



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:32 AM UTC

PDB ID : 1MMN / pdb_00001mmn
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 ⓘ 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

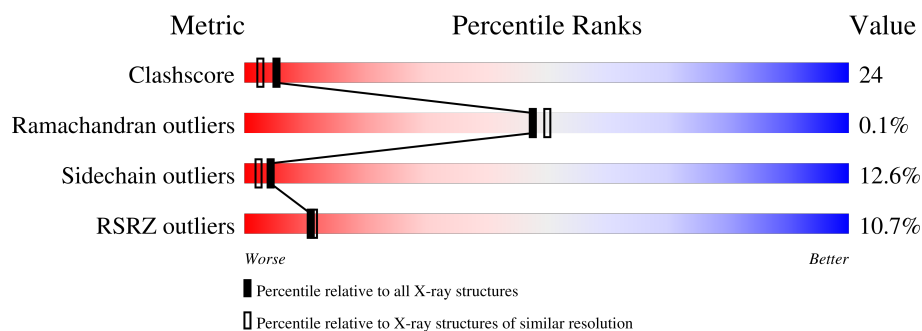
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	762	

2 Entry composition

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

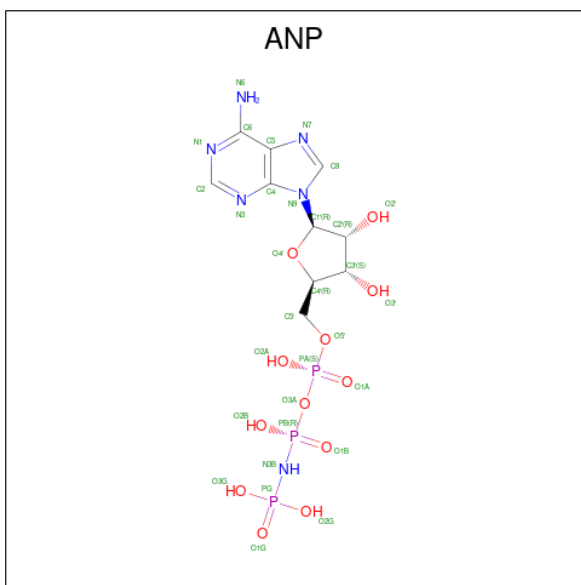
There are 8 discrepancies between the modelled and reference sequences:

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

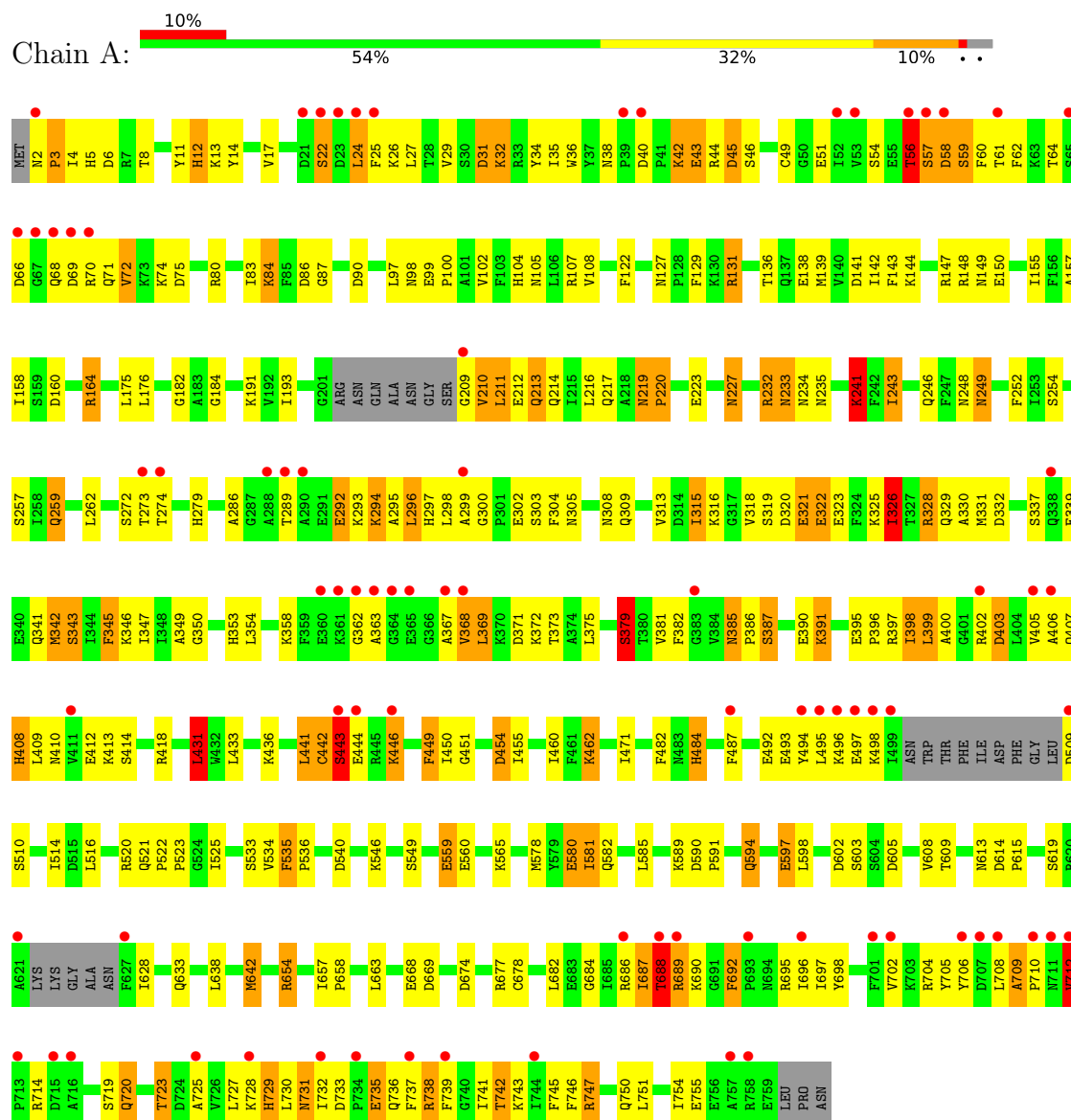
- Molecule 4 is water.

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

3 Residue-property plots

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

• Molecule 1: MYOSIN



4 Data and refinement statistics

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 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (30.00-2.10) 94.8 (30.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.44 , 155.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MG

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	1.39	10/5924 (0.2%)	1.82	94/8013 (1.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	657	ILE	CA-C	6.97	1.58	1.53
1	A	590	ASP	C-O	6.27	1.26	1.23
1	A	663	LEU	C-N	6.04	1.40	1.33
1	A	746	PHE	CA-C	-5.83	1.45	1.52
1	A	642	MET	N-CA	-5.55	1.39	1.46
1	A	326	ILE	CA-CB	-5.47	1.47	1.54
1	A	45	ASP	CA-C	-5.44	1.45	1.52
1	A	689	ARG	NE-CZ	5.30	1.38	1.33
1	A	45	ASP	CG-OD1	5.26	1.35	1.25
1	A	433	LEU	CA-C	-5.14	1.46	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	CA-CB-CG	-13.44	99.16	112.60
1	A	535	PHE	CA-CB-CG	-9.98	103.82	113.80
1	A	509	ASP	CA-CB-CG	9.20	121.80	112.60
1	A	729	HIS	CA-CB-CG	-8.56	105.24	113.80
1	A	12	HIS	CA-CB-CG	-8.22	105.58	113.80
1	A	252	PHE	CA-CB-CG	-7.97	105.83	113.80
1	A	731	ASN	CA-CB-CG	7.93	120.53	112.60
1	A	692	PHE	O-C-N	7.85	127.84	121.17
1	A	484	HIS	CA-CB-CG	-7.73	106.07	113.80
1	A	516	LEU	CA-C-O	7.72	128.74	120.55
1	A	353	HIS	CA-CB-CG	-7.63	106.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	ARG	NE-CZ-NH2	-7.59	112.37	119.20
1	A	219	ASN	CA-C-N	7.41	128.06	119.47
1	A	219	ASN	C-N-CA	7.41	128.06	119.47
1	A	692	PHE	CA-C-N	7.20	127.05	119.05
1	A	692	PHE	C-N-CA	7.20	127.05	119.05
1	A	363	ALA	N-CA-C	-7.19	103.53	111.36
1	A	233	ASN	CA-CB-CG	7.04	119.64	112.60
1	A	408	HIS	CA-CB-CG	-6.98	106.82	113.80
1	A	131	ARG	CA-C-N	6.96	128.91	122.85
1	A	131	ARG	C-N-CA	6.96	128.91	122.85
1	A	619	SER	N-CA-C	6.85	119.48	109.07
1	A	462	LYS	N-CA-C	-6.70	103.90	111.14
1	A	712	VAL	N-CA-C	6.70	114.76	107.60
1	A	160	ASP	N-CA-CB	6.65	119.65	110.01
1	A	614	ASP	CA-C-O	6.63	123.60	119.29
1	A	482	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	441	LEU	N-CA-C	6.51	121.31	113.23
1	A	442	CYS	N-CA-C	6.50	120.46	110.20
1	A	492	GLU	CB-CA-C	-6.49	100.69	110.88
1	A	210	VAL	N-CA-C	6.47	116.96	110.23
1	A	443	SER	N-CA-C	6.45	119.04	108.52
1	A	657	ILE	CB-CA-C	6.38	116.88	110.94
1	A	678	CYS	N-CA-C	6.35	119.19	111.82
1	A	22	SER	N-CA-C	6.34	119.83	109.24
1	A	227	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	345	PHE	CA-CB-CG	-6.27	107.53	113.80
1	A	449	PHE	CA-CB-CG	-6.26	107.54	113.80
1	A	454	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	746	PHE	CB-CA-C	-6.15	98.56	109.70
1	A	608	VAL	N-CA-C	6.05	116.23	110.42
1	A	315	ILE	N-CA-CB	5.91	119.29	111.25
1	A	304	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	688	THR	N-CA-CB	-5.90	101.20	110.06
1	A	450	ILE	CA-C-N	-5.82	117.15	122.80
1	A	450	ILE	C-N-CA	-5.82	117.15	122.80
1	A	279	HIS	N-CA-C	5.80	118.35	111.33
1	A	525	ILE	N-CA-C	5.79	116.44	110.36
1	A	56	THR	N-CA-C	-5.77	101.65	109.95
1	A	58	ASP	N-CA-CB	-5.74	103.26	110.90
1	A	241	LYS	CG-CD-CE	5.73	124.47	111.30
1	A	11	TYR	N-CA-C	-5.62	105.06	111.07
1	A	322	GLU	CA-C-N	5.60	127.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	GLU	C-N-CA	5.60	127.78	120.28
1	A	385	ASN	N-CA-C	5.58	118.74	108.69
1	A	367	ALA	N-CA-C	5.53	118.02	110.55
1	A	591	PRO	N-CA-C	5.51	120.14	111.38
1	A	259	GLN	CB-CG-CD	5.40	121.79	112.60
1	A	122	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	709	ALA	O-C-N	5.38	125.93	121.35
1	A	444	GLU	N-CA-C	-5.37	105.34	111.14
1	A	533	SER	N-CA-C	5.34	117.85	111.71
1	A	57	SER	CA-C-N	5.32	130.60	122.24
1	A	57	SER	C-N-CA	5.32	130.60	122.24
1	A	131	ARG	CB-CA-C	5.32	118.53	109.53
1	A	549	SER	CA-C-O	5.30	126.16	120.55
1	A	687	ILE	CB-CA-C	-5.27	105.23	111.81
1	A	597	GLU	O-C-N	5.25	127.55	122.09
1	A	688	THR	CB-CA-C	5.25	119.60	110.68
1	A	17	VAL	N-CA-C	-5.24	102.75	109.30
1	A	339	GLU	N-CA-C	-5.24	105.48	111.14
1	A	320	ASP	CB-CA-C	5.22	119.45	110.79
1	A	674	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	358	LYS	N-CA-CB	5.20	118.89	110.42
1	A	615	PRO	CB-CA-C	-5.20	104.11	112.21
1	A	431	LEU	CB-CA-C	-5.15	102.57	110.81
1	A	292	GLU	N-CA-C	-5.14	107.14	113.41
1	A	220	PRO	CB-CA-C	-5.12	103.71	112.26
1	A	259	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	493	GLU	N-CA-CB	5.08	117.55	109.82
1	A	328	ARG	CA-C-O	5.07	125.93	120.55
1	A	379	SER	CA-C-O	5.07	126.10	120.63
1	A	3	PRO	N-CA-CB	5.05	108.56	103.25
1	A	560	GLU	CA-C-O	5.05	123.06	119.32
1	A	90	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	714	ARG	O-C-N	5.04	127.33	122.09
1	A	723	THR	CA-C-N	5.04	127.97	120.31
1	A	723	THR	C-N-CA	5.04	127.97	120.31
1	A	129	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	318	VAL	O-C-N	5.03	128.50	123.07
1	A	739	PHE	CA-C-N	-5.01	116.28	122.15
1	A	739	PHE	C-N-CA	-5.01	116.28	122.15
1	A	14	TYR	N-CA-C	5.01	119.54	113.38
1	A	326	ILE	CB-CA-C	-5.01	105.38	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5812	0	5664	280	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	280	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 (280) 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
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:45:ASP:CG	1:A:677:ARG:HH22	1.87	0.82
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:84:LYS:HD2	1:A:84:LYS:C	2.07	0.79
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.18	0.79
1:A:397:ARG:HA	1:A:406:ALA:HA	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:321:GLU:H	1:A:321:GLU:CD	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:302:GLU:H	1:A:302:GLU:CD	2.07	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:342:MET:HE2	1:A:342:MET:HA	1.81	0.62
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:138:GLU:CD	1:A:138:GLU:H	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:O	1:A:332:ASP:HB2	2.05	0.56
1:A:342:MET:HA	1:A:342:MET:CE	2.34	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:410:ASN:OD1	1:A:410:ASN:C	2.50	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: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
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:45:ASP:OD2	1:A:677:ARG:NH2	2.26	0.50
1:A:331:MET:CE	1:A:345:PHE:HZ	2.24	0.50
1:A:446:LYS:HE3	1:A:449:PHE:HD2	1.75	0.50
1:A:698:TYR:CZ	1:A:720:GLN:CG	2.94	0.50
1:A:147:ARG:N	1:A:150:GLU:OE2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:ASP:C	1:A:42:LYS:HD3	2.39	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:331:MET:HE1	1:A:345:PHE:HZ	1.75	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:38:ASN:C	1:A:40:ASP:H	2.22	0.48
1:A:176:LEU:N	1:A:176:LEU:HD12	2.29	0.48
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:273:THR:C	1:A:274:THR:HG1	2.10	0.47
1:A:705:TYR:HD1	1:A:708:LEU:HD11	1.81	0.46
1:A:45:ASP:CG	1:A:677:ARG:NH2	2.67	0.46
1:A:738:ARG:N	1:A:745:PHE:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:GLU:CD	1:A:138:GLU:N	2.73	0.46
1:A:602:ASP:O	1:A:603:SER:C	2.57	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:331:MET:CE	1:A:345:PHE:CZ	2.92	0.45
1:A:727:LEU:O	1:A:731:ASN:N	2.49	0.45
1:A:295:ALA:C	1:A:296:LEU:HD23	2.41	0.45
1:A:408:HIS:C	1:A:408:HIS:CD2	2.94	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
1:A:559:GLU:HG2	1:A:578:MET:HE1	1.99	0.45
1:A:399:LEU:HD22	1:A:399:LEU:C	2.41	0.45
1:A:735:GLU:CA	1:A:738:ARG:HH22	2.30	0.44
1:A:308:ASN:C	1:A:308:ASN:OD1	2.59	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:147:ARG:H	1:A:150:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:233:ASN:HD22	1:A:233:ASN:C	2.25	0.44
1:A:399:LEU:C	1:A:399:LEU:CD2	2.91	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:343:SER:HB3	1:A:605:ASP:CG	2.44	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: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:315:ILE:HG22	1:A:316:LYS:N	2.33	0.42
1:A:750:GLN:HA	1:A:750:GLN:NE2	2.33	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: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: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:521:GLN:HA	1:A:522:PRO:C	2.45	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:741:ILE:C	1:A:742:THR:CG2	2.94	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%)	48 50

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%)	542 (87%)	78 (13%)	4 2

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	24	LEU
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	70	ARG
1	A	72	VAL
1	A	75	ASP
1	A	84	LYS
1	A	131	ARG
1	A	164	ARG
1	A	191	LYS
1	A	193	ILE
1	A	211	LEU
1	A	213	GLN
1	A	232	ARG
1	A	241	LYS
1	A	243	ILE
1	A	254	SER
1	A	257	SER
1	A	259	GLN
1	A	262	LEU
1	A	272	SER
1	A	294	LYS
1	A	296	LEU

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Mol	Chain	Res	Type
1	A	313	VAL
1	A	319	SER
1	A	321	GLU
1	A	326	ILE
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	398	ILE
1	A	399	LEU
1	A	402	ARG
1	A	403	ASP
1	A	405	VAL
1	A	412	GLU
1	A	431	LEU
1	A	436	LYS
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	559	GLU
1	A	565	LYS
1	A	580	GLU
1	A	581	ILE
1	A	594	GLN
1	A	669	ASP
1	A	686	ARG
1	A	688	THR
1	A	690	LYS
1	A	712	VAL
1	A	720	GLN
1	A	735	GLU
1	A	738	ARG
1	A	742	THR

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Mol	Chain	Res	Type
1	A	747	ARG
1	A	751	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	105	ASN
1	A	149	ASN
1	A	188	ASN
1	A	213	GLN
1	A	219	ASN
1	A	233	ASN
1	A	234	ASN
1	A	259	GLN
1	A	283	GLN
1	A	309	GLN
1	A	329	GLN
1	A	376	ASN
1	A	439	ASN
1	A	480	GLN
1	A	511	GLN
1	A	550	HIS
1	A	594	GLN
1	A	649	ASN

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

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	33,33,33	1.53	7 (21%)	45,52,52	1.49	6 (13%)

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	-	4/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ANP	PG-O1G	3.18	1.51	1.46
3	A	999	ANP	PB-O3A	2.68	1.62	1.59
3	A	999	ANP	C8-N9	-2.62	1.33	1.37
3	A	999	ANP	C6-N6	-2.51	1.27	1.34
3	A	999	ANP	O4'-C1'	-2.42	1.36	1.42
3	A	999	ANP	C2'-C3'	-2.05	1.47	1.53
3	A	999	ANP	PG-O2G	-2.03	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ANP	C2-N1-C6	4.13	125.51	118.73
3	A	999	ANP	O1G-PG-N3B	-3.54	106.56	111.77
3	A	999	ANP	C5-C6-N6	2.94	130.57	123.29
3	A	999	ANP	N3-C2-N1	-2.91	124.17	128.58
3	A	999	ANP	C5-C6-N1	-2.56	111.00	117.51
3	A	999	ANP	O4'-C1'-N9	2.34	112.59	108.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

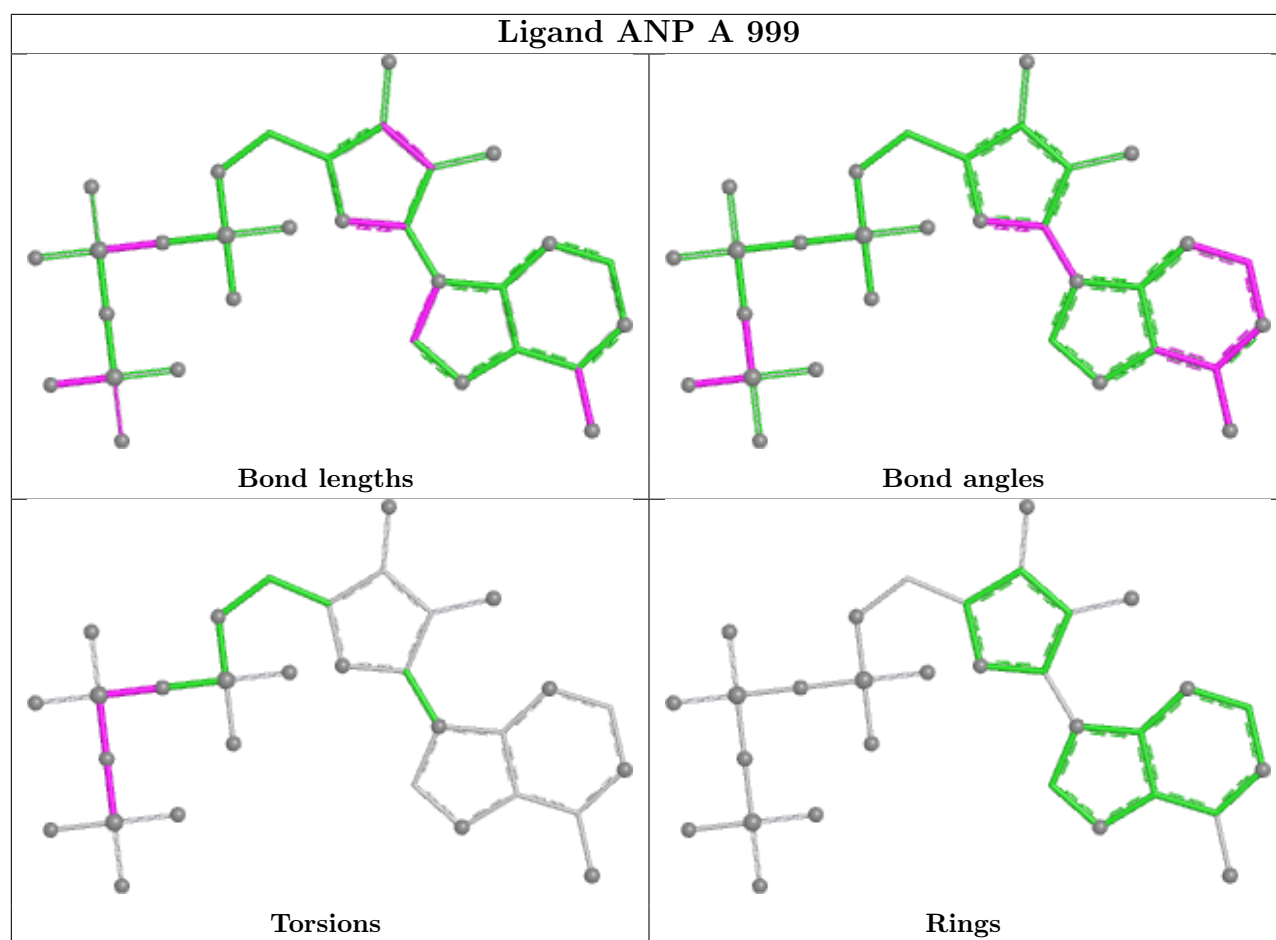
Mol	Chain	Res	Type	Atoms
3	A	999	ANP	PB-N3B-PG-O1G
3	A	999	ANP	PG-N3B-PB-O1B
3	A	999	ANP	PA-O3A-PB-O2B
3	A	999	ANP	PA-O3A-PB-O1B

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 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	737/762 (96%)	0.35	79 (10%)	11 11	10, 33, 78, 100	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	TYR	5.2
1	A	368	VAL	5.2
1	A	627	PHE	5.1
1	A	621	ALA	5.0
1	A	53	VAL	4.5
1	A	757	ALA	4.3
1	A	25	PHE	4.1
1	A	362	GLY	3.8
1	A	443	SER	3.8
1	A	758	ARG	3.6
1	A	499	ILE	3.6
1	A	363	ALA	3.6
1	A	67	GLY	3.6
1	A	288	ALA	3.6
1	A	23	ASP	3.5
1	A	273	THR	3.4
1	A	712	VAL	3.4
1	A	209	GLY	3.4
1	A	701	PHE	3.4
1	A	58	ASP	3.3
1	A	22	SER	3.3
1	A	68	GLN	3.3
1	A	290	ALA	3.2
1	A	706	TYR	3.2
1	A	24	LEU	3.1
1	A	707	ASP	3.0
1	A	715	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	361	LYS	3.0
1	A	495	LEU	3.0
1	A	402	ARG	2.9
1	A	498	LYS	2.9
1	A	21	ASP	2.9
1	A	56	THR	2.9
1	A	39	PRO	2.8
1	A	734	PRO	2.8
1	A	405	VAL	2.8
1	A	69	ASP	2.7
1	A	364	GLY	2.7
1	A	497	GLU	2.7
1	A	711	ASN	2.6
1	A	40	ASP	2.6
1	A	65	SER	2.6
1	A	716	ALA	2.6
1	A	383	GLY	2.6
1	A	367	ALA	2.6
1	A	57	SER	2.5
1	A	2	ASN	2.5
1	A	299	ALA	2.5
1	A	702	VAL	2.4
1	A	444	GLU	2.4
1	A	411	VAL	2.4
1	A	509	ASP	2.4
1	A	710	PRO	2.4
1	A	686	ARG	2.4
1	A	274	THR	2.4
1	A	70	ARG	2.3
1	A	696	ILE	2.3
1	A	61	THR	2.3
1	A	739	PHE	2.3
1	A	732	ILE	2.3
1	A	725	ALA	2.3
1	A	708	LEU	2.3
1	A	688	THR	2.2
1	A	689	ARG	2.2
1	A	496	LYS	2.2
1	A	52	ILE	2.2
1	A	365	GLU	2.2
1	A	744	ILE	2.2
1	A	360	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	737	PHE	2.1
1	A	406	ALA	2.1
1	A	66	ASP	2.1
1	A	446	LYS	2.1
1	A	728	LYS	2.1
1	A	487	PHE	2.1
1	A	713	PRO	2.1
1	A	693	PRO	2.0
1	A	338	GLN	2.0
1	A	289	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](#)

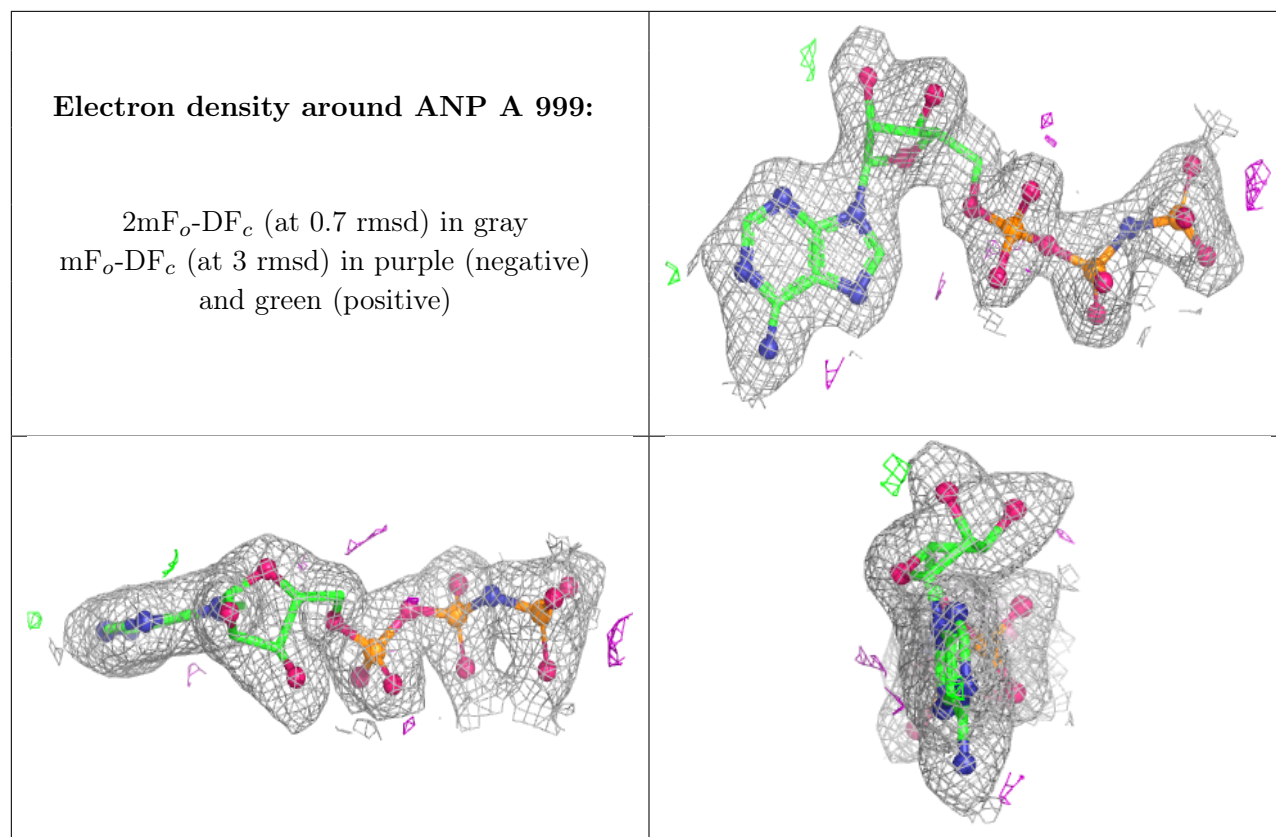
There are no oligosaccharides in this entry.

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	MG	A	998	1/1	0.98	0.03	17,17,17,17	0
3	ANP	A	999	31/31	0.99	0.05	7,19,35,47	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.