



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 AM UTC

PDB ID : 4Y21 / pdb_00004y21
Title : Crystal Structure of Munc13-1 MUN domain
Authors : Yang, X.Y.; Wang, S.; Sheng, Y.; Zhang, M.; Zou, W.J.; Wu, L.J.; Kang, L.J.;
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Deposited on : 2015-02-09
Resolution : 2.90 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

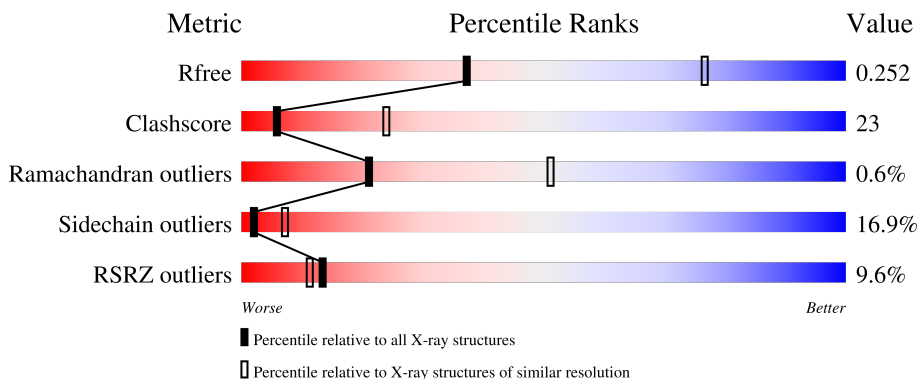
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	539	10% 58% 33% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4347 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 Protein unc-13 homolog A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4347	2773	725	821	28			

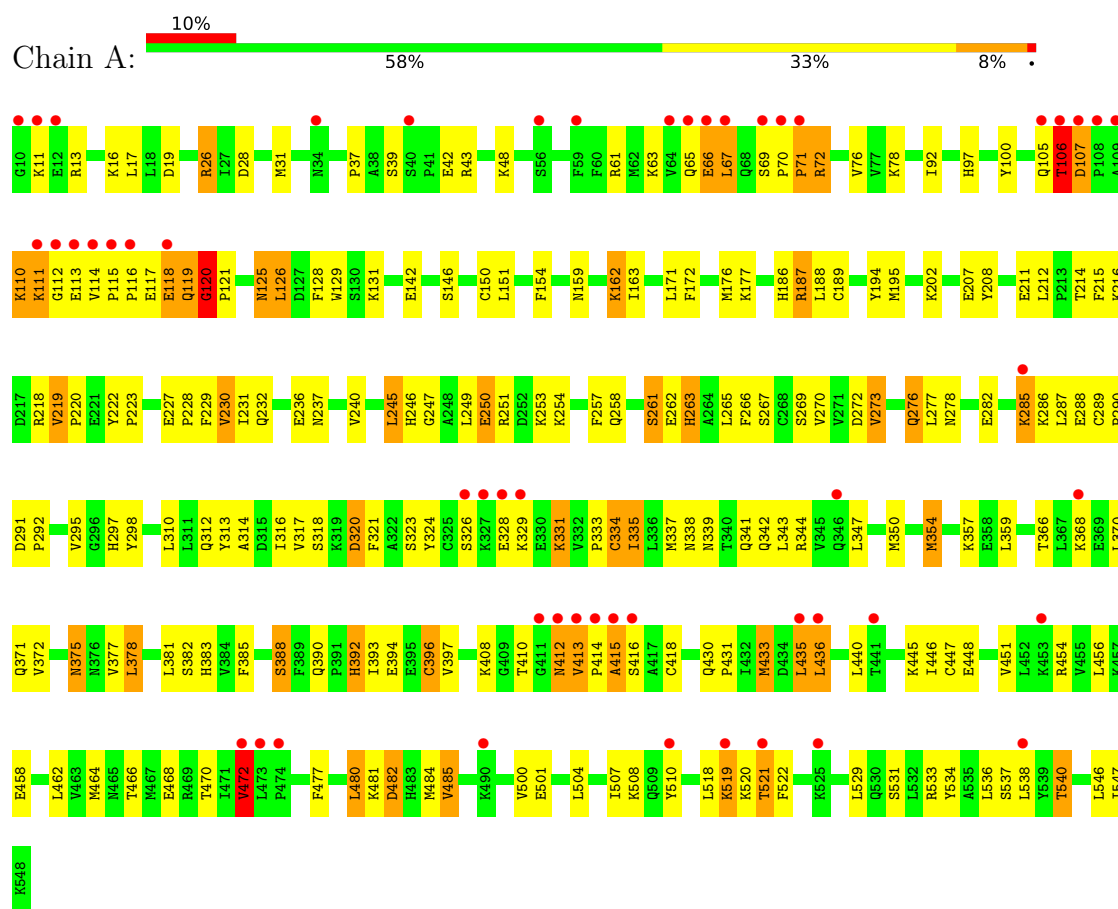
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	476	GLU	-	linker	UNP Q62768
A	477	PHE	-	linker	UNP Q62768

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: Protein unc-13 homolog A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.06Å 270.92Å 47.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.90) 99.2 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.217 , 0.252 0.218 , 0.252	Depositor DCC
R_{free} test set	1712 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.2	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	0.94	EDS
Total number of atoms	4347	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.47	0/4437	0.92	7/5995 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	120	GLY	CA-C-N	10.17	130.25	119.78
1	A	120	GLY	C-N-CA	10.17	130.25	119.78
1	A	115	PRO	CA-C-N	-9.74	109.72	119.76
1	A	115	PRO	C-N-CA	-9.74	109.72	119.76
1	A	546	LEU	N-CA-C	-6.38	101.51	110.50
1	A	115	PRO	N-CA-C	5.72	117.68	110.70
1	A	472	VAL	N-CA-C	-5.53	105.33	110.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	THR	Peptide
1	A	113	GLU	Peptide
1	A	120	GLY	Peptide

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	4347	0	4352	200	1
All	All	4347	0	4352	200	1

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 23.

All (200) 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:72:ARG:HB3	1:A:72:ARG:HH11	1.17	1.08
1:A:69:SER:C	1:A:71:PRO:HD2	1.83	1.03
1:A:72:ARG:HB3	1:A:72:ARG:NH1	1.74	1.01
1:A:69:SER:O	1:A:71:PRO:HD2	1.62	1.00
1:A:107:ASP:O	1:A:110:LYS:HG3	1.66	0.95
1:A:72:ARG:NH1	1:A:72:ARG:CB	2.30	0.94
1:A:69:SER:C	1:A:71:PRO:CD	2.43	0.91
1:A:436:LEU:C	1:A:436:LEU:HD13	1.98	0.88
1:A:116:PRO:HA	1:A:117:GLU:C	1.99	0.87
1:A:468:GLU:O	1:A:472:VAL:HG11	1.75	0.87
1:A:97:HIS:HB2	1:A:119:GLN:OE1	1.78	0.84
1:A:435:LEU:HD23	1:A:436:LEU:N	1.96	0.81
1:A:110:LYS:HD3	1:A:110:LYS:H	1.47	0.79
1:A:230:VAL:HG21	1:A:298:TYR:CZ	2.18	0.79
1:A:456:LEU:HB3	1:A:518:LEU:HD11	1.65	0.78
1:A:63:LYS:O	1:A:66:GLU:HG3	1.85	0.76
1:A:72:ARG:CZ	1:A:72:ARG:HB2	2.16	0.76
1:A:19:ASP:OD1	1:A:61:ARG:NH2	2.20	0.75
1:A:187:ARG:HH11	1:A:187:ARG:CG	2.00	0.75
1:A:105:GLN:HG3	1:A:107:ASP:HB2	1.66	0.74
1:A:187:ARG:HH11	1:A:187:ARG:HG2	1.53	0.72
1:A:341:GLN:HG2	1:A:448:GLU:HG2	1.69	0.72
1:A:120:GLY:HA2	1:A:128:PHE:CG	2.25	0.71
1:A:70:PRO:N	1:A:71:PRO:CD	2.54	0.70
1:A:468:GLU:OE1	1:A:531:SER:OG	2.08	0.70
1:A:195:MET:HE1	1:A:230:VAL:HB	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PRO:O	1:A:415:ALA:C	2.35	0.69
1:A:436:LEU:HG	1:A:510:TYR:CD2	2.28	0.68
1:A:72:ARG:HH11	1:A:72:ARG:CB	1.93	0.68
1:A:312:GLN:O	1:A:316:ILE:HG12	1.93	0.68
1:A:347:LEU:HD11	1:A:370:LEU:HD23	1.75	0.68
1:A:456:LEU:CB	1:A:518:LEU:HD11	2.23	0.68
1:A:278:ASN:OD1	1:A:350:MET:HE3	1.95	0.67
1:A:480:LEU:HB3	1:A:485:VAL:CG1	2.25	0.67
1:A:72:ARG:CB	1:A:72:ARG:CZ	2.69	0.66
1:A:97:HIS:CB	1:A:119:GLN:OE1	2.44	0.65
1:A:436:LEU:C	1:A:436:LEU:CD1	2.68	0.64
1:A:218:ARG:N	1:A:218:ARG:HD3	2.12	0.64
1:A:436:LEU:HD13	1:A:436:LEU:O	1.96	0.64
1:A:129:TRP:HB3	1:A:176:MET:HE1	1.79	0.64
1:A:468:GLU:O	1:A:472:VAL:CG1	2.45	0.64
1:A:187:ARG:HG2	1:A:187:ARG:NH1	2.11	0.63
1:A:106:THR:OG1	1:A:107:ASP:HA	1.99	0.63
1:A:477:PHE:HB3	1:A:484:MET:HG3	1.80	0.63
1:A:37:PRO:HD2	1:A:43:ARG:HG2	1.82	0.62
1:A:433:MET:HE3	1:A:510:TYR:CZ	2.34	0.62
1:A:390:GLN:HB2	1:A:462:LEU:HD21	1.81	0.62
1:A:26:ARG:HH21	1:A:76:VAL:HG13	1.65	0.61
1:A:435:LEU:HD23	1:A:436:LEU:CA	2.31	0.61
1:A:337:MET:HE1	1:A:382:SER:HA	1.81	0.61
1:A:218:ARG:N	1:A:218:ARG:CD	2.62	0.61
1:A:69:SER:C	1:A:71:PRO:HD3	2.25	0.60
1:A:313:TYR:CD1	1:A:343:LEU:HD11	2.36	0.60
1:A:125:ASN:ND2	1:A:125:ASN:C	2.59	0.60
1:A:251:ARG:NH2	1:A:272:ASP:OD2	2.34	0.60
1:A:342:GLN:HA	1:A:342:GLN:OE1	2.02	0.59
1:A:186:HIS:HB3	1:A:188:LEU:HD13	1.84	0.59
1:A:464:MET:HE1	1:A:504:LEU:HD11	1.85	0.58
1:A:333:PRO:O	1:A:337:MET:HG3	2.04	0.58
1:A:211:GLU:OE1	1:A:216:LYS:NZ	2.25	0.58
1:A:292:PRO:HA	1:A:295:VAL:HG12	1.84	0.58
1:A:383:HIS:HA	1:A:458:GLU:HG2	1.86	0.57
1:A:70:PRO:N	1:A:71:PRO:HD3	2.18	0.57
1:A:249:LEU:HD21	1:A:313:TYR:CE2	2.39	0.57
1:A:72:ARG:NH1	1:A:72:ARG:HB2	2.10	0.56
1:A:120:GLY:CA	1:A:128:PHE:CD1	2.88	0.56
1:A:414:PRO:O	1:A:416:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLY:O	1:A:251:ARG:HD3	2.06	0.56
1:A:347:LEU:C	1:A:347:LEU:HD23	2.31	0.56
1:A:430:GLN:N	1:A:431:PRO:HD2	2.21	0.56
1:A:230:VAL:CG2	1:A:298:TYR:CE1	2.89	0.56
1:A:413:VAL:O	1:A:415:ALA:HB3	2.05	0.55
1:A:230:VAL:HG21	1:A:298:TYR:CE1	2.40	0.55
1:A:118:GLU:O	1:A:120:GLY:N	2.38	0.55
1:A:410:THR:OG1	1:A:418:CYS:HB2	2.07	0.54
1:A:519:LYS:HE3	1:A:520:LYS:H	1.72	0.54
1:A:70:PRO:O	1:A:72:ARG:N	2.40	0.54
1:A:187:ARG:NH1	1:A:232:GLN:OE1	2.40	0.54
1:A:120:GLY:HA2	1:A:128:PHE:CD1	2.43	0.54
1:A:448:GLU:HB3	1:A:451:VAL:HG23	1.89	0.54
1:A:377:VAL:O	1:A:381:LEU:HB2	2.08	0.53
1:A:187:ARG:CG	1:A:187:ARG:NH1	2.66	0.53
1:A:436:LEU:CG	1:A:510:TYR:CD2	2.91	0.53
1:A:119:GLN:HE22	1:A:131:LYS:HE3	1.74	0.53
1:A:464:MET:CE	1:A:529:LEU:HD13	2.37	0.53
1:A:518:LEU:HD23	1:A:522:PHE:CD2	2.44	0.53
1:A:120:GLY:HA3	1:A:128:PHE:CE1	2.44	0.52
1:A:385:PHE:O	1:A:388:SER:HB3	2.08	0.52
1:A:245:LEU:HD12	1:A:273:VAL:HG21	1.91	0.52
1:A:106:THR:HG23	1:A:107:ASP:OD2	2.10	0.52
1:A:116:PRO:HA	1:A:118:GLU:N	2.24	0.52
1:A:436:LEU:HD11	1:A:510:TYR:CD2	2.46	0.50
1:A:540:THR:O	1:A:540:THR:HG23	2.09	0.50
1:A:331:LYS:H	1:A:331:LYS:CE	2.25	0.50
1:A:267:SER:OG	1:A:339:ASN:ND2	2.38	0.50
1:A:329:LYS:HG2	1:A:331:LYS:HZ1	1.76	0.50
1:A:519:LYS:HE3	1:A:520:LYS:N	2.26	0.50
1:A:48:LYS:HE2	1:A:150:CYS:O	2.12	0.50
1:A:261:SER:OG	1:A:263:HIS:ND1	2.45	0.49
1:A:118:GLU:OE1	1:A:119:GLN:N	2.46	0.49
1:A:125:ASN:C	1:A:125:ASN:HD22	2.20	0.49
1:A:448:GLU:HB3	1:A:451:VAL:CG2	2.42	0.49
1:A:111:LYS:HG2	1:A:112:GLY:O	2.12	0.49
1:A:262:GLU:OE1	1:A:262:GLU:N	2.43	0.49
1:A:480:LEU:HB3	1:A:485:VAL:HG11	1.93	0.49
1:A:310:LEU:HD12	1:A:370:LEU:HD21	1.95	0.49
1:A:282:GLU:O	1:A:286:LYS:HG3	2.13	0.49
1:A:236:GLU:O	1:A:240:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:MET:CE	1:A:382:SER:HA	2.43	0.48
1:A:413:VAL:HG22	1:A:414:PRO:HD2	1.95	0.48
1:A:508:LYS:NZ	1:A:533:ARG:HH22	2.10	0.48
1:A:347:LEU:HD23	1:A:347:LEU:O	2.13	0.48
1:A:334:CYS:HB3	1:A:446:ILE:HD12	1.96	0.48
1:A:317:VAL:HG23	1:A:318:SER:N	2.28	0.48
1:A:378:LEU:HD12	1:A:454:ARG:NH1	2.28	0.48
1:A:67:LEU:HD23	1:A:67:LEU:O	2.14	0.48
1:A:518:LEU:HD23	1:A:522:PHE:CE2	2.49	0.48
1:A:216:LYS:O	1:A:218:ARG:CD	2.62	0.48
1:A:435:LEU:HD23	1:A:436:LEU:HB2	1.96	0.48
1:A:202:LYS:HE2	1:A:288:GLU:OE1	2.13	0.47
1:A:212:LEU:O	1:A:216:LYS:N	2.43	0.47
1:A:186:HIS:HB3	1:A:188:LEU:CD1	2.44	0.47
1:A:249:LEU:HD13	1:A:316:ILE:HG21	1.97	0.47
1:A:186:HIS:O	1:A:188:LEU:HD12	2.14	0.47
1:A:172:PHE:CZ	1:A:176:MET:HE3	2.49	0.47
1:A:215:PHE:O	1:A:216:LYS:C	2.58	0.47
1:A:518:LEU:HD12	1:A:518:LEU:N	2.30	0.47
1:A:287:LEU:O	1:A:288:GLU:C	2.56	0.47
1:A:337:MET:HE1	1:A:382:SER:CA	2.44	0.47
1:A:436:LEU:CD2	1:A:440:LEU:HD22	2.45	0.47
1:A:436:LEU:HD22	1:A:440:LEU:HD22	1.98	0.46
1:A:219:VAL:HG23	1:A:220:PRO:HD2	1.98	0.46
1:A:100:TYR:CD2	1:A:131:LYS:HB3	2.50	0.46
1:A:335:ILE:O	1:A:338:ASN:HB2	2.16	0.46
1:A:121:PRO:HG3	1:A:129:TRP:CZ2	2.51	0.46
1:A:436:LEU:CD1	1:A:510:TYR:CD2	2.98	0.46
1:A:397:VAL:HG12	1:A:470:THR:HB	1.97	0.46
1:A:285:LYS:HD2	1:A:285:LYS:HA	1.79	0.45
1:A:277:LEU:HB3	1:A:350:MET:HE1	1.98	0.45
1:A:317:VAL:O	1:A:320:ASP:N	2.45	0.45
1:A:227:GLU:N	1:A:228:PRO:HD2	2.31	0.45
1:A:312:GLN:OE1	1:A:312:GLN:HA	2.17	0.45
1:A:534:TYR:O	1:A:537:SER:OG	2.25	0.45
1:A:537:SER:HA	1:A:540:THR:HG22	1.98	0.45
1:A:350:MET:O	1:A:354:MET:HG3	2.16	0.45
1:A:329:LYS:HG2	1:A:331:LYS:NZ	2.31	0.45
1:A:435:LEU:HD23	1:A:436:LEU:CB	2.46	0.45
1:A:482:ASP:OD1	1:A:482:ASP:N	2.30	0.45
1:A:188:LEU:HD12	1:A:188:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:O	1:A:121:PRO:C	2.60	0.44
1:A:189:CYS:HB2	1:A:194:TYR:CZ	2.52	0.44
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.82	0.44
1:A:114:VAL:O	1:A:116:PRO:HD2	2.17	0.44
1:A:317:VAL:O	1:A:321:PHE:N	2.51	0.44
1:A:519:LYS:HE3	1:A:520:LYS:HB2	2.00	0.44
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.74	0.44
1:A:195:MET:HE1	1:A:230:VAL:CB	2.45	0.43
1:A:291:ASP:HA	1:A:292:PRO:HD2	1.90	0.43
1:A:11:LYS:HD3	1:A:11:LYS:HA	1.91	0.43
1:A:413:VAL:O	1:A:415:ALA:N	2.51	0.43
1:A:396:CYS:SG	1:A:431:PRO:O	2.77	0.43
1:A:159:ASN:HB3	1:A:162:LYS:HB2	2.00	0.43
1:A:331:LYS:HB3	1:A:446:ILE:HD13	1.99	0.43
1:A:435:LEU:CD2	1:A:436:LEU:N	2.76	0.43
1:A:253:LYS:HA	1:A:257:PHE:CE1	2.53	0.42
1:A:118:GLU:O	1:A:119:GLN:C	2.62	0.42
1:A:314:ALA:O	1:A:317:VAL:HG22	2.19	0.42
1:A:216:LYS:O	1:A:218:ARG:HD3	2.20	0.42
1:A:222:TYR:CG	1:A:223:PRO:HD3	2.54	0.42
1:A:266:PHE:CE2	1:A:342:GLN:CD	2.98	0.42
1:A:118:GLU:OE1	1:A:118:GLU:HA	2.19	0.42
1:A:430:GLN:N	1:A:431:PRO:CD	2.83	0.42
1:A:436:LEU:CG	1:A:510:TYR:HD2	2.32	0.42
1:A:163:ILE:HD13	1:A:163:ILE:HA	1.82	0.42
1:A:230:VAL:CG2	1:A:298:TYR:CZ	2.96	0.42
1:A:253:LYS:HE3	1:A:324:TYR:OH	2.19	0.42
1:A:289:CYS:HA	1:A:290:PRO:HD3	1.92	0.42
1:A:519:LYS:HD3	1:A:521:THR:H	1.84	0.42
1:A:344:ARG:HD2	1:A:375:ASN:HB2	2.01	0.41
1:A:392:HIS:ND1	1:A:392:HIS:C	2.78	0.41
1:A:106:THR:HG23	1:A:107:ASP:CG	2.45	0.41
1:A:250:GLU:N	1:A:250:GLU:CD	2.79	0.41
1:A:347:LEU:HD22	1:A:371:GLN:NE2	2.36	0.41
1:A:176:MET:O	1:A:177:LYS:C	2.64	0.41
1:A:413:VAL:O	1:A:414:PRO:C	2.63	0.41
1:A:292:PRO:O	1:A:295:VAL:HG12	2.21	0.41
1:A:397:VAL:CG1	1:A:470:THR:HB	2.51	0.41
1:A:456:LEU:HB2	1:A:518:LEU:HD11	2.02	0.41
1:A:110:LYS:HD3	1:A:110:LYS:N	2.24	0.41
1:A:118:GLU:OE1	1:A:118:GLU:CA	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:HG2	1:A:466:THR:HG23	2.02	0.40
1:A:433:MET:CE	1:A:510:TYR:CE1	3.04	0.40
1:A:468:GLU:CD	1:A:531:SER:HG	2.20	0.40
1:A:354:MET:O	1:A:359:LEU:HD13	2.21	0.40
1:A:394:GLU:HA	1:A:466:THR:HG21	2.03	0.40
1:A:347:LEU:HD11	1:A:370:LEU:CD2	2.47	0.40
1:A:194:TYR:CG	1:A:229:PHE:CD2	3.09	0.40
1:A:207:GLU:HG2	1:A:208:TYR:CE2	2.57	0.40
1:A:231:ILE:HD11	1:A:297:HIS:ND1	2.36	0.40
1:A:276:GLN:HG3	1:A:277:LEU:N	2.34	0.40

All (1) 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:A:142:GLU:OE1	1:A:412:ASN:ND2[4_554]	2.11	0.09

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	537/539 (100%)	522 (97%)	12 (2%)	3 (1%)	21	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ALA
1	A	119	GLN
1	A	71	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	492/492 (100%)	409 (83%)	83 (17%)	2 7

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	16	LYS
1	A	17	LEU
1	A	26	ARG
1	A	28	ASP
1	A	31	MET
1	A	39	SER
1	A	42	GLU
1	A	65	GLN
1	A	66	GLU
1	A	67	LEU
1	A	72	ARG
1	A	78	LYS
1	A	92	ILE
1	A	106	THR
1	A	107	ASP
1	A	110	LYS
1	A	111	LYS
1	A	118	GLU
1	A	125	ASN
1	A	126	LEU
1	A	146	SER
1	A	151	LEU
1	A	154	PHE
1	A	162	LYS
1	A	171	LEU
1	A	187	ARG
1	A	214	THR
1	A	219	VAL
1	A	230	VAL

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Mol	Chain	Res	Type
1	A	237	ASN
1	A	245	LEU
1	A	246	HIS
1	A	250	GLU
1	A	254	LYS
1	A	258	GLN
1	A	261	SER
1	A	263	HIS
1	A	269	SER
1	A	270	VAL
1	A	273	VAL
1	A	276	GLN
1	A	285	LYS
1	A	320	ASP
1	A	323	SER
1	A	326	SER
1	A	328	GLU
1	A	331	LYS
1	A	334	CYS
1	A	335	ILE
1	A	354	MET
1	A	357	LYS
1	A	366	THR
1	A	368	LYS
1	A	372	VAL
1	A	375	ASN
1	A	378	LEU
1	A	388	SER
1	A	392	HIS
1	A	393	ILE
1	A	396	CYS
1	A	408	LYS
1	A	412	ASN
1	A	413	VAL
1	A	433	MET
1	A	435	LEU
1	A	436	LEU
1	A	445	LYS
1	A	447	CYS
1	A	472	VAL
1	A	480	LEU
1	A	481	LYS

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Mol	Chain	Res	Type
1	A	482	ASP
1	A	485	VAL
1	A	500	VAL
1	A	501	GLU
1	A	507	ILE
1	A	519	LYS
1	A	521	THR
1	A	536	LEU
1	A	538	LEU
1	A	540	THR
1	A	547	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	105	GLN
1	A	297	HIS

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 ⓘ

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

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	539/539 (100%)	0.44	52 (9%)	13 11	58, 96, 151, 244	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	GLY	6.7
1	A	114	VAL	6.3
1	A	111	LYS	5.8
1	A	64	VAL	5.2
1	A	115	PRO	5.1
1	A	414	PRO	5.0
1	A	11	LYS	4.8
1	A	436	LEU	4.7
1	A	65	GLN	4.5
1	A	473	LEU	4.1
1	A	106	THR	4.1
1	A	368	LYS	3.8
1	A	56	SER	3.8
1	A	472	VAL	3.7
1	A	66	GLU	3.7
1	A	413	VAL	3.6
1	A	328	GLU	3.3
1	A	40	SER	3.1
1	A	67	LEU	3.1
1	A	538	LEU	3.1
1	A	112	GLY	3.0
1	A	441	THR	3.0
1	A	70	PRO	3.0
1	A	59	PHE	2.8
1	A	327	LYS	2.7
1	A	519	LYS	2.7
1	A	525	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	474	PRO	2.7
1	A	118	GLU	2.6
1	A	510	TYR	2.6
1	A	329	LYS	2.6
1	A	415	ALA	2.6
1	A	12	GLU	2.5
1	A	435	LEU	2.5
1	A	116	PRO	2.4
1	A	326	SER	2.3
1	A	69	SER	2.3
1	A	34	ASN	2.3
1	A	109	ALA	2.3
1	A	346	GLN	2.3
1	A	490	LYS	2.3
1	A	416	SER	2.3
1	A	71	PRO	2.3
1	A	453	LYS	2.2
1	A	108	PRO	2.2
1	A	411	GLY	2.2
1	A	105	GLN	2.2
1	A	521	THR	2.2
1	A	285	LYS	2.2
1	A	412	ASN	2.1
1	A	113	GLU	2.1
1	A	107	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.