



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 24, 2025 – 10:10 am BST

PDB ID : 9Q8Y / pdb_00009q8y
Title : Structure of RNF38 RING with linchpin mutant R454Y in complex with Ubch5B-Ub
Authors : Gabrielsen, M.; Buetow, L.; Huang, D.T.
Deposited on : 2025-02-25
Resolution : 2.63 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:

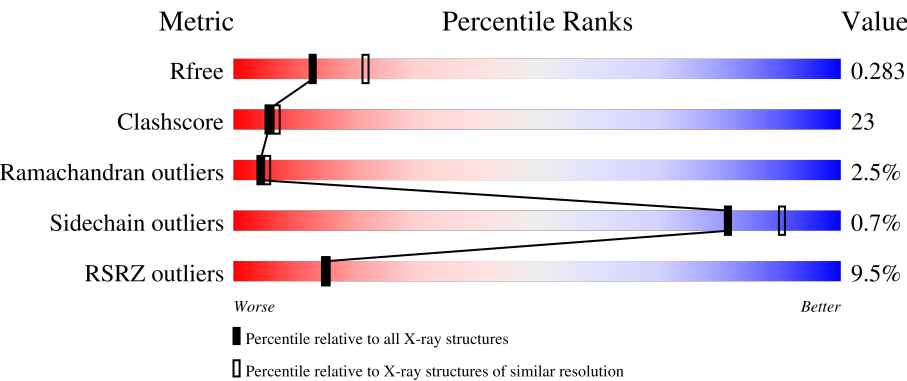
MolProbity : 4-5-2 with Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

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 2.63 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}	164625	1851 (2.66-2.62)
Clashscore	180529	1953 (2.66-2.62)
Ramachandran outliers	177936	1929 (2.66-2.62)
Sidechain outliers	177891	1929 (2.66-2.62)
RSRZ outliers	164620	1850 (2.66-2.62)

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	146	<div><div>5%</div><div><div></div><div>68%</div><div>29%</div><div>.</div></div></div>
1	B	146	<div><div>2%</div><div><div></div><div>76%</div><div>21%</div><div>.</div></div></div>
2	C	69	<div><div>6%</div><div><div></div><div>49%</div><div>45%</div><div>..</div></div></div>
2	D	69	<div><div>29%</div><div><div></div><div>48%</div><div>32%</div><div>7%</div><div>.</div><div>10%</div></div></div>
3	F	77	<div><div>13%</div><div><div></div><div>51%</div><div>42%</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	77	<p>9% 22% 23% 2% 44%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7819 atoms, of which 3763 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 Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	146	Total	C	H	N	O	S	0	0	0
			2172	721	1052	191	202	6			
1	B	146	Total	C	H	N	O	S	0	0	0
			2175	722	1057	187	203	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	SER	engineered mutation	UNP P62837
A	85	LYS	CYS	engineered mutation	UNP P62837
B	22	ARG	SER	engineered mutation	UNP P62837
B	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 2 is a protein called Isoform 2 of E3 ubiquitin-protein ligase RNF38.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	69	Total	C	H	N	O	S	0	0	0
			961	322	448	88	95	8			
2	D	62	Total	C	H	N	O	S	0	0	0
			827	275	381	80	83	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	454	TYR	ARG	engineered mutation	UNP Q9H0F5
D	454	TYR	ARG	engineered mutation	UNP Q9H0F5

- Molecule 3 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	77	Total	C	H	N	O	S	0	0	0
			1163	365	582	100	115	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	38	Total	C	H	N	O	0	0	0
			512	169	243	46	54			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	SER	-	expression tag	UNP J3QTR3
G	0	SER	-	expression tag	UNP J3QTR3

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

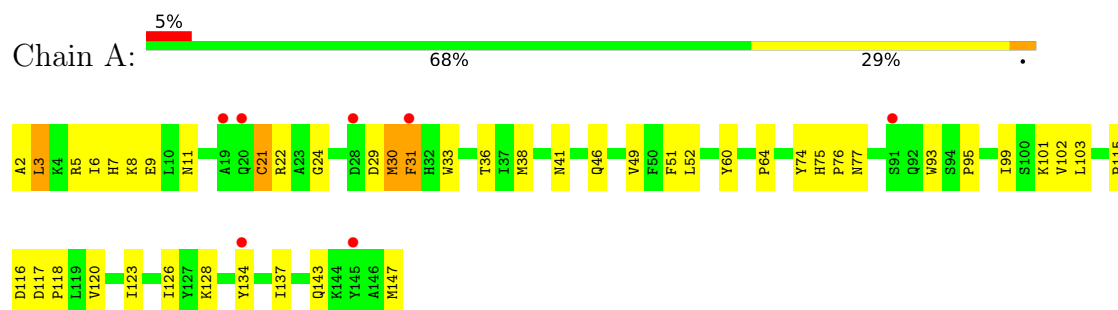
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	O	0	0
			4	4		
5	D	1	Total	O	0	0
			1	1		

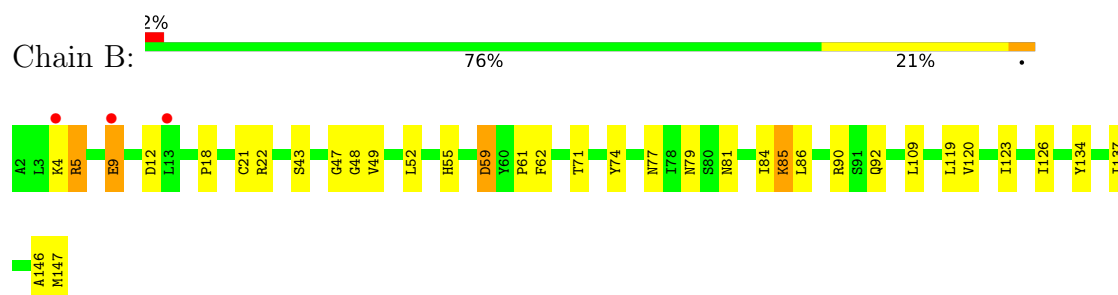
3 Residue-property plots [i](#)

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.

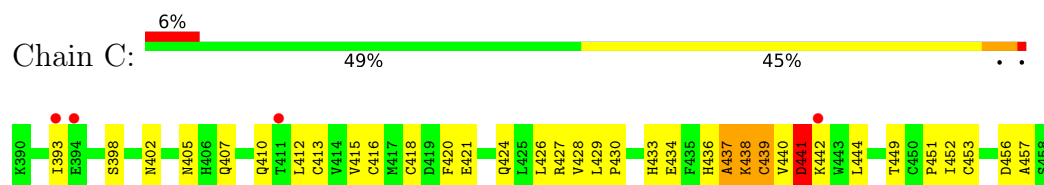
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2



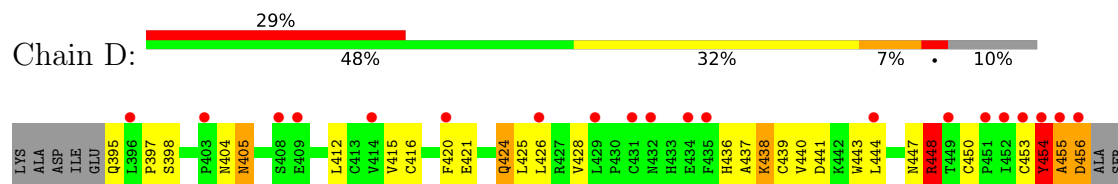
- Molecule 1: Ubiquitin-conjugating enzyme E2 D2



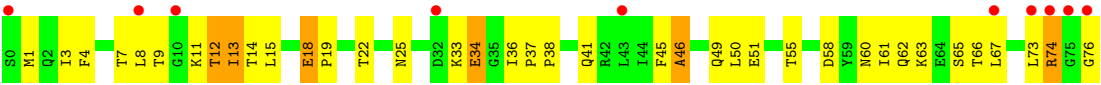
- Molecule 2: Isoform 2 of E3 ubiquitin-protein ligase RNF38



- Molecule 2: Isoform 2 of E3 ubiquitin-protein ligase RNF38



- Molecule 3: Ubiquitin-40S ribosomal protein S27a



● Molecule 3: Ubiquitin-40S ribosomal protein S27a



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	116.08 Å 116.08 Å 90.31 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.92 – 2.63 43.92 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.92-2.63) 98.9 (43.92-2.63)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.62 Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.232 , 0.275 0.244 , 0.283	Depositor DCC
R_{free} test set	1005 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 94.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7819	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	A	0.97	3/1156 (0.3%)	1.17	8/1588 (0.5%)
1	B	1.10	4/1154 (0.3%)	1.32	11/1584 (0.7%)
2	C	0.78	1/526 (0.2%)	1.04	5/721 (0.7%)
2	D	1.55	5/456 (1.1%)	1.82	13/626 (2.1%)
3	F	1.05	4/587 (0.7%)	1.32	6/795 (0.8%)
3	G	0.79	0/267	1.11	1/358 (0.3%)
All	All	1.07	17/4146 (0.4%)	1.30	44/5672 (0.8%)

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	B	0	1
2	C	0	1
2	D	0	2
3	G	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	456	ASP	CB-CG	-17.00	1.09	1.52
2	D	448	ARG	CZ-NH1	16.95	1.56	1.32
1	A	3	LEU	CG-CD2	9.38	1.83	1.52
1	A	3	LEU	CG-CD1	8.27	1.79	1.52
2	D	448	ARG	CD-NE	-7.76	1.35	1.46
1	B	77	ASN	CB-CG	7.40	1.70	1.52
3	F	18	GLU	C-N	-7.27	1.23	1.33
1	B	85	LYS	CG-CD	6.49	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	SER	CA-C	6.38	1.58	1.52
3	F	51	GLU	CD-OE1	6.11	1.36	1.25
2	D	416	CYS	CB-SG	-5.81	1.62	1.81
2	D	455	ALA	C-N	5.80	1.41	1.33
1	B	59	ASP	CA-C	-5.79	1.45	1.52
2	C	416	CYS	CB-SG	-5.20	1.64	1.81
3	F	58	ASP	CG-OD1	5.11	1.35	1.25
3	F	18	GLU	N-CA	5.08	1.54	1.45
1	A	30	MET	C-N	-5.01	1.25	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	456	ASP	CB-CG-OD2	-23.50	64.34	118.40
2	D	456	ASP	CB-CG-OD1	-16.11	81.34	118.40
3	G	40	GLN	CA-CB-CG	-11.38	91.35	114.10
1	A	3	LEU	CB-CG-CD2	9.79	140.06	110.70
1	B	85	LYS	CA-CB-CG	8.91	131.92	114.10
1	B	43	SER	O-C-N	8.40	127.08	121.71
2	D	448	ARG	CG-CD-NE	8.01	129.62	112.00
2	D	448	ARG	CA-C-N	-7.47	111.74	122.94
2	D	448	ARG	C-N-CA	-7.47	111.74	122.94
3	F	51	GLU	CB-CA-C	7.33	120.83	109.84
1	B	92	GLN	CA-CB-CG	-7.26	99.57	114.10
3	F	50	LEU	CA-C-N	6.70	130.63	121.05
3	F	50	LEU	C-N-CA	6.70	130.63	121.05
1	A	101	LYS	CA-C-N	-6.70	110.91	120.42
1	A	101	LYS	C-N-CA	-6.70	110.91	120.42
2	D	456	ASP	N-CA-CB	-6.58	99.32	110.50
2	D	456	ASP	OD1-CG-OD2	6.40	138.27	122.90
3	F	34	GLU	CA-C-N	-6.38	106.13	122.78
3	F	34	GLU	C-N-CA	-6.38	106.13	122.78
1	B	9	GLU	N-CA-CB	-6.20	101.02	110.01
2	D	448	ARG	CA-CB-CG	6.05	126.20	114.10
1	A	31	PHE	N-CA-CB	-6.01	101.02	110.46
2	D	424	GLN	CA-CB-CG	5.85	125.80	114.10
2	D	443	TRP	CA-CB-CG	5.84	124.69	113.60
1	B	9	GLU	CG-CD-OE2	5.82	131.78	118.40
3	F	51	GLU	N-CA-CB	-5.69	100.66	109.48
1	B	59	ASP	O-C-N	5.64	129.56	122.22
2	D	448	ARG	CD-NE-CZ	-5.54	116.64	124.40
1	A	3	LEU	CB-CA-C	-5.52	101.63	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	GLU	CB-CG-CD	-5.50	103.24	112.60
2	C	439	CYS	N-CA-CB	-5.47	102.06	110.16
2	D	455	ALA	O-C-N	5.38	129.49	123.19
1	B	84	ILE	CA-C-N	-5.33	115.44	122.85
1	B	84	ILE	C-N-CA	-5.33	115.44	122.85
1	B	22	ARG	CB-CA-C	5.26	121.24	109.56
2	C	441	ASP	N-CA-CB	-5.25	101.62	110.49
2	C	437	ALA	CA-C-N	5.21	131.48	121.54
2	C	437	ALA	C-N-CA	5.21	131.48	121.54
2	C	442	LYS	CA-CB-CG	5.21	124.51	114.10
1	A	21	CYS	CA-CB-SG	-5.15	102.55	114.40
2	D	448	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	2	ALA	CA-C-N	-5.10	113.44	120.28
1	A	2	ALA	C-N-CA	-5.10	113.44	120.28
1	B	9	GLU	CG-CD-OE1	-5.03	106.83	118.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	12	ASP	Sidechain
2	C	441	ASP	Sidechain
2	D	448	ARG	Sidechain
2	D	456	ASP	Sidechain
3	G	40	GLN	Sidechain

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	1120	1052	1052	45	1
1	B	1118	1057	1057	26	1
2	C	513	448	448	28	0
2	D	446	381	380	32	0
3	F	581	582	582	39	0
3	G	269	243	243	18	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2	0	0	0	0
5	B	4	0	0	0	0
5	D	1	0	0	0	0
All	All	4056	3763	3762	178	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 (178) 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:3:LEU:CG	1:A:3:LEU:CD1	1.79	1.56
1:A:3:LEU:CG	1:A:3:LEU:CD2	1.83	1.53
2:D:438:LYS:N	2:D:441:ASP:OD2	1.80	1.15
1:A:3:LEU:CD2	1:A:3:LEU:HG	1.72	1.10
3:F:22:THR:HG22	3:F:25:ASN:OD1	1.65	0.95
1:A:115:PRO:HB2	1:A:128:LYS:HE3	1.52	0.90
2:D:448:ARG:HG2	2:D:448:ARG:HH11	1.44	0.82
1:A:36:THR:HG22	1:A:51:PHE:HD1	1.45	0.82
3:F:45:PHE:CD1	3:F:67:LEU:HD22	2.15	0.81
1:A:120:VAL:HG11	1:A:123:ILE:HD12	1.65	0.79
1:A:115:PRO:O	1:A:118:PRO:HG3	1.85	0.77
2:C:440:VAL:HG22	2:C:444:LEU:HD21	1.68	0.76
3:F:11:LYS:O	3:F:12:THR:OG1	2.03	0.76
1:A:36:THR:HG22	1:A:51:PHE:CD1	2.22	0.74
2:C:438:LYS:N	2:C:441:ASP:OD2	2.22	0.73
3:F:14:THR:O	3:F:15:LEU:HD23	1.89	0.72
1:A:99:ILE:O	1:A:102:VAL:HG22	1.91	0.70
3:F:7:THR:HG22	3:F:8:LEU:H	1.57	0.70
3:F:8:LEU:O	3:F:9:THR:OG1	2.08	0.70
3:G:37:PRO:HB2	3:G:40:GLN:OE1	1.92	0.69
3:G:41:GLN:CB	3:G:69:LEU:HD12	2.22	0.69
2:D:398:SER:HB2	2:D:425:LEU:HD11	1.75	0.69
2:D:436:HIS:HB2	2:D:439:CYS:SG	2.33	0.69
2:D:450:CYS:O	2:D:454:TYR:HA	1.92	0.69
1:B:5:ARG:O	1:B:9:GLU:HG3	1.95	0.67
1:A:51:PHE:C	1:A:52:LEU:HD12	2.21	0.66
1:A:64:PRO:HB3	1:A:93:TRP:CG	2.32	0.65
2:D:437:ALA:C	2:D:441:ASP:OD2	2.39	0.65
2:D:421:GLU:H	2:D:424:GLN:NE2	1.93	0.65
3:F:73:LEU:HD23	3:F:74:ARG:C	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD22	1:A:7:HIS:HD2	1.62	0.64
1:A:3:LEU:CD1	1:A:3:LEU:CB	2.75	0.63
1:A:3:LEU:HD22	1:A:7:HIS:CD2	2.34	0.62
1:B:85:LYS:NZ	3:F:76:GLY:N	2.48	0.62
1:B:49:VAL:HG13	1:B:49:VAL:O	1.99	0.61
1:B:4:LYS:O	1:B:5:ARG:HB2	2.01	0.61
2:D:424:GLN:OE1	2:D:424:GLN:N	2.29	0.61
1:B:85:LYS:HZ2	3:F:76:GLY:C	2.09	0.60
1:B:79:ASN:OD1	1:B:81:ASN:N	2.29	0.60
3:F:33:LYS:O	3:F:34:GLU:OE2	2.20	0.59
2:C:427:ARG:HH11	2:C:427:ARG:HG3	1.68	0.59
1:A:29:ASP:OD1	1:A:31:PHE:HB2	2.01	0.58
2:D:421:GLU:N	2:D:424:GLN:HE22	2.02	0.58
3:G:7:THR:O	3:G:7:THR:HG23	2.04	0.58
1:A:74:TYR:CE1	1:A:137:ILE:HG21	2.38	0.58
3:F:1:MET:HE1	3:F:61:ILE:O	2.04	0.57
1:B:79:ASN:OD1	1:B:79:ASN:C	2.47	0.57
2:C:440:VAL:HG22	2:C:444:LEU:CD2	2.35	0.56
2:C:444:LEU:N	2:C:444:LEU:HD22	2.21	0.56
1:A:95:PRO:HB2	2:C:415:VAL:HG22	1.86	0.56
1:B:74:TYR:CZ	1:B:137:ILE:HG21	2.40	0.56
2:D:453:CYS:SG	2:D:455:ALA:HB3	2.44	0.56
3:F:45:PHE:CD1	3:F:67:LEU:CD2	2.87	0.56
3:F:12:THR:HG22	3:F:13:ILE:N	2.21	0.56
1:B:71:THR:HG21	1:B:146:ALA:HB2	1.89	0.55
3:G:69:LEU:HD23	3:G:69:LEU:H	1.71	0.55
1:A:3:LEU:CD2	1:A:7:HIS:HD2	2.20	0.55
1:A:41:ASN:OD1	1:A:46:GLN:NE2	2.39	0.55
1:B:90:ARG:HH12	3:F:73:LEU:CD2	2.19	0.55
2:C:436:HIS:HB2	2:C:439:CYS:CB	2.36	0.55
3:G:25:ASN:HA	3:G:28:ALA:HB3	1.88	0.55
3:G:36:ILE:CG2	3:G:36:ILE:O	2.55	0.54
1:B:4:LYS:O	1:B:5:ARG:CB	2.56	0.53
3:F:45:PHE:CE2	3:F:61:ILE:HG13	2.42	0.53
1:A:74:TYR:CZ	1:A:123:ILE:HG12	2.44	0.53
2:D:448:ARG:HH11	2:D:448:ARG:CG	2.17	0.53
3:F:45:PHE:O	3:F:46:ALA:C	2.51	0.53
3:F:13:ILE:HD11	3:F:34:GLU:HG3	1.91	0.52
3:F:14:THR:C	3:F:15:LEU:HD23	2.35	0.52
1:A:3:LEU:HD22	1:A:3:LEU:O	2.09	0.52
1:A:3:LEU:CD2	1:A:7:HIS:CD2	2.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:PRO:HG2	1:B:21:CYS:HB2	1.92	0.52
2:D:453:CYS:C	2:D:455:ALA:N	2.66	0.52
2:C:440:VAL:O	2:C:444:LEU:CD2	2.58	0.51
3:F:12:THR:HG22	3:F:13:ILE:H	1.75	0.51
2:D:404:ASN:O	2:D:405:ASN:CB	2.57	0.51
1:A:3:LEU:CD2	1:A:3:LEU:O	2.59	0.51
1:A:64:PRO:HB3	1:A:93:TRP:CD2	2.45	0.51
2:D:395:GLN:HA	2:D:395:GLN:OE1	2.10	0.51
2:C:421:GLU:O	2:C:424:GLN:HG3	2.10	0.50
1:A:74:TYR:CZ	1:A:137:ILE:HG21	2.46	0.50
1:A:21:CYS:SG	1:A:22:ARG:N	2.84	0.50
2:C:405:ASN:O	2:C:405:ASN:OD1	2.30	0.50
2:D:425:LEU:HG	2:D:437:ALA:HB3	1.94	0.50
2:D:425:LEU:HD12	2:D:426:LEU:N	2.27	0.49
2:D:454:TYR:N	2:D:454:TYR:CD1	2.80	0.49
3:F:8:LEU:C	3:F:9:THR:HG23	2.37	0.49
1:A:7:HIS:O	1:A:11:ASN:ND2	2.45	0.49
2:D:397:PRO:HD2	2:D:428:VAL:O	2.13	0.49
3:G:70:VAL:O	3:G:70:VAL:HG23	2.13	0.49
1:A:126:ILE:HG22	1:A:134:TYR:HB2	1.93	0.48
2:D:412:LEU:N	2:D:420:PHE:CE1	2.81	0.48
2:D:453:CYS:O	2:D:454:TYR:C	2.55	0.48
1:A:117:ASP:N	1:A:118:PRO:HD3	2.28	0.48
3:F:73:LEU:HD23	3:F:74:ARG:N	2.29	0.48
1:A:8:LYS:HE3	2:C:418:CYS:SG	2.53	0.48
1:A:75:HIS:CE1	1:A:76:PRO:HD2	2.49	0.48
1:B:85:LYS:NZ	3:F:76:GLY:C	2.71	0.48
2:C:407:GLN:HB2	3:F:49:GLN:OE1	2.14	0.47
2:D:412:LEU:N	2:D:420:PHE:HE1	2.13	0.47
2:D:440:VAL:O	2:D:444:LEU:HD23	2.13	0.47
1:B:5:ARG:NH1	2:D:415:VAL:O	2.48	0.47
3:F:1:MET:HE3	3:F:62:GLN:C	2.40	0.47
3:G:36:ILE:O	3:G:36:ILE:HG23	2.14	0.47
1:A:116:ASP:C	1:A:118:PRO:HD3	2.40	0.47
1:B:86:LEU:HD13	1:B:109:LEU:HD22	1.96	0.47
3:G:26:VAL:O	3:G:30:ILE:HD11	2.15	0.47
3:G:43:LEU:HD12	3:G:44:ILE:N	2.30	0.47
3:F:38:PRO:HA	3:F:41:GLN:NE2	2.30	0.47
3:F:73:LEU:HD23	3:F:74:ARG:O	2.15	0.47
3:F:1:MET:HE3	3:F:63:LYS:N	2.30	0.46
2:C:456:ASP:OD1	2:C:457:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:454:TYR:N	2:D:454:TYR:HD1	2.14	0.46
1:B:120:VAL:HG11	1:B:123:ILE:HD12	1.98	0.46
1:A:102:VAL:HG23	1:A:103:LEU:N	2.31	0.46
1:B:5:ARG:O	1:B:9:GLU:CG	2.63	0.45
3:F:36:ILE:HD12	3:F:36:ILE:H	1.79	0.45
1:B:90:ARG:HH12	3:F:73:LEU:HD22	1.81	0.45
1:A:103:LEU:HA	1:A:103:LEU:HD23	1.67	0.45
2:C:393:ILE:HD12	2:C:444:LEU:HB3	1.99	0.45
3:F:4:PHE:HB2	3:F:66:THR:HA	1.98	0.45
1:A:6:ILE:HD13	1:A:31:PHE:CD1	2.51	0.45
1:B:90:ARG:HH12	3:F:73:LEU:HD21	1.81	0.45
1:B:126:ILE:HG22	1:B:134:TYR:HB2	1.98	0.45
3:F:18:GLU:O	3:F:19:PRO:C	2.55	0.45
2:C:433:HIS:HE1	2:C:453:CYS:HB3	1.82	0.45
1:A:7:HIS:CD2	1:A:30:MET:HE2	2.53	0.44
2:C:436:HIS:O	2:C:440:VAL:HG12	2.16	0.44
2:C:410:GLN:HE22	2:C:452:ILE:CD1	2.30	0.44
2:C:427:ARG:HG3	2:C:427:ARG:NH1	2.30	0.44
1:B:61:PRO:HD2	1:B:62:PHE:CD1	2.53	0.43
2:C:428:VAL:HG22	2:C:434:GLU:HB3	2.00	0.43
2:C:440:VAL:O	2:C:444:LEU:HD22	2.18	0.43
2:D:453:CYS:O	2:D:455:ALA:N	2.52	0.43
3:G:36:ILE:O	3:G:37:PRO:C	2.61	0.43
3:G:43:LEU:HA	3:G:68:HIS:O	2.18	0.43
3:F:37:PRO:HA	3:F:38:PRO:HD3	1.86	0.43
3:G:39:ASP:CG	3:G:40:GLN:HE22	2.27	0.43
1:A:99:ILE:HA	1:A:99:ILE:HD13	1.83	0.43
1:A:143:GLN:OE1	1:A:147:MET:HE2	2.19	0.43
2:C:398:SER:HA	2:C:426:LEU:O	2.19	0.43
3:G:27:LYS:HA	3:G:30:ILE:HG12	2.01	0.43
3:G:61:ILE:HD12	3:G:61:ILE:N	2.34	0.43
3:F:22:THR:HG23	3:F:25:ASN:H	1.84	0.43
1:A:5:ARG:HD2	1:A:5:ARG:O	2.19	0.43
2:D:444:LEU:HA	2:D:447:ASN:O	2.18	0.43
2:C:402:ASN:OD1	2:C:402:ASN:C	2.62	0.42
2:D:421:GLU:N	2:D:424:GLN:NE2	2.61	0.42
1:A:9:GLU:OE2	1:A:60:TYR:OH	2.24	0.42
2:C:449:THR:O	2:C:451:PRO:HD3	2.19	0.42
2:D:453:CYS:SG	2:D:455:ALA:CB	3.07	0.42
2:C:412:LEU:HD23	2:C:413:CYS:C	2.45	0.42
3:F:8:LEU:O	3:F:8:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:429:LEU:HB3	2:C:430:PRO:HD2	2.01	0.42
1:A:134:TYR:CD1	1:A:134:TYR:C	2.96	0.42
2:C:433:HIS:CE1	2:C:453:CYS:HB3	2.55	0.42
2:D:448:ARG:HG2	2:D:448:ARG:NH1	2.24	0.42
3:F:65:SER:HB3	3:F:67:LEU:HD21	2.01	0.42
1:A:75:HIS:CE1	1:A:77:ASN:H	2.37	0.42
2:D:448:ARG:CG	2:D:448:ARG:NH1	2.82	0.42
3:F:8:LEU:O	3:F:9:THR:CB	2.67	0.42
3:F:22:THR:HA	3:F:55:THR:HA	2.00	0.42
2:C:420:PHE:CE1	2:C:426:LEU:HD22	2.55	0.42
3:G:36:ILE:HD12	3:G:36:ILE:HA	1.92	0.42
1:B:47:GLY:O	1:B:147:MET:SD	2.78	0.41
2:D:450:CYS:HB3	2:D:455:ALA:H	1.85	0.41
1:B:48:GLY:HA2	1:B:146:ALA:O	2.21	0.41
3:G:43:LEU:HD12	3:G:68:HIS:N	2.35	0.41
3:G:60:ASN:C	3:G:62:GLN:OE1	2.63	0.41
3:F:1:MET:HE2	3:F:3:ILE:HD11	2.01	0.41
1:A:24:GLY:O	1:A:33:TRP:HB3	2.21	0.41
1:A:3:LEU:HG	1:A:3:LEU:O	2.15	0.41
2:D:444:LEU:HA	2:D:444:LEU:HD13	1.86	0.41
1:B:119:LEU:O	1:B:119:LEU:HG	2.20	0.41
1:A:38:MET:SD	1:A:49:VAL:HG22	2.61	0.41
2:C:437:ALA:HA	2:C:441:ASP:OD2	2.21	0.41
1:B:52:LEU:HD12	1:B:52:LEU:N	2.36	0.40
1:B:85:LYS:HG3	1:B:119:LEU:HB2	2.02	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:29:ASP:OD2	1:B:59:ASP:OD2[6_665]	2.14	0.06

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	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
1	B	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	19	28
2	C	67/69 (97%)	61 (91%)	5 (8%)	1 (2%)	8	11
2	D	60/69 (87%)	51 (85%)	6 (10%)	3 (5%)	1	1
3	F	75/77 (97%)	61 (81%)	9 (12%)	5 (7%)	1	0
3	G	26/77 (34%)	19 (73%)	4 (15%)	3 (12%)	0	0
All	All	516/584 (88%)	472 (92%)	31 (6%)	13 (2%)	4	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	ARG
2	D	438	LYS
3	F	12	THR
3	F	13	ILE
2	C	438	LYS
2	D	405	ASN
2	D	454	TYR
3	F	74	ARG
3	F	60	ASN
3	G	38	PRO
3	F	46	ALA
3	G	37	PRO
3	G	42	ARG

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	116/130 (89%)	116 (100%)	0	100	100
1	B	117/130 (90%)	116 (99%)	1 (1%)	75	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	54/64 (84%)	54 (100%)	0	100	100
2	D	46/64 (72%)	45 (98%)	1 (2%)	47	67
3	F	63/69 (91%)	63 (100%)	0	100	100
3	G	27/69 (39%)	26 (96%)	1 (4%)	29	46
All	All	423/526 (80%)	420 (99%)	3 (1%)	81	90

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

Mol	Chain	Res	Type
1	B	55	HIS
2	D	454	TYR
3	G	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	11	ASN
1	B	32	HIS
2	C	405	ASN
2	D	404	ASN
2	D	406	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

Of 4 ligands modelled in this entry, 4 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

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	146/146 (100%)	0.19	7 (4%)	36 35	69, 95, 130, 156	0
1	B	146/146 (100%)	0.11	3 (2%)	63 61	66, 84, 131, 206	1 (0%)
2	C	69/69 (100%)	0.54	4 (5%)	30 29	91, 117, 185, 233	0
2	D	62/69 (89%)	1.46	20 (32%)	1 1	137, 182, 245, 271	0
3	F	77/77 (100%)	0.65	10 (12%)	9 9	86, 122, 212, 225	0
3	G	38/77 (49%)	1.16	7 (18%)	4 4	213, 252, 280, 286	0
All	All	538/584 (92%)	0.49	51 (9%)	15 15	66, 109, 246, 286	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	452	ILE	5.6
2	D	456	ASP	4.2
2	C	393	ILE	3.8
3	F	76	GLY	3.5
2	D	435	PHE	3.4
2	D	454	TYR	3.2
2	D	414	VAL	3.0
2	C	442	LYS	2.9
2	D	426	LEU	2.9
3	F	73	LEU	2.9
2	D	444	LEU	2.9
3	F	75	GLY	2.8
3	F	74	ARG	2.8
2	D	432	ASN	2.7
2	D	429	LEU	2.7
1	A	31	PHE	2.7
1	A	134	TYR	2.7
3	G	69	LEU	2.7
2	C	394	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	453	CYS	2.5
2	D	396	LEU	2.5
1	A	20	GLN	2.5
2	D	455	ALA	2.5
1	A	19	ALA	2.4
1	A	145	TYR	2.4
3	F	10	GLY	2.4
2	D	420	PHE	2.4
2	D	408	SER	2.3
1	B	13	LEU	2.3
2	C	411	THR	2.3
2	D	434	GLU	2.3
2	D	403	PRO	2.3
2	D	451	PRO	2.3
3	G	71	LEU	2.3
3	G	21	ASP	2.2
1	B	4	LYS	2.2
1	A	91	SER	2.2
1	B	9	GLU	2.2
3	F	32	ASP	2.2
2	D	449	THR	2.1
3	G	68	HIS	2.1
3	F	8	LEU	2.1
3	G	9	THR	2.1
1	A	28	ASP	2.1
3	F	43	LEU	2.1
2	D	409	GLU	2.1
3	F	0	SER	2.1
3	F	67	LEU	2.1
3	G	26	VAL	2.0
3	G	31	GLN	2.0
2	D	431	CYS	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
4	ZN	D	502	1/1	0.95	0.07	130,130,130,130	0
4	ZN	C	501	1/1	0.96	0.07	103,103,103,103	0
4	ZN	D	501	1/1	0.97	0.05	127,127,127,127	0
4	ZN	C	502	1/1	0.99	0.04	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.