



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:25 am BST

PDB ID : 5UE8  
Title : The crystal structure of Munc13-1 C1C2BMUN domain  
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Deposited on : 2016-12-29  
Resolution : 3.35 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

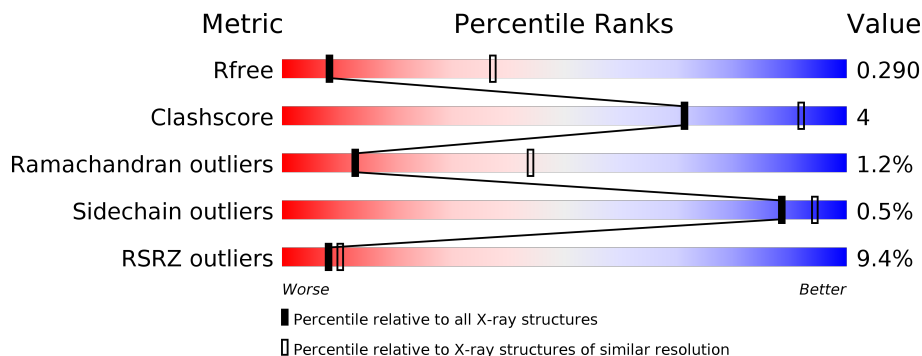
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 on 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	961	
1	B	961	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27058 atoms, of which 13455 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 Protein unc-13 homolog A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	847	13589	4342	6760	1153	1286	48	0	0	0
1	B	838	13463	4308	6695	1141	1272	47	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	756	TRP	LEU	engineered mutation	UNP Q62768
A	1450	GLU	-	linker	UNP Q62768
A	1451	PHE	-	linker	UNP Q62768
B	756	TRP	LEU	engineered mutation	UNP Q62768
B	1450	GLU	-	linker	UNP Q62768
B	1451	PHE	-	linker	UNP Q62768

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	2	Total 2	Zn 2	0	0

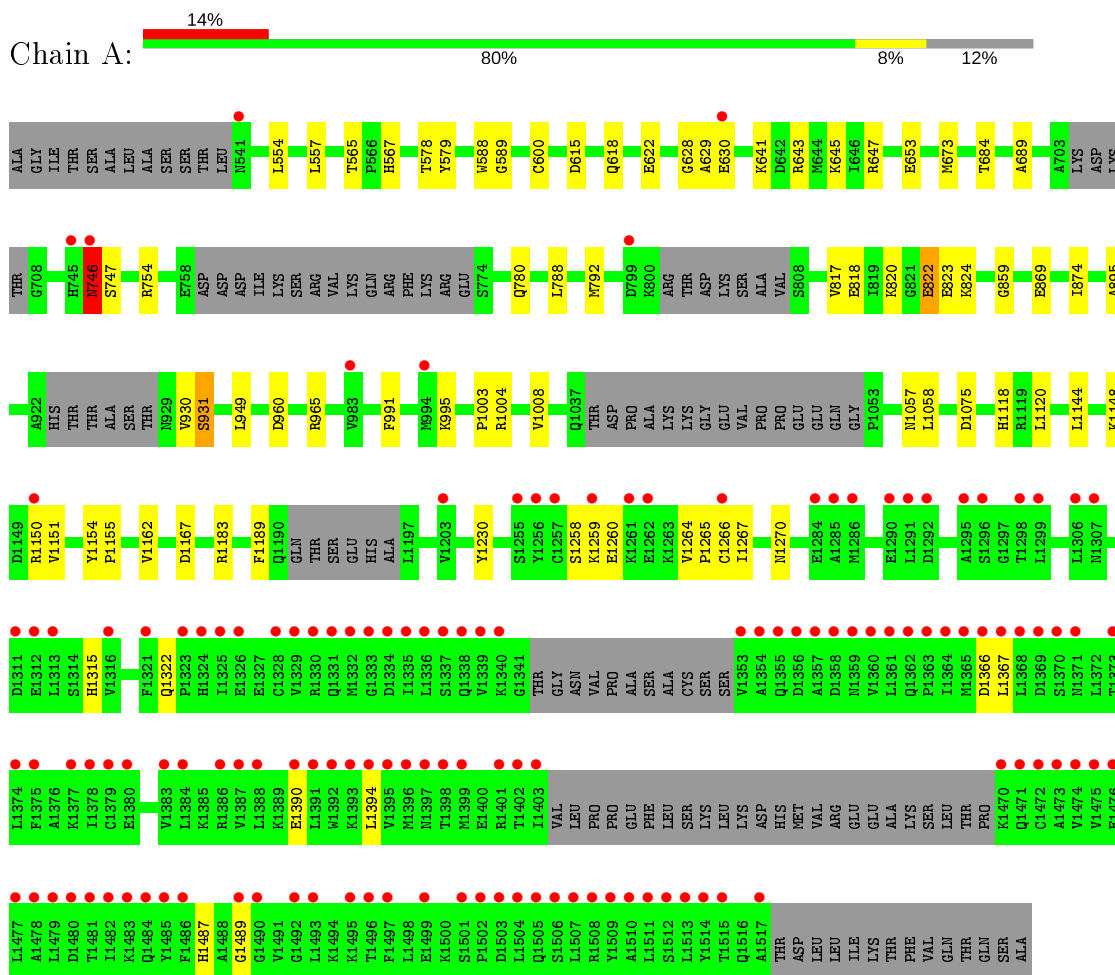
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

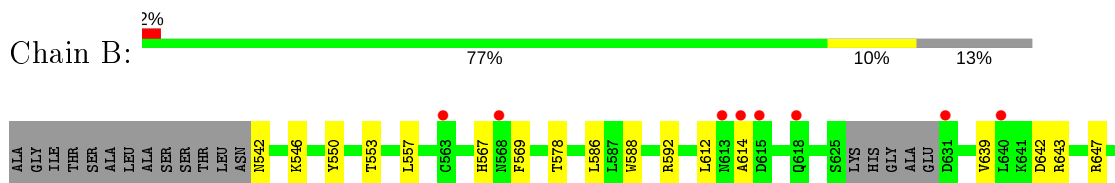
### 3 Residue-property plots

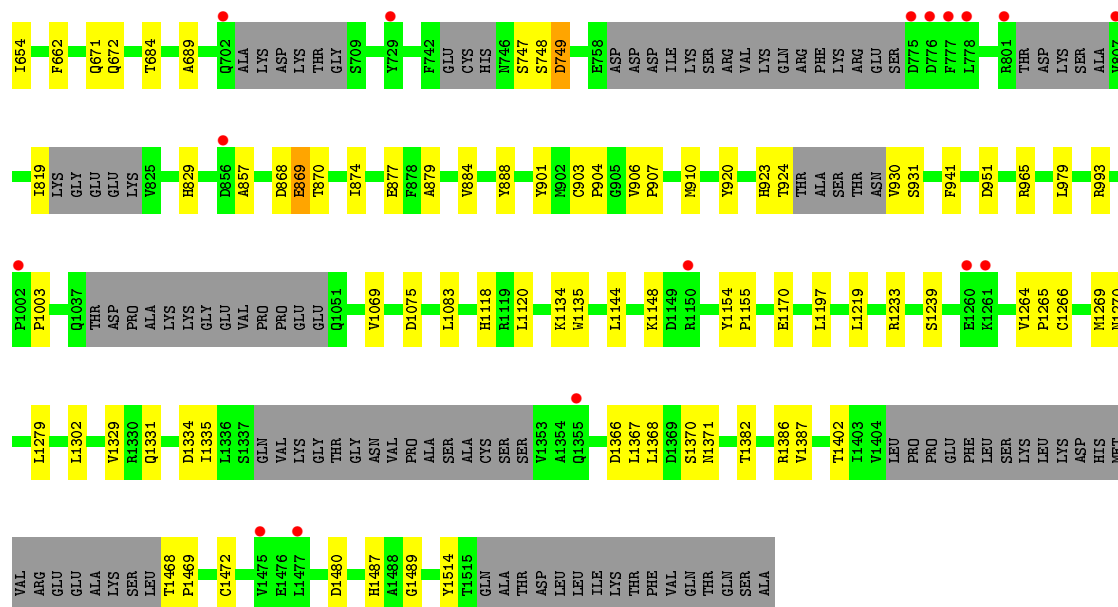
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein unc-13 homolog A



- Molecule 1: Protein unc-13 homolog A





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.15Å 86.35Å 202.14Å 90.00° 115.54° 90.00°	Depositor
Resolution (Å)	45.60 – 3.35 45.60 – 3.35	Depositor EDS
% Data completeness (in resolution range)	75.3 (45.60-3.35) 75.3 (45.60-3.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 3.32Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.252 , 0.290 0.252 , 0.290	Depositor DCC
$R_{free}$ test set	1490 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtrriage
Anisotropy	0.799	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 20.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	27058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: ZN, CL

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	0.25	0/6965	0.43	0/9403
1	B	0.27	0/6903	0.44	0/9325
All	All	0.26	0/13868	0.43	0/18728

There are no bond length outliers.

There are no bond angle outliers.

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	6829	6760	6757	40	0
1	B	6768	6695	6698	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	13603	13455	13455	95	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 (95) 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:642:ASP:OD1	1:B:643:ARG:N	2.20	0.75
1:B:868:ASP:O	1:B:870:THR:N	2.21	0.73
1:A:822:GLU:N	1:A:822:GLU:OE1	2.32	0.61
1:B:879:ALA:HA	1:B:884:VAL:HG22	1.84	0.59
1:A:1366:ASP:OD1	1:A:1367:LEU:N	2.36	0.59
1:A:628:GLY:O	1:A:630:GLU:N	2.36	0.58
1:B:923:HIS:O	1:B:923:HIS:ND1	2.36	0.57
1:A:557:LEU:HD21	1:A:874:ILE:HA	1.88	0.56
1:A:1144:LEU:O	1:A:1148:LYS:N	2.37	0.56
1:A:554:LEU:HD22	1:A:673:MET:HE1	1.88	0.56
1:B:1170:GLU:OE1	1:B:1233:ARG:NH2	2.37	0.55
1:B:557:LEU:O	1:B:647:ARG:NE	2.40	0.55
1:A:1189:PHE:HB3	1:A:1267:ILE:HD11	1.89	0.53
1:B:906:VAL:HG12	1:B:910:MET:HE2	1.92	0.52
1:B:1331:GLN:O	1:B:1335:ILE:HG13	2.10	0.52
1:A:565:THR:OG1	1:A:643:ARG:NH1	2.44	0.49
1:B:979:LEU:HG	1:B:1083:LEU:HD11	1.94	0.49
1:A:689:ALA:HA	1:A:818:GLU:O	2.13	0.49
1:B:1331:GLN:O	1:B:1334:ASP:OD1	2.30	0.48
1:A:557:LEU:O	1:A:647:ARG:NE	2.45	0.48
1:B:1144:LEU:O	1:B:1148:LYS:N	2.45	0.48
1:B:1118:HIS:HB3	1:B:1120:LEU:HD13	1.95	0.48
1:A:1258:SER:O	1:A:1260:GLU:N	2.39	0.47
1:B:557:LEU:HD21	1:B:877:GLU:HB2	1.95	0.47
1:A:822:GLU:O	1:A:824:LYS:N	2.45	0.47
1:A:1264:VAL:O	1:A:1267:ILE:HG13	2.14	0.47
1:A:1057:ASN:OD1	1:A:1058:LEU:N	2.47	0.47
1:A:1315:HIS:ND1	1:A:1390:GLU:OE2	2.47	0.47
1:B:1154:TYR:N	1:B:1155:PRO:CD	2.78	0.47
1:A:788:LEU:HB3	1:A:817:VAL:HG21	1.96	0.47
1:A:578:THR:HG22	1:A:579:TYR:N	2.30	0.46
1:A:1150:ARG:HB3	1:A:1151:VAL:HG12	1.98	0.46
1:A:567:HIS:CE1	1:A:600:CYS:SG	3.08	0.46
1:B:1197:LEU:O	1:B:1270:ASN:HB3	2.15	0.46
1:B:1329:VAL:HG12	1:B:1402:THR:OG1	2.15	0.46
1:B:903:CYS:SG	1:B:904:PRO:HD2	2.55	0.46
1:B:747:SER:C	1:B:749:ASP:H	2.18	0.46
1:A:653:GLU:OE1	1:A:653:GLU:N	2.39	0.46
1:B:869:GLU:HG3	1:B:870:THR:N	2.30	0.46
1:B:1279:LEU:HD11	1:B:1302:LEU:HD23	1.97	0.46
1:A:1162:VAL:HG21	1:A:1230:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1266:CYS:O	1:B:1270:ASN:ND2	2.49	0.46
1:B:951:ASP:OD1	1:B:993:ARG:NH2	2.49	0.46
1:A:1118:HIS:HB3	1:A:1120:LEU:HD13	1.97	0.45
1:A:1154:TYR:N	1:A:1155:PRO:CD	2.79	0.45
1:B:1334:ASP:OD1	1:B:1335:ILE:N	2.49	0.45
1:A:822:GLU:HG2	1:A:822:GLU:O	2.17	0.45
1:B:550:TYR:O	1:B:553:THR:HG22	2.17	0.45
1:B:588:TRP:H	1:B:592:ARG:HG3	1.82	0.44
1:B:1069:VAL:HG21	1:B:1135:TRP:HZ3	1.83	0.44
1:A:965:ARG:NH1	1:A:1075:ASP:OD1	2.43	0.44
1:B:689:ALA:HB2	1:B:819:ILE:HG22	2.00	0.44
1:B:1239:SER:HA	1:B:1302:LEU:HD22	1.99	0.44
1:B:1468:THR:N	1:B:1469:PRO:CD	2.81	0.44
1:B:901:TYR:O	1:B:907:PRO:HD3	2.18	0.44
1:B:639:VAL:O	1:B:642:ASP:OD1	2.36	0.44
1:A:991:PHE:CE1	1:A:995:LYS:HG3	2.53	0.43
1:A:1487:HIS:NE2	1:A:1489:GLY:O	2.50	0.43
1:A:895:ALA:HA	1:A:949:LEU:HD21	2.01	0.43
1:B:747:SER:O	1:B:749:ASP:N	2.51	0.43
1:A:1264:VAL:HB	1:A:1265:PRO:HD3	2.01	0.43
1:A:930:VAL:HG22	1:A:931:SER:N	2.34	0.43
1:A:746:ASN:ND2	1:A:747:SER:H	2.16	0.42
1:B:569:PHE:CZ	1:B:612:LEU:CD1	3.02	0.42
1:B:642:ASP:OD1	1:B:642:ASP:C	2.57	0.42
1:B:906:VAL:HG12	1:B:910:MET:CE	2.48	0.42
1:B:1134:LYS:HD2	1:B:1219:LEU:O	2.19	0.42
1:B:1487:HIS:NE2	1:B:1489:GLY:O	2.52	0.42
1:B:671:GLN:HG3	1:B:672:GLN:N	2.34	0.42
1:A:1266:CYS:O	1:A:1270:ASN:ND2	2.52	0.42
1:A:615:ASP:HB3	1:A:618:GLN:HB2	2.02	0.42
1:B:888:TYR:CE1	1:B:941:PHE:HA	2.54	0.42
1:B:829:HIS:ND1	1:B:884:VAL:HG12	2.35	0.42
1:B:567:HIS:HB2	1:B:569:PHE:CE2	2.55	0.42
1:B:557:LEU:HD11	1:B:874:ILE:HG23	2.02	0.42
1:A:641:LYS:O	1:A:645:LYS:HG2	2.20	0.42
1:B:578:THR:O	1:B:586:LEU:HD12	2.20	0.42
1:B:557:LEU:HD22	1:B:654:ILE:HD11	2.02	0.42
1:A:754:ARG:NE	1:A:780:GLN:OE1	2.53	0.41
1:B:1329:VAL:CG1	1:B:1402:THR:OG1	2.68	0.41
1:B:1269:MET:HE1	1:B:1387:VAL:CG2	2.50	0.41
1:B:1472:CYS:SG	1:B:1514:TYR:HD2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LYS:HG2	1:B:662:PHE:HD2	1.85	0.41
1:A:1322:GLN:OE1	1:A:1394:LEU:HD11	2.21	0.41
1:A:1150:ARG:HB3	1:A:1151:VAL:CG1	2.50	0.41
1:A:588:TRP:CG	1:A:589:GLY:N	2.88	0.41
1:B:1382:THR:O	1:B:1386:ARG:HG2	2.21	0.41
1:B:1264:VAL:HB	1:B:1265:PRO:HD3	2.03	0.41
1:B:923:HIS:O	1:B:924:THR:OG1	2.36	0.41
1:A:1004:ARG:O	1:A:1008:VAL:HG23	2.21	0.40
1:B:1367:LEU:O	1:B:1371:ASN:HB2	2.21	0.40
1:A:618:GLN:O	1:A:622:GLU:HG3	2.21	0.40
1:B:1366:ASP:O	1:B:1370:SER:HB3	2.22	0.40
1:B:930:VAL:O	1:B:930:VAL:HG22	2.20	0.40
1:B:965:ARG:NH1	1:B:1075:ASP:OD1	2.52	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	829/961 (86%)	761 (92%)	57 (7%)	11 (1%)	12	42
1	B	816/961 (85%)	754 (92%)	53 (6%)	9 (1%)	14	46
All	All	1645/1922 (86%)	1515 (92%)	110 (7%)	20 (1%)	13	44

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	ALA
1	B	749	ASP
1	B	869	GLU
1	A	746	ASN
1	A	820	LYS

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Mol	Chain	Res	Type
1	A	822	GLU
1	A	931	SER
1	A	1259	LYS
1	B	614	ALA
1	B	748	SER
1	B	857	ALA
1	A	823	GLU
1	A	859	GLY
1	B	684	THR
1	A	684	THR
1	A	869	GLU
1	B	931	SER
1	B	1368	LEU
1	A	1003	PRO
1	B	1003	PRO

### 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	762/861 (88%)	757 (99%)	5 (1%)	84	92
1	B	758/861 (88%)	755 (100%)	3 (0%)	91	95
All	All	1520/1722 (88%)	1512 (100%)	8 (0%)	88	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	746	ASN
1	A	792	MET
1	A	960	ASP
1	A	1167	ASP
1	A	1183	ARG
1	B	542	ASN
1	B	920	TYR
1	B	1480	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	746	ASN
1	A	1085	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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, 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	847/961 (88%)	0.90	135 (15%) <b>1</b> <b>2</b>	18, 51, 175, 205	0
1	B	838/961 (87%)	0.39	24 (2%) 51 54	13, 49, 95, 134	0
All	All	1685/1922 (87%)	0.65	159 (9%) <b>8</b> <b>10</b>	13, 51, 161, 205	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1479	LEU	12.1
1	A	1353	VAL	7.5
1	A	1337	SER	7.1
1	A	1364	ILE	7.0
1	A	1332	MET	7.0
1	A	1365	MET	6.9
1	A	1403	ILE	6.6
1	A	1392	TRP	6.4
1	A	1292	ASP	6.2
1	A	1475	VAL	5.7
1	A	1335	ILE	5.4
1	A	1391	LEU	5.4
1	A	1486	PHE	5.4
1	A	1511	LEU	5.3
1	A	1470	LYS	5.3
1	A	1502	PRO	5.3
1	A	1299	LEU	5.2
1	A	1493	LEU	5.2
1	A	1482	ILE	5.2
1	A	1339	VAL	5.1
1	A	1473	ALA	5.0
1	A	1490	GLY	5.0
1	A	1478	ALA	4.9
1	A	1477	LEU	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1514	TYR	4.9
1	A	1387	VAL	4.8
1	A	1371	ASN	4.7
1	A	1499	GLU	4.6
1	A	1375	PHE	4.6
1	A	1325	ILE	4.5
1	A	1515	THR	4.5
1	A	1378	ILE	4.5
1	A	1380	GLU	4.5
1	A	1359	ASN	4.4
1	A	1354	ALA	4.4
1	A	1395	VAL	4.4
1	A	1476	GLU	4.3
1	A	1510	ALA	4.3
1	A	1333	GLY	4.2
1	A	1336	LEU	4.1
1	A	1503	ASP	4.1
1	A	1504	LEU	4.0
1	A	1362	GLN	4.0
1	A	1355	GLN	4.0
1	A	1298	THR	3.9
1	A	1361	LEU	3.9
1	A	1328	CYS	3.9
1	A	1340	LYS	3.9
1	A	1366	ASP	3.9
1	A	1402	THR	3.9
1	A	1295	ALA	3.8
1	A	1398	THR	3.8
1	A	1290	GLU	3.7
1	A	1360	VAL	3.7
1	A	1259	LYS	3.7
1	A	1331	GLN	3.7
1	A	1481	THR	3.6
1	A	1324	HIS	3.6
1	A	1517	ALA	3.6
1	A	1399	MET	3.6
1	A	1474	VAL	3.6
1	A	1507	LEU	3.6
1	A	1483	LYS	3.5
1	A	1261	LYS	3.5
1	A	1394	LEU	3.5
1	A	1369	ASP	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1296	SER	3.5
1	A	1313	LEU	3.5
1	A	1374	LEU	3.4
1	A	1505	GLN	3.4
1	A	1396	MET	3.4
1	A	1356	ASP	3.4
1	A	1338	GLN	3.4
1	A	1388	LEU	3.3
1	A	1326	GLU	3.3
1	A	1291	LEU	3.3
1	A	1367	LEU	3.2
1	A	1489	GLY	3.2
1	A	1312	GLU	3.2
1	A	1472	CYS	3.1
1	A	1484	GLN	3.1
1	A	1330	ARG	3.1
1	A	1485	TYR	3.1
1	A	1386	ARG	3.1
1	A	1480	ASP	3.1
1	A	1323	PRO	3.0
1	A	1377	LYS	3.0
1	B	1150	ARG	3.0
1	B	563	CYS	3.0
1	A	746	ASN	2.9
1	A	1256	TYR	2.9
1	A	1286	MET	2.8
1	A	1321	PHE	2.8
1	A	1513	LEU	2.8
1	B	776	ASP	2.8
1	A	1501	SER	2.8
1	A	1307	ASN	2.8
1	A	1150	ARG	2.8
1	A	1471	GLN	2.8
1	A	1509	TYR	2.8
1	A	1379	CYS	2.7
1	B	568	ASN	2.7
1	A	1363	PRO	2.7
1	B	775	ASP	2.7
1	A	1497	PHE	2.6
1	A	1266	CYS	2.6
1	A	1383	VAL	2.5
1	B	801	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1370	SER	2.5
1	A	1492	GLY	2.5
1	B	729	TYR	2.5
1	A	1255	SER	2.5
1	B	778	LEU	2.5
1	B	1355	GLN	2.5
1	A	1390	GLU	2.5
1	A	983	VAL	2.5
1	A	1203	VAL	2.5
1	A	745	HIS	2.5
1	A	1384	LEU	2.5
1	A	1334	ASP	2.5
1	B	1477	LEU	2.5
1	A	799	ASP	2.4
1	A	1284	GLU	2.4
1	B	856	ASP	2.4
1	A	1358	ASP	2.4
1	A	1329	VAL	2.4
1	A	1401	ARG	2.4
1	B	613	ASN	2.4
1	B	1475	VAL	2.4
1	B	618	GLN	2.3
1	A	630	GLU	2.3
1	A	1508	ARG	2.3
1	A	1262	GLU	2.3
1	A	1285	ALA	2.3
1	B	777	PHE	2.3
1	B	807	VAL	2.3
1	B	702	GLN	2.3
1	B	614	ALA	2.3
1	A	1512	SER	2.3
1	B	1260	GLU	2.3
1	A	1373	THR	2.3
1	A	1368	LEU	2.2
1	A	1311	ASP	2.2
1	A	1357	ALA	2.2
1	B	640	LEU	2.2
1	B	615	ASP	2.2
1	A	1495	LYS	2.2
1	B	1261	LYS	2.2
1	B	1002	PRO	2.1
1	A	1496	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1316	VAL	2.1
1	B	631	ASP	2.1
1	A	1306	LEU	2.1
1	A	1257	CYS	2.1
1	A	1393	LYS	2.0
1	A	541	ASN	2.0
1	A	1506	SER	2.0
1	A	994	MET	2.0
1	A	1397	ASN	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 carbohydrates 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
3	CL	B	1601	1/1	0.93	0.16	8,8,8,8	0
2	ZN	A	1702	1/1	0.95	0.13	23,23,23,23	0
2	ZN	B	1602	1/1	0.95	0.07	80,80,80,80	0
3	CL	A	1703	1/1	0.96	0.19	8,8,8,8	0
2	ZN	B	1603	1/1	0.96	0.09	58,58,58,58	0
2	ZN	A	1701	1/1	0.99	0.13	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.