



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:51 AM UTC

PDB ID : 5UE8 / pdb_00005ue8
Title : The crystal structure of Munc13-1 C1C2BMUN domain
Authors : Tomchick, D.R.; Rizo, J.; Xu, J.
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

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

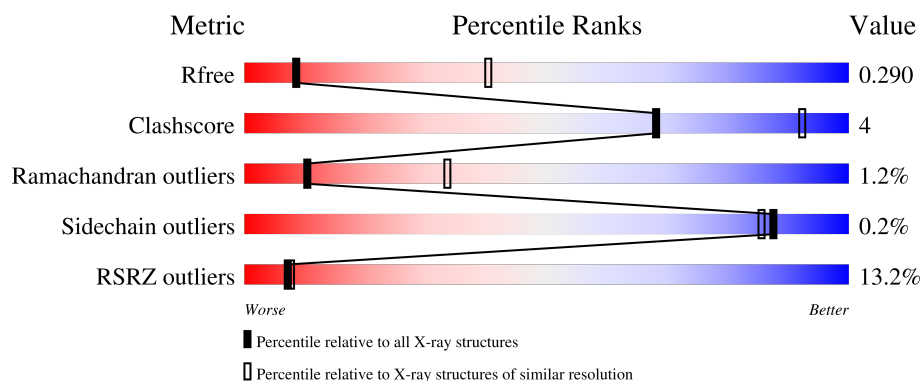
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	961	16% 80% 8% 12%
1	B	961	7% 77% 10% 13%

2 Entry composition

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
1	A	847	Total	C	H	N	O	S	0	0	0
			13589	4342	6760	1153	1286	48			
1	B	838	Total	C	H	N	O	S	0	0	0
			13463	4308	6695	1141	1272	47			

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 (CCD ID: ZN) (formula: Zn).

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

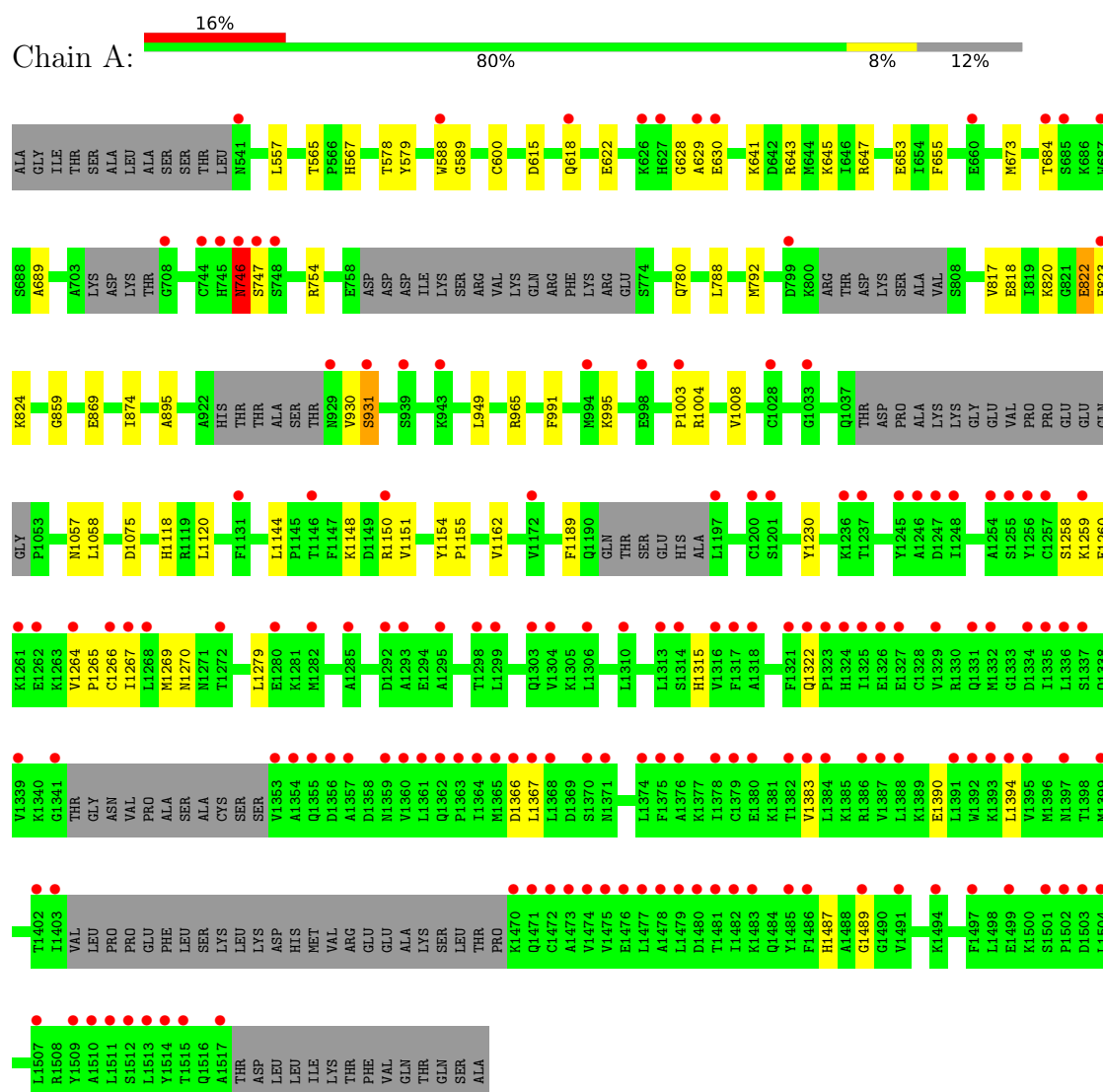
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

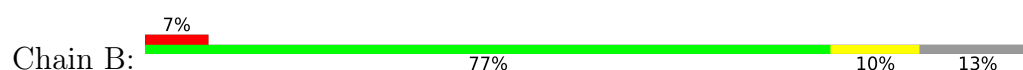
3 Residue-property plots [i](#)

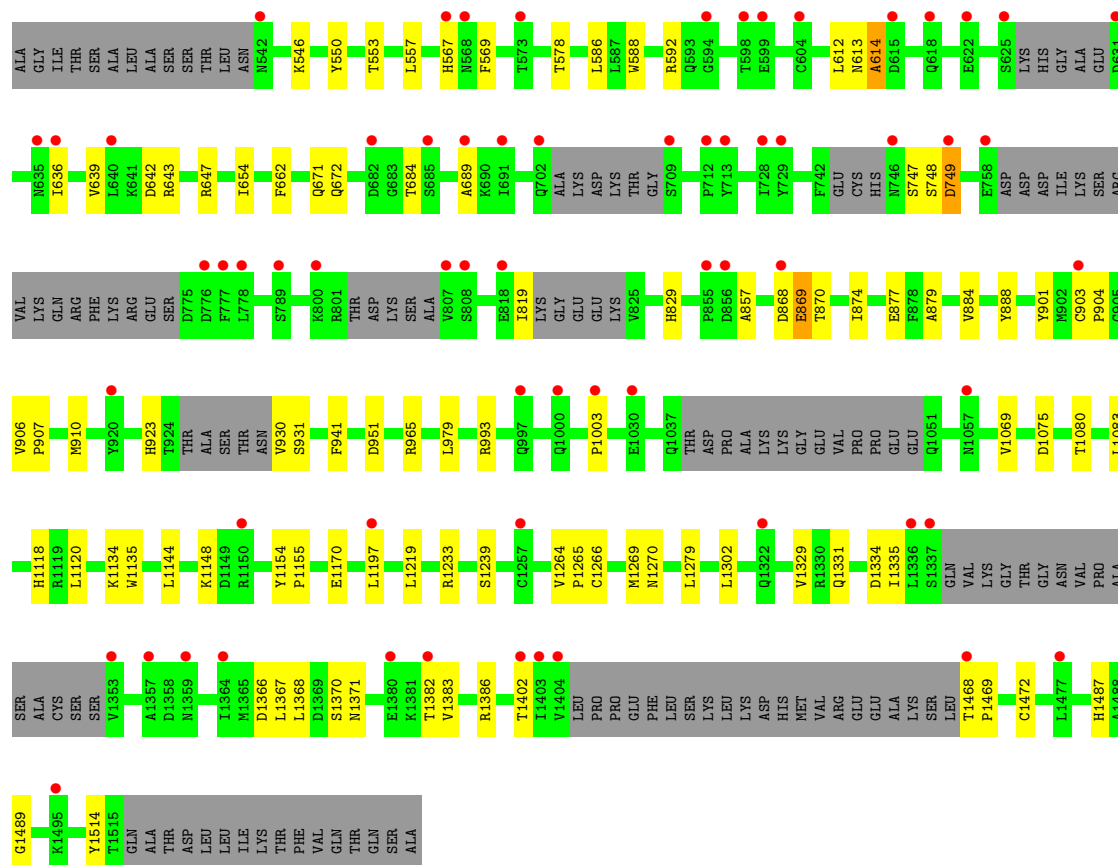
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 3.32Å)	Xtriage
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 (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	27058	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage'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.*

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

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	0.13	0/6965	0.35	0/9403
1	B	0.15	0/6903	0.36	0/9325
All	All	0.14	0/13868	0.36	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

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	42	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	97	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 (97) 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:OE1	1:A:822:GLU:N	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: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:1331:GLN:O	1:B:1335:ILE:HG13	2.10	0.52
1:B:747:SER:C	1:B:749:ASP:H	2.18	0.50
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:B:642:ASP:OD1	1:B:642:ASP:C	2.57	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:567:HIS:CE1	1:A:600:CYS:SG	3.08	0.46
1:A:1150:ARG:HB3	1:A:1151:VAL:HG12	1.98	0.46
1:B:903:CYS:SG	1:B:904:PRO:HD2	2.55	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: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
1:B:1266:CYS:O	1:B:1270:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:822:GLU:HG2	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:901:TYR:O	1:B:907:PRO:HD3	2.18	0.44
1:B:1468:THR:N	1:B:1469:PRO:CD	2.81	0.44
1:B:639:VAL:O	1:B:642:ASP:OD1	2.36	0.44
1:B:1075:ASP:O	1:B:1080:THR:OG1	2.34	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:930:VAL:HG22	1:A:931:SER:N	2.34	0.43
1:A:1264:VAL:HB	1:A:1265:PRO:HD3	2.01	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: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:1269:MET:HE2	1:B:1383:VAL:HG13	2.01	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:615:ASP:HB3	1:A:618:GLN:HB2	2.02	0.42
1:A:1266:CYS:O	1:A:1270:ASN:ND2	2.52	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:557:LEU:HD11	1:B:874:ILE:HG23	2.02	0.42
1:B:567:HIS:HB2	1:B:569:PHE:CE2	2.55	0.42
1:A:641:LYS:O	1:A:645:LYS:HG2	2.20	0.42
1:A:655:PHE:CD2	1:A:673:MET:HE1	2.55	0.42
1:B:557:LEU:HD22	1:B:654:ILE:HD11	2.02	0.42
1:B:578:THR:O	1:B:586:LEU:HD12	2.20	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: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:1279:LEU:HD23	1:A:1279:LEU:C	2.46	0.41
1:A:1322:GLN:OE1	1:A:1394:LEU:HD11	2.21	0.41
1:A:588:TRP:CG	1:A:589:GLY:N	2.88	0.41
1:A:1150:ARG:HB3	1:A:1151:VAL:CG1	2.50	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:613:ASN:O	1:B:614:ALA:C	2.63	0.41
1:A:1004:ARG:O	1:A:1008:VAL:HG23	2.21	0.40
1:A:1269:MET:HE2	1:A:1383:VAL:HG13	2.02	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:930:VAL:HG22	1:B:930:VAL:O	2.20	0.40
1:B:1366:ASP:O	1:B:1370:SER:HB3	2.22	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

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	829/961 (86%)	761 (92%)	57 (7%)	11 (1%)	9	32
1	B	816/961 (85%)	754 (92%)	53 (6%)	9 (1%)	11	36
All	All	1645/1922 (86%)	1515 (92%)	110 (7%)	20 (1%)	10	33

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	ALA
1	B	749	ASP
1	B	869	GLU

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Mol	Chain	Res	Type
1	A	746	ASN
1	A	820	LYS
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 ⓘ

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%)	760 (100%)	2 (0%)	86	84
1	B	758/861 (88%)	757 (100%)	1 (0%)	88	88
All	All	1520/1722 (88%)	1517 (100%)	3 (0%)	87	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	746	ASN
1	A	792	MET
1	B	636	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	739	ASN
1	A	889	GLN
1	A	967	ASN
1	A	1029	HIS
1	A	1085	GLN
1	A	1308	ASN
1	B	548	HIS
1	B	672	GLN
1	B	780	GLN
1	B	831	GLN
1	B	967	ASN
1	B	1029	HIS
1	B	1106	GLN
1	B	1169	ASN

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 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, 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	847/961 (88%)	1.06	158 (18%) 3 4	17, 56, 193, 227	0
1	B	838/961 (87%)	0.62	65 (7%) 19 15	11, 52, 106, 147	0
All	All	1685/1922 (87%)	0.84	223 (13%) 7 8	11, 54, 177, 227	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1364	ILE	9.1
1	A	1335	ILE	7.1
1	A	1475	VAL	7.0
1	A	746	ASN	6.8
1	A	1479	LEU	6.3
1	A	1474	VAL	5.9
1	A	1360	VAL	5.9
1	A	748	SER	5.9
1	A	1341	GLY	5.4
1	A	1374	LEU	5.4
1	B	1402	THR	5.3
1	A	1395	VAL	5.3
1	A	747	SER	5.2
1	A	1375	PHE	5.2
1	B	749	ASP	5.2
1	A	1403	ILE	5.1
1	A	1353	VAL	5.0
1	B	1403	ILE	5.0
1	A	1477	LEU	5.0
1	A	1365	MET	5.0
1	A	1507	LEU	4.9
1	A	1391	LEU	4.9
1	A	1511	LEU	4.8
1	A	1378	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1332	MET	4.7
1	A	684	THR	4.6
1	A	1316	VAL	4.4
1	A	1299	LEU	4.4
1	A	1482	ILE	4.4
1	A	1321	PHE	4.3
1	B	807	VAL	4.3
1	A	1478	ALA	4.3
1	B	778	LEU	4.1
1	A	1339	VAL	4.1
1	A	1486	PHE	4.0
1	A	1356	ASP	3.9
1	A	1497	PHE	3.9
1	A	1379	CYS	3.9
1	A	1357	ALA	3.9
1	A	1392	TRP	3.9
1	A	1517	ALA	3.9
1	A	1255	SER	3.8
1	A	1325	ILE	3.8
1	A	1513	LEU	3.7
1	A	1476	GLU	3.6
1	A	943	LYS	3.6
1	A	1336	LEU	3.6
1	A	1303	GLN	3.6
1	B	1404	VAL	3.5
1	A	1354	ALA	3.5
1	B	777	PHE	3.5
1	B	604	CYS	3.4
1	A	1399	MET	3.4
1	A	1201	SER	3.4
1	A	1256	TYR	3.4
1	A	1257	CYS	3.3
1	A	1359	ASN	3.3
1	A	1512	SER	3.3
1	A	1481	THR	3.3
1	A	1262	GLU	3.3
1	A	1503	ASP	3.3
1	A	745	HIS	3.3
1	B	618	GLN	3.2
1	A	1237	THR	3.2
1	B	800	LYS	3.2
1	A	799	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1504	LEU	3.2
1	A	744	CYS	3.2
1	A	1402	THR	3.2
1	A	1472	CYS	3.2
1	B	746	ASN	3.2
1	A	1368	LEU	3.2
1	A	1514	TYR	3.2
1	A	1491	VAL	3.2
1	B	685	SER	3.2
1	B	615	ASP	3.2
1	B	631	ASP	3.2
1	B	1030	GLU	3.2
1	A	1382	THR	3.1
1	B	789	SER	3.1
1	B	729	TYR	3.1
1	A	1131	PHE	3.1
1	A	1470	LYS	3.1
1	A	1248	ILE	3.1
1	B	702	GLN	3.0
1	A	1246	ALA	3.0
1	A	1310	LEU	3.0
1	A	1329	VAL	3.0
1	B	1337	SER	3.0
1	A	1473	ALA	3.0
1	A	1326	GLU	3.0
1	A	1388	LEU	3.0
1	A	1387	VAL	3.0
1	A	1371	ASN	3.0
1	A	1197	LEU	2.9
1	A	1393	LYS	2.9
1	B	1380	GLU	2.9
1	A	1285	ALA	2.9
1	A	1367	LEU	2.9
1	B	1477	LEU	2.9
1	B	856	ASP	2.9
1	B	1382	THR	2.9
1	A	1323	PRO	2.9
1	A	1324	HIS	2.9
1	A	1384	LEU	2.9
1	A	1366	ASP	2.9
1	A	1272	THR	2.9
1	B	1150	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1471	GLN	2.8
1	A	1370	SER	2.8
1	A	1361	LEU	2.8
1	B	920	TYR	2.8
1	A	998	GLU	2.8
1	B	635	ASN	2.8
1	A	1295	ALA	2.8
1	A	1386	ARG	2.8
1	A	1337	SER	2.7
1	A	1485	TYR	2.7
1	A	1317	PHE	2.7
1	A	1292	ASP	2.7
1	A	618	GLN	2.7
1	A	1331	GLN	2.7
1	B	997	GLN	2.7
1	A	1380	GLU	2.7
1	B	573	THR	2.7
1	A	1314	SER	2.6
1	B	728	ILE	2.6
1	A	1363	PRO	2.6
1	B	1353	VAL	2.6
1	A	685	SER	2.6
1	B	567	HIS	2.6
1	A	1003	PRO	2.6
1	B	598	THR	2.6
1	A	1282	MET	2.6
1	A	1489	GLY	2.6
1	A	1313	LEU	2.6
1	B	1468	THR	2.6
1	A	931	SER	2.6
1	A	541	ASN	2.6
1	A	1268	LEU	2.6
1	A	1499	GLU	2.6
1	A	1172	VAL	2.6
1	B	712	PRO	2.5
1	B	599	GLU	2.5
1	A	626	LYS	2.5
1	B	758	GLU	2.5
1	B	1003	PRO	2.5
1	A	1501	SER	2.5
1	B	682	ASP	2.5
1	A	1355	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1304	VAL	2.4
1	A	1298	THR	2.4
1	A	1397	ASN	2.4
1	B	542	ASN	2.4
1	B	776	ASP	2.4
1	A	1150	ARG	2.4
1	A	1280	GLU	2.4
1	A	1327	GLU	2.4
1	B	1197	LEU	2.4
1	B	1336	LEU	2.4
1	A	687	TRP	2.4
1	B	855	PRO	2.4
1	A	1510	ALA	2.4
1	A	823	GLU	2.4
1	B	709	SER	2.4
1	B	1257	CYS	2.4
1	A	1394	LEU	2.4
1	A	1200	CYS	2.4
1	A	708	GLY	2.3
1	A	1318	ALA	2.3
1	B	713	TYR	2.3
1	A	1264	VAL	2.3
1	A	1033	GLY	2.3
1	A	629	ALA	2.3
1	B	568	ASN	2.3
1	B	868	ASP	2.3
1	B	818	GLU	2.3
1	A	1494	LYS	2.3
1	A	588	TRP	2.3
1	B	691	ILE	2.3
1	A	994	MET	2.3
1	A	1480	ASP	2.3
1	A	1254	ALA	2.3
1	B	1057	ASN	2.3
1	B	1322	GLN	2.3
1	A	627	HIS	2.3
1	B	903	CYS	2.3
1	B	622	GLU	2.2
1	A	1502	PRO	2.2
1	A	939	SER	2.2
1	B	1000	GLN	2.2
1	B	1359	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1245	TYR	2.2
1	A	1247	ASP	2.2
1	A	1236	LYS	2.2
1	A	1483	LYS	2.2
1	A	1362	GLN	2.2
1	A	1266	CYS	2.2
1	A	1293	ALA	2.2
1	A	1334	ASP	2.2
1	B	636	ILE	2.2
1	A	660	GLU	2.2
1	B	594	GLY	2.2
1	B	640	LEU	2.1
1	A	1261	LYS	2.1
1	B	808	SER	2.1
1	B	1495	LYS	2.1
1	A	929	ASN	2.1
1	A	1509	TYR	2.1
1	A	1146	THR	2.1
1	A	1515	THR	2.1
1	B	1364	ILE	2.1
1	B	625	SER	2.1
1	A	1376	ALA	2.1
1	A	1259	LYS	2.1
1	A	1267	ILE	2.1
1	B	689	ALA	2.1
1	B	1357	ALA	2.1
1	A	1322	GLN	2.1
1	A	630	GLU	2.1
1	A	1383	VAL	2.0
1	A	1028	CYS	2.0
1	A	1306	LEU	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, 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($\text{\AA}^2$)	Q<0.9
3	CL	B	1601	1/1	0.85	0.11	8,8,8,8	0
3	CL	A	1703	1/1	0.87	0.08	8,8,8,8	0
2	ZN	A	1702	1/1	0.95	0.06	23,23,23,23	0
2	ZN	B	1602	1/1	0.95	0.06	80,80,80,80	0
2	ZN	B	1603	1/1	0.98	0.04	58,58,58,58	0
2	ZN	A	1701	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.