



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:45 PM UTC

PDB ID : 5E53 / pdb\_00005e53  
Title : Crystal structure of chicken CNTN1 FN1-FN3 domains  
Authors : Nikolaienko, R.M.; Bouyain, S.  
Deposited on : 2015-10-07  
Resolution : 2.50 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

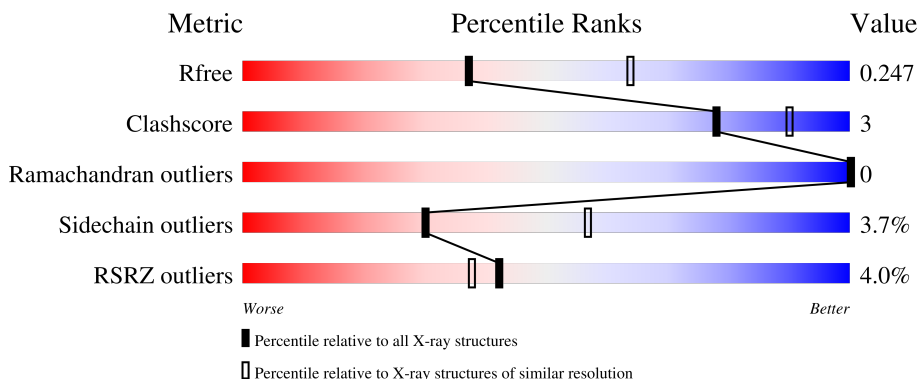
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	301	 4% 91% 5%
1	B	301	 6% 88% 10%
1	C	301	 3% 89% 8%
1	D	301	 2% 91% 9%

## 2 Entry composition [i](#)

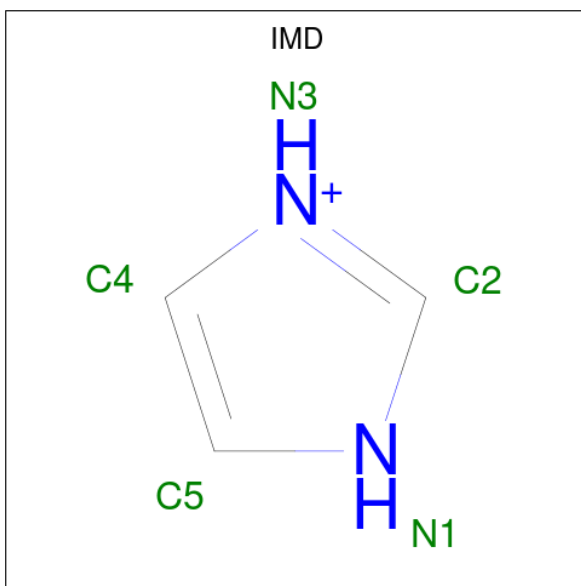
There are 3 unique types of molecules in this entry. The entry contains 9572 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Contactin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	Total 2270	C 1430	N 393	O 442	S 5	0	0	0
1	B	296	Total 2327	C 1465	N 404	O 453	S 5	0	0	0
1	C	292	Total 2304	C 1452	N 399	O 448	S 5	0	0	0
1	D	301	Total 2366	C 1488	N 411	O 462	S 5	0	0	0

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	C	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		
2	D	1	Total	C	N	0	0
			5	3	2		

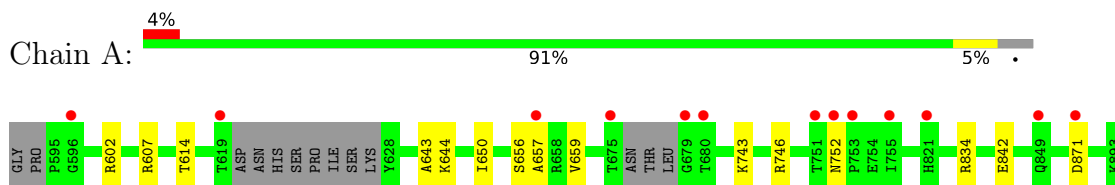
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	57	Total	O	0	0
			57	57		
3	C	53	Total	O	0	0
			53	53		
3	D	83	Total	O	0	0
			83	83		

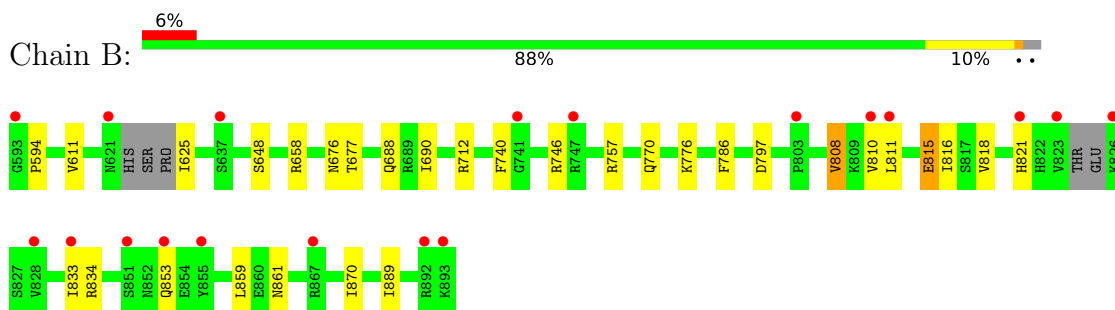
### 3 Residue-property plots [i](#)

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.

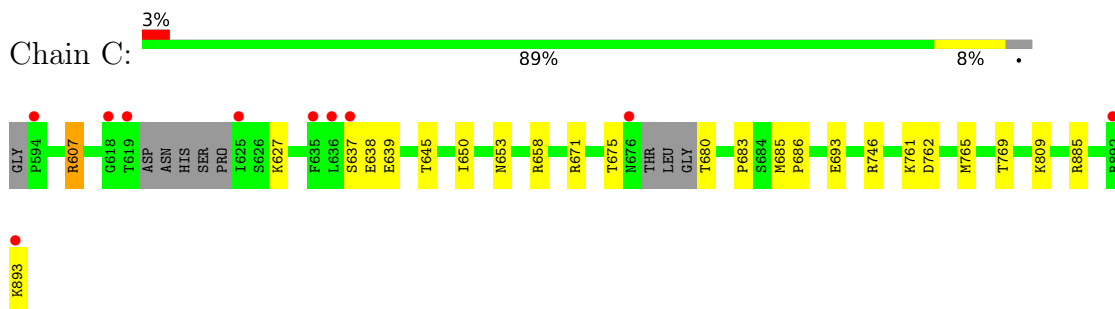
- Molecule 1: Contactin-1



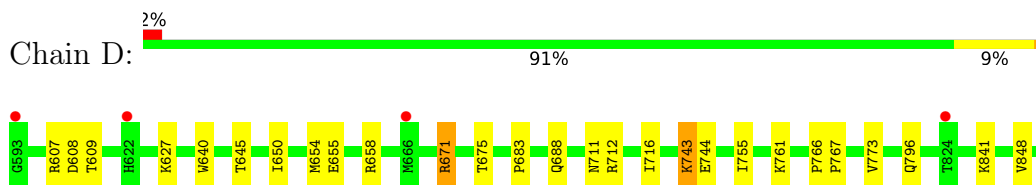
- Molecule 1: Contactin-1



- Molecule 1: Contactin-1



- Molecule 1: Contactin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.48Å 49.87Å 163.30Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	43.51 – 2.50 43.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (43.51-2.50) 95.4 (43.51-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.51Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.205 , 0.247 0.208 , 0.247	Depositor DCC
$R_{free}$ test set	2435 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.38 % 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 3.2057e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.32	0/2329	0.62	0/3165
1	B	0.35	0/2387	0.64	2/3245 (0.1%)
1	C	0.29	0/2364	0.66	1/3213 (0.0%)
1	D	0.36	1/2430 (0.0%)	0.62	0/3308
All	All	0.33	1/9510 (0.0%)	0.64	3/12931 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	658	ARG	C-O	-5.01	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	638	GLU	N-CA-C	-7.32	103.29	111.71
1	B	594	PRO	CA-C-N	5.04	125.03	119.89
1	B	594	PRO	C-N-CA	5.04	125.03	119.89

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2270	0	2195	8	0
1	B	2327	0	2254	17	0
1	C	2304	0	2234	14	0
1	D	2366	0	2288	12	0
2	A	15	0	15	0	0
2	B	10	0	10	3	0
2	C	20	0	20	0	0
2	D	30	0	30	2	0
3	A	37	0	0	0	0
3	B	57	0	0	2	0
3	C	53	0	0	3	0
3	D	83	0	0	0	0
All	All	9572	0	9046	51	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 3.

All (51) 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:637:SER:HB2	1:C:639:GLU:CD	2.17	0.69
1:A:650:ILE:HD13	1:A:657:ALA:HB2	1.80	0.64
1:C:607:ARG:NH1	1:C:693:GLU:OE1	2.34	0.60
1:B:821:HIS:HA	2:B:901:IMD:H5	1.84	0.59
1:C:637:SER:HB2	1:C:639:GLU:OE1	2.04	0.57
1:B:808:VAL:HG12	1:B:816:ILE:HD11	1.88	0.56
1:B:821:HIS:CG	2:B:901:IMD:H5	2.42	0.54
1:A:650:ILE:CD1	1:A:657:ALA:HB2	2.39	0.53
1:B:688:GLN:NE2	3:B:1002:HOH:O	2.41	0.53
1:B:833:ILE:HD11	1:B:859:LEU:HD21	1.92	0.51
1:C:658:ARG:NH2	3:C:1005:HOH:O	2.42	0.51
1:C:645:THR:HG21	1:C:650:ILE:HD11	1.93	0.50
1:D:608:ASP:OD1	1:D:609:THR:N	2.45	0.49
1:A:614:THR:HG22	1:A:656:SER:HB2	1.94	0.49
1:B:658:ARG:NH1	3:B:1007:HOH:O	2.47	0.48
1:B:816:ILE:CD1	1:B:889:ILE:HG21	2.43	0.47
1:C:637:SER:HB2	1:C:639:GLU:CG	2.44	0.47
1:D:654:MET:HG3	2:D:903:IMD:N3	2.29	0.47
1:B:712:ARG:NH1	1:B:797:ASP:OD1	2.47	0.47
1:A:614:THR:HG22	1:A:656:SER:CB	2.45	0.46
1:A:834:ARG:NH2	1:A:842:GLU:OE2	2.43	0.46
1:C:671:ARG:HH11	1:C:683:PRO:CB	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:THR:HG21	1:D:650:ILE:HD11	1.97	0.46
1:C:637:SER:HB2	1:C:639:GLU:HG2	1.98	0.44
1:D:716:ILE:HG23	1:D:773:VAL:HG21	2.01	0.43
1:A:650:ILE:HD11	1:A:657:ALA:CB	2.48	0.43
1:D:627:LYS:HE3	1:D:675:THR:HG21	2.00	0.43
1:C:762:ASP:HB3	1:C:765:MET:HE3	2.00	0.43
1:B:776:LYS:HB3	1:B:786:PHE:HA	2.01	0.43
1:B:811:LEU:HB3	1:B:815:GLU:HB3	2.01	0.43
1:B:821:HIS:CA	2:B:901:IMD:H5	2.49	0.43
1:A:650:ILE:CD1	1:A:657:ALA:CB	2.96	0.43
1:B:816:ILE:HD12	1:B:889:ILE:HG21	2.00	0.43
1:C:746:ARG:NH2	3:C:1009:HOH:O	2.52	0.42
1:C:885:ARG:NH2	3:C:1008:HOH:O	2.48	0.42
1:A:643:ALA:HB1	1:A:659:VAL:HG13	2.02	0.42
1:C:685:MET:HB3	1:C:686:PRO:HD2	2.01	0.42
1:C:671:ARG:HH11	1:C:683:PRO:HB3	1.85	0.42
1:B:690:ILE:HD12	1:B:690:ILE:C	2.45	0.42
1:B:810:VAL:HG23	1:B:889:ILE:HG12	2.02	0.42
1:B:818:VAL:HG11	1:B:833:ILE:HD12	2.02	0.42
1:D:650:ILE:HA	2:D:903:IMD:H5	2.01	0.42
1:D:743:LYS:HD2	1:D:744:GLU:HB3	2.01	0.41
1:B:861:ASN:O	1:B:861:ASN:ND2	2.53	0.41
1:B:625:ILE:HA	1:B:676:ASN:HB3	2.02	0.41
1:D:640:TRP:CE3	1:D:671:ARG:HD2	2.56	0.41
1:C:675:THR:HG22	1:C:680:THR:HG23	2.02	0.41
1:D:671:ARG:HG3	1:D:683:PRO:HB3	2.03	0.40
1:D:711:ASN:HD22	1:D:711:ASN:H	1.69	0.40
1:D:712:ARG:HH12	1:D:767:PRO:HD3	1.86	0.40
1:D:712:ARG:HH12	1:D:766:PRO:HA	1.87	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	282/301 (94%)	273 (97%)	9 (3%)	0	100	100
1	B	290/301 (96%)	277 (96%)	13 (4%)	0	100	100
1	C	286/301 (95%)	278 (97%)	8 (3%)	0	100	100
1	D	299/301 (99%)	289 (97%)	10 (3%)	0	100	100
All	All	1157/1204 (96%)	1117 (96%)	40 (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	247/259 (95%)	240 (97%)	7 (3%)	38	66
1	B	254/259 (98%)	242 (95%)	12 (5%)	23	47
1	C	252/259 (97%)	245 (97%)	7 (3%)	38	66
1	D	259/259 (100%)	248 (96%)	11 (4%)	26	52
All	All	1012/1036 (98%)	975 (96%)	37 (4%)	30	57

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

Mol	Chain	Res	Type
1	A	602	ARG
1	A	607	ARG
1	A	644	LYS
1	A	743	LYS
1	A	746	ARG
1	A	752	ASN
1	A	871	ASP
1	B	611	VAL
1	B	648	SER
1	B	677	THR
1	B	740	PHE
1	B	746	ARG
1	B	757	ARG

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Mol	Chain	Res	Type
1	B	770	GLN
1	B	808	VAL
1	B	815	GLU
1	B	834	ARG
1	B	853	GLN
1	B	870	ILE
1	C	607	ARG
1	C	627	LYS
1	C	653	ASN
1	C	761	LYS
1	C	769	THR
1	C	809	LYS
1	C	893	LYS
1	D	607	ARG
1	D	655	GLU
1	D	671	ARG
1	D	688	GLN
1	D	743	LYS
1	D	755	ILE
1	D	761	LYS
1	D	796	GLN
1	D	841	LYS
1	D	848	VAL
1	D	858	LYS

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	770	GLN
1	A	861	ASN
1	B	621	ASN
1	B	688	GLN
1	B	832	GLN
1	B	849	GLN
1	C	839	HIS
1	C	849	GLN
1	D	770	GLN

### 5.3.3 RNA

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](#)

15 ligands are 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	C	903	-	5,5,5	0.63	0	5,5,5	0.42	0
2	IMD	C	901	-	5,5,5	0.62	0	5,5,5	0.43	0
2	IMD	D	905	-	5,5,5	0.62	0	5,5,5	0.43	0
2	IMD	B	902	-	5,5,5	0.64	0	5,5,5	0.41	0
2	IMD	B	901	-	5,5,5	0.57	0	5,5,5	0.65	0
2	IMD	D	904	-	5,5,5	0.63	0	5,5,5	0.43	0
2	IMD	D	906	-	5,5,5	0.65	0	5,5,5	0.43	0
2	IMD	C	904	-	5,5,5	0.63	0	5,5,5	0.45	0
2	IMD	A	902	-	5,5,5	0.63	0	5,5,5	0.41	0
2	IMD	C	902	-	5,5,5	0.63	0	5,5,5	0.43	0
2	IMD	A	901	-	5,5,5	0.64	0	5,5,5	0.44	0
2	IMD	D	902	-	5,5,5	0.64	0	5,5,5	0.41	0
2	IMD	A	903	-	5,5,5	0.64	0	5,5,5	0.43	0
2	IMD	D	903	-	5,5,5	0.62	0	5,5,5	0.45	0
2	IMD	D	901	-	5,5,5	0.65	0	5,5,5	0.43	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	C	903	-	-	-	0/1/1/1
2	IMD	C	901	-	-	-	0/1/1/1
2	IMD	D	905	-	-	-	0/1/1/1
2	IMD	B	902	-	-	-	0/1/1/1
2	IMD	B	901	-	-	-	0/1/1/1
2	IMD	D	904	-	-	-	0/1/1/1
2	IMD	D	906	-	-	-	0/1/1/1
2	IMD	C	904	-	-	-	0/1/1/1
2	IMD	A	902	-	-	-	0/1/1/1
2	IMD	C	902	-	-	-	0/1/1/1
2	IMD	A	901	-	-	-	0/1/1/1
2	IMD	D	902	-	-	-	0/1/1/1
2	IMD	A	903	-	-	-	0/1/1/1
2	IMD	D	903	-	-	-	0/1/1/1
2	IMD	D	901	-	-	-	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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	IMD	3	0
2	D	903	IMD	2	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/301 (95%)	0.47	13 (4%) 38 33	42, 69, 106, 125	0
1	B	296/301 (98%)	0.42	19 (6%) 25 22	30, 69, 106, 181	0
1	C	292/301 (97%)	0.18	10 (3%) 48 43	33, 55, 93, 151	0
1	D	301/301 (100%)	0.04	5 (1%) 69 65	27, 52, 85, 145	0
All	All	1177/1204 (97%)	0.27	47 (3%) 42 38	27, 60, 100, 181	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	593	GLY	6.3
1	C	619	THR	4.6
1	A	679	GLY	4.1
1	B	823	VAL	4.0
1	D	666	MET	3.9
1	B	811	LEU	3.4
1	C	636	LEU	3.4
1	B	855	TYR	3.1
1	C	892	ARG	3.1
1	C	893	LYS	3.0
1	C	637	SER	2.9
1	A	657	ALA	2.8
1	B	593	GLY	2.8
1	B	826	LYS	2.8
1	C	676	ASN	2.8
1	B	893	LYS	2.8
1	A	752	ASN	2.7
1	A	675	THR	2.7
1	B	803	PRO	2.6
1	C	635	PHE	2.6
1	C	618	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	755	ILE	2.6
1	B	892	ARG	2.6
1	A	619	THR	2.6
1	C	594	PRO	2.5
1	B	741	GLY	2.5
1	D	622	HIS	2.4
1	D	893	LYS	2.4
1	A	821	HIS	2.4
1	A	680	THR	2.3
1	A	751	THR	2.3
1	A	596	GLY	2.2
1	B	851	SER	2.2
1	B	810	VAL	2.2
1	C	625	ILE	2.2
1	B	853	GLN	2.2
1	B	747	ARG	2.2
1	B	828	VAL	2.1
1	A	753	PRO	2.1
1	B	637	SER	2.1
1	A	849	GLN	2.1
1	B	621	ASN	2.1
1	D	824	THR	2.1
1	B	833	ILE	2.1
1	A	871	ASP	2.1
1	B	821	HIS	2.1
1	B	867	ARG	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, 95<sup>th</sup> 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
2	IMD	D	903	5/5	0.61	0.32	115,120,121,124	0
2	IMD	D	902	5/5	0.72	0.24	76,82,90,95	0
2	IMD	C	904	5/5	0.74	0.28	85,86,86,90	0
2	IMD	A	903	5/5	0.75	0.24	98,99,102,103	0
2	IMD	B	901	5/5	0.75	0.22	70,70,85,107	0
2	IMD	C	903	5/5	0.75	0.21	60,69,92,94	0
2	IMD	C	902	5/5	0.76	0.20	76,77,80,80	0
2	IMD	B	902	5/5	0.80	0.20	97,98,105,113	0
2	IMD	D	901	5/5	0.81	0.19	80,81,85,86	0
2	IMD	A	902	5/5	0.84	0.21	70,71,74,78	0
2	IMD	A	901	5/5	0.86	0.17	75,75,77,77	0
2	IMD	D	906	5/5	0.86	0.22	80,81,86,97	0
2	IMD	D	904	5/5	0.88	0.27	69,75,86,105	0
2	IMD	C	901	5/5	0.93	0.15	76,76,78,81	0
2	IMD	D	905	5/5	0.96	0.11	58,61,64,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.