Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 07:09 am GMT

PDB ID	:	6FG5
Title	:	Schistosoma mansoni Phosphodiesterase 4A
Authors	:	Brown, D.G.; Schroeder, S.; Gil, C.
Deposited on	:	2018-01-10
Resolution	:	2.35 Å(reported)

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

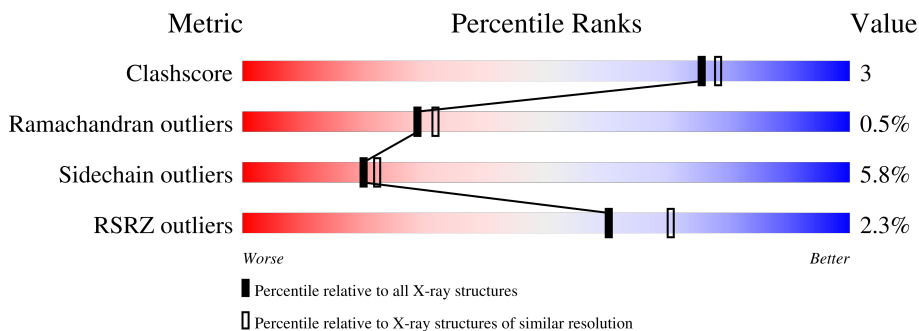|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		5.8%
RSRZ outliers		2.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

🮒 Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	370	.% 72% 16% · 10%
1	B	370	3% 71% 14% ·· 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5411 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	334	Total 2709	C 1722	N 464	O 505	S 18	0	0	0
1	B	325	Total 2643	C 1684	N 453	O 489	S 17	0	0	0

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total 35	O 35	0	0
4	B	20	Total 20	O 20	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
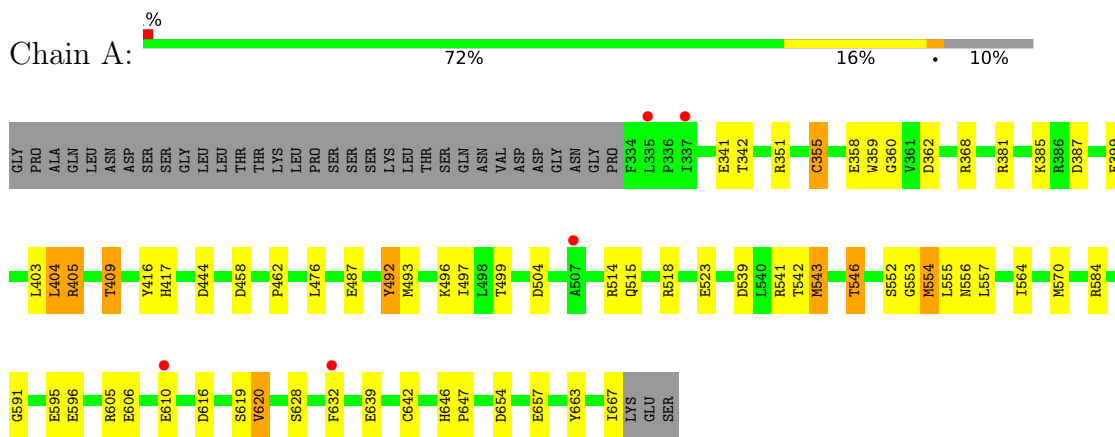
- Molecule 1: Phosphodiesterase
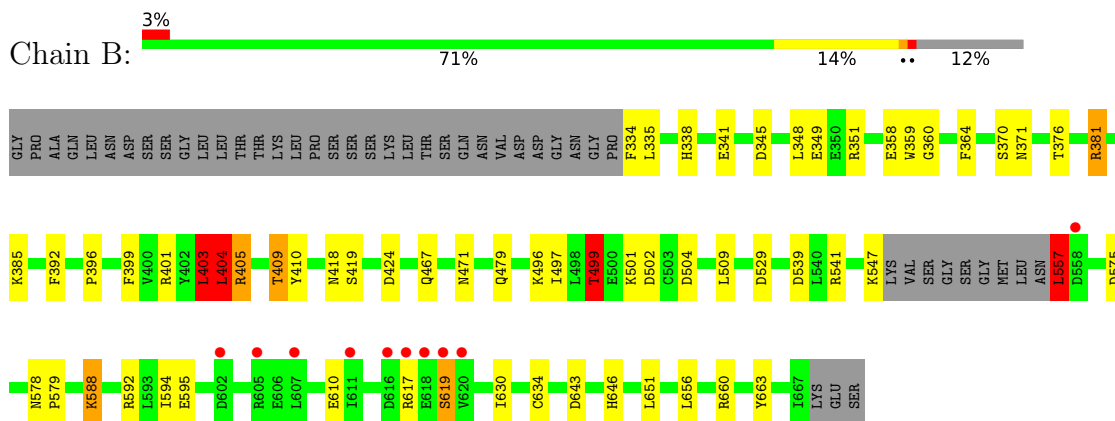
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.80Å 81.80Å 256.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.50 – 2.35 47.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.50-2.35) 96.1 (47.50-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.203 , 0.245 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5411	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, 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	1.43	22/2770 (0.8%)	1.28	22/3759 (0.6%)
1	B	1.35	13/2703 (0.5%)	1.30	23/3669 (0.6%)
All	All	1.39	35/5473 (0.6%)	1.29	45/7428 (0.6%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	GLY	N-CA	9.17	1.59	1.46
1	A	595	GLU	CD-OE2	7.68	1.34	1.25
1	A	639	GLU	CD-OE2	7.53	1.33	1.25
1	A	487	GLU	CD-OE1	-6.96	1.18	1.25
1	B	358	GLU	CG-CD	6.59	1.61	1.51
1	A	462	PRO	N-CA	6.57	1.58	1.47
1	B	341	GLU	CG-CD	6.57	1.61	1.51
1	A	663	TYR	CG-CD2	-6.41	1.30	1.39
1	B	410	TYR	CE1-CZ	6.33	1.46	1.38
1	A	595	GLU	CB-CG	6.31	1.64	1.52
1	A	610	GLU	CD-OE1	6.30	1.32	1.25
1	A	355	CYS	CB-SG	6.27	1.93	1.82
1	B	358	GLU	CD-OE1	6.21	1.32	1.25
1	A	657	GLU	CG-CD	6.08	1.61	1.51
1	B	418	ASN	C-O	6.02	1.34	1.23
1	A	362	ASP	CB-CG	5.95	1.64	1.51
1	B	419	SER	CA-CB	5.91	1.61	1.52
1	A	591	GLY	N-CA	5.82	1.54	1.46
1	B	359	TRP	CZ3-CH2	5.78	1.49	1.40
1	A	416	TYR	CZ-OH	-5.68	1.28	1.37
1	B	360	GLY	N-CA	5.55	1.54	1.46
1	B	359	TRP	CB-CG	-5.50	1.40	1.50
1	B	499	THR	C-O	-5.49	1.12	1.23
1	A	584	ARG	CZ-NH1	5.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	595	GLU	CD-OE2	5.42	1.31	1.25
1	A	654	ASP	CB-CG	5.32	1.62	1.51
1	B	341	GLU	CD-OE2	5.22	1.31	1.25
1	A	523	GLU	CD-OE1	5.21	1.31	1.25
1	A	606	GLU	CD-OE2	5.19	1.31	1.25
1	A	610	GLU	CG-CD	5.16	1.59	1.51
1	A	492	TYR	CE1-CZ	5.11	1.45	1.38
1	B	424	ASP	CB-CG	5.07	1.62	1.51
1	A	358	GLU	CD-OE2	5.06	1.31	1.25
1	A	632	PHE	CG-CD1	5.01	1.46	1.38
1	A	642	CYS	CB-SG	5.00	1.90	1.82

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	ARG	NE-CZ-NH2	-12.62	113.99	120.30
1	B	541	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	B	351	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	B	529	ASP	CB-CG-OD1	10.21	127.49	118.30
1	A	458	ASP	CB-CG-OD1	9.96	127.27	118.30
1	B	592	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	B	351	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	359	TRP	C-N-CA	-8.52	104.41	122.30
1	A	654	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	381	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	B	541	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	643	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	A	654	ASP	CB-CG-OD1	7.47	125.02	118.30
1	B	660	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	539	ASP	CB-CG-OD1	7.35	124.92	118.30
1	B	404	LEU	CB-CG-CD1	7.31	123.43	111.00
1	A	539	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	351	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	381	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	401	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	539	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	A	570	MET	CG-SD-CE	-6.66	89.55	100.20
1	B	403	LEU	CA-CB-CG	-6.50	100.34	115.30
1	A	458	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	504	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	514	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	381	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	385	LYS	CD-CE-NZ	-5.83	98.29	111.70
1	A	368	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	359	TRP	C-N-CA	-5.68	110.38	122.30
1	A	404	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	605	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	502	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	588	LYS	CD-CE-NZ	-5.48	99.09	111.70
1	B	575	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	405	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	405	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	476	LEU	CB-CG-CD2	5.31	120.03	111.00
1	B	529	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	557	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	A	518	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	444	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	B	504	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	381	ARG	CG-CD-NE	-5.03	101.25	111.80
1	A	359	TRP	O-C-N	-5.01	114.67	123.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2709	0	2637	16	0
1	B	2643	0	2568	17	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
4	A	35	0	0	2	0
4	B	20	0	0	0	0
All	All	5411	0	5205	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (33) 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:355:CYS:HB2	4:A:831:HOH:O	1.59	1.00
1:A:543:MET:HG3	1:A:555:LEU:HD21	1.69	0.75
1:B:467:GLN:HE21	1:B:471:ASN:HD21	1.35	0.72
1:B:496:LYS:O	1:B:499:THR:HB	1.97	0.65
1:A:552:SER:O	1:A:554:MET:N	2.33	0.62
1:B:557:LEU:HD23	1:B:557:LEU:N	2.16	0.61
1:B:349:GLU:OE2	1:B:381:ARG:NH2	2.26	0.57
1:B:467:GLN:HE21	1:B:471:ASN:ND2	2.03	0.56
1:A:409:THR:HG21	1:A:497:ILE:HD11	1.88	0.54
1:A:616:ASP:O	1:A:620:VAL:HG13	2.06	0.54
1:A:399:PHE:CE2	1:A:403:LEU:HD11	2.44	0.52
1:B:348:LEU:HD11	1:B:370:SER:HB3	1.96	0.48
1:B:338:HIS:HE1	1:B:345:ASP:O	1.98	0.47
1:A:355:CYS:CB	4:A:831:HOH:O	2.38	0.46
1:A:405:ARG:O	1:A:409:THR:HG22	2.15	0.46
1:A:492:TYR:CE2	1:A:493:MET:CE	2.98	0.46
1:A:496:LYS:O	1:A:499:THR:HB	2.17	0.45
1:A:542:THR:O	1:A:546:THR:HG23	2.16	0.45
1:B:335:LEU:CD2	1:B:396:PRO:HB2	2.47	0.45
1:B:364:PHE:CG	1:B:588:LYS:HE3	2.52	0.45
1:B:557:LEU:N	1:B:557:LEU:CD2	2.80	0.44
1:B:409:THR:HG21	1:B:497:ILE:HD11	2.00	0.44
1:A:543:MET:HG3	1:A:555:LEU:CD2	2.44	0.43
1:B:399:PHE:CE2	1:B:403:LEU:HD13	2.53	0.43
1:A:564:ILE:HD12	1:A:564:ILE:HA	1.88	0.42
1:B:392:PHE:HB3	1:B:509:LEU:HD11	2.01	0.41
1:B:405:ARG:O	1:B:409:THR:HG23	2.21	0.41
1:A:646:HIS:HA	1:A:647:PRO:HA	1.92	0.41
1:A:417:HIS:ND1	1:A:596:GLU:OE2	2.41	0.41
1:B:578:ASN:HB2	1:B:579:PRO:HD3	2.03	0.41
1:B:376:THR:HG21	1:B:404:LEU:HD13	2.03	0.40
1:B:630:ILE:HG23	1:B:656:LEU:HD11	2.02	0.40
1:A:492:TYR:CD2	1:A:493:MET:CE	3.04	0.40

There are no symmetry-related clashes.

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	332/370 (90%)	321 (97%)	10 (3%)	1 (0%)	41	47
1	B	321/370 (87%)	304 (95%)	15 (5%)	2 (1%)	25	27
All	All	653/740 (88%)	625 (96%)	25 (4%)	3 (0%)	29	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	GLY
1	B	619	SER
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	299/332 (90%)	283 (95%)	16 (5%)	22	25
1	B	290/332 (87%)	272 (94%)	18 (6%)	18	19
All	All	589/664 (89%)	555 (94%)	34 (6%)	20	22

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	GLU
1	A	342	THR
1	A	387	ASP

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	409	THR
1	A	515	GLN
1	A	541	ARG
1	A	543	MET
1	A	546	THR
1	A	554	MET
1	A	556	ASN
1	A	557	LEU
1	A	619	SER
1	A	620	VAL
1	A	628	SER
1	A	667	ILE
1	B	334	PHE
1	B	371	ASN
1	B	385	LYS
1	B	403	LEU
1	B	404	LEU
1	B	409	THR
1	B	479	GLN
1	B	499	THR
1	B	501	LYS
1	B	547	LYS
1	B	557	LEU
1	B	594	ILE
1	B	610	GLU
1	B	617	ARG
1	B	619	SER
1	B	634	CYS
1	B	651	LEU
1	B	663	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	565	GLN
1	B	338	HIS
1	B	371	ASN
1	B	434	GLN
1	B	471	ASN
1	B	515	GLN

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Mol	Chain	Res	Type
1	B	559	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	334/370 (90%)	-0.16	5 (1%)	73	81	35, 53, 80, 124	0
1	B	325/370 (87%)	0.01	10 (3%)	49	61	34, 56, 100, 119	0
All	All	659/740 (89%)	-0.07	15 (2%)	60	70	34, 54, 91, 124	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	607	LEU	5.0
1	B	558	ASP	3.7
1	B	620	VAL	3.2
1	B	616	ASP	3.2
1	B	611	ILE	3.1
1	A	507	ALA	2.6
1	A	337	ILE	2.4
1	B	605	ARG	2.4
1	B	618	GLU	2.4
1	B	617	ARG	2.3
1	A	335	LEU	2.3
1	A	610	GLU	2.2
1	B	602	ASP	2.1
1	A	632	PHE	2.1
1	B	619	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	702	1/1	0.87	0.06	52,52,52,52	0
3	MG	B	702	1/1	0.95	0.06	50,50,50,50	0
2	ZN	A	701	1/1	1.00	0.09	41,41,41,41	0
2	ZN	B	701	1/1	1.00	0.11	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.