



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:35 PM EDT

PDB ID : 3DPL / pdb_00003dpl
Title : Structural Insights into NEDD8 Activation of Cullin-RING Ligases: Conformational Control of Conjugation.
Authors : Duda, D.M.; Schulman, B.A.
Deposited on : 2008-07-08
Resolution : 2.60 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

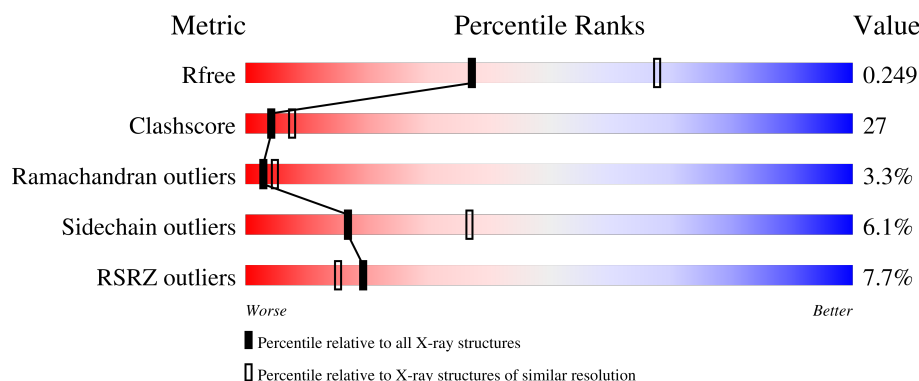
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	C	382	
2	R	106	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3932 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 Cullin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	378	Total	C	N	O	S	0	0	0
			3132	1999	544	574	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	399	GLY	-	expression tag	UNP Q93034
C	400	SER	-	expression tag	UNP Q93034
C	407	GLU	LEU	engineered mutation	UNP Q93034
C	439	LYS	LEU	engineered mutation	UNP Q93034
C	440	LYS	VAL	engineered mutation	UNP Q93034

- Molecule 2 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	87	Total	C	N	O	S	0	0	0
			724	460	134	121	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	3	GLY	-	expression tag	UNP P62877
R	4	SER	-	expression tag	UNP P62877

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	3	Total	Zn	0	0
			3	3		

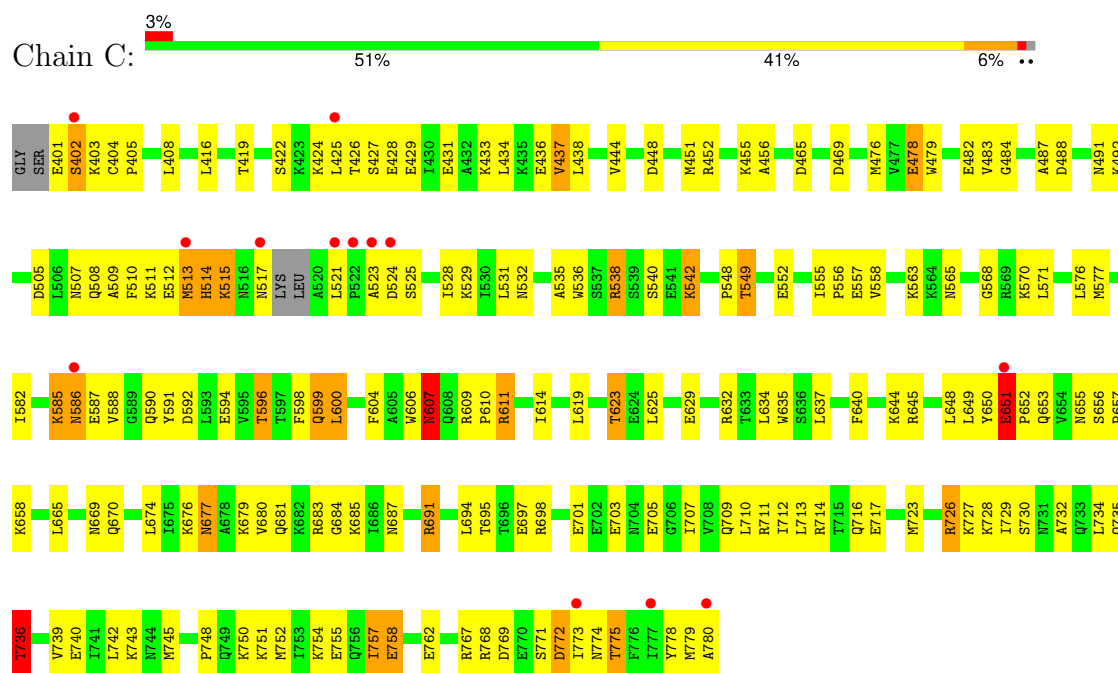
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	61	Total 61	O 61	0	0
4	R	12	Total 12	O 12	0	0

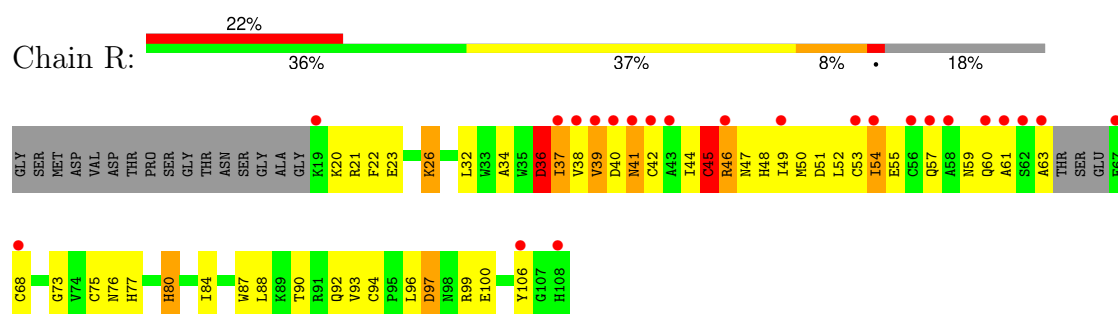
3 Residue-property plots [i](#)

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: Cullin-5



• Molecule 2: RING-box protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.97Å 65.51Å 141.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.60) 95.3 (50.00-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.277 0.245 , 0.249	Depositor DCC
R_{free} test set	906 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3932	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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

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	C	0.50	0/3186	1.00	15/4281 (0.4%)
2	R	0.47	0/745	1.03	7/1007 (0.7%)
All	All	0.49	0/3931	1.00	22/5288 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	726	ARG	N-CA-C	-9.04	95.94	110.32
1	C	651	GLU	CA-C-N	-7.69	110.22	119.84
1	C	651	GLU	C-N-CA	-7.69	110.22	119.84
2	R	60	GLN	N-CA-C	-7.59	104.93	112.97
1	C	607	ASN	N-CA-C	7.16	119.94	111.71
2	R	97	ASP	N-CA-C	-6.76	99.56	109.63
1	C	540	SER	N-CA-C	-6.71	105.13	113.38
1	C	587	GLU	N-CA-C	-6.56	102.82	113.19
1	C	505	ASP	N-CA-C	-6.38	104.25	111.14
2	R	106	TYR	N-CA-C	-6.22	106.00	113.97
1	C	437	VAL	N-CA-C	-6.04	107.01	111.90
1	C	515	LYS	N-CA-C	-5.88	105.60	112.89
1	C	640	PHE	CA-C-N	5.86	127.17	119.84
1	C	640	PHE	C-N-CA	5.86	127.17	119.84
2	R	36	ASP	N-CA-C	5.85	123.25	110.80
2	R	44	ILE	N-CA-C	-5.66	104.81	110.30
1	C	599	GLN	N-CA-C	-5.53	105.17	111.14
2	R	80	HIS	N-CA-C	-5.51	102.12	110.28
1	C	736	THR	N-CA-C	5.39	117.23	111.36
2	R	90	THR	N-CA-C	-5.28	104.43	112.04
1	C	727	LYS	N-CA-C	-5.09	107.11	113.38
1	C	521	LEU	N-CA-C	5.09	112.80	108.22

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	C	3132	0	3219	165	0
2	R	724	0	680	54	0
3	R	3	0	0	0	0
4	C	61	0	0	4	0
4	R	12	0	0	1	0
All	All	3932	0	3899	211	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 27.

All (211) 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:691:ARG:HD2	1:C:694:LEU:HD12	1.34	1.05
1:C:651:GLU:HB3	1:C:652:PRO:CD	1.91	0.98
1:C:651:GLU:HB3	1:C:652:PRO:HD2	1.45	0.98
2:R:41:ASN:HB3	2:R:47:ASN:C	1.99	0.87
1:C:596:THR:HG22	1:C:599:GLN:H	1.40	0.84
2:R:20:LYS:HG3	2:R:21:ARG:H	1.42	0.84
1:C:576:LEU:HG	1:C:577:MET:HE3	1.63	0.81
1:C:651:GLU:HA	1:C:651:GLU:OE1	1.80	0.80
1:C:652:PRO:HG2	4:C:54:HOH:O	1.83	0.79
2:R:41:ASN:HB3	2:R:47:ASN:O	1.82	0.79
2:R:77:HIS:CD2	2:R:96:LEU:HD12	2.18	0.79
1:C:429:GLU:O	1:C:433:LYS:HG3	1.83	0.79
1:C:542:LYS:H	1:C:542:LYS:HD3	1.50	0.76
1:C:542:LYS:HD3	1:C:542:LYS:N	2.01	0.75
2:R:87:TRP:HZ3	2:R:93:VAL:O	1.70	0.75
1:C:455:LYS:HG2	1:C:538:ARG:HH21	1.53	0.73
1:C:701:GLU:O	1:C:705:GLU:HG3	1.87	0.73
2:R:53:CYS:HB3	2:R:80:HIS:CD2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:LEU:HD22	1:C:476:MET:HE1	1.71	0.73
1:C:751:LYS:O	1:C:755:GLU:HG3	1.89	0.71
1:C:448:ASP:HA	1:C:451:MET:HE3	1.73	0.70
1:C:478:GLU:O	1:C:482:GLU:HG3	1.91	0.70
1:C:594:GLU:HB3	1:C:687:ASN:HA	1.75	0.69
1:C:683:ARG:HG2	1:C:683:ARG:HH21	1.58	0.68
1:C:723:MET:HE1	1:C:729:ILE:HG22	1.74	0.68
1:C:623:THR:HG23	1:C:625:LEU:H	1.59	0.67
1:C:419:THR:H	1:C:422:SER:HB3	1.59	0.67
1:C:456:ALA:HA	1:C:538:ARG:HE	1.59	0.67
1:C:455:LYS:HG2	1:C:538:ARG:NH2	2.09	0.66
1:C:767:ARG:HD2	1:C:768:ARG:H	1.61	0.66
1:C:712:ILE:O	1:C:716:GLN:HG3	1.97	0.65
1:C:676:LYS:O	1:C:677:ASN:HB2	1.97	0.65
2:R:20:LYS:CG	2:R:21:ARG:H	2.09	0.65
2:R:37:ILE:O	2:R:38:VAL:HG23	1.96	0.65
1:C:425:LEU:HA	1:C:429:GLU:OE1	1.97	0.64
1:C:577:MET:HE2	1:C:577:MET:HA	1.80	0.64
1:C:596:THR:CG2	1:C:599:GLN:H	2.11	0.64
2:R:38:VAL:O	2:R:40:ASP:N	2.27	0.64
1:C:570:LYS:HB2	2:R:36:ASP:HA	1.79	0.63
2:R:40:ASP:O	2:R:49:ILE:HG13	1.99	0.62
2:R:23:GLU:HG3	4:R:205:HOH:O	1.98	0.62
1:C:734:LEU:HD23	1:C:757:ILE:HD11	1.83	0.61
1:C:651:GLU:CB	1:C:652:PRO:CD	2.74	0.61
1:C:754:LYS:O	1:C:758:GLU:HB2	2.00	0.61
1:C:723:MET:O	1:C:726:ARG:O	2.18	0.61
1:C:734:LEU:CD2	1:C:757:ILE:HD11	2.31	0.61
1:C:774:ASN:O	1:C:775:THR:C	2.44	0.60
2:R:39:VAL:HG12	2:R:39:VAL:O	2.01	0.60
2:R:40:ASP:OD1	2:R:41:ASN:N	2.31	0.60
1:C:711:ARG:HB3	1:C:752:MET:HE1	1.85	0.59
2:R:84:ILE:O	2:R:88:LEU:HG	2.02	0.59
1:C:592:ASP:HB2	1:C:685:LYS:HG2	1.85	0.58
1:C:582:ILE:HG21	1:C:600:LEU:HD22	1.85	0.58
1:C:635:TRP:CG	1:C:657:PRO:HG3	2.39	0.58
1:C:714:ARG:HG3	1:C:745:MET:HE1	1.86	0.57
1:C:488:ASP:O	1:C:492:LYS:HG2	2.04	0.57
2:R:39:VAL:O	2:R:48:HIS:HE1	1.87	0.57
1:C:426:THR:N	1:C:429:GLU:OE1	2.34	0.57
2:R:34:ALA:HA	2:R:76:ASN:ND2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:36:ASP:O	2:R:37:ILE:C	2.48	0.57
1:C:767:ARG:HB2	1:C:779:MET:SD	2.44	0.56
1:C:713:LEU:O	1:C:717:GLU:HG3	2.05	0.56
2:R:87:TRP:CZ3	2:R:93:VAL:O	2.55	0.56
1:C:426:THR:OG1	1:C:429:GLU:HG3	2.05	0.56
1:C:596:THR:HG22	1:C:599:GLN:N	2.17	0.56
1:C:651:GLU:O	1:C:652:PRO:C	2.44	0.56
1:C:691:ARG:HD2	1:C:694:LEU:CD1	2.24	0.55
1:C:531:LEU:O	2:R:32:LEU:HA	2.06	0.55
1:C:683:ARG:HG2	1:C:683:ARG:NH2	2.19	0.55
1:C:452:ARG:HD3	1:C:703:GLU:HG3	1.88	0.55
1:C:779:MET:O	1:C:780:ALA:HB3	2.05	0.55
1:C:691:ARG:HB3	1:C:691:ARG:HH11	1.71	0.55
1:C:416:LEU:HD21	1:C:434:LEU:HD11	1.89	0.54
2:R:48:HIS:HB3	2:R:51:ASP:OD2	2.08	0.54
2:R:41:ASN:HA	2:R:48:HIS:HA	1.90	0.54
2:R:20:LYS:HG3	2:R:21:ARG:N	2.19	0.54
1:C:714:ARG:HD2	1:C:745:MET:HE1	1.90	0.53
1:C:452:ARG:HD2	1:C:707:ILE:HG13	1.90	0.53
1:C:650:TYR:CE2	1:C:653:GLN:HA	2.44	0.53
1:C:714:ARG:CG	1:C:745:MET:HE1	2.38	0.53
2:R:52:LEU:HB2	2:R:57:GLN:HB2	1.91	0.53
1:C:629:GLU:OE2	1:C:632:ARG:NH2	2.38	0.53
1:C:623:THR:CG2	1:C:625:LEU:H	2.22	0.53
1:C:767:ARG:HD2	1:C:768:ARG:N	2.23	0.53
1:C:596:THR:HG22	1:C:599:GLN:HG3	1.91	0.52
1:C:635:TRP:CD2	1:C:657:PRO:HG3	2.44	0.52
1:C:531:LEU:HB3	1:C:536:TRP:CD1	2.44	0.52
1:C:714:ARG:CD	1:C:745:MET:HE1	2.39	0.52
2:R:26:LYS:HB2	2:R:26:LYS:HZ2	1.74	0.52
2:R:26:LYS:HB2	2:R:26:LYS:NZ	2.24	0.52
1:C:644:LYS:O	1:C:645:ARG:HG2	2.10	0.52
1:C:431:GLU:HG3	1:C:479:TRP:CH2	2.46	0.51
1:C:740:GLU:O	1:C:743:LYS:HB2	2.10	0.51
1:C:416:LEU:HD11	1:C:476:MET:HE2	1.92	0.51
1:C:434:LEU:O	1:C:438:LEU:HG	2.10	0.51
1:C:433:LYS:HA	1:C:436:GLU:HG2	1.91	0.51
1:C:512:GLU:HA	1:C:515:LYS:HE2	1.93	0.51
1:C:568:GLY:C	2:R:36:ASP:HB2	2.35	0.51
1:C:723:MET:HG3	1:C:778:TYR:HB2	1.92	0.50
1:C:508:GLN:C	1:C:510:PHE:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:607:ASN:O	2:R:20:LYS:HG2	2.11	0.50
1:C:705:GLU:O	1:C:709:GLN:HG3	2.11	0.50
1:C:428:GLU:H	1:C:428:GLU:CD	2.19	0.50
1:C:767:ARG:HB3	1:C:779:MET:HE3	1.94	0.50
1:C:773:ILE:HG22	1:C:773:ILE:O	2.12	0.50
1:C:405:PRO:HG3	1:C:444:VAL:HG13	1.94	0.49
1:C:408:LEU:HD22	1:C:437:VAL:HG13	1.93	0.49
1:C:425:LEU:HD22	1:C:429:GLU:HB3	1.94	0.49
1:C:512:GLU:C	1:C:514:HIS:N	2.68	0.49
1:C:619:LEU:HD13	1:C:634:LEU:HD21	1.94	0.49
2:R:20:LYS:CG	2:R:21:ARG:N	2.76	0.49
1:C:507:ASN:HD21	1:C:511:LYS:HE3	1.78	0.49
1:C:735:GLN:O	1:C:739:VAL:HG23	2.12	0.49
1:C:774:ASN:O	1:C:775:THR:O	2.30	0.49
1:C:405:PRO:HG3	1:C:444:VAL:CG1	2.43	0.49
1:C:769:ASP:HB3	1:C:772:ASP:HB3	1.95	0.49
1:C:585:LYS:C	1:C:585:LYS:HE2	2.37	0.49
1:C:637:LEU:CB	1:C:648:LEU:HD12	2.43	0.49
1:C:742:LEU:HD12	1:C:748:PRO:HG3	1.94	0.49
1:C:552:GLU:HG2	1:C:555:ILE:HD12	1.95	0.48
1:C:586:ASN:HB3	1:C:588:VAL:H	1.78	0.48
2:R:38:VAL:C	2:R:40:ASP:N	2.69	0.48
2:R:41:ASN:OD1	2:R:48:HIS:HA	2.13	0.48
2:R:42:CYS:HB2	2:R:80:HIS:ND1	2.28	0.48
1:C:596:THR:HG23	1:C:598:PHE:H	1.77	0.48
1:C:401:GLU:HG3	1:C:402:SER:N	2.29	0.48
1:C:482:GLU:C	1:C:484:GLY:H	2.21	0.48
2:R:42:CYS:SG	2:R:45:CYS:N	2.83	0.47
1:C:656:SER:OG	1:C:658:LYS:HG2	2.15	0.47
2:R:34:ALA:HA	2:R:76:ASN:HD21	1.79	0.47
1:C:623:THR:HG23	1:C:625:LEU:N	2.27	0.47
1:C:677:ASN:C	1:C:679:LYS:H	2.23	0.47
1:C:611:ARG:HH21	1:C:670:GLN:HG3	1.80	0.47
1:C:674:LEU:HD12	1:C:684:GLY:HA3	1.97	0.47
1:C:609:ARG:N	1:C:610:PRO:HD3	2.29	0.47
1:C:507:ASN:ND2	1:C:511:LYS:HE3	2.29	0.47
1:C:424:LYS:O	1:C:425:LEU:HG	2.15	0.46
1:C:576:LEU:O	1:C:577:MET:HE2	2.14	0.46
1:C:607:ASN:HD21	2:R:22:PHE:H	1.62	0.46
1:C:677:ASN:O	1:C:679:LYS:HG3	2.14	0.46
1:C:710:LEU:HB3	4:C:25:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:TYR:CD1	1:C:591:TYR:N	2.83	0.46
1:C:513:MET:HE2	1:C:513:MET:C	2.41	0.46
1:C:762:GLU:HG3	2:R:63:ALA:HB1	1.97	0.46
1:C:767:ARG:HB3	1:C:779:MET:CE	2.46	0.46
2:R:52:LEU:CB	2:R:57:GLN:HB2	2.46	0.46
1:C:431:GLU:HG3	1:C:479:TRP:CZ2	2.51	0.45
1:C:649:LEU:HG	1:C:669:ASN:HB2	1.97	0.45
1:C:651:GLU:HB2	1:C:665:LEU:H	1.82	0.45
1:C:676:LYS:O	1:C:677:ASN:CB	2.62	0.45
2:R:94:CYS:O	2:R:97:ASP:O	2.35	0.45
2:R:48:HIS:CD2	2:R:50:MET:H	2.34	0.45
1:C:586:ASN:HD22	1:C:588:VAL:HB	1.81	0.45
1:C:732:ALA:O	1:C:736:THR:HG22	2.16	0.45
1:C:465:ASP:OD2	1:C:529:LYS:NZ	2.47	0.45
1:C:482:GLU:O	1:C:484:GLY:N	2.50	0.44
1:C:548:PRO:O	1:C:549:THR:C	2.59	0.44
1:C:676:LYS:HB2	1:C:681:GLN:OE1	2.18	0.44
2:R:53:CYS:O	2:R:54:ILE:C	2.61	0.44
1:C:607:ASN:HD22	1:C:607:ASN:HA	1.62	0.44
1:C:513:MET:CE	1:C:514:HIS:ND1	2.81	0.44
1:C:555:ILE:N	1:C:556:PRO:HD2	2.32	0.43
1:C:426:THR:O	1:C:427:SER:C	2.61	0.43
2:R:41:ASN:HA	2:R:49:ILE:H	1.83	0.43
2:R:88:LEU:HB3	2:R:92:GLN:NE2	2.33	0.43
1:C:487:ALA:O	1:C:491:ASN:HB2	2.18	0.43
1:C:570:LYS:HD3	1:C:571:LEU:N	2.34	0.43
1:C:679:LYS:O	1:C:680:VAL:C	2.61	0.43
2:R:37:ILE:O	2:R:38:VAL:CG2	2.64	0.43
1:C:508:GLN:O	1:C:510:PHE:N	2.52	0.43
1:C:538:ARG:HG2	1:C:538:ARG:HH11	1.84	0.43
1:C:538:ARG:HG2	1:C:538:ARG:NH1	2.34	0.43
2:R:39:VAL:O	2:R:48:HIS:CE1	2.70	0.43
1:C:596:THR:HG21	4:C:23:HOH:O	2.19	0.43
1:C:637:LEU:HB3	1:C:648:LEU:HD12	2.00	0.43
1:C:434:LEU:HD23	1:C:434:LEU:HA	1.93	0.42
2:R:41:ASN:CA	2:R:48:HIS:HA	2.49	0.42
1:C:525:SER:O	2:R:26:LYS:HG3	2.18	0.42
1:C:769:ASP:OD1	1:C:771:SER:N	2.50	0.42
1:C:650:TYR:HA	1:C:665:LEU:O	2.19	0.42
2:R:48:HIS:HD2	2:R:50:MET:HB3	1.83	0.42
2:R:53:CYS:O	2:R:55:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:99:ARG:O	2:R:100:GLU:C	2.63	0.42
1:C:513:MET:HE1	1:C:514:HIS:ND1	2.34	0.42
1:C:512:GLU:O	1:C:513:MET:C	2.61	0.42
1:C:524:ASP:OD1	1:C:524:ASP:O	2.37	0.42
1:C:525:SER:HA	2:R:26:LYS:HE3	2.01	0.42
1:C:685:LYS:NZ	4:C:57:HOH:O	2.53	0.42
1:C:730:SER:HA	1:C:775:THR:HA	2.01	0.42
1:C:528:ILE:HD13	1:C:558:VAL:CG1	2.50	0.42
2:R:37:ILE:HG22	2:R:38:VAL:N	2.34	0.42
2:R:73:GLY:C	2:R:75:CYS:N	2.75	0.42
1:C:515:LYS:HD3	1:C:515:LYS:HA	1.90	0.42
1:C:677:ASN:C	1:C:679:LYS:N	2.78	0.41
1:C:532:ASN:OD1	1:C:535:ALA:HB3	2.20	0.41
1:C:779:MET:O	1:C:780:ALA:CB	2.69	0.41
1:C:735:GLN:NE2	1:C:750:LYS:HG2	2.35	0.41
2:R:59:ASN:C	2:R:61:ALA:H	2.28	0.41
1:C:582:ILE:CG2	1:C:600:LEU:HD22	2.48	0.41
1:C:606:TRP:CE2	1:C:614:ILE:HD12	2.55	0.41
2:R:41:ASN:CB	2:R:46:ARG:O	2.69	0.41
1:C:508:GLN:O	1:C:509:ALA:C	2.63	0.41
1:C:600:LEU:HD13	1:C:604:PHE:CD1	2.56	0.41
1:C:697:GLU:HG3	1:C:698:ARG:N	2.36	0.41
1:C:728:LYS:HB2	1:C:728:LYS:HE3	1.82	0.41
1:C:563:LYS:C	1:C:565:ASN:H	2.29	0.40
1:C:674:LEU:CD1	1:C:684:GLY:HA3	2.52	0.40
1:C:723:MET:CE	1:C:729:ILE:HG22	2.48	0.40
1:C:670:GLN:OE1	1:C:670:GLN:HA	2.22	0.40
1:C:404:CYS:HA	1:C:405:PRO:HD3	1.86	0.40
1:C:590:GLN:HG2	1:C:683:ARG:NE	2.36	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	C	374/382 (98%)	338 (90%)	28 (8%)	8 (2%)	5	11
2	R	83/106 (78%)	63 (76%)	13 (16%)	7 (8%)	0	0
All	All	457/488 (94%)	401 (88%)	41 (9%)	15 (3%)	3	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	523	ALA
1	C	651	GLU
1	C	775	THR
2	R	37	ILE
1	C	402	SER
1	C	483	VAL
1	C	586	ASN
1	C	677	ASN
2	R	39	VAL
2	R	46	ARG
2	R	54	ILE
2	R	68	CYS
2	R	36	ASP
2	R	45	CYS
1	C	772	ASP

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	C	349/352 (99%)	326 (93%)	23 (7%)	15	34
2	R	76/90 (84%)	73 (96%)	3 (4%)	28	55
All	All	425/442 (96%)	399 (94%)	26 (6%)	17	37

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	403	LYS

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Mol	Chain	Res	Type
1	C	469	ASP
1	C	478	GLU
1	C	513	MET
1	C	514	HIS
1	C	517	ASN
1	C	538	ARG
1	C	542	LYS
1	C	549	THR
1	C	557	GLU
1	C	585	LYS
1	C	596	THR
1	C	600	LEU
1	C	607	ASN
1	C	611	ARG
1	C	623	THR
1	C	651	GLU
1	C	655	ASN
1	C	691	ARG
1	C	695	THR
1	C	736	THR
1	C	757	ILE
1	C	758	GLU
2	R	26	LYS
2	R	41	ASN
2	R	45	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	491	ASN
1	C	574	HIS
1	C	586	ASN
1	C	607	ASN
1	C	618	ASN
1	C	704	ASN
1	C	763	HIS
2	R	48	HIS

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](#)

Of 3 ligands modelled in this entry, 3 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	C	378/382 (98%)	0.25	13 (3%)	48 42	18, 43, 74, 96	0
2	R	87/106 (82%)	1.06	23 (26%)	1 1	27, 45, 105, 132	0
All	All	465/488 (95%)	0.40	36 (7%)	19 15	18, 43, 84, 132	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	63	ALA	5.8
2	R	39	VAL	5.3
2	R	61	ALA	4.5
2	R	38	VAL	4.0
2	R	62	SER	3.9
2	R	37	ILE	3.9
1	C	773	ILE	3.7
2	R	42	CYS	3.7
2	R	54	ILE	3.6
1	C	402	SER	3.5
1	C	523	ALA	3.4
2	R	106	TYR	3.3
2	R	68	CYS	3.2
1	C	524	ASP	3.2
2	R	56	CYS	3.2
1	C	586	ASN	3.1
2	R	53	CYS	3.1
1	C	425	LEU	2.9
2	R	58	ALA	2.8
2	R	49	ILE	2.8
2	R	40	ASP	2.7
2	R	60	GLN	2.7
2	R	43	ALA	2.6
2	R	19	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	R	46	ARG	2.4
1	C	521	LEU	2.3
1	C	517	ASN	2.3
2	R	57	GLN	2.3
2	R	41	ASN	2.3
1	C	780	ALA	2.2
2	R	67	GLU	2.2
1	C	522	PRO	2.2
2	R	108	HIS	2.1
1	C	777	ILE	2.1
1	C	513	MET	2.1
1	C	651	GLU	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(Å ²)	Q<0.9
3	ZN	R	203	1/1	0.94	0.07	65,65,65,65	0
3	ZN	R	201	1/1	0.95	0.06	57,57,57,57	0
3	ZN	R	202	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.