



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 PM UTC

PDB ID : 6EZU / pdb_00006ezu
Title : Schistosoma mansoni Phosphodiesterase 4A
Authors : Brown, D.G.; Schroeder, S.; Gil, C.
Deposited on : 2017-11-16
Resolution : 2.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

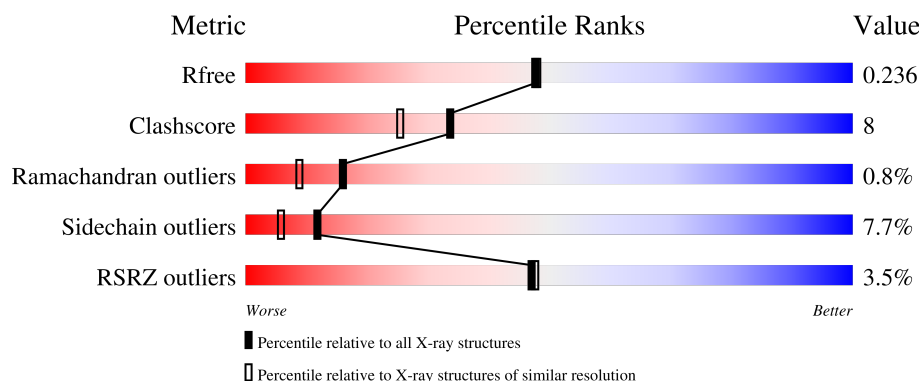
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	371	2% 52% 30% 6% 10%
1	B	371	4% 53% 27% 6% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5340 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 Phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2677	1701	459	500	17			
1	B	324	Total	C	N	O	S	0	0	0
			2558	1634	432	475	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	GLY	-	expression tag	UNP G4VPI6
A	302	PRO	-	expression tag	UNP G4VPI6
B	301	GLY	-	expression tag	UNP G4VPI6
B	302	PRO	-	expression tag	UNP G4VPI6

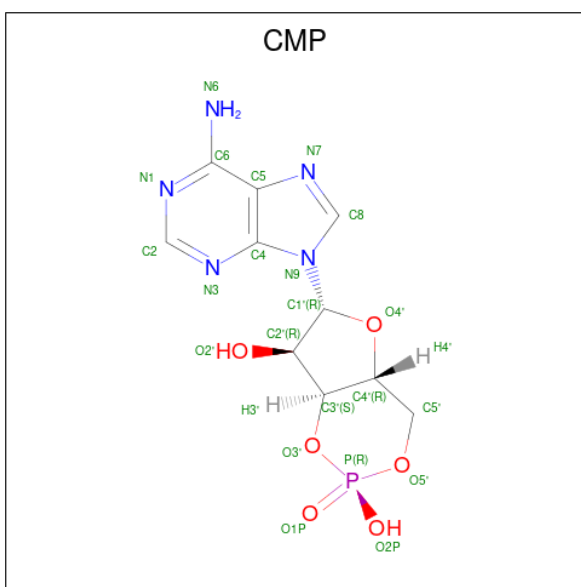
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

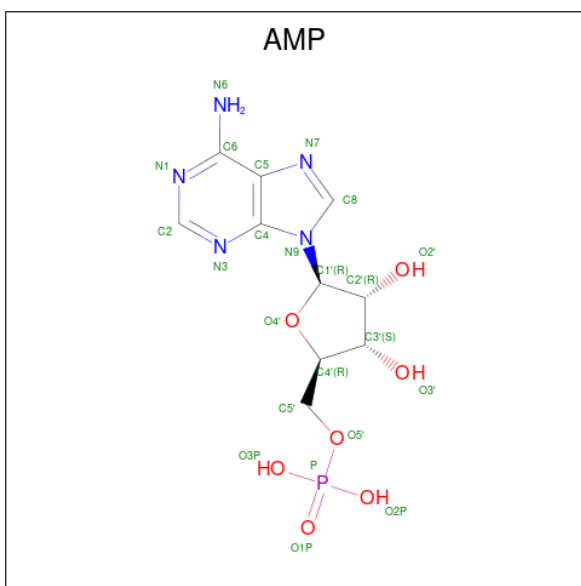
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: C₁₀H₁₂N₅O₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

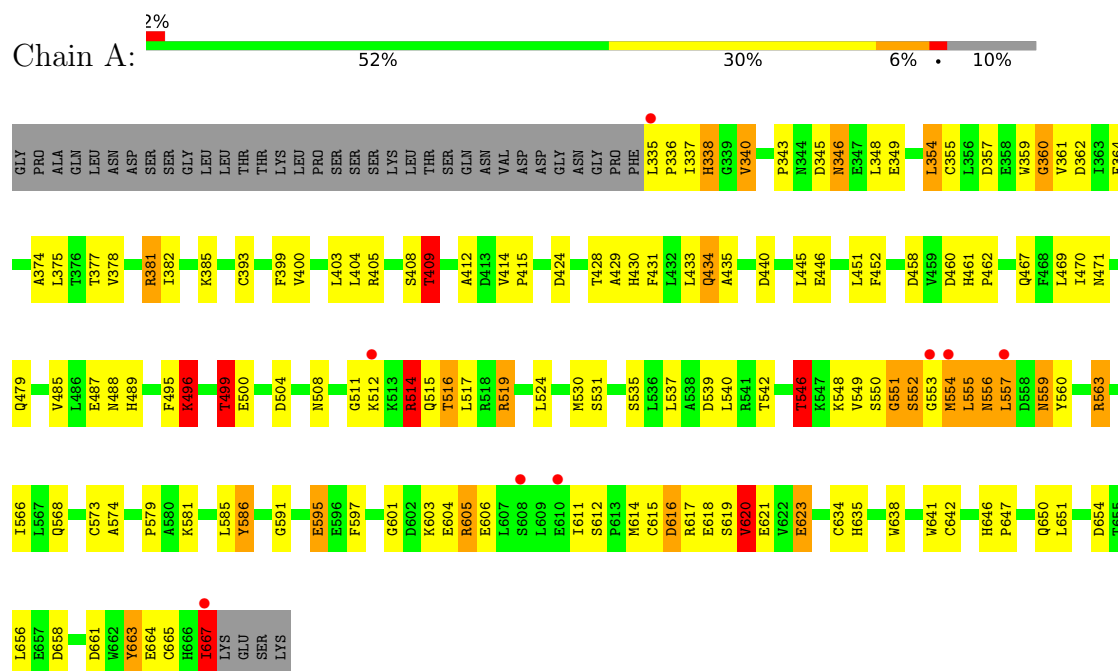
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total 34	O 34	0	0
6	B	22	Total 22	O 22	0	0

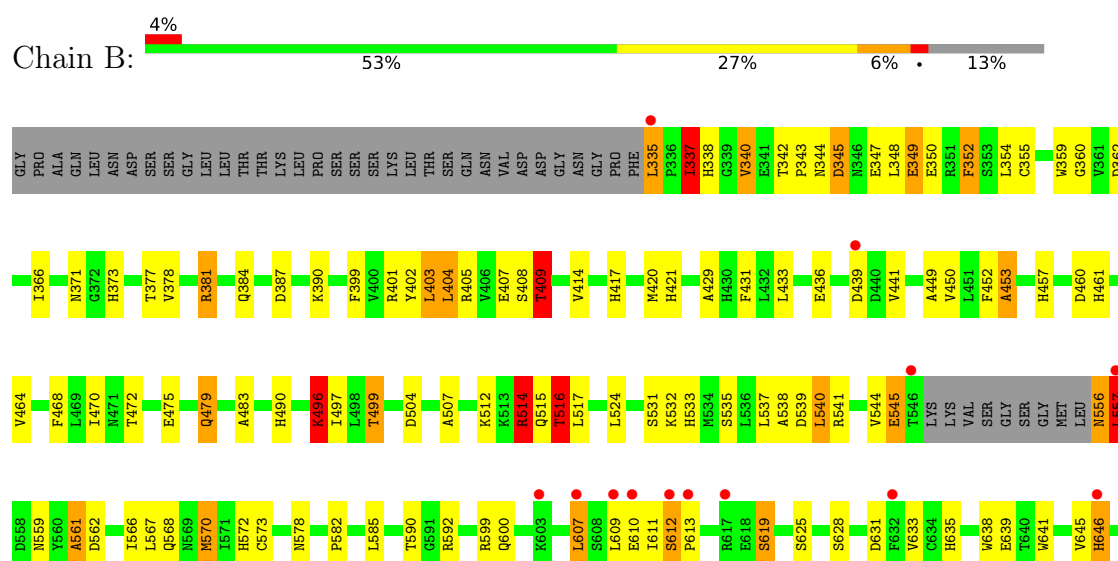
3 Residue-property plots

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

• Molecule 1: Phosphodiesterase



• Molecule 1: Phosphodiesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.55Å 81.55Å 255.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.44 – 2.04 85.29 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.44-2.04) 99.9 (85.29-2.04)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.199 , 0.233 0.205 , 0.236	Depositor DCC
R_{free} test set	3043 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5340	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	2.11	93/2737 (3.4%)	1.74	52/3720 (1.4%)
1	B	2.10	83/2616 (3.2%)	1.69	51/3562 (1.4%)
All	All	2.10	176/5353 (3.3%)	1.71	103/7282 (1.4%)

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	0	3
1	B	0	1
All	All	0	4

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	360	GLY	N-CA	13.92	1.65	1.45
1	A	360	GLY	N-CA	13.14	1.64	1.45
1	A	651	LEU	CA-C	11.37	1.68	1.52
1	A	364	PHE	N-CA	10.87	1.59	1.46
1	B	612	SER	CA-C	10.61	1.67	1.53
1	A	546	THR	CB-CG2	-9.27	1.22	1.52
1	B	344	ASN	CA-CB	9.26	1.60	1.53
1	B	661	ASP	N-CA	8.30	1.56	1.46
1	B	449	ALA	C-O	8.04	1.33	1.24
1	A	546	THR	CA-C	7.95	1.63	1.52
1	B	355	CYS	C-O	-7.95	1.13	1.24
1	B	578	ASN	N-CA	-7.84	1.39	1.46
1	B	408	SER	CA-C	7.81	1.63	1.52
1	A	616	ASP	CA-C	-7.69	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	540	LEU	CA-C	7.67	1.62	1.52
1	A	619	SER	CB-OG	-7.66	1.26	1.42
1	A	355	CYS	CA-CB	7.54	1.64	1.53
1	A	451	LEU	CA-C	7.48	1.62	1.52
1	B	612	SER	C-O	7.47	1.33	1.23
1	B	572	HIS	C-O	7.43	1.32	1.24
1	A	597	PHE	C-O	7.39	1.32	1.24
1	B	349	GLU	CA-C	7.39	1.62	1.52
1	A	499	THR	N-CA	7.28	1.55	1.46
1	B	613	PRO	N-CA	7.18	1.55	1.47
1	B	646	HIS	N-CA	7.14	1.56	1.46
1	B	561	ALA	C-O	7.12	1.32	1.24
1	A	470	ILE	CA-C	7.11	1.61	1.52
1	B	362	ASP	CA-C	7.00	1.61	1.53
1	A	360	GLY	C-O	-6.96	1.14	1.23
1	A	586	TYR	CA-C	6.95	1.61	1.52
1	A	462	PRO	N-CA	6.91	1.52	1.47
1	B	659	ASN	C-O	6.87	1.32	1.24
1	A	621	GLU	C-O	6.76	1.31	1.24
1	A	495	PHE	CA-C	6.75	1.61	1.52
1	A	424	ASP	N-CA	6.74	1.54	1.46
1	B	342	THR	N-CA	6.71	1.50	1.46
1	A	654	ASP	C-O	-6.70	1.16	1.24
1	B	499	THR	N-CA	6.69	1.55	1.46
1	B	625	SER	C-O	-6.66	1.16	1.24
1	B	657	GLU	N-CA	6.62	1.54	1.46
1	B	490	HIS	N-CA	-6.60	1.38	1.46
1	B	612	SER	CB-OG	6.59	1.55	1.42
1	B	515	GLN	N-CA	6.58	1.54	1.46
1	A	414	VAL	CA-C	6.56	1.59	1.52
1	B	352	PHE	C-O	-6.54	1.16	1.24
1	B	514	ARG	CZ-NH1	6.53	1.41	1.32
1	A	343	PRO	C-O	-6.49	1.15	1.24
1	A	642	CYS	CA-C	6.47	1.61	1.52
1	A	462	PRO	C-O	-6.47	1.15	1.24
1	B	499	THR	CB-CG2	-6.47	1.31	1.52
1	A	591	GLY	N-CA	6.46	1.54	1.45
1	A	415	PRO	CA-C	6.44	1.61	1.52
1	B	650	GLN	C-O	6.43	1.31	1.24
1	A	618	GLU	CA-CB	6.41	1.64	1.53
1	A	382	ILE	N-CA	6.41	1.54	1.46
1	B	609	LEU	N-CA	6.40	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	638	TRP	N-CA	6.39	1.54	1.46
1	B	373	HIS	CA-C	6.35	1.61	1.53
1	A	548	LYS	N-CA	6.23	1.53	1.46
1	A	362	ASP	CA-C	6.22	1.60	1.53
1	B	545	GLU	C-O	-6.18	1.16	1.24
1	A	552	SER	CA-C	-6.16	1.45	1.52
1	B	612	SER	CA-CB	6.15	1.61	1.53
1	B	599	ARG	N-CA	6.13	1.53	1.46
1	A	551	GLY	N-CA	6.13	1.54	1.45
1	A	658	ASP	C-O	-6.13	1.17	1.24
1	B	453	ALA	C-O	6.12	1.31	1.24
1	B	439	ASP	CA-C	6.08	1.60	1.52
1	A	556	ASN	N-CA	6.08	1.53	1.46
1	B	635	HIS	CA-C	6.04	1.59	1.52
1	B	420	MET	N-CA	6.04	1.53	1.46
1	A	496	LYS	N-CA	6.01	1.53	1.46
1	A	566	ILE	N-CA	-6.00	1.39	1.46
1	A	661	ASP	C-O	-5.98	1.17	1.24
1	B	387	ASP	N-CA	5.98	1.54	1.46
1	B	348	LEU	N-CA	-5.96	1.39	1.46
1	A	375	LEU	N-CA	-5.94	1.39	1.46
1	A	614	MET	N-CA	-5.93	1.38	1.46
1	B	639	GLU	C-O	5.92	1.31	1.24
1	A	623	GLU	N-CA	-5.91	1.39	1.46
1	A	458	ASP	N-CA	5.91	1.53	1.46
1	A	557	LEU	CA-C	5.88	1.60	1.52
1	B	461	HIS	CA-C	5.88	1.59	1.53
1	A	431	PHE	C-O	-5.88	1.17	1.24
1	A	434	GLN	C-O	-5.87	1.16	1.24
1	A	603	LYS	C-O	5.86	1.30	1.24
1	B	377	THR	N-CA	5.86	1.53	1.46
1	A	428	THR	N-CA	-5.84	1.39	1.46
1	B	359	TRP	N-CA	5.83	1.53	1.46
1	A	361	VAL	C-N	-5.82	1.26	1.33
1	B	340	VAL	CA-C	-5.81	1.45	1.52
1	B	585	LEU	N-CA	5.79	1.53	1.46
1	A	434	GLN	CD-NE2	-5.79	1.21	1.33
1	A	429	ALA	C-O	5.79	1.30	1.24
1	A	563	ARG	CA-C	5.78	1.60	1.52
1	A	537	LEU	CA-C	5.78	1.60	1.52
1	A	374	ALA	CA-CB	-5.78	1.44	1.53
1	B	613	PRO	CA-C	5.77	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	559	ASN	CA-C	5.77	1.59	1.52
1	A	658	ASP	CA-C	5.71	1.60	1.52
1	A	460	ASP	CA-C	-5.70	1.45	1.52
1	B	628	SER	CA-C	5.69	1.60	1.52
1	A	537	LEU	C-O	-5.68	1.17	1.24
1	A	487	GLU	N-CA	5.66	1.53	1.46
1	A	604	GLU	C-O	5.66	1.30	1.24
1	B	360	GLY	C-O	-5.65	1.16	1.23
1	B	483	ALA	CA-C	5.64	1.59	1.52
1	B	538	ALA	CA-C	5.62	1.60	1.52
1	A	647	PRO	N-CA	5.62	1.56	1.47
1	A	606	GLU	C-O	-5.61	1.17	1.24
1	A	551	GLY	C-O	-5.60	1.16	1.24
1	A	377	THR	N-CA	5.59	1.53	1.46
1	B	452	PHE	C-O	5.58	1.30	1.24
1	B	421	HIS	CA-C	-5.58	1.45	1.52
1	A	552	SER	N-CA	5.57	1.53	1.46
1	B	573	CYS	N-CA	5.57	1.53	1.46
1	B	660	ARG	N-CA	5.57	1.52	1.46
1	B	345	ASP	CA-C	5.57	1.59	1.52
1	A	378	VAL	CA-CB	-5.56	1.47	1.54
1	B	378	VAL	N-CA	-5.56	1.39	1.46
1	B	468	PHE	C-O	5.55	1.30	1.24
1	A	489	HIS	N-CA	5.53	1.53	1.46
1	A	469	LEU	N-CA	5.53	1.53	1.46
1	B	610	GLU	N-CA	5.52	1.53	1.46
1	A	620	VAL	C-O	-5.51	1.18	1.24
1	B	504	ASP	CB-CG	5.48	1.65	1.52
1	B	350	GLU	CA-C	5.48	1.60	1.52
1	B	429	ALA	N-CA	5.47	1.52	1.46
1	B	535	SER	CA-C	5.46	1.59	1.52
1	B	590	THR	N-CA	5.43	1.53	1.46
1	A	381	ARG	CA-C	5.42	1.59	1.52
1	B	436	GLU	C-O	5.41	1.30	1.24
1	B	483	ALA	CA-CB	5.41	1.60	1.53
1	B	609	LEU	CA-C	5.40	1.60	1.53
1	A	635	HIS	N-CA	-5.39	1.38	1.46
1	A	617	ARG	CZ-NH2	-5.37	1.26	1.33
1	B	408	SER	CA-CB	5.37	1.62	1.53
1	A	445	LEU	C-O	-5.34	1.17	1.24
1	A	519	ARG	N-CA	5.33	1.52	1.46
1	A	646	HIS	C-O	-5.33	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	THR	CA-CB	5.31	1.61	1.53
1	B	401	ARG	C-O	-5.28	1.18	1.24
1	B	402	TYR	CZ-OH	5.26	1.49	1.38
1	B	431	PHE	N-CA	-5.25	1.40	1.46
1	A	554	MET	CA-C	5.22	1.59	1.52
1	A	511	GLY	C-O	-5.21	1.17	1.23
1	A	357	ASP	CA-C	-5.18	1.45	1.52
1	B	568	GLN	CA-C	-5.17	1.46	1.52
1	A	574	ALA	C-O	5.17	1.30	1.24
1	B	475	GLU	CA-C	5.16	1.59	1.52
1	B	633	VAL	N-CA	5.16	1.52	1.46
1	B	347	GLU	CA-C	5.14	1.59	1.52
1	B	567	LEU	CA-CB	-5.14	1.44	1.53
1	A	364	PHE	C-O	-5.12	1.18	1.24
1	A	616	ASP	N-CA	-5.12	1.39	1.46
1	A	336	PRO	CA-C	5.11	1.59	1.52
1	B	407	GLU	CA-C	-5.10	1.46	1.52
1	A	433	LEU	N-CA	5.10	1.53	1.46
1	A	585	LEU	CA-C	-5.10	1.46	1.52
1	A	546	THR	CA-CB	5.09	1.61	1.53
1	B	460	ASP	C-O	-5.09	1.16	1.23
1	B	533	HIS	CA-C	5.08	1.59	1.52
1	B	663	TYR	N-CA	5.07	1.52	1.46
1	A	535	SER	C-O	-5.07	1.18	1.24
1	A	429	ALA	CA-C	5.06	1.59	1.52
1	B	362	ASP	CG-OD2	-5.05	1.15	1.25
1	A	452	PHE	C-O	5.05	1.29	1.24
1	A	531	SER	N-CA	-5.04	1.39	1.46
1	A	656	LEU	C-O	5.04	1.30	1.24
1	B	362	ASP	CA-CB	5.04	1.59	1.52
1	A	488	ASN	C-O	5.04	1.30	1.24
1	B	631	ASP	C-O	5.01	1.30	1.24
1	A	568	GLN	CD-OE1	-5.01	1.14	1.23
1	A	461	HIS	N-CA	5.00	1.51	1.45
1	A	560	TYR	C-O	-5.00	1.18	1.24
1	A	650	GLN	CA-CB	5.00	1.61	1.53

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	612	SER	CB-CA-C	9.55	129.99	110.31
1	B	340	VAL	CB-CA-C	-9.44	96.28	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	TRP	CA-C-N	-9.32	103.15	121.41
1	A	359	TRP	C-N-CA	-9.32	103.15	121.41
1	B	408	SER	CA-CB-OG	-9.30	92.50	111.10
1	A	530	MET	N-CA-C	9.04	123.32	111.75
1	B	359	TRP	CA-C-N	-8.74	104.29	121.41
1	B	359	TRP	C-N-CA	-8.74	104.29	121.41
1	A	646	HIS	CA-C-O	-8.23	112.01	119.75
1	B	359	TRP	O-C-N	-8.03	114.07	123.22
1	A	619	SER	CB-CA-C	-8.03	96.11	110.23
1	B	337	ILE	CB-CA-C	-7.74	99.72	112.26
1	B	665	CYS	N-CA-C	7.72	120.67	111.33
1	A	514	ARG	CG-CD-NE	-7.50	95.50	112.00
1	A	499	THR	CB-CA-C	-7.47	98.34	110.74
1	A	440	ASP	N-CA-C	7.40	121.65	112.47
1	A	563	ARG	N-CA-CB	-7.17	99.25	109.94
1	A	461	HIS	CA-C-N	-7.16	112.78	120.94
1	A	461	HIS	C-N-CA	-7.16	112.78	120.94
1	B	404	LEU	CB-CG-CD1	7.10	132.01	110.70
1	B	651	LEU	CA-CB-CG	7.10	141.15	116.30
1	A	552	SER	N-CA-C	-7.01	97.81	108.96
1	A	620	VAL	N-CA-C	6.71	119.29	109.63
1	A	524	LEU	N-CA-C	6.70	118.37	111.14
1	B	655	THR	N-CA-C	-6.67	103.48	111.69
1	B	592	ARG	NE-CZ-NH2	-6.66	113.20	119.20
1	B	496	LYS	N-CA-C	-6.64	104.12	111.82
1	A	555	LEU	CA-C-O	-6.63	113.30	120.92
1	B	499	THR	CA-CB-CG2	6.61	121.74	110.50
1	B	592	ARG	N-CA-C	6.55	118.08	111.07
1	A	408	SER	CB-CA-C	-6.52	98.57	110.63
1	B	649	ALA	CA-C-O	6.46	126.23	119.51
1	A	605	ARG	CD-NE-CZ	6.43	133.41	124.40
1	A	359	TRP	O-C-N	-6.42	114.86	122.96
1	A	550	SER	CA-C-N	-6.41	111.25	122.09
1	A	550	SER	C-N-CA	-6.41	111.25	122.09
1	A	354	LEU	N-CA-C	6.39	121.27	112.90
1	B	409	THR	CB-CA-C	6.36	123.28	109.99
1	B	401	ARG	NE-CZ-NH2	-6.35	113.48	119.20
1	A	470	ILE	N-CA-C	-6.32	104.48	110.42
1	B	619	SER	N-CA-C	6.31	124.23	110.80
1	A	516	THR	N-CA-CB	6.28	120.02	110.28
1	A	634	CYS	N-CA-C	6.16	117.80	111.14
1	A	409	THR	CB-CA-C	6.12	121.98	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	GLY	N-CA-C	6.10	123.45	115.40
1	A	338	HIS	N-CA-C	6.03	119.69	112.93
1	B	470	ILE	CA-C-O	-5.99	114.72	120.95
1	B	403	LEU	CB-CG-CD1	-5.93	92.89	110.70
1	B	514	ARG	NE-CZ-NH1	5.90	127.40	121.50
1	A	512	LYS	N-CA-C	-5.89	104.99	111.82
1	A	560	TYR	N-CA-C	-5.80	104.96	111.28
1	B	340	VAL	CG1-CB-CG2	5.78	123.51	110.80
1	B	401	ARG	CG-CD-NE	-5.77	99.31	112.00
1	A	663	TYR	N-CA-C	5.76	118.30	111.33
1	B	441	VAL	N-CA-C	5.75	116.76	111.81
1	A	430	HIS	CA-C-N	5.73	127.89	120.44
1	A	430	HIS	C-N-CA	5.73	127.89	120.44
1	A	665	CYS	N-CA-C	5.72	119.07	111.75
1	B	540	LEU	N-CA-C	-5.71	104.98	111.14
1	A	546	THR	CA-CB-CG2	5.70	120.20	110.50
1	B	504	ASP	N-CA-CB	5.68	118.76	110.58
1	A	340	VAL	CB-CA-C	-5.68	103.65	111.49
1	A	623	GLU	N-CA-C	-5.66	105.02	111.14
1	A	667	ILE	CB-CG1-CD1	5.66	125.69	113.80
1	B	409	THR	CA-CB-OG1	5.64	118.06	109.60
1	A	612	SER	N-CA-C	5.63	122.26	109.81
1	B	479	GLN	N-CA-C	5.63	117.42	111.28
1	A	485	VAL	N-CA-C	5.61	116.06	110.23
1	B	516	THR	N-CA-CB	5.60	118.92	110.30
1	B	499	THR	OG1-CB-CG2	5.57	120.45	109.30
1	B	409	THR	OG1-CB-CG2	5.56	120.41	109.30
1	B	654	ASP	N-CA-C	5.48	117.25	111.28
1	B	381	ARG	NE-CZ-NH2	-5.44	114.30	119.20
1	A	620	VAL	CG1-CB-CG2	5.44	122.77	110.80
1	A	641	TRP	N-CA-C	-5.37	105.33	111.07
1	B	651	LEU	N-CA-CB	5.37	118.48	110.22
1	B	490	HIS	N-CA-CB	5.34	117.75	110.01
1	A	385	LYS	N-CA-CB	5.30	118.39	110.22
1	B	535	SER	CA-CB-OG	-5.30	100.50	111.10
1	B	343	PRO	CA-C-N	-5.29	112.19	122.62
1	B	343	PRO	C-N-CA	-5.29	112.19	122.62
1	B	570	MET	N-CA-C	5.29	116.73	111.07
1	A	539	ASP	N-CA-CB	5.26	117.86	110.12
1	B	631	ASP	O-C-N	5.26	128.14	122.15
1	B	599	ARG	CA-C-N	5.24	127.25	120.44
1	B	599	ARG	C-N-CA	5.24	127.25	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	GLN	CB-CA-C	-5.22	102.13	110.79
1	B	531	SER	CA-CB-OG	-5.21	100.67	111.10
1	A	642	CYS	CA-C-N	5.21	127.26	120.28
1	A	642	CYS	C-N-CA	5.21	127.26	120.28
1	A	337	ILE	N-CA-CB	5.21	116.98	110.47
1	B	612	SER	N-CA-CB	-5.16	103.17	110.04
1	B	612	SER	N-CA-C	-5.15	101.53	109.87
1	A	496	LYS	CB-CA-C	-5.14	102.81	110.88
1	B	514	ARG	CD-NE-CZ	5.13	131.58	124.40
1	B	611	ILE	CB-CA-C	-5.12	102.89	111.29
1	A	595	GLU	CB-CG-CD	5.11	121.29	112.60
1	B	337	ILE	N-CA-CB	5.10	120.00	110.77
1	A	412	ALA	N-CA-C	5.09	118.60	112.38
1	A	511	GLY	N-CA-C	5.08	118.78	112.64
1	A	348	LEU	N-CA-C	-5.07	105.46	111.69
1	A	554	MET	O-C-N	-5.04	117.30	123.19
1	B	414	VAL	CB-CA-C	5.01	116.54	110.78

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	THR	Peptide
1	A	551	GLY	Peptide
1	A	605	ARG	Sidechain
1	B	619	SER	Peptide

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	2677	0	2578	39	0
1	B	2558	0	2426	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	11	2	0
5	B	23	0	12	2	0
6	A	34	0	0	1	1
6	B	22	0	0	1	0
All	All	5340	0	5027	79	1

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 8.

All (79) 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)
4:A:703:CMC:H2	4:A:703:CMC:C2	0.97	1.48
1:B:405:ARG:O	1:B:409:THR:HG23	1.81	0.81
1:B:349:GLU:OE2	1:B:381:ARG:NH2	2.15	0.78
1:A:405:ARG:O	1:A:409:THR:HG23	1.83	0.78
1:A:611:ILE:HG21	1:A:616:ASP:HB2	1.71	0.73
1:B:559:ASN:HD21	1:B:562:ASP:CG	1.98	0.72
1:A:542:THR:O	1:A:546:THR:HG23	1.91	0.70
1:A:446:GLU:OE1	1:A:563:ARG:NH1	2.25	0.69
1:B:559:ASN:ND2	1:B:562:ASP:H	1.90	0.69
1:B:399:PHE:CE2	1:B:403:LEU:HD11	2.31	0.66
1:A:664:GLU:O	1:A:667:ILE:HG13	1.95	0.65
1:B:417:HIS:NE2	5:B:703:AMP:O1P	2.30	0.64
1:B:556:ASN:ND2	1:B:556:ASN:C	2.55	0.63
1:A:400:VAL:O	1:A:404:LEU:HD23	1.98	0.63
1:A:552:SER:O	1:A:552:SER:OG	2.18	0.61
1:A:499:THR:HG22	1:A:500:GLU:HA	1.83	0.60
1:B:496:LYS:O	1:B:499:THR:HB	2.01	0.59
1:B:335:LEU:C	1:B:335:LEU:HD13	2.28	0.58
1:A:399:PHE:CE2	1:A:403:LEU:HD11	2.39	0.58
1:A:496:LYS:O	1:A:499:THR:HB	2.04	0.57
5:B:703:AMP:P	6:B:801:HOH:O	2.62	0.57
1:B:556:ASN:HD22	1:B:557:LEU:N	2.02	0.56
1:A:479:GLN:NE2	1:B:479:GLN:CD	2.63	0.56
1:A:517:LEU:C	1:A:517:LEU:HD23	2.31	0.54
1:B:607:LEU:HD23	1:B:607:LEU:O	2.09	0.52
1:A:616:ASP:O	1:A:620:VAL:HG13	2.09	0.52
1:A:504:ASP:OD2	1:A:514:ARG:NH2	2.44	0.51
1:B:399:PHE:CE2	1:B:403:LEU:CD1	2.93	0.51
1:B:433:LEU:HD23	1:B:570:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HD22	1:B:566:ILE:HD11	1.95	0.49
1:A:405:ARG:O	1:A:409:THR:CG2	2.55	0.49
1:B:399:PHE:CZ	1:B:403:LEU:HD11	2.48	0.49
1:B:337:ILE:HD11	1:B:345:ASP:HB3	1.95	0.49
1:A:346:ASN:H	1:A:346:ASN:HD22	1.61	0.47
1:A:611:ILE:CG2	1:A:616:ASP:HB2	2.43	0.47
1:B:650:GLN:HE21	1:B:654:ASP:CG	2.22	0.47
1:B:559:ASN:HD21	1:B:562:ASP:CB	2.28	0.47
1:A:579:PRO:HA	1:A:586:TYR:CD1	2.50	0.46
1:B:559:ASN:ND2	1:B:562:ASP:N	2.60	0.46
1:A:346:ASN:H	1:A:346:ASN:ND2	2.13	0.46
1:B:641:TRP:O	1:B:645:VAL:HG22	2.15	0.46
1:B:409:THR:HG21	1:B:497:ILE:HD11	1.97	0.46
1:B:556:ASN:C	1:B:556:ASN:HD22	2.22	0.45
1:A:552:SER:O	1:A:554:MET:N	2.49	0.45
1:B:464:VAL:HG12	1:B:600:GLN:HG3	1.96	0.45
1:A:349:GLU:OE1	1:A:381:ARG:NH2	2.49	0.45
1:A:399:PHE:CE2	1:A:403:LEU:CD1	3.00	0.45
1:B:514:ARG:HH11	1:B:514:ARG:HG2	1.80	0.45
1:A:573:CYS:HB3	1:A:638:TRP:CH2	2.52	0.45
1:A:623:GLU:HG3	1:A:663:TYR:CD1	2.52	0.44
1:B:559:ASN:HD22	1:B:561:ALA:HB3	1.82	0.44
1:B:556:ASN:ND2	1:B:557:LEU:N	2.64	0.44
1:B:512:LYS:O	1:B:516:THR:HG23	2.17	0.44
1:A:338:HIS:HE1	1:A:345:ASP:O	2.00	0.44
1:B:433:LEU:CD2	1:B:570:MET:HE1	2.47	0.44
1:B:335:LEU:C	1:B:335:LEU:CD1	2.91	0.43
1:B:337:ILE:HD13	1:B:338:HIS:CE1	2.53	0.43
1:B:650:GLN:NE2	1:B:654:ASP:OD1	2.50	0.43
1:A:446:GLU:CD	1:A:563:ARG:NH1	2.77	0.43
1:A:479:GLN:HE21	1:B:479:GLN:NE2	2.17	0.43
1:A:601:GLY:HA3	1:A:615:CYS:O	2.19	0.43
1:A:360:GLY:HA2	1:A:581:LYS:HD2	2.01	0.43
1:B:450:VAL:HA	1:B:524:LEU:HD13	2.00	0.42
1:A:552:SER:C	1:A:554:MET:H	2.28	0.42
1:B:338:HIS:HE1	1:B:345:ASP:O	2.03	0.42
1:B:556:ASN:O	1:B:557:LEU:HD23	2.19	0.42
1:A:400:VAL:O	1:A:404:LEU:CD2	2.68	0.42
1:A:667:ILE:C	1:A:667:ILE:CD1	2.93	0.42
1:A:393:CYS:HB3	1:A:508:ASN:HD22	1.85	0.41
1:A:434:GLN:O	1:A:435:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ALA:O	1:B:457:HIS:HB3	2.20	0.41
1:A:479:GLN:NE2	1:B:479:GLN:NE2	2.69	0.41
1:A:467:GLN:HG3	1:A:471:ASN:ND2	2.36	0.41
1:A:499:THR:HG22	1:A:500:GLU:CA	2.51	0.41
1:A:623:GLU:HG3	1:A:663:TYR:HD1	1.85	0.41
4:A:703:CMP:P	6:A:802:HOH:O	2.78	0.41
1:B:352:PHE:HE1	1:B:366:ILE:HD13	1.86	0.41
1:A:399:PHE:CZ	1:A:403:LEU:HD11	2.56	0.40
1:B:537:LEU:CD2	1:B:541:ARG:NH2	2.84	0.40

All (1) 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)
6:A:832:HOH:O	6:A:832:HOH:O[5_554]	1.46	0.74

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	331/371 (89%)	311 (94%)	19 (6%)	1 (0%)	36	30
1	B	320/371 (86%)	304 (95%)	12 (4%)	4 (1%)	9	3
All	All	651/742 (88%)	615 (94%)	31 (5%)	5 (1%)	16	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	GLU
1	B	507	ALA
1	A	553	GLY
1	B	557	LEU

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Mol	Chain	Res	Type
1	B	646	HIS

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	290/333 (87%)	270 (93%)	20 (7%)	14	8
1	B	270/333 (81%)	247 (92%)	23 (8%)	10	4
All	All	560/666 (84%)	517 (92%)	43 (8%)	12	6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
1	A	340	VAL
1	A	346	ASN
1	A	354	LEU
1	A	409	THR
1	A	496	LYS
1	A	514	ARG
1	A	515	GLN
1	A	516	THR
1	A	519	ARG
1	A	540	LEU
1	A	546	THR
1	A	549	VAL
1	A	555	LEU
1	A	556	ASN
1	A	557	LEU
1	A	559	ASN
1	A	595	GLU
1	A	620	VAL
1	A	667	ILE
1	B	335	LEU
1	B	337	ILE

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Mol	Chain	Res	Type
1	B	340	VAL
1	B	354	LEU
1	B	371	ASN
1	B	390	LYS
1	B	404	LEU
1	B	409	THR
1	B	472	THR
1	B	496	LYS
1	B	514	ARG
1	B	516	THR
1	B	517	LEU
1	B	532	LYS
1	B	539	ASP
1	B	540	LEU
1	B	544	VAL
1	B	556	ASN
1	B	557	LEU
1	B	582	PRO
1	B	607	LEU
1	B	612	SER
1	B	651	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	346	ASN
1	A	371	ASN
1	A	434	GLN
1	A	467	GLN
1	A	479	GLN
1	A	508	ASN
1	A	556	ASN
1	A	565	GLN
1	B	338	HIS
1	B	371	ASN
1	B	384	GLN
1	B	434	GLN
1	B	556	ASN
1	B	559	ASN
1	B	650	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
5	AMP	B	703	3,2	25,25,25	1.95	6 (24%)	37,38,38	2.05	12 (32%)
4	CMP	A	703	3,2	25,25,25	4.96	11 (44%)	37,39,39	6.63	18 (48%)

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
5	AMP	B	703	3,2	-	1/10/26/26	0/3/3/3
4	CMP	A	703	3,2	-	0/4/31/31	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	CMP	P-O3'	16.43	1.84	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	CMP	O3'-C3'	11.79	1.62	1.44
4	A	703	CMP	P-O5'	7.54	1.66	1.57
4	A	703	CMP	C8-N7	6.14	1.43	1.31
5	B	703	AMP	C5-C4	5.38	1.48	1.39
4	A	703	CMP	C2'-C3'	4.19	1.62	1.53
4	A	703	CMP	P-O1P	4.17	1.65	1.50
4	A	703	CMP	C2'-C1'	3.64	1.64	1.53
5	B	703	AMP	P-O3P	3.60	1.68	1.54
4	A	703	CMP	C5-C4	3.51	1.45	1.39
4	A	703	CMP	C1'-N9	3.23	1.55	1.46
4	A	703	CMP	O4'-C4'	3.13	1.51	1.45
4	A	703	CMP	O5'-C5'	-3.04	1.41	1.46
5	B	703	AMP	C5-C6	3.04	1.49	1.41
5	B	703	AMP	P-O1P	2.91	1.59	1.50
5	B	703	AMP	O4'-C4'	2.49	1.50	1.45
5	B	703	AMP	P-O5'	2.49	1.68	1.60

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	CMP	O3'-C3'-C2'	30.93	145.94	115.61
4	A	703	CMP	O5'-P-O3'	-14.99	85.63	105.70
4	A	703	CMP	O3'-P-O1P	9.14	129.96	110.39
4	A	703	CMP	C2'-C3'-C4'	-7.39	90.30	103.24
4	A	703	CMP	O2'-C2'-C1'	-6.56	87.50	110.10
4	A	703	CMP	O3'-C3'-C4'	6.23	115.41	110.71
4	A	703	CMP	C2'-C1'-N9	5.53	127.03	113.30
4	A	703	CMP	O2'-C2'-C3'	5.16	125.63	111.19
4	A	703	CMP	N6-C6-N1	5.02	129.56	118.38
4	A	703	CMP	N3-C2-N1	-4.75	121.39	128.58
5	B	703	AMP	C2-N1-C6	4.23	125.67	118.73
5	B	703	AMP	N3-C2-N1	-3.97	122.57	128.58
4	A	703	CMP	O2P-P-O1P	3.87	120.44	108.56
4	A	703	CMP	C2-N1-C6	3.86	125.07	118.73
4	A	703	CMP	C5-C6-N6	-3.80	113.89	123.29
5	B	703	AMP	N3-C4-N9	3.67	133.40	127.17
5	B	703	AMP	C5-C4-N3	-3.53	121.85	126.72
4	A	703	CMP	O2P-P-O5'	-3.48	98.67	107.16
5	B	703	AMP	O3'-C3'-C4'	3.08	119.92	111.08
5	B	703	AMP	O5'-P-O1P	-2.81	98.86	106.44
4	A	703	CMP	O4'-C4'-C3'	2.77	110.77	104.92
5	B	703	AMP	C2-N3-C4	2.72	118.47	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	703	AMP	C4-N9-C1'	-2.64	120.47	126.63
5	B	703	AMP	O3P-P-O5'	2.41	112.96	106.67
5	B	703	AMP	C4-N9-C8	2.40	108.25	105.74
4	A	703	CMP	C4-C5-N7	2.37	113.29	110.58
5	B	703	AMP	N6-C6-N1	2.34	123.60	118.38
4	A	703	CMP	C4-N9-C1'	-2.31	121.23	126.63
4	A	703	CMP	C2-N3-C4	2.29	117.43	111.83
5	B	703	AMP	O4'-C4'-C5'	-2.18	102.36	109.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

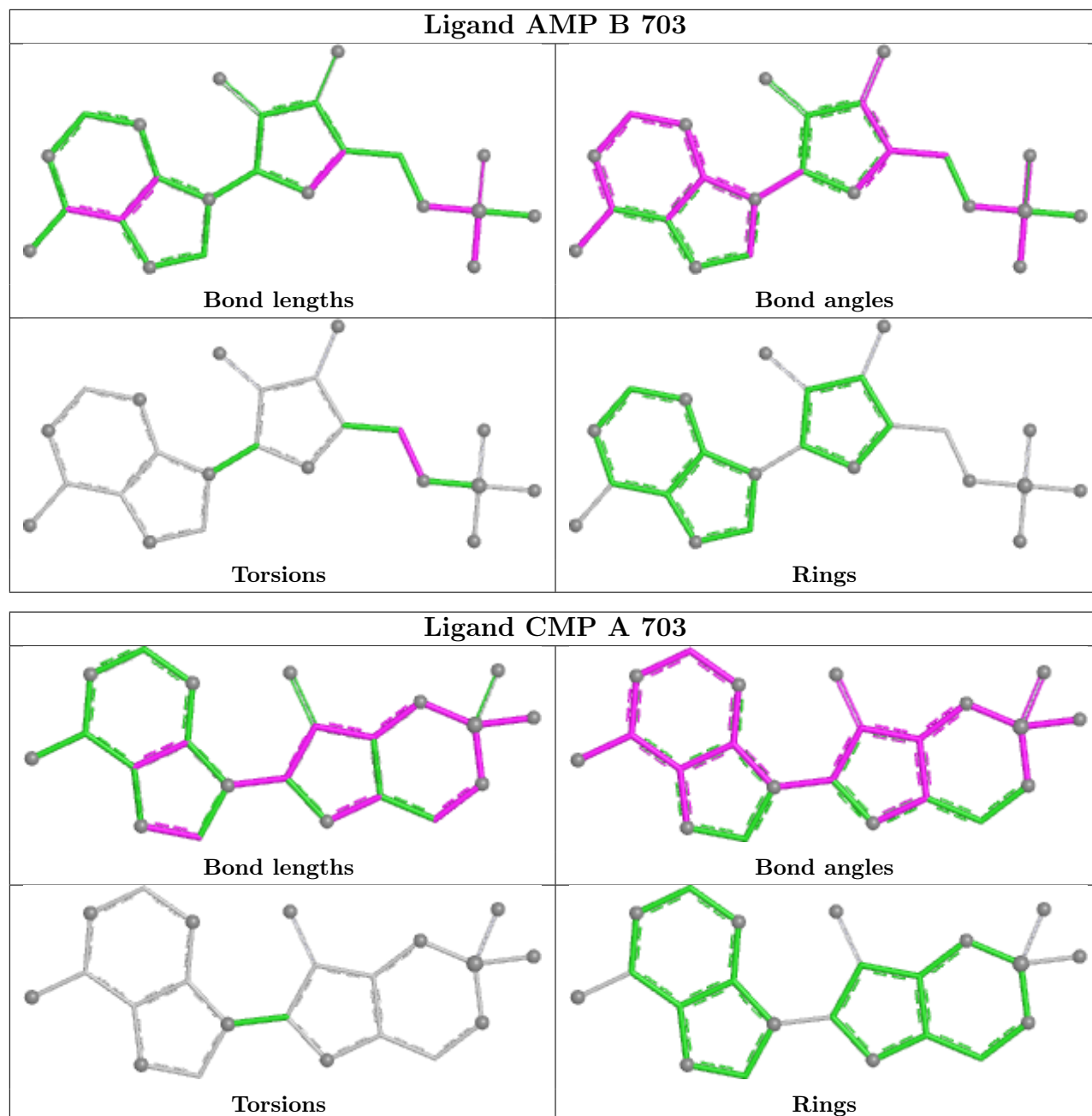
Mol	Chain	Res	Type	Atoms
5	B	703	AMP	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	703	AMP	2	0
4	A	703	CMP	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

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	333/371 (89%)	0.20	8 (2%) 59 61	37, 56, 82, 93	0
1	B	324/371 (87%)	0.40	15 (4%) 37 37	39, 61, 104, 132	0
All	All	657/742 (88%)	0.30	23 (3%) 47 48	37, 58, 92, 132	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	667	ILE	5.0
1	B	667	ILE	4.9
1	B	546	THR	4.3
1	B	335	LEU	3.4
1	B	603	LYS	3.3
1	B	610	GLU	2.8
1	B	651	LEU	2.8
1	A	553	GLY	2.7
1	B	613	PRO	2.6
1	A	554	MET	2.6
1	B	612	SER	2.6
1	A	608	SER	2.4
1	B	632	PHE	2.4
1	B	617	ARG	2.4
1	A	557	LEU	2.3
1	A	335	LEU	2.3
1	A	512	LYS	2.3
1	B	557	LEU	2.2
1	A	610	GLU	2.1
1	B	609	LEU	2.1
1	B	646	HIS	2.1
1	B	607	LEU	2.1
1	B	439	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](#)

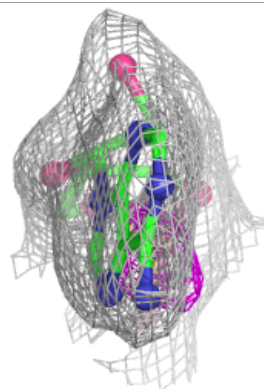
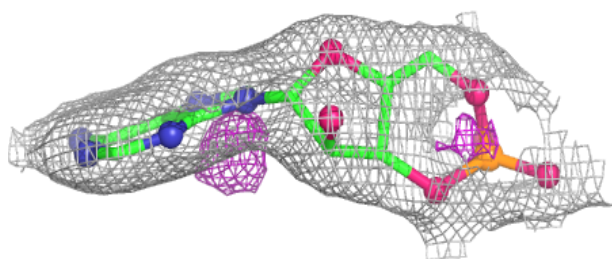
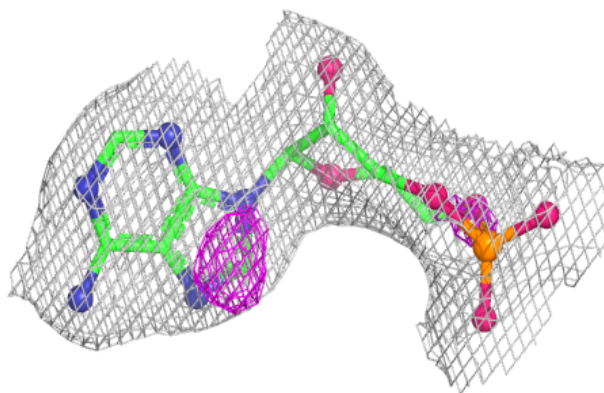
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CMP	A	703	22/22	0.95	0.08	43,51,63,69	0
5	AMP	B	703	23/23	0.97	0.07	49,64,70,71	0
3	MG	B	702	1/1	0.99	0.04	44,44,44,44	0
2	ZN	A	701	1/1	1.00	0.01	43,43,43,43	0
2	ZN	B	701	1/1	1.00	0.02	47,47,47,47	0
3	MG	A	702	1/1	1.00	0.02	40,40,40,40	0

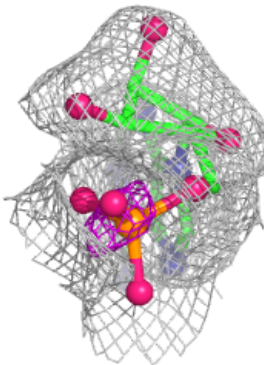
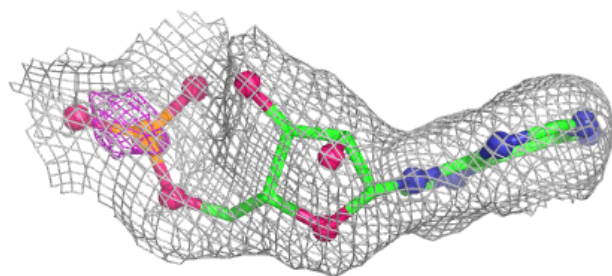
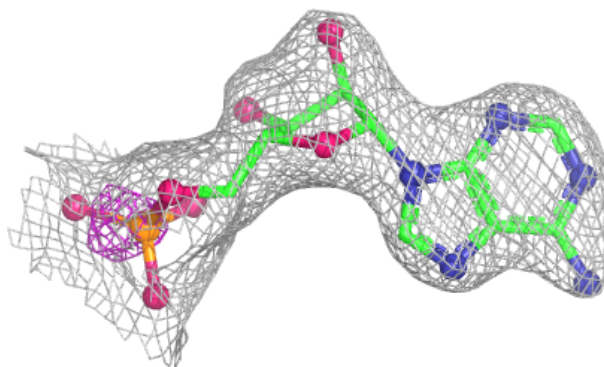
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CMP A 703:

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

**Electron density around AMP B 703:**

$2mF_o-DF_c$ (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.