



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:52 PM UTC

PDB ID : 4IL1 / pdb_00004il1
Title : Crystal Structure of the Rat Calcineurin
Authors : Ye, Q.; Faucher, F.; Jia, Z.
Deposited on : 2012-12-28
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

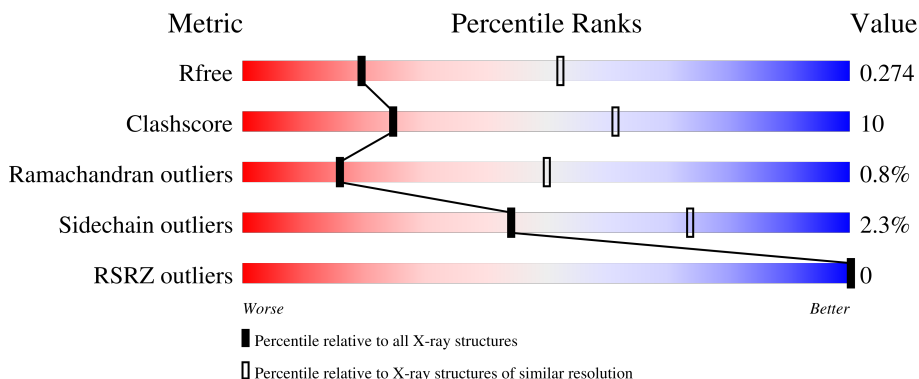
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	823	50% 13% • 36%
1	B	823	51% 12% • 36%
1	C	823	50% 13% • 36%
1	D	823	48% 14% • 36%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17255 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 Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4280	2737	718	796	29			
1	B	528	Total	C	N	O	S	0	0	0
			4277	2734	720	795	28			
1	C	529	Total	C	N	O	S	0	0	0
			4281	2739	718	796	28			
1	D	528	Total	C	N	O	S	0	0	0
			4277	2734	720	795	28			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	GLY	-	linker	UNP P62161
A	151	GLY	-	linker	UNP P62161
A	152	GLY	-	linker	UNP P62161
A	153	GLY	-	linker	UNP P62161
A	154	GLY	-	linker	UNP P62161
A	155	GLY	-	linker	UNP P62161
A	156	GLY	-	linker	UNP P62161
A	157	GLY	-	linker	UNP P62161
A	158	GLY	-	linker	UNP P62161
A	328	GLY	-	linker	UNP P63100
A	329	GLY	-	linker	UNP P63100
A	330	GLY	-	linker	UNP P63100
A	331	GLY	-	linker	UNP P63100
A	332	GLY	-	linker	UNP P63100
A	333	GLY	-	linker	UNP P63100
A	816	LEU	-	expression tag	UNP P63329
A	817	GLU	-	expression tag	UNP P63329
A	818	HIS	-	expression tag	UNP P63329
A	819	HIS	-	expression tag	UNP P63329
A	820	HIS	-	expression tag	UNP P63329

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Chain	Residue	Modelled	Actual	Comment	Reference
A	821	HIS	-	expression tag	UNP P63329
A	822	HIS	-	expression tag	UNP P63329
A	823	HIS	-	expression tag	UNP P63329
B	150	GLY	-	linker	UNP P62161
B	151	GLY	-	linker	UNP P62161
B	152	GLY	-	linker	UNP P62161
B	153	GLY	-	linker	UNP P62161
B	154	GLY	-	linker	UNP P62161
B	155	GLY	-	linker	UNP P62161
B	156	GLY	-	linker	UNP P62161
B	157	GLY	-	linker	UNP P62161
B	158	GLY	-	linker	UNP P62161
B	328	GLY	-	linker	UNP P63100
B	329	GLY	-	linker	UNP P63100
B	330	GLY	-	linker	UNP P63100
B	331	GLY	-	linker	UNP P63100
B	332	GLY	-	linker	UNP P63100
B	333	GLY	-	linker	UNP P63100
B	816	LEU	-	expression tag	UNP P63329
B	817	GLU	-	expression tag	UNP P63329
B	818	HIS	-	expression tag	UNP P63329
B	819	HIS	-	expression tag	UNP P63329
B	820	HIS	-	expression tag	UNP P63329
B	821	HIS	-	expression tag	UNP P63329
B	822	HIS	-	expression tag	UNP P63329
B	823	HIS	-	expression tag	UNP P63329
C	150	GLY	-	linker	UNP P62161
C	151	GLY	-	linker	UNP P62161
C	152	GLY	-	linker	UNP P62161
C	153	GLY	-	linker	UNP P62161
C	154	GLY	-	linker	UNP P62161
C	155	GLY	-	linker	UNP P62161
C	156	GLY	-	linker	UNP P62161
C	157	GLY	-	linker	UNP P62161
C	158	GLY	-	linker	UNP P62161
C	328	GLY	-	linker	UNP P63100
C	329	GLY	-	linker	UNP P63100
C	330	GLY	-	linker	UNP P63100
C	331	GLY	-	linker	UNP P63100
C	332	GLY	-	linker	UNP P63100
C	333	GLY	-	linker	UNP P63100
C	816	LEU	-	expression tag	UNP P63329

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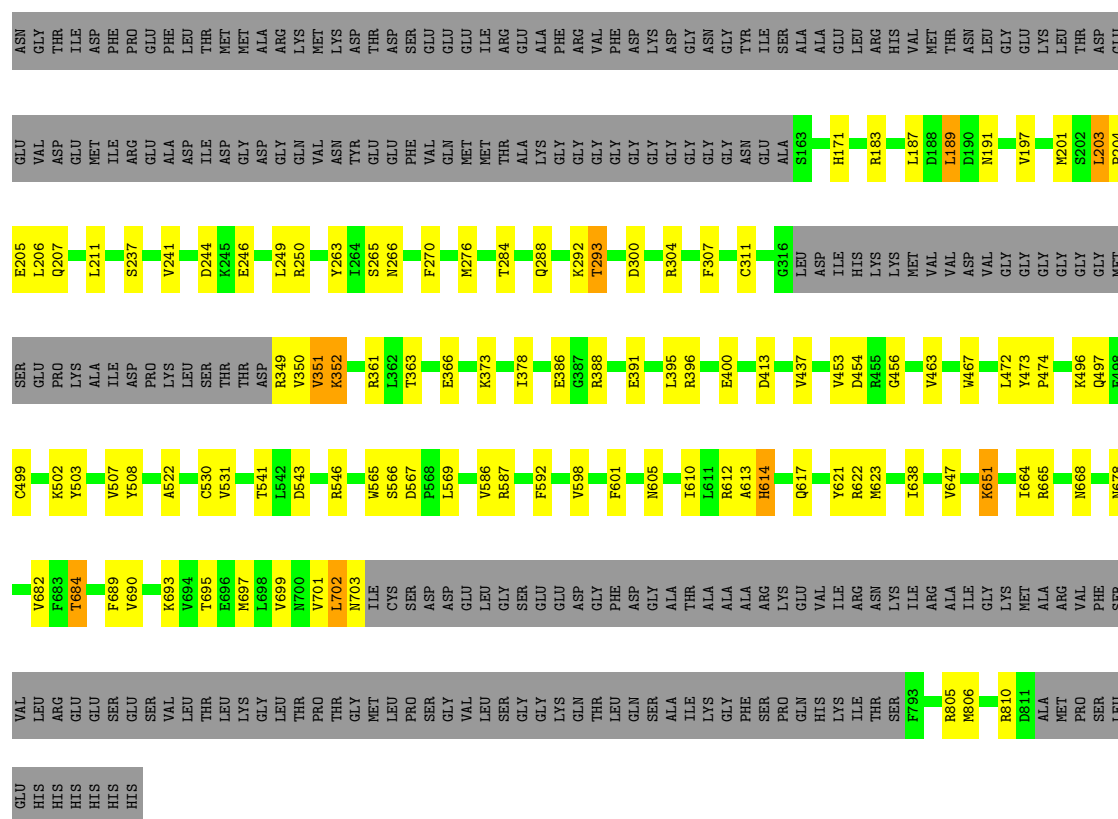
Chain	Residue	Modelled	Actual	Comment	Reference
C	817	GLU	-	expression tag	UNP P63329
C	818	HIS	-	expression tag	UNP P63329
C	819	HIS	-	expression tag	UNP P63329
C	820	HIS	-	expression tag	UNP P63329
C	821	HIS	-	expression tag	UNP P63329
C	822	HIS	-	expression tag	UNP P63329
C	823	HIS	-	expression tag	UNP P63329
D	150	GLY	-	linker	UNP P62161
D	151	GLY	-	linker	UNP P62161
D	152	GLY	-	linker	UNP P62161
D	153	GLY	-	linker	UNP P62161
D	154	GLY	-	linker	UNP P62161
D	155	GLY	-	linker	UNP P62161
D	156	GLY	-	linker	UNP P62161
D	157	GLY	-	linker	UNP P62161
D	158	GLY	-	linker	UNP P62161
D	328	GLY	-	linker	UNP P63100
D	329	GLY	-	linker	UNP P63100
D	330	GLY	-	linker	UNP P63100
D	331	GLY	-	linker	UNP P63100
D	332	GLY	-	linker	UNP P63100
D	333	GLY	-	linker	UNP P63100
D	816	LEU	-	expression tag	UNP P63329
D	817	GLU	-	expression tag	UNP P63329
D	818	HIS	-	expression tag	UNP P63329
D	819	HIS	-	expression tag	UNP P63329
D	820	HIS	-	expression tag	UNP P63329
D	821	HIS	-	expression tag	UNP P63329
D	822	HIS	-	expression tag	UNP P63329
D	823	HIS	-	expression tag	UNP P63329

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total 4 Ca 4	0	0
2	B	4	Total 4 Ca 4	0	0
2	C	4	Total 4 Ca 4	0	0
2	D	4	Total 4 Ca 4	0	0

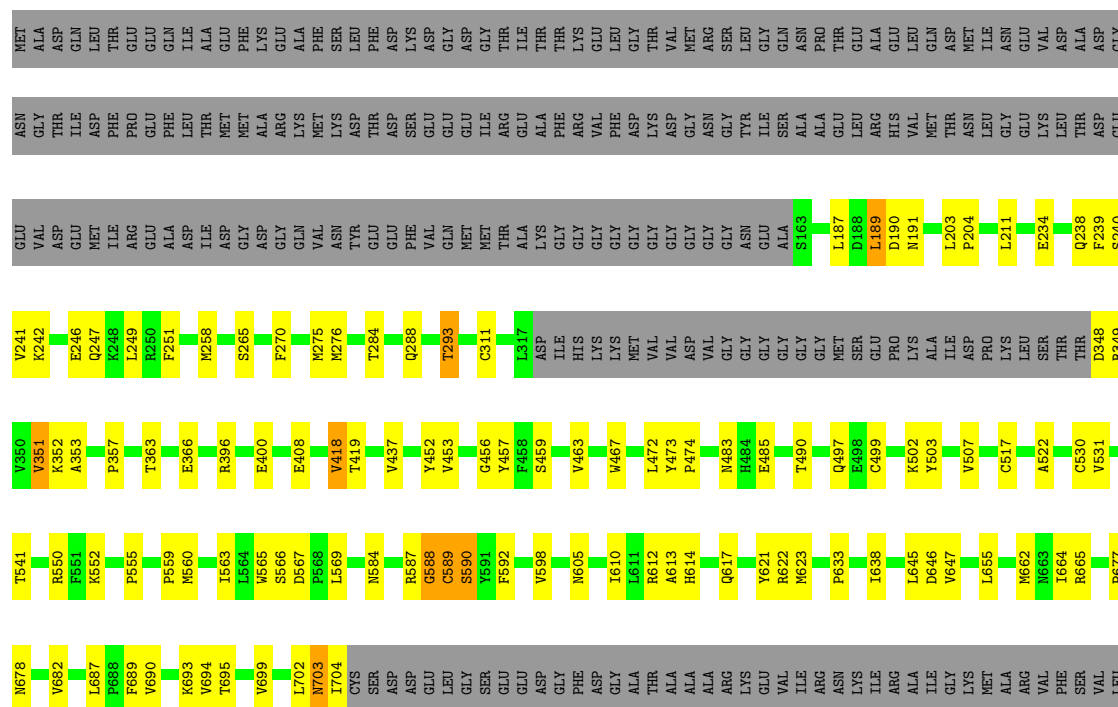
- Molecule 3 is water.

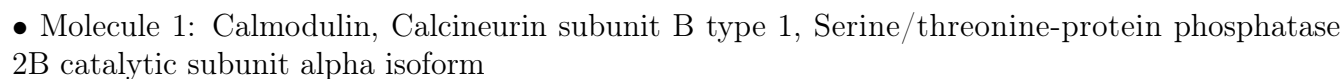
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	26	Total 26	O 26	0	0
3	C	34	Total 34	O 34	0	0
3	D	35	Total 35	O 35	0	0



- Molecule 1: Calmodulin, Calcineurin subunit B type 1, Serine/threonine-protein phosphatase 2B catalytic subunit alpha isoform

Chain C: 50% 13% 36%



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 193.85Å 107.82Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (10.00-3.00) 99.5 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.241 , 0.273 0.243 , 0.274	Depositor DCC
R_{free} test set	2034 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 16.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2090e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.81	1/4379 (0.0%)	1.00	6/5914 (0.1%)
1	B	0.83	1/4376 (0.0%)	0.98	5/5909 (0.1%)
1	C	0.82	1/4380 (0.0%)	0.99	6/5916 (0.1%)
1	D	0.83	0/4376	1.00	8/5909 (0.1%)
All	All	0.82	3/17511 (0.0%)	0.99	25/23648 (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	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	VAL	CA-C	5.39	1.59	1.52
1	A	351	VAL	CA-C	5.18	1.58	1.53
1	C	589	CYS	CA-C	5.09	1.58	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	VAL	N-CA-C	-9.86	101.26	110.53
1	D	442	ALA	N-CA-C	-8.69	95.95	109.25
1	B	352	LYS	N-CA-C	7.43	120.53	108.34
1	C	588	GLY	N-CA-C	-7.34	100.35	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	ASP	N-CA-C	6.04	123.67	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	452	TYR	Peptide
1	D	449	LEU	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	4280	0	4186	96	0
1	B	4277	0	4183	65	0
1	C	4281	0	4187	79	0
1	D	4277	0	4182	95	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	29	0	0	2	0
3	B	26	0	0	1	0
3	C	34	0	0	1	0
3	D	35	0	0	1	0
All	All	17255	0	16738	333	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 10.

The worst 5 of 333 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:C:453:VAL:O	1:C:459:SER:OG	1.62	1.15
1:A:187:LEU:HD23	1:A:195:LEU:HD21	1.26	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ARG:HD3	1:A:644:TYR:OH	1.61	1.00
1:C:517:CYS:O	1:C:550:ARG:NH1	1.96	0.98
1:D:579:GLU:O	1:D:594:SER:OG	1.81	0.98

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	523/823 (64%)	494 (94%)	24 (5%)	5 (1%)	12	45
1	B	522/823 (63%)	499 (96%)	21 (4%)	2 (0%)	30	65
1	C	523/823 (64%)	496 (95%)	23 (4%)	4 (1%)	16	50
1	D	522/823 (63%)	492 (94%)	25 (5%)	5 (1%)	12	45
All	All	2090/3292 (64%)	1981 (95%)	93 (4%)	16 (1%)	16	50

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	ASP
1	A	590	SER
1	C	703	ASN
1	D	239	PHE
1	D	454	ASP

5.3.2 Protein sidechains [i](#)

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	472/708 (67%)	457 (97%)	15 (3%)	34	67
1	B	471/708 (66%)	459 (98%)	12 (2%)	42	72
1	C	471/708 (66%)	464 (98%)	7 (2%)	57	80
1	D	471/708 (66%)	461 (98%)	10 (2%)	47	75
All	All	1885/2832 (67%)	1841 (98%)	44 (2%)	44	74

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	240	SER
1	D	221	THR
1	C	293	THR
1	C	804	GLU
1	D	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	614	HIS
1	D	425	HIS
1	D	191	ASN
1	D	483	ASN
1	B	247	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 16 ligands modelled in this entry, 16 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 [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	529/823 (64%)	-1.79	0 100 100	32, 59, 96, 154	0
1	B	528/823 (64%)	-1.79	0 100 100	33, 61, 100, 149	0
1	C	529/823 (64%)	-1.80	0 100 100	34, 58, 99, 144	0
1	D	528/823 (64%)	-1.78	0 100 100	35, 61, 95, 134	0
All	All	2114/3292 (64%)	-1.79	0 100 100	32, 60, 98, 154	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	CA	A	901	1/1	1.00	0.01	109,109,109,109	0
2	CA	A	902	1/1	1.00	0.01	65,65,65,65	0
2	CA	A	903	1/1	1.00	0.01	59,59,59,59	0
2	CA	A	904	1/1	1.00	0.01	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	901	1/1	1.00	0.01	85,85,85,85	0
2	CA	B	902	1/1	1.00	0.01	66,66,66,66	0
2	CA	B	903	1/1	1.00	0.01	67,67,67,67	0
2	CA	B	904	1/1	1.00	0.03	80,80,80,80	0
2	CA	C	901	1/1	1.00	0.01	102,102,102,102	0
2	CA	C	902	1/1	1.00	0.01	70,70,70,70	0
2	CA	C	903	1/1	1.00	0.00	65,65,65,65	0
2	CA	C	904	1/1	1.00	0.01	70,70,70,70	0
2	CA	D	901	1/1	1.00	0.01	91,91,91,91	0
2	CA	D	902	1/1	1.00	0.02	69,69,69,69	0
2	CA	D	903	1/1	1.00	0.01	69,69,69,69	0
2	CA	D	904	1/1	1.00	0.01	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.