



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:26 AM UTC

PDB ID : 1MMG / pdb_00001mmg
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

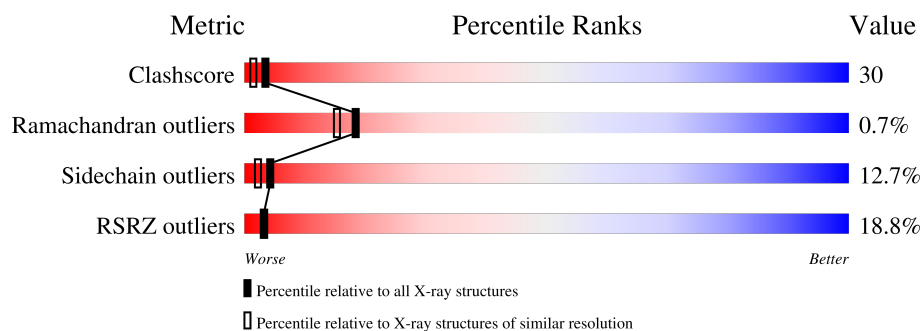
1 Overall quality at a glance

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 6234 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
1	A	741	Total	C	N	O	S	0	0	0
			5865	3724	1011	1114	16			

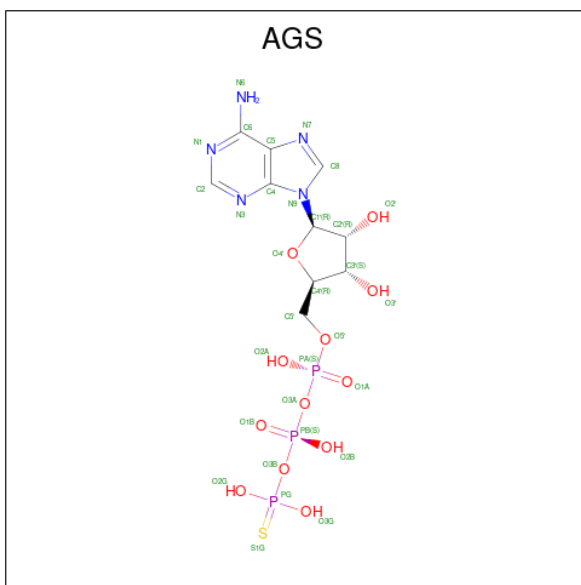
There are 11 discrepancies between the modelled and reference sequences:

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	322	ASP	GLU	conflict	UNP P08799
A	443	SER	GLN	conflict	UNP P08799
A	489	VAL	LEU	conflict	UNP P08799
A	628	LEU	ILE	conflict	UNP P08799
A	684	ALA	GLY	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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

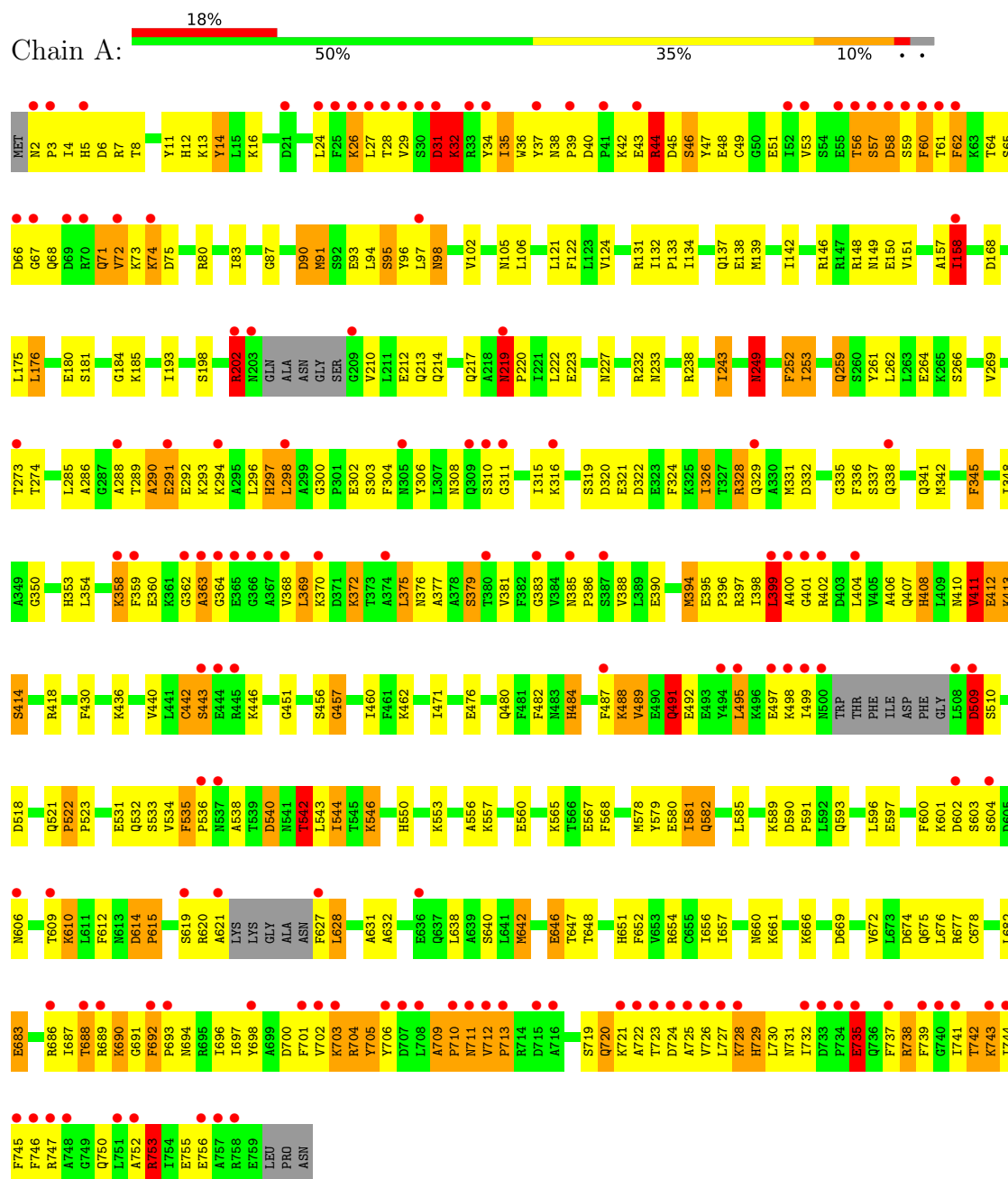
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	337	Total O 337 337	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	103.80Å 179.90Å 54.00Å 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) 96.9 (30.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.198 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 123.2	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	0.93	EDS
Total number of atoms	6234	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.45	20/5975 (0.3%)	1.88	125/8071 (1.5%)

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	1	0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	GLY	CA-C	6.50	1.60	1.51
1	A	540	ASP	CG-OD1	6.36	1.37	1.25
1	A	326	ILE	CA-CB	-6.33	1.47	1.54
1	A	480	GLN	CA-C	6.23	1.60	1.52
1	A	168	ASP	N-CA	-6.01	1.39	1.46
1	A	522	PRO	C-N	-5.88	1.25	1.33
1	A	648	THR	CA-C	-5.43	1.46	1.52
1	A	430	PHE	N-CA	-5.38	1.40	1.46
1	A	212	GLU	CD-OE2	5.27	1.35	1.25
1	A	460	ILE	C-O	-5.26	1.18	1.24
1	A	642	MET	N-CA	-5.24	1.39	1.46
1	A	75	ASP	CG-OD2	5.22	1.35	1.25
1	A	253	ILE	CA-C	-5.15	1.46	1.52
1	A	678	CYS	CA-C	-5.12	1.45	1.52
1	A	638	LEU	CA-CB	5.10	1.61	1.53
1	A	320	ASP	CG-OD1	5.08	1.34	1.25
1	A	131	ARG	NE-CZ	5.06	1.38	1.33
1	A	440	VAL	N-CA	-5.04	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	ASN	CA-CB	5.02	1.61	1.53
1	A	157	ALA	N-CA	-5.01	1.40	1.46

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	PHE	CA-CB-CG	-13.52	100.28	113.80
1	A	249	ASN	CA-CB-CG	-12.32	100.28	112.60
1	A	729	HIS	CA-CB-CG	-12.25	101.55	113.80
1	A	345	PHE	CA-CB-CG	-10.41	103.39	113.80
1	A	712	VAL	N-CA-C	9.22	119.11	108.96
1	A	484	HIS	CA-CB-CG	-9.12	104.68	113.80
1	A	131	ARG	CA-C-N	8.68	130.40	122.85
1	A	131	ARG	C-N-CA	8.68	130.40	122.85
1	A	180	GLU	N-CA-C	8.60	120.99	110.41
1	A	509	ASP	N-CA-C	-8.56	101.44	112.23
1	A	627	PHE	CA-C-N	8.32	132.69	120.87
1	A	627	PHE	C-N-CA	8.32	132.69	120.87
1	A	202	ARG	CB-CA-C	8.15	124.86	111.41
1	A	489	VAL	CB-CA-C	8.07	122.61	112.04
1	A	687	ILE	CB-CA-C	-8.02	101.52	112.02
1	A	674	ASP	CA-CB-CG	-7.94	104.66	112.60
1	A	731	ASN	CA-CB-CG	7.43	120.03	112.60
1	A	358	LYS	N-CA-CB	7.38	122.16	110.57
1	A	606	ASN	CA-CB-CG	-7.37	105.23	112.60
1	A	31	ASP	CA-C-N	7.25	131.13	120.90
1	A	31	ASP	C-N-CA	7.25	131.13	120.90
1	A	411	VAL	N-CA-C	7.06	117.06	110.42
1	A	12	HIS	CA-CB-CG	-7.00	106.80	113.80
1	A	692	PHE	CA-C-N	6.99	126.81	119.05
1	A	692	PHE	C-N-CA	6.99	126.81	119.05
1	A	489	VAL	N-CA-CB	6.91	119.11	110.47
1	A	297	HIS	CA-CB-CG	-6.79	107.01	113.80
1	A	600	PHE	CA-CB-CG	-6.79	107.01	113.80
1	A	35	ILE	CA-CB-CG2	6.57	121.67	110.50
1	A	735	GLU	N-CA-CB	6.57	121.30	110.39
1	A	582	GLN	CB-CG-CD	6.53	123.70	112.60
1	A	711	ASN	CA-C-N	6.53	132.84	119.72
1	A	711	ASN	C-N-CA	6.53	132.84	119.72
1	A	755	GLU	N-CA-C	-6.52	104.17	111.28
1	A	688	THR	CB-CA-C	6.42	120.97	110.88
1	A	491	GLN	CB-CG-CD	-6.41	101.70	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	556	ALA	N-CA-C	6.32	120.08	112.38
1	A	534	VAL	N-CA-C	6.30	117.08	110.72
1	A	58	ASP	CB-CA-C	-6.29	99.15	110.35
1	A	252	PHE	CA-CB-CG	-6.29	107.51	113.80
1	A	542	THR	N-CA-CB	-6.28	100.91	110.01
1	A	26	LYS	N-CA-C	6.25	118.09	111.28
1	A	168	ASP	N-CA-CB	6.14	118.97	110.07
1	A	98	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	60	PHE	CA-C-N	-6.07	114.22	122.77
1	A	60	PHE	C-N-CA	-6.07	114.22	122.77
1	A	121	LEU	CA-C-N	-6.05	111.73	122.74
1	A	121	LEU	C-N-CA	-6.05	111.73	122.74
1	A	688	THR	N-CA-CB	-6.00	101.30	110.01
1	A	310	SER	CA-C-N	-6.00	113.70	122.46
1	A	310	SER	C-N-CA	-6.00	113.70	122.46
1	A	298	LEU	N-CA-C	5.98	118.62	110.55
1	A	489	VAL	N-CA-C	5.97	117.43	110.62
1	A	44	ARG	CD-NE-CZ	5.96	132.74	124.40
1	A	48	GLU	N-CA-C	-5.89	100.45	109.41
1	A	394	MET	CA-C-N	-5.88	116.06	122.59
1	A	394	MET	C-N-CA	-5.88	116.06	122.59
1	A	713	PRO	N-CA-CB	5.87	109.42	103.25
1	A	326	ILE	CB-CA-C	-5.79	104.56	111.97
1	A	615	PRO	CB-CA-C	-5.77	103.65	111.85
1	A	614	ASP	CA-C-O	5.76	123.04	119.29
1	A	259	GLN	CB-CG-CD	5.73	122.34	112.60
1	A	628	LEU	N-CA-CB	-5.71	101.57	109.97
1	A	358	LYS	CA-CB-CG	-5.71	102.69	114.10
1	A	11	TYR	CA-C-O	5.70	126.46	120.42
1	A	399	LEU	N-CA-C	5.69	117.34	109.15
1	A	219	ASN	CA-CB-CG	-5.64	106.95	112.60
1	A	661	LYS	CA-C-N	-5.64	114.22	122.40
1	A	661	LYS	C-N-CA	-5.64	114.22	122.40
1	A	67	GLY	N-CA-C	-5.64	107.48	115.43
1	A	443	SER	N-CA-CB	5.61	119.36	110.55
1	A	315	ILE	N-CA-CB	5.61	118.88	111.25
1	A	672	VAL	CA-C-N	5.60	128.05	120.38
1	A	672	VAL	C-N-CA	5.60	128.05	120.38
1	A	660	ASN	CA-CB-CG	-5.58	107.02	112.60
1	A	710	PRO	N-CA-C	-5.58	100.97	112.47
1	A	704	ARG	CA-C-N	-5.58	113.48	122.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	ARG	C-N-CA	-5.58	113.48	122.23
1	A	509	ASP	O-C-N	5.55	129.77	122.33
1	A	652	PHE	N-CA-C	5.51	117.51	108.52
1	A	326	ILE	CA-CB-CG2	-5.49	101.17	110.50
1	A	678	CYS	CA-C-O	-5.47	113.68	119.97
1	A	35	ILE	CB-CA-C	-5.46	102.25	110.55
1	A	74	LYS	N-CA-C	-5.45	104.73	111.33
1	A	90	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	683	GLU	CB-CG-CD	5.34	121.67	112.60
1	A	442	CYS	N-CA-C	5.33	118.17	110.28
1	A	482	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	518	ASP	N-CA-C	5.32	119.88	113.17
1	A	57	SER	N-CA-CB	-5.32	101.50	110.49
1	A	476	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	408	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	39	PRO	CA-C-O	5.31	124.97	118.92
1	A	338	GLN	O-C-N	5.29	127.73	122.12
1	A	542	THR	N-CA-C	-5.29	105.41	111.07
1	A	91	MET	CA-C-O	5.29	125.89	119.49
1	A	709	ALA	O-C-N	5.29	126.10	121.39
1	A	62	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	262	LEU	CB-CA-C	-5.28	104.39	111.89
1	A	122	PHE	CB-CA-C	-5.22	101.18	109.80
1	A	402	ARG	N-CA-C	-5.22	105.03	111.40
1	A	148	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	A	678	CYS	O-C-N	5.17	128.63	122.27
1	A	620	ARG	CA-C-N	-5.17	112.40	121.70
1	A	620	ARG	C-N-CA	-5.17	112.40	121.70
1	A	14	TYR	N-CA-C	5.16	119.72	113.38
1	A	647	THR	CA-CB-OG1	5.16	117.34	109.60
1	A	631	ALA	CB-CA-C	-5.15	102.24	110.79
1	A	158	ILE	CA-CB-CG1	-5.13	101.68	110.40
1	A	492	GLU	CB-CA-C	-5.12	102.62	110.81
1	A	176	LEU	O-C-N	5.12	129.14	123.05
1	A	462	LYS	CB-CA-C	-5.11	103.09	110.96
1	A	335	GLY	CA-C-N	-5.10	114.99	122.19
1	A	335	GLY	C-N-CA	-5.10	114.99	122.19
1	A	311	GLY	CA-C-N	-5.10	115.91	123.05
1	A	311	GLY	C-N-CA	-5.10	115.91	123.05
1	A	705	TYR	N-CA-C	5.09	121.19	114.12
1	A	560	GLU	N-CA-C	-5.08	103.36	109.72
1	A	675	GLN	OE1-CD-NE2	5.08	127.68	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	692	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	353	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	32	LYS	N-CA-C	5.04	117.35	110.24
1	A	753	ARG	CA-C-N	5.01	126.87	120.56
1	A	753	ARG	C-N-CA	5.01	126.87	120.56

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	489	VAL	CA

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	5865	0	5757	349	0
2	A	1	0	0	0	0
3	A	31	0	12	3	0
4	A	337	0	0	6	0
All	All	6234	0	5769	349	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 30.

All (349) 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:61:THR:HG23	1:A:71:GLN:HG2	1.17	1.10
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.35	1.07
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.19	1.02
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.42	1.01
1:A:735:GLU:HA	1:A:738:ARG:NH2	1.76	1.01
1:A:532:GLN:HE22	1:A:542:THR:CG2	1.75	0.98
1:A:219:ASN:N	1:A:220:PRO:HD2	1.82	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:HE1	1:A:72:VAL:HG12	1.34	0.92
1:A:286:ALA:HB1	1:A:321:GLU:HG3	1.48	0.91
1:A:742:THR:HG22	1:A:743:LYS:HD2	1.51	0.91
1:A:654:ARG:NH1	4:A:8067:HOH:O	2.02	0.91
1:A:735:GLU:CA	1:A:738:ARG:HH21	1.83	0.90
1:A:139:MET:HA	1:A:142:ILE:HD12	1.54	0.90
1:A:16:LYS:NZ	4:A:8221:HOH:O	2.05	0.89
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.07	0.89
1:A:412:GLU:HG3	1:A:413:LYS:N	1.88	0.89
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.11	0.85
1:A:202:ARG:HH11	1:A:252:PHE:HB3	1.41	0.84
1:A:202:ARG:HH11	1:A:252:PHE:CB	1.91	0.82
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.15	0.82
1:A:61:THR:CG2	1:A:71:GLN:HG2	2.06	0.81
1:A:286:ALA:HB1	1:A:321:GLU:CG	2.11	0.81
1:A:286:ALA:CB	1:A:321:GLU:HG3	2.10	0.81
1:A:532:GLN:NE2	1:A:542:THR:CG2	2.42	0.81
1:A:61:THR:HG23	1:A:71:GLN:CG	2.08	0.81
1:A:730:LEU:HB2	1:A:732:ILE:HD12	1.62	0.81
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.11	0.81
1:A:538:ALA:HB1	1:A:542:THR:HG21	1.62	0.80
1:A:40:ASP:OD1	1:A:42:LYS:HB2	1.82	0.80
1:A:692:PHE:CE1	1:A:747:ARG:HG3	2.15	0.80
1:A:509:ASP:OD2	1:A:557:LYS:NZ	2.13	0.80
1:A:87:GLY:H	1:A:105:ASN:ND2	1.79	0.79
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.82	0.79
1:A:580:GLU:HG3	1:A:582:GLN:OE1	1.82	0.79
1:A:395:GLU:HA	1:A:407:GLN:O	1.82	0.79
1:A:59:SER:CA	1:A:74:LYS:HG3	2.14	0.78
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.14	0.78
1:A:146:ARG:HD3	1:A:151:VAL:HG13	1.66	0.78
1:A:497:GLU:OE2	1:A:742:THR:HB	1.84	0.78
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.65	0.77
1:A:62:PHE:CE1	1:A:72:VAL:HG12	2.18	0.77
1:A:289:THR:HB	1:A:291:GLU:CD	2.10	0.77
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.91	0.76
1:A:358:LYS:HG2	1:A:359:PHE:N	1.98	0.75
1:A:735:GLU:CA	1:A:738:ARG:NH2	2.45	0.75
1:A:397:ARG:HA	1:A:406:ALA:HA	1.68	0.75
1:A:210:VAL:O	1:A:214:GLN:HG3	1.88	0.74
1:A:385:ASN:OD1	1:A:386:PRO:HD2	1.85	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:O	1:A:293:LYS:HE2	1.87	0.74
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.15	0.74
1:A:396:PRO:O	1:A:398:ILE:HD12	1.88	0.74
1:A:399:LEU:HD11	1:A:401:GLY:O	1.86	0.74
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.23	0.73
1:A:742:THR:CG2	1:A:743:LYS:HD2	2.17	0.73
1:A:412:GLU:HG3	1:A:413:LYS:H	1.54	0.73
1:A:732:ILE:HG22	1:A:737:PHE:CE2	2.24	0.73
1:A:35:ILE:HD12	1:A:35:ILE:O	1.88	0.73
1:A:692:PHE:CD1	1:A:747:ARG:HG2	2.25	0.72
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.19	0.71
1:A:300:GLY:HA3	1:A:302:GLU:OE2	1.90	0.71
1:A:27:LEU:O	4:A:8229:HOH:O	2.09	0.71
1:A:732:ILE:HG22	1:A:737:PHE:HE2	1.55	0.71
1:A:683:GLU:HG3	1:A:686:ARG:NH1	2.05	0.70
1:A:289:THR:HB	1:A:291:GLU:OE2	1.91	0.70
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.58	0.69
1:A:290:ALA:HA	1:A:293:LYS:CD	2.20	0.69
1:A:532:GLN:HE22	1:A:542:THR:HG21	1.57	0.69
1:A:40:ASP:HB3	1:A:43:GLU:HG2	1.73	0.68
1:A:319:SER:OG	1:A:322:ASP:HB2	1.94	0.68
1:A:532:GLN:NE2	1:A:542:THR:HG22	2.10	0.67
1:A:60:PHE:CD2	1:A:74:LYS:HA	2.29	0.67
1:A:399:LEU:HD12	1:A:401:GLY:H	1.59	0.66
1:A:692:PHE:CD1	1:A:747:ARG:CG	2.78	0.66
1:A:703:LYS:HD3	1:A:704:ARG:N	2.11	0.66
1:A:692:PHE:CZ	1:A:738:ARG:HG2	2.31	0.66
1:A:273:THR:O	1:A:274:THR:OG1	2.09	0.65
1:A:686:ARG:HA	1:A:689:ARG:NH1	2.11	0.65
1:A:491:GLN:O	1:A:495:LEU:HD22	1.96	0.65
1:A:532:GLN:HE22	1:A:538:ALA:HB1	1.62	0.65
1:A:51:GLU:O	1:A:62:PHE:HB2	1.98	0.64
1:A:249:ASN:ND2	1:A:249:ASN:H	1.74	0.64
1:A:72:VAL:HG22	1:A:73:LYS:O	1.97	0.64
1:A:329:GLN:O	1:A:332:ASP:HB2	1.96	0.64
1:A:87:GLY:H	1:A:105:ASN:HD21	1.45	0.64
1:A:45:ASP:CG	1:A:677:ARG:NH2	2.56	0.63
1:A:710:PRO:HG2	1:A:729:HIS:CE1	2.33	0.63
1:A:710:PRO:HD2	1:A:729:HIS:CE1	2.33	0.63
1:A:336:PHE:O	1:A:341:GLN:NE2	2.30	0.62
1:A:98:ASN:O	1:A:102:VAL:HG23	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.79	0.62
1:A:614:ASP:OD1	1:A:615:PRO:HD2	1.99	0.62
1:A:181:SER:OG	3:A:999:AGS:O2G	2.14	0.62
1:A:64:THR:HG23	1:A:68:GLN:O	1.99	0.62
1:A:124:VAL:HG13	1:A:656:ILE:HD12	1.81	0.61
1:A:698:TYR:CE1	1:A:720:GLN:HG2	2.36	0.61
1:A:498:LYS:O	1:A:498:LYS:HG2	1.99	0.60
1:A:59:SER:N	1:A:74:LYS:HG3	2.16	0.60
1:A:59:SER:HA	1:A:74:LYS:HG3	1.84	0.60
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.84	0.60
1:A:742:THR:HG22	1:A:743:LYS:CD	2.27	0.60
1:A:137:GLN:HG3	1:A:137:GLN:O	2.02	0.59
1:A:484:HIS:O	1:A:487:PHE:HB3	2.02	0.59
1:A:34:TYR:CD1	1:A:51:GLU:HA	2.38	0.59
1:A:567:GLU:HB3	1:A:578:MET:CE	2.32	0.59
1:A:337:SER:O	1:A:341:GLN:HG3	2.02	0.59
1:A:289:THR:C	1:A:291:GLU:N	2.60	0.59
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.84	0.59
1:A:735:GLU:C	1:A:738:ARG:HH21	2.10	0.58
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.84	0.58
1:A:37:TYR:O	1:A:47:TYR:HA	2.03	0.58
1:A:62:PHE:HE1	1:A:72:VAL:CG1	2.13	0.58
1:A:397:ARG:HD2	1:A:404:LEU:CD2	2.33	0.58
1:A:753:ARG:O	1:A:756:GLU:HB2	2.03	0.58
1:A:491:GLN:O	1:A:495:LEU:HD13	2.02	0.58
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.85	0.58
1:A:202:ARG:NH1	1:A:252:PHE:CB	2.66	0.58
1:A:523:PRO:HD2	4:A:8295:HOH:O	2.03	0.58
1:A:696:ILE:O	1:A:743:LYS:HA	2.03	0.58
1:A:703:LYS:CD	1:A:704:ARG:N	2.67	0.58
1:A:372:LYS:HE3	1:A:390:GLU:OE2	2.04	0.57
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.18	0.57
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.33	0.57
1:A:31:ASP:N	1:A:31:ASP:OD1	2.37	0.57
1:A:726:VAL:O	1:A:730:LEU:HG	2.04	0.57
1:A:399:LEU:HD12	1:A:401:GLY:N	2.20	0.57
1:A:59:SER:HB2	1:A:72:VAL:O	2.05	0.57
1:A:2:ASN:ND2	1:A:5:HIS:CE1	2.73	0.57
1:A:213:GLN:O	1:A:217:GLN:HG2	2.06	0.56
1:A:724:ASP:O	1:A:728:LYS:HB2	2.05	0.56
1:A:296:LEU:O	1:A:297:HIS:HB2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:HD22	1:A:5:HIS:CE1	2.24	0.56
1:A:146:ARG:HD3	1:A:151:VAL:CG1	2.34	0.56
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.35	0.55
1:A:289:THR:O	1:A:291:GLU:N	2.39	0.55
1:A:487:PHE:O	1:A:491:GLN:HB2	2.06	0.55
1:A:289:THR:C	1:A:291:GLU:H	2.12	0.55
1:A:567:GLU:HB3	1:A:578:MET:HE2	1.89	0.55
1:A:383:GLY:HA3	1:A:604:SER:OG	2.07	0.55
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.89	0.55
1:A:223:GLU:O	1:A:227:ASN:HB2	2.07	0.54
1:A:542:THR:HG22	1:A:543:LEU:N	2.22	0.54
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.42	0.54
1:A:692:PHE:CD1	1:A:747:ARG:HG3	2.43	0.54
1:A:697:ILE:HB	1:A:700:ASP:OD2	2.07	0.54
1:A:6:ASP:C	1:A:8:THR:H	2.16	0.54
1:A:243:ILE:O	1:A:451:GLY:HA2	2.07	0.54
1:A:730:LEU:CB	1:A:732:ILE:HD12	2.35	0.54
1:A:139:MET:HA	1:A:142:ILE:CD1	2.34	0.54
1:A:642:MET:O	1:A:646:GLU:OE1	2.26	0.54
1:A:698:TYR:OH	1:A:739:PHE:HD1	1.91	0.54
1:A:319:SER:CB	1:A:322:ASP:HB2	2.38	0.54
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.27	0.53
1:A:723:THR:HG22	1:A:739:PHE:CZ	2.43	0.53
1:A:725:ALA:O	1:A:729:HIS:N	2.34	0.53
1:A:176:LEU:N	1:A:176:LEU:HD12	2.24	0.53
1:A:698:TYR:HE1	1:A:739:PHE:CE1	2.26	0.53
1:A:532:GLN:NE2	1:A:538:ALA:HB1	2.23	0.53
1:A:533:SER:O	1:A:589:LYS:HE3	2.09	0.53
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.26	0.53
1:A:397:ARG:HD2	1:A:404:LEU:HD21	1.91	0.53
1:A:60:PHE:N	1:A:72:VAL:O	2.33	0.52
1:A:308:ASN:C	1:A:308:ASN:OD1	2.53	0.52
1:A:732:ILE:CG2	1:A:737:PHE:HE2	2.21	0.52
1:A:43:GLU:O	1:A:43:GLU:HG3	2.10	0.52
1:A:72:VAL:CG2	1:A:73:LYS:N	2.72	0.52
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.92	0.52
1:A:59:SER:OG	1:A:71:GLN:OE1	2.27	0.52
1:A:184:GLY:HA2	3:A:999:AGS:O1A	2.10	0.52
1:A:217:GLN:O	1:A:220:PRO:HG2	2.09	0.52
1:A:35:ILE:HD13	1:A:37:TYR:HB3	1.92	0.51
1:A:700:ASP:O	1:A:703:LYS:HD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:HA	1:A:298:LEU:HD12	1.93	0.51
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.44	0.51
1:A:730:LEU:CB	1:A:732:ILE:CD1	2.88	0.51
1:A:735:GLU:HB3	1:A:738:ARG:HH22	1.74	0.51
1:A:354:LEU:O	1:A:418:ARG:HD3	2.10	0.51
1:A:710:PRO:HD2	1:A:729:HIS:NE2	2.26	0.51
1:A:692:PHE:CE1	1:A:747:ARG:CG	2.88	0.51
1:A:730:LEU:CD1	1:A:732:ILE:HD11	2.41	0.51
1:A:26:LYS:HA	1:A:29:VAL:HG23	1.92	0.51
1:A:410:ASN:C	1:A:410:ASN:OD1	2.54	0.51
1:A:730:LEU:HB2	1:A:732:ILE:CD1	2.39	0.50
1:A:738:ARG:N	1:A:745:PHE:O	2.37	0.50
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.47	0.50
1:A:544:ILE:O	1:A:544:ILE:HG13	2.12	0.50
1:A:202:ARG:NH1	1:A:252:PHE:HB2	2.27	0.50
1:A:362:GLY:O	1:A:363:ALA:C	2.54	0.50
1:A:497:GLU:CD	1:A:742:THR:HB	2.37	0.50
1:A:535:PHE:CD2	1:A:535:PHE:N	2.76	0.50
1:A:181:SER:HA	3:A:999:AGS:S1G	2.52	0.49
1:A:289:THR:HG1	1:A:292:GLU:HG3	1.75	0.49
1:A:597:GLU:OE1	1:A:612:PHE:HD2	1.94	0.49
1:A:456:SER:OG	1:A:457:GLY:O	2.29	0.49
1:A:43:GLU:O	1:A:43:GLU:CG	2.60	0.49
1:A:375:LEU:O	1:A:379:SER:OG	2.30	0.49
1:A:756:GLU:OE2	4:A:8220:HOH:O	2.20	0.49
1:A:538:ALA:CB	1:A:542:THR:HG21	2.38	0.49
1:A:698:TYR:O	1:A:702:VAL:HG23	2.12	0.49
1:A:737:PHE:HB3	1:A:746:PHE:CD1	2.48	0.49
1:A:59:SER:HA	1:A:74:LYS:H	1.78	0.49
1:A:538:ALA:HB1	1:A:542:THR:CG2	2.39	0.49
1:A:202:ARG:HH11	1:A:252:PHE:HB2	1.76	0.48
1:A:385:ASN:O	1:A:388:VAL:N	2.45	0.48
1:A:750:GLN:O	1:A:750:GLN:NE2	2.45	0.48
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.48	0.48
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.95	0.48
1:A:602:ASP:O	1:A:603:SER:C	2.56	0.48
1:A:37:TYR:OH	1:A:65:SER:N	2.41	0.48
1:A:532:GLN:OE1	1:A:542:THR:HG23	2.13	0.48
1:A:90:ASP:HB3	1:A:93:GLU:HG3	1.94	0.48
1:A:202:ARG:NH1	1:A:253:ILE:O	2.46	0.48
1:A:97:LEU:HB2	1:A:689:ARG:HD3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:ILE:HD13	1:A:676:LEU:HD21	1.95	0.48
1:A:36:TRP:NE1	1:A:80:ARG:HG3	2.29	0.48
1:A:146:ARG:CD	1:A:151:VAL:CG1	2.92	0.48
1:A:495:LEU:CD1	1:A:495:LEU:N	2.75	0.48
1:A:726:VAL:O	1:A:729:HIS:HB3	2.14	0.48
1:A:682:LEU:O	1:A:686:ARG:HG3	2.14	0.47
1:A:2:ASN:O	1:A:5:HIS:N	2.41	0.47
1:A:732:ILE:CG2	1:A:737:PHE:CE2	2.93	0.47
1:A:53:VAL:HG23	1:A:62:PHE:HA	1.96	0.47
1:A:60:PHE:O	1:A:71:GLN:HA	2.13	0.47
1:A:35:ILE:CD1	1:A:37:TYR:HD2	2.28	0.47
1:A:149:ASN:H	1:A:149:ASN:ND2	2.10	0.47
1:A:738:ARG:HA	1:A:738:ARG:HD3	1.54	0.47
1:A:696:ILE:N	1:A:696:ILE:HD12	2.30	0.47
1:A:35:ILE:HD11	1:A:37:TYR:HD2	1.80	0.47
1:A:185:LYS:HE3	1:A:456:SER:HA	1.97	0.47
1:A:32:LYS:HB3	1:A:34:TYR:CE2	2.50	0.46
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.50	0.46
1:A:521:GLN:HA	1:A:522:PRO:C	2.41	0.46
1:A:698:TYR:CD1	1:A:720:GLN:HA	2.50	0.46
1:A:35:ILE:HD12	1:A:35:ILE:C	2.40	0.46
1:A:385:ASN:HB3	1:A:388:VAL:HG21	1.97	0.46
1:A:217:GLN:C	1:A:220:PRO:HG2	2.41	0.46
1:A:238:ARG:HD3	1:A:264:GLU:OE1	2.15	0.46
1:A:410:ASN:O	1:A:414:SER:HB2	2.15	0.46
1:A:386:PRO:O	1:A:390:GLU:HB2	2.16	0.46
1:A:59:SER:C	1:A:74:LYS:HG3	2.41	0.46
1:A:62:PHE:CE1	1:A:72:VAL:CG1	2.95	0.46
1:A:341:GLN:O	1:A:345:PHE:CD2	2.69	0.46
1:A:358:LYS:NZ	1:A:359:PHE:O	2.38	0.46
1:A:289:THR:CB	1:A:291:GLU:CD	2.86	0.46
1:A:181:SER:O	1:A:657:ILE:HD12	2.16	0.46
1:A:139:MET:CA	1:A:142:ILE:HD12	2.36	0.45
1:A:397:ARG:HD2	1:A:404:LEU:HD23	1.97	0.45
1:A:546:LYS:O	1:A:550:HIS:HD2	1.98	0.45
1:A:686:ARG:O	1:A:689:ARG:HB3	2.17	0.45
1:A:532:GLN:HE21	1:A:532:GLN:HB3	1.29	0.45
1:A:372:LYS:O	1:A:376:ASN:CG	2.59	0.45
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.69	0.45
1:A:628:LEU:HD11	1:A:632:ALA:HB1	1.98	0.45
1:A:60:PHE:HD2	1:A:74:LYS:HA	1.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:CD	1:A:138:GLU:H	2.25	0.45
1:A:377:ALA:O	1:A:381:VAL:HG22	2.16	0.45
1:A:362:GLY:O	1:A:364:GLY:N	2.50	0.45
1:A:710:PRO:CD	1:A:729:HIS:CE1	2.99	0.45
1:A:710:PRO:CG	1:A:729:HIS:CE1	3.00	0.45
1:A:735:GLU:O	1:A:738:ARG:NH2	2.50	0.45
1:A:590:ASP:N	1:A:591:PRO:HD3	2.32	0.45
1:A:324:PHE:O	1:A:328:ARG:HB2	2.17	0.45
1:A:345:PHE:HD1	1:A:345:PHE:HA	1.56	0.45
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.98	0.44
1:A:696:ILE:HG22	1:A:697:ILE:O	2.16	0.44
1:A:37:TYR:O	1:A:47:TYR:CA	2.65	0.44
1:A:2:ASN:HA	1:A:3:PRO:HD2	1.79	0.44
1:A:124:VAL:CG1	1:A:656:ILE:HD12	2.46	0.44
1:A:683:GLU:HG3	1:A:686:ARG:HH12	1.80	0.44
1:A:719:SER:HA	1:A:722:ALA:HB3	2.00	0.44
1:A:597:GLU:O	1:A:601:LYS:HG3	2.17	0.44
1:A:293:LYS:O	1:A:297:HIS:N	2.51	0.44
1:A:621:ALA:HB2	1:A:628:LEU:HB2	2.00	0.44
1:A:698:TYR:CE2	1:A:720:GLN:CG	3.01	0.44
1:A:358:LYS:CG	1:A:359:PHE:N	2.74	0.44
1:A:408:HIS:C	1:A:408:HIS:ND1	2.76	0.44
1:A:585:LEU:O	1:A:589:LYS:HG3	2.17	0.44
1:A:692:PHE:CE2	1:A:738:ARG:HG2	2.52	0.44
1:A:87:GLY:N	1:A:105:ASN:HD21	2.12	0.43
1:A:628:LEU:HD12	1:A:628:LEU:HA	1.43	0.43
1:A:34:TYR:HE1	1:A:51:GLU:HB2	1.73	0.43
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.58	0.43
1:A:202:ARG:HD3	1:A:252:PHE:CB	2.48	0.43
1:A:319:SER:HB3	1:A:322:ASP:HB2	2.00	0.43
1:A:737:PHE:HB3	1:A:746:PHE:CE1	2.53	0.43
1:A:273:THR:C	1:A:274:THR:HG1	2.14	0.43
1:A:690:LYS:HE2	1:A:690:LYS:HB3	1.45	0.43
1:A:701:PHE:CE1	1:A:705:TYR:CD2	3.06	0.43
1:A:6:ASP:O	1:A:8:THR:N	2.52	0.43
1:A:399:LEU:HD11	1:A:401:GLY:C	2.44	0.43
1:A:568:PHE:C	1:A:578:MET:CE	2.92	0.43
1:A:597:GLU:OE1	1:A:612:PHE:CD2	2.72	0.43
1:A:38:ASN:C	1:A:40:ASP:H	2.26	0.43
1:A:691:GLY:O	1:A:747:ARG:CD	2.67	0.43
1:A:710:PRO:HG2	1:A:729:HIS:HE1	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:CA	1:A:381:VAL:HG21	2.49	0.43
1:A:698:TYR:CE1	1:A:739:PHE:CE1	3.07	0.43
1:A:96:TYR:OH	1:A:753:ARG:CZ	2.67	0.43
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.84	0.43
1:A:38:ASN:HA	1:A:46:SER:O	2.19	0.42
1:A:94:LEU:O	1:A:97:LEU:HD11	2.19	0.42
1:A:146:ARG:HD2	1:A:151:VAL:HG11	2.01	0.42
1:A:698:TYR:CZ	1:A:720:GLN:CG	3.00	0.42
1:A:610:LYS:HB3	1:A:610:LYS:HE2	1.67	0.42
1:A:132:ILE:HG22	1:A:134:ILE:HG23	2.00	0.42
1:A:219:ASN:H	1:A:220:PRO:HD2	1.78	0.42
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.72	0.42
1:A:399:LEU:HD12	1:A:400:ALA:N	2.34	0.42
1:A:302:GLU:H	1:A:302:GLU:CD	2.27	0.42
1:A:60:PHE:CD2	1:A:74:LYS:HG2	2.55	0.42
1:A:232:ARG:NH1	1:A:232:ARG:HG2	2.34	0.42
1:A:348:ILE:HD13	1:A:348:ILE:HA	1.86	0.42
1:A:385:ASN:HB3	1:A:388:VAL:HG23	2.01	0.42
1:A:568:PHE:CA	1:A:578:MET:HE1	2.50	0.42
1:A:395:GLU:HG2	1:A:408:HIS:HA	2.00	0.42
1:A:712:VAL:HG21	1:A:725:ALA:HB3	2.00	0.42
1:A:394:MET:HG2	1:A:414:SER:OG	2.19	0.42
1:A:693:PRO:HD2	1:A:747:ARG:HA	2.02	0.42
1:A:56:THR:OG1	1:A:58:ASP:OD1	2.29	0.42
1:A:300:GLY:O	1:A:304:PHE:CD2	2.72	0.42
1:A:495:LEU:HD13	1:A:495:LEU:H	1.84	0.42
1:A:95:SER:HB3	1:A:752:ALA:HB2	2.02	0.42
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.49	0.42
1:A:688:THR:HA	4:A:8198:HOH:O	2.20	0.42
1:A:91:MET:CE	1:A:106:LEU:HD13	2.50	0.41
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.79	0.41
1:A:369:LEU:O	1:A:372:LYS:NZ	2.34	0.41
1:A:491:GLN:HE21	1:A:491:GLN:HB3	1.55	0.41
1:A:750:GLN:NE2	1:A:750:GLN:HA	2.35	0.41
1:A:399:LEU:HD12	1:A:399:LEU:C	2.45	0.41
1:A:728:LYS:O	1:A:729:HIS:C	2.63	0.41
1:A:158:ILE:HG22	1:A:175:LEU:HD21	2.03	0.41
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.55	0.41
1:A:495:LEU:HD13	1:A:495:LEU:N	2.35	0.41
1:A:289:THR:O	1:A:292:GLU:N	2.54	0.41
1:A:385:ASN:HA	1:A:386:PRO:HD3	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LYS:HE3	1:A:488:LYS:HB2	1.84	0.41
1:A:693:PRO:HD2	1:A:746:PHE:O	2.20	0.41
1:A:289:THR:HB	1:A:291:GLU:OE1	2.20	0.41
1:A:698:TYR:CE1	1:A:739:PHE:CD1	3.09	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG11	2.03	0.41
1:A:542:THR:CG2	1:A:543:LEU:N	2.84	0.40
1:A:567:GLU:HA	1:A:579:TYR:O	2.22	0.40
1:A:175:LEU:HG	1:A:651:HIS:HB2	2.03	0.40
1:A:40:ASP:HB3	1:A:43:GLU:CG	2.48	0.40
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.56	0.40
1:A:289:THR:O	1:A:290:ALA:C	2.63	0.40
1:A:704:ARG:HG2	1:A:705:TYR:CZ	2.57	0.40
1:A:292:GLU:O	1:A:296:LEU:N	2.55	0.40
1:A:442:CYS:SG	1:A:443:SER:N	2.95	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	733/762 (96%)	695 (95%)	33 (4%)	5 (1%)	18 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ALA
1	A	711	ASN
1	A	7	ARG
1	A	290	ALA
1	A	713	PRO

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	629/666 (94%)	549 (87%)	80 (13%)	4 2

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	24	LEU
1	A	28	THR
1	A	31	ASP
1	A	32	LYS
1	A	44	ARG
1	A	46	SER
1	A	56	THR
1	A	57	SER
1	A	66	ASP
1	A	71	GLN
1	A	72	VAL
1	A	83	ILE
1	A	95	SER
1	A	150	GLU
1	A	158	ILE
1	A	193	ILE
1	A	198	SER
1	A	202	ARG
1	A	219	ASN
1	A	243	ILE
1	A	249	ASN
1	A	266	SER
1	A	285	LEU
1	A	291	GLU
1	A	294	LYS
1	A	303	SER
1	A	316	LYS
1	A	326	ILE
1	A	328	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	342	MET
1	A	360	GLU
1	A	368	VAL
1	A	369	LEU
1	A	370	LYS
1	A	372	LYS
1	A	375	LEU
1	A	379	SER
1	A	399	LEU
1	A	411	VAL
1	A	412	GLU
1	A	413	LYS
1	A	414	SER
1	A	436	LYS
1	A	446	LYS
1	A	471	ILE
1	A	488	LYS
1	A	489	VAL
1	A	491	GLN
1	A	495	LEU
1	A	499	ILE
1	A	509	ASP
1	A	510	SER
1	A	531	GLU
1	A	542	THR
1	A	544	ILE
1	A	546	LYS
1	A	553	LYS
1	A	565	LYS
1	A	581	ILE
1	A	609	THR
1	A	610	LYS
1	A	619	SER
1	A	640	SER
1	A	646	GLU
1	A	666	LYS
1	A	669	ASP
1	A	690	LYS
1	A	703	LYS
1	A	720	GLN
1	A	721	LYS
1	A	727	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	728	LYS
1	A	735	GLU
1	A	738	ARG
1	A	741	ILE
1	A	742	THR
1	A	743	LYS
1	A	744	ILE
1	A	753	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	105	ASN
1	A	149	ASN
1	A	188	ASN
1	A	217	GLN
1	A	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	329	GLN
1	A	439	ASN
1	A	491	GLN
1	A	532	GLN
1	A	594	GLN
1	A	606	ASN
1	A	613	ASN
1	A	649	ASN
1	A	662	GLN
1	A	729	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	AGS	A	999	2	32,33,33	1.73	7 (21%)	45,52,52	1.48	9 (20%)

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	AGS	A	999	2	-	3/21/38/38	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	AGS	PG-S1G	5.28	2.02	1.90
3	A	999	AGS	PA-O3A	-4.18	1.55	1.59
3	A	999	AGS	C6-N6	-3.49	1.25	1.34
3	A	999	AGS	PB-O3B	2.30	1.62	1.59
3	A	999	AGS	O4'-C1'	-2.23	1.36	1.42
3	A	999	AGS	PA-O1A	2.13	1.58	1.50
3	A	999	AGS	C2-N1	2.08	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AGS	C2-N1-C6	4.03	125.35	118.73
3	A	999	AGS	N3-C2-N1	-3.05	123.96	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AGS	C2'-C3'-C4'	-2.80	97.21	102.61
3	A	999	AGS	O3'-C3'-C2'	2.78	120.73	111.82
3	A	999	AGS	C4-N9-C1'	-2.55	120.67	126.63
3	A	999	AGS	O3G-PG-O3B	2.54	113.12	104.64
3	A	999	AGS	C1'-N9-C8	2.19	131.95	127.09
3	A	999	AGS	C5-C6-N1	-2.13	112.11	117.51
3	A	999	AGS	O4'-C1'-N9	2.06	112.04	108.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

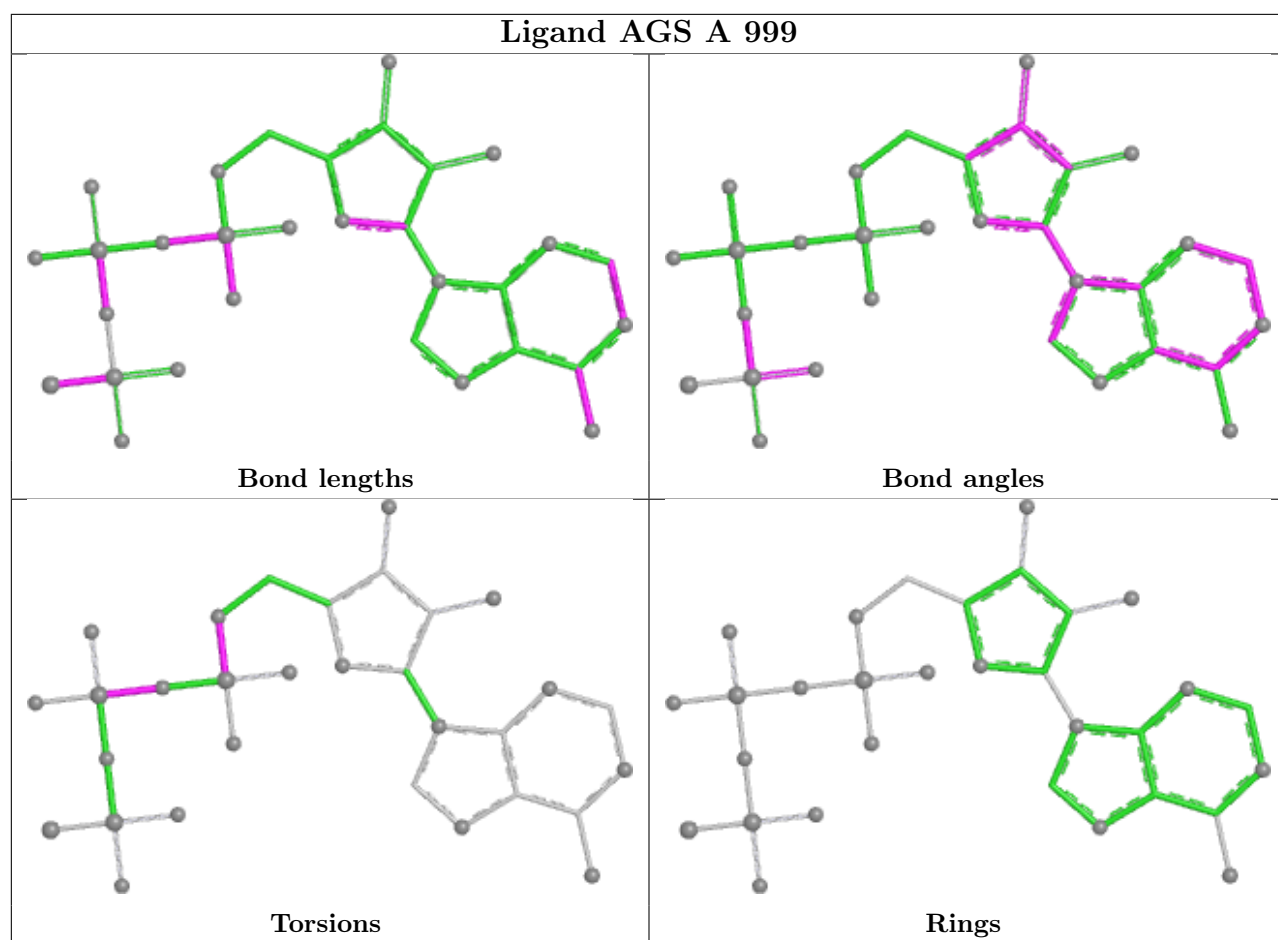
Mol	Chain	Res	Type	Atoms
3	A	999	AGS	C5'-O5'-PA-O1A
3	A	999	AGS	PA-O3A-PB-O2B
3	A	999	AGS	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	AGS	3	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	741/762 (97%)	0.67	139 (18%) 3 3	12, 37, 84, 100	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	627	PHE	5.8
1	A	748	ALA	5.6
1	A	494	TYR	5.4
1	A	25	PHE	5.0
1	A	363	ALA	4.9
1	A	725	ALA	4.7
1	A	715	ASP	4.7
1	A	734	PRO	4.6
1	A	495	LEU	4.5
1	A	710	PRO	4.4
1	A	737	PHE	4.3
1	A	621	ALA	4.3
1	A	52	ILE	4.3
1	A	53	VAL	4.3
1	A	500	ASN	4.3
1	A	498	LYS	4.2
1	A	757	ALA	4.1
1	A	203	ASN	4.0
1	A	59	SER	4.0
1	A	744	ILE	4.0
1	A	739	PHE	3.9
1	A	536	PRO	3.9
1	A	443	SER	3.9
1	A	364	GLY	3.8
1	A	367	ALA	3.8
1	A	383	GLY	3.8
1	A	399	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	745	PHE	3.6
1	A	400	ALA	3.6
1	A	368	VAL	3.6
1	A	707	ASP	3.5
1	A	39	PRO	3.4
1	A	706	TYR	3.4
1	A	61	THR	3.4
1	A	716	ALA	3.4
1	A	708	LEU	3.4
1	A	508	LEU	3.4
1	A	751	LEU	3.4
1	A	202	ARG	3.3
1	A	209	GLY	3.3
1	A	60	PHE	3.3
1	A	602	ASP	3.3
1	A	487	PHE	3.3
1	A	509	ASP	3.3
1	A	746	PHE	3.2
1	A	728	LYS	3.2
1	A	499	ILE	3.2
1	A	711	ASN	3.2
1	A	56	THR	3.1
1	A	743	LYS	3.1
1	A	366	GLY	3.1
1	A	402	ARG	3.1
1	A	365	GLU	3.1
1	A	294	LYS	3.1
1	A	404	LEU	3.1
1	A	3	PRO	3.0
1	A	741	ILE	3.0
1	A	26	LYS	3.0
1	A	693	PRO	3.0
1	A	758	ARG	2.9
1	A	219	ASN	2.9
1	A	28	THR	2.9
1	A	701	PHE	2.9
1	A	27	LEU	2.9
1	A	298	LEU	2.9
1	A	311	GLY	2.9
1	A	273	THR	2.9
1	A	380	THR	2.9
1	A	362	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	727	LEU	2.8
1	A	688	THR	2.8
1	A	69	ASP	2.8
1	A	721	LYS	2.8
1	A	752	ALA	2.7
1	A	41	PRO	2.7
1	A	713	PRO	2.7
1	A	726	VAL	2.7
1	A	97	LEU	2.6
1	A	21	ASP	2.6
1	A	33	ARG	2.6
1	A	329	GLN	2.6
1	A	70	ARG	2.6
1	A	66	ASP	2.5
1	A	733	ASP	2.5
1	A	37	TYR	2.5
1	A	756	GLU	2.5
1	A	401	GLY	2.5
1	A	29	VAL	2.5
1	A	724	ASP	2.5
1	A	43	GLU	2.5
1	A	692	PHE	2.5
1	A	2	ASN	2.5
1	A	385	ASN	2.5
1	A	732	ILE	2.5
1	A	497	GLU	2.4
1	A	723	THR	2.4
1	A	305	ASN	2.4
1	A	158	ILE	2.4
1	A	74	LYS	2.4
1	A	604	SER	2.4
1	A	445	ARG	2.3
1	A	72	VAL	2.3
1	A	309	GLN	2.3
1	A	537	ASN	2.3
1	A	444	GLU	2.3
1	A	722	ALA	2.3
1	A	55	GLU	2.3
1	A	703	LYS	2.3
1	A	698	TYR	2.3
1	A	359	PHE	2.2
1	A	735	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	619	SER	2.2
1	A	609	THR	2.2
1	A	291	GLU	2.2
1	A	686	ARG	2.2
1	A	62	PHE	2.2
1	A	387	SER	2.2
1	A	747	ARG	2.2
1	A	606	ASN	2.2
1	A	712	VAL	2.1
1	A	338	GLN	2.1
1	A	740	GLY	2.1
1	A	288	ALA	2.1
1	A	57	SER	2.1
1	A	316	LYS	2.1
1	A	5	HIS	2.1
1	A	702	VAL	2.1
1	A	24	LEU	2.1
1	A	358	LYS	2.1
1	A	370	LYS	2.1
1	A	30	SER	2.1
1	A	310	SER	2.1
1	A	689	ARG	2.1
1	A	374	ALA	2.1
1	A	34	TYR	2.1
1	A	67	GLY	2.1
1	A	31	ASP	2.0
1	A	636	GLU	2.0
1	A	58	ASP	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.

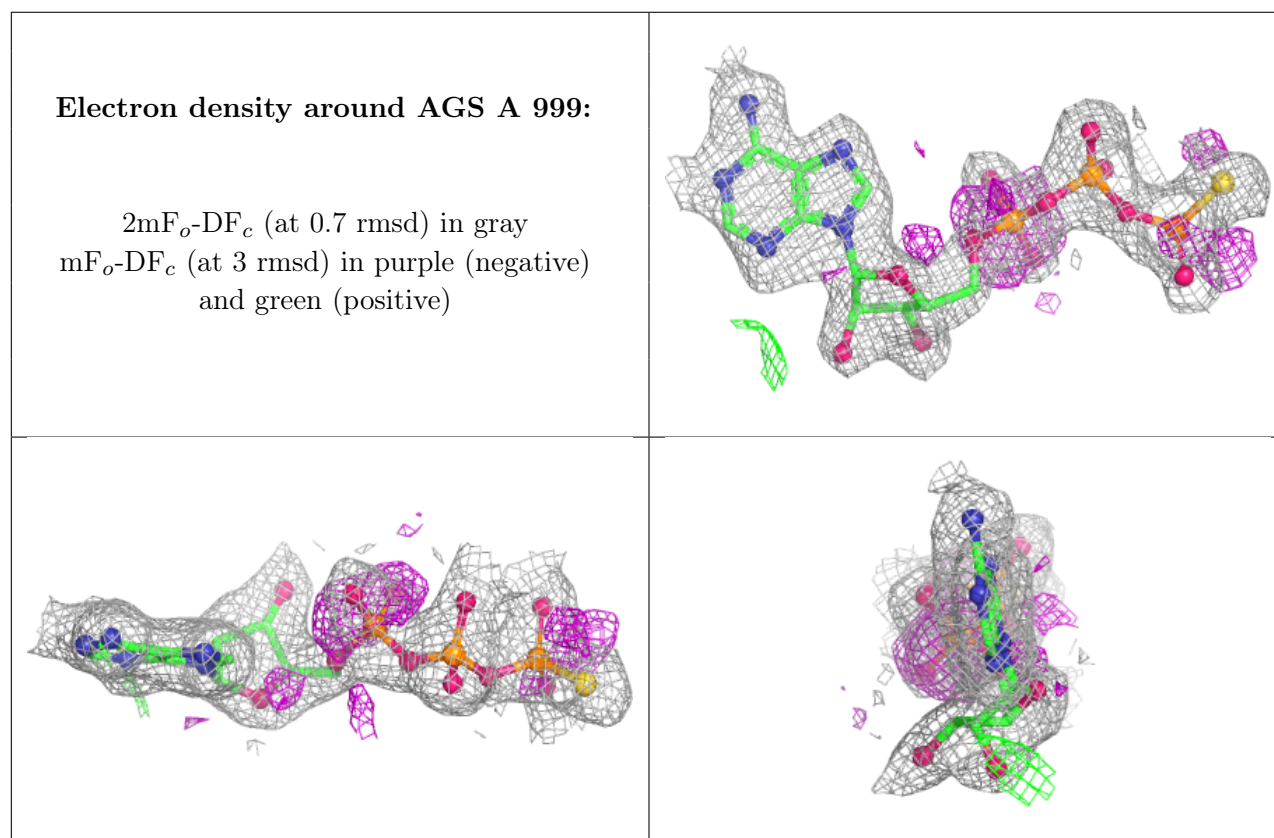
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	AGS	A	999	31/31	0.96	0.11	11,38,100,100	0
2	MG	A	998	1/1	0.98	0.02	19,19,19,19	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.