



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:36 AM GMT

PDB ID : 2FSH
Title : Complex SecA:AMP-PNP from Escherichia coli
Authors : Papanikolau, Y.; Petratos, K.; Economou, A.
Deposited on : 2006-01-23
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

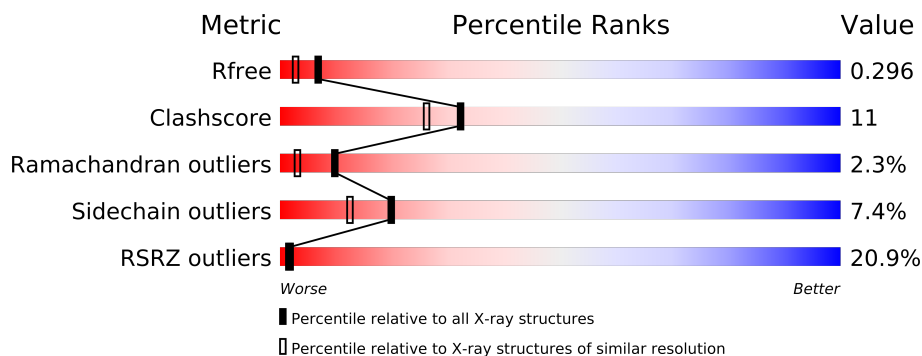
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	853	
1	B	853	

2 Entry composition i

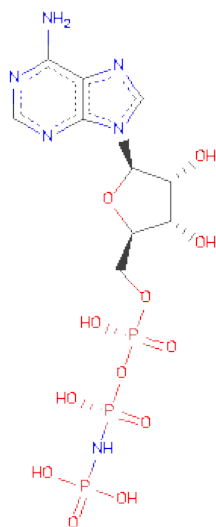
There are 3 unique types of molecules in this entry. The entry contains 11728 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

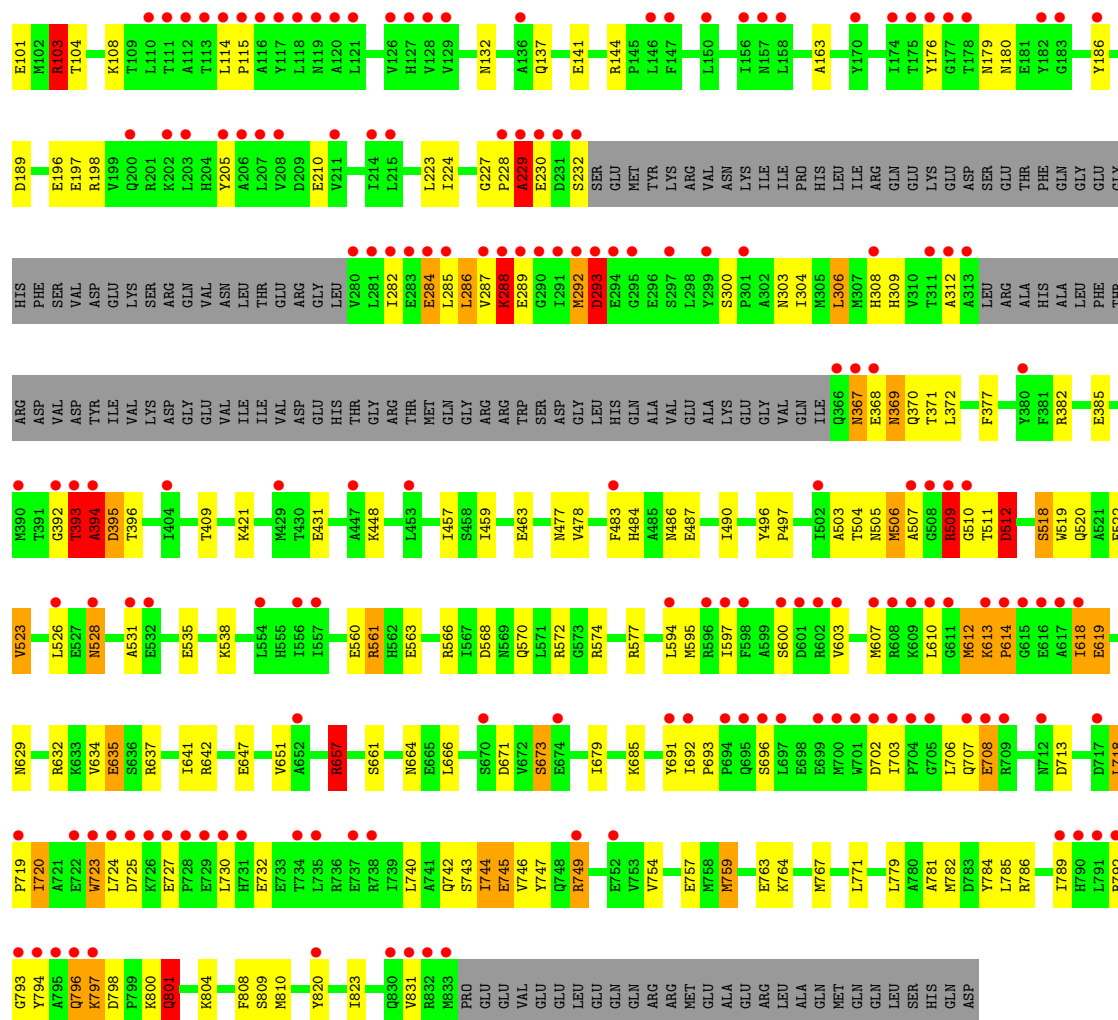
- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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) 90.5 (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 , 0.296	Depositor DCC
R_{free} test set	6535 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.8	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 130193 reflections	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.

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	1.19	15/5590 (0.3%)	1.00	15/7542 (0.2%)
1	B	1.29	33/5827 (0.6%)	1.07	17/7861 (0.2%)
All	All	1.25	48/11417 (0.4%)	1.04	32/15403 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	GLU	C-O	17.67	1.56	1.23
1	A	699	GLU	CD-OE2	14.21	1.41	1.25
1	A	98	CYS	CB-SG	-11.81	1.62	1.82
1	B	23	LYS	CE-NZ	10.56	1.75	1.49
1	A	696	SER	CB-OG	10.43	1.55	1.42
1	A	752	GLU	CG-CD	8.55	1.64	1.51
1	B	210	GLU	CG-CD	7.92	1.63	1.51
1	A	697	LEU	C-N	7.18	1.50	1.34
1	B	448	LYS	CE-NZ	7.17	1.67	1.49
1	B	393	THR	CA-CB	6.96	1.71	1.53
1	B	512	ASP	CB-CG	6.87	1.66	1.51
1	B	503	ALA	CA-CB	-6.85	1.38	1.52
1	A	96	GLU	CD-OE2	6.85	1.33	1.25
1	A	802	GLU	CG-CD	6.80	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	CYS	CB-SG	-6.77	1.70	1.82
1	B	394	ALA	CA-CB	6.54	1.66	1.52
1	B	186	TYR	CE1-CZ	-6.52	1.30	1.38
1	A	96	GLU	CG-CD	6.49	1.61	1.51
1	B	103	ARG	CG-CD	6.44	1.68	1.51
1	B	809	SER	CB-OG	-6.08	1.34	1.42
1	B	176	TYR	CE1-CZ	-6.06	1.30	1.38
1	A	693	PRO	C-O	6.03	1.35	1.23
1	A	560	GLU	CG-CD	5.98	1.60	1.51
1	B	393	THR	N-CA	5.87	1.58	1.46
1	B	76	LYS	CE-NZ	5.86	1.63	1.49
1	B	197	GLU	CD-OE2	5.74	1.31	1.25
1	B	572	ARG	CB-CG	-5.72	1.37	1.52
1	A	816	GLU	CG-CD	5.71	1.60	1.51
1	B	66	GLU	CD-OE2	5.68	1.31	1.25
1	B	421	LYS	CE-NZ	5.66	1.63	1.49
1	B	49	GLU	CB-CG	-5.60	1.41	1.52
1	B	141	GLU	CG-CD	5.57	1.60	1.51
1	B	385	GLU	CD-OE2	5.57	1.31	1.25
1	B	96	GLU	CG-CD	5.55	1.60	1.51
1	B	661	SER	CB-OG	-5.53	1.35	1.42
1	B	23	LYS	CG-CD	5.49	1.71	1.52
1	B	478	VAL	CB-CG2	-5.48	1.41	1.52
1	B	560	GLU	CG-CD	5.44	1.60	1.51
1	B	41	GLU	CG-CD	5.36	1.59	1.51
1	A	460	GLU	CD-OE1	5.35	1.31	1.25
1	B	210	GLU	CD-OE2	5.35	1.31	1.25
1	B	61	GLU	CD-OE1	5.25	1.31	1.25
1	B	163	ALA	CA-CB	5.25	1.63	1.52
1	B	635	GLU	CD-OE1	5.22	1.31	1.25
1	A	697	LEU	C-O	5.20	1.33	1.23
1	B	205	TYR	CD1-CE1	5.17	1.47	1.39
1	A	176	TYR	CD1-CE1	5.09	1.47	1.39
1	B	808	PHE	CB-CG	-5.02	1.42	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	657	ARG	NE-CZ-NH2	11.13	125.87	120.30
1	A	72	ARG	NE-CZ-NH2	8.82	124.71	120.30
1	B	23	LYS	CD-CE-NZ	8.12	130.37	111.70
1	A	805	ARG	NE-CZ-NH2	-7.96	116.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	B	561	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	B	144	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	B	572	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	577	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	382	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	801	GLN	N-CA-CB	6.16	121.68	110.60
1	B	749	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	699	GLU	OE1-CD-OE2	5.97	130.46	123.30
1	A	82	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	82	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	81	MET	CG-SD-CE	5.76	109.41	100.20
1	A	798	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	709	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	85	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	418	MET	CG-SD-CE	5.43	108.89	100.20
1	A	577	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	657	ARG	CG-CD-NE	5.43	123.19	111.80
1	B	786	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	A	697	LEU	O-C-N	5.41	131.36	122.70
1	B	189	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	610	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	657	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	B	40	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	805	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	144	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	572	ARG	CG-CD-NE	-5.11	101.06	111.80
1	B	568	ASP	CB-CG-OD1	5.02	122.82	118.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5500	0	5481	107	0
1	B	5735	0	5724	152	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	256	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (256) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	1.24
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:369:ASN:C	1:B:369:ASN:ND2	2.18	0.96
1:A:799:PRO:O	1:A:800:LYS:HB3	1.67	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: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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:598:PHE:O	1:A:600:SER:N	2.24	0.70
1:A:428:TYR:HB3	1:A:433:GLU:HG3	1.72	0.70
1:A:609:LYS:HB2	3:A:1080:HOH:O	1.90	0.70
1:A:742:GLN:HE21	1:A:742:GLN:HA	1.56	0.70
1:B:395:ASP:CB	3:B:925:HOH:O	2.39	0.69
1:A:594:LEU:O	1:A:594:LEU:HD23	1.92	0.68
1:B:227:GLY:HA3	1:B:372:LEU:HD11	1.73	0.68
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
1:B:522:GLU:HB2	3:B:1087:HOH:O	1.94	0.66
1:A:395:ASP:CG	1:A:396:THR:N	2.49	0.66
1:B:104:THR:HG21	1:B:577:ARG:NH2	2.11	0.66
1:A:618:ILE:O	1:A:619:GLU:HB2	1.98	0.64
1:B:523:VAL:HG22	3:B:1094:HOH:O	1.96	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:782:MET:HE3	1:B:810:MET:HE3	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:282:ILE:O	1:B:286:LEU:HB2	2.02	0.59
1:B:651:VAL:HG21	1:B:804:LYS:HG2	1.85	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:B:104:THR:HG23	1:B:509:ARG:HE	1.72	0.54
1:A:519:TRP:HA	1:A:522:GLU:OE1	2.07	0.54
1:B:613:LYS:HB3	1:B:614:PRO:CD	2.37	0.54
1:A:17:THR:O	1:A:21:MET:HG3	2.08	0.54
1:A:31:MET:CE	1:A:66:GLU:HG2	2.38	0.54
1:B:519:TRP:CH2	1:B:538:LYS:HE2	2.43	0.54
1:A:797:LYS:HD2	3:A:1048:HOH:O	2.08	0.54
1:B:137:GLN:CD	3:B:1081:HOH:O	2.47	0.54
1:A:531:ALA:O	1:A:534:ILE:HG13	2.08	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
1:A:471:LYS:HE2	3:A:1078:HOH:O	2.07	0.54
1:A:591:GLU:O	1:A:592:ASP:C	2.46	0.54
2:A:900:ANP:O2G	2:A:900:ANP:O1A	2.25	0.53
1:A:395:ASP:CG	1:A:396:THR:H	2.12	0.53
1:B:293:ASP:OD2	1:B:293:ASP:N	2.40	0.53
1:B:713:ASP:OD2	1:B:820:TYR:OH	2.22	0.53
1:A:722:GLU:HG2	1:A:726:LYS:HZ1	1.74	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:B:782:MET:CE	1:B:810:MET:HE3	2.39	0.53
1:A:669:VAL:HG22	1:A:670:SER:N	2.24	0.53
1:A:409:THR:HG23	3:A:924:HOH:O	2.08	0.53
1:B:18:LEU:HD23	1:B:21:MET:CE	2.39	0.53
1:B:518:SER:C	1:B:520:GLN:H	2.12	0.52
1:B:792:ARG:HB2	3:B:1142:HOH:O	2.08	0.52
1:B:137:GLN:NE2	3:B:1081:HOH:O	2.42	0.52
1:A:99:ILE:HB	1:A:409:THR:HB	1.89	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:HH11	1:B:103:ARG:HG3	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:789:ILE:O	1:B:789:ILE:HG22	2.11	0.51
1:A:395:ASP:N	3:A:1045:HOH:O	2.43	0.51
1:A:531:ALA:O	1:A:533:GLN:N	2.44	0.51
1:A:397:GLU:OE1	1:A:566:ARG:NH2	2.44	0.51
1:B:393:THR:O	1:B:395:ASP:N	2.44	0.51
1:B:759:MET:CE	1:B:759:MET:HA	2.41	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:31:MET:HE3	1:A:66:GLU:HG2	1.91	0.50
1:A:531:ALA:O	1:A:532:GLU:C	2.49	0.50
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
1:B:522:GLU:N	3:B:1087:HOH:O	2.44	0.50
1:B:284:GLU:HA	1:B:287:VAL:HG12	1.93	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:101:GLU:CD	1:B:393:THR:HA	2.32	0.49
1:B:73:GLU:O	1:B:77:ARG:HG3	2.12	0.49
1:B:693:PRO:O	1:B:696:SER:CB	2.57	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:A:594:LEU:C	1:A:596:ARG:H	2.16	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
2:B:901:ANP:O3A	2:B:901:ANP:O3G	2.31	0.49
1:B:657:ARG:HH21	1:B:657:ARG:HG3	1.76	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:538:LYS:HZ3	1:B:528:ASN:HD21	1.61	0.47
1:A:531:ALA:HA	1:A:534:ILE:HD11	1.96	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:801:GLN:HA	1:B:801:GLN:OE1	2.14	0.47
1:B:724:LEU:CD2	1:B:730:LEU:HD11	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:782:MET:CE	1:B:810:MET:CE	2.93	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:647:GLU:OE2	1:B:800:LYS:CE	2.61	0.46
1:B:308:HIS:CE1	1:B:784:TYR:CZ	3.03	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:392:GLY:C	1:A:394:ALA:N	2.69	0.46
1:A:800:LYS:H	1:A:803:TYR:H	1.64	0.46
1:B:79:PHE:HB3	1:B:81:MET:HE2	1.98	0.46
1:A:679:ILE:HG13	1:A:823:ILE:HD11	1.97	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:731:HIS:NE2	1:A:734:THR:HG23	2.31	0.45
1:A:367:ASN:O	1:A:368:GLU:O	2.33	0.45
1:B:300:SER:OG	1:B:303:ASN:ND2	2.49	0.45
1:B:757:GLU:HB2	3:B:1069:HOH:O	2.15	0.45
1:B:518:SER:CB	1:B:520:GLN:NE2	2.79	0.45
1:B:520:GLN:N	3:B:1087:HOH:O	2.50	0.45
1:A:531:ALA:O	1:A:534:ILE:CG1	2.65	0.45
1:B:103:ARG:CD	3:B:1095:HOH:O	2.65	0.45
1:A:529:PRO:HA	1:A:533:GLN:HE21	1.81	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:B:771:LEU:HD23	1:B:771:LEU:C	2.37	0.45
1:B:104:THR:CG2	1:B:577:ARG:CZ	2.93	0.44
1:A:642:ARG:NH1	3:A:945:HOH:O	2.48	0.44
1:B:496:TYR:CD2	1:B:497:PRO:HD2	2.52	0.44
1:B:303:ASN:HA	3:B:1125:HOH:O	2.18	0.44
1:B:224:ILE:HG23	1:B:371:THR:HG23	2.00	0.44
1:B:519:TRP:C	3:B:1087:HOH:O	2.56	0.44
1:A:692:ILE:O	1:A:692:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:796:GLN:OE1	1:B:797:LYS:N	2.50	0.44
1:A:101:GLU:OE2	1:A:395:ASP:HB2	2.18	0.44
1:A:460:GLU:H	1:A:460:GLU:CD	2.21	0.43
1:B:720:ILE:HG13	1:B:723:TRP:CD1	2.53	0.43
1:B:395:ASP:HA	3:B:925:HOH:O	2.16	0.43
1:A:742:GLN:O	1:A:746:VAL:HG23	2.18	0.43
1:A:230:GLU:HB3	1:A:367:ASN:HB3	2.01	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:B:108:LYS:HB2	2:B:901:ANP:HNB1	1.78	0.43
1:B:103:ARG:NH1	1:B:103:ARG:HG3	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:B:782:MET:HE1	1:B:810:MET:CE	2.49	0.42
1:B:369:ASN:O	1:B:369:ASN:ND2	2.45	0.42
1:A:594:LEU:HD21	1:A:597:ILE:HD11	2.01	0.42
1:B:180:ASN:H	1:B:180:ASN:ND2	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:B:99:ILE:HB	1:B:409:THR:HG22	2.00	0.42
1:A:786:ARG:O	1:A:789:ILE:HG22	2.19	0.42
1:B:282:ILE:CG1	1:B:286:LEU:HD12	2.50	0.42
1:B:504:THR:O	1:B:505:ASN:C	2.58	0.42
1:B:637:ARG:O	1:B:641:ILE:HD12	2.19	0.42
1:A:89:LEU:O	1:A:93:VAL:HG23	2.20	0.42
1:B:486:ASN:O	1:B:490:ILE:HG13	2.20	0.42
1:B:800:LYS:O	1:B:801:GLN:HB2	2.20	0.42
1:A:692:ILE:O	1:A:693:PRO:C	2.57	0.42
1:A:167:ARG:HG2	1:A:199:VAL:HA	2.01	0.42
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: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:A:395:ASP:O	1:A:396:THR:OG1	2.35	0.41
1:B:789:ILE:HA	3:B:1142:HOH:O	2.20	0.41
1:A:719:PRO:HB2	1:A:722:GLU:HB2	2.01	0.41
1:A:103:ARG:NH1	1:A:573:GLY:O	2.53	0.41
1:B:798:ASP:CG	1:B:800:LYS:O	2.59	0.41
1:B:79:PHE:HB3	1:B:81:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:751:GLU:HA	1:A:759:MET:HG3	2.03	0.41
1:A:144:ARG:HG3	1:A:148:GLU:OE1	2.17	0.41
1:A:32:GLU:OE1	1:A:82:ARG:NH1	2.53	0.41
1:B:108:LYS:CB	2:B:901:ANP:HNB1	2.33	0.41
1:B:509:ARG:CZ	1:B:509:ARG:HB2	2.50	0.41
1:A:574:ARG:HG3	3:A:1032:HOH:O	2.21	0.41
1:B:483:PHE:HB3	1:B:486:ASN:ND2	2.35	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:B:18:LEU:HD23	1:B:21:MET:HE3	2.04	0.40
1:A:418:MET:HE3	1:A:420:ARG:H	1.86	0.40
1:A:835:GLU:HG2	1:A:836:GLU:N	2.37	0.40
1:B:747:TYR:HH	1:B:763:GLU:CD	2.08	0.40
1:B:782:MET:HE1	1:B:810:MET:HE1	2.03	0.40
1:A:722:GLU:HB3	1:A:726:LYS:HZ2	1.86	0.40
1:B:17:THR:HG22	1:B:21:MET:CE	2.51	0.40
3:A:1047:HOH:O	1:B:477:ASN:ND2	2.54	0.40
1:A:523:VAL:O	1:A:524:ALA:C	2.60	0.40
1:A:435:ILE:O	1:A:439:ILE:HG12	2.21	0.40
1:B:763:GLU:O	1:B:767:MET:HG3	2.21	0.40
1:A:742:GLN:CA	1:A:742:GLN:HE21	2.30	0.40
1:A:741:ALA:HB2	3:A:1046:HOH:O	2.21	0.40
1:B:306:LEU:O	1:B:309:HIS:HB2	2.22	0.40
1:B:114:LEU:HB2	1:B:115:PRO:CD	2.51	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	Distance(Å)	Clash(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

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	687/853 (80%)	640 (93%)	32 (5%)	15 (2%)	10	3
1	B	716/853 (84%)	661 (92%)	38 (5%)	17 (2%)	9	3
All	All	1403/1706 (82%)	1301 (93%)	70 (5%)	32 (2%)	10	3

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%)	549 (94%)	37 (6%)	25	18
1	B	612/728 (84%)	560 (92%)	52 (8%)	15	9
All	All	1198/1456 (82%)	1109 (93%)	89 (7%)	20	12

All (89) 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	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	461	LYS
1	A	506	MET
1	A	509	ARG
1	A	512	ASP
1	A	530	THR
1	A	535	GLU
1	A	563	GLU
1	A	592	ASP
1	A	661	SER
1	A	674	GLU
1	A	698	GLU
1	A	722	GLU
1	A	725	ASP
1	A	727	GLU

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Mol	Chain	Res	Type
1	A	731	HIS
1	A	735	LEU
1	A	742	GLN
1	A	759	MET
1	A	797	LYS
1	A	800	LYS
1	A	816	GLU
1	A	817	SER
1	B	13	ARG
1	B	37	LYS
1	B	38	LEU
1	B	103	ARG
1	B	196	GLU
1	B	232	SER
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	367	ASN
1	B	368	GLU
1	B	369	ASN
1	B	393	THR
1	B	431	GLU
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
1	B	528	ASN
1	B	595	MET
1	B	607	MET
1	B	612	MET
1	B	618	ILE
1	B	642	ARG
1	B	657	ARG
1	B	673	SER
1	B	685	LYS

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Mol	Chain	Res	Type
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	754	VAL
1	B	759	MET
1	B	779	LEU
1	B	785	LEU
1	B	794	TYR
1	B	797	LYS
1	B	831	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	HIS
1	A	486	ASN
1	A	533	GLN
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	B	180	ASN
1	B	303	ASN
1	B	369	ASN
1	B	484	HIS
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

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Mol	Chain	Res	Type
1	B	742	GLN
1	B	761	HIS
1	B	787	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	A	900	-	33,33,33	4.85	7 (21%)	51,52,52	2.44	19 (37%)
2	ANP	B	901	-	33,33,33	6.69	15 (45%)	51,52,52	3.48	21 (41%)

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	A	900	-	-	0/18/38/38	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	B	901	-	-	0/18/38/38	0/1/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ANP	PG-N3B	30.60	1.91	1.64
2	A	900	ANP	PG-N3B	19.21	1.81	1.64
2	B	901	ANP	PG-O1G	18.90	1.69	1.46
2	A	900	ANP	PB-N3B	16.65	1.78	1.64
2	A	900	ANP	PG-O1G	6.71	1.54	1.46
2	B	901	ANP	PB-N3B	6.09	1.69	1.64
2	A	900	ANP	PA-O3A	5.19	1.69	1.59
2	A	900	ANP	O4'-C1'	4.67	1.48	1.41
2	B	901	ANP	PG-O2G	4.28	1.67	1.55
2	B	901	ANP	PB-O3A	4.10	1.64	1.59
2	B	901	ANP	O4'-C1'	3.85	1.47	1.41
2	B	901	ANP	PB-O1B	3.81	1.50	1.46
2	B	901	ANP	PA-O5'	3.75	1.76	1.59
2	A	900	ANP	C5-C4	3.73	1.48	1.40
2	B	901	ANP	C5'-C4'	3.28	1.62	1.51
2	B	901	ANP	PB-O2B	-3.23	1.45	1.55
2	B	901	ANP	PA-O3A	3.01	1.65	1.59
2	B	901	ANP	C5-C4	2.56	1.46	1.40
2	B	901	ANP	O4'-C4'	2.36	1.50	1.45
2	B	901	ANP	PG-O3G	2.31	1.62	1.55
2	B	901	ANP	C2-N3	2.08	1.36	1.32
2	A	900	ANP	C2-N3	2.03	1.36	1.32

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ANP	PB-N3B-PG	-10.77	111.96	130.07
2	B	901	ANP	O2B-PB-N3B	7.86	127.95	106.61
2	A	900	ANP	N3-C2-N1	-7.69	122.28	128.71
2	A	900	ANP	N3-C4-N9	7.42	138.84	125.43
2	B	901	ANP	O3A-PB-N3B	-6.72	87.95	106.59
2	B	901	ANP	O1G-PG-N3B	6.61	121.81	111.83
2	B	901	ANP	N3-C2-N1	-6.41	123.35	128.71
2	B	901	ANP	N3-C4-N9	6.35	136.90	125.43
2	B	901	ANP	C4'-O4'-C1'	5.81	116.06	109.75
2	A	900	ANP	PA-O3A-PB	-4.86	115.22	131.81
2	B	901	ANP	O2G-PG-N3B	-4.73	93.76	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ANP	C5-C4-N3	-4.44	116.03	125.70
2	B	901	ANP	O5'-C5'-C4'	4.43	125.21	108.94
2	B	901	ANP	O3G-PG-O2G	4.43	120.35	107.66
2	B	901	ANP	O4'-C1'-C2'	-4.35	100.11	106.77
2	A	900	ANP	C4'-O4'-C1'	4.22	114.33	109.75
2	B	901	ANP	C5-C4-N3	-4.07	116.84	125.70
2	B	901	ANP	O4'-C4'-C3'	-3.99	97.08	105.17
2	B	901	ANP	O3'-C3'-C2'	-3.57	100.22	111.83
2	B	901	ANP	O1B-PB-N3B	-3.49	106.56	111.83
2	B	901	ANP	O4'-C4'-C5'	3.41	121.54	109.36
2	A	900	ANP	C2-N3-C4	3.33	123.48	114.01
2	B	901	ANP	O2B-PB-O1B	3.27	117.43	109.89
2	B	901	ANP	C2-N3-C4	3.21	123.16	114.01
2	B	901	ANP	C2'-C3'-C4'	3.14	108.91	102.65
2	A	900	ANP	O3A-PA-O5'	-3.05	89.79	103.41
2	A	900	ANP	O4'-C1'-C2'	-3.04	102.12	106.77
2	A	900	ANP	O1G-PG-N3B	-2.77	107.65	111.83
2	B	901	ANP	N6-C6-N1	2.62	124.51	119.36
2	A	900	ANP	O3G-PG-O2G	2.61	115.16	107.66
2	A	900	ANP	O2B-PB-O1B	-2.48	104.15	109.89
2	A	900	ANP	O2G-PG-O1G	-2.41	107.41	113.60
2	A	900	ANP	C8-N9-C1'	-2.32	121.82	126.38
2	A	900	ANP	O2B-PB-O3A	2.24	115.75	105.14
2	A	900	ANP	N6-C6-N1	2.22	123.72	119.36
2	A	900	ANP	C1'-N9-C4	2.21	130.45	126.64
2	A	900	ANP	O3A-PB-N3B	-2.17	100.56	106.59
2	A	900	ANP	O4'-C4'-C5'	2.07	116.73	109.36
2	A	900	ANP	O1B-PB-N3B	2.06	114.94	111.83
2	B	901	ANP	C5-C6-N6	-2.03	116.13	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	691/853 (81%)	0.85	113 (16%) 2 2	36, 50, 81, 93	0
1	B	722/853 (84%)	1.30	182 (25%) 1 1	34, 51, 83, 98	0
All	All	1413/1706 (82%)	1.08	295 (20%) 1 2	34, 50, 82, 98	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	789	ILE	11.7
1	B	728	PRO	10.4
1	B	794	TYR	10.2
1	A	229	ALA	9.3
1	A	791	LEU	9.1
1	B	791	LEU	9.0
1	B	614	PRO	9.0
1	B	290	GLY	8.3
1	B	795	ALA	8.1
1	B	697	LEU	7.7
1	A	792	ARG	7.6
1	A	366	GLN	7.6
1	B	615	GLY	7.3
1	B	291	ILE	7.2
1	B	833	MET	7.2
1	A	794	TYR	7.1
1	A	367	ASN	7.1
1	B	695	GLN	7.0
1	B	729	GLU	7.0
1	B	796	GLN	7.0
1	B	618	ILE	7.0
1	B	229	ALA	6.8
1	B	730	LEU	6.6
1	A	796	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	232	SER	6.5
1	A	614	PRO	6.3
1	B	292	MET	6.3
1	A	836	GLU	6.3
1	B	700	MET	6.3
1	B	508	GLY	6.2
1	A	835	GLU	6.2
1	A	597	ILE	6.2
1	B	367	ASN	6.1
1	B	295	GLY	6.1
1	A	532	GLU	6.1
1	B	366	GLN	6.0
1	B	280	VAL	6.0
1	B	299	TYR	6.0
1	B	603	VAL	5.9
1	B	793	GLY	5.8
1	A	615	GLY	5.8
1	A	616	GLU	5.8
1	A	795	ALA	5.8
1	A	728	PRO	5.7
1	B	312	ALA	5.6
1	B	313	ALA	5.5
1	A	14	ASN	5.5
1	B	294	GLU	5.5
1	A	834	PRO	5.5
1	B	610	LEU	5.5
1	B	507	ALA	5.4
1	B	231	ASP	5.4
1	B	731	HIS	5.4
1	A	232	SER	5.3
1	A	15	ASP	5.2
1	B	281	LEU	5.2
1	B	611	GLY	5.1
1	B	704	PRO	5.1
1	B	71	VAL	5.1
1	A	789	ILE	5.1
1	A	368	GLU	5.1
1	A	784	TYR	5.1
1	B	727	GLU	5.0
1	B	287	VAL	4.9
1	A	231	ASP	4.9
1	A	604	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	792	ARG	4.8
1	A	612	MET	4.8
1	A	394	ALA	4.7
1	B	738	ARG	4.7
1	B	532	GLU	4.6
1	A	13	ARG	4.6
1	B	696	SER	4.6
1	B	694	PRO	4.6
1	A	596	ARG	4.5
1	B	602	ARG	4.5
1	B	790	HIS	4.4
1	B	126	VAL	4.4
1	A	610	LEU	4.3
1	B	832	ARG	4.3
1	B	722	GLU	4.3
1	B	617	ALA	4.3
1	A	602	ARG	4.2
1	A	790	HIS	4.2
1	B	608	ARG	4.2
1	B	114	LEU	4.2
1	A	230	GLU	4.2
1	A	228	PRO	4.1
1	B	230	GLU	4.1
1	A	613	LYS	4.1
1	B	831	VAL	4.1
1	B	699	GLU	4.1
1	B	596	ARG	4.0
1	A	832	ARG	4.0
1	B	116	ALA	4.0
1	B	707	GLN	3.9
1	B	282	ILE	3.9
1	A	731	HIS	3.9
1	A	603	VAL	3.9
1	B	510	GLY	3.8
1	B	483	PHE	3.8
1	A	16	ARG	3.8
1	B	289	GLU	3.8
1	B	726	LYS	3.8
1	B	170	TYR	3.8
1	B	206	ALA	3.8
1	B	509	ARG	3.7
1	B	719	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	117	TYR	3.6
1	B	616	GLU	3.6
1	B	111	THR	3.6
1	A	793	GLY	3.6
1	B	725	ASP	3.6
1	B	724	LEU	3.6
1	B	113	THR	3.5
1	B	598	PHE	3.5
1	B	368	GLU	3.5
1	B	293	ASP	3.5
1	A	723	TRP	3.5
1	A	509	ARG	3.5
1	B	207	LEU	3.5
1	B	283	GLU	3.4
1	B	749	ARG	3.4
1	B	182	TYR	3.4
1	B	67	ALA	3.4
1	B	74	ALA	3.4
1	A	175	THR	3.4
1	B	301	PRO	3.3
1	B	110	LEU	3.3
1	B	393	THR	3.3
1	A	601	ASP	3.3
1	B	308	HIS	3.3
1	B	528	ASN	3.2
1	B	128	VAL	3.2
1	B	709	ARG	3.2
1	B	708	GLU	3.2
1	B	703	ILE	3.2
1	A	704	PRO	3.2
1	B	601	ASP	3.2
1	A	729	GLU	3.2
1	B	609	LYS	3.2
1	B	453	LEU	3.2
1	B	70	VAL	3.2
1	B	208	VAL	3.2
1	B	176	TYR	3.1
1	B	136	ALA	3.1
1	B	288	LYS	3.1
1	A	454	VAL	3.1
1	A	525	ALA	3.1
1	B	150	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	527	GLU	3.1
1	B	174	ILE	3.1
1	A	530	THR	3.1
1	B	734	THR	3.1
1	B	127	HIS	3.0
1	B	89	LEU	3.0
1	B	68	PHE	3.0
1	B	205	TYR	3.0
1	A	557	ILE	3.0
1	B	311	THR	2.9
1	B	177	GLY	2.9
1	A	618	ILE	2.9
1	B	69	ALA	2.9
1	B	556	ILE	2.9
1	B	156	ILE	2.9
1	B	284	GLU	2.9
1	B	147	PHE	2.9
1	A	393	THR	2.9
1	B	186	TYR	2.9
1	A	611	GLY	2.8
1	B	90	GLY	2.8
1	A	127	HIS	2.8
1	B	526	LEU	2.8
1	A	608	ARG	2.8
1	B	175	THR	2.8
1	A	797	LYS	2.8
1	A	176	TYR	2.8
1	A	70	VAL	2.8
1	A	717	ASP	2.8
1	B	554	LEU	2.8
1	A	833	MET	2.8
1	A	182	TYR	2.8
1	B	691	TYR	2.8
1	A	727	GLU	2.8
1	A	508	GLY	2.8
1	A	594	LEU	2.8
1	A	170	TYR	2.8
1	B	394	ALA	2.8
1	B	701	TRP	2.7
1	B	735	LEU	2.7
1	A	113	THR	2.7
1	A	126	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	228	PRO	2.7
1	A	745	GLU	2.7
1	B	607	MET	2.7
1	B	91	GLY	2.7
1	B	670	SER	2.7
1	B	613	LYS	2.7
1	B	531	ALA	2.7
1	B	830	GLN	2.7
1	B	129	VAL	2.7
1	A	554	LEU	2.7
1	B	121	LEU	2.7
1	B	100	ALA	2.6
1	A	831	VAL	2.6
1	A	617	ALA	2.6
1	A	511	THR	2.6
1	A	30	ALA	2.6
1	A	609	LYS	2.6
1	B	702	ASP	2.6
1	A	453	LEU	2.6
1	B	88	LEU	2.6
1	B	146	LEU	2.6
1	B	797	LYS	2.6
1	A	114	LEU	2.6
1	A	705	GLY	2.6
1	B	115	PRO	2.5
1	B	118	LEU	2.5
1	A	405	TYR	2.5
1	B	215	LEU	2.5
1	A	71	VAL	2.5
1	B	211	VAL	2.5
1	B	178	THR	2.5
1	A	116	ALA	2.5
1	A	206	ALA	2.5
1	B	392	GLY	2.4
1	A	112	ALA	2.4
1	B	63	LEU	2.4
1	B	737	GLU	2.4
1	A	19	ARG	2.4
1	B	597	ILE	2.4
1	A	754	VAL	2.4
1	B	723	TRP	2.4
1	A	169	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	447	ALA	2.4
1	A	208	VAL	2.4
1	B	297	SER	2.4
1	A	700	MET	2.4
1	A	37	LYS	2.4
1	A	605	GLY	2.4
1	B	557	ILE	2.4
1	B	86	VAL	2.3
1	A	725	ASP	2.3
1	A	177	GLY	2.3
1	A	510	GLY	2.3
1	B	94	LEU	2.3
1	B	183	GLY	2.3
1	A	507	ALA	2.3
1	B	120	ALA	2.3
1	A	150	LEU	2.3
1	B	99	ILE	2.3
1	B	717	ASP	2.3
1	A	39	SER	2.2
1	A	215	LEU	2.2
1	A	556	ILE	2.2
1	A	724	LEU	2.2
1	B	600	SER	2.2
1	A	607	MET	2.2
1	B	429	MET	2.2
1	B	119	ASN	2.2
1	A	524	ALA	2.2
1	A	117	TYR	2.2
1	B	157	ASN	2.2
1	A	719	PRO	2.2
1	B	502	ILE	2.2
1	A	674	GLU	2.2
1	A	128	VAL	2.2
1	B	203	LEU	2.1
1	B	594	LEU	2.1
1	A	733	GLU	2.1
1	B	820	TYR	2.1
1	A	369	ASN	2.1
1	B	112	ALA	2.1
1	B	214	ILE	2.1
1	A	452	VAL	2.1
1	B	285	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	129	VAL	2.1
1	B	200	GLN	2.1
1	B	390	MET	2.1
1	B	692	ILE	2.1
1	B	652	ALA	2.1
1	B	93	VAL	2.1
1	B	712	ASN	2.0
1	A	502	ILE	2.0
1	A	726	LYS	2.0
1	B	202	LYS	2.0
1	B	404	ILE	2.0
1	A	715	ASP	2.0
1	B	92	MET	2.0
1	B	674	GLU	2.0
1	B	752	GLU	2.0
1	A	670	SER	2.0
1	B	705	GLY	2.0
1	B	380	TYR	2.0
1	B	158	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ANP	A	900	31/31	0.25	1.34	39,57,62,63	0
2	ANP	B	901	31/31	0.20	-0.02	25,47,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.