	119.83
1	A	158	LEU	C-N-CA	5.97	126.27	119.83
1	B	669	VAL	CB-CA-C	5.96	119.71	110.83
1	B	392	GLY	CA-C-N	5.95	132.05	120.99
1	B	392	GLY	C-N-CA	5.95	132.05	120.99
1	B	613	LYS	CA-C-N	5.95	127.27	119.84
1	B	613	LYS	C-N-CA	5.95	127.27	119.84
1	B	99	ILE	CB-CA-C	-5.91	102.80	110.84
1	A	567	ILE	N-CA-C	5.89	116.07	110.42
1	B	411	VAL	CB-CA-C	-5.84	103.84	111.25
1	A	754	VAL	CB-CA-C	-5.78	104.50	112.24
1	B	23	LYS	CD-CE-NZ	5.77	130.37	111.90
1	A	673	SER	CB-CA-C	-5.77	101.16	110.74
1	A	613	LYS	CA-C-N	5.73	127.00	119.84
1	A	613	LYS	C-N-CA	5.73	127.00	119.84
1	A	210	GLU	CB-CA-C	-5.73	103.10	111.23
1	B	139	ASP	N-CA-C	5.68	117.47	111.28
1	B	547	ALA	N-CA-C	5.65	117.44	111.28
1	B	607	MET	N-CA-C	-5.60	105.18	111.28
1	A	639	PHE	N-CA-C	5.51	117.36	111.36
1	B	393	THR	CA-C-O	5.42	125.93	119.10
1	B	639	PHE	N-CA-C	5.38	117.90	111.71
1	B	121	LEU	N-CA-C	5.34	117.10	111.28
1	A	674	GLU	N-CA-C	-5.28	105.60	111.36
1	A	368	GLU	N-CA-C	5.20	121.87	110.80
1	B	517	GLY	N-CA-C	-5.18	106.76	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	VAL	N-CA-C	-5.15	107.81	112.96
1	B	657	ARG	CG-CD-NE	5.09	123.19	112.00
1	B	416	ARG	CA-C-N	-5.06	114.55	119.76
1	B	416	ARG	C-N-CA	-5.06	114.55	119.76
1	A	90	GLY	N-CA-C	-5.03	106.33	112.77
1	B	642	ARG	N-CA-C	5.02	116.75	111.28
1	B	650	ASP	N-CA-C	-5.01	106.67	112.89

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLN	Peptide
1	A	393	THR	Peptide
1	A	800	LYS	Peptide
1	B	229	ALA	Peptide
1	B	393	THR	Peptide
1	B	394	ALA	Peptide
1	B	613	LYS	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	5500	0	5481	112	0
1	B	5735	0	5724	158	0
2	A	31	0	13	1	0
2	B	31	0	13	7	0
3	A	189	0	0	18	1
3	B	242	0	0	25	1
All	All	11728	0	11231	267	2

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 12.

All (267) 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:B:23:LYS:CE	1:B:23:LYS:NZ	1.75	1.49
1:B:369:ASN:C	1:B:369:ASN:HD22	1.39	1.29
1:B:757:GLU:HG3	3:B:1056:HOH:O	1.51	1.08
1:A:731:HIS:CE1	1:A:733:GLU:HB3	1.94	1.01
1:B:782:MET:HE1	1:B:810:MET:CE	1.97	0.94
1:B:369:ASN:C	1:B:369:ASN:ND2	2.18	0.93
1:A:799:PRO:O	1:A:800:LYS:HB3	1.67	0.92
1:A:31:MET:HE1	1:A:66:GLU:HG2	1.49	0.92
1:A:144:ARG:HG2	1:A:148:GLU:OE1	1.67	0.92
1:A:657:ARG:HD3	3:A:1026:HOH:O	1.72	0.90
1:B:782:MET:HE1	1:B:810:MET:HE3	1.53	0.89
1:B:520:GLN:HA	3:B:1094:HOH:O	1.74	0.86
1:A:144:ARG:CG	1:A:148:GLU:OE1	2.24	0.85
1:B:693:PRO:O	1:B:696:SER:HB2	1.79	0.82
1:B:747:TYR:OH	1:B:763:GLU:OE2	1.97	0.81
1:B:108:LYS:HB2	2:B:901:ANP:PG	2.21	0.81
1:B:369:ASN:HD22	1:B:370:GLN:N	1.83	0.77
1:B:102:MET:HE3	1:B:108:LYS:HG2	1.65	0.77
1:B:457:ILE:O	1:B:505:ASN:ND2	2.16	0.77
1:A:577:ARG:HD3	3:A:1054:HOH:O	1.85	0.76
1:B:228:PRO:O	1:B:230:GLU:OE1	2.02	0.76
1:A:799:PRO:O	1:A:800:LYS:CB	2.34	0.75
1:B:629:ASN:HD22	1:B:632:ARG:NH2	1.86	0.73
1:B:108:LYS:HB2	2:B:901:ANP:N3B	2.03	0.73
1:B:637:ARG:NH1	1:B:641:ILE:HD11	2.02	0.73
1:B:759:MET:HA	1:B:759:MET:HE3	1.69	0.73
1:B:618:ILE:O	1:B:619:GLU:HB2	1.88	0.72
1:B:104:THR:HG21	1:B:577:ARG:CZ	2.20	0.72
1:B:108:LYS:HE2	2:B:901:ANP:O1G	1.90	0.71
1:B:396:THR:N	3:B:931:HOH:O	2.22	0.71
1:B:647:GLU:OE2	1:B:800:LYS:HE3	1.91	0.70
1:A:428:TYR:HB3	1:A:433:GLU:HG3	1.72	0.70
1:A:598:PHE:O	1:A:600:SER:N	2.24	0.70
1:A:609:LYS:HB2	3:A:1080:HOH:O	1.90	0.70
1:A:742:GLN:HA	1:A:742:GLN:HE21	1.56	0.70
1:B:395:ASP:CB	3:B:925:HOH:O	2.39	0.69
1:A:594:LEU:HD23	1:A:594:LEU:O	1.92	0.68
1:B:227:GLY:HA3	1:B:372:LEU:HD11	1.73	0.68
1:A:102:MET:HE3	1:A:108:LYS:HG2	1.75	0.67
1:B:395:ASP:HB2	3:B:925:HOH:O	1.94	0.67
1:B:103:ARG:HD3	1:B:104:THR:O	1.95	0.67
1:B:369:ASN:HB2	3:B:1106:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLU:HB2	3:B:1087:HOH:O	1.94	0.66
1:B:104:THR:HG21	1:B:577:ARG:NH2	2.11	0.66
1:A:395:ASP:CG	1:A:396:THR:N	2.49	0.64
1:B:523:VAL:HG22	3:B:1094:HOH:O	1.96	0.64
1:A:618:ILE:O	1:A:619:GLU:HB2	1.98	0.64
1:B:228:PRO:O	1:B:230:GLU:N	2.30	0.64
1:B:600:SER:HB3	1:B:603:VAL:HB	1.80	0.64
1:A:15:ASP:HA	1:A:18:LEU:HB2	1.80	0.62
1:A:394:ALA:HA	3:A:1045:HOH:O	1.99	0.62
1:A:614:PRO:HA	3:A:1005:HOH:O	2.00	0.61
1:B:395:ASP:CA	3:B:925:HOH:O	2.48	0.61
1:A:429:MET:HG2	1:A:612:MET:SD	2.40	0.61
1:A:741:ALA:N	3:A:1046:HOH:O	2.33	0.61
1:B:17:THR:HG22	1:B:21:MET:HE2	1.82	0.61
1:A:29:ASN:OD1	1:A:72:ARG:NH1	2.29	0.60
1:B:223:LEU:HD21	1:B:377:PHE:CZ	2.37	0.59
1:B:651:VAL:CG2	1:B:804:LYS:HG2	2.32	0.59
1:B:629:ASN:ND2	1:B:632:ARG:NH2	2.51	0.59
1:B:459:ILE:O	1:B:463:GLU:HG3	2.02	0.59
1:B:782:MET:HE1	1:B:810:MET:HE1	1.82	0.59
1:B:282:ILE:O	1:B:286:LEU:HB2	2.02	0.59
1:B:137:GLN:CD	3:B:1081:HOH:O	2.47	0.58
1:A:591:GLU:O	1:A:592:ASP:C	2.46	0.58
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.85	0.58
1:A:395:ASP:CG	1:A:396:THR:H	2.12	0.58
1:A:538:LYS:NZ	1:B:528:ASN:ND2	2.52	0.58
1:B:718:LEU:O	1:B:720:ILE:N	2.37	0.57
1:B:484:HIS:HD2	1:B:487:GLU:OE2	1.86	0.57
1:B:518:SER:CB	1:B:520:GLN:HE21	2.18	0.57
1:B:518:SER:C	1:B:520:GLN:H	2.12	0.56
1:B:229:ALA:HB3	1:B:372:LEU:HD21	1.87	0.56
1:A:72:ARG:HD2	1:A:82:ARG:HG2	1.86	0.56
1:A:722:GLU:HB3	1:A:726:LYS:HZ2	1.70	0.56
1:A:538:LYS:NZ	1:B:528:ASN:HD21	2.03	0.56
1:B:613:LYS:HB3	1:B:614:PRO:HD2	1.88	0.56
1:A:486:ASN:HD21	1:B:132:ASN:HD21	1.55	0.55
1:A:531:ALA:O	1:A:532:GLU:C	2.49	0.55
1:A:392:GLY:O	1:A:394:ALA:N	2.40	0.55
1:B:510:GLY:HA3	1:B:574:ARG:HH12	1.71	0.55
1:A:17:THR:O	1:A:21:MET:HG3	2.08	0.54
1:A:519:TRP:HA	1:A:522:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:HG23	1:B:509:ARG:HE	1.72	0.54
1:B:613:LYS:HB3	1:B:614:PRO:CD	2.37	0.54
1:B:101:GLU:CD	1:B:393:THR:HA	2.32	0.54
1:B:519:TRP:CH2	1:B:538:LYS:HE2	2.43	0.54
1:A:594:LEU:C	1:A:596:ARG:H	2.16	0.54
1:A:797:LYS:HD2	3:A:1048:HOH:O	2.08	0.54
1:A:531:ALA:O	1:A:534:ILE:HG13	2.08	0.54
1:A:471:LYS:HE2	3:A:1078:HOH:O	2.07	0.54
1:B:395:ASP:HB2	3:B:931:HOH:O	2.07	0.54
1:B:409:THR:HG23	3:B:930:HOH:O	2.08	0.54
2:A:900:ANP:O1A	2:A:900:ANP:O2G	2.25	0.53
1:B:293:ASP:N	1:B:293:ASP:OD2	2.40	0.53
1:B:713:ASP:OD2	1:B:820:TYR:OH	2.22	0.53
1:B:392:GLY:O	1:B:394:ALA:HB3	2.09	0.53
1:A:32:GLU:HB3	1:A:33:PRO:HD3	1.90	0.53
1:A:730:LEU:HD12	1:A:734:THR:OG1	2.09	0.53
1:B:179:ASN:OD1	1:B:180:ASN:ND2	2.42	0.53
1:A:409:THR:HG23	3:A:924:HOH:O	2.08	0.53
1:A:669:VAL:HG22	1:A:670:SER:N	2.24	0.53
1:B:18:LEU:HD23	1:B:21:MET:CE	2.39	0.53
1:B:792:ARG:HB2	3:B:1142:HOH:O	2.08	0.52
1:A:99:ILE:HB	1:A:409:THR:HB	1.89	0.52
1:B:137:GLN:NE2	3:B:1081:HOH:O	2.42	0.52
1:B:304:ILE:HG21	1:B:781:ALA:HB1	1.91	0.52
1:B:691:TYR:HB3	1:B:702:ASP:O	2.09	0.52
1:B:282:ILE:HG13	1:B:286:LEU:HD12	1.92	0.52
1:A:657:ARG:CD	3:A:1026:HOH:O	2.44	0.52
1:B:79:PHE:HB3	1:B:81:MET:CE	2.40	0.52
1:B:594:LEU:HG	1:B:597:ILE:HD13	1.91	0.52
1:B:103:ARG:HG3	1:B:103:ARG:HH11	1.75	0.51
1:B:789:ILE:HG22	1:B:789:ILE:O	2.11	0.51
1:A:696:SER:HG	1:A:701:TRP:CD1	2.29	0.51
1:A:395:ASP:N	3:A:1045:HOH:O	2.43	0.51
1:A:397:GLU:OE1	1:A:566:ARG:NH2	2.44	0.51
1:A:531:ALA:O	1:A:533:GLN:N	2.44	0.51
1:A:392:GLY:C	1:A:394:ALA:N	2.69	0.51
1:B:393:THR:O	1:B:395:ASP:N	2.44	0.51
1:B:394:ALA:HB3	3:B:909:HOH:O	2.11	0.51
1:B:566:ARG:O	1:B:570:GLN:HG3	2.10	0.51
1:A:519:TRP:CH2	1:A:538:LYS:HD3	2.46	0.50
1:B:287:VAL:O	1:B:288:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLU:HA	1:B:287:VAL:HG12	1.93	0.50
1:B:522:GLU:N	3:B:1087:HOH:O	2.44	0.50
1:B:745:GLU:HG2	1:B:746:VAL:N	2.27	0.50
1:A:104:THR:HG21	1:A:577:ARG:NH2	2.26	0.50
1:B:563:GLU:HG2	1:B:634:VAL:HG11	1.93	0.50
1:B:594:LEU:O	1:B:597:ILE:HG12	2.12	0.49
1:B:73:GLU:O	1:B:77:ARG:HG3	2.12	0.49
1:A:460:GLU:CD	1:A:460:GLU:H	2.21	0.49
1:B:771:LEU:C	1:B:771:LEU:HD23	2.37	0.49
1:A:519:TRP:CZ2	1:A:538:LYS:HD3	2.47	0.49
1:A:789:ILE:O	1:A:790:HIS:CG	2.65	0.49
1:B:693:PRO:O	1:B:696:SER:CB	2.57	0.49
1:B:108:LYS:HB2	2:B:901:ANP:O2G	2.11	0.49
1:B:789:ILE:O	1:B:789:ILE:CG2	2.61	0.49
1:B:519:TRP:C	3:B:1087:HOH:O	2.56	0.49
1:B:595:MET:HE2	1:B:607:MET:HE2	1.95	0.49
1:B:657:ARG:HH21	1:B:657:ARG:HG3	1.76	0.49
2:B:901:ANP:O3G	2:B:901:ANP:O3A	2.31	0.49
1:B:198:ARG:HH21	1:B:664:ASN:HD22	1.60	0.48
1:B:518:SER:HB2	1:B:520:GLN:HE21	1.78	0.48
1:B:618:ILE:HG22	1:B:619:GLU:N	2.29	0.48
1:A:13:ARG:NE	1:A:13:ARG:HA	2.28	0.48
1:A:669:VAL:HG22	1:A:671:ASP:H	1.78	0.48
1:B:506:MET:HA	3:B:1015:HOH:O	2.13	0.48
1:B:671:ASP:OD1	1:B:673:SER:OG	2.29	0.48
1:A:531:ALA:HA	1:A:534:ILE:HD11	1.96	0.47
1:A:538:LYS:HZ3	1:B:528:ASN:HD21	1.61	0.47
1:B:198:ARG:HH21	1:B:664:ASN:ND2	2.11	0.47
1:B:635:GLU:HB3	3:B:1031:HOH:O	2.13	0.47
1:A:752:GLU:HB3	3:A:1075:HOH:O	2.15	0.47
1:B:724:LEU:CD2	1:B:730:LEU:HD11	2.44	0.47
1:B:801:GLN:HA	1:B:801:GLN:OE1	2.14	0.47
1:A:229:ALA:HB3	1:A:776:LYS:HZ3	1.79	0.47
1:B:531:ALA:O	1:B:535:GLU:HB3	2.14	0.47
1:A:698:GLU:O	1:A:701:TRP:HB2	2.15	0.47
1:B:13:ARG:N	1:B:15:ASP:OD1	2.47	0.47
1:B:666:LEU:O	1:B:764:LYS:HE3	2.15	0.47
1:A:731:HIS:CD2	1:A:734:THR:HG23	2.49	0.47
1:A:457:ILE:HG22	1:A:562:HIS:CE1	2.50	0.47
1:B:308:HIS:CE1	1:B:784:TYR:CZ	3.03	0.46
1:B:504:THR:O	1:B:505:ASN:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:GLU:OE2	1:B:800:LYS:CE	2.61	0.46
1:A:101:GLU:OE2	1:A:393:THR:HA	2.14	0.46
1:A:211:VAL:HG11	1:A:389:GLY:HA3	1.97	0.46
1:A:229:ALA:O	1:A:231:ASP:N	2.48	0.46
1:A:378:GLN:O	1:A:382:ARG:HG3	2.15	0.46
1:A:800:LYS:H	1:A:803:TYR:H	1.64	0.46
1:A:679:ILE:HG13	1:A:823:ILE:HD11	1.97	0.46
1:B:79:PHE:HB3	1:B:81:MET:HE2	1.98	0.46
1:B:798:ASP:CG	1:B:800:LYS:O	2.59	0.46
1:A:618:ILE:O	1:A:619:GLU:CB	2.64	0.46
1:B:506:MET:SD	1:B:574:ARG:NE	2.89	0.46
1:A:571:LEU:O	1:A:574:ARG:HB2	2.16	0.45
1:A:367:ASN:O	1:A:368:GLU:O	2.33	0.45
1:A:731:HIS:NE2	1:A:734:THR:HG23	2.31	0.45
1:B:300:SER:OG	1:B:303:ASN:ND2	2.49	0.45
1:B:607:MET:HB3	1:B:612:MET:HE1	1.99	0.45
1:B:518:SER:CB	1:B:520:GLN:NE2	2.79	0.45
1:B:757:GLU:HB2	3:B:1069:HOH:O	2.15	0.45
1:B:759:MET:HA	1:B:759:MET:CE	2.41	0.45
1:A:531:ALA:O	1:A:534:ILE:CG1	2.65	0.45
1:B:520:GLN:N	3:B:1087:HOH:O	2.50	0.45
1:A:523:VAL:O	1:A:524:ALA:C	2.60	0.45
1:A:529:PRO:HA	1:A:533:GLN:HE21	1.81	0.45
1:B:103:ARG:CD	3:B:1095:HOH:O	2.65	0.45
1:B:747:TYR:HH	1:B:763:GLU:CD	2.08	0.45
1:A:229:ALA:HB3	1:A:776:LYS:NZ	2.31	0.45
1:A:681:GLU:HG2	1:A:740:LEU:HD21	1.99	0.45
1:B:309:HIS:O	1:B:312:ALA:HB3	2.16	0.45
1:B:369:ASN:ND2	1:B:370:GLN:N	2.57	0.45
1:A:642:ARG:NH1	3:A:945:HOH:O	2.48	0.44
1:B:104:THR:CG2	1:B:577:ARG:CZ	2.93	0.44
1:B:496:TYR:CD2	1:B:497:PRO:HD2	2.52	0.44
1:B:224:ILE:HG23	1:B:371:THR:HG23	2.00	0.44
1:B:303:ASN:HA	3:B:1125:HOH:O	2.18	0.44
1:A:749:ARG:HD3	1:A:833:MET:HE2	2.00	0.44
1:B:607:MET:C	1:B:609:LYS:H	2.26	0.44
1:A:692:ILE:O	1:A:692:ILE:HG22	2.17	0.44
1:B:796:GLN:OE1	1:B:797:LYS:N	2.50	0.44
1:A:594:LEU:HD23	1:A:594:LEU:C	2.43	0.44
1:A:101:GLU:OE2	1:A:395:ASP:HB2	2.18	0.44
1:B:393:THR:C	1:B:395:ASP:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:O	1:A:231:ASP:C	2.61	0.43
1:B:720:ILE:HG13	1:B:723:TRP:CD1	2.53	0.43
1:A:692:ILE:O	1:A:693:PRO:C	2.57	0.43
1:A:230:GLU:HB3	1:A:367:ASN:HB3	2.01	0.43
1:A:742:GLN:O	1:A:746:VAL:HG23	2.18	0.43
1:B:395:ASP:HA	3:B:925:HOH:O	2.16	0.43
1:B:679:ILE:HG13	1:B:823:ILE:HD11	2.00	0.43
1:A:731:HIS:HB3	3:A:1051:HOH:O	2.18	0.43
1:B:703:ILE:HA	1:B:706:LEU:HB3	2.00	0.43
1:A:229:ALA:O	1:A:230:GLU:C	2.62	0.43
1:B:108:LYS:HB2	2:B:901:ANP:HNB1	1.78	0.43
1:B:793:GLY:C	1:B:794:TYR:CD1	2.97	0.43
1:B:103:ARG:HG3	1:B:103:ARG:NH1	2.33	0.43
1:B:512:ASP:OD1	1:B:577:ARG:HD3	2.19	0.42
1:A:392:GLY:O	1:A:394:ALA:CA	2.67	0.42
1:B:707:GLN:CG	1:B:708:GLU:N	2.82	0.42
1:A:594:LEU:HD21	1:A:597:ILE:HD11	2.01	0.42
1:B:180:ASN:ND2	1:B:180:ASN:H	2.17	0.42
1:B:692:ILE:HG21	1:B:732:GLU:HG3	2.01	0.42
1:A:457:ILE:HA	1:A:505:ASN:OD1	2.20	0.42
1:A:24:VAL:HG13	1:A:65:PRO:HG3	2.02	0.42
1:A:786:ARG:O	1:A:789:ILE:HG22	2.19	0.42
1:B:99:ILE:HB	1:B:409:THR:HG22	2.00	0.42
1:B:282:ILE:CG1	1:B:286:LEU:HD12	2.50	0.42
1:A:89:LEU:O	1:A:93:VAL:HG23	2.20	0.42
1:A:462:SER:OG	1:A:504:THR:OG1	2.36	0.42
1:B:486:ASN:O	1:B:490:ILE:HG13	2.20	0.42
1:B:637:ARG:O	1:B:641:ILE:HD12	2.19	0.42
1:A:167:ARG:HG2	1:A:199:VAL:HA	2.01	0.42
1:B:800:LYS:O	1:B:801:GLN:HB2	2.20	0.42
1:B:394:ALA:O	1:B:395:ASP:C	2.62	0.41
1:B:457:ILE:C	1:B:505:ASN:HD21	2.17	0.41
1:A:512:ASP:OD2	3:A:1054:HOH:O	2.22	0.41
1:A:746:VAL:O	1:A:749:ARG:HG2	2.20	0.41
1:A:230:GLU:HG2	1:A:367:ASN:C	2.46	0.41
1:B:740:LEU:O	1:B:744:ILE:HG13	2.20	0.41
1:B:561:ARG:HB2	1:B:594:LEU:HD22	2.02	0.41
1:B:789:ILE:HA	3:B:1142:HOH:O	2.20	0.41
1:A:103:ARG:NH1	1:A:573:GLY:O	2.53	0.41
1:A:719:PRO:HB2	1:A:722:GLU:HB2	2.01	0.41
1:A:751:GLU:HA	1:A:759:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:PHE:HB3	1:B:81:MET:HE3	2.03	0.41
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.53	0.41
1:A:144:ARG:HG3	1:A:148:GLU:OE1	2.17	0.41
1:A:531:ALA:C	1:A:533:GLN:N	2.79	0.41
1:A:574:ARG:HG3	3:A:1032:HOH:O	2.21	0.41
1:B:108:LYS:CB	2:B:901:ANP:HNB1	2.33	0.41
1:B:483:PHE:HB3	1:B:486:ASN:ND2	2.35	0.41
1:B:509:ARG:HB2	1:B:509:ARG:CZ	2.50	0.41
1:B:756:ALA:O	1:B:757:GLU:C	2.62	0.41
1:A:511:THR:HG22	1:A:512:ASP:O	2.21	0.41
1:A:538:LYS:HZ3	1:B:528:ASN:ND2	2.18	0.41
1:B:613:LYS:CB	1:B:614:PRO:CD	2.99	0.41
1:A:835:GLU:HG2	1:A:836:GLU:N	2.37	0.40
1:A:435:ILE:O	1:A:439:ILE:HG12	2.21	0.40
3:A:1047:HOH:O	1:B:477:ASN:ND2	2.54	0.40
1:A:741:ALA:HB2	3:A:1046:HOH:O	2.21	0.40
1:A:742:GLN:HE21	1:A:742:GLN:CA	2.30	0.40
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.51	0.40
1:B:306:LEU:O	1:B:309:HIS:HB2	2.22	0.40
1:B:763:GLU:O	1:B:767:MET:HG3	2.21	0.40

All (2) 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)
3:A:972:HOH:O	3:A:999:HOH:O[1_455]	2.05	0.15
3:B:1057:HOH:O	3:B:1069: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	687/853 (80%)	640 (93%)	32 (5%)	15 (2%)	5	2
1	B	716/853 (84%)	661 (92%)	38 (5%)	17 (2%)	4	2
All	All	1403/1706 (82%)	1301 (93%)	70 (5%)	32 (2%)	5	2

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLU
1	A	368	GLU
1	A	394	ALA
1	A	532	GLU
1	A	599	ALA
1	A	835	GLU
1	B	229	ALA
1	B	289	GLU
1	B	293	ASP
1	B	394	ALA
1	B	395	ASP
1	B	509	ARG
1	B	612	MET
1	B	796	GLN
1	B	801	GLN
1	A	510	GLY
1	A	790	HIS
1	B	367	ASN
1	B	507	ALA
1	A	393	THR
1	A	592	ASP
1	A	730	LEU
1	B	288	LYS
1	B	292	MET
1	B	614	PRO
1	B	619	GLU
1	B	719	PRO
1	A	614	PRO
1	A	619	GLU
1	A	800	LYS
1	B	793	GLY
1	A	603	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	586/728 (80%)	544 (93%)	42 (7%)	13	10
1	B	612/728 (84%)	551 (90%)	61 (10%)	7	4
All	All	1198/1456 (82%)	1095 (91%)	103 (9%)	10	6

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	16	ARG
1	A	19	ARG
1	A	22	ARG
1	A	37	LYS
1	A	56	LYS
1	A	72	ARG
1	A	76	LYS
1	A	101	GLU
1	A	156	ILE
1	A	226	SER
1	A	369	ASN
1	A	393	THR
1	A	409	THR
1	A	416	ARG
1	A	418	MET
1	A	460	GLU
1	A	506	MET
1	A	509	ARG
1	A	523	VAL
1	A	530	THR
1	A	535	GLU
1	A	538	LYS
1	A	550	GLU
1	A	563	GLU
1	A	592	ASP
1	A	612	MET

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Mol	Chain	Res	Type
1	A	632	ARG
1	A	661	SER
1	A	672	VAL
1	A	674	GLU
1	A	698	GLU
1	A	722	GLU
1	A	725	ASP
1	A	727	GLU
1	A	735	LEU
1	A	742	GLN
1	A	754	VAL
1	A	797	LYS
1	A	800	LYS
1	A	805	ARG
1	A	816	GLU
1	B	37	LYS
1	B	38	LEU
1	B	196	GLU
1	B	232	SER
1	B	281	LEU
1	B	284	GLU
1	B	285	LEU
1	B	286	LEU
1	B	288	LYS
1	B	292	MET
1	B	293	ASP
1	B	306	LEU
1	B	310	VAL
1	B	367	ASN
1	B	368	GLU
1	B	369	ASN
1	B	393	THR
1	B	409	THR
1	B	431	GLU
1	B	459	ILE
1	B	506	MET
1	B	509	ARG
1	B	511	THR
1	B	512	ASP
1	B	518	SER
1	B	523	VAL
1	B	526	LEU

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Mol	Chain	Res	Type
1	B	528	ASN
1	B	556	ILE
1	B	578	GLN
1	B	594	LEU
1	B	595	MET
1	B	607	MET
1	B	610	LEU
1	B	618	ILE
1	B	625	LYS
1	B	642	ARG
1	B	657	ARG
1	B	672	VAL
1	B	673	SER
1	B	679	ILE
1	B	685	LYS
1	B	697	LEU
1	B	708	GLU
1	B	718	LEU
1	B	720	ILE
1	B	723	TRP
1	B	725	ASP
1	B	727	GLU
1	B	742	GLN
1	B	743	SER
1	B	744	ILE
1	B	745	GLU
1	B	749	ARG
1	B	750	LYS
1	B	754	VAL
1	B	759	MET
1	B	779	LEU
1	B	785	LEU
1	B	797	LYS
1	B	831	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	436	GLN
1	A	484	HIS
1	A	486	ASN

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Mol	Chain	Res	Type
1	A	533	GLN
1	A	562	HIS
1	A	629	ASN
1	A	638	ASN
1	A	662	GLN
1	A	707	GLN
1	A	731	HIS
1	A	742	GLN
1	A	748	GLN
1	B	180	ASN
1	B	303	ASN
1	B	369	ASN
1	B	467	ASN
1	B	484	HIS
1	B	486	ASN
1	B	493	GLN
1	B	520	GLN
1	B	528	ASN
1	B	578	GLN
1	B	629	ASN
1	B	638	ASN
1	B	644	GLN
1	B	664	ASN
1	B	761	HIS
1	B	787	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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ANP	B	901	-	33,33,33	4.12	16 (48%)	45,52,52	3.07	21 (46%)
2	ANP	A	900	-	33,33,33	2.87	9 (27%)	45,52,52	2.51	20 (44%)

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	ANP	B	901	-	-	4/18/38/38	0/3/3/3
2	ANP	A	900	-	-	8/18/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ANP	PG-O1G	15.49	1.69	1.46
2	B	901	ANP	PG-N3B	10.58	1.91	1.63
2	A	900	ANP	PA-O3A	9.04	1.69	1.59
2	A	900	ANP	PG-N3B	6.77	1.81	1.63
2	A	900	ANP	PB-N3B	5.92	1.78	1.63
2	A	900	ANP	C5-C4	5.51	1.48	1.39
2	A	900	ANP	PG-O1G	5.48	1.54	1.46
2	B	901	ANP	PA-O3A	5.39	1.65	1.59
2	B	901	ANP	PB-O3A	4.72	1.64	1.59
2	B	901	ANP	PA-O5'	4.28	1.76	1.59
2	B	901	ANP	PB-O2B	-4.16	1.45	1.56
2	B	901	ANP	PG-O2G	4.14	1.67	1.56
2	B	901	ANP	C5-C4	4.03	1.46	1.39
2	B	901	ANP	C5-C6	4.03	1.52	1.41
2	B	901	ANP	C5'-C4'	3.57	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ANP	PB-O1B	3.09	1.50	1.46
2	A	900	ANP	O4'-C1'	2.82	1.48	1.42
2	B	901	ANP	C1'-N9	2.70	1.53	1.46
2	A	900	ANP	C1'-N9	2.66	1.53	1.46
2	B	901	ANP	C8-N7	2.64	1.36	1.31
2	B	901	ANP	O4'-C4'	2.50	1.50	1.45
2	B	901	ANP	PB-N3B	2.40	1.69	1.63
2	A	900	ANP	C5-C6	2.33	1.47	1.41
2	A	900	ANP	C8-N7	2.29	1.36	1.31
2	B	901	ANP	O4'-C1'	2.27	1.47	1.42

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ANP	C5-C4-N3	-7.76	116.03	126.72
2	B	901	ANP	C5-C4-N3	-7.17	116.84	126.72
2	A	900	ANP	N3-C4-N9	6.86	138.84	127.17
2	B	901	ANP	O1G-PG-N3B	6.82	121.81	111.77
2	B	901	ANP	O3A-PB-N3B	-6.72	87.95	106.59
2	B	901	ANP	N3-C4-N9	5.73	136.90	127.17
2	A	900	ANP	C2-N3-C4	4.77	123.48	111.83
2	B	901	ANP	O5'-C5'-C4'	4.76	125.21	108.99
2	B	901	ANP	O2G-PG-O3G	4.75	120.35	107.59
2	B	901	ANP	C2-N3-C4	4.64	123.16	111.83
2	A	900	ANP	N3-C2-N1	-4.16	122.28	128.58
2	B	901	ANP	O4'-C4'-C3'	-4.07	97.08	105.15
2	A	900	ANP	O3A-PA-O1A	4.03	122.84	110.70
2	B	901	ANP	O4'-C4'-C5'	3.81	121.54	109.33
2	B	901	ANP	O3'-C3'-C2'	-3.62	100.22	111.82
2	B	901	ANP	O1B-PB-N3B	-3.54	106.56	111.77
2	B	901	ANP	O2B-PB-O1B	3.52	117.43	109.87
2	B	901	ANP	N3-C2-N1	-3.46	123.35	128.58
2	A	900	ANP	O2B-PB-O3A	3.33	115.75	104.64
2	B	901	ANP	C2'-C3'-C4'	3.26	108.91	102.61
2	B	901	ANP	O4'-C1'-C2'	-3.04	100.11	106.62
2	B	901	ANP	C4'-O4'-C1'	2.99	116.06	109.47
2	B	901	ANP	C5-C6-N6	-2.89	116.13	123.29
2	A	900	ANP	O2G-PG-O3G	2.81	115.16	107.59
2	A	900	ANP	O1G-PG-N3B	-2.80	107.65	111.77
2	B	901	ANP	N6-C6-N1	2.75	124.51	118.38
2	A	900	ANP	O2B-PB-O1B	-2.66	104.15	109.87
2	A	900	ANP	C5-C6-N6	-2.66	116.70	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ANP	O3A-PA-O1A	-2.42	103.44	110.70
2	A	900	ANP	O2G-PG-O1G	-2.41	107.41	113.45
2	A	900	ANP	N6-C6-N1	2.40	123.72	118.38
2	A	900	ANP	C1'-N9-C8	-2.38	121.82	127.09
2	B	901	ANP	C4-C5-N7	-2.35	107.90	110.58
2	B	901	ANP	O2A-PA-O3A	2.34	113.59	107.27
2	A	900	ANP	O4'-C4'-C5'	2.31	116.73	109.33
2	A	900	ANP	C4'-O4'-C1'	2.20	114.33	109.47
2	A	900	ANP	C4-C5-N7	-2.18	108.09	110.58
2	A	900	ANP	O3A-PB-N3B	-2.17	100.56	106.59
2	A	900	ANP	O1B-PB-N3B	2.15	114.94	111.77
2	A	900	ANP	C5-N7-C8	2.14	106.81	103.45
2	A	900	ANP	O4'-C1'-C2'	-2.10	102.12	106.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	ANP	PB-N3B-PG-O1G
2	A	900	ANP	C5'-O5'-PA-O1A
2	A	900	ANP	C5'-O5'-PA-O2A
2	A	900	ANP	C5'-O5'-PA-O3A
2	B	901	ANP	PB-N3B-PG-O1G
2	B	901	ANP	PG-N3B-PB-O1B
2	A	900	ANP	O4'-C4'-C5'-O5'
2	A	900	ANP	C3'-C4'-C5'-O5'
2	B	901	ANP	O4'-C4'-C5'-O5'
2	B	901	ANP	C3'-C4'-C5'-O5'
2	A	900	ANP	PA-O3A-PB-O1B
2	A	900	ANP	PG-N3B-PB-O3A

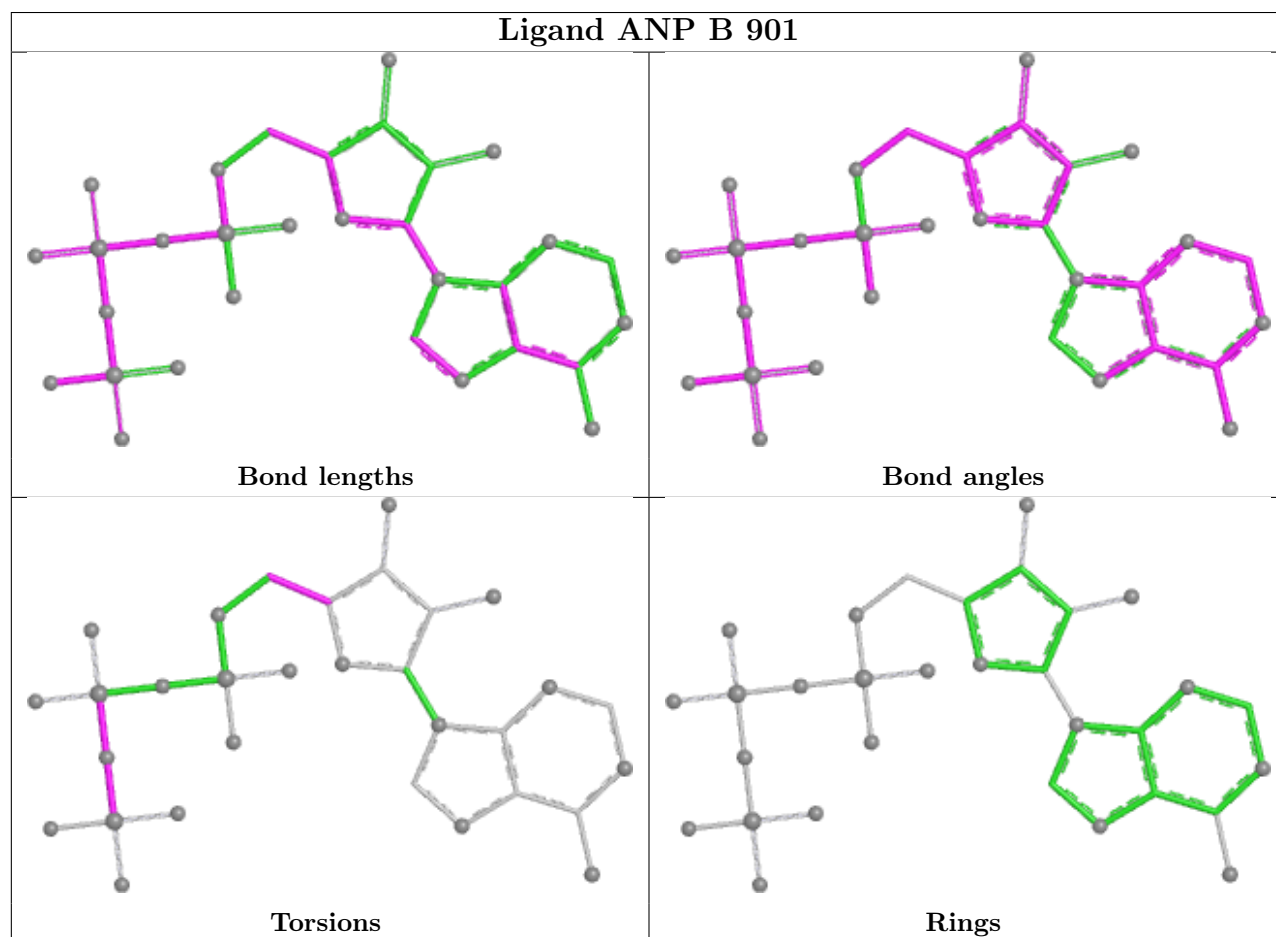
There are no ring outliers.

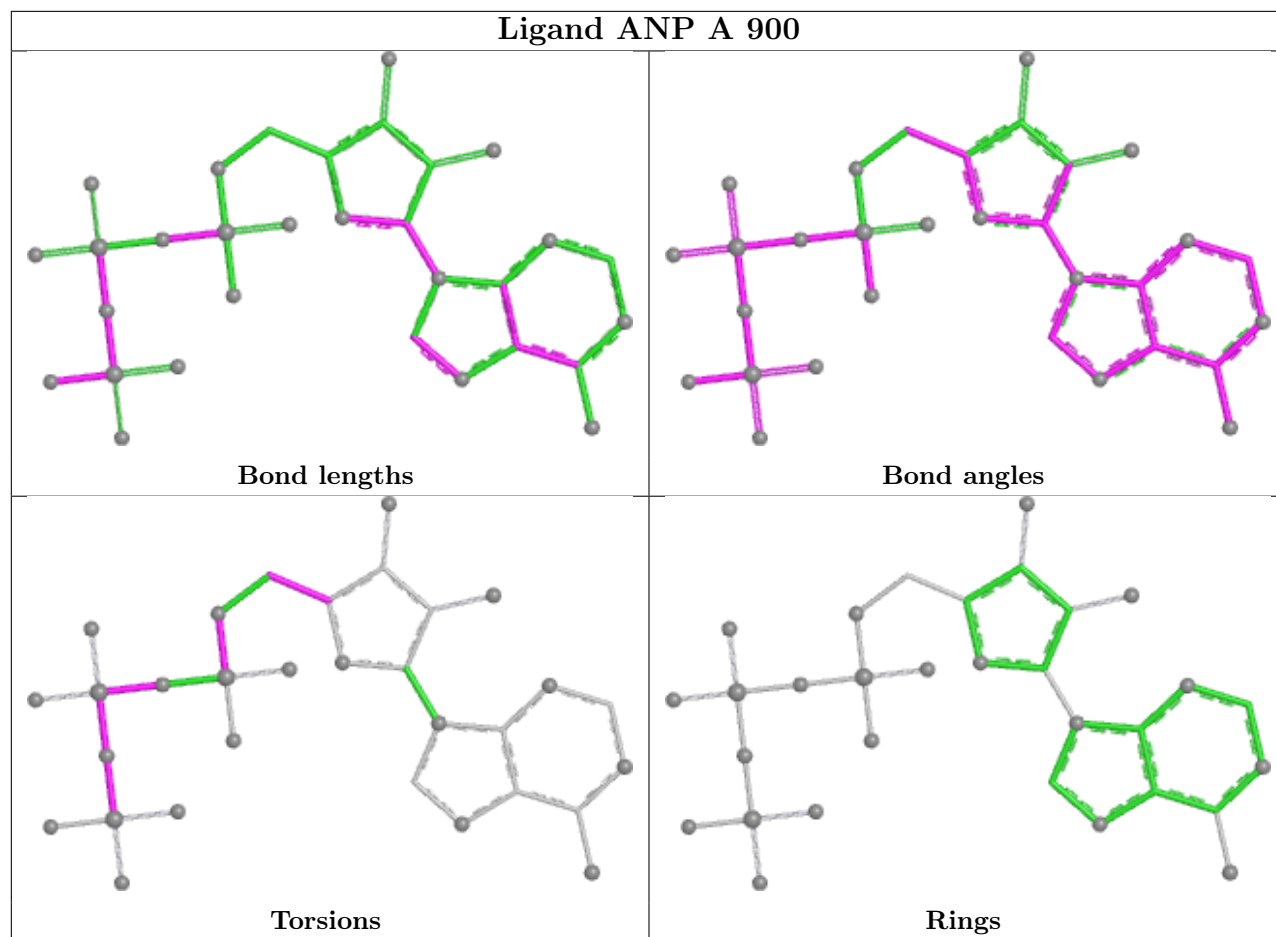
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ANP	7	0
2	A	900	ANP	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 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	691/853 (81%)	1.18	118 (17%) 4 4	36, 50, 81, 93	0
1	B	722/853 (84%)	1.55	200 (27%) 1 1	34, 51, 83, 98	0
All	All	1413/1706 (82%)	1.37	318 (22%) 2 2	34, 50, 82, 98	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	610	LEU	8.7
1	A	597	ILE	8.3
1	B	789	ILE	7.9
1	B	614	PRO	7.8
1	B	291	ILE	7.1
1	B	728	PRO	7.0
1	B	598	PHE	7.0
1	B	603	VAL	6.6
1	A	791	LEU	6.6
1	B	597	ILE	6.6
1	A	229	ALA	6.3
1	A	394	ALA	6.2
1	B	794	TYR	6.1
1	B	730	LEU	6.0
1	B	394	ALA	6.0
1	B	229	ALA	6.0
1	B	791	LEU	5.9
1	A	610	LEU	5.9
1	B	507	ALA	5.8
1	A	598	PHE	5.6
1	B	700	MET	5.6
1	B	312	ALA	5.5
1	B	703	ILE	5.4
1	B	393	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	604	SER	5.3
1	A	723	TRP	5.3
1	A	614	PRO	5.3
1	B	611	GLY	5.3
1	B	697	LEU	4.9
1	A	792	ARG	4.9
1	B	688	ILE	4.8
1	B	618	ILE	4.8
1	B	483	PHE	4.8
1	B	795	ALA	4.8
1	B	706	LEU	4.8
1	A	796	GLN	4.8
1	A	15	ASP	4.8
1	A	616	GLU	4.7
1	A	607	MET	4.7
1	B	287	VAL	4.7
1	A	393	THR	4.7
1	A	507	ALA	4.7
1	B	509	ARG	4.7
1	B	295	GLY	4.7
1	B	615	GLY	4.7
1	A	834	PRO	4.7
1	B	290	GLY	4.6
1	B	692	ILE	4.6
1	B	731	HIS	4.6
1	B	283	GLU	4.6
1	B	280	VAL	4.6
1	A	603	VAL	4.5
1	B	299	TYR	4.5
1	A	14	ASN	4.5
1	B	833	MET	4.5
1	B	281	LEU	4.5
1	B	734	THR	4.5
1	B	721	ALA	4.5
1	B	292	MET	4.4
1	B	607	MET	4.3
1	B	701	TRP	4.3
1	B	704	PRO	4.3
1	B	308	HIS	4.3
1	B	720	ILE	4.3
1	A	784	TYR	4.2
1	B	793	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	796	GLN	4.1
1	A	728	PRO	4.1
1	B	723	TRP	4.1
1	A	797	LYS	4.0
1	B	608	ARG	4.0
1	A	612	MET	4.0
1	B	716	LEU	3.9
1	B	617	ALA	3.9
1	B	727	GLU	3.9
1	B	313	ALA	3.9
1	A	532	GLU	3.9
1	B	831	VAL	3.9
1	B	714	PHE	3.9
1	B	691	TYR	3.8
1	A	594	LEU	3.8
1	A	718	LEU	3.8
1	B	735	LEU	3.8
1	B	790	HIS	3.8
1	B	684	PHE	3.8
1	A	795	ALA	3.8
1	B	724	LEU	3.8
1	A	605	GLY	3.8
1	A	615	GLY	3.8
1	B	513	ILE	3.7
1	B	718	LEU	3.7
1	A	529	PRO	3.7
1	B	695	GLN	3.7
1	B	729	GLU	3.7
1	B	670	SER	3.7
1	A	721	ALA	3.7
1	A	599	ALA	3.7
1	B	519	TRP	3.6
1	A	793	GLY	3.6
1	A	789	ILE	3.6
1	B	395	ASP	3.6
1	B	594	LEU	3.6
1	A	731	HIS	3.6
1	B	523	VAL	3.6
1	B	311	THR	3.6
1	B	508	GLY	3.6
1	B	694	PRO	3.6
1	B	710	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	103	ARG	3.6
1	B	792	ARG	3.6
1	B	832	ARG	3.6
1	A	727	GLU	3.5
1	A	704	PRO	3.5
1	A	719	PRO	3.5
1	B	510	GLY	3.5
1	B	604	SER	3.5
1	B	110	LEU	3.4
1	B	722	GLU	3.4
1	B	301	PRO	3.4
1	B	613	LYS	3.4
1	A	509	ARG	3.4
1	A	593	ALA	3.4
1	A	716	LEU	3.4
1	B	230	GLU	3.4
1	B	669	VAL	3.4
1	B	609	LYS	3.4
1	B	739	ILE	3.4
1	B	707	GLN	3.4
1	A	794	TYR	3.3
1	A	398	ALA	3.3
1	A	720	ILE	3.3
1	B	282	ILE	3.3
1	B	525	ALA	3.3
1	A	526	LEU	3.3
1	B	526	LEU	3.3
1	A	799	PRO	3.3
1	B	747	TYR	3.3
1	B	820	TYR	3.3
1	A	17	THR	3.2
1	B	719	PRO	3.2
1	B	284	GLU	3.2
1	B	71	VAL	3.2
1	B	294	GLU	3.2
1	B	532	GLU	3.2
1	A	705	GLY	3.2
1	B	136	ALA	3.1
1	A	831	VAL	3.1
1	A	519	TRP	3.1
1	B	612	MET	3.1
1	B	170	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	367	ASN	3.1
1	B	738	ARG	3.1
1	B	126	VAL	3.1
1	B	392	GLY	3.0
1	B	286	LEU	3.0
1	A	16	ARG	3.0
1	A	368	GLU	3.0
1	A	395	ASP	3.0
1	B	606	MET	3.0
1	B	599	ALA	3.0
1	A	523	VAL	3.0
1	B	600	SER	3.0
1	B	696	SER	3.0
1	B	602	ARG	3.0
1	B	367	ASN	3.0
1	B	310	VAL	3.0
1	B	156	ILE	3.0
1	A	715	ASP	3.0
1	B	715	ASP	3.0
1	B	709	ARG	2.9
1	B	749	ARG	2.9
1	B	366	GLN	2.9
1	A	602	ARG	2.9
1	A	617	ALA	2.9
1	A	530	THR	2.9
1	A	618	ILE	2.9
1	A	606	MET	2.8
1	A	790	HIS	2.8
1	A	611	GLY	2.8
1	A	798	ASP	2.8
1	B	596	ARG	2.8
1	B	708	GLU	2.8
1	A	613	LYS	2.8
1	A	832	ARG	2.8
1	A	717	ASP	2.8
1	A	754	VAL	2.8
1	A	601	ASP	2.8
1	A	203	LEU	2.8
1	B	753	VAL	2.8
1	A	596	ARG	2.7
1	B	506	MET	2.7
1	B	206	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	528	ASN	2.7
1	A	600	SER	2.7
1	A	700	MET	2.7
1	B	702	ASP	2.7
1	B	685	LYS	2.7
1	A	105	GLY	2.7
1	A	103	ARG	2.7
1	A	697	LEU	2.7
1	B	757	GLU	2.7
1	B	205	TYR	2.7
1	B	232	SER	2.7
1	A	231	ASP	2.7
1	A	30	ALA	2.6
1	A	724	LEU	2.6
1	A	170	TYR	2.6
1	B	176	TYR	2.6
1	B	202	LYS	2.6
1	A	510	GLY	2.6
1	B	605	GLY	2.6
1	A	169	ALA	2.6
1	A	595	MET	2.6
1	A	833	MET	2.6
1	B	711	LYS	2.6
1	A	230	GLU	2.6
1	B	15	ASP	2.6
1	B	725	ASP	2.6
1	B	207	LEU	2.6
1	A	835	GLU	2.5
1	A	531	ALA	2.5
1	A	366	GLN	2.5
1	B	616	GLU	2.5
1	B	534	ILE	2.5
1	B	531	ALA	2.5
1	B	754	VAL	2.5
1	A	725	ASP	2.5
1	B	289	GLU	2.5
1	B	732	GLU	2.5
1	B	690	ALA	2.5
1	B	203	LEU	2.5
1	B	595	MET	2.5
1	A	19	ARG	2.5
1	A	13	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	513	ILE	2.4
1	A	534	ILE	2.4
1	A	609	LYS	2.4
1	B	788	GLY	2.4
1	A	745	GLU	2.4
1	B	829	VAL	2.4
1	B	726	LYS	2.4
1	B	116	ALA	2.4
1	B	293	ASP	2.4
1	B	429	MET	2.4
1	A	488	ALA	2.3
1	B	150	LEU	2.3
1	A	709	ARG	2.3
1	B	797	LYS	2.3
1	A	521	ALA	2.3
1	B	160	GLY	2.3
1	B	755	GLY	2.3
1	B	512	ASP	2.3
1	A	193	PHE	2.3
1	B	491	VAL	2.3
1	B	54	LEU	2.3
1	B	114	LEU	2.3
1	B	231	ASP	2.3
1	A	156	ILE	2.3
1	A	567	ILE	2.3
1	B	129	VAL	2.3
1	B	122	THR	2.3
1	B	481	ALA	2.3
1	B	177	GLY	2.3
1	B	699	GLU	2.2
1	B	297	SER	2.2
1	B	59	VAL	2.2
1	B	409	THR	2.2
1	B	303	ASN	2.2
1	A	546	ASP	2.2
1	B	488	ALA	2.2
1	A	228	PRO	2.2
1	B	23	LYS	2.2
1	B	154	VAL	2.2
1	B	208	VAL	2.2
1	B	302	ALA	2.2
1	B	752	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	571	LEU	2.2
1	B	94	LEU	2.2
1	B	285	LEU	2.2
1	B	109	THR	2.2
1	A	208	VAL	2.2
1	A	733	GLU	2.2
1	B	521	ALA	2.2
1	B	830	GLN	2.2
1	B	209	ASP	2.2
1	B	228	PRO	2.1
1	A	639	PHE	2.1
1	A	836	GLU	2.1
1	B	214	ILE	2.1
1	B	686	ALA	2.1
1	B	741	ALA	2.1
1	B	298	LEU	2.1
1	B	479	LEU	2.1
1	B	740	LEU	2.1
1	B	111	THR	2.1
1	B	147	PHE	2.1
1	B	128	VAL	2.1
1	A	691	TYR	2.1
1	B	529	PRO	2.1
1	A	57	GLY	2.1
1	B	304	ILE	2.1
1	A	171	ALA	2.1
1	B	447	ALA	2.1
1	B	652	ALA	2.1
1	A	588	LEU	2.1
1	A	527	GLU	2.1
1	A	176	TYR	2.1
1	B	27	ILE	2.1
1	A	481	ALA	2.1
1	B	826	LEU	2.0
1	A	684	PHE	2.0
1	B	524	ALA	2.0
1	B	60	LEU	2.0
1	B	158	LEU	2.0
1	B	309	HIS	2.0
1	A	145	PRO	2.0
1	A	734	THR	2.0
1	B	693	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

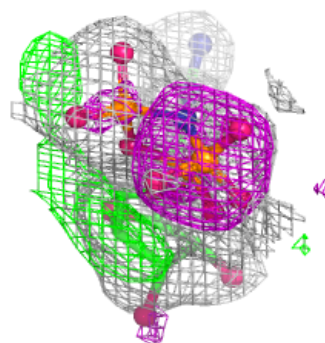
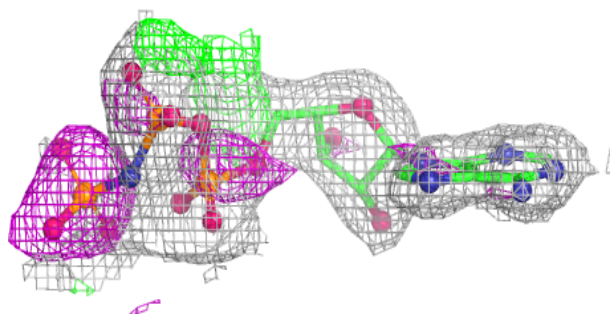
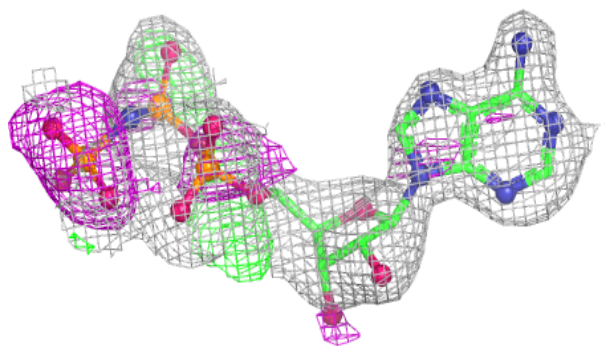
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	A	900	31/31	0.77	0.17	39,57,62,63	0
2	ANP	B	901	31/31	0.83	0.15	25,47,63,63	0

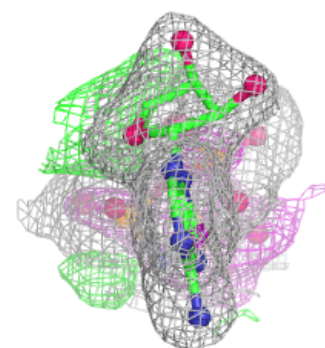
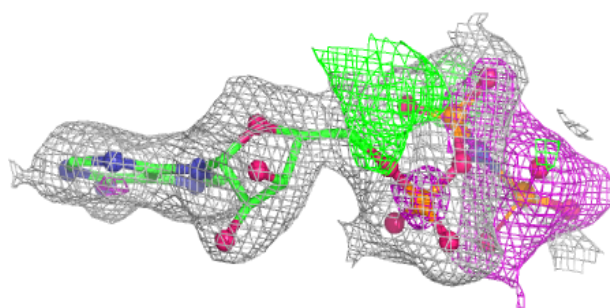
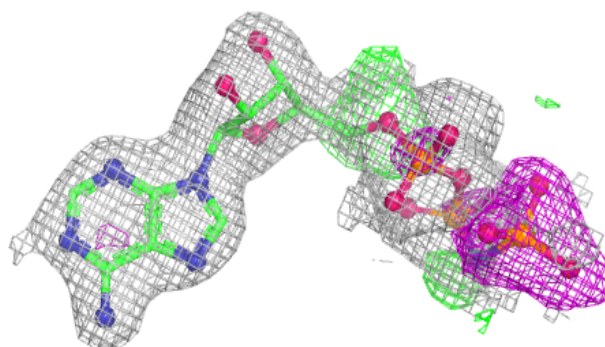
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 900:

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

**Electron density around ANP B 901:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.