



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 01:02 PM EDT

PDB ID : 4MVT
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.

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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

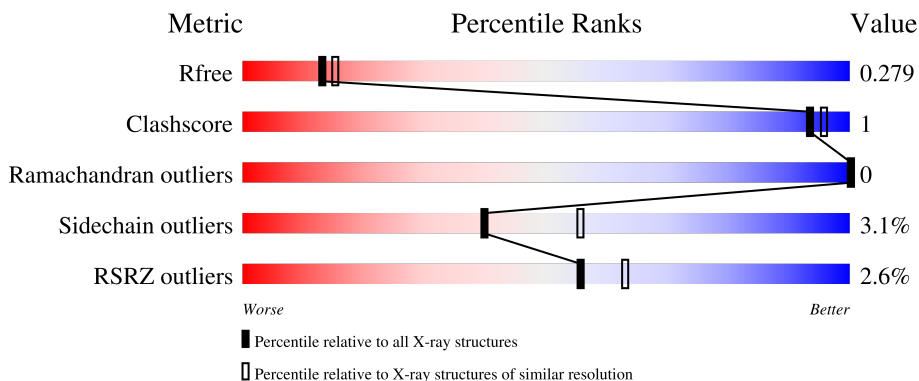
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	 2% 64% 32%
1	B	374	 % 63% 33%
1	C	374	 2% 64% 32%
1	D	374	 2% 61% 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 i

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

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

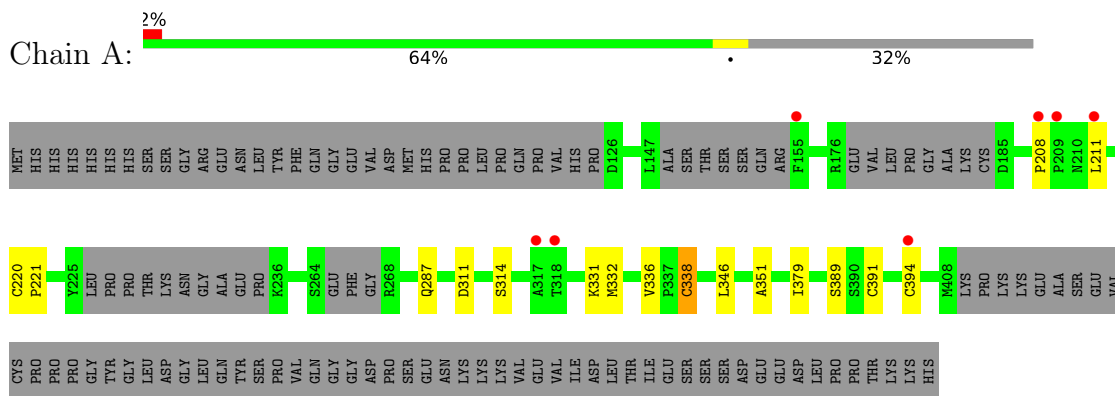
- Molecule 5 is water.

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

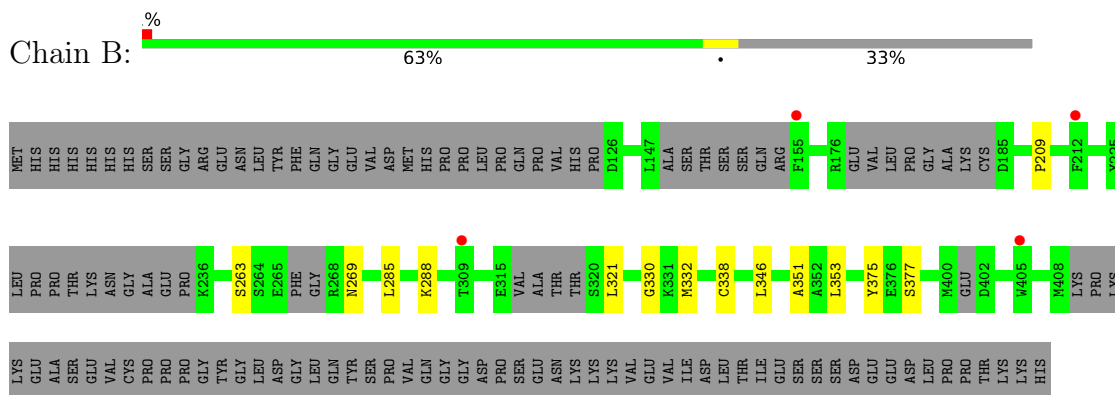
3 Residue-property plots [i](#)

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.

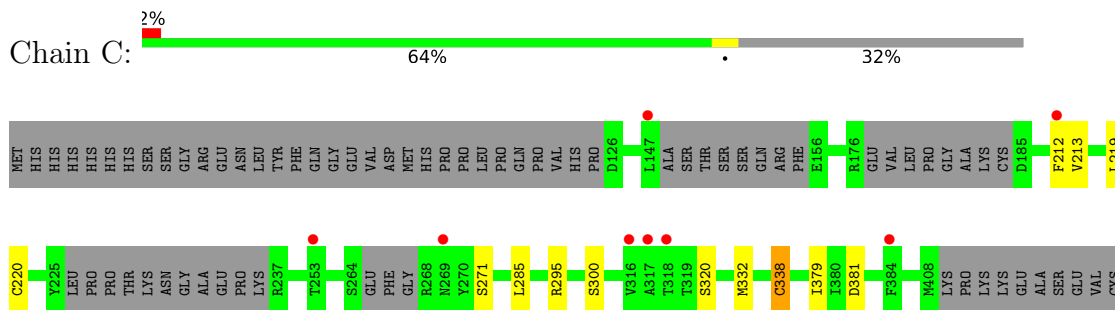
- Molecule 1: E3 SUMO-protein ligase PIAS3



- Molecule 1: E3 SUMO-protein ligase PIAS3



- Molecule 1: E3 SUMO-protein ligase PIAS3



PRO
PRO
PRO
GLY
TYR
GLY
LEU
ASP
GLY
LEU
GLN
TYR
SER
PRO
VAL
GLN
GLY
GLY
ASP
PRO
SER
SER
GLU
ASN
LYS
LYS
VAL
GLU
VAL
ILE
ILE
ASP
LEU
THR
ILE
GLU
SER
SER
SER
GLU
GLU
ASP
LEU
PRO
THR
LYS
LYS
HIS

● Molecule 1: E3 SUMO-protein ligase PIAS3

Chain D: 2% 61% 6% 33%

MET
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
ARG
GLU
GLU
ASN
LEU
TYR
PHE
GLN
GLY
GLY
GLU
VAL
ASP
MET
HIS
PRO
PRO
LEU
PRO
GLN
VAL
VAL
HIS
PRO
D126
L147
ALA
SER
THR
SER
SER
GLN
ARG
PHE
E156
I172
R176
GLU
VAL
LEU
PRO
GLY
ALA
LYS
CYS
D185
C197

R208
P209
V213
C220
Y228
LEU
PRO
THR
LYS
ASN
GLY
ALA
GLU
PRO
K236
R237
L250
S263
S264
GLU
PHE
GLY
R268
R269
R295
P312
D313
S314
E315
VAL
ALA
THR
THR
S320
L321
R322
G330
K331
M332
L346
L353
K360
I379
C394
I397

M400
GLU
D402
G403
S404
M405
C406
P407
M408
LYS
PRO
LYS
LYS
GLU
ALA
SER
GLU
VAL
CYS
PRO
PRO
PRO
GLY
TYR
GLY
LEU
GLY
LEU
GLN
TYR
SER
PRO
VAL
GLN
GLY
GLY
ASP
GLY
LEU
GLN
TYR
SER
PRO
VAL
GLU
GLU
VAL
ILE
ASP
LEU
THR
ILE
GLU
SER
SER
SER
GLU

GLU
ASP
LEU
PRO
PRO
THR
LYS
LYS
HIS

4 Data and refinement statistics i

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 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.04-2.30) 97.9 (48.04-2.29)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.29Å)	Xtrriage
Refinement program	REFMAC, BUSTER 2.10.0	Depositor
R, R_{free}	0.238 , 0.270 0.245 , 0.279	Depositor DCC
R_{free} test set	1428 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.075 for -h,-l,-k	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, CL, 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	0.51	0/1996	0.67	0/2724
1	B	0.50	0/1958	0.66	0/2667
1	C	0.49	0/1980	0.65	0/2701
1	D	0.49	0/1946	0.63	0/2649
All	All	0.50	0/7880	0.65	0/10741

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	1954	0	1904	6	0
1	B	1918	0	1871	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	22	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 1.

All (22) 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: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 [i](#)

5.3.1 Protein backbone [i](#)

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
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 [i](#)

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%)	206 (97%)	6 (3%)	43	60
1	B	208/338 (62%)	202 (97%)	6 (3%)	42	58
1	C	210/338 (62%)	204 (97%)	6 (3%)	42	58
1	D	205/338 (61%)	197 (96%)	8 (4%)	32	46
All	All	835/1352 (62%)	809 (97%)	26 (3%)	40	55

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

Mol	Chain	Res	Type
1	A	287	GLN
1	A	331	LYS

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Mol	Chain	Res	Type
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	212	PHE
1	C	219	LEU
1	C	271	SER
1	C	320	SER
1	C	332	MET
1	C	338	CYS
1	D	237	ARG
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. There are no such sidechains identified.

5.3.3 RNA [i](#)

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 monosaccharides 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%)	0.35	7 (2%) 54 62	27, 45, 72, 98	0
1	B	251/374 (67%)	0.35	4 (1%) 72 77	27, 46, 73, 100	0
1	C	253/374 (67%)	0.41	8 (3%) 47 54	29, 46, 70, 94	0
1	D	249/374 (66%)	0.43	7 (2%) 53 60	27, 46, 75, 97	0
All	All	1008/1496 (67%)	0.38	26 (2%) 56 63	27, 46, 73, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	269	ASN	4.7
1	C	318	THR	4.1
1	C	317	ALA	4.1
1	A	155	PHE	3.6
1	D	403	GLY	3.2
1	B	212	PHE	2.9
1	D	208	PRO	2.9
1	C	253	THR	2.7
1	A	211	LEU	2.6
1	A	394	CYS	2.6
1	B	155	PHE	2.5
1	C	269	ASN	2.4
1	C	316	VAL	2.4
1	A	317	ALA	2.3
1	C	384	PHE	2.3
1	B	309	THR	2.3
1	D	397	ILE	2.3
1	B	405	TRP	2.2
1	C	147	LEU	2.2
1	A	318	THR	2.1
1	A	208	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	197	CYS	2.1
1	C	212	PHE	2.1
1	D	312	PRO	2.1
1	A	209	PRO	2.0
1	D	313	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 monosaccharides 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	A	505	1/1	-0.58	1.41	300,300,300,300	0
4	UNX	A	507	1/1	-0.41	1.67	300,300,300,300	0
4	UNX	B	502	1/1	-0.41	1.30	300,300,300,300	0
4	UNX	C	505	1/1	-0.31	1.42	300,300,300,300	0
4	UNX	C	509	1/1	-0.27	1.42	300,300,300,300	0
4	UNX	A	511	1/1	-0.21	1.27	300,300,300,300	0
4	UNX	A	506	1/1	-0.18	1.40	300,300,300,300	0
4	UNX	D	503	1/1	-0.17	1.39	300,300,300,300	0
4	UNX	C	506	1/1	-0.04	1.64	300,300,300,300	0
4	UNX	A	508	1/1	0.05	1.40	300,300,300,300	0
4	UNX	B	504	1/1	0.11	1.59	300,300,300,300	0
4	UNX	A	510	1/1	0.13	1.25	299,299,299,299	0
4	UNX	D	507	1/1	0.13	1.56	297,297,297,297	0
4	UNX	C	503	1/1	0.16	1.23	269,269,269,269	0
4	UNX	C	508	1/1	0.27	1.22	300,300,300,300	0
4	UNX	B	508	1/1	0.27	1.30	300,300,300,300	0
4	UNX	B	506	1/1	0.29	1.34	300,300,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	UNX	C	510	1/1	0.37	1.46	300,300,300,300	0
4	UNX	B	507	1/1	0.37	1.38	300,300,300,300	0
4	UNX	C	507	1/1	0.37	1.45	300,300,300,300	0
4	UNX	B	505	1/1	0.38	1.28	275,275,275,275	0
4	UNX	A	512	1/1	0.40	1.54	300,300,300,300	0
4	UNX	B	503	1/1	0.40	1.43	300,300,300,300	0
4	UNX	A	509	1/1	0.42	1.46	300,300,300,300	0
4	UNX	D	502	1/1	0.42	1.38	295,295,295,295	0
4	UNX	D	504	1/1	0.48	1.25	281,281,281,281	0
4	UNX	D	505	1/1	0.51	1.43	300,300,300,300	0
4	UNX	A	504	1/1	0.54	1.25	300,300,300,300	0
4	UNX	A	503	1/1	0.55	1.48	300,300,300,300	0
4	UNX	C	504	1/1	0.56	1.54	300,300,300,300	0
4	UNX	D	506	1/1	0.67	1.38	300,300,300,300	0
4	UNX	C	511	1/1	0.74	1.69	300,300,300,300	0
3	CL	C	502	1/1	0.99	0.14	29,29,29,29	0
2	ZN	D	501	1/1	0.99	0.15	44,44,44,44	0
3	CL	A	502	1/1	0.99	0.14	29,29,29,29	0
2	ZN	C	501	1/1	1.00	0.16	44,44,44,44	0
2	ZN	A	501	1/1	1.00	0.18	41,41,41,41	0
2	ZN	B	501	1/1	1.00	0.18	43,43,43,43	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.