Full wwPDB X-ray Structure Validation Report (i)

Jul 31, 2023 – 03:18 AM EDT

PDB ID	:	1MMN
Title	:	X-RAY STRUCTURES OF THE MGADP, MGATPGAMMAS, AND MGAMPPNP COMPLEXES OF THE DICTYOSTELIUM DISCOIDEUM MYOSIN MOTOR DOMAIN
Authors	:	Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Rayment, I.
Deposited on	:	1997-07-18
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

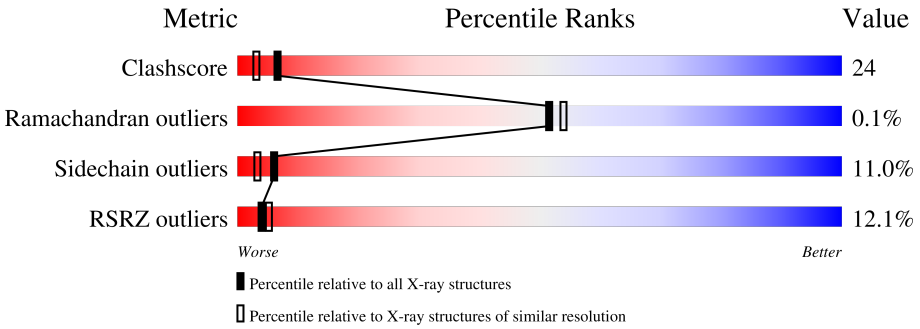
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	762	12% 53% 35% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6321 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	737	5812	3692	998	1106	16	0	0	0

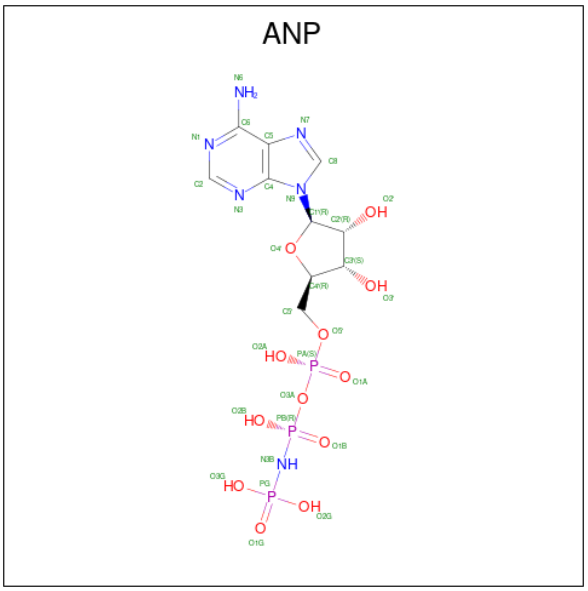
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	SER	VAL	conflict	UNP P08799
A	273	THR	GLU	conflict	UNP P08799
A	312	CYS	TYR	conflict	UNP P08799
A	321	GLU	SER	conflict	UNP P08799
A	443	SER	GLN	conflict	UNP P08799
A	489	VAL	LEU	conflict	UNP P08799
A	707	ASP	LEU	conflict	UNP P08799
A	737	PHE	TYR	conflict	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 4 is water.

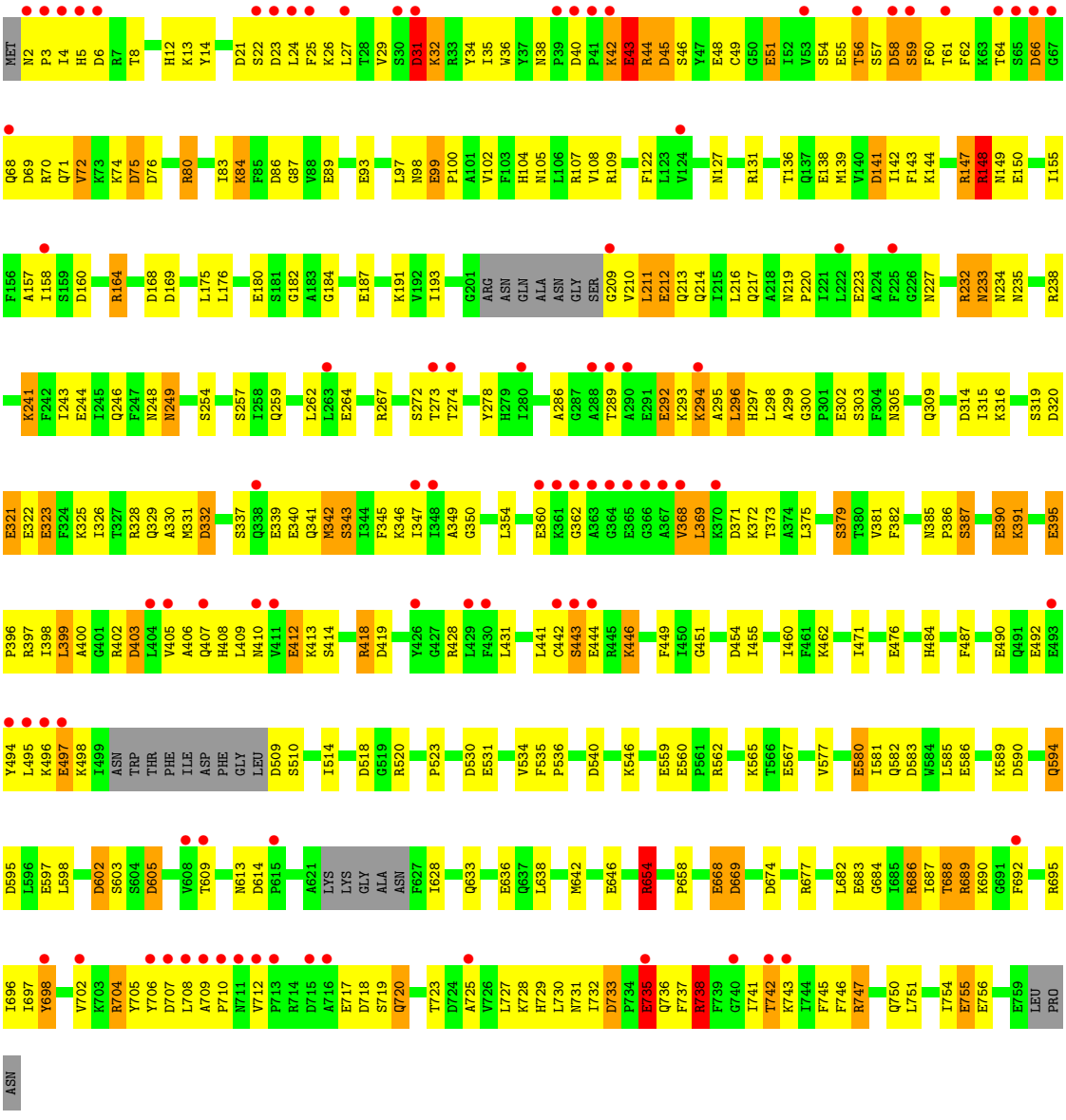
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	477	Total	O	0	0
			477	477		

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: MYOSIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.90Å 180.10Å 54.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.60 – 2.07	Depositor EDS
% Data completeness (in resolution range)	92.0 (30.00-2.10) 91.8 (29.60-2.07)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.06Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.198 , (Not available) 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 149.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6321	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.13	39/5924 (0.7%)	1.52	80/8013 (1.0%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CD-OE2	7.95	1.34	1.25
1	A	395	GLU	CD-OE1	7.56	1.33	1.25
1	A	264	GLU	CD-OE2	-7.52	1.17	1.25
1	A	492	GLU	CD-OE1	7.45	1.33	1.25
1	A	668	GLU	CD-OE2	6.96	1.33	1.25
1	A	292	GLU	CD-OE2	6.91	1.33	1.25
1	A	55	GLU	CD-OE1	6.90	1.33	1.25
1	A	51	GLU	CD-OE1	6.86	1.33	1.25
1	A	187	GLU	CD-OE1	6.80	1.33	1.25
1	A	339	GLU	CD-OE1	6.79	1.33	1.25
1	A	636	GLU	CD-OE1	6.78	1.33	1.25
1	A	340	GLU	CD-OE1	6.68	1.32	1.25
1	A	560	GLU	CD-OE2	6.66	1.32	1.25
1	A	531	GLU	CD-OE1	6.59	1.32	1.25
1	A	180	GLU	CD-OE1	6.59	1.32	1.25
1	A	360	GLU	CD-OE2	6.59	1.32	1.25
1	A	497	GLU	CD-OE1	6.56	1.32	1.25
1	A	321	GLU	CD-OE2	6.53	1.32	1.25
1	A	735	GLU	CD-OE2	6.46	1.32	1.25
1	A	490	GLU	CD-OE2	6.36	1.32	1.25
1	A	717	GLU	CD-OE1	6.20	1.32	1.25
1	A	444	GLU	CD-OE1	6.11	1.32	1.25
1	A	390	GLU	CD-OE1	6.10	1.32	1.25
1	A	48	GLU	CD-OE1	6.05	1.32	1.25
1	A	412	GLU	CD-OE1	5.99	1.32	1.25
1	A	43	GLU	CD-OE1	5.90	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	756	GLU	CD-OE1	5.90	1.32	1.25
1	A	646	GLU	CD-OE2	5.86	1.32	1.25
1	A	683	GLU	CD-OE1	5.83	1.32	1.25
1	A	244	GLU	CD-OE1	5.83	1.32	1.25
1	A	93	GLU	CD-OE1	5.76	1.31	1.25
1	A	476	GLU	CD-OE1	5.47	1.31	1.25
1	A	586	GLU	CD-OE2	5.41	1.31	1.25
1	A	99	GLU	CD-OE2	5.28	1.31	1.25
1	A	89	GLU	CD-OE1	5.23	1.31	1.25
1	A	755	GLU	CD-OE1	5.23	1.31	1.25
1	A	559	GLU	CD-OE1	5.20	1.31	1.25
1	A	323	GLU	CD-OE2	5.09	1.31	1.25
1	A	567	GLU	CD-OE2	5.08	1.31	1.25

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	654	ARG	NE-CZ-NH2	-15.86	112.37	120.30
1	A	689	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	669	ASP	CB-CG-OD2	-10.96	108.43	118.30
1	A	238	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	A	238	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	A	590	ASP	CB-CG-OD1	-9.72	109.55	118.30
1	A	614	ASP	CB-CG-OD1	8.90	126.31	118.30
1	A	738	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	562	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	A	23	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	148	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	614	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	A	669	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	530	ASP	CB-CG-OD1	-7.75	111.33	118.30
1	A	58	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	428	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	605	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	160	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	A	168	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	686	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	704	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	602	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	A	674	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	45	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	A	583	ASP	CB-CG-OD1	-6.97	112.02	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	530	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	332	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	A	518	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	733	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	141	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	602	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	518	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	419	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	707	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	278	TYR	CB-CG-CD1	-6.49	117.10	121.00
1	A	80	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	249	ASN	CA-CB-CG	-6.47	99.16	113.40
1	A	320	ASP	CB-CG-OD2	6.46	124.12	118.30
1	A	168	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	66	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	A	428	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	147	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	562	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	718	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	418	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	75	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	314	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	267	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	148	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	674	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	590	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	58	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	509	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	746	PHE	CB-CA-C	-5.92	98.56	110.40
1	A	583	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	14	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	419	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	733	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	278	TYR	CB-CG-CD2	5.67	124.40	121.00
1	A	76	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	A	707	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	A	605	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	21	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	44	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	109	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	689	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	698	TYR	CB-CG-CD2	5.32	124.19	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	45	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	654	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	A	31	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	595	ASP	CB-CG-OD1	-5.18	113.63	118.30
1	A	169	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	577	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	A	595	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	70	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	122	PHE	CB-CG-CD2	-5.11	117.23	120.80
1	A	160	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	418	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	160	ASP	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	5812	0	5664	272	0
2	A	1	0	0	0	0
3	A	31	0	13	4	0
4	A	477	0	0	17	0
All	All	6321	0	5677	272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (272) 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:A:498:LYS:H	1:A:741:ILE:HD13	0.98	1.08
1:A:286:ALA:HB1	1:A:321:GLU:HG3	1.37	1.03
1:A:141:ASP:HA	1:A:144:LYS:HD3	1.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.47	0.94
1:A:289:THR:HG22	1:A:292:GLU:CG	1.98	0.93
1:A:498:LYS:N	1:A:741:ILE:HD13	1.83	0.93
1:A:182:GLY:H	3:A:999:ANP:HNB1	1.15	0.92
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.01	0.91
1:A:300:GLY:HA3	1:A:302:GLU:OE2	1.72	0.89
1:A:22:SER:HB3	1:A:27:LEU:HD11	1.52	0.89
1:A:273:THR:O	1:A:274:THR:OG1	1.92	0.87
1:A:289:THR:HG22	1:A:292:GLU:HG3	1.57	0.85
1:A:273:THR:HG22	1:A:274:THR:HG23	1.60	0.82
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.62	0.80
1:A:42:LYS:CD	1:A:42:LYS:H	1.95	0.80
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.16	0.80
1:A:397:ARG:HA	1:A:406:ALA:HA	1.65	0.78
1:A:368:VAL:HG12	1:A:369:LEU:H	1.47	0.78
1:A:83:ILE:HD11	4:A:8032:HOH:O	1.83	0.77
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.87	0.77
1:A:139:MET:HA	1:A:142:ILE:HD12	1.65	0.77
1:A:395:GLU:HA	1:A:407:GLN:O	1.84	0.77
1:A:97:LEU:HB2	1:A:689:ARG:HD2	1.66	0.76
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.66	0.76
1:A:580:GLU:HG3	4:A:8403:HOH:O	1.85	0.75
1:A:289:THR:HG22	1:A:292:GLU:CB	2.16	0.75
1:A:38:ASN:ND2	1:A:46:SER:O	2.18	0.74
1:A:87:GLY:H	1:A:105:ASN:ND2	1.85	0.74
1:A:24:LEU:N	1:A:24:LEU:HD23	2.02	0.74
1:A:84:LYS:HD2	1:A:84:LYS:C	2.07	0.74
1:A:403:ASP:OD1	1:A:403:ASP:N	2.22	0.73
1:A:498:LYS:H	1:A:741:ILE:CD1	1.91	0.73
1:A:59:SER:HB2	1:A:72:VAL:O	1.88	0.73
1:A:219:ASN:N	1:A:220:PRO:HD2	2.02	0.73
1:A:246:GLN:OE1	1:A:443:SER:HB2	1.89	0.73
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.25	0.72
1:A:56:THR:HG23	4:A:8025:HOH:O	1.89	0.71
1:A:84:LYS:HD2	1:A:84:LYS:O	1.89	0.71
1:A:385:ASN:OD1	1:A:386:PRO:HD2	1.91	0.70
1:A:692:PHE:CE1	1:A:747:ARG:HD3	2.26	0.70
1:A:249:ASN:OD1	1:A:249:ASN:N	2.24	0.69
1:A:322:GLU:HA	1:A:325:LYS:HD2	1.75	0.69
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.72	0.69
1:A:696:ILE:O	1:A:743:LYS:HB3	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:GLU:OE2	1:A:747:ARG:NH2	2.24	0.69
1:A:232:ARG:NH1	1:A:232:ARG:HG2	2.07	0.68
1:A:687:ILE:HG22	1:A:688:THR:N	2.08	0.68
1:A:289:THR:CG2	1:A:292:GLU:HG3	2.23	0.68
1:A:32:LYS:HB3	1:A:34:TYR:CE2	2.29	0.68
1:A:286:ALA:CB	1:A:321:GLU:HG3	2.22	0.68
1:A:296:LEU:HD13	1:A:349:ALA:CB	2.24	0.67
1:A:692:PHE:CZ	1:A:747:ARG:HD3	2.28	0.67
1:A:158:ILE:HD12	1:A:175:LEU:HD21	1.77	0.67
1:A:2:ASN:N	4:A:8353:HOH:O	2.28	0.66
1:A:62:PHE:HE2	1:A:72:VAL:HG22	1.59	0.66
1:A:64:THR:HG23	1:A:68:GLN:O	1.96	0.66
1:A:289:THR:HG22	1:A:292:GLU:HB2	1.79	0.65
1:A:321:GLU:H	1:A:321:GLU:CD	2.00	0.65
1:A:184:GLY:HA2	3:A:999:ANP:O1A	1.97	0.65
1:A:212:GLU:O	1:A:216:LEU:HG	1.98	0.64
1:A:289:THR:HG23	1:A:292:GLU:N	2.11	0.64
1:A:40:ASP:CB	1:A:42:LYS:HE2	2.28	0.64
1:A:42:LYS:H	1:A:42:LYS:HD2	1.62	0.63
1:A:219:ASN:HB3	1:A:220:PRO:CD	2.24	0.63
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.33	0.63
1:A:375:LEU:O	1:A:379:SER:OG	2.17	0.63
1:A:684:GLY:O	1:A:688:THR:HB	1.99	0.62
1:A:40:ASP:CB	1:A:42:LYS:CE	2.77	0.62
1:A:372:LYS:HE2	1:A:375:LEU:HD23	1.81	0.62
1:A:147:ARG:HG3	1:A:150:GLU:OE2	2.00	0.62
1:A:484:HIS:O	1:A:487:PHE:HB3	1.99	0.62
1:A:510:SER:O	1:A:514:ILE:HG13	2.00	0.62
1:A:26:LYS:O	1:A:29:VAL:HG23	2.00	0.61
1:A:735:GLU:HA	1:A:738:ARG:HH22	1.64	0.61
1:A:706:TYR:HD2	1:A:712:VAL:O	1.83	0.61
1:A:410:ASN:OD1	1:A:413:LYS:N	2.33	0.60
1:A:98:ASN:OD1	1:A:100:PRO:HD2	2.01	0.60
1:A:698:TYR:CE2	1:A:720:GLN:HG3	2.37	0.60
1:A:386:PRO:O	1:A:390:GLU:HB2	2.02	0.60
1:A:32:LYS:HB3	1:A:34:TYR:CZ	2.37	0.60
1:A:2:ASN:O	1:A:5:HIS:N	2.29	0.59
1:A:232:ARG:NH1	4:A:8079:HOH:O	2.29	0.59
1:A:219:ASN:N	1:A:220:PRO:CD	2.66	0.59
1:A:723:THR:O	1:A:727:LEU:HG	2.03	0.59
1:A:302:GLU:H	1:A:302:GLU:CD	2.07	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD13	1:A:349:ALA:HB2	1.85	0.58
1:A:62:PHE:HE2	1:A:72:VAL:CG2	2.15	0.58
1:A:396:PRO:O	1:A:398:ILE:HD12	2.03	0.58
1:A:294:LYS:HG2	1:A:295:ALA:N	2.18	0.58
1:A:331:MET:HE3	1:A:345:PHE:HZ	1.68	0.58
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.37	0.58
1:A:40:ASP:CB	1:A:42:LYS:HZ3	2.17	0.58
1:A:628:ILE:HD11	1:A:633:GLN:HB2	1.86	0.58
1:A:56:THR:O	1:A:74:LYS:HE3	2.04	0.58
1:A:25:PHE:HE1	1:A:705:TYR:HE1	1.52	0.57
1:A:184:GLY:HA2	3:A:999:ANP:PA	2.45	0.57
1:A:209:GLY:O	1:A:213:GLN:HG2	2.04	0.57
1:A:234:ASN:ND2	4:A:8260:HOH:O	2.37	0.57
1:A:2:ASN:O	1:A:6:ASP:N	2.36	0.56
1:A:232:ARG:HG2	1:A:232:ARG:HH11	1.70	0.56
1:A:329:GLN:O	1:A:332:ASP:HB2	2.05	0.56
1:A:342:MET:CE	1:A:342:MET:HA	2.34	0.56
1:A:273:THR:C	1:A:274:THR:HG1	2.02	0.56
1:A:138:GLU:CD	1:A:138:GLU:H	2.09	0.55
1:A:698:TYR:CE1	1:A:720:GLN:HG2	2.42	0.55
1:A:219:ASN:CB	1:A:220:PRO:CD	2.83	0.55
1:A:399:LEU:HD23	1:A:403:ASP:O	2.06	0.55
1:A:248:ASN:HB3	4:A:8469:HOH:O	2.06	0.55
1:A:232:ARG:HH11	1:A:232:ARG:CG	2.19	0.54
1:A:442:CYS:SG	1:A:443:SER:N	2.81	0.54
1:A:233:ASN:ND2	1:A:235:ASN:H	2.05	0.54
1:A:217:GLN:OE1	1:A:330:ALA:HA	2.08	0.54
1:A:582:GLN:O	4:A:8201:HOH:O	2.19	0.54
1:A:698:TYR:CD2	1:A:720:GLN:HG3	2.42	0.54
1:A:42:LYS:HD3	1:A:43:GLU:H	1.73	0.53
1:A:213:GLN:NE2	1:A:213:GLN:HA	2.23	0.53
1:A:243:ILE:O	1:A:451:GLY:HA2	2.07	0.53
1:A:368:VAL:HG12	1:A:369:LEU:N	2.22	0.53
1:A:692:PHE:HB3	1:A:745:PHE:HB3	1.89	0.53
1:A:609:THR:HG22	1:A:613:ASN:OD1	2.07	0.53
1:A:331:MET:CE	1:A:345:PHE:CZ	2.92	0.53
1:A:342:MET:HA	1:A:342:MET:HE2	1.91	0.53
1:A:40:ASP:CB	1:A:42:LYS:NZ	2.72	0.52
1:A:343:SER:O	1:A:347:ILE:HG13	2.10	0.52
1:A:597:GLU:HA	1:A:597:GLU:OE1	2.09	0.52
1:A:233:ASN:HD22	1:A:234:ASN:N	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.44	0.52
1:A:704:ARG:O	1:A:704:ARG:HG2	2.08	0.52
1:A:698:TYR:O	1:A:702:VAL:HG23	2.10	0.51
1:A:25:PHE:CE1	1:A:705:TYR:HE1	2.28	0.51
1:A:732:ILE:HG22	1:A:733:ASP:N	2.26	0.51
1:A:754:ILE:HG22	1:A:755:GLU:N	2.24	0.51
1:A:59:SER:CB	1:A:72:VAL:O	2.58	0.51
1:A:158:ILE:HD12	1:A:175:LEU:CD2	2.41	0.51
1:A:354:LEU:O	1:A:418:ARG:NH1	2.43	0.51
1:A:3:PRO:O	1:A:12:HIS:HD2	1.95	0.50
1:A:341:GLN:O	1:A:345:PHE:CD2	2.64	0.50
1:A:494:TYR:O	1:A:497:GLU:O	2.29	0.50
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.27	0.50
1:A:331:MET:HE3	1:A:345:PHE:CZ	2.47	0.50
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.26	0.50
1:A:446:LYS:HE3	1:A:449:PHE:HD2	1.75	0.50
1:A:410:ASN:OD1	1:A:410:ASN:C	2.50	0.50
1:A:698:TYR:CZ	1:A:720:GLN:CG	2.94	0.50
1:A:331:MET:CE	1:A:345:PHE:HZ	2.24	0.50
1:A:147:ARG:N	1:A:150:GLU:OE2	2.28	0.50
1:A:241:LYS:HE2	1:A:454:ASP:OD2	2.12	0.50
1:A:410:ASN:O	1:A:414:SER:HB2	2.11	0.50
1:A:148:ARG:HB3	4:A:8065:HOH:O	2.11	0.50
1:A:61:THR:HG23	1:A:71:GLN:HG3	1.94	0.49
1:A:210:VAL:O	1:A:214:GLN:HG3	2.12	0.49
1:A:727:LEU:HD13	1:A:737:PHE:CD2	2.47	0.49
1:A:609:THR:CG2	1:A:613:ASN:OD1	2.61	0.49
1:A:31:ASP:N	1:A:31:ASP:OD1	2.45	0.49
1:A:408:HIS:HD2	1:A:409:LEU:N	2.11	0.49
1:A:638:LEU:O	1:A:642:MET:HG2	2.13	0.48
1:A:87:GLY:H	1:A:105:ASN:HD21	1.57	0.48
1:A:289:THR:HG23	1:A:292:GLU:H	1.75	0.48
1:A:98:ASN:O	1:A:102:VAL:HG23	2.14	0.48
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.48	0.48
1:A:182:GLY:N	3:A:999:ANP:HNB1	1.96	0.48
1:A:25:PHE:CE1	1:A:705:TYR:CE1	3.02	0.48
1:A:223:GLU:O	1:A:227:ASN:HB2	2.13	0.48
1:A:343:SER:HB3	1:A:605:ASP:OD1	2.13	0.48
1:A:710:PRO:CD	1:A:729:HIS:ND1	2.76	0.48
1:A:698:TYR:HB3	1:A:719:SER:HB3	1.96	0.48
1:A:176:LEU:N	1:A:176:LEU:HD12	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LEU:O	1:A:589:LYS:HD3	2.13	0.48
1:A:219:ASN:CB	1:A:220:PRO:HD3	2.27	0.47
1:A:398:ILE:HD12	1:A:407:GLN:HG2	1.95	0.47
1:A:61:THR:OG1	1:A:71:GLN:HG2	2.14	0.47
1:A:42:LYS:H	1:A:42:LYS:HD3	1.73	0.47
1:A:294:LYS:CG	1:A:295:ALA:N	2.77	0.47
1:A:295:ALA:O	1:A:296:LEU:HD23	2.15	0.47
1:A:709:ALA:HB1	1:A:710:PRO:HD2	1.97	0.47
1:A:594:GLN:O	1:A:598:LEU:HG	2.15	0.47
1:A:695:ARG:HG2	1:A:745:PHE:CD2	2.50	0.47
1:A:62:PHE:CE2	1:A:72:VAL:CG2	2.97	0.47
1:A:147:ARG:HB2	1:A:149:ASN:ND2	2.30	0.47
1:A:83:ILE:HD12	1:A:86:ASP:OD2	2.15	0.47
1:A:705:TYR:HD1	1:A:708:LEU:HD11	1.81	0.46
1:A:738:ARG:N	1:A:745:PHE:O	2.46	0.46
1:A:399:LEU:HD22	1:A:400:ALA:N	2.31	0.46
1:A:654:ARG:HD2	1:A:654:ARG:HA	1.47	0.46
1:A:83:ILE:HD12	1:A:83:ILE:HA	1.72	0.46
1:A:372:LYS:HD2	4:A:8292:HOH:O	2.16	0.46
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.81	0.46
1:A:728:LYS:O	1:A:731:ASN:N	2.48	0.46
1:A:732:ILE:CG2	1:A:733:ASP:N	2.78	0.46
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.56	0.46
1:A:147:ARG:HD3	4:A:8064:HOH:O	2.15	0.46
1:A:158:ILE:CD1	1:A:175:LEU:CD2	2.94	0.46
1:A:293:LYS:O	1:A:297:HIS:N	2.49	0.46
1:A:654:ARG:N	1:A:654:ARG:CD	2.76	0.45
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.57	0.45
1:A:727:LEU:O	1:A:731:ASN:N	2.49	0.45
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.97	0.45
1:A:62:PHE:O	1:A:69:ASP:HA	2.16	0.45
1:A:147:ARG:CB	1:A:149:ASN:ND2	2.79	0.45
1:A:296:LEU:HD22	1:A:381:VAL:HG11	1.98	0.45
1:A:736:GLN:HA	1:A:747:ARG:HG3	1.98	0.45
1:A:582:GLN:HB2	4:A:8403:HOH:O	2.17	0.45
1:A:496:LYS:HG2	4:A:8323:HOH:O	2.17	0.45
1:A:594:GLN:O	1:A:597:GLU:HB2	2.17	0.45
1:A:127:ASN:O	1:A:658:PRO:HG3	2.16	0.45
1:A:164:ARG:HA	1:A:164:ARG:HD3	1.89	0.45
1:A:495:LEU:O	1:A:495:LEU:HD12	2.17	0.45
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.52	0.45
1:A:735:GLU:CA	1:A:738:ARG:HH22	2.30	0.44
1:A:371:ASP:OD1	1:A:373:THR:OG1	2.17	0.44
1:A:709:ALA:HA	1:A:710:PRO:HD3	1.80	0.44
1:A:431:LEU:HA	1:A:431:LEU:HD12	1.77	0.44
1:A:296:LEU:HB3	1:A:298:LEU:HD11	1.99	0.44
1:A:323:GLU:O	1:A:326:ILE:HB	2.18	0.44
1:A:725:ALA:O	1:A:729:HIS:N	2.31	0.44
1:A:692:PHE:CE1	1:A:747:ARG:CD	3.00	0.44
1:A:706:TYR:CD2	1:A:712:VAL:O	2.69	0.44
1:A:315:ILE:HG22	1:A:316:LYS:N	2.33	0.44
1:A:3:PRO:O	1:A:12:HIS:CD2	2.71	0.43
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.51	0.43
1:A:107:ARG:NH2	4:A:8030:HOH:O	2.35	0.43
1:A:654:ARG:N	1:A:654:ARG:HD3	2.32	0.43
1:A:289:THR:CG2	1:A:292:GLU:N	2.80	0.43
1:A:299:ALA:HB3	1:A:303:SER:HB2	2.00	0.43
1:A:710:PRO:HD3	1:A:729:HIS:CG	2.53	0.43
1:A:141:ASP:CA	1:A:144:LYS:HD3	2.35	0.43
1:A:51:GLU:O	1:A:62:PHE:HB2	2.19	0.43
1:A:143:PHE:CD2	1:A:157:ALA:HB2	2.54	0.43
1:A:40:ASP:C	1:A:42:LYS:HD3	2.39	0.43
1:A:387:SER:O	1:A:391:LYS:HD2	2.18	0.43
1:A:677:ARG:HG3	1:A:682:LEU:HD12	2.01	0.43
1:A:210:VAL:O	1:A:213:GLN:HB2	2.19	0.43
1:A:750:GLN:HA	1:A:750:GLN:NE2	2.33	0.42
1:A:138:GLU:CD	1:A:138:GLU:N	2.73	0.42
1:A:455:ILE:O	1:A:455:ILE:HG13	2.17	0.42
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	0.42
1:A:38:ASN:C	1:A:40:ASP:H	2.22	0.42
1:A:42:LYS:CD	1:A:42:LYS:N	2.69	0.42
1:A:398:ILE:HD13	1:A:407:GLN:HG3	2.02	0.42
1:A:107:ARG:HD2	4:A:8038:HOH:O	2.19	0.42
1:A:296:LEU:HD22	1:A:381:VAL:CG1	2.50	0.42
1:A:343:SER:HA	1:A:346:LYS:HB2	2.00	0.42
1:A:602:ASP:O	1:A:603:SER:C	2.57	0.42
1:A:735:GLU:HA	1:A:738:ARG:NH2	2.33	0.42
1:A:395:GLU:HG2	1:A:408:HIS:HA	2.02	0.41
1:A:410:ASN:O	1:A:414:SER:CB	2.68	0.41
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.54	0.41
1:A:155:ILE:HD12	1:A:158:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:O	1:A:341:GLN:HG3	2.21	0.41
1:A:534:VAL:H	1:A:534:VAL:HG23	1.61	0.41
1:A:399:LEU:HD22	1:A:399:LEU:C	2.41	0.41
1:A:408:HIS:C	1:A:408:HIS:CD2	2.94	0.41
1:A:211:LEU:HA	1:A:214:GLN:OE1	2.20	0.41
1:A:36:TRP:NE1	1:A:80:ARG:HG3	2.36	0.41
1:A:136:THR:OG1	1:A:139:MET:HG2	2.21	0.41
1:A:138:GLU:O	1:A:142:ILE:HG13	2.21	0.41
1:A:305:ASN:O	1:A:309:GLN:HG2	2.21	0.41
1:A:398:ILE:CD1	1:A:407:GLN:HG2	2.50	0.41
1:A:494:TYR:OH	1:A:692:PHE:HB2	2.21	0.41
1:A:523:PRO:HD2	4:A:8165:HOH:O	2.20	0.41
1:A:709:ALA:HB1	1:A:710:PRO:CD	2.49	0.41
1:A:233:ASN:HD22	1:A:235:ASN:H	1.69	0.41
1:A:295:ALA:C	1:A:296:LEU:HD23	2.41	0.41
1:A:382:PHE:O	1:A:603:SER:OG	2.38	0.41
1:A:99:GLU:HG2	1:A:682:LEU:HD13	2.04	0.40
1:A:668:GLU:OE1	4:A:8210:HOH:O	2.22	0.40
1:A:696:ILE:O	1:A:743:LYS:CB	2.67	0.40
1:A:2:ASN:HA	1:A:3:PRO:HD2	1.96	0.40
1:A:22:SER:OG	1:A:24:LEU:HG	2.21	0.40
1:A:104:HIS:O	1:A:108:VAL:HG23	2.22	0.40
1:A:399:LEU:CD2	1:A:400:ALA:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	729/762 (96%)	688 (94%)	40 (6%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	620/666 (93%)	552 (89%)	68 (11%)	6 3

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	42	LYS
1	A	43	GLU
1	A	44	ARG
1	A	54	SER
1	A	56	THR
1	A	57	SER
1	A	58	ASP
1	A	59	SER
1	A	66	ASP
1	A	72	VAL
1	A	75	ASP
1	A	84	LYS
1	A	131	ARG
1	A	148	ARG
1	A	164	ARG
1	A	191	LYS
1	A	193	ILE
1	A	211	LEU
1	A	232	ARG
1	A	233	ASN
1	A	241	LYS
1	A	254	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	257	SER
1	A	259	GLN
1	A	262	LEU
1	A	272	SER
1	A	294	LYS
1	A	296	LEU
1	A	319	SER
1	A	328	ARG
1	A	342	MET
1	A	343	SER
1	A	368	VAL
1	A	369	LEU
1	A	379	SER
1	A	387	SER
1	A	391	LYS
1	A	399	LEU
1	A	402	ARG
1	A	403	ASP
1	A	405	VAL
1	A	412	GLU
1	A	441	LEU
1	A	443	SER
1	A	446	LYS
1	A	460	ILE
1	A	462	LYS
1	A	471	ILE
1	A	520	ARG
1	A	546	LYS
1	A	565	LYS
1	A	580	GLU
1	A	594	GLN
1	A	654	ARG
1	A	669	ASP
1	A	686	ARG
1	A	688	THR
1	A	690	LYS
1	A	720	GLN
1	A	735	GLU
1	A	738	ARG
1	A	742	THR
1	A	747	ARG
1	A	751	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	105	ASN
1	A	149	ASN
1	A	194	GLN
1	A	213	GLN
1	A	233	ASN
1	A	234	ASN
1	A	283	GLN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN
1	A	550	HIS
1	A	594	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\|>2$
3	ANP	A	999	2	29,33,33	1.60	5 (17%)	31,52,52	1.99	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	999	2	-	4/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ANP	C2'-C1'	-3.70	1.48	1.53
3	A	999	ANP	O4'-C1'	-3.35	1.36	1.41
3	A	999	ANP	PG-O1G	3.06	1.51	1.46
3	A	999	ANP	PB-O3A	2.65	1.62	1.59
3	A	999	ANP	C2'-C3'	-2.02	1.47	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	ANP	C5-C6-N6	6.72	130.57	120.35
3	A	999	ANP	C5-C6-N1	-4.12	111.00	120.35
3	A	999	ANP	C2-N1-C6	3.95	125.51	118.75
3	A	999	ANP	O1G-PG-N3B	-3.54	106.56	111.77
3	A	999	ANP	N3-C2-N1	-2.88	124.17	128.68
3	A	999	ANP	C1'-N9-C4	-2.02	123.09	126.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	ANP	PB-N3B-PG-O1G
3	A	999	ANP	PG-N3B-PB-O1B
3	A	999	ANP	PA-O3A-PB-O1B
3	A	999	ANP	PA-O3A-PB-O2B

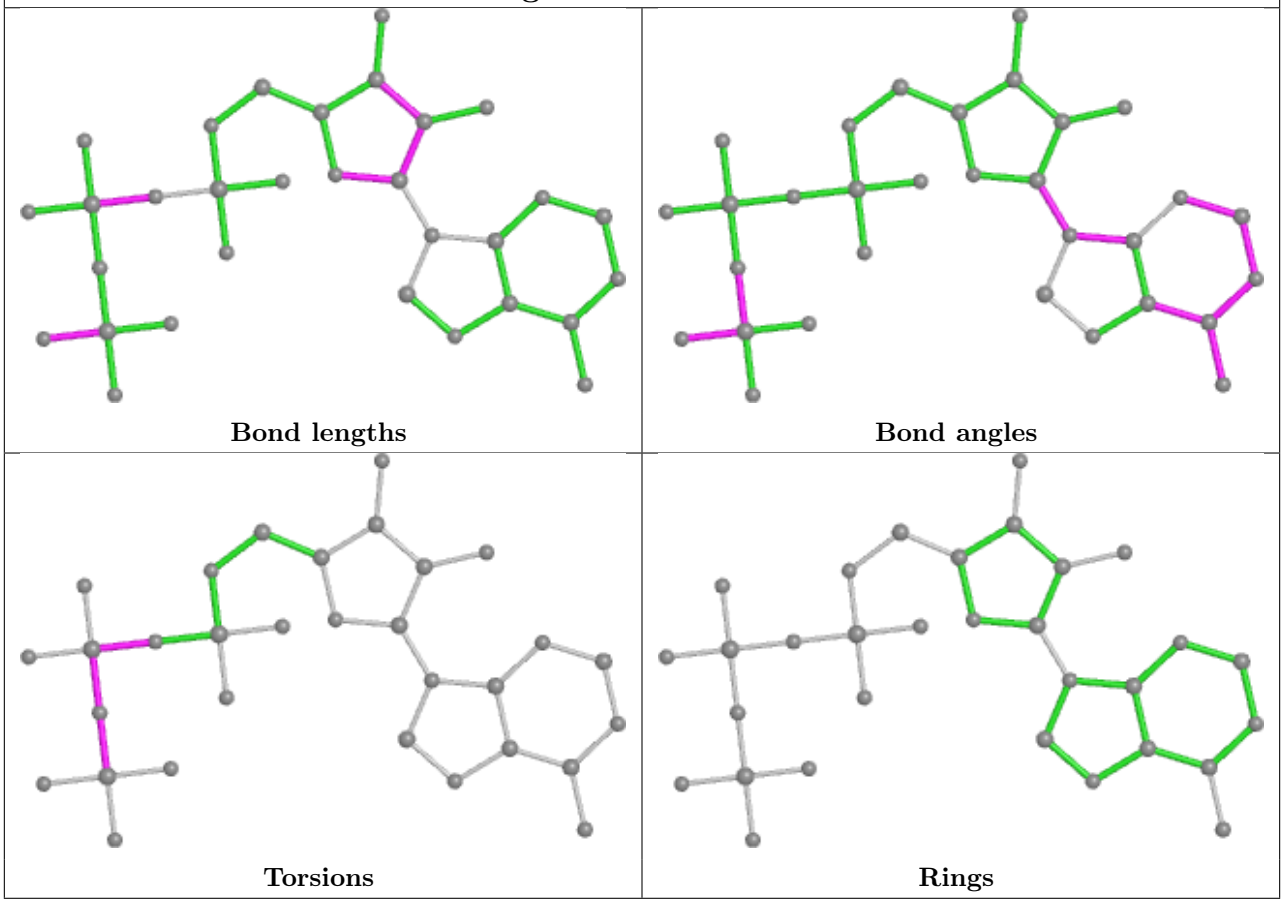
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ANP	4	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 ANP A 999



5.7 Other polymers

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, 95^{th} 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	737/762 (96%)	0.57	89 (12%) 4 5	10, 33, 78, 100	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	SER	7.3
1	A	362	GLY	6.4
1	A	68	GLN	5.8
1	A	67	GLY	5.7
1	A	25	PHE	5.4
1	A	444	GLU	5.3
1	A	712	VAL	5.1
1	A	23	ASP	5.0
1	A	495	LEU	4.8
1	A	494	TYR	4.6
1	A	706	TYR	4.5
1	A	56	THR	4.4
1	A	65	SER	4.3
1	A	368	VAL	4.2
1	A	405	VAL	4.2
1	A	3	PRO	4.1
1	A	53	VAL	4.1
1	A	66	ASP	4.0
1	A	289	THR	3.9
1	A	713	PRO	3.8
1	A	367	ALA	3.8
1	A	496	LYS	3.6
1	A	707	ASP	3.6
1	A	361	LYS	3.5
1	A	58	ASP	3.4
1	A	497	GLU	3.4
1	A	709	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	410	ASN	3.2
1	A	429	LEU	3.2
1	A	348	ILE	3.1
1	A	363	ALA	3.1
1	A	411	VAL	3.1
1	A	288	ALA	3.0
1	A	40	ASP	3.0
1	A	59	SER	3.0
1	A	64	THR	3.0
1	A	124	VAL	3.0
1	A	711	ASN	2.9
1	A	5	HIS	2.9
1	A	22	SER	2.9
1	A	366	GLY	2.8
1	A	209	GLY	2.8
1	A	27	LEU	2.8
1	A	30	SER	2.7
1	A	347	ILE	2.7
1	A	2	ASN	2.7
1	A	698	TYR	2.7
1	A	725	ALA	2.7
1	A	740	GLY	2.7
1	A	294	LYS	2.7
1	A	61	THR	2.7
1	A	24	LEU	2.7
1	A	426	TYR	2.6
1	A	290	ALA	2.6
1	A	692	PHE	2.6
1	A	39	PRO	2.6
1	A	222	LEU	2.6
1	A	715	ASP	2.5
1	A	338	GLN	2.4
1	A	364	GLY	2.4
1	A	716	ALA	2.4
1	A	42	LYS	2.4
1	A	430	PHE	2.4
1	A	742	THR	2.4
1	A	404	LEU	2.4
1	A	493	GLU	2.4
1	A	735	GLU	2.4
1	A	710	PRO	2.4
1	A	273	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	743	LYS	2.3
1	A	6	ASP	2.3
1	A	615	PRO	2.3
1	A	31	ASP	2.3
1	A	360	GLU	2.3
1	A	365	GLU	2.3
1	A	370	LYS	2.2
1	A	274	THR	2.2
1	A	702	VAL	2.2
1	A	158	ILE	2.2
1	A	442	CYS	2.2
1	A	263	LEU	2.2
1	A	225	PHE	2.2
1	A	708	LEU	2.2
1	A	280	ILE	2.1
1	A	407	GLN	2.1
1	A	41	PRO	2.0
1	A	608	VAL	2.0
1	A	4	ILE	2.0
1	A	609	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

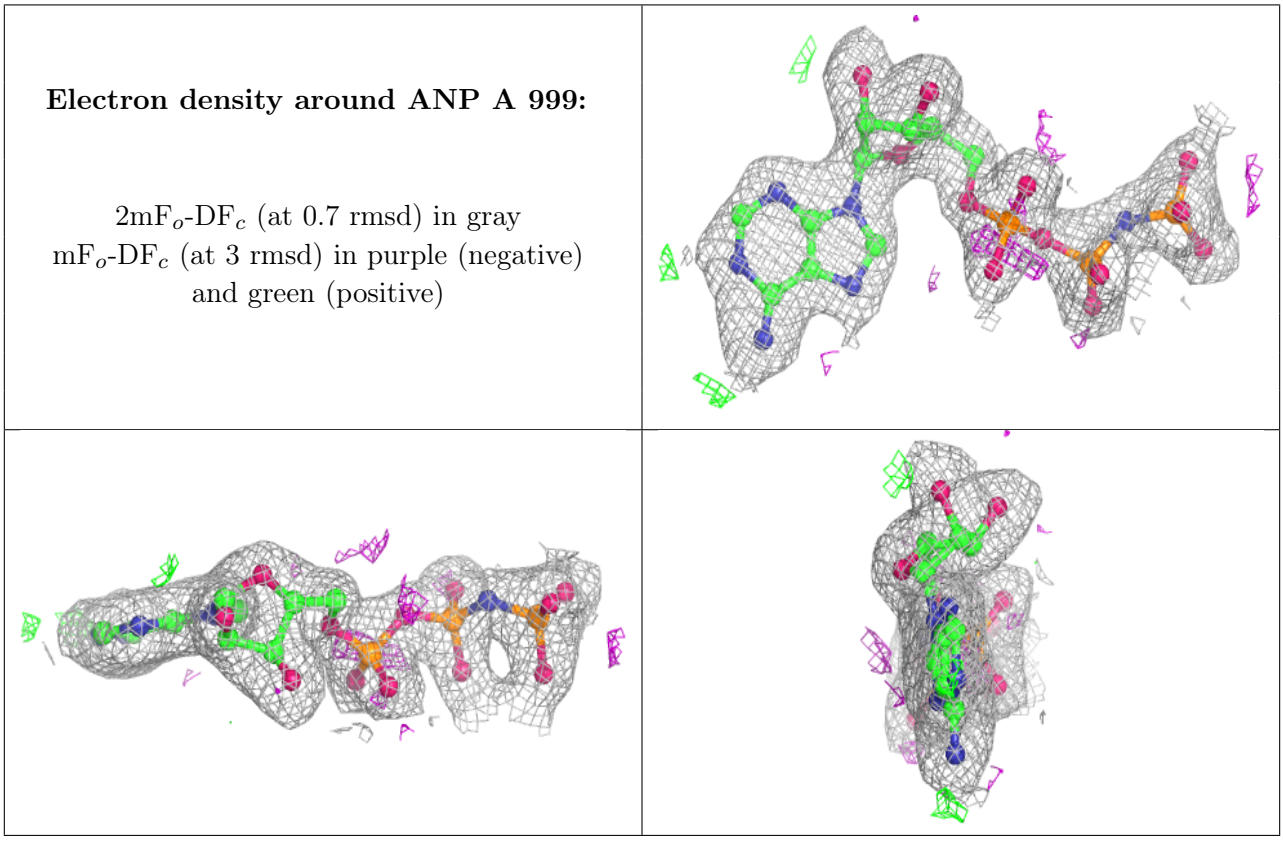
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	ANP	A	999	31/31	0.98	0.10	7,19,35,47	0
2	MG	A	998	1/1	0.99	0.06	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 ANP A 999:

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



6.5 Other polymers (i)

There are no such residues in this entry.