



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:01 PM UTC

PDB ID : 6FG5 / pdb_00006fg5
Title : Schistosoma mansoni Phosphodiesterase 4A
Authors : Brown, D.G.; Schroeder, S.; Gil, C.
Deposited on : 2018-01-10
Resolution : 2.35 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

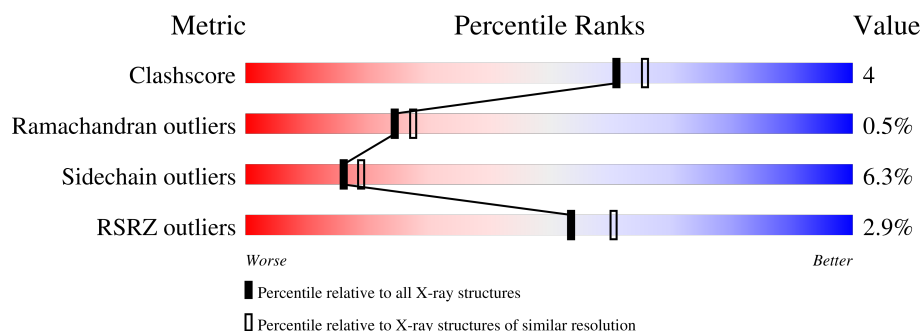
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 $\leq 5\%$. 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	370	2% 64% 24% •• 10%
1	B	370	3% 64% 20% •• 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	C	N	O	S	0	0	0
			2709	1722	464	505	18			
1	B	325	Total	C	N	O	S	0	0	0
			2643	1684	453	489	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		

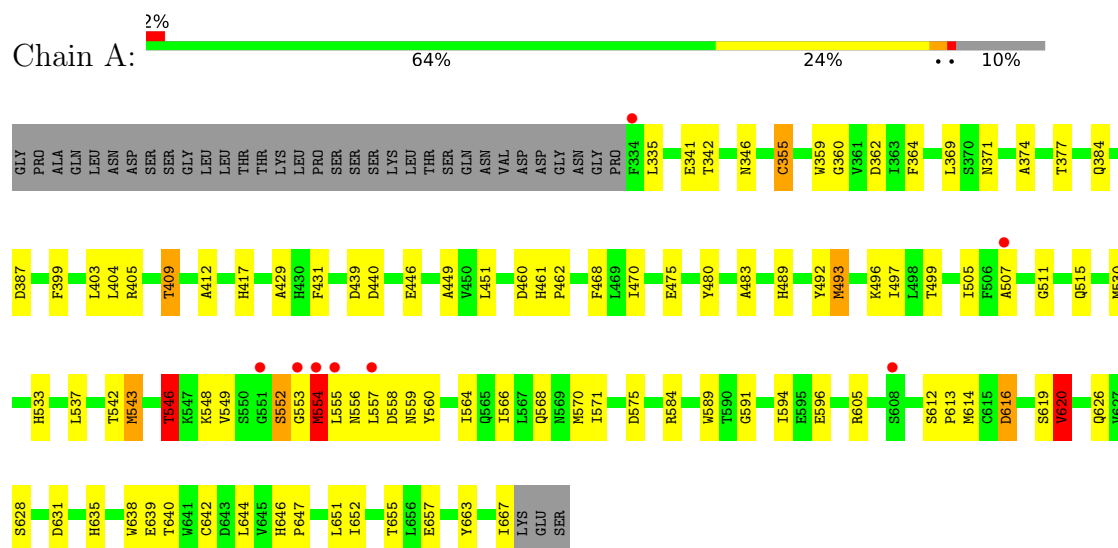
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total 35	O 35	0	0
4	B	20	Total 20	O 20	0	0

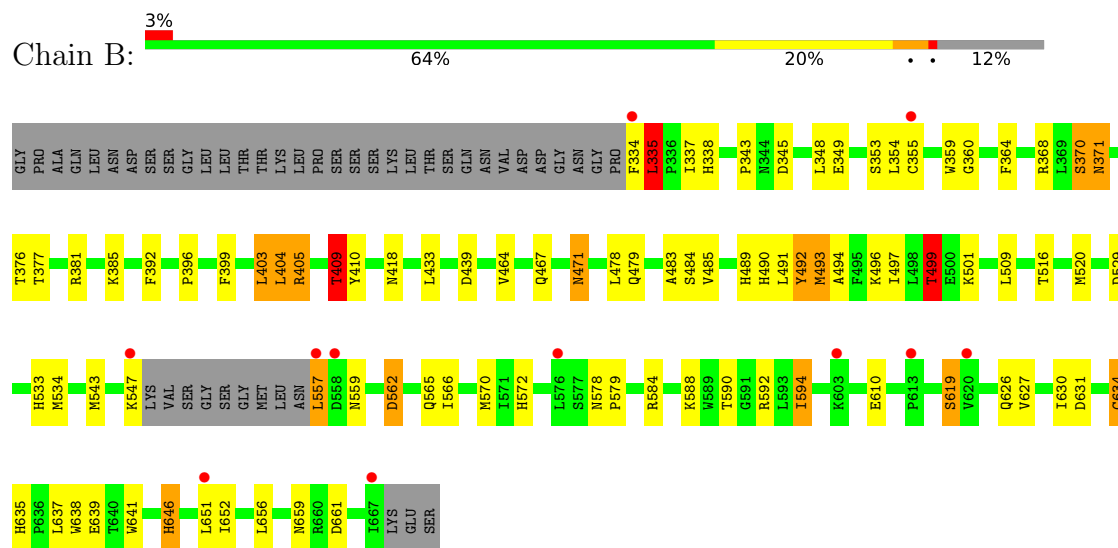
3 Residue-property plots [i](#)

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
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.203 , 0.245 (Not available) , (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)	0.32 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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

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	1.86	56/2770 (2.0%)	1.57	30/3759 (0.8%)
1	B	1.76	37/2703 (1.4%)	1.47	21/3669 (0.6%)
All	All	1.81	93/5473 (1.7%)	1.52	51/7428 (0.7%)

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	PRO	N-CA	10.86	1.58	1.47
1	A	360	GLY	N-CA	9.95	1.59	1.45
1	B	499	THR	C-O	-8.60	1.12	1.24
1	A	651	LEU	CA-C	8.40	1.64	1.52
1	B	405	ARG	CA-C	8.06	1.63	1.52
1	A	639	GLU	N-CA	-7.83	1.37	1.46
1	B	478	LEU	C-O	-7.50	1.15	1.24
1	A	480	TYR	N-CA	7.50	1.55	1.46
1	A	559	ASN	CA-C	7.36	1.62	1.52
1	B	418	ASN	C-O	7.22	1.34	1.23
1	A	355	CYS	CA-CB	7.20	1.64	1.54
1	A	470	ILE	CA-C	7.09	1.61	1.52
1	B	490	HIS	N-CA	-7.03	1.38	1.46
1	A	591	GLY	N-CA	6.95	1.54	1.45
1	A	616	ASP	N-CA	-6.92	1.37	1.46
1	A	364	PHE	N-CA	6.91	1.54	1.46
1	A	575	ASP	C-O	-6.78	1.15	1.24
1	B	485	VAL	N-CA	-6.78	1.39	1.46
1	B	631	ASP	N-CA	6.70	1.54	1.46
1	A	431	PHE	C-O	-6.68	1.16	1.24
1	A	489	HIS	N-CA	6.64	1.54	1.46
1	A	613	PRO	CA-CB	6.60	1.62	1.53
1	B	377	THR	CA-C	6.55	1.61	1.52
1	A	571	ILE	C-O	-6.51	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	PRO	C-O	-6.45	1.16	1.23
1	A	483	ALA	N-CA	6.43	1.54	1.46
1	A	589	TRP	N-CA	-6.36	1.38	1.46
1	B	661	ASP	N-CA	6.34	1.54	1.46
1	B	533	HIS	CA-C	6.34	1.61	1.52
1	A	475	GLU	CA-C	6.31	1.61	1.52
1	A	652	ILE	N-CA	-6.30	1.39	1.46
1	A	631	ASP	C-O	-6.29	1.16	1.24
1	B	360	GLY	N-CA	6.21	1.54	1.45
1	A	480	TYR	C-O	-6.18	1.15	1.24
1	A	644	LEU	C-O	6.18	1.31	1.24
1	B	464	VAL	CA-C	6.16	1.59	1.52
1	B	483	ALA	N-CA	6.14	1.53	1.46
1	A	552	SER	CA-C	-6.05	1.45	1.52
1	A	537	LEU	C-O	-5.98	1.17	1.24
1	A	360	GLY	C-O	-5.96	1.15	1.23
1	B	639	GLU	C-O	5.94	1.30	1.24
1	A	446	GLU	C-O	-5.93	1.17	1.24
1	A	384	GLN	C-O	-5.89	1.17	1.24
1	B	529	ASP	CA-C	5.83	1.60	1.52
1	B	584	ARG	N-CA	-5.81	1.38	1.46
1	B	492	TYR	N-CA	-5.81	1.39	1.46
1	B	353	SER	C-O	-5.78	1.16	1.24
1	B	471	ASN	N-CA	5.75	1.53	1.46
1	A	546	THR	CA-C	5.74	1.60	1.52
1	B	646	HIS	N-CA	5.73	1.54	1.46
1	A	507	ALA	CA-C	5.73	1.60	1.52
1	A	594	ILE	C-O	-5.65	1.17	1.24
1	A	554	MET	N-CA	5.64	1.53	1.45
1	A	369	LEU	C-O	-5.59	1.17	1.24
1	A	655	THR	N-CA	-5.57	1.39	1.46
1	A	546	THR	CA-CB	5.56	1.63	1.53
1	A	570	MET	SD-CE	-5.51	1.65	1.79
1	B	409	THR	C-O	-5.48	1.16	1.24
1	A	493	MET	SD-CE	-5.45	1.66	1.79
1	A	429	ALA	C-O	5.44	1.30	1.24
1	A	642	CYS	C-O	-5.43	1.17	1.24
1	B	343	PRO	CA-C	5.43	1.57	1.52
1	A	362	ASP	CA-C	5.42	1.59	1.53
1	B	659	ASN	C-O	5.41	1.30	1.24
1	B	637	LEU	CA-C	-5.41	1.46	1.52
1	B	354	LEU	C-O	-5.41	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	ILE	CA-C	-5.39	1.46	1.52
1	A	616	ASP	CA-C	-5.39	1.46	1.52
1	A	568	GLN	C-O	5.37	1.30	1.24
1	B	337	ILE	C-O	-5.32	1.18	1.24
1	B	572	HIS	C-O	5.31	1.30	1.24
1	A	468	PHE	C-O	-5.29	1.18	1.24
1	B	635	HIS	CA-C	5.25	1.59	1.52
1	A	584	ARG	CZ-NH1	5.25	1.40	1.32
1	B	370	SER	N-CA	-5.25	1.39	1.46
1	B	491	LEU	C-O	-5.19	1.18	1.24
1	A	612	SER	C-N	5.17	1.40	1.33
1	B	534	MET	N-CA	5.14	1.52	1.46
1	B	627	VAL	CA-C	5.14	1.59	1.52
1	A	626	GLN	CA-C	-5.14	1.46	1.52
1	A	439	ASP	C-O	5.13	1.29	1.23
1	A	449	ALA	N-CA	-5.13	1.40	1.46
1	B	652	ILE	C-O	5.13	1.29	1.24
1	A	640	THR	N-CA	-5.12	1.40	1.46
1	A	638	TRP	C-O	-5.10	1.17	1.24
1	B	484	SER	CA-C	5.09	1.59	1.53
1	B	439	ASP	N-CA	5.06	1.52	1.46
1	B	493	MET	SD-CE	-5.06	1.66	1.79
1	B	368	ARG	N-CA	-5.05	1.40	1.46
1	A	614	MET	CA-C	5.04	1.59	1.52
1	A	620	VAL	N-CA	-5.01	1.40	1.46
1	A	460	ASP	N-CA	5.01	1.53	1.46
1	A	451	LEU	CA-C	5.00	1.59	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	TRP	CA-C-N	-8.67	104.41	121.41
1	A	359	TRP	C-N-CA	-8.67	104.41	121.41
1	A	560	TYR	N-CA-C	-7.82	102.71	111.71
1	B	355	CYS	N-CA-C	7.63	122.69	113.23
1	A	461	HIS	CA-C-N	-7.50	112.31	121.00
1	A	461	HIS	C-N-CA	-7.50	112.31	121.00
1	B	641	TRP	N-CA-C	-7.33	103.23	111.14
1	A	635	HIS	CA-C-N	-6.98	111.79	119.19
1	A	635	HIS	C-N-CA	-6.98	111.79	119.19
1	A	359	TRP	O-C-N	-6.71	114.67	122.93
1	B	359	TRP	O-C-N	-6.70	115.56	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLY	N-CA-C	6.58	120.60	112.64
1	B	562	ASP	N-CA-C	6.53	119.37	111.40
1	A	657	GLU	N-CA-C	6.48	118.35	111.28
1	A	558	ASP	N-CA-C	-6.47	105.55	113.50
1	A	655	THR	N-CA-C	-6.26	104.53	111.36
1	B	409	THR	CB-CA-C	6.25	121.72	109.72
1	B	335	LEU	N-CA-C	6.23	118.45	109.48
1	B	359	TRP	N-CA-C	-6.22	100.44	110.32
1	B	634	CYS	N-CA-C	6.14	117.85	111.03
1	A	663	TYR	N-CA-C	6.12	118.75	111.71
1	B	490	HIS	N-CA-CB	6.07	118.88	110.07
1	B	635	HIS	CA-C-O	6.07	124.22	118.34
1	B	494	ALA	N-CA-C	6.03	118.34	111.11
1	A	620	VAL	N-CA-C	5.99	118.58	109.12
1	B	410	TYR	N-CA-C	-5.92	101.73	110.48
1	A	371	ASN	N-CA-C	5.91	119.79	111.52
1	B	594	ILE	N-CA-C	-5.86	104.80	110.72
1	B	592	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	A	552	SER	N-CA-C	-5.77	97.77	107.99
1	A	642	CYS	CA-C-N	5.72	128.41	120.29
1	A	642	CYS	C-N-CA	5.72	128.41	120.29
1	B	359	TRP	CA-C-N	-5.63	110.38	121.41
1	B	359	TRP	C-N-CA	-5.63	110.38	121.41
1	B	590	THR	N-CA-C	5.54	116.99	111.07
1	A	374	ALA	N-CA-C	5.47	117.68	111.11
1	A	440	ASP	N-CA-C	5.46	119.11	111.90
1	A	412	ALA	N-CA-C	5.39	117.90	111.71
1	A	377	THR	N-CA-C	5.31	116.87	111.14
1	A	605	ARG	CA-C-N	5.25	129.48	120.72
1	A	605	ARG	C-N-CA	5.25	129.48	120.72
1	A	530	MET	N-CA-C	5.21	118.42	111.75
1	A	346	ASN	N-CA-CB	5.18	117.82	110.16
1	A	591	GLY	N-CA-C	-5.17	106.52	112.73
1	B	371	ASN	N-CA-C	5.16	118.75	111.52
1	B	626	GLN	N-CA-C	5.16	116.71	111.14
1	B	638	TRP	CA-C-O	5.16	125.89	120.42
1	A	570	MET	CG-SD-CE	-5.16	89.55	100.90
1	A	533	HIS	CA-C-N	5.14	127.59	120.29
1	A	533	HIS	C-N-CA	5.14	127.59	120.29
1	B	359	TRP	N-CA-CB	-5.03	102.21	110.41

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	18	0
1	B	2643	0	2568	26	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	44	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 4.

All (44) 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:489:HIS:CE1	1:B:493:MET:HE3	2.36	0.60
1:B:492:TYR:CE2	1:B:493:MET:HE2	2.38	0.59
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:B:492:TYR:CD2	1:B:493:MET:HE2	2.41	0.55
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:433:LEU:CD2	1:B:570:MET:HE1	2.39	0.52
1:B:433:LEU:HD23	1:B:570:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:THR:HG22	1:B:520:MET:HE2	1.91	0.52
1:B:489:HIS:HE1	1:B:493:MET:HE3	1.75	0.51
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:B:543:MET:HE1	1:B:566:ILE:HG13	1.97	0.47
1:A:492:TYR:CD2	1:A:493:MET:HE2	2.50	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:B:559:ASN:HD21	1:B:562:ASP:CG	2.27	0.43
1:A:564:ILE:HD12	1:A:564:ILE:HA	1.88	0.42
1:A:543:MET:HE2	1:A:543:MET:HB2	1.92	0.41
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 [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	332/370 (90%)	321 (97%)	10 (3%)	1 (0%)	36	43
1	B	321/370 (87%)	304 (95%)	15 (5%)	2 (1%)	21	24
All	All	653/740 (88%)	625 (96%)	25 (4%)	3 (0%)	24	27

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%)	280 (94%)	19 (6%)	16	18
1	B	290/332 (87%)	272 (94%)	18 (6%)	16	19
All	All	589/664 (89%)	552 (94%)	37 (6%)	16	19

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
1	A	341	GLU
1	A	342	THR
1	A	387	ASP
1	A	404	LEU
1	A	409	THR
1	A	505	ILE
1	A	515	GLN
1	A	543	MET
1	A	546	THR
1	A	548	LYS
1	A	549	VAL
1	A	554	MET

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Mol	Chain	Res	Type
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	335	LEU
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	565	GLN
1	B	594	ILE
1	B	610	GLU
1	B	619	SER
1	B	634	CYS
1	B	651	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	384	GLN
1	A	467	GLN
1	A	471	ASN
1	A	565	GLN
1	A	626	GLN
1	B	338	HIS
1	B	371	ASN
1	B	434	GLN
1	B	467	GLN
1	B	471	ASN
1	B	559	ASN
1	B	626	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/370 (90%)	0.15	8 (2%) 59 66	35, 53, 80, 124	0
1	B	325/370 (87%)	0.23	11 (3%) 48 55	34, 56, 100, 119	0
All	All	659/740 (89%)	0.19	19 (2%) 53 60	34, 54, 91, 124	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	557	LEU	5.7
1	B	667	ILE	5.0
1	A	334	PHE	4.9
1	B	334	PHE	4.3
1	A	553	GLY	4.0
1	B	547	LYS	3.8
1	A	554	MET	3.8
1	B	651	LEU	3.7
1	A	555	LEU	3.5
1	B	613	PRO	2.8
1	A	551	GLY	2.5
1	A	608	SER	2.3
1	B	603	LYS	2.1
1	B	558	ASP	2.1
1	B	620	VAL	2.1
1	A	507	ALA	2.0
1	A	557	LEU	2.0
1	B	576	LEU	2.0
1	B	355	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	702	1/1	0.96	0.12	52,52,52,52	0
3	MG	B	702	1/1	0.97	0.14	50,50,50,50	0
2	ZN	A	701	1/1	1.00	0.02	41,41,41,41	0
2	ZN	B	701	1/1	1.00	0.03	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.