Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 04:05 PM EDT

PDB ID	:	8ESF
Title	:	Crystal structure of human Nischarin PX and LRR domains with engineered mutations
Authors	:	Eldershaw, D.E.; Collins, B.M.
Deposited on	:	2022-10-13
Resolution	:	2.56 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:

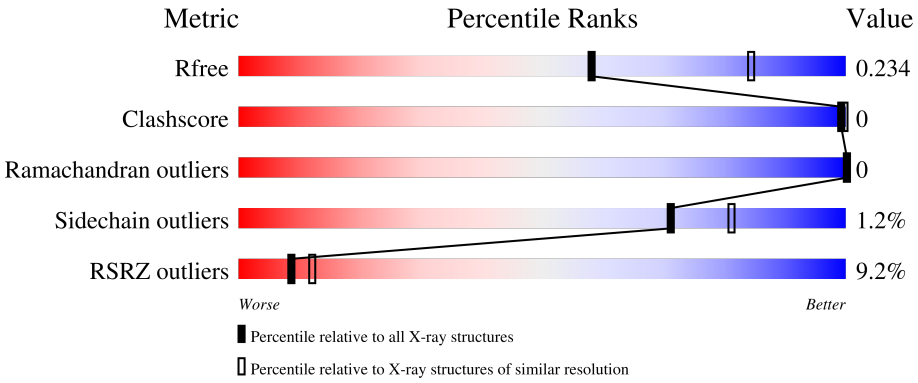
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	502	3% 82% . 16%
1	B	502	13% 83% . 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13745 atoms, of which 6937 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 Nischarin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	420	Total	C	H	N	O	S	0	0	0
			6783	2148	3425	570	630	10			
1	B	427	Total	C	H	N	O	S	0	0	0
			6868	2184	3451	575	649	9			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP Q9Y2I1
A	-32	GLY	-	expression tag	UNP Q9Y2I1
A	-31	SER	-	expression tag	UNP Q9Y2I1
A	-30	SER	-	expression tag	UNP Q9Y2I1
A	-29	HIS	-	expression tag	UNP Q9Y2I1
A	-28	HIS	-	expression tag	UNP Q9Y2I1
A	-27	HIS	-	expression tag	UNP Q9Y2I1
A	-26	HIS	-	expression tag	UNP Q9Y2I1
A	-25	HIS	-	expression tag	UNP Q9Y2I1
A	-24	HIS	-	expression tag	UNP Q9Y2I1
A	-23	SER	-	expression tag	UNP Q9Y2I1
A	-22	SER	-	expression tag	UNP Q9Y2I1
A	-21	GLY	-	expression tag	UNP Q9Y2I1
A	-20	LEU	-	expression tag	UNP Q9Y2I1
A	-19	VAL	-	expression tag	UNP Q9Y2I1
A	-18	PRO	-	expression tag	UNP Q9Y2I1
A	-17	ARG	-	expression tag	UNP Q9Y2I1
A	-16	GLY	-	expression tag	UNP Q9Y2I1
A	-15	SER	-	expression tag	UNP Q9Y2I1
A	-14	HIS	-	expression tag	UNP Q9Y2I1
A	-13	MET	-	expression tag	UNP Q9Y2I1
A	-12	ALA	-	expression tag	UNP Q9Y2I1
A	-11	SER	-	expression tag	UNP Q9Y2I1
A	-10	MET	-	expression tag	UNP Q9Y2I1
A	-9	THR	-	expression tag	UNP Q9Y2I1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q9Y2I1
A	-7	GLY	-	expression tag	UNP Q9Y2I1
A	-6	GLN	-	expression tag	UNP Q9Y2I1
A	-5	GLN	-	expression tag	UNP Q9Y2I1
A	-4	MET	-	expression tag	UNP Q9Y2I1
A	-3	GLY	-	expression tag	UNP Q9Y2I1
A	-2	ARG	-	expression tag	UNP Q9Y2I1
A	-1	GLY	-	expression tag	UNP Q9Y2I1
A	0	SER	-	expression tag	UNP Q9Y2I1
A	29	ASN	THR	conflict	UNP Q9Y2I1
A	38	ARG	THR	conflict	UNP Q9Y2I1
A	39	VAL	ASP	conflict	UNP Q9Y2I1
A	43	LYS	GLU	conflict	UNP Q9Y2I1
A	64	HIS	ARG	conflict	UNP Q9Y2I1
A	89	ARG	GLU	conflict	UNP Q9Y2I1
A	102	TYR	ALA	conflict	UNP Q9Y2I1
A	119	LYS	PHE	conflict	UNP Q9Y2I1
A	127	GLN	ALA	conflict	UNP Q9Y2I1
A	142	GLN	GLY	conflict	UNP Q9Y2I1
A	148	GLU	ALA	conflict	UNP Q9Y2I1
A	150	THR	GLY	conflict	UNP Q9Y2I1
A	184	CYS	THR	conflict	UNP Q9Y2I1
A	192	ILE	VAL	conflict	UNP Q9Y2I1
A	193	GLN	SER	conflict	UNP Q9Y2I1
A	205	ILE	GLN	conflict	UNP Q9Y2I1
A	208	GLN	LEU	conflict	UNP Q9Y2I1
A	230	ARG	LYS	conflict	UNP Q9Y2I1
A	233	TYR	ARG	conflict	UNP Q9Y2I1
A	236	GLU	VAL	conflict	UNP Q9Y2I1
A	251	THR	ALA	conflict	UNP Q9Y2I1
A	298	CYS	SER	conflict	UNP Q9Y2I1
A	299	ILE	VAL	variant	UNP Q9Y2I1
A	301	CYS	GLU	conflict	UNP Q9Y2I1
A	321	GLU	GLY	conflict	UNP Q9Y2I1
A	345	THR	SER	conflict	UNP Q9Y2I1
A	385	SER	ARG	conflict	UNP Q9Y2I1
A	386	ASN	ASP	conflict	UNP Q9Y2I1
A	397	HIS	SER	conflict	UNP Q9Y2I1
A	406	TYR	HIS	conflict	UNP Q9Y2I1
A	407	LEU	VAL	conflict	UNP Q9Y2I1
A	410	THR	LEU	conflict	UNP Q9Y2I1
A	414	VAL	LEU	conflict	UNP Q9Y2I1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	415	THR	SER	conflict	UNP Q9Y2I1
A	416	THR	ILE	conflict	UNP Q9Y2I1
A	430	ASP	GLU	conflict	UNP Q9Y2I1
A	440	GLU	THR	conflict	UNP Q9Y2I1
A	444	GLN	GLU	conflict	UNP Q9Y2I1
B	-33	MET	-	expression tag	UNP Q9Y2I1
B	-32	GLY	-	expression tag	UNP Q9Y2I1
B	-31	SER	-	expression tag	UNP Q9Y2I1
B	-30	SER	-	expression tag	UNP Q9Y2I1
B	-29	HIS	-	expression tag	UNP Q9Y2I1
B	-28	HIS	-	expression tag	UNP Q9Y2I1
B	-27	HIS	-	expression tag	UNP Q9Y2I1
B	-26	HIS	-	expression tag	UNP Q9Y2I1
B	-25	HIS	-	expression tag	UNP Q9Y2I1
B	-24	HIS	-	expression tag	UNP Q9Y2I1
B	-23	SER	-	expression tag	UNP Q9Y2I1
B	-22	SER	-	expression tag	UNP Q9Y2I1
B	-21	GLY	-	expression tag	UNP Q9Y2I1
B	-20	LEU	-	expression tag	UNP Q9Y2I1
B	-19	VAL	-	expression tag	UNP Q9Y2I1
B	-18	PRO	-	expression tag	UNP Q9Y2I1
B	-17	ARG	-	expression tag	UNP Q9Y2I1
B	-16	GLY	-	expression tag	UNP Q9Y2I1
B	-15	SER	-	expression tag	UNP Q9Y2I1
B	-14	HIS	-	expression tag	UNP Q9Y2I1
B	-13	MET	-	expression tag	UNP Q9Y2I1
B	-12	ALA	-	expression tag	UNP Q9Y2I1
B	-11	SER	-	expression tag	UNP Q9Y2I1
B	-10	MET	-	expression tag	UNP Q9Y2I1
B	-9	THR	-	expression tag	UNP Q9Y2I1
B	-8	GLY	-	expression tag	UNP Q9Y2I1
B	-7	GLY	-	expression tag	UNP Q9Y2I1
B	-6	GLN	-	expression tag	UNP Q9Y2I1
B	-5	GLN	-	expression tag	UNP Q9Y2I1
B	-4	MET	-	expression tag	UNP Q9Y2I1
B	-3	GLY	-	expression tag	UNP Q9Y2I1
B	-2	ARG	-	expression tag	UNP Q9Y2I1
B	-1	GLY	-	expression tag	UNP Q9Y2I1
B	0	SER	-	expression tag	UNP Q9Y2I1
B	29	ASN	THR	conflict	UNP Q9Y2I1
B	38	ARG	THR	conflict	UNP Q9Y2I1
B	39	VAL	ASP	conflict	UNP Q9Y2I1

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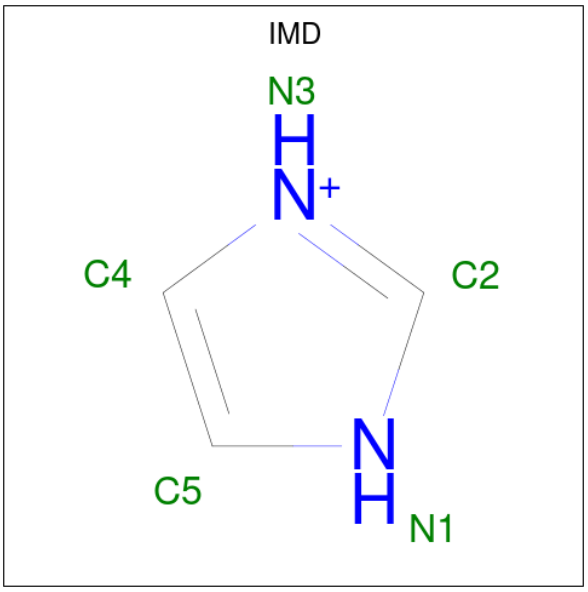
Chain	Residue	Modelled	Actual	Comment	Reference
B	43	LYS	GLU	conflict	UNP Q9Y2I1
B	64	HIS	ARG	conflict	UNP Q9Y2I1
B	89	ARG	GLU	conflict	UNP Q9Y2I1
B	102	TYR	ALA	conflict	UNP Q9Y2I1
B	119	LYS	PHE	conflict	UNP Q9Y2I1
B	127	GLN	ALA	conflict	UNP Q9Y2I1
B	142	GLN	GLY	conflict	UNP Q9Y2I1
B	148	GLU	ALA	conflict	UNP Q9Y2I1
B	150	THR	GLY	conflict	UNP Q9Y2I1
B	184	CYS	THR	conflict	UNP Q9Y2I1
B	192	ILE	VAL	conflict	UNP Q9Y2I1
B	193	GLN	SER	conflict	UNP Q9Y2I1
B	205	ILE	GLN	conflict	UNP Q9Y2I1
B	208	GLN	LEU	conflict	UNP Q9Y2I1
B	230	ARG	LYS	conflict	UNP Q9Y2I1
B	233	TYR	ARG	conflict	UNP Q9Y2I1
B	236	GLU	VAL	conflict	UNP Q9Y2I1
B	251	THR	ALA	conflict	UNP Q9Y2I1
B	298	CYS	SER	conflict	UNP Q9Y2I1
B	299	ILE	VAL	variant	UNP Q9Y2I1
B	301	CYS	GLU	conflict	UNP Q9Y2I1
B	321	GLU	GLY	conflict	UNP Q9Y2I1
B	345	THR	SER	conflict	UNP Q9Y2I1
B	385	SER	ARG	conflict	UNP Q9Y2I1
B	386	ASN	ASP	conflict	UNP Q9Y2I1
B	397	HIS	SER	conflict	UNP Q9Y2I1
B	406	TYR	HIS	conflict	UNP Q9Y2I1
B	407	LEU	VAL	conflict	UNP Q9Y2I1
B	410	THR	LEU	conflict	UNP Q9Y2I1
B	414	VAL	LEU	conflict	UNP Q9Y2I1
B	415	THR	SER	conflict	UNP Q9Y2I1
B	416	THR	ILE	conflict	UNP Q9Y2I1
B	430	ASP	GLU	conflict	UNP Q9Y2I1
B	440	GLU	THR	conflict	UNP Q9Y2I1
B	444	GLN	GLU	conflict	UNP Q9Y2I1

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H N 10 3 5 2	0	0

- Molecule 3 is water.

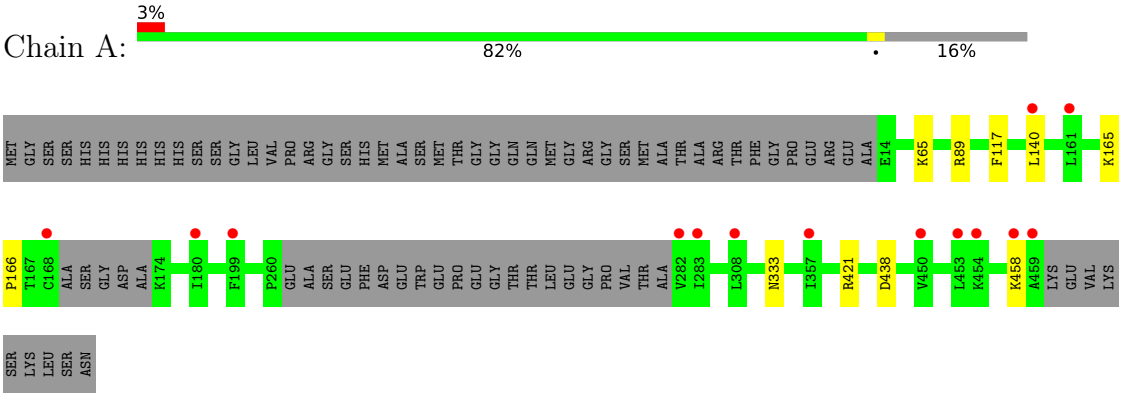
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	20	Total H O 60 40 20	0	0
3	B	8	Total H O 24 16 8	0	0

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.

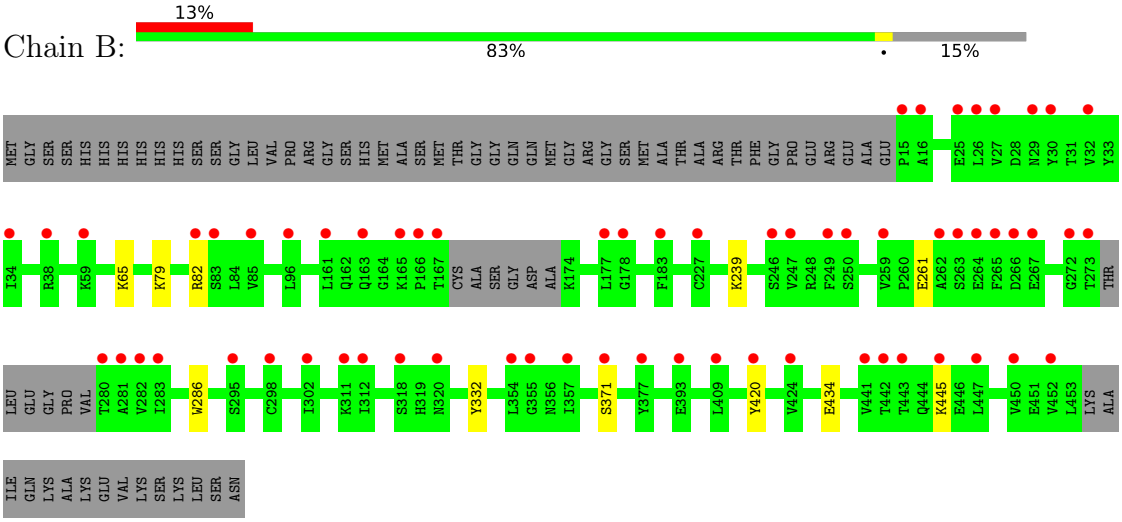
• Molecule 1: Nischarin

Chain A:



• Molecule 1: Nischarin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.17Å 83.31Å 90.83Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	43.96 – 2.56 43.96 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.96-2.56) 99.0 (43.96-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.215 , 0.243 0.208 , 0.234	Depositor DCC
R_{free} test set	2009 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13745	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.52	0/3421	0.79	4/4636 (0.1%)
1	B	0.55	0/3484	0.80	0/4725
All	All	0.54	0/6905	0.80	4/9361 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	117	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	117	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	89	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	3358	3425	3421	1	2
1	B	3417	3451	3448	1	5
2	A	5	5	5	0	1
3	A	20	40	0	0	0
3	B	8	16	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6808	6937	6874	2	6

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 0.

All (2) 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:B:239:LYS:HE2	1:B:286:TRP:CE2	2.56	0.41
1:A:165:LYS:HA	1:A:166:PRO:HD3	1.97	0.41

All (6) 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)
1:B:79:LYS:HZ1	1:B:434:GLU:O[2_546]	0.69	0.91
1:B:79:LYS:NZ	1:B:434:GLU:O[2_546]	1.46	0.74
1:A:333:ASN:HD22	1:B:332:TYR:HH[1_655]	1.29	0.31
1:B:79:LYS:CE	1:B:434:GLU:O[2_546]	2.13	0.07
1:B:79:LYS:HZ1	1:B:434:GLU:C[2_546]	1.55	0.05
1:A:438:ASP:OD2	2:A:501:IMD:H2[2_555]	1.56	0.04

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	414/502 (82%)	400 (97%)	14 (3%)	0	100	100
1	B	421/502 (84%)	400 (95%)	21 (5%)	0	100	100
All	All	835/1004 (83%)	800 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	383/446 (86%)	380 (99%)	3 (1%)	81 88
1	B	389/446 (87%)	383 (98%)	6 (2%)	65 77
All	All	772/892 (86%)	763 (99%)	9 (1%)	71 81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	140	LEU
1	A	458	LYS
1	B	65	LYS
1	B	82	ARG
1	B	261	GLU
1	B	371	SER
1	B	420	TYR
1	B	445	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	IMD	A	501	-	3,5,5	0.26	0	4,5,5	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	A	501	-	-	-	0/1/1/1

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.

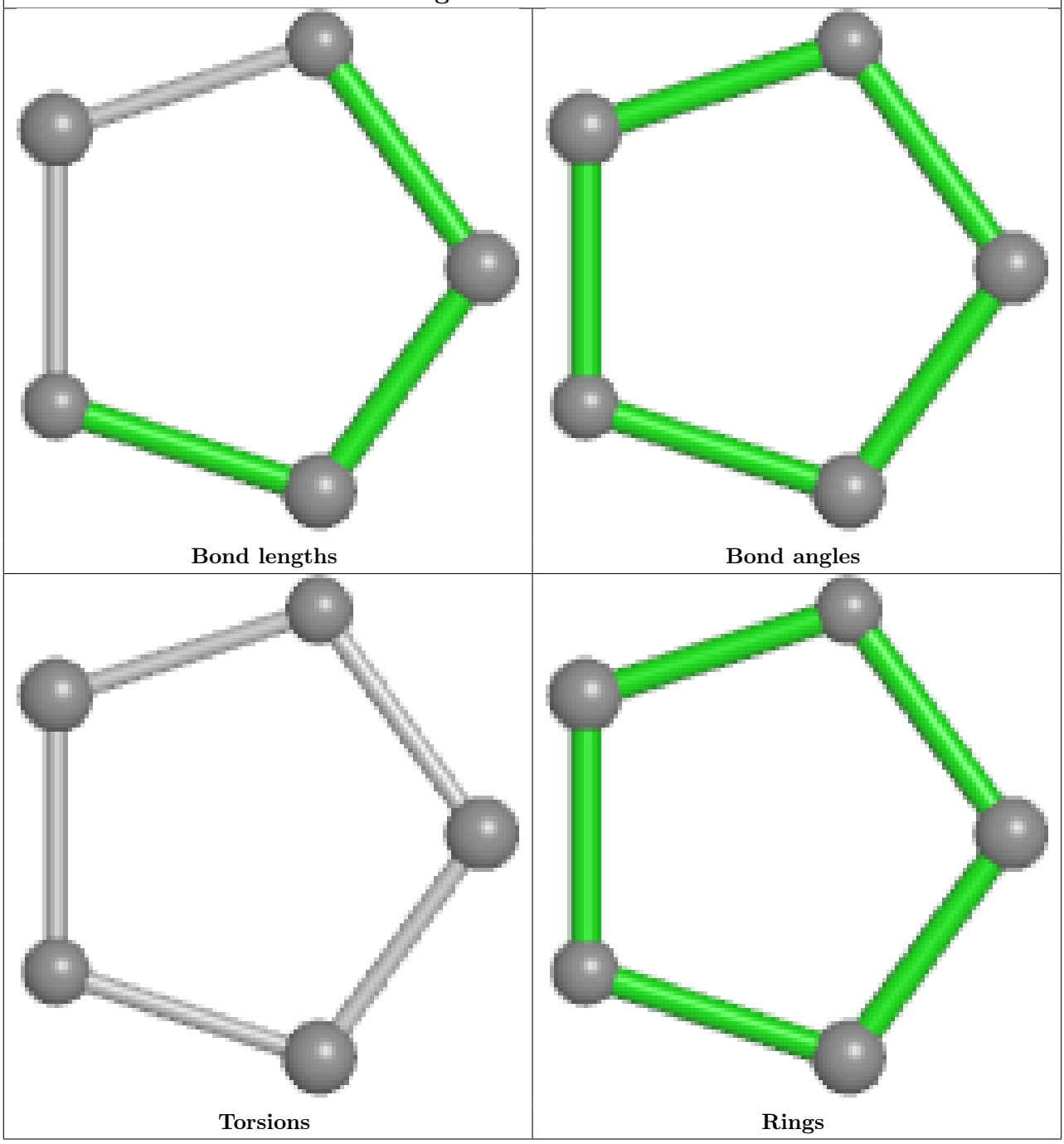
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	IMD	0	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IMD A 501



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, 95^{th} 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	420/502 (83%)	0.67	14 (3%) 46 56	54, 70, 94, 129	0
1	B	427/502 (85%)	1.10	64 (14%) 2 3	52, 79, 113, 146	0
All	All	847/1004 (84%)	0.89	78 (9%) 9 12	52, 74, 106, 146	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	PHE	6.5
1	B	262	ALA	6.1
1	B	266	ASP	5.5
1	B	452	VAL	4.6
1	B	281	ALA	4.6
1	A	458	LYS	4.5
1	B	27	VAL	4.4
1	B	273	THR	4.3
1	B	442	THR	4.3
1	B	30	TYR	4.3
1	B	15	PRO	4.3
1	B	165	LYS	4.0
1	A	459	ALA	3.7
1	B	280	THR	3.7
1	A	283	ILE	3.4
1	B	82	ARG	3.4
1	A	282	VAL	3.3
1	B	167	THR	3.2
1	A	140	LEU	3.2
1	B	420	TYR	3.1
1	B	177	LEU	3.1
1	B	26	LEU	3.0
1	A	453	LEU	3.0
1	B	85	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	38	ARG	3.0
1	B	267	GLU	2.9
1	B	264	GLU	2.9
1	B	450	VAL	2.9
1	B	178	GLY	2.8
1	B	227	CYS	2.8
1	B	443	THR	2.8
1	A	180	ILE	2.7
1	A	357	ILE	2.7
1	B	354	LEU	2.7
1	B	29	ASN	2.7
1	B	272	GLY	2.7
1	B	371	SER	2.7
1	A	168	CYS	2.6
1	B	441	VAL	2.6
1	B	445	LYS	2.6
1	B	16	ALA	2.6
1	B	355	GLY	2.6
1	B	163	GLN	2.5
1	B	409	LEU	2.4
1	B	263	SER	2.4
1	B	161	LEU	2.4
1	B	250	SER	2.4
1	A	199	PHE	2.4
1	B	83	SER	2.4
1	B	96	LEU	2.4
1	B	318	SER	2.3
1	B	282	VAL	2.3
1	A	161	LEU	2.3
1	B	295	SER	2.3
1	B	283	ILE	2.3
1	A	308	LEU	2.3
1	B	32	VAL	2.2
1	B	25	GLU	2.2
1	B	34	ILE	2.2
1	B	302	ILE	2.2
1	B	59	LYS	2.2
1	A	450	VAL	2.2
1	B	447	LEU	2.2
1	A	454	LYS	2.2
1	B	377	TYR	2.2
1	B	259	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	249	PHE	2.2
1	B	424	VAL	2.2
1	B	298	CYS	2.2
1	B	320	ASN	2.2
1	B	166	PRO	2.1
1	B	357	ILE	2.1
1	B	246	SER	2.1
1	B	247	VAL	2.1
1	B	312	ILE	2.1
1	B	393	GLU	2.1
1	B	311	LYS	2.1
1	B	183	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

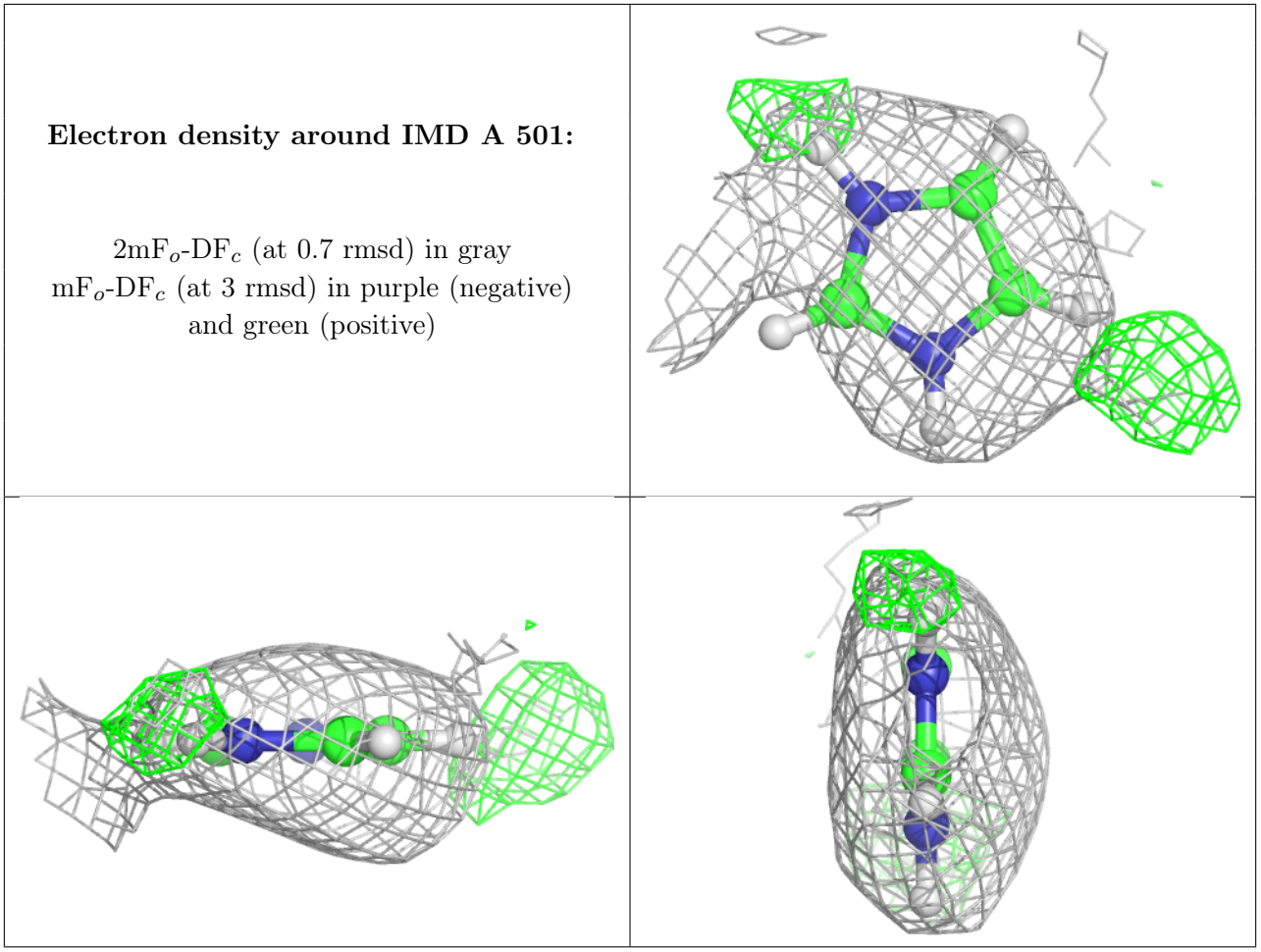
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	IMD	A	501	5/5	0.86	0.15	57,77,97,99	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around IMD A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.