



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:46 AM GMT

PDB ID : 4B9K
Title : pVHL-ELOB-ELOC complex_(2S,4R)-1-(3-amino-2-methylbenzoyl)-4-hydroxy-N-(4-(4-methylthiazol-5-yl)benzyl)pyrrolidine-2-carboxamidebound
Authors : Buckley, D.L.; Gustafson, J.L.; VanMolle, I.; Roth, A.G.; SeopTae, H.; Gareiss, P.C.; Jorgensen, W.L.; Ciulli, A.; Crews, C.M.
Deposited on : 2012-09-05
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

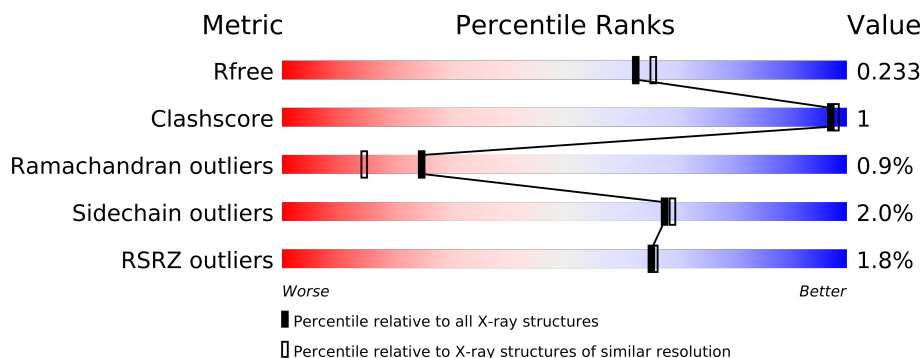
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	104	
1	D	104	
1	G	104	
1	J	104	
2	B	97	
2	H	97	
2	K	97	
3	C	171	
3	F	171	
3	I	171	
3	L	171	
4	E	97	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	ACT	F	1205	-	X
6	ACT	H	1114	-	X
6	ACT	I	1209	-	X
6	ACT	L	1208	-	X
6	ACT	L	1210	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11711 atoms, of which 0 are hydrogen and 0 are deuterium.

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	103	Total	As	C	N	O	S	0	1	0
			811	3	516	137	150	5			
1	D	101	Total	As	C	N	O	S	0	2	0
			803	3	509	137	150	4			
1	G	103	Total	As	C	N	O	S	0	1	0
			827	2	523	140	157	5			
1	J	103	Total	As	C	N	O	S	0	0	0
			810	2	515	136	152	5			

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	1	0
			698	452	113	127	6			
2	H	89	Total	C	N	O	S	0	1	0
			693	449	110	128	6			
2	K	91	Total	C	N	O	S	0	0	0
			714	461	112	134	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	EXPRESSION TAG	UNP Q15369
H	16	MET	-	EXPRESSION TAG	UNP Q15369
K	16	MET	-	EXPRESSION TAG	UNP Q15369

- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	138	Total	As	C	N	O	S	0	2	0
			1119	1	717	198	201	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	143	Total	As	C	N	O	S	0	2	0
			1157	1	738	206	210	2			
3	I	147	Total	As	C	N	O	S	0	1	0
			1172	1	751	206	212	2			
3	L	146	Total	As	C	N	O	S	0	0	0
			1164	1	742	212	207	2			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	43	SER	-	EXPRESSION TAG	UNP P40337
C	44	MET	-	EXPRESSION TAG	UNP P40337
C	45	SER	-	EXPRESSION TAG	UNP P40337
C	46	GLU	-	EXPRESSION TAG	UNP P40337
C	47	ASN	-	EXPRESSION TAG	UNP P40337
C	48	LEU	-	EXPRESSION TAG	UNP P40337
C	49	TYR	-	EXPRESSION TAG	UNP P40337
C	50	PHE	-	EXPRESSION TAG	UNP P40337
C	51	GLN	-	EXPRESSION TAG	UNP P40337
C	52	GLY	-	EXPRESSION TAG	UNP P40337
C	53	SER	-	EXPRESSION TAG	UNP P40337
F	43	SER	-	EXPRESSION TAG	UNP P40337
F	44	MET	-	EXPRESSION TAG	UNP P40337
F	45	SER	-	EXPRESSION TAG	UNP P40337
F	46	GLU	-	EXPRESSION TAG	UNP P40337
F	47	ASN	-	EXPRESSION TAG	UNP P40337
F	48	LEU	-	EXPRESSION TAG	UNP P40337
F	49	TYR	-	EXPRESSION TAG	UNP P40337
F	50	PHE	-	EXPRESSION TAG	UNP P40337
F	51	GLN	-	EXPRESSION TAG	UNP P40337
F	52	GLY	-	EXPRESSION TAG	UNP P40337
F	53	SER	-	EXPRESSION TAG	UNP P40337
I	43	SER	-	EXPRESSION TAG	UNP P40337
I	44	MET	-	EXPRESSION TAG	UNP P40337
I	45	SER	-	EXPRESSION TAG	UNP P40337
I	46	GLU	-	EXPRESSION TAG	UNP P40337
I	47	ASN	-	EXPRESSION TAG	UNP P40337
I	48	LEU	-	EXPRESSION TAG	UNP P40337
I	49	TYR	-	EXPRESSION TAG	UNP P40337
I	50	PHE	-	EXPRESSION TAG	UNP P40337
I	51	GLN	-	EXPRESSION TAG	UNP P40337
I	52	GLY	-	EXPRESSION TAG	UNP P40337

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	53	SER	-	EXPRESSION TAG	UNP P40337
L	43	SER	-	EXPRESSION TAG	UNP P40337
L	44	MET	-	EXPRESSION TAG	UNP P40337
L	45	SER	-	EXPRESSION TAG	UNP P40337
L	46	GLU	-	EXPRESSION TAG	UNP P40337
L	47	ASN	-	EXPRESSION TAG	UNP P40337
L	48	LEU	-	EXPRESSION TAG	UNP P40337
L	49	TYR	-	EXPRESSION TAG	UNP P40337
L	50	PHE	-	EXPRESSION TAG	UNP P40337
L	51	GLN	-	EXPRESSION TAG	UNP P40337
L	52	GLY	-	EXPRESSION TAG	UNP P40337
L	53	SER	-	EXPRESSION TAG	UNP P40337

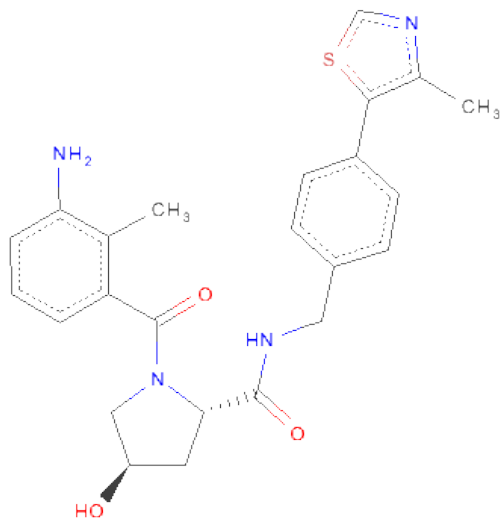
- Molecule 4 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	E	87	Total	As	C	N	O	S	0	0	0
			690	1	446	109	128	6			

There is a discrepancy between the modelled and reference sequences:

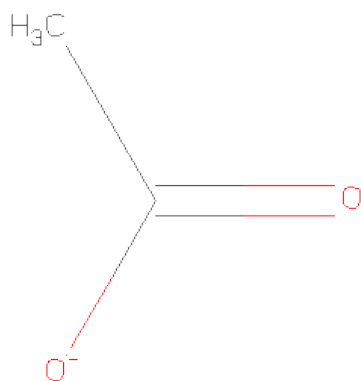
Chain	Residue	Modelled	Actual	Comment	Reference
E	16	MET	-	EXPRESSION TAG	UNP Q15369

- Molecule 5 is (2S,4R)-1-(3-AMINO-2-METHYLBENZOYL)-4-HYDROXY-N-(4-(4-METHYLTHIAZOL-5-YL)BENZYL)PYRROLIDINE-2-CARBOXAMIDE (three-letter code: TG0) (formula: C₂₄H₂₆N₄O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			32	24	4	3	1		
5	F	1	Total	C	N	O	S	0	0
			32	24	4	3	1		
5	I	1	Total	C	N	O	S	0	0
			32	24	4	3	1		
5	L	1	Total	C	N	O	S	0	0
			32	24	4	3	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	I	1	Total C O 4 2 2	0	0
6	K	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

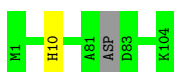
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	96	Total O 96 96	0	0
7	B	41	Total O 41 41	0	0
7	C	85	Total O 85 85	0	0
7	D	58	Total O 58 58	0	0
7	E	33	Total O 33 33	0	0
7	F	82	Total O 82 82	0	0
7	G	82	Total O 82 82	0	0
7	H	60	Total O 60 60	0	0
7	I	93	Total O 93 93	0	0
7	J	105	Total O 105 105	0	0
7	K	58	Total O 58 58	0	0
7	L	100	Total O 100 100	0	0

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 errors 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.

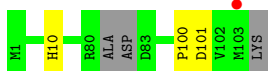
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain A: 



- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain D: 



- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain G: 



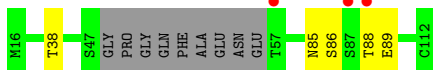
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain J: 



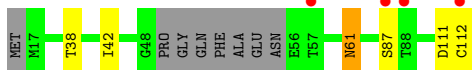
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain B: 



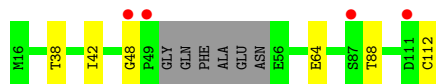
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain H: 



- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain K: 



- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain C: 



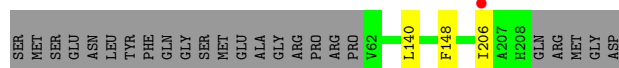
- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain F: 



- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain I: 



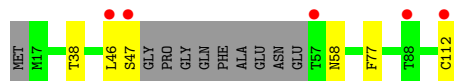
- Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain L: 



- Molecule 4: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.86Å 92.86Å 364.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.06 – 2.00 46.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.06-2.00) 100.0 (46.06-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.189 , 0.220 0.200 , 0.233	Depositor DCC
R_{free} test set	5443 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	14 of 108859 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11711	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 29.64 % 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 1.4981e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, TG0, ACT

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	0.48	0/797	0.67	0/1073
1	D	0.44	0/788	0.69	1/1063 (0.1%)
1	G	0.47	0/823	0.69	0/1110
1	J	0.50	0/806	0.67	0/1087
2	B	0.49	0/712	0.69	0/961
2	H	0.53	0/707	0.63	0/956
2	K	0.54	0/729	0.71	0/984
3	C	0.46	0/1138	0.68	1/1555 (0.1%)
3	F	0.46	0/1177	0.67	0/1609
3	I	0.47	0/1192	0.65	0/1629
3	L	0.48	0/1184	0.70	0/1618
4	E	0.48	0/694	0.64	0/938
All	All	0.48	0/10747	0.67	2/14583 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	103	PRO	N-CA-C	5.39	126.12	112.10
1	D	100	PRO	N-CA-CB	5.06	109.37	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	811	0	0	0	0
1	D	803	0	0	0	0
1	G	827	0	0	0	0
1	J	810	0	0	1	0
2	B	698	0	0	0	0
2	H	693	0	0	1	0
2	K	714	0	0	1	0
3	C	1119	0	0	2	0
3	F	1157	0	0	1	0
3	I	1172	0	0	0	0
3	L	1164	0	0	3	0
4	E	690	0	7	2	0
5	C	32	0	26	0	0
5	F	32	0	26	0	0
5	I	32	0	26	0	0
5	L	32	0	26	0	0
6	F	8	0	6	0	0
6	H	8	0	6	0	0
6	I	4	0	3	0	0
6	K	4	0	3	0	0
6	L	8	0	6	0	0
7	A	96	0	0	0	0
7	B	41	0	0	0	0
7	C	85	0	0	0	0
7	D	58	0	0	0	0
7	E	33	0	0	0	0
7	F	82	0	0	0	0
7	G	82	0	0	0	0
7	H	60	0	0	1	0
7	I	93	0	0	0	0
7	J	105	0	0	1	0
7	K	58	0	0	0	0
7	L	100	0	0	1	0
All	All	11711	0	135	10	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 1.

All (10) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:120[B]:ARG:NH1	3:C:197:ASP:OD2	2.28	0.66
3:C:107[B]:ARG:NH1	2:K:64:GLU:OE2	2.28	0.66
4:E:77:PHE:CE1	4:E:112:CAS:AS	3.11	0.64
2:H:61:ASN:ND2	7:H:2007:HOH:O	2.37	0.57
4:E:47:SER:OG	4:E:47:SER:O	2.34	0.45
3:F:120[A]:ARG:NH1	3:F:197:ASP:OD2	2.50	0.45
1:J:68:ARG:NE	7:J:2076:HOH:O	2.49	0.44
3:L:79:ARG:NE	3:L:150:ASN:OD1	2.52	0.43
3:L:120:ARG:NE	7:L:2054:HOH:O	2.52	0.43
3:L:115:HIS:O	3:L:138:PRO:CD	2.68	0.41

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	97/104 (93%)	94 (97%)	3 (3%)	0	100	100
1	D	96/104 (92%)	92 (96%)	3 (3%)	1 (1%)	22	12
1	G	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
1	J	99/104 (95%)	96 (97%)	3 (3%)	0	100	100
2	B	85/97 (88%)	80 (94%)	2 (2%)	3 (4%)	6	1
2	H	86/97 (89%)	84 (98%)	2 (2%)	0	100	100
2	K	87/97 (90%)	83 (95%)	2 (2%)	2 (2%)	10	3
3	C	135/171 (79%)	130 (96%)	4 (3%)	1 (1%)	30	20
3	F	142/171 (83%)	138 (97%)	4 (3%)	0	100	100
3	I	145/171 (85%)	140 (97%)	4 (3%)	1 (1%)	30	20
3	L	143/171 (84%)	134 (94%)	6 (4%)	3 (2%)	11	3
4	E	83/97 (86%)	82 (99%)	1 (1%)	0	100	100
All	All	1298/1488 (87%)	1250 (96%)	37 (3%)	11 (1%)	25	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	142	VAL
3	L	180	ILE
2	B	89	GLU
3	I	206	ILE
2	K	88	THR
2	B	85	ASN
2	B	86	SER
1	D	101	ASP
3	L	144	GLY
3	C	103	PRO
2	K	48	GLY

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	83/90 (92%)	82 (99%)	1 (1%)	82	84
1	D	80/90 (89%)	79 (99%)	1 (1%)	80	82
1	G	89/90 (99%)	88 (99%)	1 (1%)	84	86
1	J	86/90 (96%)	86 (100%)	0	100	100
2	B	74/86 (86%)	72 (97%)	2 (3%)	57	56
2	H	76/86 (88%)	70 (92%)	6 (8%)	18	11
2	K	79/86 (92%)	76 (96%)	3 (4%)	44	39
3	C	121/156 (78%)	120 (99%)	1 (1%)	89	92
3	F	125/156 (80%)	123 (98%)	2 (2%)	75	77
3	I	125/156 (80%)	123 (98%)	2 (2%)	75	77
3	L	126/156 (81%)	124 (98%)	2 (2%)	75	77
4	E	75/85 (88%)	72 (96%)	3 (4%)	42	36
All	All	1139/1327 (86%)	1115 (98%)	24 (2%)	68	67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	38	THR
2	B	88	THR
3	C	201	LEU
1	D	10	HIS
4	E	38	THR
4	E	46	LEU
4	E	58	ASN
3	F	107[A]	ARG
3	F	107[B]	ARG
1	G	3	VAL
2	H	38	THR
2	H	42	ILE
2	H	61	ASN
2	H	87	SER
2	H	111	ASP
2	H	112	CYS
3	I	140	LEU
3	I	148	PHE
2	K	38	THR
2	K	42	ILE
2	K	112	CYS
3	L	63	LEU
3	L	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

15 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	60	1	8,8,9	8.55	3 (37%)	7,9,11	3.35	4 (57%)
1	CAS	A	89[A]	1	8,8,9	6.18	2 (25%)	7,9,11	4.38	4 (57%)
1	CAS	A	89[B]	1	8,8,9	6.27	1 (12%)	7,9,11	2.49	3 (42%)
3	CAS	C	77	3	8,8,9	7.07	2 (25%)	7,9,11	2.97	3 (42%)
1	CAS	D	60	1	8,8,9	6.44	3 (37%)	7,9,11	3.81	3 (42%)
1	CAS	D	89[A]	1	8,8,9	6.24	2 (25%)	7,9,11	4.51	4 (57%)
1	CAS	D	89[B]	1	8,8,9	6.20	2 (25%)	7,9,11	2.85	3 (42%)
4	CAS	E	112	4	9,9,9	3.41	1 (11%)	11,11,11	4.77	5 (45%)
3	CAS	F	77	3	8,8,9	6.76	3 (37%)	7,9,11	2.68	2 (28%)
1	CAS	G	60	1	8,8,9	6.04	3 (37%)	7,9,11	3.52	4 (57%)
1	CAS	G	89	1	8,8,9	6.56	4 (50%)	7,9,11	7.87	5 (71%)
3	CAS	I	77	3	8,8,9	6.21	2 (25%)	7,9,11	5.03	4 (57%)
1	CAS	J	60	1	8,8,9	6.81	3 (37%)	7,9,11	2.84	3 (42%)
1	CAS	J	89	1	8,8,9	6.78	3 (37%)	7,9,11	4.04	4 (57%)
3	CAS	L	77	3	8,8,9	6.98	3 (37%)	7,9,11	4.24	4 (57%)

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	60	1	-	0/2/7/9	0/0/0/0
1	CAS	A	89[A]	1	-	0/2/7/9	0/0/0/0
1	CAS	A	89[B]	1	-	0/2/7/9	0/0/0/0
3	CAS	C	77	3	-	0/2/7/9	0/0/0/0
1	CAS	D	60	1	-	0/2/7/9	0/0/0/0
1	CAS	D	89[A]	1	-	0/2/7/9	0/0/0/0
1	CAS	D	89[B]	1	-	0/2/7/9	0/0/0/0
4	CAS	E	112	4	-	0/6/9/9	0/0/0/0
3	CAS	F	77	3	-	0/2/7/9	0/0/0/0
1	CAS	G	60	1	-	0/2/7/9	0/0/0/0
1	CAS	G	89	1	-	0/2/7/9	0/0/0/0
3	CAS	I	77	3	-	0/2/7/9	0/0/0/0
1	CAS	J	60	1	-	0/2/7/9	0/0/0/0
1	CAS	J	89	1	-	0/2/7/9	0/0/0/0
3	CAS	L	77	3	-	0/2/7/9	0/0/0/0

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	77	CAS	O-C	18.31	1.24	1.11
1	A	60	CAS	O-C	17.83	1.23	1.11
1	G	89	CAS	O-C	17.52	1.23	1.11
1	A	89[B]	CAS	O-C	17.47	1.23	1.11
1	D	89[B]	CAS	O-C	17.32	1.23	1.11
1	D	89[A]	CAS	O-C	17.31	1.23	1.11
3	F	77	CAS	O-C	17.26	1.23	1.11
1	A	89[A]	CAS	O-C	17.23	1.23	1.11
1	J	89	CAS	O-C	16.92	1.23	1.11
3	I	77	CAS	O-C	16.28	1.22	1.11
1	G	60	CAS	O-C	16.22	1.22	1.11
1	D	60	CAS	O-C	16.08	1.22	1.11
3	L	77	CAS	O-C	16.07	1.22	1.11
1	A	60	CAS	AS-SG	16.03	2.36	2.26
1	J	60	CAS	O-C	15.95	1.22	1.11
3	L	77	CAS	AS-SG	-11.08	2.18	2.26
1	J	60	CAS	AS-SG	10.23	2.32	2.26
4	E	112	CAS	AS-SG	-9.77	2.19	2.26
1	J	89	CAS	AS-SG	-8.23	2.20	2.26
1	D	60	CAS	AS-SG	8.04	2.31	2.26
3	C	77	CAS	AS-SG	-7.66	2.21	2.26
3	F	77	CAS	AS-SG	-7.60	2.21	2.26
3	I	77	CAS	AS-SG	-6.16	2.22	2.26
1	G	89	CAS	AS-SG	-4.96	2.22	2.26
1	G	60	CAS	CA-C	3.84	1.55	1.48
1	G	60	CAS	AS-SG	3.43	2.28	2.26
1	J	60	CAS	CA-C	2.88	1.53	1.48
1	J	89	CAS	CA-C	2.66	1.53	1.48
1	D	60	CAS	CA-C	2.57	1.53	1.48
1	A	60	CAS	CA-C	2.41	1.52	1.48
3	L	77	CAS	CA-C	2.35	1.52	1.48
3	F	77	CAS	CA-C	2.25	1.52	1.48
1	G	89	CAS	CA-C	2.23	1.52	1.48
1	D	89[A]	CAS	CA-C	2.20	1.52	1.48
1	G	89	CAS	CB-SG	-2.19	1.77	1.84
1	D	89[B]	CAS	CA-C	2.12	1.52	1.48
1	A	89[A]	CAS	CA-C	2.07	1.52	1.48

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	89	CAS	CE2-AS-CE1	13.69	118.12	96.77
1	G	89	CAS	AS-SG-CB	-12.92	80.70	102.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	77	CAS	CE2-AS-CE1	11.19	114.22	96.77
4	E	112	CAS	CE2-AS-CE1	10.42	113.01	96.77
4	E	112	CAS	AS-SG-CB	-9.99	85.59	102.24
1	D	89[A]	CAS	CE2-AS-CE1	9.75	111.97	96.77
1	A	89[A]	CAS	CE2-AS-CE1	9.14	111.01	96.77
3	L	77	CAS	CE2-AS-CE1	8.38	109.84	96.77
1	D	60	CAS	CE2-AS-CE1	8.31	109.73	96.77
1	J	89	CAS	CE2-AS-CE1	7.84	109.00	96.77
1	G	60	CAS	CE2-AS-CE1	7.36	108.24	96.77
1	G	89	CAS	CE1-AS-SG	6.24	119.69	96.44
1	A	60	CAS	CE2-AS-CE1	5.82	105.84	96.77
1	D	89[B]	CAS	CE2-AS-CE1	5.51	105.37	96.77
3	C	77	CAS	C-CA-N	-5.51	108.32	113.83
3	F	77	CAS	C-CA-N	-5.36	108.48	113.83
1	J	89	CAS	C-CA-N	-5.20	108.64	113.83
3	L	77	CAS	CE1-AS-SG	5.08	115.38	96.44
1	G	89	CAS	CE2-AS-SG	4.96	114.92	96.44
3	I	77	CAS	C-CA-N	-4.83	109.01	113.83
1	J	60	CAS	CE2-AS-CE1	4.78	104.21	96.77
1	D	60	CAS	CE1-AS-SG	4.69	113.93	96.44
1	A	60	CAS	CE2-AS-SG	4.61	113.63	96.44
3	I	77	CAS	CE1-AS-SG	4.55	113.39	96.44
1	J	60	CAS	CE2-AS-SG	4.51	113.26	96.44
1	A	89[B]	CAS	CE2-AS-CE1	4.40	103.63	96.77
3	L	77	CAS	C-CA-N	-4.28	109.56	113.83
4	E	112	CAS	CE1-AS-SG	4.25	112.30	96.44
3	C	77	CAS	CE2-AS-CE1	4.16	103.26	96.77
1	D	89[A]	CAS	C-CA-N	-4.16	109.68	113.83
1	A	89[A]	CAS	CE1-AS-SG	4.13	111.85	96.44
1	A	89[A]	CAS	C-CA-N	-4.13	109.70	113.83
4	E	112	CAS	C-CA-N	4.10	116.15	109.36
1	A	60	CAS	AS-SG-CB	4.08	109.05	102.24
1	A	89[A]	CAS	CE2-AS-SG	3.99	111.30	96.44
3	F	77	CAS	CE2-AS-CE1	3.88	102.82	96.77
1	D	89[A]	CAS	CE2-AS-SG	3.85	110.79	96.44
1	J	89	CAS	CE2-AS-SG	3.84	110.78	96.44
1	D	89[A]	CAS	CE1-AS-SG	3.74	110.37	96.44
1	A	89[B]	CAS	C-CA-N	-3.66	110.18	113.83
1	D	89[B]	CAS	C-CA-N	-3.65	110.18	113.83
1	G	89	CAS	C-CA-N	-3.53	110.30	113.83
1	G	60	CAS	CE1-AS-SG	3.52	109.57	96.44
1	G	60	CAS	C-CA-N	-3.28	110.55	113.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	89	CAS	AS-SG-CB	-2.85	97.50	102.24
1	D	89[B]	CAS	CE1-AS-SG	2.61	106.17	96.44
3	L	77	CAS	CB-CA-N	-2.55	105.94	110.27
4	E	112	CAS	CE2-AS-SG	2.45	105.56	96.44
1	J	60	CAS	AS-SG-CB	2.44	106.30	102.24
3	I	77	CAS	CB-CA-N	-2.38	106.22	110.27
1	D	60	CAS	AS-SG-CB	2.38	106.21	102.24
1	A	60	CAS	CA-CB-SG	-2.16	103.34	111.64
1	G	60	CAS	AS-SG-CB	2.15	105.83	102.24
3	C	77	CAS	AS-SG-CB	-2.14	98.67	102.24
1	A	89[B]	CAS	CE2-AS-SG	2.06	104.13	96.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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
5	TG0	C	1203	-	35,35,35	2.11	8 (22%)	49,50,50	1.81	7 (14%)
6	ACT	F	1205	-	1,3,3	4.14	1 (100%)	0,3,3	0.00	-
5	TG0	F	1206	-	35,35,35	2.12	7 (20%)	49,50,50	1.80	9 (18%)
6	ACT	F	1207	-	1,3,3	4.25	1 (100%)	0,3,3	0.00	-
6	ACT	H	1113	-	1,3,3	4.47	1 (100%)	0,3,3	0.00	-
6	ACT	H	1114	-	1,3,3	3.81	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	I	1209	-	1,3,3	4.54	1 (100%)	0,3,3	0.00	-
5	TG0	I	1210	-	35,35,35	2.22	8 (22%)	49,50,50	1.78	10 (20%)
6	ACT	K	1113	-	1,3,3	3.86	1 (100%)	0,3,3	0.00	-
6	ACT	L	1208	-	1,3,3	4.95	1 (100%)	0,3,3	0.00	-
5	TG0	L	1209	-	35,35,35	1.99	7 (20%)	49,50,50	1.86	9 (18%)
6	ACT	L	1210	-	1,3,3	2.12	1 (100%)	0,3,3	0.00	-

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
5	TG0	C	1203	-	-	0/21/33/33	0/4/4/4
6	ACT	F	1205	-	-	0/0/0/0	0/0/0/0
5	TG0	F	1206	-	-	0/21/33/33	0/4/4/4
6	ACT	F	1207	-	-	0/0/0/0	0/0/0/0
6	ACT	H	1113	-	-	0/0/0/0	0/0/0/0
6	ACT	H	1114	-	-	0/0/0/0	0/0/0/0
6	ACT	I	1209	-	-	0/0/0/0	0/0/0/0
5	TG0	I	1210	-	-	0/21/33/33	0/4/4/4
6	ACT	K	1113	-	-	0/0/0/0	0/0/0/0
6	ACT	L	1208	-	-	0/0/0/0	0/0/0/0
5	TG0	L	1209	-	-	0/21/33/33	0/4/4/4
6	ACT	L	1210	-	-	0/0/0/0	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1203	TG0	C06-N07	7.54	1.45	1.35
5	I	1210	TG0	C06-N07	7.20	1.45	1.35
5	F	1206	TG0	C06-N07	6.96	1.44	1.35
5	L	1209	TG0	C06-N07	6.04	1.43	1.35
5	I	1210	TG0	C09-N10	5.77	1.46	1.33
5	L	1209	TG0	C09-N10	5.40	1.45	1.33
5	C	1203	TG0	C09-N10	5.04	1.44	1.33
6	L	1208	ACT	CH3-C	4.95	1.55	1.48
5	F	1206	TG0	C09-N10	4.90	1.44	1.33
5	I	1210	TG0	C15-C16	4.85	1.52	1.48
6	I	1209	ACT	CH3-C	4.54	1.55	1.48
6	H	1113	ACT	CH3-C	4.47	1.55	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1206	TG0	C15-C16	4.40	1.52	1.48
5	I	1210	TG0	C17-N19	4.37	1.48	1.36
6	F	1207	ACT	CH3-C	4.25	1.54	1.48
5	L	1209	TG0	C17-N19	4.19	1.47	1.36
5	F	1206	TG0	C17-N19	4.15	1.47	1.36
6	F	1205	ACT	CH3-C	4.14	1.54	1.48
5	C	1203	TG0	C17-N19	4.08	1.47	1.36
5	L	1209	TG0	C15-C16	3.87	1.52	1.48
6	K	1113	ACT	CH3-C	3.86	1.54	1.48
6	H	1114	ACT	CH3-C	3.81	1.54	1.48
5	C	1203	TG0	C15-C16	3.39	1.51	1.48
5	I	1210	TG0	C16-C17	2.99	1.45	1.37
5	F	1206	TG0	C16-C17	2.96	1.45	1.37
5	C	1203	TG0	C16-S21	-2.92	1.62	1.74
5	L	1209	TG0	C16-C17	2.87	1.44	1.37
5	I	1210	TG0	C16-S21	-2.74	1.63	1.74
5	C	1203	TG0	C16-C17	2.70	1.44	1.37
5	F	1206	TG0	C16-S21	-2.60	1.63	1.74
5	L	1209	TG0	C16-S21	-2.50	1.64	1.74
5	F	1206	TG0	C02-N01	2.24	1.45	1.38
5	I	1210	TG0	C02-N01	2.16	1.45	1.38
5	C	1203	TG0	C25-C26	-2.15	1.47	1.52
6	L	1210	ACT	CH3-C	2.12	1.51	1.48
5	L	1209	TG0	C25-C08	-2.07	1.49	1.53
5	C	1203	TG0	C02-N01	2.07	1.44	1.38
5	I	1210	TG0	C25-C26	-2.00	1.48	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1203	TG0	C20-S21-C16	5.78	99.36	91.07
5	I	1210	TG0	C20-S21-C16	5.63	99.14	91.07
5	F	1206	TG0	C20-S21-C16	5.59	99.08	91.07
5	L	1209	TG0	C20-S21-C16	5.55	99.02	91.07
5	C	1203	TG0	C15-C16-S21	5.12	125.40	116.01
5	L	1209	TG0	C15-C16-S21	5.07	125.31	116.01
5	I	1210	TG0	C15-C16-S21	4.91	125.03	116.01
5	F	1206	TG0	C15-C16-S21	4.80	124.82	116.01
5	F	1206	TG0	C20-N19-C17	4.51	112.86	104.23
5	L	1209	TG0	C20-N19-C17	4.46	112.76	104.23
5	C	1203	TG0	C20-N19-C17	4.32	112.48	104.23
5	L	1209	TG0	C30-C05-C03	4.26	123.43	120.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1210	TG0	C20-N19-C17	3.97	111.81	104.23
5	C	1203	TG0	C11-N10-C09	-3.83	116.92	122.31
5	I	1210	TG0	C25-C08-N07	3.72	109.08	103.19
5	I	1210	TG0	C16-C17-N19	3.51	109.73	108.42
5	I	1210	TG0	C25-C26-C28	3.27	108.19	103.53
5	L	1209	TG0	C25-C26-C28	3.12	107.99	103.53
5	F	1206	TG0	C11-N10-C09	-3.03	118.05	122.31
5	F	1206	TG0	C25-C26-C28	2.87	107.63	103.53
5	L	1209	TG0	C12-C11-N10	-2.77	106.46	112.89
5	C	1203	TG0	C25-C08-N07	2.71	107.47	103.19
5	L	1209	TG0	C03-C02-N01	2.68	123.74	120.21
5	F	1206	TG0	C03-C02-N01	2.61	123.65	120.21
5	C	1203	TG0	C22-C15-C16	-2.51	119.01	120.94
5	F	1206	TG0	C25-C08-N07	2.51	107.15	103.19
5	L	1209	TG0	C25-C08-N07	2.43	107.03	103.19
5	F	1206	TG0	C12-C11-N10	-2.33	107.48	112.89
5	F	1206	TG0	C14-C15-C16	-2.33	119.15	120.94
5	I	1210	TG0	C12-C11-N10	-2.24	107.68	112.89
5	I	1210	TG0	C03-C02-N01	2.23	123.14	120.21
5	I	1210	TG0	C28-N07-C08	-2.21	108.07	111.58
5	L	1209	TG0	O24-C09-N10	-2.17	118.63	123.05
5	I	1210	TG0	C18-C17-C16	-2.13	127.17	129.68
5	C	1203	TG0	C16-C17-N19	2.04	109.18	108.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	103/104 (99%)	-0.29	0 100 100	27, 38, 65, 85	1 (0%)
1	D	101/104 (97%)	-0.01	1 (0%) 79 80	30, 50, 82, 112	1 (0%)
1	G	103/104 (99%)	-0.19	1 (0%) 79 80	28, 42, 62, 73	2 (1%)
1	J	103/104 (99%)	-0.30	0 100 100	24, 33, 56, 70	2 (1%)
2	B	88/97 (90%)	-0.05	3 (3%) 43 43	26, 40, 72, 86	0
2	H	89/97 (91%)	-0.06	4 (4%) 32 31	26, 37, 62, 82	0
2	K	91/97 (93%)	0.11	4 (4%) 33 32	24, 36, 68, 83	0
3	C	138/171 (80%)	-0.12	0 100 100	27, 39, 61, 107	1 (0%)
3	F	143/171 (83%)	-0.08	1 (0%) 84 85	26, 39, 65, 117	1 (0%)
3	I	147/171 (85%)	-0.06	1 (0%) 84 85	28, 41, 61, 129	0
3	L	146/171 (85%)	-0.03	4 (2%) 52 52	23, 37, 74, 121	1 (0%)
4	E	87/97 (89%)	0.09	5 (5%) 23 22	27, 45, 71, 85	1 (1%)
All	All	1339/1488 (89%)	-0.08	24 (1%) 65 66	23, 40, 71, 129	10 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	48	GLY	4.9
2	B	87	SER	4.6
3	I	206	ILE	4.5
2	K	49	PRO	4.1
4	E	57	THR	3.7
2	H	57	THR	3.4
4	E	47	SER	3.2
1	D	103	MET	3.2
4	E	88	THR	3.2
3	L	207	ALA	3.1
2	B	57	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	143	ASP	2.9
3	F	201	LEU	2.9
2	B	88	THR	2.7
1	G	89	CAS	2.6
2	K	111	ASP	2.6
2	K	87	SER	2.5
4	E	112	CAS	2.5
2	H	88	THR	2.4
3	L	181	VAL	2.4
2	H	87	SER	2.3
4	E	46	LEU	2.2
2	H	112	CYS	2.2
3	L	206	ILE	2.1

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CAS	E	112	10/10	0.20	6.41	45,55,58,63	3
1	CAS	G	89	9/10	0.20	6.20	32,39,59,60	3
1	CAS	A	89[A]	9/10	0.15	3.45	43,46,62,63	9
1	CAS	A	89[B]	9/10	0.15	3.21	44,46,60,62	9
1	CAS	J	89	9/10	0.13	2.83	32,34,44,45	3
3	CAS	L	77	9/10	0.12	0.49	26,29,43,45	3
3	CAS	C	77	9/10	0.14	0.42	33,38,51,54	3
1	CAS	G	60	9/10	0.12	0.21	38,40,47,49	3
1	CAS	J	60	9/10	0.12	0.16	34,38,48,49	3
1	CAS	D	89[A]	9/10	0.14	0.15	60,62,76,76	9
1	CAS	D	89[B]	9/10	0.14	0.04	60,62,74,78	9
3	CAS	I	77	9/10	0.11	-0.01	31,35,49,49	3
1	CAS	A	60	9/10	0.12	-0.11	31,34,42,42	3
3	CAS	F	77	9/10	0.10	-0.46	29,32,45,47	3
1	CAS	D	60	9/10	0.10	-0.96	36,38,49,50	3

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	ACT	L	1210	4/4	0.25	24.96	43,50,55,59	0
6	ACT	F	1205	4/4	0.23	15.43	66,69,69,71	0
6	ACT	L	1208	4/4	0.37	10.94	59,60,61,62	0
6	ACT	H	1114	4/4	0.37	5.90	64,64,64,65	0
6	ACT	I	1209	4/4	0.14	2.08	53,65,66,67	0
6	ACT	K	1113	4/4	0.13	1.52	52,54,55,61	0
6	ACT	H	1113	4/4	0.15	1.29	61,61,63,64	0
5	TG0	I	1210	32/32	0.13	0.36	31,35,40,42	0
5	TG0	L	1209	32/32	0.10	-0.03	23,28,31,31	0
5	TG0	C	1203	32/32	0.10	-0.30	23,32,42,43	0
5	TG0	F	1206	32/32	0.10	-0.54	24,31,35,36	0
6	ACT	F	1207	4/4	0.12	-0.60	75,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.