



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:25 AM EDT

PDB ID : 1D0Z / pdb_00001d0z
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH P-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

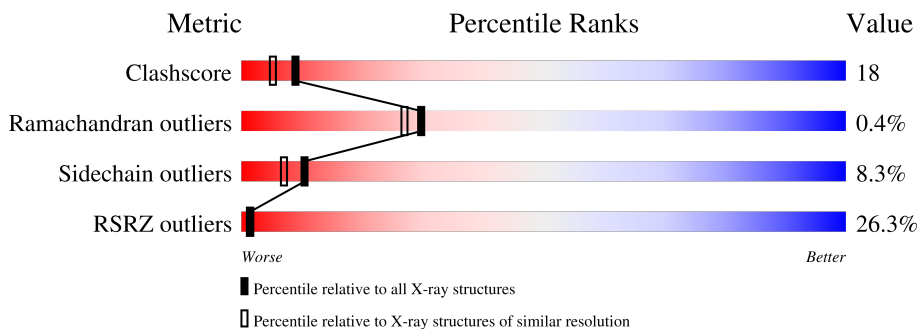
1 Overall quality at a glance

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 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
1	A	742	Total	C	N	O	S	0	0	0
			5869	3729	1009	1115	16			

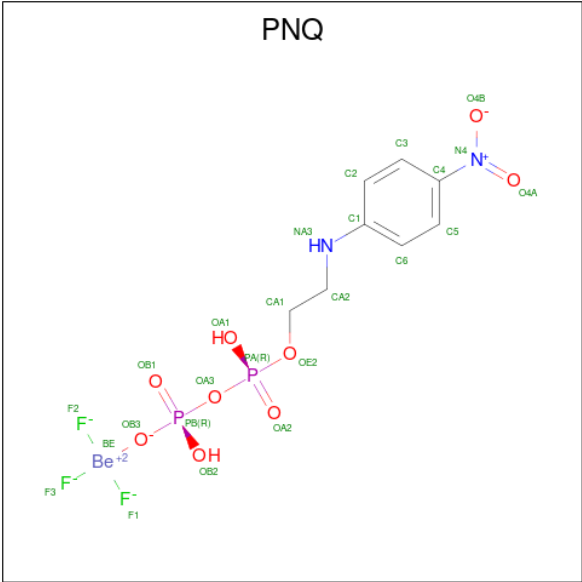
There are 3 discrepancies between the modelled and reference sequences:

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 P-NITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE (CCD ID: 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

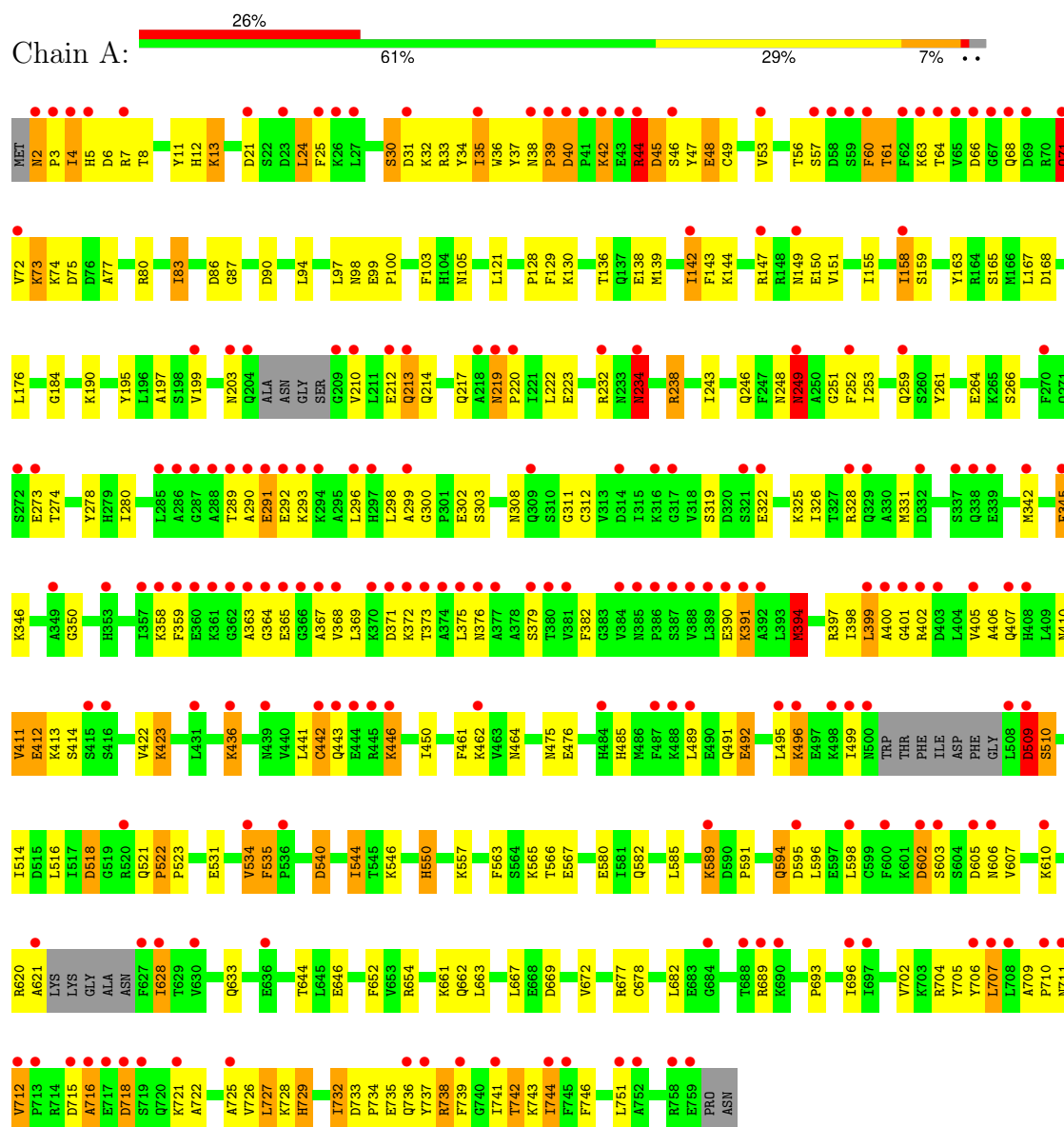
- Molecule 4 is water.

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 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (25.00-2.00) 91.6 (25.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.00Å)	Xtriage
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	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 89.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	1.42	19/5980 (0.3%)	1.79	93/8081 (1.2%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	ASN	CG-OD1	13.34	1.48	1.23
1	A	628	ILE	C-N	9.35	1.45	1.33
1	A	40	ASP	CG-OD2	5.97	1.36	1.25
1	A	40	ASP	N-CA	-5.89	1.40	1.46
1	A	45	ASP	CA-C	-5.86	1.45	1.52
1	A	86	ASP	CA-CB	5.66	1.60	1.53
1	A	414	SER	N-CA	-5.61	1.39	1.46
1	A	238	ARG	CD-NE	-5.57	1.38	1.46
1	A	652	PHE	CA-CB	5.51	1.60	1.53
1	A	326	ILE	CA-CB	-5.43	1.48	1.54
1	A	39	PRO	C-N	-5.28	1.28	1.33
1	A	165	SER	C-N	-5.25	1.27	1.33
1	A	644	THR	C-O	-5.25	1.18	1.24
1	A	663	LEU	C-N	5.23	1.39	1.33
1	A	71	GLN	CA-C	-5.21	1.46	1.52
1	A	550	HIS	CE1-NE2	5.19	1.37	1.32
1	A	522	PRO	C-N	-5.16	1.26	1.33
1	A	550	HIS	CA-C	-5.07	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ASP	CG-OD2	5.04	1.34	1.25

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASN	OD1-CG-ND2	20.56	143.16	122.60
1	A	234	ASN	CB-CG-OD1	-17.51	85.78	120.80
1	A	234	ASN	CA-CB-CG	-17.44	95.16	112.60
1	A	234	ASN	CB-CG-ND2	-14.22	95.06	116.40
1	A	628	ILE	O-C-N	11.61	135.23	122.93
1	A	249	ASN	CA-CB-CG	-10.90	101.70	112.60
1	A	509	ASP	N-CA-C	-10.47	99.04	112.23
1	A	402	ARG	N-CA-C	-9.84	100.93	113.72
1	A	712	VAL	N-CA-C	8.15	126.50	108.88
1	A	464	ASN	CA-CB-CG	-7.58	105.02	112.60
1	A	252	PHE	CA-CB-CG	-7.28	106.52	113.80
1	A	2	ASN	N-CA-CB	7.22	122.78	110.50
1	A	442	CYS	N-CA-C	7.20	120.76	109.96
1	A	450	ILE	CA-C-N	-7.17	115.63	122.66
1	A	450	ILE	C-N-CA	-7.17	115.63	122.66
1	A	12	HIS	CA-CB-CG	-7.12	106.67	113.80
1	A	535	PHE	CA-CB-CG	-7.09	106.71	113.80
1	A	729	HIS	CA-CB-CG	-7.08	106.72	113.80
1	A	540	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	620	ARG	CA-C-N	-6.76	109.53	121.70
1	A	620	ARG	C-N-CA	-6.76	109.53	121.70
1	A	30	SER	CA-C-N	6.74	132.15	120.68
1	A	30	SER	C-N-CA	6.74	132.15	120.68
1	A	363	ALA	N-CA-C	-6.74	102.33	112.04
1	A	234	ASN	N-CA-CB	6.59	121.33	110.39
1	A	45	ASP	CA-CB-CG	-6.45	106.15	112.60
1	A	128	PRO	CB-CA-C	-6.44	100.93	111.56
1	A	475	ASN	CA-CB-CG	-6.41	106.19	112.60
1	A	739	PHE	CA-C-N	-6.36	114.91	122.16
1	A	739	PHE	C-N-CA	-6.36	114.91	122.16
1	A	364	GLY	N-CA-C	-6.35	98.12	113.18
1	A	718	ASP	N-CA-CB	6.33	118.25	110.53
1	A	312	CYS	CA-C-N	-6.25	115.11	122.36
1	A	312	CYS	C-N-CA	-6.25	115.11	122.36
1	A	441	LEU	N-CA-C	6.23	119.35	111.69
1	A	495	LEU	N-CA-CB	6.20	119.06	110.07
1	A	25	PHE	CA-CB-CG	6.10	119.90	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PHE	CA-CB-CG	-6.06	107.74	113.80
1	A	142	ILE	CB-CA-C	-6.03	104.00	112.14
1	A	11	TYR	N-CA-C	-6.02	104.63	111.07
1	A	144	LYS	N-CA-C	5.98	119.49	110.64
1	A	567	GLU	N-CA-CB	-5.86	102.11	111.43
1	A	461	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	394	MET	CA-C-N	-5.82	116.37	122.89
1	A	394	MET	C-N-CA	-5.82	116.37	122.89
1	A	243	ILE	CA-C-N	-5.80	115.31	122.84
1	A	243	ILE	C-N-CA	-5.80	115.31	122.84
1	A	60	PHE	CA-CB-CG	5.71	119.51	113.80
1	A	535	PHE	CA-C-O	5.68	122.98	119.29
1	A	702	VAL	CB-CA-C	-5.68	104.47	112.14
1	A	98	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	143	PHE	CA-CB-CG	-5.62	108.19	113.80
1	A	516	LEU	CA-C-O	5.61	126.44	120.10
1	A	678	CYS	N-CA-C	5.55	118.26	111.82
1	A	712	VAL	O-C-N	5.51	127.38	121.10
1	A	48	GLU	N-CA-C	-5.51	100.92	109.24
1	A	44	ARG	CD-NE-CZ	5.47	132.05	124.40
1	A	398	ILE	N-CA-C	5.44	115.73	108.11
1	A	249	ASN	CA-C-O	5.44	126.24	120.10
1	A	591	PRO	N-CA-C	5.42	119.99	111.38
1	A	168	ASP	N-CA-C	5.41	116.98	111.14
1	A	365	GLU	N-CA-C	-5.40	105.36	113.89
1	A	2	ASN	CA-C-N	5.36	126.54	119.84
1	A	2	ASN	C-N-CA	5.36	126.54	119.84
1	A	238	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	A	248	ASN	CA-C-N	5.31	127.93	120.28
1	A	248	ASN	C-N-CA	5.31	127.93	120.28
1	A	628	ILE	N-CA-CB	5.30	119.35	110.86
1	A	566	THR	CA-C-N	-5.30	113.91	122.82
1	A	566	THR	C-N-CA	-5.30	113.91	122.82
1	A	75	ASP	CB-CA-C	5.30	120.17	110.11
1	A	249	ASN	N-CA-CB	-5.29	102.07	110.22
1	A	476	GLU	CB-CA-C	-5.27	101.89	110.85
1	A	219	ASN	O-C-N	5.23	124.51	120.38
1	A	103	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	367	ALA	N-CA-C	5.20	117.39	110.53
1	A	661	LYS	CA-C-N	-5.15	114.94	122.40
1	A	661	LYS	C-N-CA	-5.15	114.94	122.40
1	A	595	ASP	N-CA-CB	5.14	118.14	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	712	VAL	CA-C-N	5.13	126.25	119.84
1	A	712	VAL	C-N-CA	5.13	126.25	119.84
1	A	149	ASN	CA-C-N	-5.12	114.11	122.26
1	A	149	ASN	C-N-CA	-5.12	114.11	122.26
1	A	266	SER	CA-C-O	5.12	125.89	120.10
1	A	21	ASP	CA-CB-CG	-5.11	107.49	112.60
1	A	606	ASN	CA-CB-CG	-5.11	107.49	112.60
1	A	238	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	A	462	LYS	CB-CA-C	-5.06	102.39	110.79
1	A	582	GLN	N-CA-C	5.03	117.63	110.24
1	A	518	ASP	N-CA-C	5.02	120.03	113.30
1	A	602	ASP	CB-CA-C	-5.02	101.71	110.09
1	A	492	GLU	CB-CA-C	-5.00	103.02	110.88

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

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	215	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	215	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 (215) 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	0.98
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
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:331:MET:HE1	1:A:345:PHE:HZ	1.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:GLU:H	1:A:138:GLU:CD	2.03	0.66
1:A:369:LEU:HG	1:A:394:MET:HE1	1.77	0.66
1:A:710:PRO:HD2	1:A:729:HIS:CE1	2.31	0.65
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.30	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:147:ARG:HB2	1:A:150:GLU:CD	2.23	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:718:ASP:CG	1:A:721:LYS:HB2	2.26	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:328:ARG:HA	1:A:331:MET:HE3	1.83	0.60
1:A:523:PRO:HD2	4:A:1121:HOH:O	2.02	0.59
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:544:ILE:HG13	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:399:LEU:C	1:A:399:LEU:CD2	2.79	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:540:ASP:OD2	4:A:1437:HOH:O	2.19	0.52
1:A:60:PHE:O	1:A:71:GLN:HG2	2.09	0.52
1:A:369:LEU:HG	1:A:394:MET:HE2	1.89	0.52
1:A:308:ASN:OD1	1:A:308:ASN:C	2.52	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:705:TYR:O	1:A:706:TYR:C	2.53	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:138:GLU:N	1:A:138:GLU:CD	2.66	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:410:ASN:OD1	1:A:410:ASN:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:H	1:A:302:GLU:CD	2.19	0.50
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:273:GLU:C	1:A:274:THR:HG23	2.36	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:158:ILE:HD12	1:A:158:ILE:C	2.36	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:99:GLU:N	1:A:100:PRO:HD2	2.28	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:669:ASP:CG	4:A:1313:HOH:O	2.58	0.47
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.62	0.47
1:A:163:TYR:OH	1:A:251:GLY:O	2.33	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
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:399:LEU:C	1:A:399:LEU:HD23	2.40	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: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:158:ILE:C	1:A:158:ILE:CD1	2.90	0.45
1:A:289:THR:HG23	1:A:289:THR:O	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASP:CG	1:A:557:LYS:HZ1	2.25	0.45
1:A:13:LYS:HZ2	1:A:13:LYS:HG3	1.56	0.45
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:40:ASP:C	1:A:42:LYS:N	2.75	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:509:ASP:CG	1:A:557:LYS:NZ	2.76	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:32:LYS:C	1:A:33:ARG:HD3	2.43	0.43
1:A:40:ASP:OD2	1:A:40:ASP:C	2.61	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:602:ASP:O	1:A:603:SER:C	2.59	0.42
1:A:628:ILE:CD1	1:A:633:GLN:CB	2.91	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: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
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:521:GLN:HA	1:A:522:PRO:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASP:OD1	1:A:518:ASP:C	2.63	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:696:ILE:O	1:A:743:LYS:HA	2.21	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	30 27

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 ⓘ

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%)	575 (92%)	52 (8%)	10 7

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	13	LYS
1	A	24	LEU
1	A	31	ASP
1	A	35	ILE
1	A	42	LYS
1	A	44	ARG
1	A	57	SER
1	A	61	THR
1	A	66	ASP
1	A	71	GLN
1	A	73	LYS
1	A	83	ILE
1	A	158	ILE
1	A	203	ASN
1	A	213	GLN
1	A	232	ARG
1	A	234	ASN
1	A	249	ASN
1	A	291	GLU
1	A	319	SER
1	A	358	LYS
1	A	375	LEU
1	A	379	SER
1	A	391	LYS
1	A	394	MET
1	A	399	LEU
1	A	405	VAL
1	A	407	GLN
1	A	411	VAL

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Mol	Chain	Res	Type
1	A	412	GLU
1	A	422	VAL
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	689	ARG
1	A	707	LEU
1	A	727	LEU
1	A	728	LYS
1	A	732	ILE
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 (31) 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	112	GLN
1	A	149	ASN
1	A	188	ASN
1	A	203	ASN
1	A	213	GLN
1	A	249	ASN
1	A	259	GLN
1	A	271	GLN
1	A	283	GLN
1	A	407	GLN

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Mol	Chain	Res	Type
1	A	439	ASN
1	A	483	ASN
1	A	491	GLN
1	A	532	GLN
1	A	550	HIS
1	A	593	GLN
1	A	594	GLN
1	A	633	GLN
1	A	649	ASN
1	A	660	ASN
1	A	662	GLN
1	A	720	GLN
1	A	729	HIS
1	A	731	ASN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PNQ	A	999	2	23,25,25	1.71	3 (13%)	23,37,37	1.29	2 (8%)

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	-	3/16/24/24	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	-5.94	1.34	1.45
3	A	999	PNQ	C1-NA3	2.57	1.46	1.38
3	A	999	PNQ	O4B-N4	-2.49	1.18	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PNQ	PA-OE2-CA1	-2.19	110.85	121.26
3	A	999	PNQ	C3-C2-C1	-2.07	117.92	120.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PNQ	CA1-OE2-PA-OA2
3	A	999	PNQ	PA-OA3-PB-OB2
3	A	999	PNQ	PA-OA3-PB-OB1

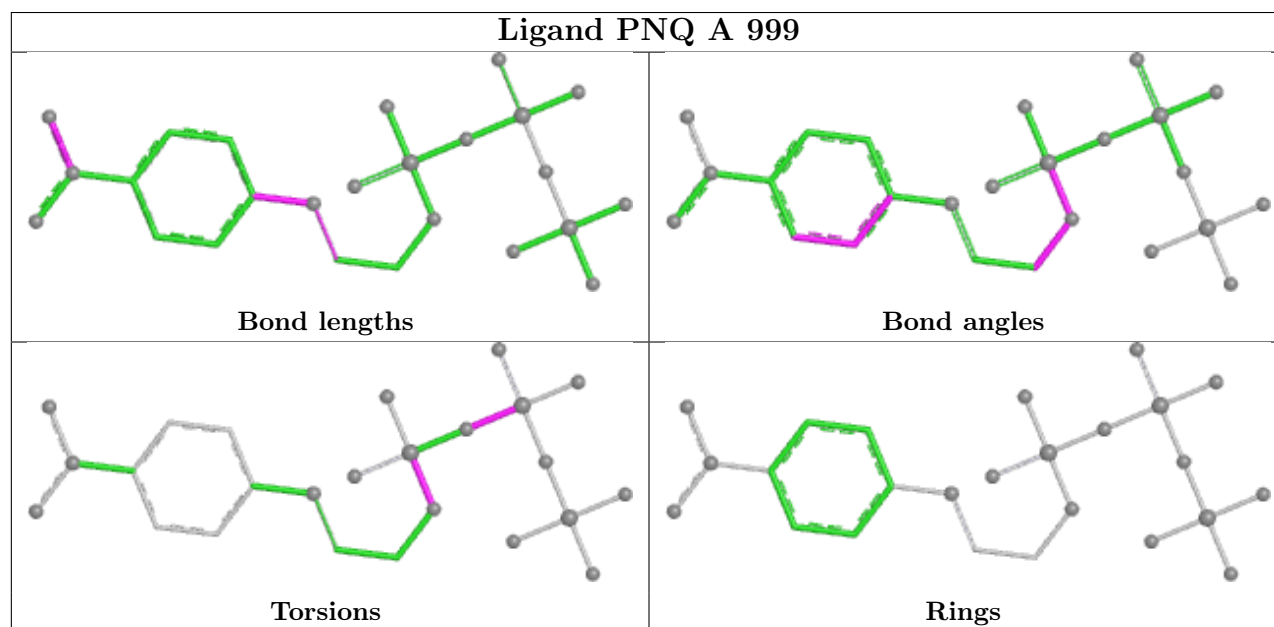
There are no ring outliers.

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%)	1.41	195 (26%) 1 1	7, 27, 66, 97	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	ASP	6.8
1	A	627	PHE	6.5
1	A	710	PRO	6.3
1	A	362	GLY	5.6
1	A	290	ALA	5.3
1	A	621	ALA	5.2
1	A	711	ASN	5.1
1	A	509	ASP	4.9
1	A	316	LYS	4.8
1	A	363	ALA	4.8
1	A	366	GLY	4.7
1	A	210	VAL	4.5
1	A	297	HIS	4.5
1	A	53	VAL	4.4
1	A	405	VAL	4.4
1	A	368	VAL	4.3
1	A	443	GLN	4.3
1	A	322	GLU	4.2
1	A	737	TYR	4.2
1	A	364	GLY	4.1
1	A	69	ASP	4.1
1	A	43	GLU	4.1
1	A	487	PHE	4.1
1	A	360	GLU	4.1
1	A	203	ASN	4.1
1	A	209	GLY	4.1
1	A	294	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	401	GLY	4.0
1	A	361	LYS	4.0
1	A	371	ASP	4.0
1	A	741	ILE	4.0
1	A	292	GLU	3.9
1	A	299	ALA	3.9
1	A	65	VAL	3.9
1	A	508	LEU	3.9
1	A	60	PHE	3.9
1	A	500	ASN	3.8
1	A	380	THR	3.8
1	A	329	GLN	3.8
1	A	431	LEU	3.8
1	A	399	LEU	3.7
1	A	199	VAL	3.7
1	A	602	ASP	3.6
1	A	496	LYS	3.6
1	A	534	VAL	3.6
1	A	370	LYS	3.6
1	A	35	ILE	3.5
1	A	367	ALA	3.5
1	A	376	ASN	3.5
1	A	234	ASN	3.4
1	A	64	THR	3.4
1	A	3	PRO	3.4
1	A	400	ALA	3.4
1	A	328	ARG	3.4
1	A	67	GLY	3.4
1	A	721	LYS	3.3
1	A	386	PRO	3.3
1	A	339	GLU	3.3
1	A	717	GLU	3.3
1	A	41	PRO	3.3
1	A	357	ILE	3.3
1	A	375	LEU	3.3
1	A	288	ALA	3.3
1	A	444	GLU	3.3
1	A	57	SER	3.2
1	A	439	ASN	3.2
1	A	716	ALA	3.2
1	A	706	TYR	3.2
1	A	365	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	3.2
1	A	725	ALA	3.2
1	A	58	ASP	3.2
1	A	232	ARG	3.2
1	A	219	ASN	3.2
1	A	445	ARG	3.1
1	A	66	ASP	3.1
1	A	5	HIS	3.1
1	A	402	ARG	3.1
1	A	391	LYS	3.0
1	A	286	ALA	3.0
1	A	373	THR	3.0
1	A	68	GLN	3.0
1	A	388	VAL	3.0
1	A	495	LEU	3.0
1	A	259	GLN	2.9
1	A	291	GLU	2.9
1	A	358	LYS	2.9
1	A	690	LYS	2.9
1	A	349	ALA	2.9
1	A	499	ILE	2.9
1	A	42	LYS	2.9
1	A	285	LEU	2.8
1	A	4	ILE	2.8
1	A	598	LEU	2.8
1	A	7	ARG	2.8
1	A	71	GLN	2.8
1	A	436	LYS	2.8
1	A	21	ASP	2.8
1	A	62	PHE	2.8
1	A	600	PHE	2.8
1	A	158	ILE	2.8
1	A	204	GLN	2.7
1	A	345	PHE	2.7
1	A	39	PRO	2.7
1	A	744	ILE	2.7
1	A	314	ASP	2.7
1	A	63	LYS	2.7
1	A	44	ARG	2.7
1	A	758	ARG	2.7
1	A	712	VAL	2.7
1	A	372	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	296	LEU	2.6
1	A	309	GLN	2.6
1	A	149	ASN	2.6
1	A	606	ASN	2.6
1	A	489	LEU	2.6
1	A	745	PHE	2.6
1	A	384	VAL	2.6
1	A	697	ILE	2.6
1	A	759	GLU	2.6
1	A	289	THR	2.6
1	A	403	ASP	2.6
1	A	407	GLN	2.6
1	A	628	ILE	2.6
1	A	218	ALA	2.6
1	A	688	THR	2.6
1	A	31	ASP	2.5
1	A	40	ASP	2.5
1	A	72	VAL	2.5
1	A	2	ASN	2.5
1	A	272	SER	2.5
1	A	38	ASN	2.5
1	A	636	GLU	2.5
1	A	59	SER	2.4
1	A	293	LYS	2.4
1	A	520	ARG	2.4
1	A	536	PRO	2.4
1	A	147	ARG	2.4
1	A	707	LEU	2.4
1	A	317	GLY	2.4
1	A	142	ILE	2.4
1	A	488	LYS	2.4
1	A	408	HIS	2.4
1	A	392	ALA	2.3
1	A	462	LYS	2.3
1	A	321	SER	2.3
1	A	442	CYS	2.3
1	A	736	GLN	2.3
1	A	708	LEU	2.3
1	A	342	MET	2.3
1	A	446	LYS	2.3
1	A	252	PHE	2.3
1	A	377	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	610	LYS	2.3
1	A	212	GLU	2.2
1	A	595	ASP	2.2
1	A	387	SER	2.2
1	A	603	SER	2.2
1	A	25	PHE	2.2
1	A	689	ARG	2.2
1	A	27	LEU	2.2
1	A	719	SER	2.2
1	A	23	ASP	2.2
1	A	630	VAL	2.2
1	A	353	HIS	2.2
1	A	389	LEU	2.2
1	A	337	SER	2.2
1	A	220	PRO	2.1
1	A	718	ASP	2.2
1	A	696	ILE	2.1
1	A	415	SER	2.1
1	A	498	LYS	2.1
1	A	589	LYS	2.1
1	A	273	GLU	2.1
1	A	287	GLY	2.1
1	A	684	GLY	2.1
1	A	374	ALA	2.1
1	A	26	LYS	2.1
1	A	751	LEU	2.1
1	A	739	PHE	2.1
1	A	379	SER	2.1
1	A	385	ASN	2.1
1	A	338	GLN	2.1
1	A	484	HIS	2.1
1	A	713	PRO	2.1
1	A	46	SER	2.1
1	A	416	SER	2.1
1	A	249	ASN	2.0
1	A	213	GLN	2.0
1	A	332	ASP	2.0
1	A	270	PHE	2.0
1	A	359	PHE	2.0
1	A	390	GLU	2.0
1	A	752	ALA	2.0
1	A	605	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](#)

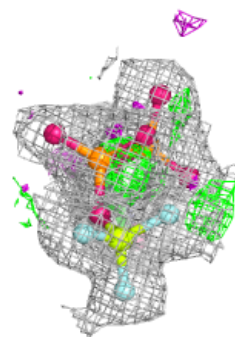
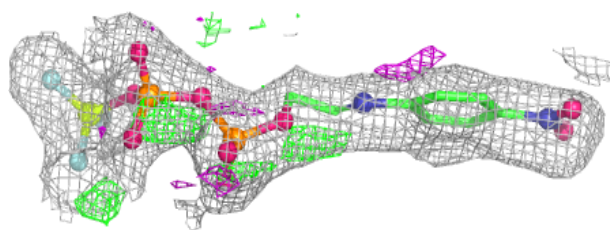
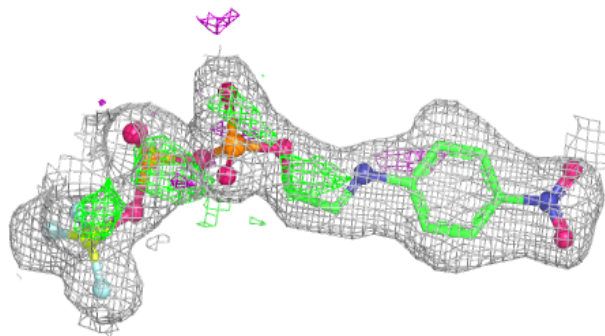
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	998	1/1	0.82	0.05	10,10,10,10	0
3	PNQ	A	999	25/25	0.94	0.11	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.

Electron density around PNQ A 999:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.