Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:26 pm BST

PDB ID	:	6GMN
Title	:	pVHL:EloB:EloC in complex with methyl 4H-furo[3,2-b]pyrrole-5-carboxylate
Authors	:	Van Molle, I.; Lucas, X.; Ciulli, A.
Deposited on	:	2018-05-27
Resolution	:	1.94 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 following versions of software and data (see references ⓘ) were used in the production of this report:

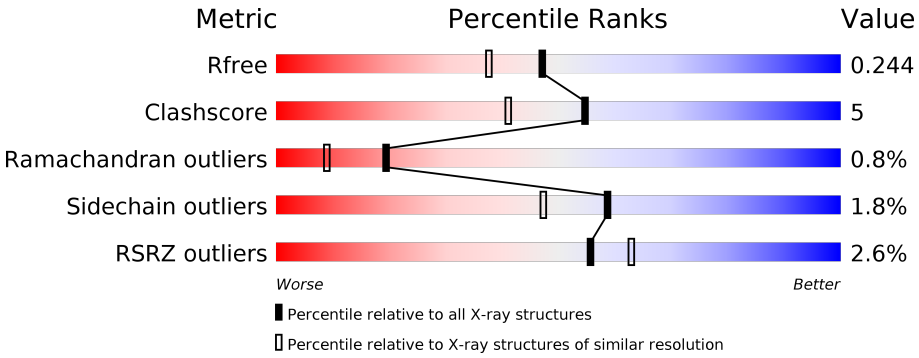
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 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 <=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	88% 11%
2	B	97	86% 10%
2	E	97	80% 7% 10%
2	H	97	6% 79% 9% 11%
2	K	97	3% 73% 13% 10%
3	C	162	4% 70% 12% 15%

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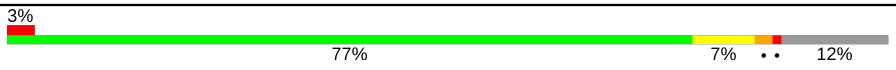
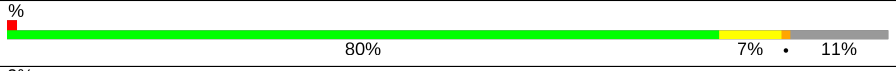
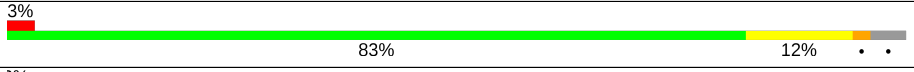
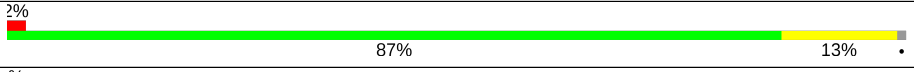
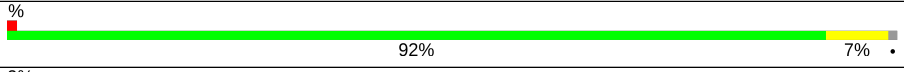
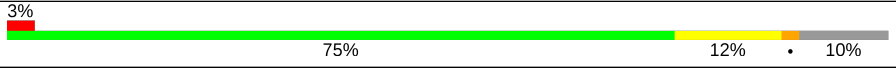
Mol	Chain	Length	Quality of chain
3	F	162	
3	L	162	
4	D	104	
4	G	104	
4	J	104	
5	I	162	

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
7	F4E	K	201	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11441 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 Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	103	Total	As	C	N	O	S	0	0	0
			800	1	509	136	150	4			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			688	445	110	127	6			
2	E	87	Total	C	N	O	S	0	1	0
			695	448	112	129	6			
2	H	86	Total	C	N	O	S	0	0	0
			687	443	110	128	6			
2	K	87	Total	C	N	O	S	0	0	0
			696	449	111	129	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	137	Total	As	C	N	O	S	0	0	0
			1099	1	702	195	199	2			
3	F	142	Total	As	C	N	O	S	0	3	0
			1165	1	742	210	210	2			
3	L	144	Total	As	C	N	O	S	0	1	0
			1173	1	746	212	212	2			

There are 6 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
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	100	Total	As	C	N	O	S	0	0	0
			779	2	496	133	145	3			
4	G	103	Total	As	C	N	O	S	0	0	0
			809	2	513	135	154	5			
4	J	103	Total	As	C	N	O	S	0	0	0
			809	2	514	136	152	5			

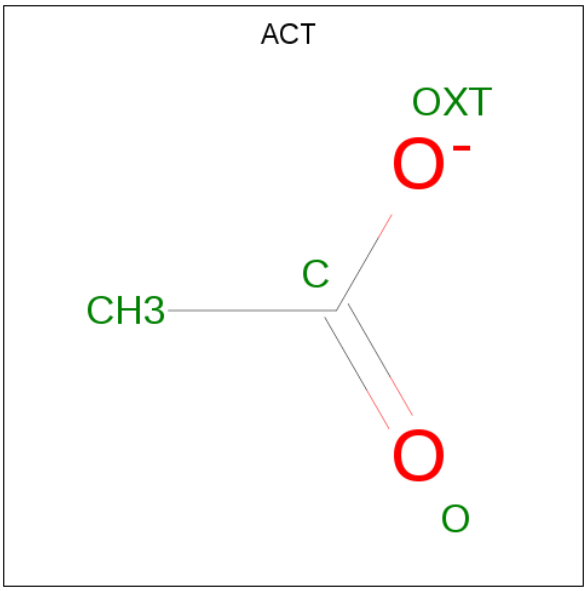
- Molecule 5 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	145	Total	C	N	O	S	0	0	0
			1158	737	208	211	2			

There are 2 discrepancies between the modelled and reference sequences:

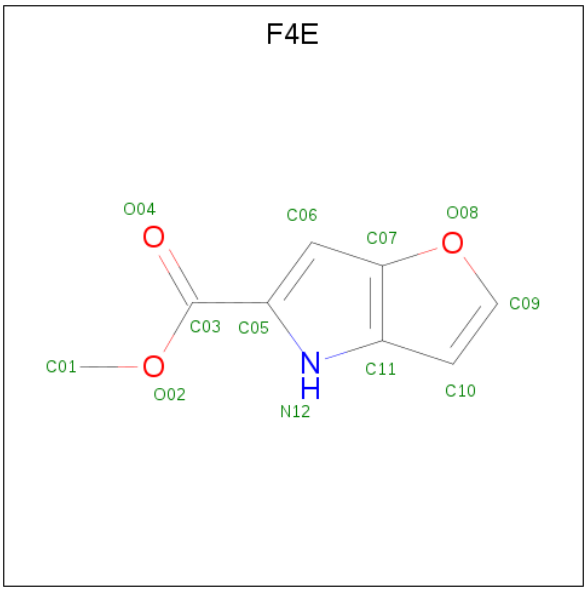
Chain	Residue	Modelled	Actual	Comment	Reference
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is methyl 4 {H}-furo[3,2-b]pyrrole-5-carboxylate (three-letter code: F4E) (formula: $C_8H_7NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 12 8 1 3	0	0
7	K	1	Total C N O 12 8 1 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	103	Total O 103 103	0	0
8	B	52	Total O 52 52	0	0
8	C	59	Total O 59 59	0	0
8	D	45	Total O 45 45	0	0
8	E	46	Total O 46 46	0	0
8	F	54	Total O 54 54	0	0
8	G	59	Total O 59 59	0	0
8	H	46	Total O 46 46	0	0
8	I	78	Total O 78 78	0	0
8	J	119	Total O 119 119	0	0

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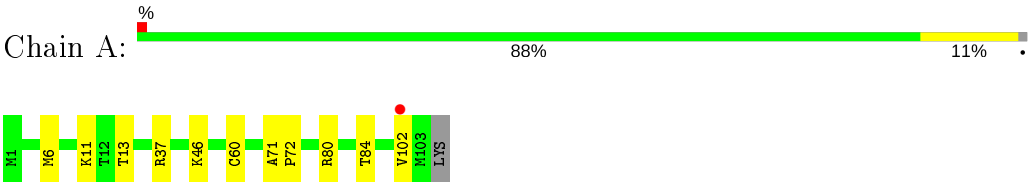
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	66	Total O 66 66	0	0
8	L	112	Total O 112 112	0	0

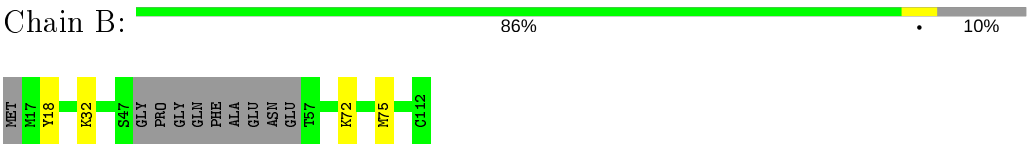
3 Residue-property plots (i)

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.

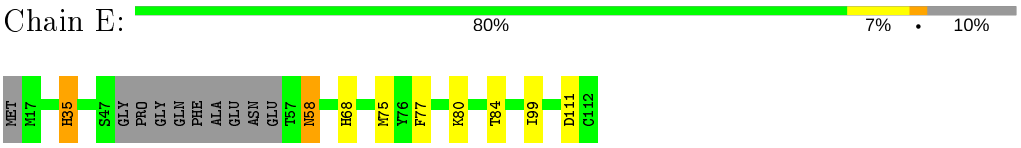
- Molecule 1: Elongin-B



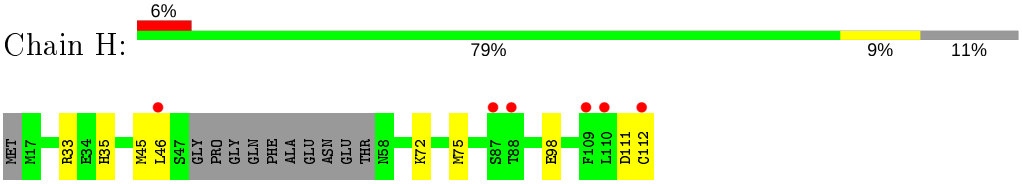
- Molecule 2: Elongin-C



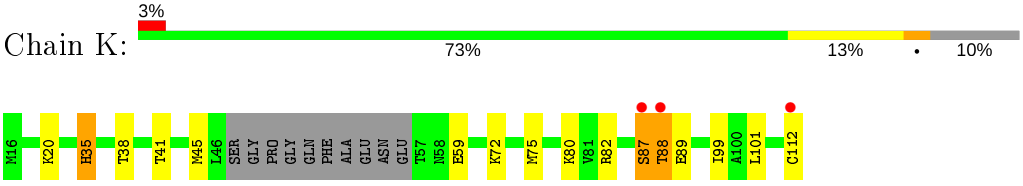
- Molecule 2: Elongin-C



- Molecule 2: Elongin-C

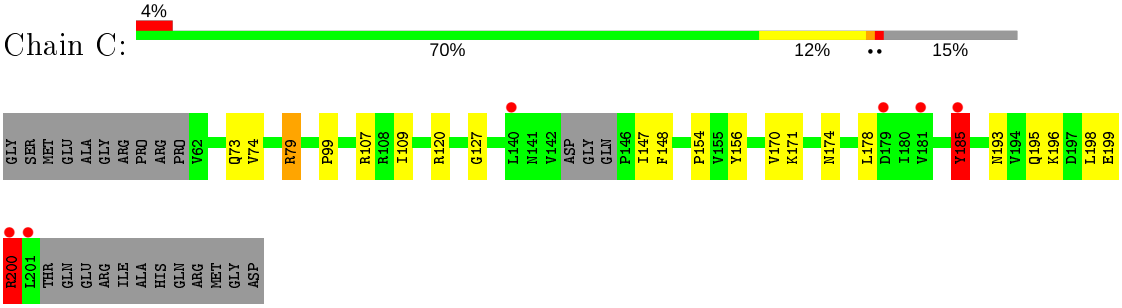


- Molecule 2: Elongin-C



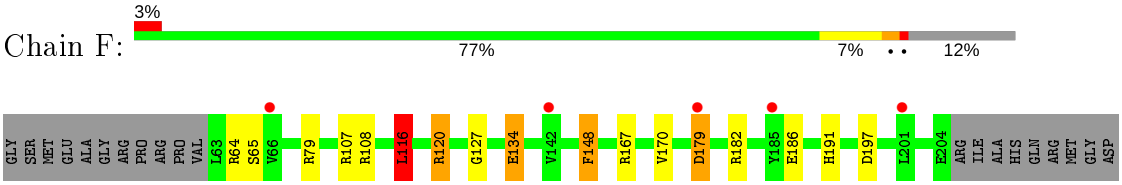
- Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C:



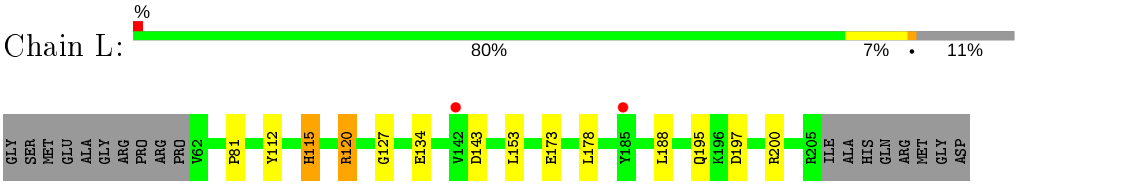
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:



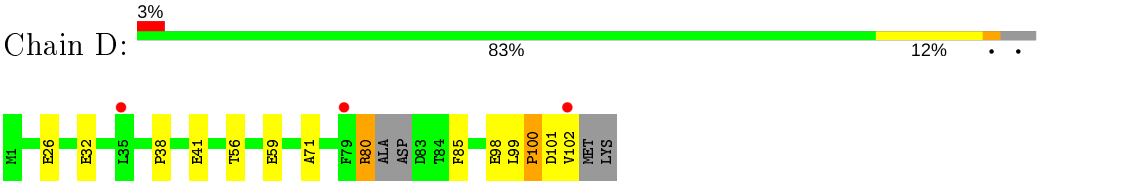
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain L:



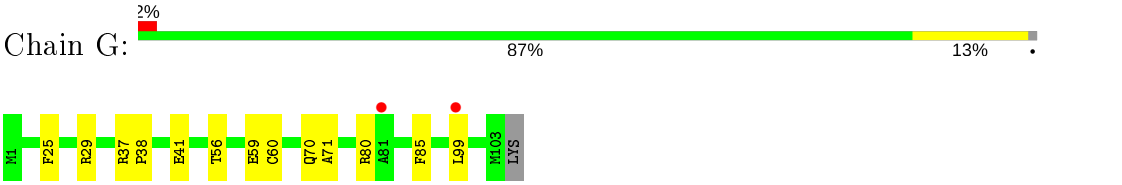
• Molecule 4: Elongin-B

Chain D:



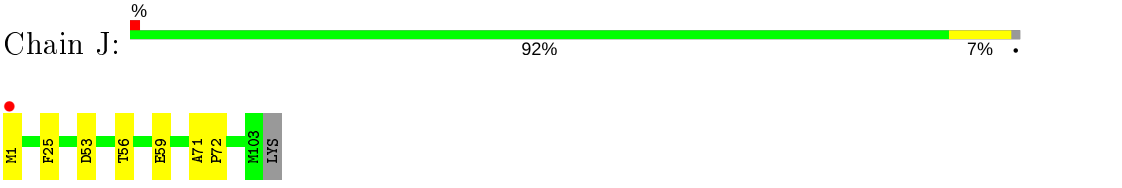
• Molecule 4: Elongin-B

Chain G:



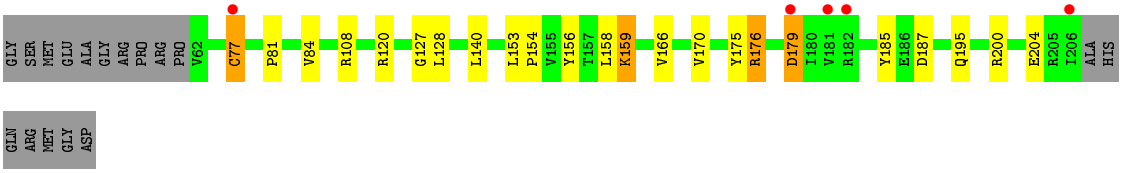
• Molecule 4: Elongin-B

Chain J:



• Molecule 5: von Hippel-Lindau disease tumor suppressor

Chain I:


GLY
SER
MET
GLU
ALA
GLY
ARG
PRO
ARG
PRO
V62
C77
P81
V84
R108
R120
G127
L128
L140
L153
P154
V155
Y156
T157
L158
K159
V166
V170
Y175
R176
D179
I180
V181
R182
Y185
E186
D187
Q195
R200
E204
R205
I206
ALA
HIS
GLN
ARG
MET
GLY
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.71Å 93.71Å 364.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.47 – 1.94 49.06 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.47-1.94) 99.2 (49.06-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.203 , 0.244 0.203 , 0.244	Depositor DCC
R_{free} test set	6006 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11441	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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 30.51 % 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 1.2911e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, F4E, 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	0.45	0/806	0.63	0/1090
2	B	0.46	0/702	0.62	0/948
2	E	0.42	0/709	0.62	0/956
2	H	0.43	0/701	0.58	0/945
2	K	0.49	0/710	0.64	0/957
3	C	0.49	1/1118 (0.1%)	0.77	4/1527 (0.3%)
3	F	0.55	1/1186 (0.1%)	0.93	8/1622 (0.5%)
3	L	0.42	0/1193	0.63	0/1628
4	D	0.38	0/773	0.68	3/1042 (0.3%)
4	G	0.44	0/805	0.61	0/1087
4	J	0.47	0/805	0.66	0/1086
5	I	0.52	1/1187 (0.1%)	0.70	2/1624 (0.1%)
All	All	0.47	3/10695 (0.0%)	0.69	17/14512 (0.1%)

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
3	C	0	1
3	F	0	1
4	G	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	77	CYS	CB-SG	10.25	1.99	1.82
3	F	134	GLU	CG-CD	-8.37	1.39	1.51
3	C	185	TYR	CE1-CZ	5.42	1.45	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	79	ARG	NE-CZ-NH1	-12.09	114.26	120.30
3	F	79	ARG	CB-CG-CD	-10.07	85.42	111.60
3	C	200	ARG	NE-CZ-NH2	-9.98	115.31	120.30
5	I	179	ASP	CB-CG-OD2	-9.65	109.61	118.30
3	F	116	LEU	CB-CG-CD2	-8.41	96.69	111.00
5	I	179	ASP	CB-CG-OD1	8.32	125.78	118.30
3	F	79	ARG	CD-NE-CZ	8.27	135.18	123.60
3	F	134	GLU	CA-CB-CG	7.77	130.49	113.40
4	D	100	PRO	N-CA-CB	7.36	112.14	103.30
3	F	134	GLU	CB-CA-C	7.09	124.59	110.40
3	C	185	TYR	CB-CG-CD2	-6.90	116.86	121.00
3	C	200	ARG	CA-CB-CG	6.66	128.05	113.40
4	D	80	ARG	CB-CG-CD	-6.52	94.64	111.60
4	D	80	ARG	NE-CZ-NH2	-6.12	117.24	120.30
3	C	200	ARG	NE-CZ-NH1	6.03	123.32	120.30
3	F	79	ARG	CG-CD-NE	5.78	123.93	111.80
3	F	179	ASP	CB-CG-OD1	-5.19	113.63	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	185	TYR	Sidechain
3	F	134	GLU	Sidechain
4	G	60	CAS	Mainchain

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	800	0	793	11	0
2	B	688	0	683	7	0
2	E	695	0	687	6	0
2	H	687	0	688	11	0
2	K	696	0	699	19	0
3	C	1099	0	1063	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1165	0	1129	10	0
3	L	1173	0	1149	8	1
4	D	779	0	764	8	0
4	G	809	0	793	15	0
4	J	809	0	800	9	0
5	I	1158	0	1139	15	0
6	A	4	0	3	1	0
6	C	4	0	3	0	0
6	F	4	0	3	0	0
6	I	4	0	3	0	0
6	L	4	0	3	0	0
7	B	12	0	0	0	0
7	K	12	0	0	0	0
8	A	103	0	0	1	0
8	B	52	0	0	0	0
8	C	59	0	0	2	0
8	D	45	0	0	1	0
8	E	46	0	0	2	0
8	F	54	0	0	1	0
8	G	59	0	0	0	0
8	H	46	0	0	1	0
8	I	78	0	0	3	0
8	J	119	0	0	2	0
8	K	66	0	0	3	0
8	L	112	0	0	0	1
All	All	11441	0	10402	109	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (109) 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)
4:G:25:PHE:CZ	4:G:29:ARG:NH1	2.19	1.11
4:G:25:PHE:HZ	4:G:29:ARG:NH1	1.60	0.99
3:F:182:ARG:O	3:F:186:GLU:OE1	1.83	0.94
4:G:25:PHE:CE2	4:G:29:ARG:NH1	2.39	0.87
4:G:25:PHE:HE2	4:G:29:ARG:HH11	1.21	0.86
3:F:107:ARG:NH2	8:F:401:HOH:O	2.08	0.85
1:A:6:MET:HE3	1:A:13:THR:HG21	1.67	0.76
4:J:72:PRO:HD2	2:K:75:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:NE2	8:C:401:HOH:O	2.17	0.76
8:J:224:HOH:O	2:K:75:MET:HE1	1.85	0.76
3:C:195:GLN:NE2	8:C:402:HOH:O	2.21	0.74
8:A:315:HOH:O	2:B:75:MET:HE1	1.89	0.73
2:K:87:SER:HA	2:K:88:THR:O	1.89	0.73
4:G:99:LEU:HD11	2:H:98:GLU:HG3	1.71	0.72
4:J:72:PRO:HD2	2:K:75:MET:HE2	1.71	0.72
4:D:26:GLU:OE2	8:D:201:HOH:O	2.07	0.71
3:F:65:SER:HA	3:F:116:LEU:HD12	1.69	0.71
4:G:25:PHE:HZ	4:G:29:ARG:HH12	1.39	0.70
4:G:99:LEU:CD1	2:H:98:GLU:HG3	2.22	0.69
3:L:120[B]:ARG:HD3	3:L:127:GLY:HA2	1.73	0.68
2:K:82:ARG:HH12	2:K:88:THR:HG21	1.58	0.67
2:E:35:HIS:HB3	2:E:77:PHE:HB3	1.79	0.65
1:A:72:PRO:HD2	2:B:75:MET:CE	2.26	0.65
1:A:37:ARG:NH2	1:A:80:ARG:O	2.30	0.63
2:E:111:ASP:OD1	8:E:201:HOH:O	2.16	0.62
3:F:120[A]:ARG:NH2	3:F:197:ASP:OD2	2.31	0.62
1:A:72:PRO:HD2	2:B:75:MET:HE2	1.82	0.61
4:D:102:VAL:HA	3:F:170:VAL:HG22	1.86	0.58
2:K:35:HIS:HE1	8:K:347:HOH:O	1.86	0.57
3:F:120[B]:ARG:HD3	3:F:127:GLY:HA2	1.84	0.57
1:A:71:ALA:HA	2:B:75:MET:CE	2.35	0.57
2:E:68:HIS:HD2	2:E:99:ILE:HG22	1.71	0.56
4:J:71:ALA:HA	2:K:75:MET:CE	2.36	0.56
5:I:159:LYS:NZ	5:I:187:ASP:OD2	2.38	0.56
2:K:38:THR:HG23	2:K:80:LYS:HD3	1.88	0.56
3:C:170:VAL:HG21	3:C:178:LEU:HD11	1.88	0.55
1:A:6:MET:CE	1:A:13:THR:HG21	2.36	0.55
3:C:74:VAL:HG12	3:C:147:ILE:HB	1.90	0.54
4:D:41:GLU:HG2	4:D:80:ARG:HE	1.73	0.54
2:K:20:LYS:HB3	2:K:59:GLU:HG2	1.90	0.54
3:L:120[A]:ARG:NH2	3:L:197:ASP:OD2	2.41	0.53
4:J:72:PRO:HD2	2:K:75:MET:HE3	1.91	0.53
2:E:75:MET:HE1	8:E:203:HOH:O	2.08	0.52
5:I:166:VAL:O	5:I:170:VAL:HG22	2.09	0.52
5:I:195:GLN:NE2	8:I:403:HOH:O	2.43	0.52
3:L:81:PRO:HD2	3:L:153:LEU:HG	1.92	0.51
4:J:56:THR:OG1	4:J:59:GLU:HG3	2.10	0.51
4:G:70:GLN:O	2:H:75:MET:HE3	2.10	0.50
1:A:102:VAL:O	1:A:102:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:154:PRO:HG2	5:I:156:TYR:CE1	2.47	0.49
3:C:120:ARG:HD3	3:C:127:GLY:HA2	1.94	0.49
2:H:112:CYS:HB2	5:I:158:LEU:HB3	1.94	0.49
4:D:56:THR:OG1	4:D:59:GLU:HG3	2.12	0.49
4:G:70:GLN:O	2:H:75:MET:CE	2.60	0.49
2:K:38:THR:CG2	2:K:80:LYS:HD3	2.42	0.49
3:C:193:ASN:OD1	3:C:196:LYS:N	2.32	0.49
4:G:99:LEU:HD11	2:H:98:GLU:HA	1.94	0.49
2:H:75:MET:HE1	8:H:223:HOH:O	2.12	0.49
3:L:134:GLU:OE2	3:L:200:ARG:NH2	2.46	0.49
5:I:81:PRO:HD2	5:I:153:LEU:HG	1.95	0.48
4:J:71:ALA:HA	2:K:75:MET:HE2	1.95	0.48
3:C:154:PRO:HG2	3:C:156:TYR:CE1	2.47	0.48
5:I:170:VAL:HG23	5:I:175:TYR:CE1	2.49	0.48
5:I:120:ARG:HD3	5:I:127:GLY:HA2	1.95	0.47
2:K:89:GLU:HA	8:K:325:HOH:O	2.15	0.46
4:G:71:ALA:HA	2:H:75:MET:HE3	1.98	0.46
3:L:120[A]:ARG:NH1	3:L:197:ASP:OD2	2.49	0.46
4:D:80:ARG:HA	4:D:85:PHE:HA	1.99	0.45
3:C:171:LYS:HB2	3:C:174:ASN:HD22	1.81	0.45
2:E:80:LYS:O	2:E:84:THR:HG23	2.17	0.45
5:I:140:LEU:HD12	8:I:442:HOH:O	2.17	0.45
2:H:33:ARG:NH1	2:H:46:LEU:HB3	2.32	0.45
4:D:80:ARG:HD3	4:D:85:PHE:CE2	2.52	0.45
5:I:108:ARG:NH2	8:I:405:HOH:O	2.50	0.44
5:I:170:VAL:HG23	5:I:175:TYR:HE1	1.82	0.44
3:L:173:GLU:H	3:L:173:GLU:HG3	1.48	0.44
5:I:179:ASP:O	5:I:179:ASP:OD1	2.35	0.44
3:F:64:ARG:O	3:F:116:LEU:HD13	2.17	0.44
2:B:18:TYR:CE1	2:B:32:LYS:HG2	2.52	0.44
3:C:74:VAL:HG23	3:C:109:ILE:HB	2.00	0.44
3:F:148:PHE:HZ	2:H:45:MET:HG2	1.83	0.44
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.85	0.43
3:C:79:ARG:HG3	3:C:79:ARG:HH11	1.83	0.43
3:L:112:TYR:HB2	3:L:115:HIS:CE1	2.53	0.43
5:I:176:ARG:NH1	5:I:185:TYR:CB	2.81	0.43
3:F:108[A]:ARG:NE	2:H:111:ASP:HB2	2.34	0.42
2:K:35:HIS:HD2	8:K:313:HOH:O	2.01	0.42
4:J:1:MET:HE3	8:J:231:HOH:O	2.18	0.42
1:A:72:PRO:HD2	2:B:75:MET:HE3	2.01	0.42
2:K:101:LEU:HD11	3:L:178:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:PRO:O	3:C:107:ARG:NH2	2.43	0.42
1:A:11:LYS:HB2	6:A:201:ACT:H1	2.01	0.42
3:C:199:GLU:O	3:C:200:ARG:HB3	2.20	0.42
4:G:56:THR:OG1	4:G:59:GLU:HG2	2.20	0.41
4:G:80:ARG:HA	4:G:85:PHE:HA	2.02	0.41
4:G:38:PRO:HD2	4:G:41:GLU:OE1	2.20	0.41
5:I:84:VAL:HG22	5:I:128:LEU:CD1	2.50	0.41
1:A:71:ALA:HA	2:B:75:MET:HE2	2.02	0.41
2:K:101:LEU:HD23	2:K:101:LEU:HA	1.96	0.41
4:D:32:GLU:OE2	4:D:38:PRO:HA	2.21	0.41
3:F:167:ARG:HD3	3:F:191[A]:HIS:CD2	2.56	0.41
5:I:200:ARG:HG2	5:I:204:GLU:OE1	2.20	0.41
4:J:72:PRO:CD	2:K:75:MET:HE2	2.45	0.41
4:D:71:ALA:HA	2:E:75:MET:CE	2.51	0.41
4:J:25:PHE:HB2	4:J:53:ASP:HB3	2.03	0.41
1:A:46:LYS:HD2	1:A:60:CAS:O	2.21	0.40
4:G:37:ARG:NH2	4:G:80:ARG:O	2.53	0.40
2:K:72:LYS:HG3	2:K:99:ILE:CD1	2.51	0.40
2:K:41:THR:O	2:K:45:MET:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:195:GLN:OE1	8:L:431:HOH:O[5_555]	2.18	0.02

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%)	95 (95%)	4 (4%)	1 (1%)	15 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	83/97 (86%)	82 (99%)	1 (1%)	0	100 100
2	E	84/97 (87%)	82 (98%)	1 (1%)	1 (1%)	13 4
2	H	82/97 (84%)	82 (100%)	0	0	100 100
2	K	83/97 (86%)	81 (98%)	0	2 (2%)	6 0
3	C	132/162 (82%)	127 (96%)	4 (3%)	1 (1%)	19 9
3	F	142/162 (88%)	137 (96%)	5 (4%)	0	100 100
3	L	142/162 (88%)	135 (95%)	6 (4%)	1 (1%)	22 11
4	D	94/104 (90%)	87 (93%)	3 (3%)	4 (4%)	2 0
4	G	99/104 (95%)	95 (96%)	4 (4%)	0	100 100
4	J	99/104 (95%)	96 (97%)	3 (3%)	0	100 100
5	I	143/162 (88%)	139 (97%)	4 (3%)	0	100 100
All	All	1283/1452 (88%)	1238 (96%)	35 (3%)	10 (1%)	19 9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	THR
4	D	98	GLU
4	D	100	PRO
2	K	88	THR
2	E	58	ASN
2	K	87	SER
3	L	143	ASP
3	C	200	ARG
4	D	99	LEU
4	D	101	ASP

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	85/91 (93%)	85 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	76/86 (88%)	75 (99%)	1 (1%)	69 62
2	E	77/86 (90%)	75 (97%)	2 (3%)	46 32
2	H	78/86 (91%)	76 (97%)	2 (3%)	46 32
2	K	79/86 (92%)	77 (98%)	2 (2%)	47 35
3	C	121/147 (82%)	117 (97%)	4 (3%)	38 24
3	F	128/147 (87%)	123 (96%)	5 (4%)	32 17
3	L	130/147 (88%)	126 (97%)	4 (3%)	40 26
4	D	81/90 (90%)	81 (100%)	0	100 100
4	G	86/90 (96%)	86 (100%)	0	100 100
4	J	86/90 (96%)	86 (100%)	0	100 100
5	I	130/148 (88%)	127 (98%)	3 (2%)	50 38
All	All	1157/1294 (89%)	1134 (98%)	23 (2%)	59 42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	72	LYS
3	C	79	ARG
3	C	148	PHE
3	C	185	TYR
3	C	200	ARG
2	E	35	HIS
2	E	58	ASN
3	F	116	LEU
3	F	120[A]	ARG
3	F	120[B]	ARG
3	F	148	PHE
3	F	179	ASP
2	H	35	HIS
2	H	72	LYS
5	I	77	CYS
5	I	159	LYS
5	I	176	ARG
2	K	35	HIS
2	K	112	CYS
3	L	115	HIS
3	L	120[A]	ARG
3	L	120[B]	ARG

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Mol	Chain	Res	Type
3	L	188	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	150	ASN
3	C	174	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

10 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	$\#\|Z\| > 2$
4	CAS	D	89	4	5,8,9	1.13	0	1,9,11	0.42	0
1	CAS	A	60	1	5,8,9	0.95	0	1,9,11	0.73	0
3	CAS	C	77	3	5,8,9	1.06	0	1,9,11	0.37	0
4	CAS	G	89	4	5,8,9	1.01	0	1,9,11	0.37	0
4	CAS	J	60	4	5,8,9	0.89	0	1,9,11	0.61	0
4	CAS	D	60	4	5,8,9	0.95	0	1,9,11	1.19	0
3	CAS	F	77	3	5,8,9	0.83	0	1,9,11	1.08	0
4	CAS	G	60	4	5,8,9	0.93	0	1,9,11	0.95	0
3	CAS	L	77	3	5,8,9	0.73	0	1,9,11	0.13	0
4	CAS	J	89	4	5,8,9	1.09	0	1,9,11	0.89	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	CAS	D	89	4	-	0/0/7/9	-
1	CAS	A	60	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
4	CAS	G	89	4	-	0/0/7/9	-
4	CAS	J	60	4	-	0/0/7/9	-
4	CAS	D	60	4	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
4	CAS	G	60	4	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
4	CAS	J	89	4	-	0/0/7/9	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	60	CAS	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
6	ACT	I	301	-	1,3,3	6.84	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	F4E	B	201	-	9,13,13	1.41	2 (22%)	8,18,18	2.00	3 (37%)
7	F4E	K	201	-	9,13,13	1.34	2 (22%)	8,18,18	2.16	4 (50%)
6	ACT	L	301	-	1,3,3	7.52	1 (100%)	0,3,3	0.00	-
6	ACT	C	301	-	1,3,3	7.76	1 (100%)	0,3,3	0.00	-
6	ACT	A	201	-	1,3,3	7.30	1 (100%)	0,3,3	0.00	-
6	ACT	F	301	-	1,3,3	6.49	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
7	F4E	B	201	-	-	4/6/6/6	0/2/2/2
7	F4E	K	201	-	-	2/6/6/6	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	301	ACT	CH3-C	7.76	1.58	1.48
6	L	301	ACT	CH3-C	7.52	1.58	1.48
6	A	201	ACT	CH3-C	7.30	1.58	1.48
6	I	301	ACT	CH3-C	6.84	1.57	1.48
6	F	301	ACT	CH3-C	6.49	1.57	1.48
7	B	201	F4E	O02-C01	-2.95	1.38	1.45
7	K	201	F4E	O02-C01	-2.89	1.38	1.45
7	B	201	F4E	O02-C03	2.27	1.38	1.33
7	K	201	F4E	O02-C03	2.03	1.37	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	201	F4E	O02-C03-C05	4.55	119.87	112.49
7	B	201	F4E	O02-C03-C05	3.94	118.89	112.49
7	B	201	F4E	C01-O02-C03	2.62	120.88	115.83
7	K	201	F4E	C05-N12-C11	2.46	109.58	104.45
7	B	201	F4E	C05-N12-C11	2.35	109.36	104.45
7	K	201	F4E	C01-O02-C03	2.09	119.87	115.83
7	K	201	F4E	O02-C03-O04	-2.06	119.42	123.45

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	201	F4E	O04-C03-C05-C06
7	K	201	F4E	C05-C03-O02-C01
7	K	201	F4E	O04-C03-O02-C01
7	B	201	F4E	O04-C03-C05-N12
7	B	201	F4E	O02-C03-C05-N12
7	B	201	F4E	O02-C03-C05-C06

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	201	ACT	1	0

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, 95^{th} 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	102/104 (98%)	0.11	1 (0%) 82 86	27, 38, 72, 103	1 (0%)
2	B	87/97 (89%)	0.15	0 100 100	29, 40, 88, 102	0
2	E	87/97 (89%)	0.31	0 100 100	30, 48, 86, 97	1 (1%)
2	H	86/97 (88%)	0.39	6 (6%) 16 22	33, 47, 91, 115	0
2	K	87/97 (89%)	0.22	3 (3%) 45 53	27, 39, 80, 95	0
3	C	136/162 (83%)	0.23	6 (4%) 34 41	30, 46, 79, 116	0
3	F	141/162 (87%)	0.27	5 (3%) 44 51	31, 48, 81, 119	0
3	L	143/162 (88%)	0.14	2 (1%) 75 80	25, 37, 72, 90	0
4	D	98/104 (94%)	0.38	3 (3%) 49 56	31, 50, 84, 102	0
4	G	101/104 (97%)	0.08	2 (1%) 65 71	32, 48, 76, 80	0
4	J	101/104 (97%)	0.08	1 (0%) 82 86	26, 35, 61, 73	0
5	I	145/162 (89%)	0.16	5 (3%) 45 53	30, 43, 73, 96	0
All	All	1314/1452 (90%)	0.20	34 (2%) 56 63	25, 44, 80, 119	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	TYR	5.0
2	H	46	LEU	4.9
3	F	185	TYR	4.7
2	H	110	LEU	4.4
2	H	112	CYS	4.2
3	F	201	LEU	3.8
4	D	102	VAL	3.6
2	K	88	THR	3.4
3	C	200	ARG	3.4
4	J	1	MET	3.3
1	A	102	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	109	PHE	3.2
4	D	79	PHE	3.2
3	F	179	ASP	3.1
5	I	181	VAL	3.0
3	C	179	ASP	3.0
4	G	81	ALA	3.0
3	F	66	VAL	2.9
3	F	142	VAL	2.9
5	I	179	ASP	2.8
3	L	142	VAL	2.8
4	G	99	LEU	2.7
5	I	77	CYS	2.7
5	I	182	ARG	2.7
3	C	140	LEU	2.6
2	K	87	SER	2.5
3	C	201	LEU	2.4
5	I	206	ILE	2.4
2	K	112	CYS	2.2
3	C	181	VAL	2.2
2	H	87	SER	2.1
3	L	185	TYR	2.1
4	D	35	LEU	2.1
2	H	88	THR	2.0

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. The B-factors column lists the minimum, median, 95^{th} 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	CAS	D	89	9/10	0.90	0.11	44,54,124,125	9
4	CAS	J	60	9/10	0.91	0.14	28,33,94,94	9
1	CAS	A	60	9/10	0.93	0.16	26,30,103,108	0
4	CAS	D	60	9/10	0.93	0.12	26,35,85,92	0
3	CAS	F	77	9/10	0.93	0.12	33,37,82,94	9
3	CAS	L	77	9/10	0.93	0.15	24,31,102,115	0
4	CAS	G	89	9/10	0.95	0.10	29,36,125,126	0
3	CAS	C	77	9/10	0.96	0.14	32,37,85,104	9
4	CAS	J	89	9/10	0.96	0.10	26,31,94,102	0
4	CAS	G	60	9/10	0.97	0.11	38,43,76,87	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. The B-factors column lists the minimum, median, 95^{th} 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
7	F4E	B	201	12/12	0.61	0.33	90,103,107,111	0
6	ACT	C	301	4/4	0.67	0.17	61,62,71,72	0
6	ACT	I	301	4/4	0.71	0.15	56,61,65,66	0
7	F4E	K	201	12/12	0.72	0.41	108,115,118,119	0
6	ACT	L	301	4/4	0.80	0.15	42,70,71,75	0
6	ACT	F	301	4/4	0.88	0.18	52,61,61,67	0
6	ACT	A	201	4/4	0.95	0.11	51,64,64,78	0

6.5 Other polymers (i)

There are no such residues in this entry.