



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:03 am GMT

PDB ID : 4W9F
Title : pVHL:EloB:EloC in complex with (2S,4R)-1-(3,3-dimethylbutanoyl)-4-hydroxy-N-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamide (ligand 5)
Authors : van Molle, I.; Hewitt, S.; Galdeano, C.; Gadd, M.S.; Ciulli, A.
Deposited on : 2014-08-27
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

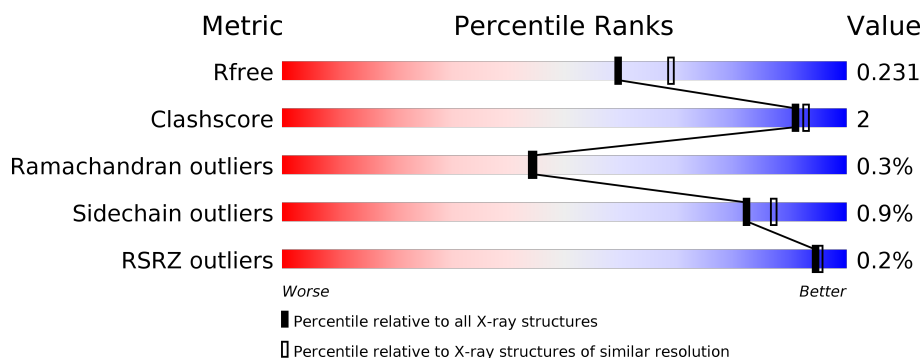
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	104	<div> <div>95%</div> <div>5%</div> </div>
1	D	104	<div> <div>93%</div> <div>5%</div> </div>
1	G	104	<div> <div>96%</div> <div>5%</div> </div>
1	J	104	<div> <div>95%</div> <div>5%</div> </div>
2	B	97	<div> <div>87%</div> <div>10%</div> </div>
2	E	97	<div> <div>88%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	97	<div><div></div><div>86%</div><div><div></div><div></div><div></div></div><div>10%</div></div>
2	K	97	<div>%<div><div></div><div></div><div></div></div><div>77%</div><div>10%</div><div><div></div><div></div><div></div></div><div>10%</div></div>
3	C	162	<div><div></div><div>81%</div><div><div></div><div></div><div></div></div><div>6%</div><div>13%</div></div>
3	F	162	<div><div></div><div>83%</div><div><div></div><div></div><div></div></div><div>5%</div><div>12%</div></div>
3	I	162	<div>%<div><div></div><div></div><div></div></div><div>86%</div><div><div></div><div></div><div></div></div><div>11%</div></div>
3	L	162	<div><div></div><div>76%</div><div><div></div><div></div><div></div></div><div>6%</div><div>18%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10937 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 Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	104	Total	As	C	N	O	S	0	0	0
			802	1	511	137	148	5			
1	D	99	Total	As	C	N	O	S	0	0	0
			731	1	470	120	137	3			
1	G	103	Total	As	C	N	O	S	0	0	0
			788	1	502	130	151	4			
1	J	103	Total	As	C	N	O	S	0	0	0
			789	1	502	132	150	4			

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	87	Total	As	C	N	O	S	0	0	0
			678	1	441	107	124	5			
2	E	87	Total	As	C	N	O	S	0	0	0
			677	1	439	108	123	6			
2	H	87	Total		C	N	O	S	0	0	0
			665		435	106	119	5			
2	K	87	Total	As	C	N	O	S	0	0	0
			682	1	443	108	123	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369
H	16	MET	-	initiating methionine	UNP Q15369
K	16	MET	-	initiating methionine	UNP Q15369

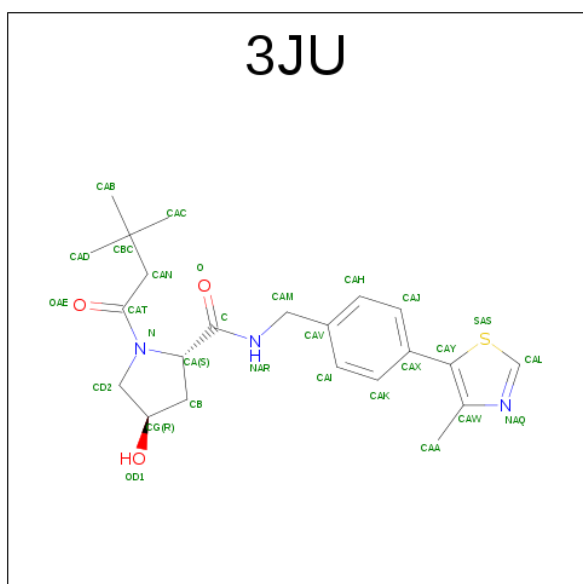
- Molecule 3 is a protein called Von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	141	Total 1098	As 1	C 703	N 197	O 195	S 2	0	1	0
3	F	142	Total 1124	As 1	C 720	N 202	O 199	S 2	0	2	0
3	I	144	Total 1132	As 1	C 727	N 200	O 202	S 2	0	0	0
3	L	133	Total 1052	As 1	C 672	N 191	O 186	S 2	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

- Molecule 4 is (4R)-1-(3,3-dimethylbutanoyl)-4-hydroxy-N-[4-(4-methyl-1,3-thiazol-5-yl)benzyl]-L-prolinamide (three-letter code: 3JU) (formula: C₂₂H₂₉N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			29	22	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	S	0	0
			29	22	3	3	1		
4	I	1	Total	C	N	O	S	0	0
			29	22	3	3	1		
4	L	1	Total	C	N	O	S	0	0
			29	22	3	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	41	Total	O	0	2
			43	43		
5	C	69	Total	O	0	0
			69	69		
5	D	30	Total	O	0	0
			30	30		
5	E	25	Total	O	0	1
			26	26		
5	F	57	Total	O	0	0
			57	57		
5	G	42	Total	O	0	0
			42	42		
5	H	38	Total	O	0	0
			38	38		
5	I	61	Total	O	0	0
			61	61		
5	J	64	Total	O	0	0
			64	64		
5	K	47	Total	O	0	0
			47	47		
5	L	57	Total	O	0	0
			57	57		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

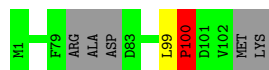
- Molecule 1: Transcription elongation factor B polypeptide 2

Chain A: 



- Molecule 1: Transcription elongation factor B polypeptide 2

Chain D: 



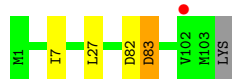
- Molecule 1: Transcription elongation factor B polypeptide 2

Chain G: 




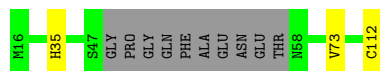
- Molecule 1: Transcription elongation factor B polypeptide 2

Chain J: 




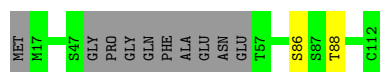
- Molecule 2: Transcription elongation factor B polypeptide 1

Chain B: 



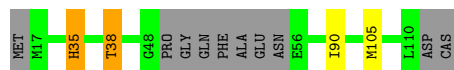
- Molecule 2: Transcription elongation factor B polypeptide 1

Chain E: 



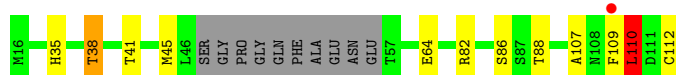
- Molecule 2: Transcription elongation factor B polypeptide 1

Chain H: 86% 10%



- Molecule 2: Transcription elongation factor B polypeptide 1

Chain K: 77% 10% 10%



- Molecule 3: Von Hippel-Lindau disease tumor suppressor

Chain C: 81% 6% 13%



- Molecule 3: Von Hippel-Lindau disease tumor suppressor

Chain F: 83% 5% 12%



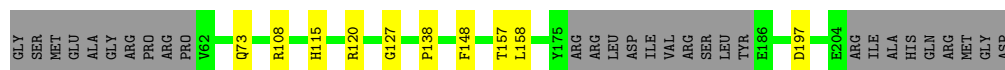
- Molecule 3: Von Hippel-Lindau disease tumor suppressor

Chain I: 86% 11%



- Molecule 3: Von Hippel-Lindau disease tumor suppressor

Chain L: 76% 6% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.68Å 92.68Å 364.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.68 – 2.10 48.71 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.68-2.10) 100.0 (48.71-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.205 , 0.229 0.210 , 0.231	Depositor DCC
R_{free} test set	4704 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10937	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.87 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7104e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CAS, 3JU

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	0.35	0/808	0.59	0/1091
1	D	0.34	0/735	0.60	1/998 (0.1%)
1	G	0.32	0/794	0.56	0/1077
1	J	0.35	0/795	0.57	0/1076
2	B	0.34	0/682	0.51	0/924
2	E	0.32	0/681	0.49	0/923
2	H	0.32	0/679	0.49	0/919
2	K	0.36	0/686	0.53	0/927
3	C	0.33	0/1116	0.58	0/1527
3	F	0.33	0/1144	0.60	0/1568
3	I	0.33	0/1152	0.61	0/1578
3	L	0.37	0/1070	0.64	0/1464
All	All	0.34	0/10342	0.57	1/14072 (0.0%)

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
2	K	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	PRO	N-CA-CB	7.70	112.54	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	110	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	802	0	794	5	0
1	D	731	0	679	1	0
1	G	788	0	761	1	0
1	J	789	0	762	2	0
2	B	678	0	654	2	0
2	E	677	0	655	1	0
2	H	665	0	656	3	0
2	K	682	0	667	12	0
3	C	1098	0	1043	9	0
3	F	1124	0	1078	4	0
3	I	1132	0	1094	2	0
3	L	1052	0	1011	6	0
4	C	29	0	29	0	0
4	F	29	0	29	0	0
4	I	29	0	29	0	0
4	L	29	0	29	0	0
5	A	69	0	0	0	0
5	B	43	0	0	0	0
5	C	69	0	0	0	0
5	D	30	0	0	0	0
5	E	26	0	0	0	0
5	F	57	0	0	0	0
5	G	42	0	0	0	0
5	H	38	0	0	0	0
5	I	61	0	0	3	0
5	J	64	0	0	0	0
5	K	47	0	0	0	0
5	L	57	0	0	0	0
All	All	10937	0	9970	41	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 (41) 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)
2:K:112:CAS:AS	3:L:157:THR:HB	2.24	0.97
3:F:73:GLN:OE1	3:F:108:ARG:NH1	1.99	0.95
2:K:41:THR:OG1	2:K:110:LEU:HA	1.78	0.81
2:K:107:ALA:O	2:K:112:CAS:SG	2.41	0.79
1:A:89:CAS:C	1:A:90:ILE:N	2.53	0.72
2:B:73:VAL:HG13	2:B:112:CAS:CE2	2.20	0.72
1:J:7:ILE:HD11	1:J:27:LEU:HD22	1.74	0.69
2:K:112:CAS:HB3	3:L:158:LEU:HB3	1.80	0.64
1:A:89:CAS:O	1:A:90:ILE:N	2.32	0.63
3:L:120[A]:ARG:NH2	3:L:197:ASP:OD2	2.27	0.61
3:C:120[B]:ARG:NH2	3:C:197:ASP:OD2	2.33	0.59
3:C:73:GLN:OE1	3:C:108:ARG:NH1	2.35	0.59
1:A:102:VAL:CG1	3:C:170:VAL:HG13	2.35	0.57
2:B:112:CAS:OXT	3:C:158:LEU:N	2.39	0.56
2:K:109:PHE:O	2:K:110:LEU:CB	2.56	0.54
1:J:82:ASP:O	1:J:83:ASP:CB	2.56	0.53
3:C:107:ARG:HD3	2:K:109:PHE:CZ	2.43	0.53
1:G:80:ARG:HA	1:G:85:PHE:HA	1.92	0.51
1:D:99:LEU:O	1:D:100:PRO:CB	2.58	0.51
2:E:86:SER:OG	2:E:88:THR:HG22	2.11	0.50
2:H:35:HIS:O	2:H:38:THR:HB	2.12	0.50
3:I:120:ARG:HD3	3:I:127:GLY:HA2	1.95	0.49
2:K:41:THR:HG1	2:K:110:LEU:HA	1.79	0.47
2:H:90:ILE:HD12	5:I:443:HOH:O	2.17	0.45
3:I:107:ARG:HD2	5:I:415:HOH:O	2.16	0.45
3:F:84:VAL:HG22	3:F:128:LEU:CD1	2.46	0.45
3:L:73:GLN:HG2	3:L:108:ARG:HH12	1.82	0.44
2:K:107:ALA:HA	2:K:112:CAS:HB2	1.99	0.44
2:K:41:THR:HG22	2:K:45:MET:SD	2.57	0.44
2:K:35:HIS:O	2:K:38:THR:HB	2.20	0.42
1:A:102:VAL:HG12	3:C:170:VAL:HG13	2.01	0.42
3:C:73:GLN:OE1	3:C:108:ARG:CZ	2.68	0.42
1:A:80:ARG:HA	1:A:85:PHE:HA	2.02	0.42
3:C:107:ARG:NH1	2:K:64:GLU:OE2	2.46	0.41
2:K:82:ARG:HH22	2:K:88:THR:HG21	1.85	0.41
3:L:120[B]:ARG:HD3	3:L:127:GLY:HA2	2.03	0.41
3:L:115:HIS:O	3:L:138:PRO:HD2	2.21	0.41
3:F:76:PHE:O	3:F:106:GLY:HA2	2.21	0.41
3:F:120[B]:ARG:HD3	3:F:127:GLY:HA2	2.02	0.41
2:H:105:MET:HG2	5:I:425:HOH:O	2.21	0.41
3:C:120[A]:ARG:HD3	3:C:127:GLY:HA2	2.04	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	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
1	D	94/104 (90%)	90 (96%)	3 (3%)	1 (1%)	17	11
1	G	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
1	J	100/104 (96%)	95 (95%)	4 (4%)	1 (1%)	18	12
2	B	83/97 (86%)	81 (98%)	2 (2%)	0	100	100
2	E	83/97 (86%)	81 (98%)	2 (2%)	0	100	100
2	H	83/97 (86%)	83 (100%)	0	0	100	100
2	K	83/97 (86%)	81 (98%)	1 (1%)	1 (1%)	15	9
3	C	137/162 (85%)	133 (97%)	3 (2%)	1 (1%)	25	20
3	F	141/162 (87%)	139 (99%)	2 (1%)	0	100	100
3	I	141/162 (87%)	138 (98%)	3 (2%)	0	100	100
3	L	129/162 (80%)	124 (96%)	5 (4%)	0	100	100
All	All	1274/1452 (88%)	1239 (97%)	31 (2%)	4 (0%)	44	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	100	PRO
2	K	110	LEU
3	C	200	ARG
1	J	83	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	A	84/91 (92%)	84 (100%)	0	100	100
1	D	69/91 (76%)	69 (100%)	0	100	100
1	G	82/91 (90%)	81 (99%)	1 (1%)	75	81
1	J	81/91 (89%)	81 (100%)	0	100	100
2	B	70/85 (82%)	69 (99%)	1 (1%)	71	78
2	E	71/85 (84%)	71 (100%)	0	100	100
2	H	70/85 (82%)	68 (97%)	2 (3%)	48	51
2	K	72/85 (85%)	70 (97%)	2 (3%)	49	52
3	C	114/147 (78%)	113 (99%)	1 (1%)	82	87
3	F	119/147 (81%)	119 (100%)	0	100	100
3	I	121/147 (82%)	119 (98%)	2 (2%)	66	72
3	L	112/147 (76%)	111 (99%)	1 (1%)	82	87
All	All	1065/1292 (82%)	1055 (99%)	10 (1%)	82	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	35	HIS
3	C	173	GLU
1	G	3	VAL
2	H	35	HIS
2	H	38	THR
3	I	63	LEU
3	I	148	PHE
2	K	38	THR
2	K	86	SER
3	L	148	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	96	GLN
3	F	174	ASN
3	I	73	GLN
3	I	110	HIS
3	L	145	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CAS	A	89	1	6,8,9	1.00	0	2,9,11	1.54	0
2	CAS	B	112	2	3,9,9	1.07	0	1,11,11	1.32	0
3	CAS	C	77	3	6,8,9	0.67	0	2,9,11	1.25	0
1	CAS	D	89	1	6,8,9	0.82	0	2,9,11	1.12	0
2	CAS	E	112	2	3,9,9	1.35	0	1,11,11	1.26	0
3	CAS	F	77	3	6,8,9	0.57	0	2,9,11	1.14	0
1	CAS	G	89	1	6,8,9	1.08	0	2,9,11	0.99	0
3	CAS	I	77	3	6,8,9	0.65	0	2,9,11	1.08	0
1	CAS	J	89	1	6,8,9	0.81	0	2,9,11	1.10	0
2	CAS	K	112	2	3,9,9	1.64	1 (33%)	1,11,11	1.37	0
3	CAS	L	77	3	6,8,9	0.71	0	2,9,11	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	A	89	1	-	0/0/7/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CAS	B	112	2	-	0/2/9/9	0/0/0/0
3	CAS	C	77	3	-	0/0/7/9	0/0/0/0
1	CAS	D	89	1	-	0/0/7/9	0/0/0/0
2	CAS	E	112	2	-	0/2/9/9	0/0/0/0
3	CAS	F	77	3	-	0/0/7/9	0/0/0/0
1	CAS	G	89	1	-	0/0/7/9	0/0/0/0
3	CAS	I	77	3	-	0/0/7/9	0/0/0/0
1	CAS	J	89	1	-	0/0/7/9	0/0/0/0
2	CAS	K	112	2	-	0/2/9/9	0/0/0/0
3	CAS	L	77	3	-	0/0/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	112	CAS	AS-CE2	2.13	2.01	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	89	CAS	2	0
2	B	112	CAS	2	0
2	K	112	CAS	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	3JU	C	301	-	28,31,31	2.92	4 (14%)	33,45,45	0.82	0
4	3JU	F	301	-	28,31,31	2.81	5 (17%)	33,45,45	0.71	0
4	3JU	I	301	-	28,31,31	2.94	5 (17%)	33,45,45	0.95	2 (6%)
4	3JU	L	301	-	28,31,31	2.94	6 (21%)	33,45,45	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3JU	C	301	-	-	0/22/34/34	0/3/3/3
4	3JU	F	301	-	-	0/22/34/34	0/3/3/3
4	3JU	I	301	-	-	0/22/34/34	0/3/3/3
4	3JU	L	301	-	-	0/22/34/34	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	3JU	CAX-CAY	-13.09	1.35	1.48
4	C	301	3JU	CAX-CAY	-12.44	1.36	1.48
4	F	301	3JU	CAX-CAY	-12.43	1.36	1.48
4	I	301	3JU	CAX-CAY	-12.42	1.36	1.48
4	I	301	3JU	CA-C	-6.51	1.38	1.52
4	C	301	3JU	CA-C	-5.21	1.41	1.52
4	L	301	3JU	CA-C	-5.02	1.42	1.52
4	F	301	3JU	CA-C	-4.86	1.42	1.52
4	C	301	3JU	CAM-CAV	-4.02	1.42	1.51
4	I	301	3JU	CAM-CAV	-3.44	1.43	1.51
4	F	301	3JU	CAM-CAV	-3.37	1.43	1.51
4	L	301	3JU	CAM-CAV	-3.06	1.44	1.51
4	L	301	3JU	CAL-SAS	-2.12	1.62	1.68
4	F	301	3JU	CAA-CAW	2.01	1.54	1.50
4	I	301	3JU	CAA-CAW	2.01	1.54	1.50
4	L	301	3JU	CAA-CAW	2.19	1.54	1.50
4	F	301	3JU	CAN-CAT	3.90	1.56	1.51
4	I	301	3JU	CAN-CAT	3.94	1.56	1.51
4	L	301	3JU	CAN-CAT	3.98	1.56	1.51
4	C	301	3JU	CAN-CAT	4.54	1.56	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	301	3JU	CD2-N-CA	-2.23	108.31	111.69
4	I	301	3JU	CG-CD2-N	2.05	105.34	103.08

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	89:CAS	C	90:ILE	N	2.53

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	103/104 (99%)	-0.42	0 100 100	28, 39, 66, 79	0
1	D	98/104 (94%)	-0.28	0 100 100	34, 52, 77, 86	0
1	G	102/104 (98%)	-0.32	0 100 100	34, 52, 66, 72	0
1	J	102/104 (98%)	-0.38	1 (0%) 82 85	27, 37, 61, 84	0
2	B	86/97 (88%)	-0.35	0 100 100	30, 39, 72, 98	2 (2%)
2	E	86/97 (88%)	-0.34	0 100 100	31, 47, 74, 81	1 (1%)
2	H	87/97 (89%)	-0.28	0 100 100	32, 45, 70, 87	1 (1%)
2	K	86/97 (88%)	-0.09	1 (1%) 79 82	27, 40, 72, 87	0
3	C	140/162 (86%)	-0.39	0 100 100	28, 41, 74, 95	0
3	F	141/162 (87%)	-0.41	0 100 100	28, 41, 66, 90	0
3	I	143/162 (88%)	-0.30	1 (0%) 87 89	33, 44, 64, 80	1 (0%)
3	L	132/162 (81%)	-0.21	0 100 100	26, 38, 74, 87	0
All	All	1306/1452 (89%)	-0.32	3 (0%) 94 95	26, 43, 72, 98	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	102	VAL	3.2
2	K	109	PHE	3.1
3	I	182	ARG	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CAS	C	77	9/10	0.97	0.07	-	34,37,63,63	0
3	CAS	F	77	9/10	0.98	0.08	-	31,34,58,59	0
2	CAS	K	112	10/10	0.50	0.32	-	41,77,142,147	0
3	CAS	I	77	9/10	0.98	0.07	-	34,36,57,58	0
2	CAS	E	112	10/10	0.90	0.21	-	52,63,97,103	0
1	CAS	D	89	9/10	0.86	0.14	-	59,71,116,120	0
3	CAS	L	77	9/10	0.98	0.09	-	28,30,48,49	0
1	CAS	J	89	9/10	0.96	0.10	-	34,37,67,68	9
1	CAS	A	89	9/10	0.87	0.19	-	49,59,99,100	0
1	CAS	G	89	9/10	0.92	0.10	-	42,50,103,107	0
2	CAS	B	112	10/10	0.93	0.25	-	60,69,95,104	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	3JU	L	301	29/29	0.96	0.12	0.93	28,31,42,44	0
4	3JU	C	301	29/29	0.95	0.11	0.55	27,37,43,48	0
4	3JU	I	301	29/29	0.96	0.10	0.25	32,37,51,54	0
4	3JU	F	301	29/29	0.96	0.10	-0.22	28,35,50,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.