



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 03:03 PM EDT

PDB ID : 1D0Z
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH P-NITROPHENYL AMINOETHYLDIPHOSPHATE
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

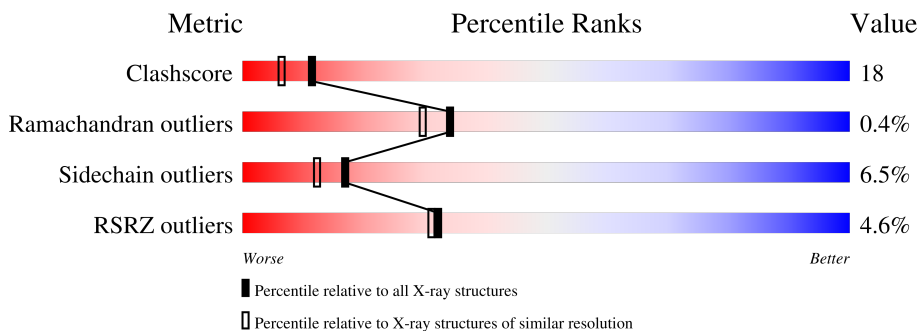
1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6349 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	742	5869	3729	1009	1115	16	0	0	0

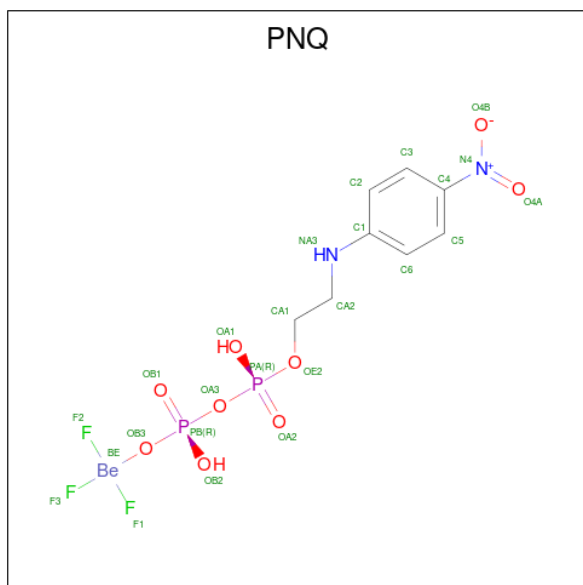
There are 3 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is P-NITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE (three-letter code: PNQ) (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

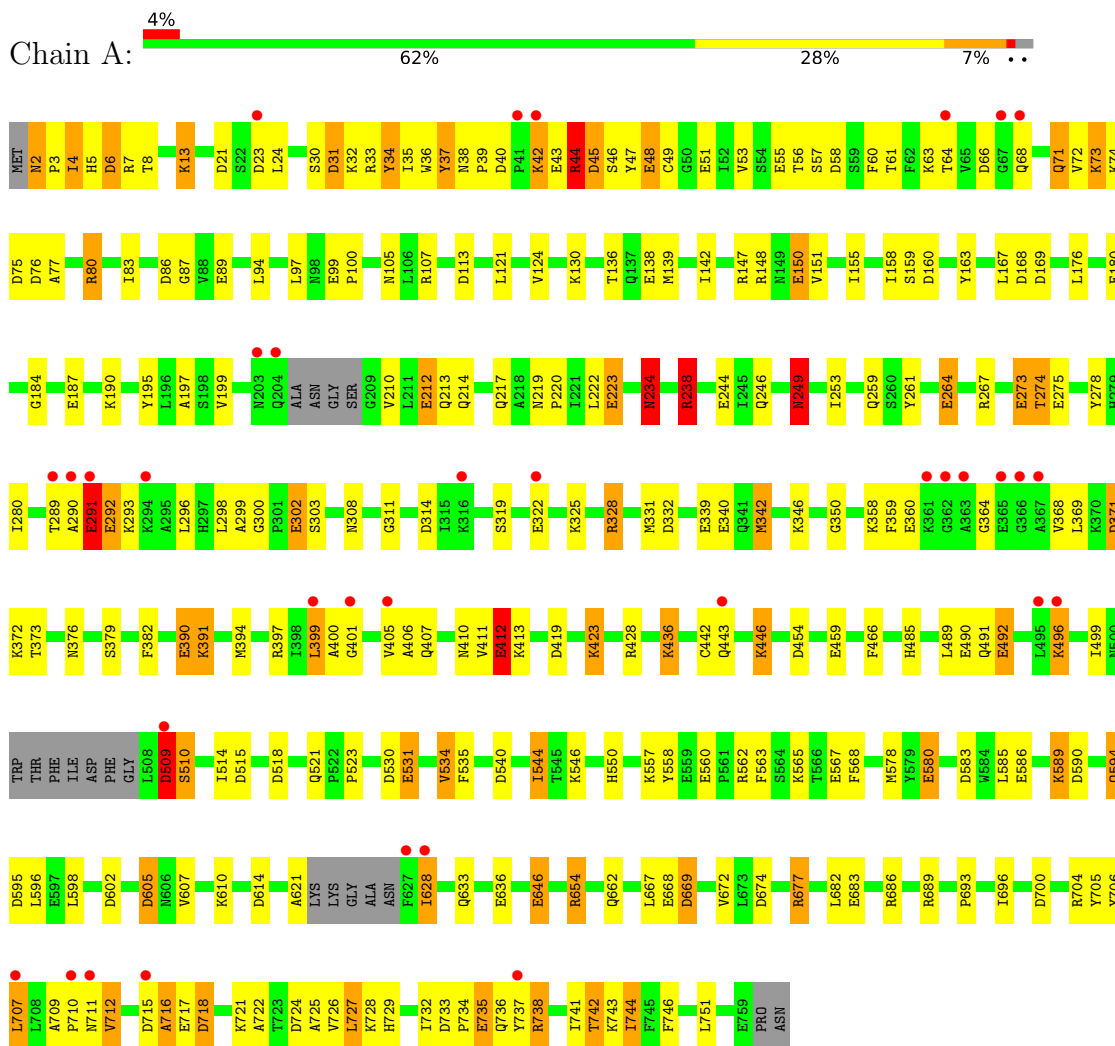
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	454	Total	O	0	0
			454	454		

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	103.99Å 180.85Å 54.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 29.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (25.00-2.00) 91.7 (29.19-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.00Å)	Xtrriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.193 , (Not available) 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 85.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6349	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PNQ, 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	1.14	39/5980 (0.7%)	1.51	92/8081 (1.1%)

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	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ASN	CG-OD1	11.34	1.48	1.24
1	A	89	GLU	CD-OE2	8.20	1.34	1.25
1	A	244	GLU	CD-OE2	8.20	1.34	1.25
1	A	567	GLU	CD-OE2	7.91	1.34	1.25
1	A	275	GLU	CD-OE2	7.70	1.34	1.25
1	A	683	GLU	CD-OE2	7.37	1.33	1.25
1	A	668	GLU	CD-OE2	7.28	1.33	1.25
1	A	531	GLU	CD-OE2	7.10	1.33	1.25
1	A	51	GLU	CD-OE2	6.58	1.32	1.25
1	A	390	GLU	CD-OE2	6.51	1.32	1.25
1	A	360	GLU	CD-OE2	6.41	1.32	1.25
1	A	339	GLU	CD-OE2	6.39	1.32	1.25
1	A	490	GLU	CD-OE2	6.38	1.32	1.25
1	A	291	GLU	CD-OE2	6.34	1.32	1.25
1	A	340	GLU	CD-OE2	6.28	1.32	1.25
1	A	580	GLU	CD-OE2	6.27	1.32	1.25
1	A	459	GLU	CD-OE2	6.25	1.32	1.25
1	A	492	GLU	CD-OE2	6.14	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	GLU	CD-OE2	6.09	1.32	1.25
1	A	273	GLU	CD-OE2	5.97	1.32	1.25
1	A	586	GLU	CD-OE2	5.91	1.32	1.25
1	A	717	GLU	CD-OE2	5.88	1.32	1.25
1	A	180	GLU	CD-OE2	5.85	1.32	1.25
1	A	636	GLU	CD-OE2	5.82	1.32	1.25
1	A	244	GLU	CD-OE1	-5.78	1.19	1.25
1	A	264	GLU	CD-OE1	-5.75	1.19	1.25
1	A	212	GLU	CD-OE2	5.74	1.31	1.25
1	A	302	GLU	CD-OE2	5.68	1.31	1.25
1	A	560	GLU	CD-OE1	-5.60	1.19	1.25
1	A	412	GLU	CD-OE2	5.58	1.31	1.25
1	A	55	GLU	CD-OE2	5.56	1.31	1.25
1	A	735	GLU	CD-OE2	5.48	1.31	1.25
1	A	646	GLU	CD-OE2	5.29	1.31	1.25
1	A	150	GLU	CD-OE2	5.29	1.31	1.25
1	A	43	GLU	CD-OE2	5.25	1.31	1.25
1	A	292	GLU	CD-OE2	5.23	1.31	1.25
1	A	223	GLU	CD-OE2	5.22	1.31	1.25
1	A	187	GLU	CD-OE2	5.14	1.31	1.25
1	A	628	ILE	C-N	5.04	1.45	1.34

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASN	CB-CG-OD1	-17.91	85.78	121.60
1	A	238	ARG	NE-CZ-NH1	13.03	126.82	120.30
1	A	238	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	590	ASP	CB-CG-OD2	-10.12	109.19	118.30
1	A	428	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	234	ASN	OD1-CG-ND2	9.24	143.16	121.90
1	A	267	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	234	ASN	CB-CG-ND2	-9.02	95.06	116.70
1	A	419	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	A	44	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	A	674	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	A	234	ASN	CA-CB-CG	-8.29	95.16	113.40
1	A	80	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	614	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	332	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	A	44	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	602	ASP	CB-CG-OD2	-8.00	111.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ASP	CB-CG-OD1	7.94	125.45	118.30
1	A	76	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	628	ILE	O-C-N	7.83	135.23	122.70
1	A	605	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	686	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	148	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	700	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	677	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	267	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	21	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	590	ASP	CB-CG-OD1	7.16	124.75	118.30
1	A	558	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	614	ASP	CB-CG-OD1	7.08	124.67	118.30
1	A	45	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	31	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	700	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	168	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	718	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	2	ASN	N-CA-CB	6.77	122.78	110.60
1	A	107	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	371	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	428	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	558	TYR	CB-CG-CD2	6.60	124.96	121.00
1	A	595	ASP	CB-CG-OD1	6.58	124.23	118.30
1	A	371	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	454	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	168	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	A	314	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	76	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	169	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	724	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	37	TYR	CB-CG-CD1	6.29	124.78	121.00
1	A	23	ASP	CB-CG-OD1	6.25	123.92	118.30
1	A	332	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	605	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	509	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	6	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	44	ARG	CD-NE-CZ	6.04	132.05	123.60
1	A	66	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	66	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	364	GLY	N-CA-C	-5.99	98.12	113.10
1	A	234	ASN	N-CA-CB	5.96	121.33	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	34	TYR	CB-CG-CD2	5.87	124.52	121.00
1	A	602	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	509	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	595	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	75	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	31	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	58	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	674	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	712	VAL	N-CA-C	5.74	126.50	111.00
1	A	328	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	113	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	148	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	21	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	530	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	454	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	466	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	A	562	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	86	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	518	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	75	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	160	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	669	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	249	ASN	CA-CB-CG	-5.32	101.70	113.40
1	A	628	ILE	CA-C-N	-5.31	105.52	117.20
1	A	530	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	669	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	45	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	274	THR	CA-CB-CG2	-5.14	105.21	112.40
1	A	234	ASN	CB-CA-C	5.08	120.56	110.40
1	A	124	VAL	CA-CB-CG1	-5.05	103.33	110.90
1	A	515	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	113	ASP	N-CA-CB	5.01	119.63	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ASN	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5869	0	5744	206	1
2	A	1	0	0	0	0
3	A	25	0	9	3	0
4	A	454	0	0	12	2
All	All	6349	0	5753	206	2

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 18.

All (206) 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:45:ASP:CG	1:A:677:ARG:HH22	1.71	0.94
1:A:289:THR:HG23	1:A:292:GLU:H	1.33	0.93
1:A:234:ASN:N	1:A:234:ASN:OD1	1.91	0.92
1:A:4:ILE:HD11	1:A:151:VAL:HG12	1.53	0.90
1:A:289:THR:HG22	1:A:292:GLU:HB2	1.53	0.90
1:A:628:ILE:HD11	1:A:633:GLN:HB2	1.56	0.88
1:A:289:THR:HG22	1:A:292:GLU:CB	2.05	0.86
1:A:139:MET:HA	1:A:142:ILE:HD12	1.56	0.86
1:A:139:MET:HA	1:A:142:ILE:CD1	2.07	0.83
1:A:628:ILE:CD1	1:A:633:GLN:HB2	2.08	0.83
1:A:24:LEU:N	1:A:24:LEU:HD23	1.92	0.83
1:A:158:ILE:HD12	1:A:159:SER:N	1.93	0.82
1:A:249:ASN:ND2	1:A:249:ASN:H	1.67	0.81
1:A:61:THR:OG1	1:A:71:GLN:HG3	1.81	0.80
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.17	0.79
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.66	0.78
1:A:147:ARG:HB2	1:A:150:GLU:OE1	1.86	0.76
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.67	0.76
1:A:289:THR:CG2	1:A:292:GLU:H	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:HG23	1:A:68:GLN:O	1.85	0.75
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.69	0.75
1:A:737:TYR:O	1:A:738:ARG:HD3	1.88	0.73
1:A:369:LEU:HG	1:A:394:MET:CE	2.17	0.72
1:A:707:LEU:H	1:A:707:LEU:CD2	2.02	0.72
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.20	0.72
1:A:138:GLU:OE2	1:A:138:GLU:N	2.20	0.72
1:A:289:THR:HG22	1:A:292:GLU:CG	2.20	0.72
1:A:45:ASP:OD1	1:A:677:ARG:NH1	2.23	0.71
1:A:38:ASN:ND2	1:A:46:SER:O	2.22	0.71
1:A:397:ARG:HA	1:A:406:ALA:HA	1.71	0.71
1:A:707:LEU:N	1:A:707:LEU:HD23	2.06	0.71
1:A:707:LEU:H	1:A:707:LEU:HD23	1.55	0.71
1:A:246:GLN:HG2	1:A:446:LYS:HD2	1.71	0.70
1:A:289:THR:HG23	1:A:292:GLU:N	2.06	0.70
1:A:368:VAL:HG12	1:A:369:LEU:N	2.07	0.69
1:A:219:ASN:N	1:A:220:PRO:HD2	2.07	0.69
1:A:158:ILE:HD12	1:A:159:SER:H	1.57	0.69
1:A:369:LEU:HG	1:A:394:MET:HE1	1.74	0.69
1:A:155:ILE:HD12	1:A:158:ILE:HD11	1.74	0.69
1:A:210:VAL:O	1:A:214:GLN:HG3	1.92	0.69
1:A:299:ALA:HB3	1:A:303:SER:OG	1.94	0.68
1:A:2:ASN:ND2	1:A:5:HIS:HD2	1.91	0.68
1:A:40:ASP:OD2	1:A:42:LYS:HB2	1.94	0.68
1:A:176:LEU:HD12	1:A:176:LEU:N	2.10	0.67
1:A:39:PRO:HD2	4:A:1174:HOH:O	1.94	0.67
1:A:372:LYS:NZ	1:A:390:GLU:OE1	2.24	0.67
1:A:710:PRO:HD2	1:A:729:HIS:CE1	2.31	0.65
1:A:139:MET:CA	1:A:142:ILE:HD12	2.27	0.65
1:A:654:ARG:NH1	4:A:1192:HOH:O	2.22	0.64
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.81	0.63
1:A:213:GLN:O	1:A:217:GLN:HG2	1.99	0.62
1:A:372:LYS:O	1:A:376:ASN:ND2	2.32	0.62
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.34	0.62
1:A:53:VAL:CG2	1:A:61:THR:HG22	2.28	0.62
1:A:56:THR:O	1:A:74:LYS:HE3	1.99	0.62
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.30	0.61
1:A:138:GLU:H	1:A:138:GLU:CD	2.03	0.61
1:A:399:LEU:HD21	1:A:401:GLY:O	2.00	0.61
1:A:4:ILE:CD1	1:A:151:VAL:HG12	2.29	0.60
1:A:523:PRO:HD2	4:A:1121:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.19	0.59
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.02	0.59
1:A:710:PRO:HD2	1:A:729:HIS:ND1	2.17	0.59
1:A:147:ARG:HB2	1:A:150:GLU:CD	2.23	0.58
1:A:289:THR:CG2	1:A:292:GLU:N	2.65	0.58
1:A:53:VAL:HG11	1:A:63:LYS:HD2	1.85	0.58
1:A:30:SER:O	1:A:33:ARG:NH1	2.34	0.58
1:A:197:ALA:HA	1:A:253:ILE:HD11	1.84	0.58
1:A:693:PRO:HD2	1:A:746:PHE:O	2.03	0.58
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.39	0.57
1:A:37:TYR:OH	1:A:64:THR:HB	2.04	0.57
1:A:138:GLU:O	1:A:142:ILE:HD12	2.05	0.57
1:A:733:ASP:O	1:A:736:GLN:HB2	2.04	0.57
1:A:718:ASP:CG	1:A:721:LYS:HB2	2.26	0.56
1:A:39:PRO:HG3	1:A:48:GLU:HG3	1.88	0.56
1:A:710:PRO:CD	1:A:729:HIS:CE1	2.88	0.56
1:A:2:ASN:ND2	1:A:5:HIS:CD2	2.72	0.56
1:A:2:ASN:HD22	1:A:5:HIS:HD2	1.51	0.55
1:A:499:ILE:HD12	1:A:738:ARG:HB3	1.87	0.55
1:A:412:GLU:OE2	1:A:413:LYS:HG3	2.06	0.55
1:A:544:ILE:HG13	1:A:544:ILE:O	2.06	0.55
1:A:87:GLY:H	1:A:105:ASN:ND2	2.04	0.55
1:A:534:VAL:HG13	1:A:535:PHE:CE2	2.41	0.55
1:A:290:ALA:HA	1:A:293:LYS:CD	2.35	0.55
1:A:130:LYS:HA	3:A:999:PNQ:O4A	2.07	0.54
1:A:280:ILE:HG13	1:A:280:ILE:O	2.07	0.54
1:A:37:TYR:O	1:A:47:TYR:HA	2.06	0.54
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.37	0.54
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.89	0.54
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.43	0.54
1:A:621:ALA:HB2	1:A:628:ILE:HG13	1.89	0.54
1:A:436:LYS:HB3	1:A:436:LYS:NZ	2.23	0.54
1:A:39:PRO:HG3	1:A:48:GLU:CG	2.38	0.53
1:A:155:ILE:O	1:A:158:ILE:HD12	2.08	0.53
1:A:531:GLU:O	1:A:531:GLU:HG3	2.09	0.53
1:A:744:ILE:CD1	1:A:746:PHE:CZ	2.92	0.53
1:A:13:LYS:HZ3	1:A:13:LYS:HB2	1.73	0.53
1:A:722:ALA:O	1:A:725:ALA:HB3	2.08	0.53
1:A:485:HIS:NE2	1:A:489:LEU:HD11	2.23	0.52
1:A:328:ARG:HA	1:A:331:MET:HE2	1.91	0.52
1:A:540:ASP:OD2	4:A:1437:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:O	1:A:71:GLN:HG2	2.09	0.52
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.42	0.52
1:A:509:ASP:OD2	1:A:557:LYS:NZ	2.43	0.52
1:A:238:ARG:HD3	1:A:264:GLU:OE2	2.11	0.51
1:A:371:ASP:OD2	1:A:373:THR:OG1	2.25	0.51
1:A:413:LYS:HD2	4:A:1382:HOH:O	2.09	0.51
1:A:195:TYR:CE2	1:A:199:VAL:HG11	2.45	0.51
1:A:368:VAL:CG1	1:A:369:LEU:N	2.74	0.51
1:A:399:LEU:HD23	1:A:400:ALA:N	2.25	0.51
1:A:249:ASN:ND2	1:A:249:ASN:N	2.49	0.51
1:A:368:VAL:HG12	1:A:369:LEU:H	1.75	0.51
1:A:735:GLU:O	1:A:735:GLU:HG3	2.10	0.51
1:A:83:ILE:HD11	4:A:1054:HOH:O	2.10	0.51
1:A:423:LYS:HE3	4:A:1217:HOH:O	2.11	0.50
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.12	0.50
1:A:399:LEU:C	1:A:399:LEU:CD2	2.79	0.50
1:A:40:ASP:OD2	1:A:42:LYS:N	2.36	0.49
1:A:311:GLY:N	4:A:1222:HOH:O	2.41	0.49
1:A:646:GLU:HG3	4:A:1390:HOH:O	2.10	0.49
1:A:369:LEU:HG	1:A:394:MET:HE2	1.92	0.49
1:A:130:LYS:CA	3:A:999:PNQ:O4A	2.60	0.49
1:A:289:THR:O	1:A:292:GLU:N	2.45	0.48
1:A:73:LYS:HB2	4:A:1177:HOH:O	2.11	0.48
1:A:510:SER:O	1:A:514:ILE:HG13	2.13	0.48
1:A:585:LEU:O	1:A:589:LYS:HD2	2.13	0.48
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.79	0.48
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.96	0.48
1:A:715:ASP:O	1:A:716:ALA:HB2	2.13	0.48
1:A:289:THR:HG23	1:A:289:THR:O	2.13	0.48
1:A:99:GLU:N	1:A:100:PRO:HD2	2.28	0.47
1:A:308:ASN:OD1	1:A:308:ASN:C	2.52	0.47
1:A:531:GLU:O	1:A:534:VAL:HG12	2.14	0.47
1:A:662:GLN:NE2	4:A:1198:HOH:O	2.48	0.47
1:A:136:THR:HB	1:A:138:GLU:OE2	2.15	0.47
1:A:598:LEU:HA	1:A:598:LEU:HD23	1.67	0.47
1:A:492:GLU:O	1:A:496:LYS:HG2	2.15	0.47
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.62	0.47
1:A:705:TYR:O	1:A:706:TYR:C	2.53	0.47
1:A:138:GLU:N	1:A:138:GLU:CD	2.66	0.46
1:A:184:GLY:HA2	3:A:999:PNQ:PA	2.54	0.46
1:A:32:LYS:N	1:A:32:LYS:HD3	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD21	1:A:346:LYS:HG2	1.97	0.46
1:A:296:LEU:HB3	1:A:298:LEU:HD21	1.97	0.46
1:A:73:LYS:HA	1:A:73:LYS:HD3	1.66	0.46
1:A:60:PHE:CE1	1:A:74:LYS:HG2	2.51	0.46
1:A:44:ARG:O	1:A:44:ARG:HG2	2.16	0.46
1:A:359:PHE:CB	1:A:411:VAL:HG22	2.46	0.46
1:A:410:ASN:OD1	1:A:410:ASN:C	2.54	0.46
1:A:190:LYS:CE	1:A:223:GLU:OE2	2.65	0.45
1:A:442:CYS:SG	1:A:443:GLN:N	2.89	0.45
1:A:87:GLY:H	1:A:105:ASN:HD21	1.64	0.45
1:A:302:GLU:H	1:A:302:GLU:CD	2.19	0.45
1:A:273:GLU:C	1:A:274:THR:HG23	2.36	0.45
1:A:322:GLU:O	1:A:325:LYS:HB2	2.16	0.45
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.51	0.45
1:A:13:LYS:HZ2	1:A:13:LYS:HG3	1.56	0.45
1:A:158:ILE:HD12	1:A:158:ILE:C	2.36	0.44
1:A:158:ILE:CD1	1:A:159:SER:N	2.75	0.44
1:A:147:ARG:HD2	1:A:150:GLU:OE1	2.18	0.44
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.76	0.44
1:A:53:VAL:CG1	1:A:63:LYS:HD2	2.48	0.44
1:A:72:VAL:HG22	1:A:73:LYS:N	2.33	0.44
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.18	0.44
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.58	0.44
1:A:94:LEU:O	1:A:97:LEU:HD11	2.18	0.44
1:A:212:GLU:OE1	1:A:212:GLU:N	2.49	0.43
1:A:53:VAL:HG11	1:A:63:LYS:CD	2.49	0.43
1:A:289:THR:CG2	1:A:292:GLU:CG	2.95	0.43
1:A:289:THR:CG2	1:A:289:THR:O	2.66	0.43
1:A:696:ILE:HD11	1:A:751:LEU:HD22	2.01	0.43
1:A:53:VAL:HG22	1:A:61:THR:O	2.19	0.43
1:A:696:ILE:O	1:A:743:LYS:HB3	2.19	0.42
1:A:546:LYS:NZ	1:A:550:HIS:HE1	2.17	0.42
1:A:735:GLU:O	1:A:735:GLU:CG	2.67	0.42
1:A:628:ILE:CD1	1:A:633:GLN:CB	2.91	0.42
1:A:669:ASP:CG	4:A:1313:HOH:O	2.58	0.42
1:A:491:GLN:HE21	1:A:491:GLN:HB3	1.51	0.42
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.76	0.42
1:A:399:LEU:HD23	1:A:399:LEU:C	2.40	0.42
1:A:563:PHE:O	1:A:565:LYS:NZ	2.53	0.42
1:A:121:LEU:CD1	1:A:489:LEU:HD12	2.49	0.42
1:A:99:GLU:HB2	1:A:100:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:N	1:A:100:PRO:CD	2.84	0.41
1:A:121:LEU:HD11	1:A:489:LEU:HD12	2.03	0.41
1:A:605:ASP:OD1	1:A:607:VAL:N	2.44	0.41
1:A:704:ARG:O	1:A:707:LEU:HD21	2.20	0.41
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.51	0.41
1:A:13:LYS:HZ3	1:A:13:LYS:CB	2.33	0.41
1:A:296:LEU:CD2	1:A:346:LYS:HG2	2.51	0.41
1:A:391:LYS:HA	1:A:391:LYS:HD3	1.88	0.41
1:A:711:ASN:HB2	1:A:712:VAL:HG23	2.01	0.41
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.56	0.41
1:A:289:THR:OG1	1:A:291:GLU:OE2	2.36	0.41
1:A:531:GLU:O	1:A:534:VAL:CG1	2.69	0.41
1:A:190:LYS:HE2	1:A:223:GLU:OE2	2.21	0.41
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.90	0.41
1:A:71:GLN:HE21	1:A:71:GLN:HB3	1.53	0.40
1:A:667:LEU:HD11	1:A:672:VAL:HG21	2.03	0.40
1:A:732:ILE:HG22	1:A:733:ASP:N	2.36	0.40
1:A:568:PHE:O	1:A:578:MET:HE3	2.20	0.40
1:A:696:ILE:O	1:A:743:LYS:HA	2.21	0.40
1:A:40:ASP:C	1:A:42:LYS:N	2.75	0.40
1:A:238:ARG:HB2	1:A:278:TYR:HE1	1.86	0.40
1:A:732:ILE:CG2	1:A:733:ASP:N	2.85	0.40
1:A:733:ASP:HA	1:A:734:PRO:HD3	1.91	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLN:OE1	4:A:1183:HOH:O[4_456]	1.86	0.34
4:A:1121:HOH:O	4:A:1184:HOH:O[4_456]	2.10	0.10

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	734/761 (96%)	706 (96%)	25 (3%)	3 (0%)	34 30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	716	ALA
1	A	3	PRO

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	627/665 (94%)	586 (94%)	41 (6%)	17 12

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	13	LYS
1	A	31	ASP
1	A	42	LYS
1	A	44	ARG
1	A	57	SER
1	A	71	GLN
1	A	73	LYS
1	A	234	ASN
1	A	238	ARG
1	A	249	ASN
1	A	291	GLU
1	A	319	SER
1	A	342	MET
1	A	358	LYS
1	A	379	SER
1	A	391	LYS

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Mol	Chain	Res	Type
1	A	399	LEU
1	A	405	VAL
1	A	407	GLN
1	A	412	GLU
1	A	423	LYS
1	A	436	LYS
1	A	446	LYS
1	A	496	LYS
1	A	509	ASP
1	A	510	SER
1	A	534	VAL
1	A	544	ILE
1	A	580	GLU
1	A	589	LYS
1	A	594	GLN
1	A	610	LYS
1	A	654	ARG
1	A	689	ARG
1	A	707	LEU
1	A	727	LEU
1	A	728	LYS
1	A	738	ARG
1	A	742	THR
1	A	744	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	2	ASN
1	A	5	HIS
1	A	68	GLN
1	A	71	GLN
1	A	79	GLN
1	A	105	ASN
1	A	149	ASN
1	A	203	ASN
1	A	213	GLN
1	A	249	ASN
1	A	259	GLN
1	A	283	GLN
1	A	376	ASN
1	A	439	ASN

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	532	GLN
1	A	550	HIS
1	A	594	GLN
1	A	662	GLN
1	A	720	GLN
1	A	729	HIS
1	A	731	ASN
1	A	736	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	PNQ	A	999	2	20,25,25	1.69	3 (15%)	21,37,37	1.48	5 (23%)

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	PNQ	A	999	2	-	5/18/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PNQ	CA2-NA3	-5.69	1.34	1.45
3	A	999	PNQ	C1-NA3	2.48	1.46	1.38
3	A	999	PNQ	C4-N4	2.25	1.49	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PNQ	O4B-N4-C4	2.94	120.88	114.72
3	A	999	PNQ	C5-C4-N4	2.21	121.05	119.35
3	A	999	PNQ	C3-C4-N4	-2.19	117.67	119.35
3	A	999	PNQ	PA-OE2-CA1	-2.18	110.85	121.59
3	A	999	PNQ	C3-C2-C1	-2.06	117.92	120.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PNQ	CA1-OE2-PA-OA2
3	A	999	PNQ	C5-C4-N4-O4B
3	A	999	PNQ	C3-C4-N4-O4B
3	A	999	PNQ	PA-OA3-PB-OB2
3	A	999	PNQ	PA-OA3-PB-OB1

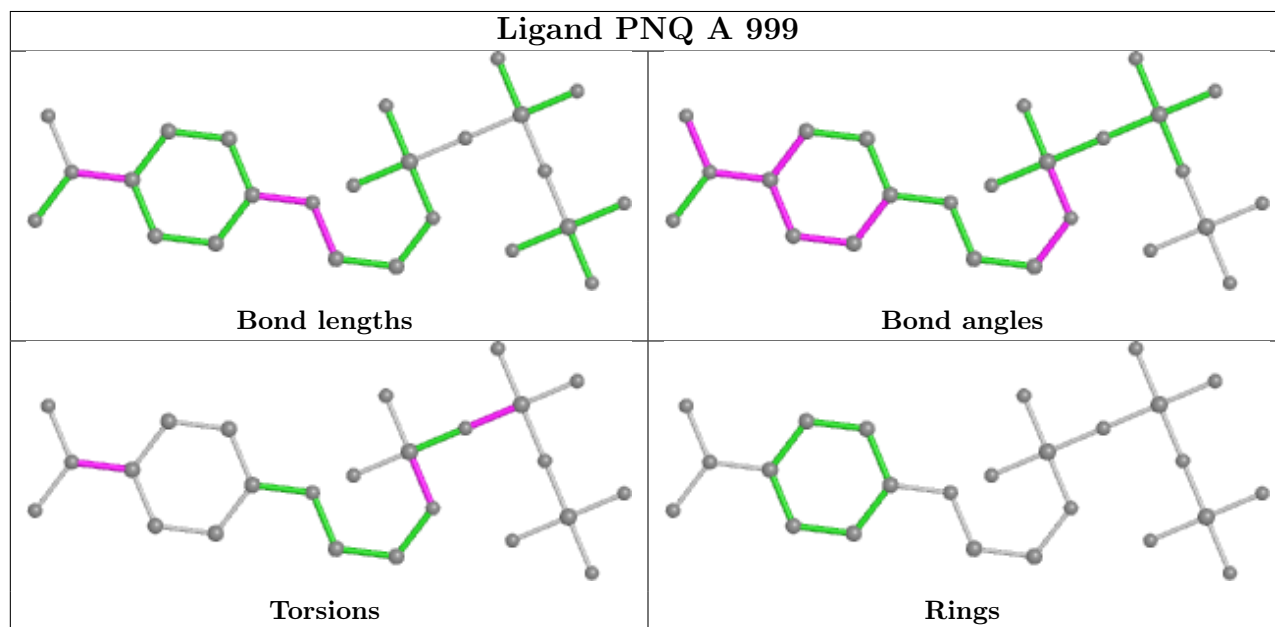
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PNQ	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	742/761 (97%)	0.51	34 (4%) 32 31	7, 27, 66, 97	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	GLN	5.0
1	A	290	ALA	4.1
1	A	715	ASP	4.0
1	A	710	PRO	3.7
1	A	365	GLU	3.6
1	A	737	TYR	3.6
1	A	627	PHE	3.4
1	A	362	GLY	3.4
1	A	711	ASN	2.9
1	A	294	LYS	2.8
1	A	322	GLU	2.8
1	A	68	GLN	2.8
1	A	42	LYS	2.7
1	A	495	LEU	2.7
1	A	509	ASP	2.7
1	A	405	VAL	2.6
1	A	399	LEU	2.6
1	A	316	LYS	2.5
1	A	203	ASN	2.5
1	A	707	LEU	2.4
1	A	23	ASP	2.4
1	A	64	THR	2.4
1	A	204	GLN	2.4
1	A	366	GLY	2.4
1	A	361	LYS	2.3
1	A	496	LYS	2.3
1	A	289	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	628	ILE	2.3
1	A	67	GLY	2.2
1	A	367	ALA	2.2
1	A	401	GLY	2.1
1	A	41	PRO	2.1
1	A	363	ALA	2.1
1	A	291	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

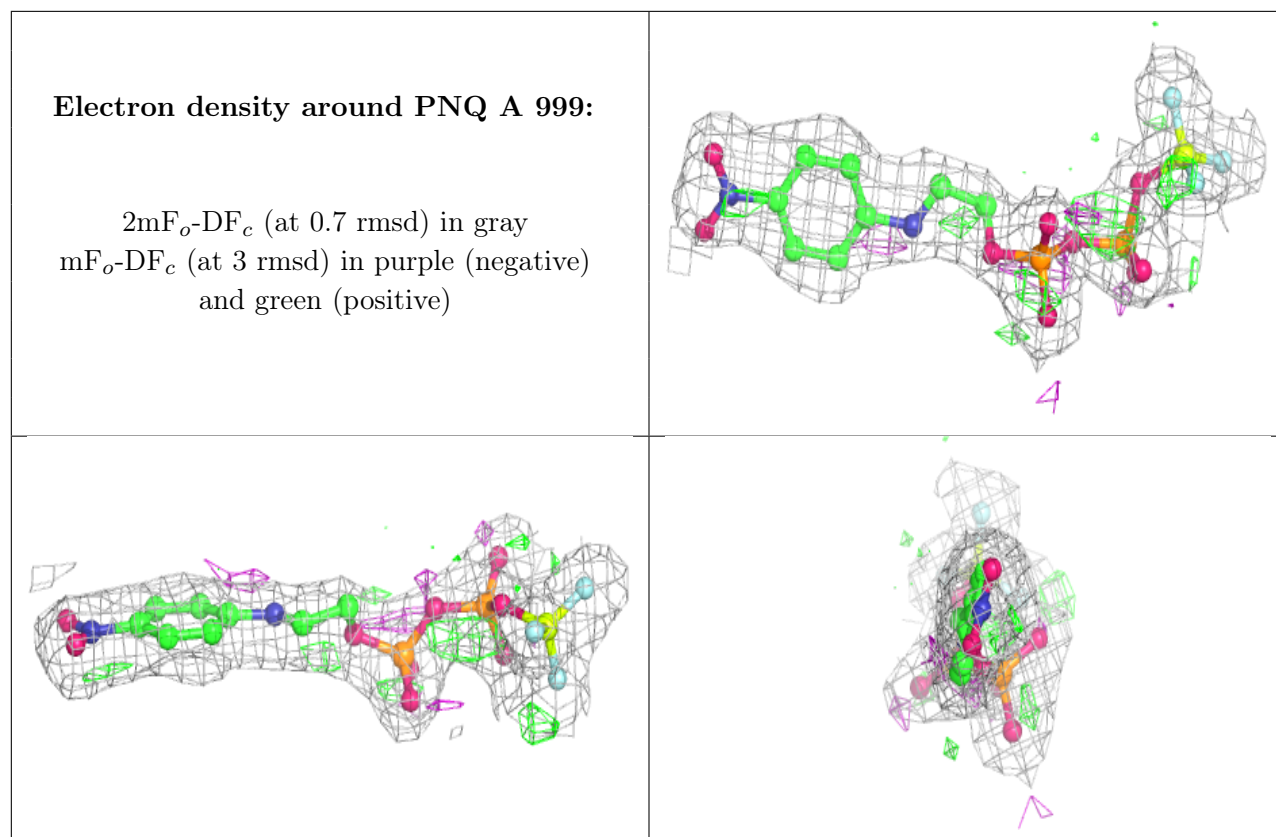
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	MG	A	998	1/1	0.93	0.07	10,10,10,10	0
3	PNQ	A	999	25/25	0.94	0.14	8,14,28,86	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.