



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:39 PM UTC

PDB ID : 4AFY / pdb_00004afy
Title : Crystal structure of the FimX EAL domain in complex with reaction product pGpG
Authors : Robert-Paganin, J.; Nonin-Lecomte, S.; Rety, S.
Deposited on : 2012-01-23
Resolution : 2.01 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

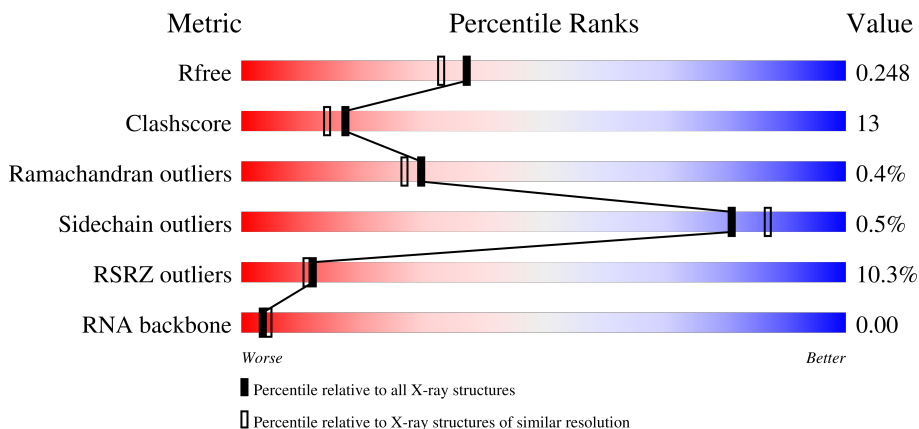
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
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)
RNA backbone	3983	1000 (2.36-1.64)

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	274	10% 70% 20% 9%
1	B	274	7% 77% 14% 8%
2	C	2	100% 50% 50%
2	D	2	100% 50% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4277 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 FIMX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	1
			1951	1253	334	360	4			
1	B	251	Total	C	N	O	S	0	0	1
			1961	1259	337	361	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	MET	-	expression tag	UNP Q02F59
A	419	GLY	-	expression tag	UNP Q02F59
A	420	SER	-	expression tag	UNP Q02F59
A	421	SER	-	expression tag	UNP Q02F59
A	422	HIS	-	expression tag	UNP Q02F59
A	423	HIS	-	expression tag	UNP Q02F59
A	424	HIS	-	expression tag	UNP Q02F59
A	425	HIS	-	expression tag	UNP Q02F59
A	426	HIS	-	expression tag	UNP Q02F59
A	427	HIS	-	expression tag	UNP Q02F59
A	428	SER	-	expression tag	UNP Q02F59
A	429	SER	-	expression tag	UNP Q02F59
A	430	GLY	-	expression tag	UNP Q02F59
A	431	LEU	-	expression tag	UNP Q02F59
A	432	VAL	-	expression tag	UNP Q02F59
A	433	PRO	-	expression tag	UNP Q02F59
A	434	ARG	-	expression tag	UNP Q02F59
A	435	GLY	-	expression tag	UNP Q02F59
A	436	SER	-	expression tag	UNP Q02F59
A	437	HIS	-	expression tag	UNP Q02F59
A	438	MET	-	expression tag	UNP Q02F59
B	418	MET	-	expression tag	UNP Q02F59
B	419	GLY	-	expression tag	UNP Q02F59
B	420	SER	-	expression tag	UNP Q02F59
B	421	SER	-	expression tag	UNP Q02F59

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	HIS	-	expression tag	UNP Q02F59
B	423	HIS	-	expression tag	UNP Q02F59
B	424	HIS	-	expression tag	UNP Q02F59
B	425	HIS	-	expression tag	UNP Q02F59
B	426	HIS	-	expression tag	UNP Q02F59
B	427	HIS	-	expression tag	UNP Q02F59
B	428	SER	-	expression tag	UNP Q02F59
B	429	SER	-	expression tag	UNP Q02F59
B	430	GLY	-	expression tag	UNP Q02F59
B	431	LEU	-	expression tag	UNP Q02F59
B	432	VAL	-	expression tag	UNP Q02F59
B	433	PRO	-	expression tag	UNP Q02F59
B	434	ARG	-	expression tag	UNP Q02F59
B	435	GLY	-	expression tag	UNP Q02F59
B	436	SER	-	expression tag	UNP Q02F59
B	437	HIS	-	expression tag	UNP Q02F59
B	438	MET	-	expression tag	UNP Q02F59

- Molecule 2 is a RNA chain called 5'-R(*GP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			
2	D	2	Total	C	N	O	P	0	0	0
			46	20	10	14	2			

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

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

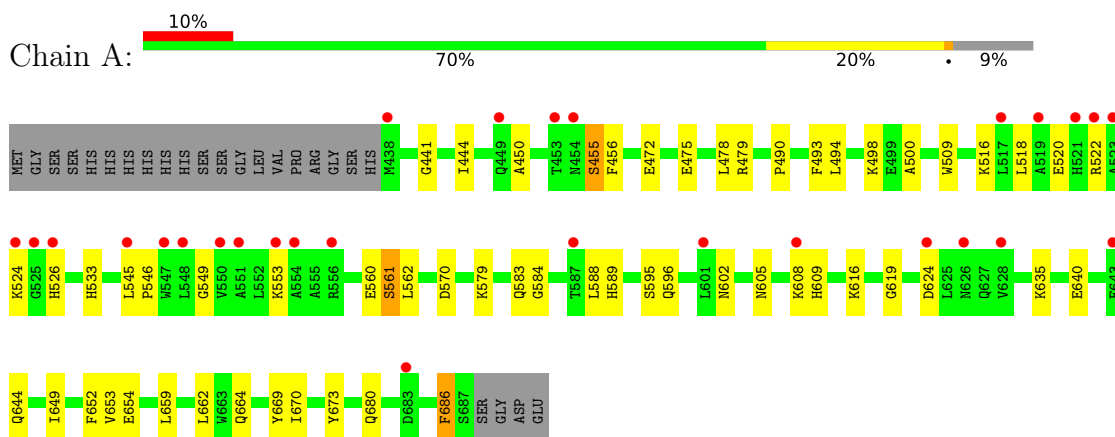
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total 136	O 136	0	0
5	B	125	Total 125	O 125	0	0
5	C	4	Total 4	O 4	0	0
5	D	3	Total 3	O 3	0	0

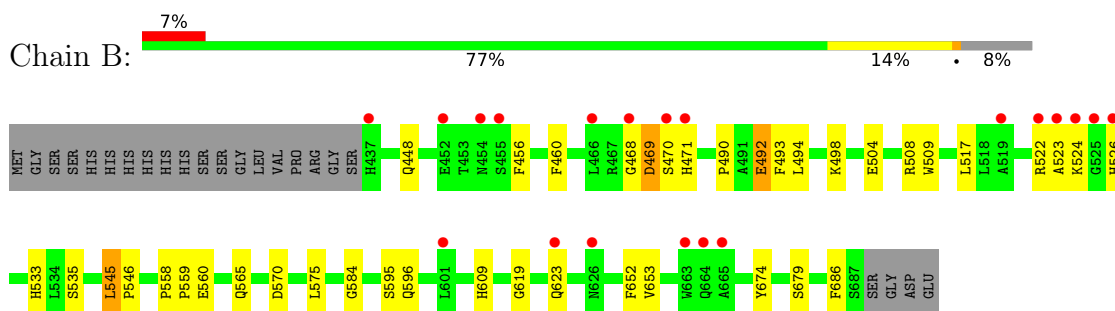
3 Residue-property plots [i](#)

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.

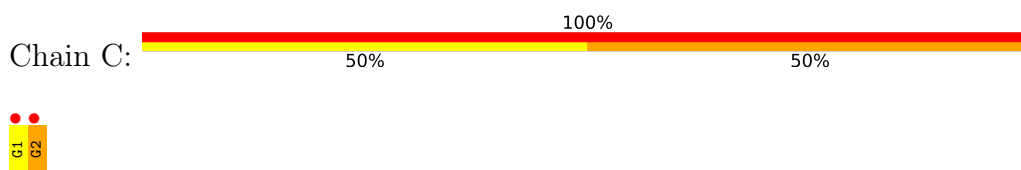
• Molecule 1: FIMX



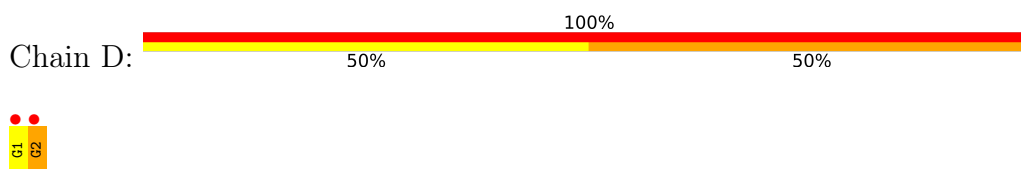
• Molecule 1: FIMX



• Molecule 2: 5'-R(*GP*GP)-3'



• Molecule 2: 5'-R(*GP*GP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.33Å 104.33Å 154.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.21 – 2.01 43.21 – 2.01	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.21-2.01) 99.9 (43.21-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 2.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.208 , 0.239 (Not available) , 0.248	Depositor DCC
R_{free} test set	2890 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4277	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, NA

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	0.85	2/1992 (0.1%)	0.90	1/2705 (0.0%)
1	B	0.83	2/2003 (0.1%)	0.90	3/2720 (0.1%)
2	C	1.08	0/51	0.78	0/78
2	D	1.18	0/51	0.76	0/78
All	All	0.85	4/4097 (0.1%)	0.90	4/5581 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	686	PHE	C-N	-6.46	1.24	1.33
1	B	686	PHE	C-N	-6.41	1.24	1.33
1	B	653	VAL	CA-C	-6.09	1.47	1.53
1	A	664	GLN	CG-CD	-5.28	1.38	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ALA	N-CA-C	-5.66	105.19	111.36
1	B	492	GLU	CA-CB-CG	5.34	124.79	114.10
1	B	545	LEU	CA-C-N	-5.05	113.84	119.19
1	B	545	LEU	C-N-CA	-5.05	113.84	119.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	HIS	Peptide

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	1951	0	1967	55	0
1	B	1961	0	1974	49	0
2	C	46	0	23	15	0
2	D	46	0	23	16	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
5	A	136	0	0	12	1
5	B	125	0	0	7	1
5	C	4	0	0	1	0
5	D	3	0	0	0	0
All	All	4277	0	3987	101	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 13.

All (101) 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:640:GLU:OE1	5:A:2104:HOH:O	1.87	0.92
1:B:468:GLY:O	5:B:2024:HOH:O	1.89	0.88
1:B:448:GLN:OE1	5:B:2010:HOH:O	1.96	0.83
1:A:560:GLU:OE2	5:A:2059:HOH:O	2.06	0.72
1:A:522:ARG:NH1	1:A:561:SER:OG	2.22	0.72
1:B:565:GLN:NE2	2:D:2:G:OP1	2.23	0.72
1:B:560:GLU:OE1	5:B:2072:HOH:O	2.07	0.72
1:B:470:SER:O	5:B:2026:HOH:O	2.08	0.70
1:A:545:LEU:HD21	1:A:584:GLY:HA3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:TYR:HB2	1:B:492:GLU:HG2	1.74	0.69
1:B:596:GLN:OE1	2:D:1:G:H2'	1.92	0.69
5:A:2045:HOH:O	1:B:623:GLN:HG3	1.93	0.69
1:B:504:GLU:OE2	1:B:508:ARG:NH1	2.26	0.69
1:A:596:GLN:OE1	2:C:1:G:H2'	1.93	0.68
1:B:595:SER:HG	2:D:2:G:HO3'	1.41	0.67
1:A:624:ASP:OD1	5:A:2091:HOH:O	2.12	0.66
1:A:475:GLU:OE2	2:C:2:G:OP1	2.13	0.66
1:A:533:HIS:CE1	2:C:2:G:H5'	2.30	0.66
1:A:619:GLY:H	2:C:1:G:H8	1.41	0.66
1:B:652:PHE:CE2	2:D:1:G:O4'	2.50	0.65
1:A:673:TYR:HB2	1:B:492:GLU:CG	2.27	0.64
1:A:533:HIS:HB3	2:C:2:G:H2'	1.78	0.64
1:A:518:LEU:CD1	1:A:562:LEU:HD13	2.28	0.63
5:B:2073:HOH:O	2:D:2:G:N2	2.27	0.63
5:A:2045:HOH:O	1:B:623:GLN:CG	2.46	0.60
1:B:595:SER:OG	2:D:2:G:O3'	2.12	0.60
1:B:533:HIS:CG	2:D:2:G:H2'	2.37	0.59
1:A:455:SER:O	5:A:2013:HOH:O	2.17	0.59
1:B:522:ARG:HE	1:B:558:PRO:HG2	1.68	0.58
1:B:619:GLY:H	2:D:1:G:H8	1.51	0.58
1:A:624:ASP:HB2	5:A:2092:HOH:O	2.03	0.58
1:A:659:LEU:C	1:A:659:LEU:HD23	2.28	0.58
1:A:498:LYS:HD2	1:B:623:GLN:NE2	2.19	0.57
1:A:456:PHE:HB3	1:A:478:LEU:HD11	1.85	0.57
1:A:570:ASP:OD2	2:C:2:G:N2	2.37	0.57
2:C:1:G:N2	5:C:2003:HOH:O	2.26	0.56
1:B:498:LYS:NZ	2:D:2:G:O6	2.38	0.55
1:A:518:LEU:HD11	1:A:562:LEU:HD13	1.87	0.55
1:A:545:LEU:HB3	1:A:546:PRO:HD3	1.86	0.55
1:A:588:LEU:O	1:A:589:HIS:HB2	2.06	0.54
1:A:533:HIS:CG	2:C:2:G:H2'	2.43	0.53
1:B:522:ARG:C	1:B:524:LYS:N	2.66	0.53
1:A:498:LYS:NZ	5:A:2044:HOH:O	2.42	0.53
1:A:602:ASN:O	5:A:2079:HOH:O	2.19	0.52
1:A:608:LYS:HG3	1:A:609:HIS:ND1	2.24	0.52
1:B:679:SER:HB3	5:B:2020:HOH:O	2.09	0.52
5:A:2045:HOH:O	1:B:623:GLN:NE2	2.23	0.51
1:B:522:ARG:C	1:B:524:LYS:H	2.18	0.51
1:B:575:LEU:O	1:B:575:LEU:HD13	2.09	0.51
1:A:653:VAL:HG22	1:A:662:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLY:O	1:B:469:ASP:C	2.53	0.50
1:A:652:PHE:CZ	2:C:1:G:H5''	2.46	0.50
1:A:616:LYS:HE2	2:C:1:G:H4'	1.93	0.50
1:B:533:HIS:CE1	2:D:2:G:H5'	2.47	0.49
1:B:533:HIS:HB3	2:D:2:G:H2'	1.94	0.49
1:A:652:PHE:CE2	2:C:1:G:O4'	2.67	0.48
1:B:570:ASP:OD2	2:D:2:G:N2	2.46	0.48
1:A:490:PRO:O	1:A:494:LEU:HG	2.14	0.48
1:B:570:ASP:OD2	2:D:2:G:C2	2.67	0.48
1:A:516:LYS:HE2	1:A:520:GLU:CD	2.39	0.48
1:A:516:LYS:HE2	1:A:520:GLU:OE2	2.14	0.48
1:A:579:LYS:O	1:A:583:GLN:HG3	2.14	0.47
1:A:524:LYS:HB2	1:A:526:HIS:CD2	2.49	0.47
1:B:575:LEU:HD11	1:B:609:HIS:HB2	1.97	0.46
1:B:524:LYS:HB2	1:B:526:HIS:HD2	1.80	0.46
1:A:441:GLY:O	1:B:674:TYR:HA	2.16	0.46
1:A:533:HIS:CB	2:C:2:G:H2'	2.45	0.45
1:B:623:GLN:HA	1:B:623:GLN:OE1	2.15	0.45
1:A:444:ILE:HG23	1:A:500:ALA:HB2	1.98	0.44
1:A:608:LYS:HG3	1:A:609:HIS:CG	2.52	0.44
1:A:680:GLN:OE1	1:A:680:GLN:N	2.43	0.44
1:A:649:ILE:HG12	1:A:669:TYR:HB2	2.00	0.44
1:B:559:PRO:C	1:B:560:GLU:HG2	2.42	0.44
1:A:472:GLU:HG2	1:A:686:PHE:CD1	2.53	0.44
1:A:493:PHE:CD1	1:A:493:PHE:C	2.95	0.44
1:A:653:VAL:HG21	1:A:670:ILE:HB	2.00	0.44
1:B:545:LEU:HB3	1:B:546:PRO:CD	2.48	0.44
1:A:635:LYS:NZ	5:A:2096:HOH:O	2.35	0.44
1:B:522:ARG:O	1:B:524:LYS:N	2.51	0.43
1:A:596:GLN:OE1	2:C:1:G:C2'	2.64	0.43
1:A:624:ASP:CB	5:A:2092:HOH:O	2.65	0.43
1:B:522:ARG:O	5:B:2054:HOH:O	2.21	0.43
1:A:619:GLY:N	2:C:1:G:H8	2.12	0.43
1:A:640:GLU:O	1:A:644:GLN:HG2	2.19	0.43
1:B:456:PHE:HB2	1:B:509:TRP:CH2	2.54	0.42
1:B:490:PRO:HA	1:B:493:PHE:CE2	2.54	0.42
1:B:460:PHE:CZ	1:B:517:LEU:HD23	2.54	0.42
1:B:460:PHE:HZ	1:B:517:LEU:HD23	1.82	0.42
1:A:549:GLY:O	1:A:553:LYS:HG2	2.19	0.42
1:B:545:LEU:HB3	1:B:546:PRO:HD3	2.02	0.42
1:B:596:GLN:OE1	2:D:1:G:C2'	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ASN:O	1:A:608:LYS:HG2	2.20	0.41
1:A:654:GLU:OE2	1:B:492:GLU:OE2	2.38	0.41
1:B:545:LEU:HD21	1:B:584:GLY:HA3	2.02	0.41
1:B:535:SER:HA	2:D:2:G:C6	2.55	0.41
1:A:478:LEU:O	1:A:479:ARG:HD3	2.20	0.41
1:A:595:SER:OG	2:C:2:G:O3'	2.22	0.41
1:A:456:PHE:HB2	1:A:509:TRP:CH2	2.55	0.41
1:B:490:PRO:O	1:B:494:LEU:HG	2.20	0.41
1:B:565:GLN:HE21	2:D:2:G:H3'	1.85	0.41
1:B:524:LYS:C	1:B:526:HIS:H	2.29	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)
5:A:2119:HOH:O	5:B:2115:HOH:O[6_545]	2.00	0.20

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	248/274 (90%)	239 (96%)	9 (4%)	0	100	100
1	B	249/274 (91%)	241 (97%)	6 (2%)	2 (1%)	16	11
All	All	497/548 (91%)	480 (97%)	15 (3%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	523	ALA
1	B	469	ASP

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	209/230 (91%)	207 (99%)	2 (1%)	68	75
1	B	210/230 (91%)	210 (100%)	0	100	100
All	All	419/460 (91%)	417 (100%)	2 (0%)	81	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	455	SER
1	A	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	GLN
1	A	495	HIS
1	A	526	HIS
1	A	623	GLN
1	B	484	GLN
1	B	540	GLN
1	B	565	GLN
1	B	580	GLN
1	B	642	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	1/2 (50%)	1 (100%)	0
2	D	1/2 (50%)	1 (100%)	0
All	All	2/4 (50%)	2 (100%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	G
2	D	2	G

There are no RNA pucker outliers to report.

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 5 ligands modelled in this entry, 5 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

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	250/274 (91%)	0.66	28 (11%) 10 9	23, 41, 66, 105	0
1	B	251/274 (91%)	0.39	20 (7%) 18 17	23, 37, 66, 97	0
2	C	2/2 (100%)	3.43	2 (100%) 0 0	58, 58, 58, 70	0
2	D	2/2 (100%)	3.13	2 (100%) 0 0	58, 58, 58, 60	0
All	All	505/552 (91%)	0.55	52 (10%) 12 11	23, 39, 67, 105	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	523	ALA	6.8
1	A	523	ALA	5.6
1	A	522	ARG	4.8
1	B	522	ARG	4.8
1	A	519	ALA	4.5
1	B	468	GLY	4.0
1	A	521	HIS	4.0
1	A	524	LYS	3.7
1	B	525	GLY	3.5
1	B	663	TRP	3.5
1	A	547	TRP	3.5
2	C	2	G	3.5
1	B	524	LYS	3.4
1	A	525	GLY	3.4
2	C	1	G	3.4
1	B	623	GLN	3.4
1	A	587	THR	3.2
2	D	1	G	3.2
1	B	470	SER	3.2
1	A	624	ASP	3.1
1	A	643	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	2	G	3.1
1	B	526	HIS	3.1
1	A	683	ASP	3.0
1	B	626	ASN	2.9
1	A	545	LEU	2.9
1	B	437	HIS	2.9
1	B	455	SER	2.8
1	A	449	GLN	2.7
1	A	626	ASN	2.7
1	B	665	ALA	2.7
1	A	628	VAL	2.6
1	B	664	GLN	2.6
1	B	601	LEU	2.6
1	A	454	ASN	2.6
1	A	550	VAL	2.5
1	A	608	LYS	2.5
1	A	601	LEU	2.4
1	A	551	ALA	2.4
1	A	526	HIS	2.4
1	B	519	ALA	2.3
1	A	517	LEU	2.3
1	B	454	ASN	2.3
1	A	554	ALA	2.2
1	A	438	MET	2.2
1	A	453	THR	2.2
1	A	548	LEU	2.2
1	B	471	HIS	2.1
1	B	452	GLU	2.1
1	B	466	LEU	2.1
1	A	556	ARG	2.1
1	A	553	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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	NA	A	803	1/1	0.93	0.12	50,50,50,50	0
3	MG	A	802	1/1	0.95	0.15	51,51,51,51	0
4	NA	A	804	1/1	0.95	0.11	39,39,39,39	0
3	MG	A	801	1/1	0.98	0.13	40,40,40,40	0
3	MG	B	801	1/1	0.98	0.14	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.