



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:46 PM EDT

PDB ID : 1D0X / pdb_00001d0x
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH M-NITROPHENYL AMINOETHYLDIPHOSPHA
TE BERYLLIUM TRIFLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

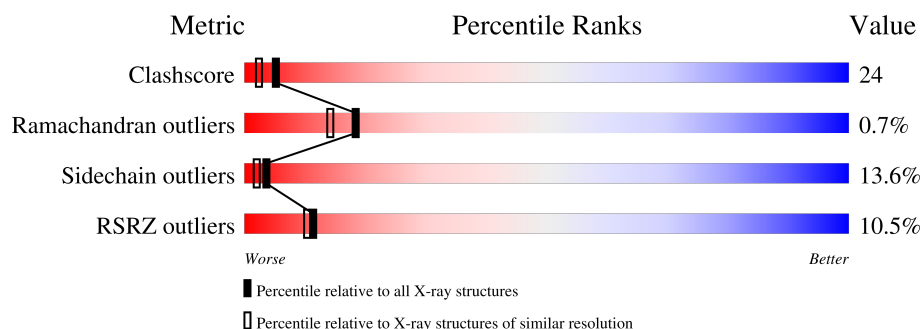
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

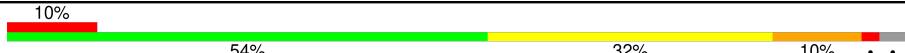
The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6643 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 S1DC MOTOR DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	35	0
			5887	3744	1017	1110	16			

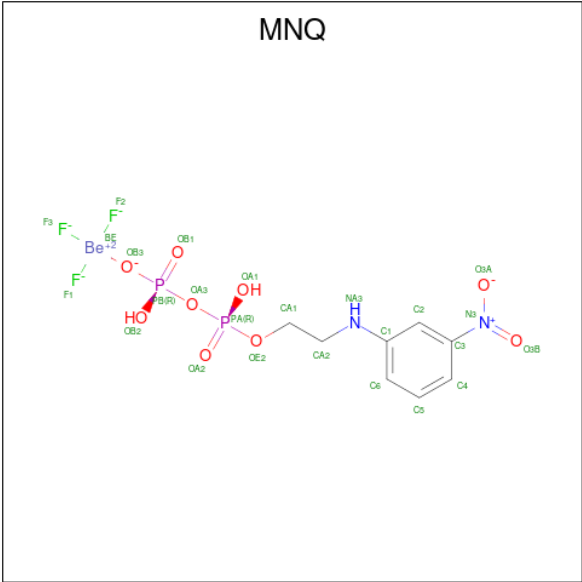
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	SEE REMARK 999	UNP P08799
A	760	PRO	GLN	engineered mutation	UNP P08799
A	761	ASN	ARG	engineered mutation	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 M-NITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRI-FLUORIDE (CCD ID: MNQ) (formula: C₈H₁₁BeF₃N₂O₉P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	25	1	8	3	2	9	2	0	0

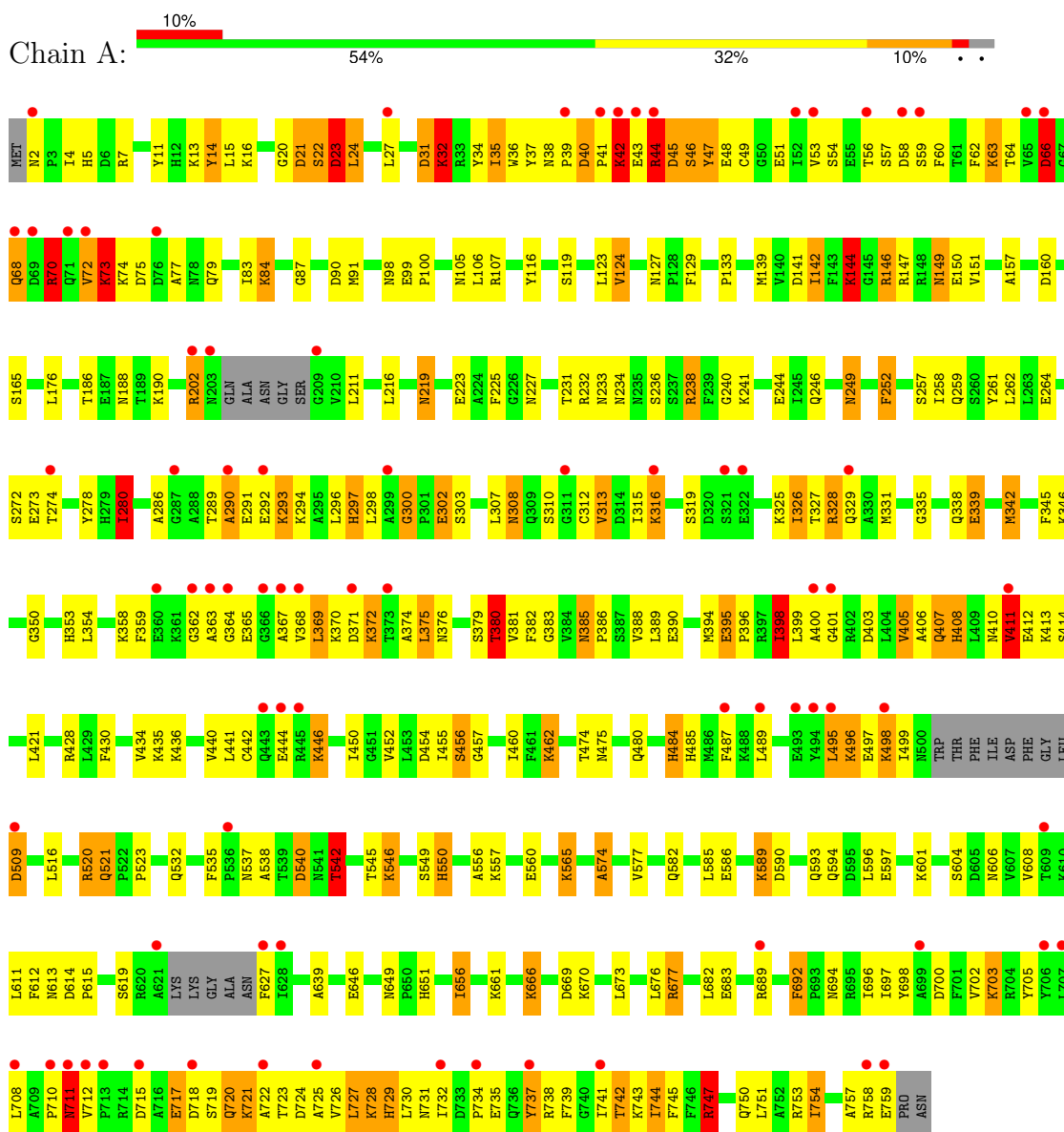
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	730	Total	O	0	0
			730	730		

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 S1DC MOTOR DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.00Å 180.50Å 54.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.00-2.00) 94.8 (25.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.01Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.187 , (Not available) 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 135.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6643	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: MG, MNQ

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	1.40	21/5999 (0.4%)	1.95	126/8097 (1.6%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	ASP	C-O	-7.18	1.20	1.23
1	A	326	ILE	CA-CB	-6.44	1.46	1.54
1	A	737	TYR	C-N	6.22	1.41	1.33
1	A	639	ALA	CA-C	6.07	1.60	1.52
1	A	90	ASP	CG-OD2	5.95	1.36	1.25
1	A	238[A]	ARG	CD-NE	-5.92	1.38	1.46
1	A	232[A]	ARG	CA-C	5.85	1.60	1.52
1	A	649	ASN	CA-C	5.80	1.59	1.52
1	A	70[A]	ARG	NE-CZ	5.76	1.39	1.33
1	A	73	LYS	N-CA	-5.70	1.39	1.46
1	A	475	ASN	C-N	5.69	1.41	1.33
1	A	165	SER	C-N	-5.47	1.26	1.33
1	A	560	GLU	CA-C	5.45	1.59	1.52
1	A	440	VAL	C-O	-5.31	1.18	1.24
1	A	550	HIS	CA-C	-5.31	1.45	1.52
1	A	157	ALA	N-CA	-5.28	1.40	1.46
1	A	452	VAL	CA-C	5.25	1.58	1.52
1	A	21	ASP	CG-OD2	5.12	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	GLU	CD-OE2	5.08	1.35	1.25
1	A	47	TYR	CA-C	-5.01	1.46	1.52
1	A	550	HIS	CE1-NE2	5.00	1.37	1.32

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	CA-CB-CG	-12.65	99.95	112.60
1	A	45	ASP	CA-CB-CG	-9.44	103.16	112.60
1	A	711	ASN	CA-CB-CG	9.20	121.80	112.60
1	A	280	ILE	N-CA-C	8.98	120.86	110.62
1	A	731	ASN	CA-CB-CG	8.79	121.39	112.60
1	A	729	HIS	CA-CB-CG	-8.78	105.02	113.80
1	A	238[A]	ARG	NE-CZ-NH2	-8.26	111.76	119.20
1	A	129	PHE	CA-CB-CG	-8.15	105.65	113.80
1	A	403	ASP	CA-CB-CG	7.98	120.58	112.60
1	A	41	PRO	CA-C-N	7.79	135.59	122.65
1	A	41	PRO	C-N-CA	7.79	135.59	122.65
1	A	606	ASN	N-CA-C	7.62	120.66	111.82
1	A	516	LEU	CA-C-O	7.58	128.81	120.63
1	A	747[A]	ARG	CD-NE-CZ	-7.38	114.06	124.40
1	A	705	TYR	N-CA-C	7.38	122.47	113.17
1	A	219	ASN	CB-CA-C	7.35	126.43	112.76
1	A	712	VAL	N-CA-C	7.29	124.63	108.88
1	A	456	SER	CA-C-O	-7.27	113.44	121.87
1	A	21	ASP	CA-CB-CG	-7.21	105.39	112.60
1	A	380	THR	N-CA-CB	7.18	120.74	109.82
1	A	540	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	238[A]	ARG	CD-NE-CZ	7.13	134.39	124.40
1	A	297	HIS	CA-CB-CG	-7.02	106.78	113.80
1	A	677[A]	ARG	O-C-N	-6.94	114.24	122.15
1	A	11	TYR	N-CA-C	-6.92	103.67	111.07
1	A	737	TYR	O-C-N	6.88	131.09	123.25
1	A	41	PRO	N-CA-CB	6.87	110.46	103.25
1	A	661	LYS	CA-C-N	-6.76	112.61	122.40
1	A	661	LYS	C-N-CA	-6.76	112.61	122.40
1	A	608	VAL	N-CA-CB	6.73	117.98	110.51
1	A	238[A]	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	A	606	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	712	VAL	CA-C-N	6.70	127.70	120.13
1	A	712	VAL	C-N-CA	6.70	127.70	120.13
1	A	747[A]	ARG	NE-CZ-NH1	-6.67	114.83	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	ALA	N-CA-C	6.64	120.87	110.32
1	A	537	ASN	CA-CB-CG	-6.61	106.00	112.60
1	A	44[A]	ARG	CD-NE-CZ	6.55	133.57	124.40
1	A	22	SER	N-CA-CB	6.55	120.25	110.29
1	A	408	HIS	CA-CB-CG	-6.46	107.34	113.80
1	A	42	LYS	N-CA-C	-6.45	105.71	112.93
1	A	141	ASP	N-CA-C	6.35	118.20	111.28
1	A	313	VAL	N-CA-CB	6.34	120.44	112.26
1	A	24	LEU	N-CA-C	6.28	119.59	110.42
1	A	262	LEU	N-CA-CB	-6.27	102.42	111.70
1	A	535	PHE	CA-C-N	6.27	126.47	119.32
1	A	535	PHE	C-N-CA	6.27	126.47	119.32
1	A	14	TYR	N-CA-C	6.25	120.97	113.23
1	A	405	VAL	N-CA-C	6.13	116.76	108.17
1	A	677[A]	ARG	CA-C-O	6.13	126.92	120.42
1	A	233	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	188	ASN	CA-CB-CG	-6.09	106.51	112.60
1	A	475	ASN	CA-CB-CG	-6.08	106.52	112.60
1	A	23	ASP	N-CA-CB	-6.04	102.87	110.90
1	A	441	LEU	N-CA-C	6.03	119.11	111.69
1	A	656	ILE	N-CA-CB	-6.01	101.59	111.44
1	A	244	GLU	CB-CA-C	-5.98	101.21	110.78
1	A	452	VAL	CA-C-N	-5.96	114.71	123.05
1	A	452	VAL	C-N-CA	-5.96	114.71	123.05
1	A	142	ILE	CB-CA-C	-5.91	102.68	112.26
1	A	252	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	313	VAL	N-CA-C	-5.88	107.25	112.90
1	A	549	SER	CA-CB-OG	-5.86	99.37	111.10
1	A	651	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	75	ASP	CA-CB-CG	-5.80	106.80	112.60
1	A	90	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	98	ASN	N-CA-CB	-5.77	101.64	110.42
1	A	286	ALA	CA-C-N	5.77	127.61	120.34
1	A	286	ALA	C-N-CA	5.77	127.61	120.34
1	A	565	LYS	CA-C-N	-5.69	113.60	122.37
1	A	565	LYS	C-N-CA	-5.69	113.60	122.37
1	A	411	VAL	N-CA-C	5.68	115.87	110.42
1	A	300	GLY	CA-C-O	-5.67	116.96	122.46
1	A	715	ASP	N-CA-CB	5.62	116.65	110.35
1	A	339	GLU	N-CA-C	-5.61	104.85	110.97
1	A	119	SER	N-CA-CB	5.61	121.22	110.90
1	A	574	ALA	N-CA-CB	-5.54	101.45	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LEU	CA-C-N	-5.53	113.91	122.59
1	A	15	LEU	C-N-CA	-5.53	113.91	122.59
1	A	44[A]	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	A	542	THR	CB-CA-C	-5.51	102.23	110.88
1	A	66	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	692	PHE	O-C-N	5.49	126.22	121.34
1	A	606	ASN	CB-CA-C	5.47	121.17	110.67
1	A	712	VAL	O-C-N	5.43	127.29	121.10
1	A	738[A]	ARG	N-CA-CB	5.41	119.58	110.77
1	A	219	ASN	CA-CB-CG	5.40	118.00	112.60
1	A	398	ILE	CA-CB-CG1	5.39	119.57	110.40
1	A	456	SER	O-C-N	5.38	128.92	122.79
1	A	677[A]	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	A	385	ASN	CA-C-N	5.37	125.18	119.28
1	A	385	ASN	C-N-CA	5.37	125.18	119.28
1	A	107[A]	ARG	CG-CD-NE	-5.36	100.20	112.00
1	A	717	GLU	CB-CA-C	5.34	118.94	109.65
1	A	216	LEU	N-CA-CB	5.33	118.06	110.16
1	A	739	PHE	N-CA-CB	5.32	118.28	109.88
1	A	405	VAL	N-CA-CB	-5.31	104.03	111.25
1	A	484	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	381	VAL	N-CA-C	5.30	116.03	110.62
1	A	442	CYS	N-CA-C	5.28	118.10	110.28
1	A	32	LYS	N-CA-CB	5.28	117.77	109.69
1	A	307	LEU	CA-C-N	-5.27	114.38	122.60
1	A	307	LEU	C-N-CA	-5.27	114.38	122.60
1	A	160	ASP	N-CA-CB	5.27	117.64	110.01
1	A	310	SER	N-CA-C	5.25	118.95	112.54
1	A	144	LYS	N-CA-C	5.24	118.16	110.30
1	A	521	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	A	538	ALA	N-CA-CB	5.19	117.68	110.26
1	A	556	ALA	N-CA-C	5.17	118.68	112.38
1	A	717	GLU	N-CA-CB	5.17	118.23	110.53
1	A	41	PRO	O-C-N	5.16	129.60	122.64
1	A	737	TYR	CA-C-N	-5.15	114.77	122.39
1	A	737	TYR	C-N-CA	-5.15	114.77	122.39
1	A	231	THR	CA-C-O	5.14	125.73	119.05
1	A	457	GLY	CA-C-O	-5.13	116.53	121.92
1	A	523	PRO	CA-C-N	-5.13	117.86	122.43
1	A	523	PRO	C-N-CA	-5.13	117.86	122.43
1	A	365	GLU	CA-C-N	5.12	126.87	121.45
1	A	365	GLU	C-N-CA	5.12	126.87	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ILE	N-CA-C	-5.10	98.68	107.24
1	A	545	THR	O-C-N	5.08	127.51	122.12
1	A	124	VAL	CA-CB-CG2	-5.07	101.79	110.40
1	A	474	THR	CA-C-O	5.05	126.31	120.90
1	A	560	GLU	N-CA-C	-5.04	103.31	109.65
1	A	480	GLN	N-CA-C	-5.02	105.89	111.36
1	A	308	ASN	CA-CB-CG	-5.01	107.59	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	606	ASN	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	5887	0	5597	280	0
2	A	1	0	0	0	0
3	A	25	0	9	2	0
4	A	730	0	0	39	0
All	All	6643	0	5606	283	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 (283) 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:4:ILE:HD11	1:A:142:ILE:HG23	1.24	1.17
1:A:45:ASP:HB2	1:A:670:LYS:HD3	1.17	1.15
1:A:45:ASP:HB2	1:A:670:LYS:CD	1.76	1.13
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.24	1.09
1:A:398:ILE:HG12	1:A:407:GLN:HG3	1.31	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:HB3	1:A:42:LYS:HB2	1.45	0.98
1:A:45:ASP:CG	1:A:677[A]:ARG:HH22	1.73	0.96
1:A:485:HIS:NE2	1:A:489:LEU:HD11	1.84	0.93
1:A:62:PHE:HE2	1:A:72:VAL:HG22	1.34	0.93
1:A:35:ILE:HD11	1:A:77:ALA:CB	1.98	0.92
1:A:398:ILE:HG12	1:A:407:GLN:CG	2.01	0.91
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.53	0.90
1:A:45:ASP:CB	1:A:670:LYS:HD3	2.01	0.89
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.56	0.88
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.55	0.87
1:A:127:ASN:HD21	3:A:999:MNQ:HA21	1.37	0.86
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.05	0.86
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.58	0.84
1:A:53:VAL:HG11	1:A:63:LYS:HD2	1.58	0.84
1:A:249:ASN:ND2	4:A:1086:HOH:O	2.04	0.82
1:A:149:ASN:HD22	1:A:150:GLU:N	1.78	0.82
1:A:2:ASN:HB3	1:A:5:HIS:HD2	1.45	0.81
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.10	0.81
1:A:64:THR:HG23	1:A:68:GLN:O	1.81	0.81
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.14	0.81
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.11	0.80
1:A:149:ASN:HD22	1:A:149:ASN:C	1.90	0.78
1:A:249:ASN:ND2	1:A:249:ASN:H	1.79	0.77
1:A:40:ASP:C	1:A:42:LYS:H	1.90	0.76
1:A:280:ILE:HG13	1:A:280:ILE:O	1.85	0.76
1:A:698:TYR:CZ	1:A:720:GLN:HG3	2.21	0.75
1:A:698:TYR:CE1	1:A:720:GLN:HG3	2.22	0.74
1:A:718:ASP:CG	1:A:721:LYS:HB2	2.12	0.74
1:A:289:THR:HG23	1:A:292:GLU:OE2	1.87	0.74
1:A:99:GLU:OE2	4:A:1670:HOH:O	2.05	0.74
1:A:62:PHE:CE2	1:A:72:VAL:HG22	2.19	0.74
1:A:399:LEU:HD12	1:A:400:ALA:N	2.03	0.73
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.71	0.72
1:A:219:ASN:HB3	4:A:1724:HOH:O	1.89	0.72
1:A:45:ASP:HB2	1:A:670:LYS:HD2	1.67	0.72
1:A:302:GLU:H	1:A:302:GLU:CD	1.97	0.72
1:A:498:LYS:O	1:A:498:LYS:HG2	1.88	0.72
1:A:521:GLN:OE1	4:A:1657:HOH:O	2.08	0.72
1:A:40:ASP:CB	1:A:42:LYS:HB2	2.19	0.71
1:A:495:LEU:HD12	4:A:1654:HOH:O	1.90	0.71
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:MET:HG3	1:A:346:LYS:CE	2.20	0.70
1:A:2:ASN:HB3	1:A:5:HIS:CD2	2.27	0.70
1:A:342:MET:HE3	1:A:342:MET:HA	1.74	0.69
1:A:87:GLY:H	1:A:105:ASN:ND2	1.89	0.69
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.28	0.68
1:A:372:LYS:O	1:A:376:ASN:ND2	2.27	0.68
1:A:273:GLU:O	1:A:274:THR:OG1	2.12	0.68
1:A:249:ASN:H	1:A:249:ASN:HD22	1.41	0.67
1:A:574:ALA:HA	4:A:1583:HOH:O	1.93	0.67
1:A:399:LEU:HD11	1:A:401:GLY:C	2.19	0.67
1:A:710:PRO:O	1:A:711:ASN:ND2	2.27	0.67
1:A:497:GLU:OE1	1:A:742:THR:HG23	1.95	0.67
1:A:697:ILE:HD13	1:A:743:LYS:CG	2.23	0.67
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.57	0.67
1:A:542:THR:HG23	4:A:1661:HOH:O	1.94	0.67
1:A:219:ASN:ND2	4:A:1274:HOH:O	2.27	0.66
1:A:62:PHE:HE2	1:A:72:VAL:CG2	2.06	0.66
1:A:289:THR:O	1:A:291:GLU:N	2.27	0.66
1:A:697:ILE:HB	1:A:700:ASP:OD1	1.96	0.66
1:A:225:PHE:CZ	1:A:280:ILE:HD13	2.31	0.66
1:A:509:ASP:OD2	1:A:557:LYS:NZ	2.22	0.66
1:A:238[A]:ARG:HD3	1:A:264:GLU:OE2	1.95	0.65
1:A:31:ASP:OD2	1:A:31:ASP:N	2.21	0.65
1:A:42:LYS:O	1:A:43:GLU:HG3	1.96	0.65
1:A:395:GLU:HA	1:A:407:GLN:O	1.96	0.65
1:A:485:HIS:NE2	1:A:489:LEU:CD1	2.58	0.65
1:A:710:PRO:HD3	1:A:729:HIS:ND1	2.11	0.65
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.28	0.64
1:A:546:LYS:NZ	4:A:1450:HOH:O	2.30	0.63
1:A:139:MET:HA	1:A:142:ILE:HD12	1.81	0.63
1:A:435:LYS:HG3	4:A:1505:HOH:O	1.99	0.63
1:A:241:LYS:NZ	1:A:454:ASP:OD1	2.29	0.63
1:A:646:GLU:HG3	4:A:1653:HOH:O	1.98	0.62
1:A:710:PRO:HD3	1:A:729:HIS:CG	2.34	0.62
1:A:410:ASN:C	1:A:410:ASN:OD1	2.42	0.62
1:A:290:ALA:HA	1:A:293:LYS:CD	2.30	0.62
1:A:62:PHE:CE2	1:A:72:VAL:CG2	2.82	0.62
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.36	0.61
1:A:399:LEU:HD11	1:A:401:GLY:O	2.00	0.61
1:A:710:PRO:HG3	1:A:729:HIS:CE1	2.35	0.61
1:A:718:ASP:OD1	1:A:721:LYS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520[A]:ARG:NE	4:A:1702:HOH:O	2.34	0.61
1:A:399:LEU:HD12	1:A:400:ALA:H	1.66	0.60
1:A:385:ASN:OD1	1:A:386:PRO:HD2	2.02	0.60
1:A:40:ASP:OD2	1:A:42:LYS:HB2	2.02	0.59
1:A:176:LEU:N	1:A:176:LEU:HD12	2.16	0.59
1:A:328[A]:ARG:HD2	4:A:1207:HOH:O	2.02	0.59
1:A:45:ASP:H	1:A:670:LYS:HE2	1.67	0.59
1:A:45:ASP:CB	1:A:670:LYS:CD	2.68	0.59
1:A:312:CYS:HB2	4:A:1638:HOH:O	2.02	0.59
1:A:542:THR:CB	4:A:1661:HOH:O	2.50	0.59
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.29	0.59
1:A:722:ALA:O	1:A:725:ALA:HB3	2.02	0.59
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.16	0.59
1:A:289:THR:O	1:A:292:GLU:N	2.36	0.58
1:A:38:ASN:C	1:A:40:ASP:H	2.10	0.58
1:A:289:THR:C	1:A:291:GLU:N	2.62	0.58
1:A:296:LEU:O	1:A:297:HIS:HB2	2.04	0.58
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.34	0.57
1:A:683:GLU:HG3	4:A:1365:HOH:O	2.04	0.57
1:A:601:LYS:HG2	1:A:613:ASN:ND2	2.19	0.57
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.86	0.57
1:A:710:PRO:HD3	1:A:729:HIS:CE1	2.40	0.57
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.34	0.56
1:A:726:VAL:O	1:A:730:LEU:HG	2.06	0.56
1:A:59:SER:HB2	1:A:72:VAL:O	2.06	0.56
1:A:698:TYR:CZ	1:A:720:GLN:CG	2.89	0.56
1:A:91:MET:CE	1:A:106:LEU:HD13	2.36	0.56
1:A:542:THR:CG2	4:A:1661:HOH:O	2.54	0.55
1:A:371:ASP:OD2	1:A:372:LYS:N	2.39	0.55
1:A:24:LEU:N	1:A:24:LEU:HD23	2.22	0.55
1:A:289:THR:C	1:A:291:GLU:H	2.14	0.55
1:A:732:ILE:HD12	1:A:750:GLN:NE2	2.22	0.54
1:A:396:PRO:HG2	1:A:398:ILE:HD11	1.88	0.54
1:A:58:ASP:N	1:A:58:ASP:OD2	2.40	0.54
1:A:498:LYS:C	1:A:499:ILE:HG13	2.33	0.54
1:A:79:GLN:HB2	4:A:1089:HOH:O	2.06	0.54
1:A:540:ASP:OD2	4:A:1511:HOH:O	2.19	0.54
1:A:582:GLN:HG3	4:A:1325:HOH:O	2.07	0.53
1:A:124:VAL:HG13	1:A:656:ILE:HD12	1.90	0.53
1:A:697:ILE:O	1:A:700:ASP:HB2	2.08	0.53
1:A:149:ASN:C	1:A:149:ASN:ND2	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:HA	1:A:298:LEU:HD12	1.91	0.53
1:A:51:GLU:O	1:A:53:VAL:HG13	2.09	0.52
1:A:40:ASP:C	1:A:42:LYS:N	2.64	0.51
1:A:45:ASP:HB3	1:A:673:LEU:HD12	1.92	0.51
1:A:190:LYS:HE2	1:A:223:GLU:OE2	2.11	0.51
1:A:362:GLY:O	1:A:364:GLY:N	2.44	0.51
1:A:37:TYR:O	1:A:47:TYR:HA	2.11	0.51
1:A:79:GLN:HG3	4:A:1260:HOH:O	2.10	0.50
1:A:127:ASN:ND2	3:A:999:MNQ:HA21	2.18	0.50
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.45	0.50
1:A:290:ALA:N	1:A:293:LYS:HD2	2.27	0.50
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.94	0.50
1:A:383:GLY:O	1:A:604:SER:N	2.37	0.50
1:A:737:TYR:HB2	1:A:744:ILE:HD11	1.94	0.50
1:A:87:GLY:H	1:A:105:ASN:HD21	1.57	0.49
1:A:297:HIS:HB2	1:A:353:HIS:NE2	2.27	0.49
1:A:708:LEU:HD23	1:A:759:GLU:HA	1.93	0.49
1:A:45:ASP:H	1:A:670:LYS:CE	2.25	0.49
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.94	0.49
1:A:219:ASN:CB	4:A:1724:HOH:O	2.54	0.49
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.48	0.49
1:A:498:LYS:O	1:A:499:ILE:HG13	2.12	0.49
1:A:38:ASN:C	1:A:40:ASP:N	2.71	0.49
1:A:550:HIS:HD2	4:A:1303:HOH:O	1.95	0.49
1:A:532:GLN:OE1	1:A:542:THR:HB	2.12	0.48
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.53	0.48
1:A:40:ASP:OD2	1:A:42:LYS:HG3	2.15	0.47
1:A:149:ASN:ND2	1:A:150:GLU:HG3	2.29	0.47
1:A:227:ASN:HA	1:A:236:SER:O	2.14	0.47
1:A:354:LEU:HD13	1:A:421:LEU:HD23	1.97	0.47
1:A:342:MET:CG	1:A:346:LYS:CE	2.93	0.47
1:A:327:THR:HG22	1:A:331:MET:HE2	1.97	0.47
1:A:38:ASN:ND2	1:A:46:SER:O	2.35	0.46
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.51	0.46
1:A:40:ASP:CG	1:A:42:LYS:HB2	2.39	0.46
1:A:408:HIS:ND1	1:A:408:HIS:C	2.73	0.46
1:A:614:ASP:OD1	1:A:614:ASP:C	2.58	0.46
1:A:32:LYS:HB2	1:A:34:TYR:CE2	2.51	0.46
1:A:335:GLY:HA3	4:A:1640:HOH:O	2.16	0.46
1:A:362:GLY:C	1:A:364:GLY:N	2.74	0.46
1:A:35:ILE:HD13	4:A:1087:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PRO:HG3	1:A:48:GLU:HG3	1.98	0.45
1:A:40:ASP:HB3	1:A:42:LYS:CB	2.30	0.45
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.44	0.45
1:A:359:PHE:CB	1:A:411:VAL:HG22	2.46	0.45
1:A:585:LEU:O	1:A:589:LYS:HD2	2.16	0.45
1:A:99:GLU:HB2	1:A:100:PRO:HD3	1.97	0.45
1:A:462:LYS:HD2	1:A:462:LYS:HA	1.57	0.45
1:A:83:ILE:HD11	4:A:1044:HOH:O	2.16	0.45
1:A:249:ASN:ND2	1:A:249:ASN:N	2.49	0.45
1:A:614:ASP:OD1	1:A:615:PRO:HD2	2.17	0.45
1:A:698:TYR:CE2	1:A:720:GLN:HG3	2.51	0.45
1:A:455:ILE:O	1:A:455:ILE:HG13	2.15	0.45
1:A:338:GLN:NE2	4:A:1289:HOH:O	2.50	0.45
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.52	0.44
1:A:484:HIS:O	1:A:487:PHE:HB3	2.17	0.44
1:A:84:LYS:HB3	4:A:1261:HOH:O	2.17	0.44
1:A:720:GLN:O	1:A:723:THR:HB	2.18	0.44
1:A:462:LYS:HG2	4:A:1649:HOH:O	2.18	0.44
1:A:22:SER:OG	1:A:23:ASP:N	2.51	0.44
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.66	0.44
1:A:223:GLU:O	1:A:227:ASN:HB2	2.18	0.44
1:A:16:LYS:NZ	4:A:1223:HOH:O	2.51	0.44
1:A:144:LYS:HD3	4:A:1619:HOH:O	2.16	0.43
1:A:696:ILE:O	1:A:744:ILE:N	2.44	0.43
1:A:293:LYS:H	1:A:293:LYS:HG3	1.63	0.43
1:A:293:LYS:O	1:A:297:HIS:N	2.51	0.43
1:A:589:LYS:NZ	4:A:1255:HOH:O	2.50	0.43
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.17	0.43
1:A:656:ILE:HD13	1:A:676:LEU:HD21	2.01	0.43
1:A:240:GLY:HA3	1:A:455:ILE:HG22	1.99	0.43
1:A:724:ASP:O	1:A:728:LYS:HB2	2.18	0.43
1:A:698:TYR:HB3	1:A:719:SER:HB3	2.00	0.43
1:A:53:VAL:HG22	1:A:62:PHE:HA	2.01	0.43
1:A:116:TYR:HB3	1:A:123:LEU:HD11	2.01	0.43
1:A:727:LEU:HA	1:A:727:LEU:HD12	1.69	0.43
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.89	0.43
1:A:246:GLN:HG2	1:A:446:LYS:HD3	2.00	0.43
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.18	0.43
1:A:374:ALA:O	1:A:375:LEU:C	2.61	0.42
1:A:44[A]:ARG:HD3	1:A:45:ASP:OD2	2.19	0.42
1:A:60:PHE:CE1	1:A:74:LYS:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ILE:O	1:A:757:ALA:HB3	2.19	0.42
1:A:308:ASN:C	1:A:308:ASN:OD1	2.61	0.42
1:A:586:GLU:HB2	4:A:1514:HOH:O	2.19	0.42
1:A:597:GLU:OE1	1:A:612:PHE:CD2	2.73	0.42
1:A:410:ASN:OD1	1:A:413:LYS:N	2.46	0.42
1:A:289:THR:C	1:A:293:LYS:HD2	2.44	0.42
1:A:289:THR:O	1:A:289:THR:OG1	2.37	0.42
1:A:64:THR:OG1	1:A:66:ASP:OD1	2.31	0.42
1:A:593:GLN:NE2	4:A:1572:HOH:O	2.42	0.41
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.78	0.41
1:A:708:LEU:CD2	1:A:758:ARG:O	2.68	0.41
1:A:258:ILE:HD13	1:A:258:ILE:HG21	1.82	0.41
1:A:376:ASN:O	1:A:380:THR:HG22	2.21	0.41
1:A:485:HIS:CD2	1:A:489:LEU:CD1	3.03	0.41
1:A:273:GLU:C	1:A:274:THR:HG1	2.18	0.41
1:A:23:ASP:N	1:A:23:ASP:OD1	2.52	0.41
1:A:60:PHE:N	1:A:72:VAL:O	2.49	0.41
1:A:186:THR:HG22	1:A:190:LYS:HE3	2.03	0.41
1:A:428[A]:ARG:HD3	1:A:611:LEU:O	2.21	0.41
1:A:56:THR:OG1	1:A:58:ASP:OD2	2.23	0.41
1:A:289:THR:O	1:A:290:ALA:C	2.64	0.41
1:A:702:VAL:O	1:A:703:LYS:C	2.64	0.41
1:A:146[A]:ARG:HD3	1:A:151:VAL:CG1	2.51	0.41
1:A:146[A]:ARG:HD3	1:A:151:VAL:HG13	2.01	0.41
1:A:430:PHE:O	1:A:434:VAL:HG23	2.21	0.41
1:A:698:TYR:CD2	1:A:720:GLN:HA	2.56	0.41
1:A:747[A]:ARG:HH11	1:A:747[A]:ARG:HD3	1.54	0.41
1:A:21:ASP:N	1:A:21:ASP:OD2	2.54	0.40
1:A:99:GLU:N	1:A:100:PRO:HD2	2.36	0.40
1:A:375:LEU:HD12	1:A:389:LEU:HD23	2.03	0.40
1:A:460:ILE:HG12	1:A:577:VAL:HG22	2.02	0.40
1:A:698:TYR:CD1	1:A:720:GLN:HG3	2.56	0.40
1:A:20:GLY:N	4:A:1385:HOH:O	2.27	0.40
1:A:234:ASN:OD1	1:A:315:ILE:HG23	2.20	0.40
1:A:399:LEU:HD12	1:A:399:LEU:C	2.43	0.40
1:A:34:TYR:CD1	1:A:51:GLU:HB2	2.56	0.40
1:A:39:PRO:HG3	1:A:48:GLU:CG	2.52	0.40
1:A:142:ILE:CG2	1:A:142:ILE:O	2.69	0.40
1:A:372:LYS:HB2	1:A:372:LYS:HE3	1.52	0.40
1:A:386:PRO:O	1:A:390:GLU:HB2	2.22	0.40
1:A:496:LYS:NZ	1:A:496:LYS:HB3	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LYS:HE2	4:A:1217:HOH:O	2.21	0.40
1:A:710:PRO:CG	1:A:729:HIS:CE1	3.05	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	732/761 (96%)	698 (95%)	29 (4%)	5 (1%)	18 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44[A]	ARG
1	A	290	ALA
1	A	363	ALA
1	A	711	ASN
1	A	7[A]	ARG

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	632/665 (95%)	546 (86%)	86 (14%)	3 2

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	23	ASP
1	A	27	LEU
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	40	ASP
1	A	42	LYS
1	A	44[A]	ARG
1	A	46	SER
1	A	54	SER
1	A	57	SER
1	A	63	LYS
1	A	66	ASP
1	A	68	GLN
1	A	70[A]	ARG
1	A	72	VAL
1	A	73	LYS
1	A	84	LYS
1	A	144	LYS
1	A	146[A]	ARG
1	A	147[A]	ARG
1	A	149	ASN
1	A	202[A]	ARG
1	A	211	LEU
1	A	257	SER
1	A	272	SER
1	A	280	ILE
1	A	293	LYS
1	A	294	LYS
1	A	302	GLU
1	A	303	SER
1	A	313	VAL
1	A	316	LYS
1	A	319	SER
1	A	325	LYS
1	A	326	ILE
1	A	328[A]	ARG
1	A	329	GLN
1	A	339	GLU
1	A	342	MET
1	A	358	LYS

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Mol	Chain	Res	Type
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	380	THR
1	A	394	MET
1	A	398	ILE
1	A	405	VAL
1	A	407	GLN
1	A	411	VAL
1	A	412	GLU
1	A	414	SER
1	A	436	LYS
1	A	444	GLU
1	A	446	LYS
1	A	456	SER
1	A	462	LYS
1	A	495	LEU
1	A	496	LYS
1	A	498	LYS
1	A	509	ASP
1	A	520[A]	ARG
1	A	542	THR
1	A	546	LYS
1	A	565	LYS
1	A	589	LYS
1	A	594	GLN
1	A	666	LYS
1	A	669	ASP
1	A	689[A]	ARG
1	A	703	LYS
1	A	711	ASN
1	A	717	GLU
1	A	720	GLN
1	A	721	LYS
1	A	727	LEU
1	A	728	LYS
1	A	742	THR
1	A	744	ILE
1	A	747[A]	ARG

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Mol	Chain	Res	Type
1	A	751	LEU
1	A	754	ILE

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

Mol	Chain	Res	Type
1	A	68	GLN
1	A	78	ASN
1	A	105	ASN
1	A	149	ASN
1	A	188	ASN
1	A	219	ASN
1	A	249	ASN
1	A	259	GLN
1	A	283	GLN
1	A	329	GLN
1	A	376	ASN
1	A	408	HIS
1	A	439	ASN
1	A	479	GLN
1	A	480	GLN
1	A	491	GLN
1	A	511	GLN
1	A	521	GLN
1	A	550	HIS
1	A	594	GLN
1	A	616	ASN
1	A	662	GLN
1	A	736	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 [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	MNQ	A	999	2	23,25,25	2.17	6 (26%)	23,37,37	3.51	8 (34%)

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	MNQ	A	999	2	-	2/16/24/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	MNQ	O3B-N3	6.17	1.33	1.22
3	A	999	MNQ	C5-C6	4.89	1.47	1.38
3	A	999	MNQ	C4-C3	2.90	1.44	1.38
3	A	999	MNQ	CA2-NA3	2.75	1.51	1.45
3	A	999	MNQ	C5-C4	-2.51	1.34	1.38
3	A	999	MNQ	C6-C1	2.40	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	MNQ	C4-C3-N3	9.89	127.98	119.34
3	A	999	MNQ	CA2-NA3-C1	-8.47	104.19	122.92
3	A	999	MNQ	C2-C3-N3	-8.41	111.49	118.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	MNQ	C3-C2-C1	3.48	122.13	118.47
3	A	999	MNQ	C5-C6-C1	-2.71	116.61	119.73
3	A	999	MNQ	C2-C1-NA3	-2.52	114.00	120.78
3	A	999	MNQ	CA1-CA2-NA3	2.18	116.31	111.22
3	A	999	MNQ	C6-C1-NA3	2.04	125.57	120.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

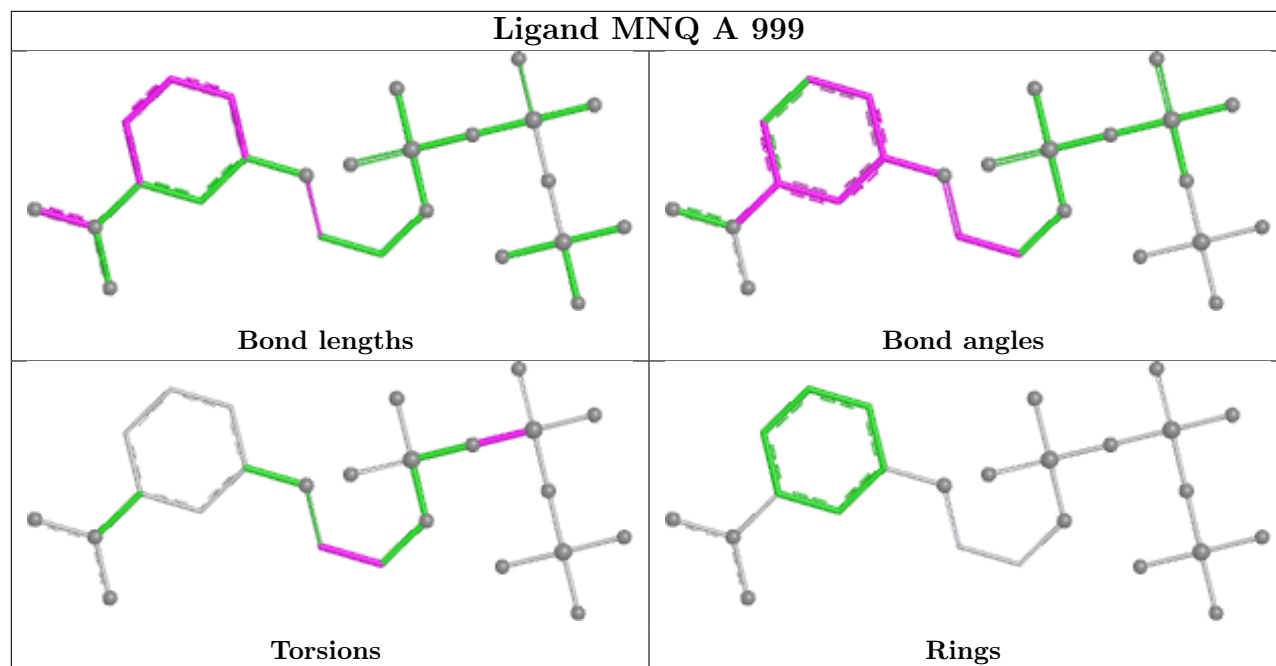
Mol	Chain	Res	Type	Atoms
3	A	999	MNQ	OE2-CA1-CA2-NA3
3	A	999	MNQ	PA-OA3-PB-OB2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	MNQ	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	740/761 (97%)	0.32	78 (10%)	11 10	12, 32, 74, 100	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	VAL	9.4
1	A	627	PHE	7.2
1	A	707	LEU	7.1
1	A	737	TYR	5.9
1	A	362	GLY	5.6
1	A	363	ALA	4.8
1	A	364	GLY	4.7
1	A	39	PRO	4.5
1	A	708	LEU	4.4
1	A	495	LEU	4.2
1	A	321	SER	4.2
1	A	367	ALA	4.0
1	A	713	PRO	3.9
1	A	368	VAL	3.8
1	A	41	PRO	3.8
1	A	489	LEU	3.8
1	A	53	VAL	3.6
1	A	209	GLY	3.6
1	A	401	GLY	3.6
1	A	290	ALA	3.5
1	A	72	VAL	3.5
1	A	322	GLU	3.3
1	A	493	GLU	3.3
1	A	69	ASP	3.2
1	A	59	SER	3.2
1	A	311	GLY	3.2
1	A	443	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	3.0
1	A	202[A]	ARG	2.9
1	A	2	ASN	2.9
1	A	329	GLN	2.8
1	A	718	ASP	2.8
1	A	445	ARG	2.7
1	A	712	VAL	2.7
1	A	66	ASP	2.7
1	A	366	GLY	2.7
1	A	725	ALA	2.7
1	A	203	ASN	2.7
1	A	699	ALA	2.6
1	A	706	TYR	2.6
1	A	536	PRO	2.6
1	A	444	GLU	2.6
1	A	58	ASP	2.6
1	A	487	PHE	2.6
1	A	498	LYS	2.6
1	A	43	GLU	2.5
1	A	371	ASP	2.5
1	A	509	ASP	2.5
1	A	316	LYS	2.5
1	A	494	TYR	2.5
1	A	734	PRO	2.5
1	A	759	GLU	2.4
1	A	621	ALA	2.4
1	A	722	ALA	2.4
1	A	411	VAL	2.4
1	A	274	THR	2.4
1	A	689[A]	ARG	2.4
1	A	52	ILE	2.4
1	A	715	ASP	2.3
1	A	732	ILE	2.3
1	A	76	ASP	2.3
1	A	758	ARG	2.3
1	A	711	ASN	2.3
1	A	710	PRO	2.3
1	A	628	ILE	2.2
1	A	287	GLY	2.2
1	A	741	ILE	2.1
1	A	44[A]	ARG	2.1
1	A	68	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	292	GLU	2.1
1	A	56	THR	2.1
1	A	71	GLN	2.1
1	A	373	THR	2.1
1	A	299	ALA	2.1
1	A	609	THR	2.1
1	A	360	GLU	2.0
1	A	27	LEU	2.0
1	A	42	LYS	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](#)

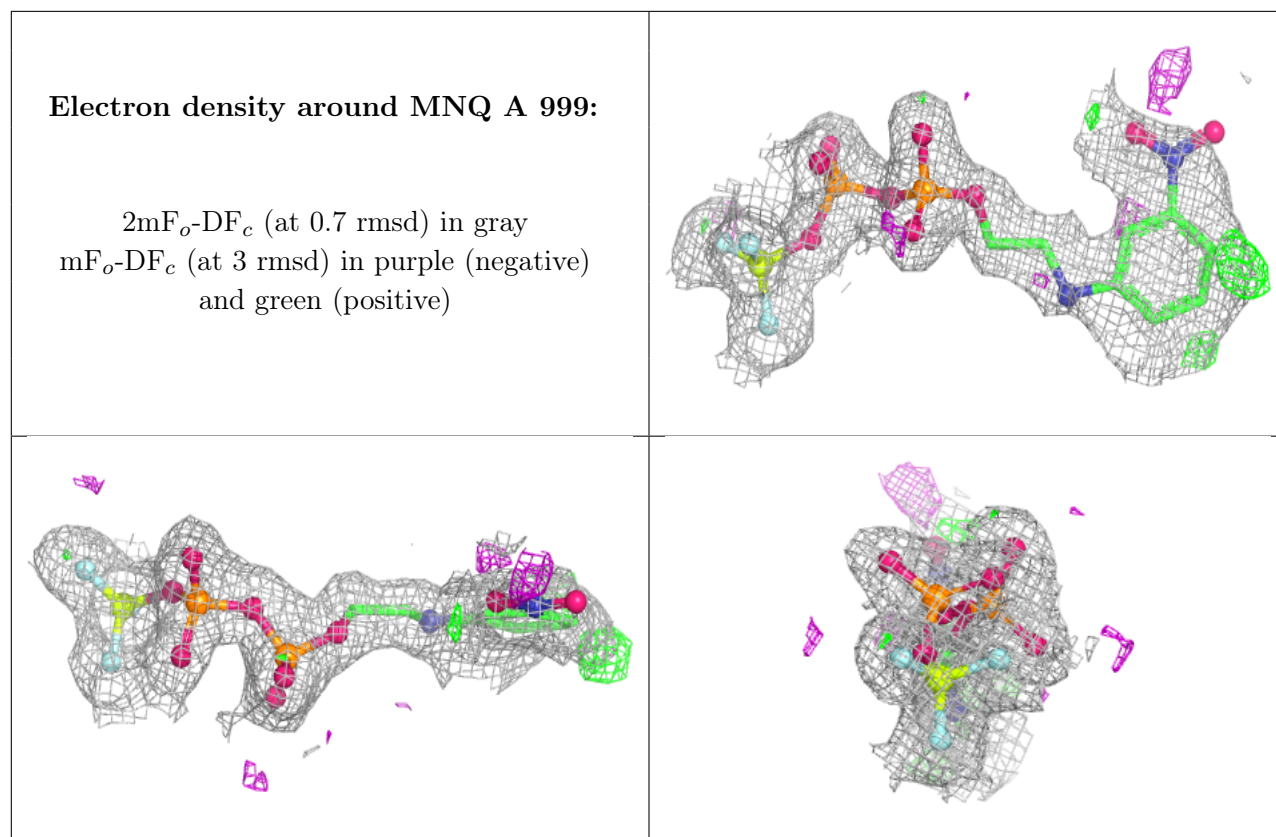
There are no oligosaccharides in this entry.

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
3	MNQ	A	999	25/25	0.97	0.10	12,22,98,100	0
2	MG	A	998	1/1	0.99	0.02	20,20,20,20	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.