



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:05 AM UTC

PDB ID : 4MVT / pdb_00004mvt
Title : Crystal structure of SUMO E3 Ligase PIAS3
Authors : Dong, A.; Hu, J.; Li, Y.; Tempel, W.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Tong, Y.; Structural Genomics Consortium (SGC)
Deposited on : 2013-09-24
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

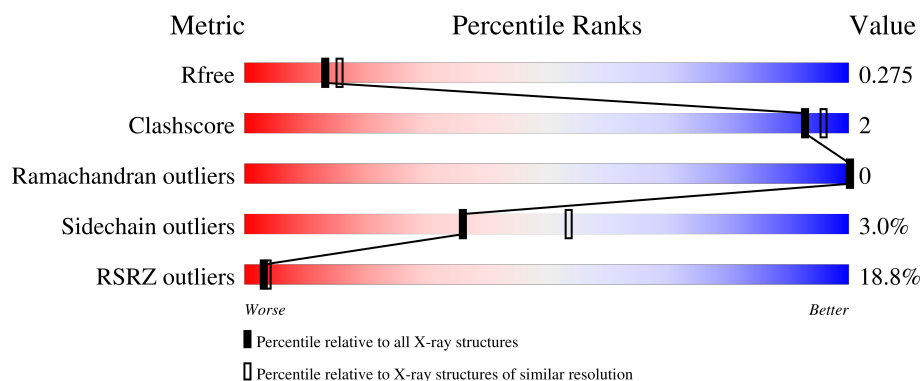
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	374	10% 63% 5% 32%
1	B	374	13% 62% 5% 33%
1	C	374	14% 63% 5% 32%
1	D	374	13% 60% 6% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	A	503	-	-	-	X
4	UNX	A	504	-	-	-	X
4	UNX	A	505	-	-	-	X
4	UNX	A	506	-	-	-	X
4	UNX	A	507	-	-	-	X
4	UNX	A	508	-	-	-	X
4	UNX	A	509	-	-	-	X
4	UNX	A	510	-	-	-	X
4	UNX	A	511	-	-	-	X
4	UNX	A	512	-	-	-	X
4	UNX	B	502	-	-	-	X
4	UNX	B	503	-	-	-	X
4	UNX	B	504	-	-	-	X
4	UNX	B	505	-	-	-	X
4	UNX	B	506	-	-	-	X
4	UNX	B	507	-	-	-	X
4	UNX	B	508	-	-	-	X
4	UNX	C	503	-	-	-	X
4	UNX	C	504	-	-	-	X
4	UNX	C	505	-	-	-	X
4	UNX	C	506	-	-	-	X
4	UNX	C	507	-	-	-	X
4	UNX	C	508	-	-	-	X
4	UNX	C	509	-	-	-	X
4	UNX	C	510	-	-	-	X
4	UNX	C	511	-	-	-	X
4	UNX	D	502	-	-	-	X
4	UNX	D	503	-	-	-	X
4	UNX	D	504	-	-	-	X
4	UNX	D	505	-	-	-	X
4	UNX	D	506	-	-	-	X
4	UNX	D	507	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7900 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 E3 SUMO-protein ligase PIAS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	1	0
			1954	1253	322	360	19			
1	B	251	Total	C	N	O	S	0	0	0
			1918	1236	312	351	19			
1	C	253	Total	C	N	O	S	0	0	0
			1937	1249	317	352	19			
1	D	249	Total	C	N	O	S	0	0	0
			1905	1226	319	341	19			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MET	-	expression tag	UNP Q9Y6X2
A	95	HIS	-	expression tag	UNP Q9Y6X2
A	96	HIS	-	expression tag	UNP Q9Y6X2
A	97	HIS	-	expression tag	UNP Q9Y6X2
A	98	HIS	-	expression tag	UNP Q9Y6X2
A	99	HIS	-	expression tag	UNP Q9Y6X2
A	100	HIS	-	expression tag	UNP Q9Y6X2
A	101	SER	-	expression tag	UNP Q9Y6X2
A	102	SER	-	expression tag	UNP Q9Y6X2
A	103	GLY	-	expression tag	UNP Q9Y6X2
A	104	ARG	-	expression tag	UNP Q9Y6X2
A	105	GLU	-	expression tag	UNP Q9Y6X2
A	106	ASN	-	expression tag	UNP Q9Y6X2
A	107	LEU	-	expression tag	UNP Q9Y6X2
A	108	TYR	-	expression tag	UNP Q9Y6X2
A	109	PHE	-	expression tag	UNP Q9Y6X2
A	110	GLN	-	expression tag	UNP Q9Y6X2
A	111	GLY	-	expression tag	UNP Q9Y6X2
B	94	MET	-	expression tag	UNP Q9Y6X2
B	95	HIS	-	expression tag	UNP Q9Y6X2
B	96	HIS	-	expression tag	UNP Q9Y6X2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	97	HIS	-	expression tag	UNP Q9Y6X2
B	98	HIS	-	expression tag	UNP Q9Y6X2
B	99	HIS	-	expression tag	UNP Q9Y6X2
B	100	HIS	-	expression tag	UNP Q9Y6X2
B	101	SER	-	expression tag	UNP Q9Y6X2
B	102	SER	-	expression tag	UNP Q9Y6X2
B	103	GLY	-	expression tag	UNP Q9Y6X2
B	104	ARG	-	expression tag	UNP Q9Y6X2
B	105	GLU	-	expression tag	UNP Q9Y6X2
B	106	ASN	-	expression tag	UNP Q9Y6X2
B	107	LEU	-	expression tag	UNP Q9Y6X2
B	108	TYR	-	expression tag	UNP Q9Y6X2
B	109	PHE	-	expression tag	UNP Q9Y6X2
B	110	GLN	-	expression tag	UNP Q9Y6X2
B	111	GLY	-	expression tag	UNP Q9Y6X2
C	94	MET	-	expression tag	UNP Q9Y6X2
C	95	HIS	-	expression tag	UNP Q9Y6X2
C	96	HIS	-	expression tag	UNP Q9Y6X2
C	97	HIS	-	expression tag	UNP Q9Y6X2
C	98	HIS	-	expression tag	UNP Q9Y6X2
C	99	HIS	-	expression tag	UNP Q9Y6X2
C	100	HIS	-	expression tag	UNP Q9Y6X2
C	101	SER	-	expression tag	UNP Q9Y6X2
C	102	SER	-	expression tag	UNP Q9Y6X2
C	103	GLY	-	expression tag	UNP Q9Y6X2
C	104	ARG	-	expression tag	UNP Q9Y6X2
C	105	GLU	-	expression tag	UNP Q9Y6X2
C	106	ASN	-	expression tag	UNP Q9Y6X2
C	107	LEU	-	expression tag	UNP Q9Y6X2
C	108	TYR	-	expression tag	UNP Q9Y6X2
C	109	PHE	-	expression tag	UNP Q9Y6X2
C	110	GLN	-	expression tag	UNP Q9Y6X2
C	111	GLY	-	expression tag	UNP Q9Y6X2
D	94	MET	-	expression tag	UNP Q9Y6X2
D	95	HIS	-	expression tag	UNP Q9Y6X2
D	96	HIS	-	expression tag	UNP Q9Y6X2
D	97	HIS	-	expression tag	UNP Q9Y6X2
D	98	HIS	-	expression tag	UNP Q9Y6X2
D	99	HIS	-	expression tag	UNP Q9Y6X2
D	100	HIS	-	expression tag	UNP Q9Y6X2
D	101	SER	-	expression tag	UNP Q9Y6X2
D	102	SER	-	expression tag	UNP Q9Y6X2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	103	GLY	-	expression tag	UNP Q9Y6X2
D	104	ARG	-	expression tag	UNP Q9Y6X2
D	105	GLU	-	expression tag	UNP Q9Y6X2
D	106	ASN	-	expression tag	UNP Q9Y6X2
D	107	LEU	-	expression tag	UNP Q9Y6X2
D	108	TYR	-	expression tag	UNP Q9Y6X2
D	109	PHE	-	expression tag	UNP Q9Y6X2
D	110	GLN	-	expression tag	UNP Q9Y6X2
D	111	GLY	-	expression tag	UNP Q9Y6X2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- 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	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	X	0	0
			10	10		
4	B	7	Total	X	0	0
			7	7		
4	C	9	Total	X	0	0
			9	9		
4	D	6	Total	X	0	0
			6	6		

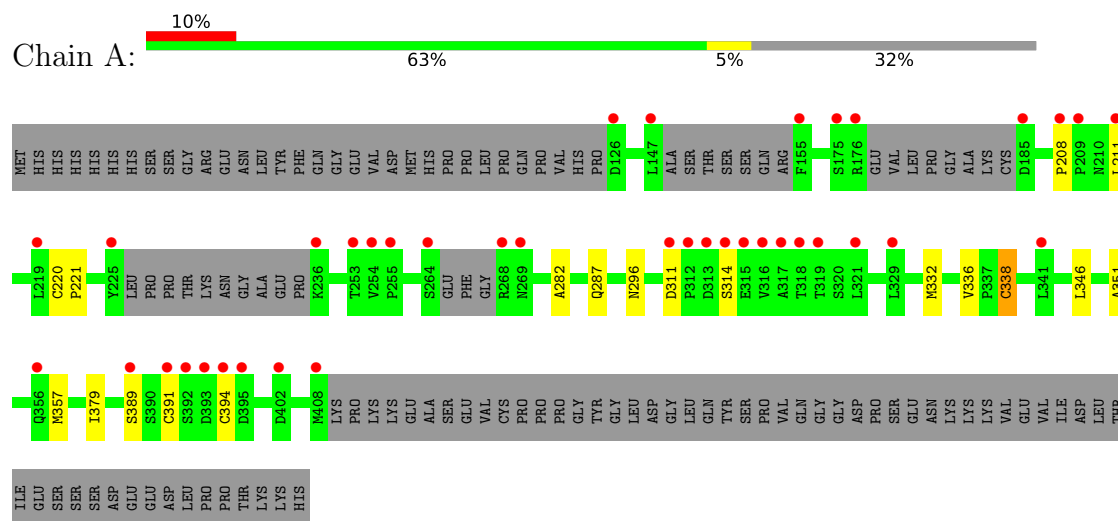
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total 39	O 39	0	0
5	B	37	Total 37	O 37	0	0
5	C	34	Total 35	O 35	0	1
5	D	36	Total 37	O 37	0	1

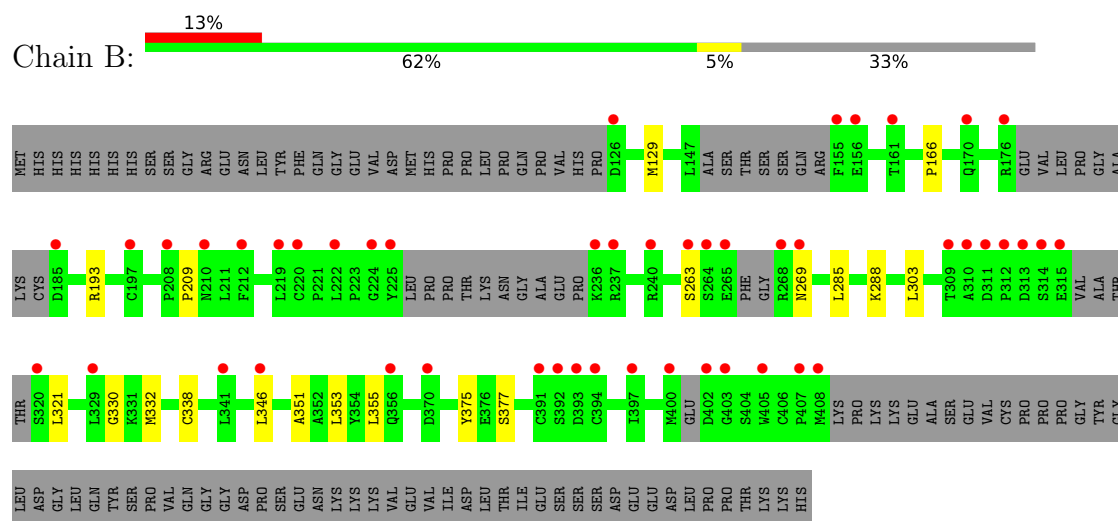
3 Residue-property plots [i](#)

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: E3 SUMO-protein ligase PIAS3

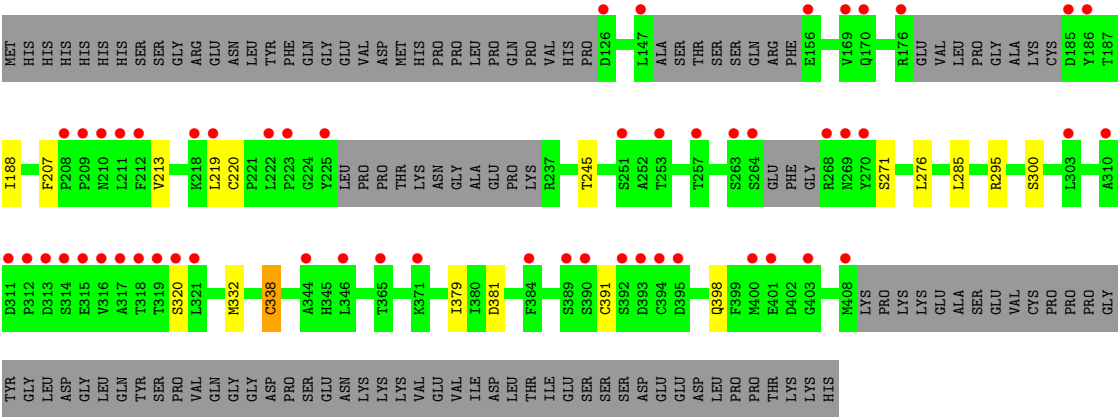


• Molecule 1: E3 SUMO-protein ligase PIAS3

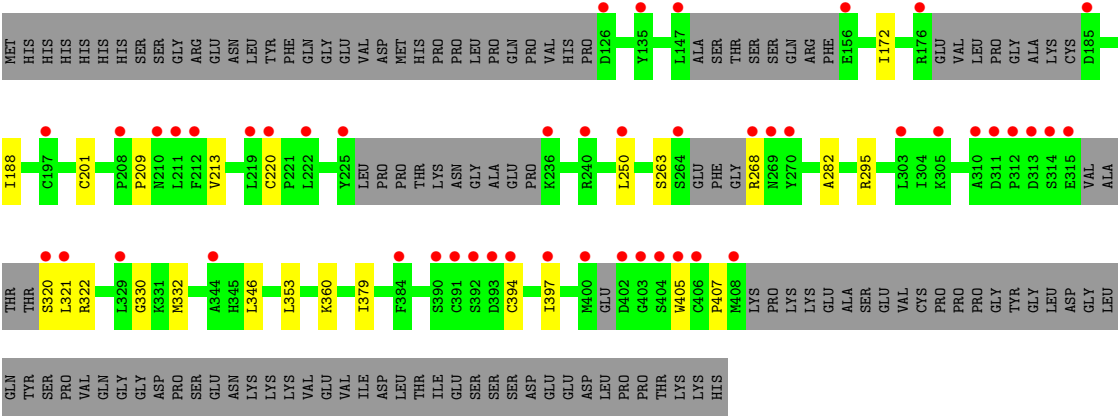


• Molecule 1: E3 SUMO-protein ligase PIAS3





● Molecule 1: E3 SUMO-protein ligase PIAS3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.45Å 85.44Å 89.53Å 83.08° 86.57° 86.14°	Depositor
Resolution (Å)	48.04 – 2.30 48.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.04-2.30) 98.3 (48.04-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC, BUSTER 2.10.0	Depositor
R, R_{free}	0.238 , 0.270 0.245 , 0.275	Depositor DCC
R_{free} test set	1428 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.075 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: CL, UNX, 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	0.88	1/1996 (0.1%)	1.17	3/2724 (0.1%)
1	B	0.86	0/1958	1.18	6/2667 (0.2%)
1	C	0.85	0/1980	1.18	5/2701 (0.2%)
1	D	0.84	0/1946	1.14	4/2649 (0.2%)
All	All	0.86	1/7880 (0.0%)	1.17	18/10741 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	MET	SD-CE	5.40	1.93	1.79

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	CYS	CA-C-N	5.72	128.26	120.54
1	C	391	CYS	C-N-CA	5.72	128.26	120.54
1	D	282	ALA	CA-C-N	5.52	126.10	119.98
1	D	282	ALA	C-N-CA	5.52	126.10	119.98
1	D	201	CYS	N-CA-C	5.46	113.14	108.22
1	A	296	ASN	CA-CB-CG	5.41	118.01	112.60
1	C	276	LEU	N-CA-C	-5.25	100.17	108.73
1	B	303	LEU	CA-C-N	5.24	127.27	120.56
1	B	303	LEU	C-N-CA	5.24	127.27	120.56
1	B	355	LEU	CA-C-N	5.18	127.22	120.28
1	B	355	LEU	C-N-CA	5.18	127.22	120.28
1	D	188	ILE	N-CA-CB	5.15	116.87	111.00
1	C	207	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	282	ALA	CA-C-N	5.11	125.65	119.98
1	A	282	ALA	C-N-CA	5.11	125.65	119.98
1	C	188	ILE	N-CA-CB	5.08	116.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	PRO	CA-C-N	5.05	127.47	120.29
1	B	166	PRO	C-N-CA	5.05	127.47	120.29

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	1954	0	1904	6	0
1	B	1918	0	1871	5	0
1	C	1937	0	1902	5	0
1	D	1905	0	1865	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	10	0	0	0	0
4	B	7	0	0	0	0
4	C	9	0	0	0	0
4	D	6	0	0	0	0
5	A	39	0	0	0	0
5	B	37	0	0	0	0
5	C	35	0	0	0	0
5	D	37	0	0	0	0
All	All	7900	0	7542	23	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 2.

All (23) 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:285:LEU:HD22	1:B:375:TYR:CZ	2.38	0.57
1:B:330:GLY:HA3	1:B:353:LEU:CD2	2.41	0.50
1:A:208:PRO:HD2	1:A:211:LEU:HD13	1.93	0.50
1:A:338:CYS:HB2	1:A:379:ILE:O	2.12	0.49
1:B:129:MET:HE2	1:B:193:ARG:HB3	1.95	0.47
1:A:336:VAL:HB	1:A:351:ALA:HB3	1.97	0.46
1:A:391:CYS:SG	1:A:394:CYS:HB3	2.55	0.46
1:C:295:ARG:HD3	1:C:379:ILE:HD13	1.98	0.45
1:D:330:GLY:HA3	1:D:353:LEU:CD2	2.47	0.45
1:A:311:ASP:HB3	1:A:314:SER:HB2	1.98	0.45
1:D:209:PRO:HG2	1:D:263:SER:O	2.19	0.43
1:C:213:VAL:HB	1:C:220:CYS:HB3	2.01	0.43
1:D:397:ILE:HD12	1:D:405:TRP:CZ3	2.54	0.42
1:A:220:CYS:HA	1:A:221:PRO:HD3	1.95	0.41
1:C:300:SER:OG	1:C:381:ASP:OD2	2.36	0.41
1:B:209:PRO:HG2	1:B:263:SER:O	2.20	0.41
1:D:213:VAL:HB	1:D:220:CYS:HB3	2.01	0.41
1:D:172:ILE:HG21	1:D:250:LEU:HD22	2.03	0.41
1:C:338:CYS:HB2	1:C:379:ILE:O	2.21	0.40
1:B:338:CYS:HB2	1:B:351:ALA:HB2	2.02	0.40
1:D:394:CYS:SG	1:D:407:PRO:HB3	2.61	0.40
1:C:285:LEU:HD12	1:C:285:LEU:HA	1.89	0.40
1:D:295:ARG:HD3	1:D:379:ILE:HD13	2.03	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	245/374 (66%)	238 (97%)	7 (3%)	0	100	100
1	B	237/374 (63%)	234 (99%)	3 (1%)	0	100	100
1	C	243/374 (65%)	236 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	235/374 (63%)	229 (97%)	6 (3%)	0	100	100
All	All	960/1496 (64%)	937 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	212/338 (63%)	207 (98%)	5 (2%)	43	62
1	B	208/338 (62%)	202 (97%)	6 (3%)	37	55
1	C	210/338 (62%)	203 (97%)	7 (3%)	33	50
1	D	205/338 (61%)	198 (97%)	7 (3%)	32	49
All	All	835/1352 (62%)	810 (97%)	25 (3%)	36	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	332	MET
1	A	338	CYS
1	A	346	LEU
1	A	389	SER
1	B	269	ASN
1	B	288	LYS
1	B	321	LEU
1	B	332	MET
1	B	346	LEU
1	B	377	SER
1	C	219	LEU
1	C	245	THR
1	C	271	SER
1	C	320	SER
1	C	332	MET

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Mol	Chain	Res	Type
1	C	338	CYS
1	C	398	GLN
1	D	268	ARG
1	D	320	SER
1	D	321	LEU
1	D	322	ARG
1	D	332	MET
1	D	346	LEU
1	D	360	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	279	GLN
1	B	171	GLN
1	B	203	GLN
1	B	269	ASN
1	B	398	GLN
1	C	171	GLN
1	C	203	GLN
1	C	356	GLN
1	D	171	GLN
1	D	279	GLN

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 [i](#)

Of 38 ligands modelled in this entry, 6 are monoatomic and 32 are unknown - 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	255/374 (68%)	0.98	39 (15%) 5 6	27, 45, 72, 98	1 (0%)
1	B	251/374 (67%)	1.01	48 (19%) 3 4	27, 46, 73, 100	0
1	C	253/374 (67%)	1.22	54 (21%) 2 3	29, 46, 70, 94	0
1	D	249/374 (66%)	1.22	48 (19%) 3 3	27, 46, 75, 97	0
All	All	1008/1496 (67%)	1.11	189 (18%) 3 4	27, 46, 73, 100	1 (0%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	ALA	8.9
1	D	264	SER	7.0
1	C	264	SER	6.9
1	D	176	ARG	6.4
1	A	264	SER	6.1
1	A	225	TYR	5.7
1	B	176	ARG	5.6
1	A	126[A]	ASP	5.6
1	D	402	ASP	5.5
1	B	265	GLU	5.4
1	C	318	THR	5.4
1	B	225	TYR	5.2
1	A	176	ARG	5.2
1	C	176	ARG	5.2
1	A	155	PHE	5.1
1	D	311	ASP	4.9
1	D	313	ASP	4.8
1	D	236	LYS	4.7
1	C	316	VAL	4.6
1	C	313	ASP	4.6
1	A	236	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	225	TYR	4.2
1	A	317	ALA	4.2
1	A	394	CYS	4.2
1	A	393	ASP	4.2
1	D	269	ASN	4.2
1	C	401	GLU	4.2
1	D	390	SER	4.1
1	A	313	ASP	4.1
1	C	268	ARG	4.0
1	D	315	GLU	4.0
1	C	314	SER	4.0
1	D	408	MET	3.9
1	D	126	ASP	3.9
1	D	403	GLY	3.8
1	C	225	TYR	3.7
1	C	147	LEU	3.7
1	D	312	PRO	3.7
1	B	155	PHE	3.7
1	D	156	GLU	3.7
1	D	400	MET	3.7
1	D	394	CYS	3.6
1	A	318	THR	3.6
1	C	156	GLU	3.6
1	D	314	SER	3.6
1	B	236	LYS	3.6
1	B	402	ASP	3.6
1	A	312	PRO	3.6
1	D	405	TRP	3.6
1	C	321	LEU	3.5
1	C	390	SER	3.4
1	B	408	MET	3.3
1	B	313	ASP	3.3
1	B	219	LEU	3.3
1	B	268	ARG	3.3
1	B	400	MET	3.2
1	A	316	VAL	3.2
1	C	408	MET	3.2
1	D	321	LEU	3.2
1	B	403	GLY	3.2
1	D	393	ASP	3.2
1	C	384	PHE	3.1
1	C	394	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	356	GLN	3.1
1	B	185	ASP	3.1
1	A	208	PRO	3.1
1	A	392	SER	3.0
1	C	392	SER	3.0
1	B	341	LEU	3.0
1	B	405	TRP	3.0
1	A	389	SER	3.0
1	C	210	ASN	3.0
1	D	310	ALA	3.0
1	D	147	LEU	3.0
1	B	264	SER	3.0
1	C	263	SER	3.0
1	C	219	LEU	3.0
1	B	210	ASN	3.0
1	C	303	LEU	2.9
1	D	197	CYS	2.9
1	D	404	SER	2.9
1	A	311	ASP	2.9
1	B	269	ASN	2.9
1	D	185	ASP	2.9
1	D	270	TYR	2.9
1	B	329	LEU	2.9
1	C	253	THR	2.9
1	D	320	SER	2.8
1	B	312	PRO	2.8
1	B	240	ARG	2.8
1	B	156	GLU	2.8
1	B	394	CYS	2.8
1	A	147	LEU	2.8
1	D	329	LEU	2.8
1	B	309	THR	2.8
1	D	208	PRO	2.8
1	C	310	ALA	2.8
1	D	222	LEU	2.7
1	C	320	SER	2.7
1	B	356	GLN	2.7
1	C	312	PRO	2.7
1	D	305	LYS	2.7
1	C	212	PHE	2.7
1	A	185	ASP	2.7
1	B	310	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	208	PRO	2.6
1	B	126	ASP	2.6
1	A	253	THR	2.6
1	B	392	SER	2.6
1	D	240	ARG	2.6
1	B	311	ASP	2.6
1	D	397	ILE	2.6
1	B	393	ASP	2.6
1	C	126	ASP	2.6
1	C	319	THR	2.6
1	B	237	ARG	2.5
1	D	391	CYS	2.5
1	C	311	ASP	2.5
1	B	314	SER	2.5
1	A	268	ARG	2.5
1	A	341	LEU	2.5
1	D	210	ASN	2.5
1	A	254	VAL	2.5
1	D	303	LEU	2.5
1	A	391	CYS	2.4
1	B	320	SER	2.4
1	A	321	LEU	2.4
1	D	135	TYR	2.4
1	A	402	ASP	2.4
1	B	391	CYS	2.4
1	A	408	MET	2.4
1	C	186	TYR	2.4
1	B	370	ASP	2.4
1	C	209	PRO	2.4
1	C	344	ALA	2.4
1	C	400	MET	2.4
1	A	395	ASP	2.3
1	A	319	THR	2.3
1	B	212	PHE	2.3
1	A	314	SER	2.3
1	C	371	LYS	2.3
1	D	384	PHE	2.3
1	D	219	LEU	2.3
1	A	269	ASN	2.3
1	A	209	PRO	2.3
1	D	212	PHE	2.2
1	C	395	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	175	SER	2.2
1	C	211	LEU	2.2
1	C	346	LEU	2.2
1	C	393	ASP	2.2
1	B	407	PRO	2.2
1	C	403	GLY	2.2
1	C	315	GLU	2.2
1	B	397	ILE	2.2
1	B	222	LEU	2.2
1	D	268	ARG	2.2
1	C	223	PRO	2.2
1	A	315	GLU	2.2
1	C	389	SER	2.2
1	D	392	SER	2.2
1	D	211	LEU	2.1
1	C	170	GLN	2.1
1	B	220	CYS	2.1
1	C	257	THR	2.1
1	A	219	LEU	2.1
1	C	222	LEU	2.1
1	C	169	VAL	2.1
1	D	220	CYS	2.1
1	B	315	GLU	2.1
1	B	346	LEU	2.1
1	C	185	ASP	2.1
1	C	269	ASN	2.1
1	B	170	GLN	2.1
1	B	263	SER	2.1
1	C	365	THR	2.1
1	D	406	CYS	2.1
1	D	344	ALA	2.1
1	A	211	LEU	2.1
1	A	329	LEU	2.1
1	A	255	PRO	2.1
1	B	208	PRO	2.1
1	C	270	TYR	2.1
1	B	224	GLY	2.1
1	D	250	LEU	2.0
1	B	161	THR	2.0
1	C	251	SER	2.0
1	B	197	CYS	2.0
1	C	218	LYS	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	UNX	C	505	1/1	-0.32	0.47	300,300,300,300	0
4	UNX	A	507	1/1	-0.08	0.49	300,300,300,300	0
4	UNX	C	511	1/1	-0.08	0.41	300,300,300,300	0
4	UNX	B	507	1/1	0.07	0.61	300,300,300,300	0
4	UNX	B	503	1/1	0.16	0.77	300,300,300,300	0
4	UNX	A	504	1/1	0.19	0.70	300,300,300,300	0
4	UNX	C	509	1/1	0.22	0.64	300,300,300,300	0
4	UNX	A	508	1/1	0.27	0.52	300,300,300,300	0
4	UNX	A	503	1/1	0.27	0.90	300,300,300,300	0
4	UNX	C	510	1/1	0.33	0.62	300,300,300,300	0
4	UNX	A	512	1/1	0.33	0.53	300,300,300,300	0
4	UNX	C	508	1/1	0.35	0.49	300,300,300,300	0
4	UNX	D	506	1/1	0.36	0.64	300,300,300,300	0
4	UNX	B	504	1/1	0.37	0.70	300,300,300,300	0
4	UNX	A	509	1/1	0.37	0.67	300,300,300,300	0
4	UNX	D	503	1/1	0.40	0.62	300,300,300,300	0
4	UNX	C	506	1/1	0.40	0.70	300,300,300,300	0
4	UNX	C	504	1/1	0.41	0.66	300,300,300,300	0
4	UNX	D	502	1/1	0.41	0.59	295,295,295,295	0
4	UNX	D	504	1/1	0.42	0.61	281,281,281,281	0
4	UNX	C	507	1/1	0.43	0.56	300,300,300,300	0
4	UNX	C	503	1/1	0.43	0.61	269,269,269,269	0
4	UNX	B	505	1/1	0.43	0.59	275,275,275,275	0
4	UNX	A	506	1/1	0.46	0.46	300,300,300,300	0
4	UNX	A	510	1/1	0.46	0.55	299,299,299,299	0
4	UNX	D	505	1/1	0.48	0.58	300,300,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UNX	B	508	1/1	0.49	0.61	300,300,300,300	0
4	UNX	A	511	1/1	0.53	0.55	300,300,300,300	0
4	UNX	A	505	1/1	0.55	0.51	300,300,300,300	0
4	UNX	D	507	1/1	0.55	0.51	297,297,297,297	0
4	UNX	B	502	1/1	0.60	0.50	300,300,300,300	0
4	UNX	B	506	1/1	0.62	0.49	300,300,300,300	0
3	CL	A	502	1/1	0.98	0.07	29,29,29,29	0
3	CL	C	502	1/1	0.98	0.06	29,29,29,29	0
2	ZN	C	501	1/1	1.00	0.03	44,44,44,44	0
2	ZN	D	501	1/1	1.00	0.02	44,44,44,44	0
2	ZN	A	501	1/1	1.00	0.04	41,41,41,41	0
2	ZN	B	501	1/1	1.00	0.05	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.