



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:01 PM UTC

PDB ID : 6FPT / pdb_00006fpt
Title : Crystal structure of Danio rerio Lin41 filamin-NHL domains
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Deposited on : 2018-02-12
Resolution : 2.60 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

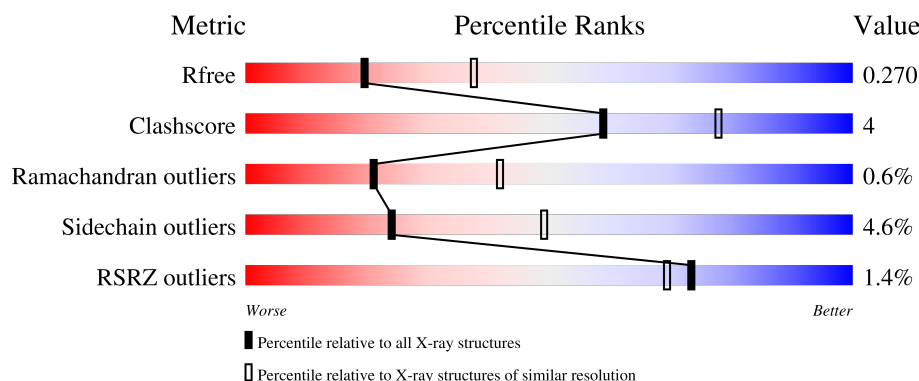
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	409	
1	B	409	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6217 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 E3 ubiquitin-protein ligase TRIM71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			3012	1891	547	562	12			
1	B	388	Total	C	N	O	S	0	1	0
			2990	1878	541	559	12			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	MET	-	initiating methionine	UNP E7FAM5
A	417	ALA	-	expression tag	UNP E7FAM5
A	418	HIS	-	expression tag	UNP E7FAM5
A	419	HIS	-	expression tag	UNP E7FAM5
A	420	HIS	-	expression tag	UNP E7FAM5
A	421	HIS	-	expression tag	UNP E7FAM5
A	422	HIS	-	expression tag	UNP E7FAM5
A	423	HIS	-	expression tag	UNP E7FAM5
A	424	SER	-	expression tag	UNP E7FAM5
A	425	SER	-	expression tag	UNP E7FAM5
A	426	GLY	-	expression tag	UNP E7FAM5
A	427	LEU	-	expression tag	UNP E7FAM5
A	428	GLU	-	expression tag	UNP E7FAM5
A	429	VAL	-	expression tag	UNP E7FAM5
A	430	LEU	-	expression tag	UNP E7FAM5
A	431	PHE	-	expression tag	UNP E7FAM5
A	432	GLN	-	expression tag	UNP E7FAM5
A	433	GLY	-	expression tag	UNP E7FAM5
A	434	PRO	-	expression tag	UNP E7FAM5
B	416	MET	-	initiating methionine	UNP E7FAM5
B	417	ALA	-	expression tag	UNP E7FAM5
B	418	HIS	-	expression tag	UNP E7FAM5
B	419	HIS	-	expression tag	UNP E7FAM5
B	420	HIS	-	expression tag	UNP E7FAM5
B	421	HIS	-	expression tag	UNP E7FAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	422	HIS	-	expression tag	UNP E7FAM5
B	423	HIS	-	expression tag	UNP E7FAM5
B	424	SER	-	expression tag	UNP E7FAM5
B	425	SER	-	expression tag	UNP E7FAM5
B	426	GLY	-	expression tag	UNP E7FAM5
B	427	LEU	-	expression tag	UNP E7FAM5
B	428	GLU	-	expression tag	UNP E7FAM5
B	429	VAL	-	expression tag	UNP E7FAM5
B	430	LEU	-	expression tag	UNP E7FAM5
B	431	PHE	-	expression tag	UNP E7FAM5
B	432	GLN	-	expression tag	UNP E7FAM5
B	433	GLY	-	expression tag	UNP E7FAM5
B	434	PRO	-	expression tag	UNP E7FAM5

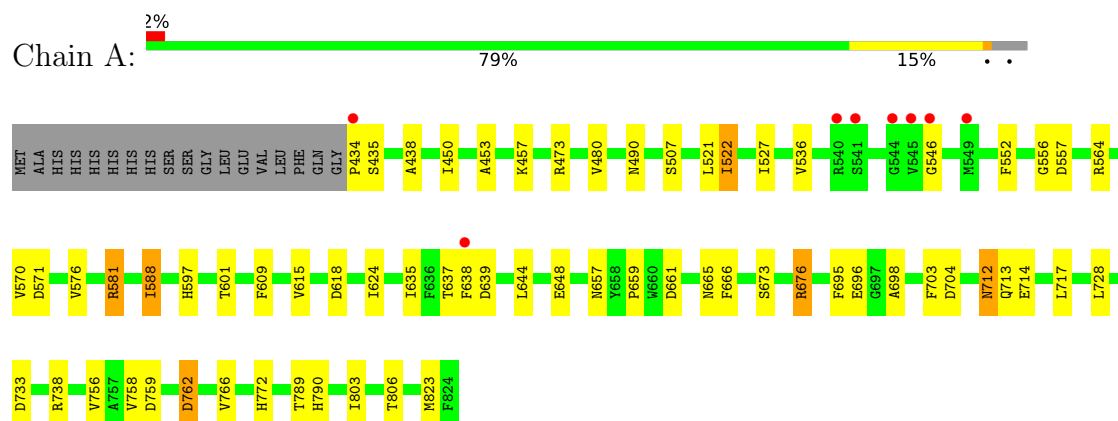
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	99	Total 99	O 99	0	0
2	B	116	Total 116	O 116	0	0

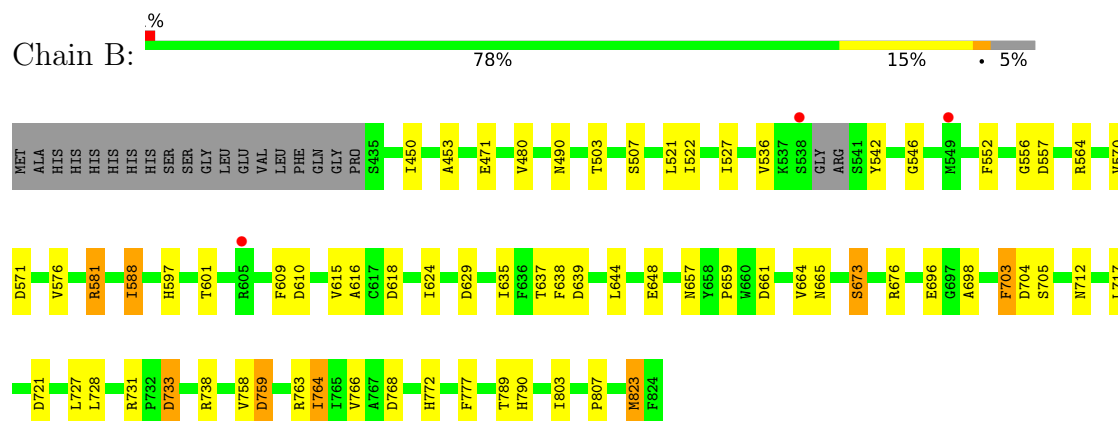
3 Residue-property plots

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: E3 ubiquitin-protein ligase TRIM71



• Molecule 1: E3 ubiquitin-protein ligase TRIM71



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.80Å 90.59Å 131.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 2.60 46.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.43-2.60) 95.3 (46.43-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.244 0.199 , 0.270	Depositor DCC
R_{free} test set	1182 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.993	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6217	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 44.78 % 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 1.4536e-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

5.1 Standard geometry

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	0/3086	1.33	24/4165 (0.6%)
1	B	0.84	3/3062 (0.1%)	1.30	22/4132 (0.5%)
All	All	0.85	3/6148 (0.0%)	1.32	46/8297 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	704	ASP	CA-C	5.94	1.55	1.52
1	B	823	MET	SD-CE	-5.48	1.65	1.79
1	B	705	SER	CA-C	5.04	1.58	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	GLU	N-CA-C	7.34	121.48	112.23
1	B	696	GLU	N-CA-C	7.24	121.35	112.23
1	B	759	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	762	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	637	THR	N-CA-C	-6.80	101.75	110.53
1	A	637	THR	N-CA-C	-6.74	101.83	110.53
1	A	712	ASN	CA-CB-CG	6.51	119.11	112.60
1	B	610	ASP	CA-CB-CG	6.50	119.11	112.60
1	A	759	ASP	CA-CB-CG	6.50	119.10	112.60
1	B	571	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	703	PHE	CA-C-N	6.25	129.14	121.64
1	B	703	PHE	C-N-CA	6.25	129.14	121.64
1	B	618	ASP	CA-C-N	6.20	128.88	120.38
1	B	618	ASP	C-N-CA	6.20	128.88	120.38
1	A	618	ASP	CA-C-N	6.15	128.81	120.38
1	A	618	ASP	C-N-CA	6.15	128.81	120.38
1	B	557	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	665	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	556	GLY	CA-C-N	5.56	130.09	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	GLY	C-N-CA	5.56	130.09	120.58
1	B	665	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	733	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	557	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	661	ASP	CA-CB-CG	5.43	118.03	112.60
1	B	768	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	733	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	571	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	766	VAL	N-CA-C	5.28	115.50	108.11
1	A	556	GLY	N-CA-C	5.26	118.25	110.63
1	B	571	ASP	CA-C-N	5.24	127.61	120.54
1	B	571	ASP	C-N-CA	5.24	127.61	120.54
1	A	434	PRO	CA-C-N	5.22	131.51	121.54
1	A	434	PRO	C-N-CA	5.22	131.51	121.54
1	B	556	GLY	CA-C-N	5.21	129.53	120.68
1	B	556	GLY	C-N-CA	5.21	129.53	120.68
1	A	738	ARG	N-CA-C	-5.18	102.10	110.14
1	A	618	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	522	ILE	N-CA-CB	5.16	117.96	111.46
1	B	556	GLY	N-CA-C	5.15	118.09	110.63
1	A	695	PHE	CA-C-N	5.09	129.33	120.68
1	A	695	PHE	C-N-CA	5.09	129.33	120.68
1	B	721	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	609	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	609	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	704	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	618	ASP	CA-CB-CG	5.00	117.60	112.60

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	3012	0	2890	27	0
1	B	2990	0	2865	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	99	0	0	0	0
2	B	116	0	0	2	0
All	All	6217	0	5755	52	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 (52) 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:570:VAL:HG11	1:A:806:THR:HG22	1.64	0.78
1:B:490:ASN:HB2	2:B:1002:HOH:O	1.94	0.67
1:B:588:ILE:HG21	1:B:638[B]:PHE:CZ	2.33	0.63
1:A:490:ASN:HB2	1:B:738:ARG:HE	1.63	0.63
1:B:552:PHE:CE2	1:B:823:MET:HE3	2.34	0.63
1:A:576:VAL:HG21	1:A:823:MET:HE2	1.83	0.61
1:B:588:ILE:HD12	1:B:597:HIS:HB3	1.82	0.61
1:A:552:PHE:CE1	1:A:823:MET:HE3	2.36	0.61
1:A:588:ILE:HD12	1:A:597:HIS:HB3	1.82	0.60
1:A:453:ALA:HB3	1:A:536:VAL:HG22	1.85	0.59
1:A:564:ARG:O	1:A:581:ARG:HB2	2.02	0.59
1:B:564:ARG:O	1:B:581:ARG:HB2	2.03	0.59
1:A:552:PHE:HE1	1:A:823:MET:HE3	1.69	0.57
1:A:698:ALA:HB3	1:B:521:LEU:HD21	1.85	0.57
1:B:552:PHE:HE2	1:B:823:MET:HE3	1.68	0.56
1:B:576:VAL:HG21	1:B:823:MET:HE2	1.86	0.56
1:A:756:VAL:HG23	1:A:766:VAL:HG22	1.88	0.56
1:A:522:ILE:HG12	1:A:527:ILE:CG2	2.36	0.55
1:B:453:ALA:HB3	1:B:536:VAL:HG22	1.88	0.54
1:B:570:VAL:HG12	1:B:576:VAL:HG22	1.89	0.54
1:B:712:ASN:HA	1:B:758:VAL:HG11	1.90	0.54
1:A:521:LEU:HD21	1:B:698:ALA:HB3	1.90	0.53
1:B:659:PRO:HA	1:B:673:SER:O	2.08	0.53
1:A:712:ASN:HA	1:A:758:VAL:HG11	1.91	0.52
1:B:807:PRO:HD2	2:B:921:HOH:O	2.09	0.51
1:B:616:ALA:HB1	1:B:664:VAL:HG12	1.92	0.51
1:B:764:ILE:HG13	1:B:777:PHE:HB2	1.93	0.51
1:A:657:ASN:HB3	1:A:676:ARG:HB2	1.92	0.51
1:A:713:GLN:HB2	1:A:762:ASP:OD1	2.11	0.51
1:B:657:ASN:HB3	1:B:676:ARG:HB2	1.93	0.50
1:A:570:VAL:HG22	1:A:576:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:VAL:HG21	1:B:823:MET:CE	2.45	0.47
1:B:772:HIS:CE1	1:B:790:HIS:HD2	2.33	0.47
1:A:576:VAL:HG21	1:A:823:MET:CE	2.44	0.47
1:A:714:GLU:CD	1:B:731:ARG:HH22	2.24	0.46
1:A:666:PHE:CE1	1:B:733:ASP:HA	2.50	0.46
1:B:703:PHE:HB2	1:B:728:LEU:HD21	2.01	0.43
1:A:624:ILE:HG23	1:A:635:ILE:CD1	2.49	0.43
1:A:772:HIS:CE1	1:A:790:HIS:HD2	2.36	0.43
1:A:703:PHE:HB2	1:A:728:LEU:HD21	2.00	0.43
1:A:588:ILE:HG21	1:A:638[B]:PHE:CZ	2.54	0.43
1:B:624:ILE:HG23	1:B:635:ILE:CD1	2.49	0.42
1:B:542:TYR:HE2	1:B:759:ASP:OD2	2.02	0.42
1:A:659:PRO:HA	1:A:673:SER:O	2.20	0.42
1:B:727:LEU:CD2	1:B:764:ILE:HD13	2.49	0.42
1:B:480:VAL:HG22	1:B:522:ILE:HD12	2.01	0.42
1:A:624:ILE:HG23	1:A:635:ILE:HD13	2.02	0.42
1:A:480:VAL:HG22	1:A:522:ILE:HD12	2.02	0.41
1:B:661:ASP:H	1:B:673:SER:HB2	1.85	0.41
1:B:759:ASP:CG	1:B:763:ARG:HB2	2.45	0.41
1:B:522:ILE:HG12	1:B:527:ILE:CG2	2.51	0.40
1:A:438:ALA:N	1:A:473:ARG:HD2	2.36	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	390/409 (95%)	365 (94%)	22 (6%)	3 (1%)	16	34
1	B	385/409 (94%)	357 (93%)	26 (7%)	2 (0%)	24	46
All	All	775/818 (95%)	722 (93%)	48 (6%)	5 (1%)	21	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	SER
1	A	581	ARG
1	B	546	GLY
1	B	581	ARG
1	A	546	GLY

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	319/333 (96%)	306 (96%)	13 (4%)	27	54
1	B	317/333 (95%)	301 (95%)	16 (5%)	22	46
All	All	636/666 (96%)	607 (95%)	29 (5%)	24	49

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	450	ILE
1	A	457	LYS
1	A	507	SER
1	A	588	ILE
1	A	601	THR
1	A	615	VAL
1	A	639	ASP
1	A	644	LEU
1	A	648	GLU
1	A	676	ARG
1	A	717	LEU
1	A	789	THR
1	A	803	ILE
1	B	450	ILE
1	B	471	GLU
1	B	503	THR
1	B	507	SER
1	B	588	ILE

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Mol	Chain	Res	Type
1	B	601	THR
1	B	615	VAL
1	B	629	ASP
1	B	639	ASP
1	B	644	LEU
1	B	648	GLU
1	B	673	SER
1	B	717	LEU
1	B	764	ILE
1	B	789	THR
1	B	803	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	490	ASN
1	A	561	GLN
1	A	702	HIS
1	A	713	GLN
1	A	716	HIS
1	A	790	HIS
1	B	490	ASN
1	B	561	GLN
1	B	678	HIS
1	B	735	GLN
1	B	790	HIS

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

There are no ligands in this entry.

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	391/409 (95%)	-0.16	8 (2%) 65 60	15, 30, 49, 83	1 (0%)
1	B	388/409 (94%)	-0.22	3 (0%) 82 80	12, 28, 46, 69	1 (0%)
All	All	779/818 (95%)	-0.19	11 (1%) 73 69	12, 29, 48, 83	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	PRO	3.1
1	A	546	GLY	3.1
1	A	549	MET	2.7
1	A	638[A]	PHE	2.5
1	A	540	ARG	2.4
1	A	541	SER	2.3
1	A	545	VAL	2.3
1	A	544	GLY	2.2
1	B	605	ARG	2.1
1	B	538	SER	2.1
1	B	549	MET	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.