Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2020 – 10:34 pm BST

PDB ID	:	6GMQ
Title	:	pVHL:EloB:EloC in complex with (4-(1H-pyrrol-1-yl)phenyl)methanol
Authors	:	Van Molle, I.; Lucas, X.; Ciulli, A.
Deposited on	:	2018-05-28
Resolution	:	2.75 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

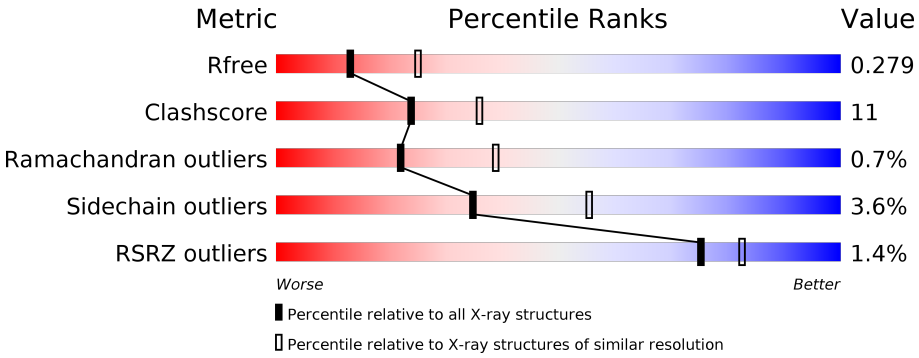
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	73% 25% •
1	D	104	2% 64% 26% • • 7%
1	G	104	3% 72% 25% • •
1	J	104	76% 23% •
2	B	97	% 72% 16% • 10%
2	E	97	% 64% 24% • 10%

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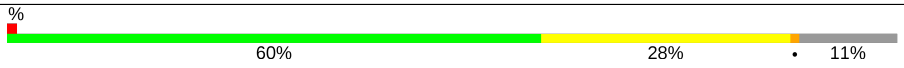
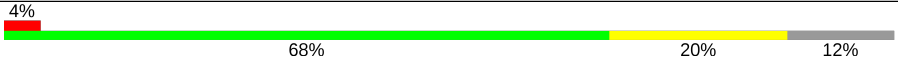
Mol	Chain	Length	Quality of chain
3	C	162	
3	F	162	
3	I	162	
3	L	162	
4	H	97	
4	K	97	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10650 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	102	Total	As	C	N	O	S	0	0	0
			802	2	509	135	151	5			
1	D	97	Total	As	C	N	O	S	0	0	0
			738	2	470	120	143	3			
1	G	103	Total	As	C	N	O	S	0	0	0
			815	2	515	135	158	5			
1	J	103	Total	As	C	N	O	S	0	0	0
			809	2	513	135	154	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	87	Total	As	C	N	O	S	0	0	0
			686	1	444	107	128	6			
2	E	87	Total	As	C	N	O	S	0	0	0
			686	1	444	111	124	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
B	112	CAS	-	expression tag	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369
E	112	CAS	-	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	135	Total	As	C	N	O	S	0	0	0
			1069	1	687	184	195	2			
3	F	141	Total	As	C	N	O	S	0	0	0
			1116	1	711	197	205	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	144	Total	As	C	N	O	S	0	0	0
			1158	1	738	204	213	2			
3	L	144	Total	As	C	N	O	S	0	0	0
			1166	1	744	208	211	2			

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

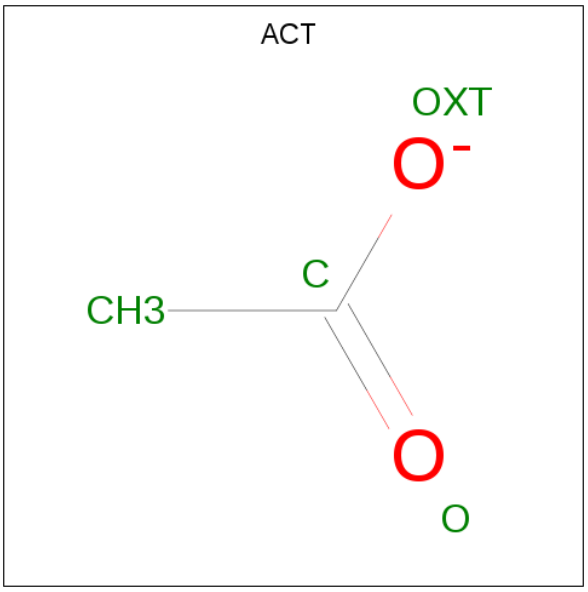
- Molecule 4 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	85	Total	C	N	O	S	0	0	0
			664	429	106	123	6			
4	K	85	Total	C	N	O	S	0	0	0
			683	442	109	125	7			

There are 2 discrepancies between the modelled and reference sequences:

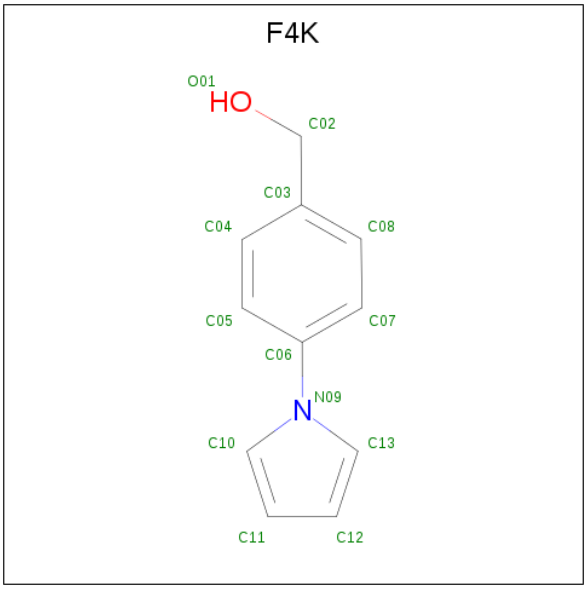
Chain	Residue	Modelled	Actual	Comment	Reference
H	16	MET	-	initiating methionine	UNP Q15369
K	16	MET	-	initiating methionine	UNP Q15369

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is (4-pyrrol-1-ylphenyl)methanol (three-letter code: F4K) (formula: $C_{11}H_{11}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total C N O 13 11 1 1	0	0

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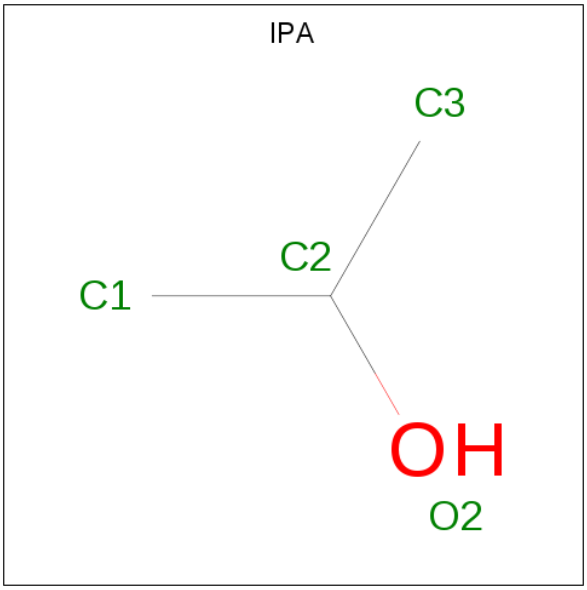
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 13 11 1 1	0	0

- Molecule 7 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	1	Total C O 4 3 1	0	0
7	L	1	Total C O 4 3 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	33	Total O 33 33	0	0
8	B	7	Total O 7 7	0	0
8	C	16	Total O 16 16	0	0
8	D	10	Total O 10 10	0	0
8	E	6	Total O 6 6	0	0
8	F	9	Total O 9 9	0	0

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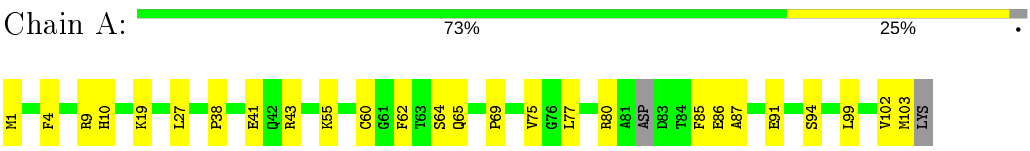
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	12	Total O 12 12	0	0
8	H	9	Total O 9 9	0	0
8	I	20	Total O 20 20	0	0
8	J	36	Total O 36 36	0	0
8	K	23	Total O 23 23	0	0
8	L	31	Total O 31 31	0	0

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.

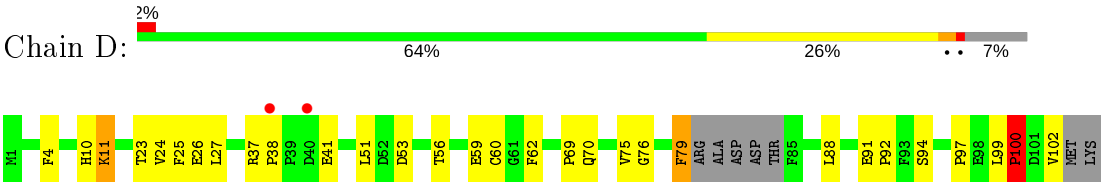
- Molecule 1: Elongin-B

Chain A:



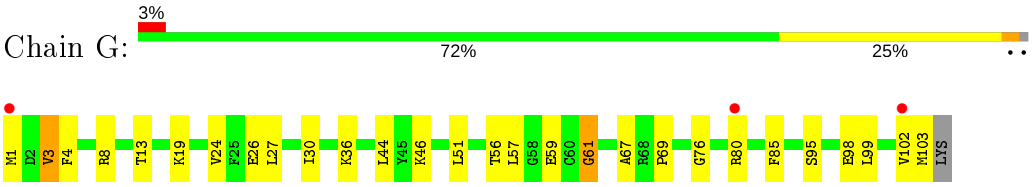
- Molecule 1: Elongin-B

Chain D:



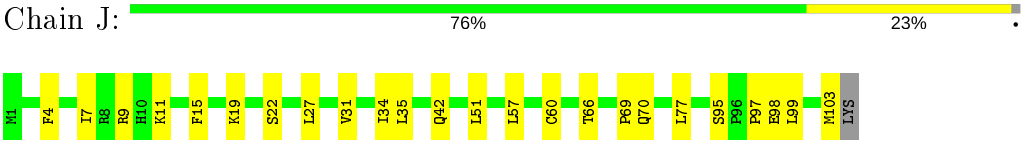
- Molecule 1: Elongin-B

Chain G:



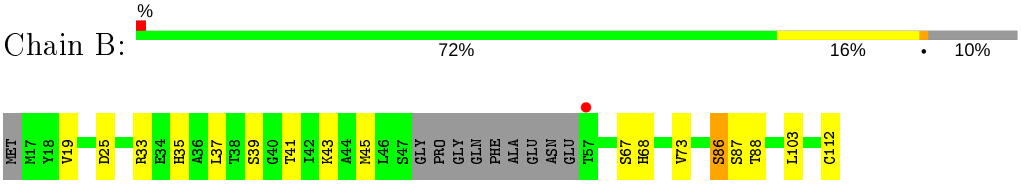
- Molecule 1: Elongin-B

Chain J:



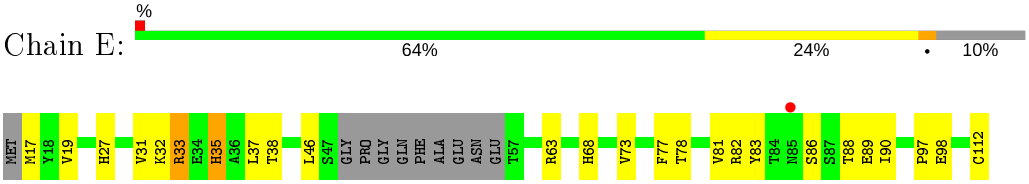
- Molecule 2: Elongin-C

Chain B:



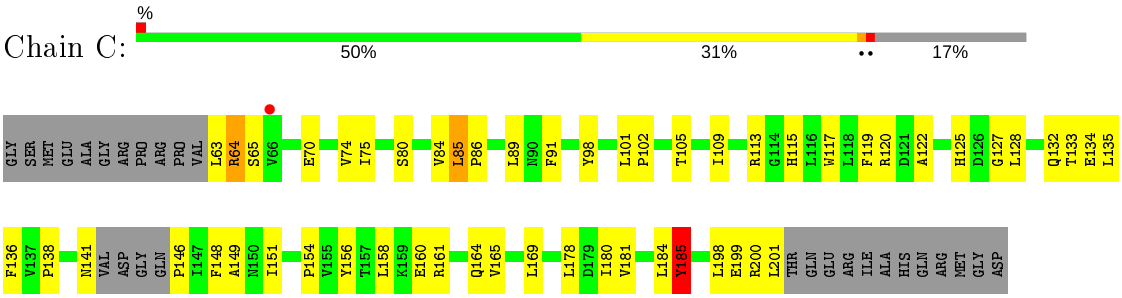
- Molecule 2: Elongin-C

Chain E:



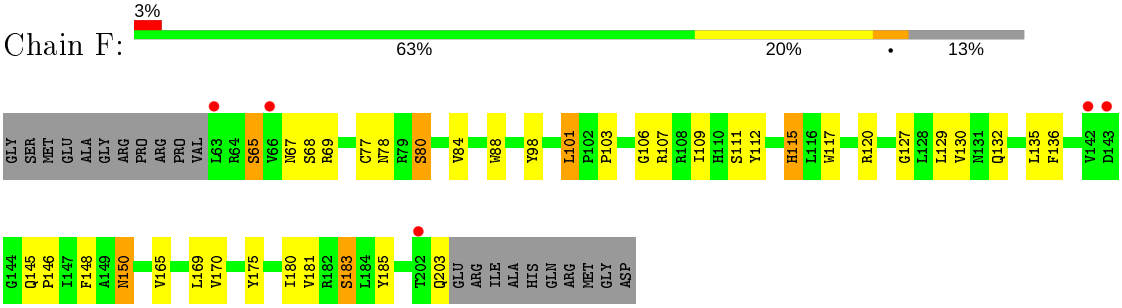
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C:



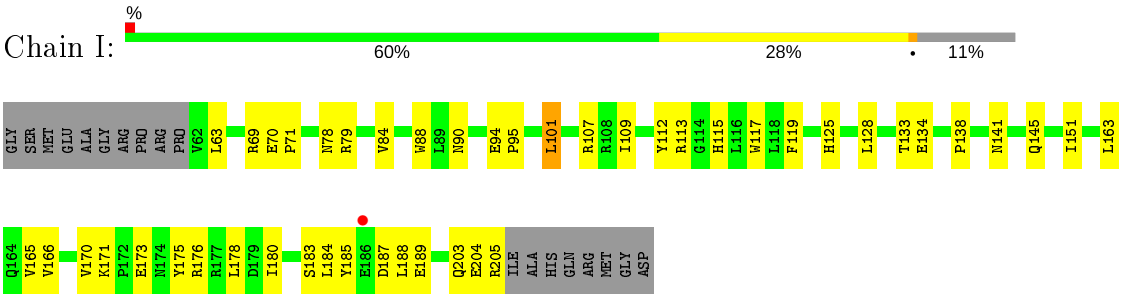
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:



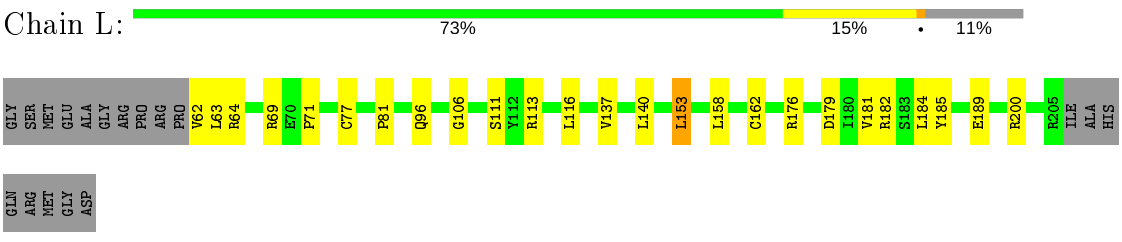
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain I:



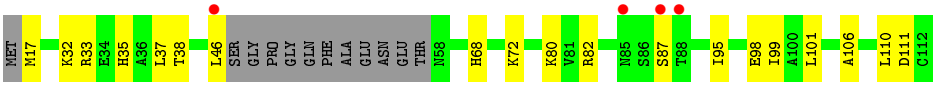
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain L:



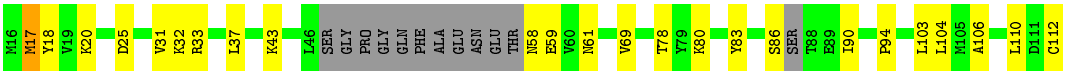
• Molecule 4: Elongin-C

Chain H:



- Molecule 4: Elongin-C

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.83Å 93.83Å 363.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 2.75 29.67 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.67-2.75) 99.5 (29.67-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.74 (at 2.76Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.205 , 0.279 0.206 , 0.279	Depositor DCC
R_{free} test set	2150 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 28.8	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	0.94	EDS
Total number of atoms	10650	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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 31.05 % 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 1.1800e-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, F4K, IPA, 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	0.52	0/797	0.75	0/1073
1	D	0.65	2/732 (0.3%)	0.84	3/990 (0.3%)
1	G	0.48	0/811	0.70	0/1095
1	J	0.50	0/805	0.78	2/1087 (0.2%)
2	B	0.53	0/690	0.60	0/934
2	E	0.56	0/690	0.67	0/933
3	C	0.57	1/1088 (0.1%)	0.79	1/1489 (0.1%)
3	F	0.50	0/1136	0.87	2/1556 (0.1%)
3	I	0.50	0/1178	0.85	2/1611 (0.1%)
3	L	0.49	0/1186	0.73	2/1619 (0.1%)
4	H	0.51	0/677	0.78	3/915 (0.3%)
4	K	0.53	0/696	0.60	0/936
All	All	0.53	3/10486 (0.0%)	0.76	15/14238 (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
1	D	0	1
3	C	0	2
4	H	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	11	LYS	CE-NZ	8.10	1.69	1.49
1	D	41	GLU	CD-OE1	5.48	1.31	1.25
3	C	185	TYR	CB-CG	-5.25	1.43	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	101	LEU	CB-CG-CD1	-16.92	82.24	111.00
3	F	101	LEU	CB-CG-CD1	-12.92	89.03	111.00
3	F	101	LEU	CB-CG-CD2	8.96	126.24	111.00
3	I	101	LEU	CB-CG-CD2	8.17	124.88	111.00
1	D	41	GLU	CA-CB-CG	7.71	130.37	113.40
4	H	32	LYS	CB-CG-CD	7.03	129.89	111.60
3	L	153	LEU	CA-CB-CG	6.59	130.47	115.30
3	L	153	LEU	CB-CG-CD1	-6.44	100.05	111.00
4	H	32	LYS	CA-CB-CG	6.28	127.22	113.40
1	J	97	PRO	C-N-CA	-6.04	106.59	121.70
1	J	98	GLU	CA-CB-CG	5.91	126.39	113.40
1	D	11	LYS	CB-CG-CD	-5.52	97.25	111.60
4	H	46	LEU	CA-CB-CG	-5.35	102.99	115.30
3	C	134	GLU	N-CA-CB	-5.33	101.00	110.60
1	D	100	PRO	N-CA-CB	5.15	109.48	103.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	185	TYR	Sidechain
3	C	64	ARG	Sidechain
1	D	100	PRO	Peptide
4	H	87	SER	Peptide

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	802	0	790	16	2
1	D	738	0	695	24	0
1	G	815	0	797	17	0
1	J	809	0	793	13	0
2	B	686	0	673	11	0
2	E	686	0	677	20	0
3	C	1069	0	1022	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1116	0	1068	27	0
3	I	1158	0	1126	40	1
3	L	1166	0	1148	17	0
4	H	664	0	658	10	0
4	K	683	0	686	15	0
5	F	4	0	3	0	0
5	I	4	0	3	0	0
5	L	4	0	3	0	0
6	I	13	0	0	1	0
6	L	13	0	0	0	0
7	I	4	0	8	2	0
7	L	4	0	8	0	0
8	A	33	0	0	3	1
8	B	7	0	0	1	0
8	C	16	0	0	3	0
8	D	10	0	0	0	0
8	E	6	0	0	1	0
8	F	9	0	0	1	0
8	G	12	0	0	0	0
8	H	9	0	0	0	0
8	I	20	0	0	0	0
8	J	36	0	0	1	0
8	K	23	0	0	1	0
8	L	31	0	0	0	0
All	All	10650	0	10158	229	3

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 11.

All (229) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:LYS:NZ	1:D:11:LYS:CE	1.69	1.55
4:H:106:ALA:O	4:H:110:LEU:HD12	1.49	1.12
3:I:101:LEU:HD12	3:I:101:LEU:C	1.77	1.05
3:I:101:LEU:HD12	3:I:101:LEU:O	1.55	1.04
3:F:180:ILE:HG13	3:F:185:TYR:HE1	1.39	0.87
3:F:101:LEU:C	3:F:101:LEU:HD12	2.01	0.80
3:F:101:LEU:O	3:F:101:LEU:HD12	1.83	0.79
4:H:106:ALA:O	4:H:110:LEU:CD1	2.29	0.79
3:C:180:ILE:HD12	3:C:184:LEU:HB3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:70:GLU:OE2	3:I:113:ARG:NH1	2.17	0.76
3:F:67:ASN:O	3:F:69:ARG:N	2.19	0.75
4:K:69:VAL:HG13	4:K:103:LEU:HD23	1.70	0.73
2:E:83:TYR:HB3	2:E:90:ILE:HD13	1.71	0.72
3:F:203:GLN:OE1	3:F:203:GLN:N	2.24	0.71
1:G:98:GLU:HG3	1:G:99:LEU:H	1.57	0.69
2:E:17:MET:N	8:E:201:HOH:O	2.26	0.69
3:F:180:ILE:HG13	3:F:185:TYR:CE1	2.26	0.68
3:I:171:LYS:HB3	3:I:173:GLU:OE2	1.93	0.68
3:C:64:ARG:HD2	3:C:91:PHE:O	1.94	0.68
3:I:203:GLN:C	3:I:205:ARG:H	1.95	0.68
3:F:135:LEU:O	8:F:401:HOH:O	2.12	0.68
1:G:4:PHE:CE1	1:G:69:PRO:HG3	2.29	0.68
3:F:120:ARG:HD3	3:F:127:GLY:HA2	1.76	0.67
3:L:181:VAL:HG22	3:L:184:LEU:HG	1.78	0.66
2:E:97:PRO:HB3	3:F:169:LEU:HD21	1.78	0.65
1:A:10:HIS:HD2	8:A:225:HOH:O	1.81	0.64
3:C:120:ARG:HD3	3:C:127:GLY:HA2	1.80	0.63
1:D:94:SER:HG	2:E:68:HIS:HD1	1.39	0.63
3:C:180:ILE:HD12	3:C:184:LEU:CB	2.29	0.63
2:E:77:PHE:HE1	2:E:112:CAS:CE1	2.12	0.62
3:C:178:LEU:O	3:C:185:TYR:OH	2.17	0.62
3:L:176:ARG:NH1	3:L:189:GLU:OE1	2.33	0.61
1:G:102:VAL:HG21	3:I:178:LEU:HD23	1.83	0.61
2:B:33:ARG:NH1	8:B:201:HOH:O	2.31	0.60
3:F:107:ARG:HG2	3:F:109:ILE:HG12	1.84	0.59
3:F:112:TYR:HB2	3:F:115:HIS:CE1	2.37	0.59
1:G:56:THR:OG1	1:G:59:GLU:HG2	2.03	0.59
1:G:103:MET:HG2	3:I:170:VAL:HG12	1.84	0.59
3:C:63:LEU:HD23	3:C:198:LEU:HD22	1.84	0.58
4:K:106:ALA:O	4:K:110:LEU:HD12	2.03	0.58
1:A:91:GLU:OE1	8:A:201:HOH:O	2.17	0.58
1:D:56:THR:OG1	1:D:59:GLU:HG3	2.03	0.58
1:D:76:GLY:HA3	1:D:88:LEU:HD11	1.86	0.58
1:A:9:ARG:HB2	1:A:77:LEU:O	2.04	0.58
1:D:25:PHE:HB2	1:D:53:ASP:HB3	1.85	0.58
2:E:33:ARG:HE	2:E:37:LEU:HD11	1.68	0.58
3:I:133:THR:HG22	3:I:134:GLU:H	1.68	0.58
2:E:86:SER:OG	2:E:88:THR:HB	2.04	0.57
3:I:203:GLN:O	3:I:205:ARG:N	2.37	0.57
1:G:98:GLU:CG	1:G:99:LEU:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:84:VAL:HG22	3:I:128:LEU:HD13	1.86	0.57
3:I:203:GLN:C	3:I:205:ARG:N	2.58	0.57
4:K:112:CYS:HB3	3:L:158:LEU:HB3	1.87	0.57
3:C:75:ILE:HD12	3:C:146:PRO:HB2	1.87	0.56
1:J:7:ILE:HD11	1:J:27:LEU:HD22	1.86	0.56
1:D:10:HIS:NE2	1:D:79:PHE:HZ	2.04	0.56
3:C:98:TYR:CE2	3:C:117:TRP:CH2	2.93	0.56
1:A:99:LEU:HD22	1:A:103:MET:HB2	1.87	0.55
1:D:10:HIS:CE1	1:D:79:PHE:HE1	2.25	0.55
3:L:181:VAL:HG23	3:L:184:LEU:H	1.70	0.55
3:I:101:LEU:C	3:I:101:LEU:CD1	2.60	0.55
3:I:173:GLU:CD	3:I:173:GLU:H	2.09	0.55
4:H:101:LEU:HD21	3:I:178:LEU:HD13	1.88	0.54
3:L:113:ARG:HD2	3:L:140:LEU:HD13	1.90	0.54
1:G:46:LYS:NZ	1:G:61:GLY:HA3	2.23	0.53
1:A:9:ARG:HH11	1:A:9:ARG:HG2	1.73	0.53
3:I:112:TYR:CE2	7:I:303:IPA:H11	2.43	0.53
1:D:11:LYS:HB3	2:E:27:HIS:CD2	2.43	0.53
3:C:180:ILE:HB	3:C:184:LEU:HD12	1.90	0.53
3:F:78:ASN:OD1	3:F:80:SER:HB3	2.09	0.53
1:D:10:HIS:CE1	1:D:79:PHE:CE1	2.97	0.53
1:D:24:VAL:HG21	1:D:51:LEU:HB3	1.91	0.53
1:J:4:PHE:CE1	1:J:69:PRO:HG3	2.44	0.52
1:D:10:HIS:HE2	1:D:79:PHE:HZ	1.56	0.52
3:I:94:GLU:OE1	3:I:95:PRO:HD2	2.08	0.52
3:C:120:ARG:HD2	3:C:125:HIS:O	2.09	0.52
3:I:163:LEU:HD22	3:I:188:LEU:HD23	1.90	0.52
2:E:33:ARG:NE	2:E:37:LEU:HD11	2.25	0.52
3:I:79:ARG:HG3	3:I:79:ARG:HH11	1.74	0.52
3:C:74:VAL:HG23	3:C:109:ILE:HB	1.92	0.51
1:D:102:VAL:CB	3:F:169:LEU:HB3	2.40	0.51
1:G:3:VAL:HG22	1:G:67:ALA:HB3	1.93	0.51
1:A:1:MET:HG3	1:A:64:SER:HB3	1.93	0.51
3:I:166:VAL:CG2	3:I:188:LEU:HD21	2.41	0.51
3:F:77:CAS:CE2	3:F:106:GLY:HA2	2.41	0.51
1:A:4:PHE:CE1	1:A:69:PRO:HG3	2.46	0.51
4:H:33:ARG:O	4:H:37:LEU:HD13	2.11	0.51
2:B:19:VAL:HG13	2:B:33:ARG:HG2	1.93	0.50
2:E:35:HIS:O	2:E:38:THR:HB	2.10	0.50
1:G:24:VAL:HG21	1:G:51:LEU:HB3	1.93	0.50
3:F:98:TYR:CE2	3:F:117:TRP:CH2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:GLU:O	1:G:30:ILE:HD12	2.12	0.50
4:K:83:TYR:HB3	4:K:90:ILE:HG12	1.94	0.50
3:I:176:ARG:HA	3:I:185:TYR:CE1	2.46	0.50
4:K:20:LYS:HB3	4:K:59:GLU:HG2	1.94	0.50
1:D:11:LYS:NZ	1:D:11:LYS:CD	2.62	0.49
3:C:84:VAL:HG21	3:C:151:ILE:HG21	1.95	0.49
2:B:41:THR:O	2:B:45:MET:HG3	2.11	0.49
3:I:112:TYR:HE2	7:I:303:IPA:H11	1.76	0.49
3:C:98:TYR:CE2	3:C:117:TRP:HH2	2.30	0.49
1:J:99:LEU:HD22	1:J:103:MET:HB2	1.95	0.49
3:I:134:GLU:HB3	6:I:302:F4K:C11	2.42	0.49
1:A:80:ARG:HB3	1:A:85:PHE:CD1	2.48	0.49
1:J:19:LYS:O	1:J:22:SER:HB3	2.13	0.49
3:C:141:ASN:ND2	3:C:146:PRO:HA	2.28	0.49
1:D:10:HIS:NE2	1:D:79:PHE:CZ	2.80	0.49
1:J:15:PHE:HB2	4:K:31:VAL:HG12	1.95	0.48
1:D:70:GLN:N	1:D:70:GLN:OE1	2.34	0.48
8:J:205:HOH:O	4:K:32:LYS:HG2	2.13	0.48
3:L:62:VAL:O	3:L:63:LEU:HB2	2.13	0.48
2:B:25:ASP:OD1	2:B:25:ASP:N	2.44	0.48
1:D:11:LYS:HD3	1:D:91:GLU:HB2	1.95	0.48
3:L:81:PRO:HD2	3:L:153:LEU:HG	1.96	0.47
2:B:103:LEU:HD11	3:C:158:LEU:HD21	1.97	0.47
3:I:180:ILE:HD12	3:I:184:LEU:HB3	1.96	0.47
3:I:175:TYR:HD2	3:I:189:GLU:HG2	1.78	0.47
3:C:135:LEU:HB2	8:C:304:HOH:O	2.15	0.47
1:J:27:LEU:HD12	1:J:57:LEU:HD21	1.96	0.47
3:I:119:PHE:CG	3:I:151:ILE:HD12	2.49	0.47
4:H:95:ILE:HB	3:I:165:VAL:HG21	1.96	0.47
2:B:39:SER:HB2	2:B:112:CAS:CE2	2.44	0.47
1:D:23:THR:OG1	1:D:26:GLU:HG3	2.15	0.47
3:C:70:GLU:OE1	3:C:113:ARG:NH1	2.48	0.47
4:K:104:LEU:HG	3:L:184:LEU:HD13	1.97	0.47
3:I:188:LEU:HA	3:I:188:LEU:HD23	1.69	0.47
4:H:72:LYS:HG3	4:H:99:ILE:CD1	2.46	0.46
3:C:133:THR:HG22	8:C:304:HOH:O	2.15	0.46
3:C:65:SER:OG	3:C:89:LEU:O	2.22	0.46
4:H:38:THR:HG23	4:H:80:LYS:HD3	1.97	0.46
3:L:116:LEU:HD12	3:L:137:VAL:HG22	1.97	0.46
1:A:38:PRO:HD2	1:A:41:GLU:OE1	2.15	0.46
3:C:86:PRO:HB3	3:C:119:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:PHE:CZ	1:D:75:VAL:HG22	2.51	0.46
3:L:69:ARG:O	3:L:71:PRO:HD3	2.16	0.46
1:A:43:ARG:HG3	1:A:85:PHE:CE1	2.50	0.46
3:C:180:ILE:HD11	3:C:185:TYR:CE1	2.51	0.46
2:E:35:HIS:CE1	2:E:81:VAL:HG21	2.51	0.46
3:L:64:ARG:HE	3:L:64:ARG:HB2	1.58	0.46
3:C:160:GLU:O	3:C:164:GLN:HG3	2.15	0.45
3:F:78:ASN:ND2	3:F:103:PRO:HA	2.31	0.45
2:B:73:VAL:HG13	2:B:112:CAS:CE1	2.46	0.45
4:K:17:MET:SD	4:K:33:ARG:HD2	2.57	0.45
2:B:37:LEU:HD22	2:B:43:LYS:HG3	1.98	0.45
3:C:133:THR:CG2	8:C:304:HOH:O	2.65	0.45
1:J:51:LEU:HD22	1:J:60:CAS:SG	2.57	0.45
3:C:101:LEU:HD22	3:C:101:LEU:N	2.32	0.45
3:I:115:HIS:O	3:I:138:PRO:HD2	2.17	0.45
3:C:98:TYR:HE2	3:C:117:TRP:CH2	2.32	0.45
3:L:181:VAL:CG2	3:L:184:LEU:HG	2.46	0.45
3:C:154:PRO:HG2	3:C:156:TYR:CE1	2.52	0.45
1:D:4:PHE:CE1	1:D:69:PRO:HG3	2.52	0.45
3:F:165:VAL:O	3:F:169:LEU:HD13	2.16	0.45
3:C:199:GLU:O	3:C:201:LEU:HG	2.17	0.45
4:K:58:ASN:ND2	8:K:203:HOH:O	2.44	0.45
3:I:184:LEU:HA	3:I:187:ASP:HB2	1.99	0.45
1:A:10:HIS:O	1:A:91:GLU:HB3	2.17	0.45
3:C:115:HIS:O	3:C:138:PRO:HD2	2.17	0.45
1:J:99:LEU:HA	1:J:99:LEU:HD23	1.86	0.44
2:E:73:VAL:HG13	2:E:112:CAS:CE2	2.47	0.44
3:I:180:ILE:HD12	3:I:184:LEU:CB	2.47	0.44
2:E:19:VAL:HG21	2:E:46:LEU:HD11	2.00	0.44
3:I:173:GLU:N	3:I:173:GLU:OE2	2.28	0.44
3:I:69:ARG:O	3:I:71:PRO:HD3	2.18	0.44
3:I:90:ASN:HD21	3:I:94:GLU:HB2	1.82	0.44
3:I:88:TRP:HB2	3:I:117:TRP:CZ3	2.53	0.44
3:L:77:CAS:CE2	3:L:106:GLY:HA3	2.47	0.44
1:A:62:PHE:CZ	1:A:75:VAL:HG22	2.52	0.43
1:J:34:ILE:HD11	4:K:18:TYR:CZ	2.52	0.43
3:F:117:TRP:HB2	3:F:136:PHE:HB3	2.00	0.43
2:E:77:PHE:O	2:E:81:VAL:HG23	2.19	0.43
3:L:182:ARG:HA	3:L:185:TYR:CD2	2.54	0.43
3:I:107:ARG:HG2	3:I:109:ILE:HD11	1.99	0.43
3:I:185:TYR:O	3:I:189:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:25:ASP:N	4:K:25:ASP:OD1	2.42	0.43
3:F:130:VAL:HA	3:F:150:ASN:O	2.19	0.43
1:G:8:ARG:HG2	1:G:13:THR:HG23	1.99	0.43
3:C:85:LEU:HB2	3:C:122:ALA:HB2	2.00	0.43
2:E:88:THR:HG22	2:E:89:GLU:O	2.19	0.43
3:C:136:PHE:CE2	3:C:149:ALA:HB2	2.54	0.42
2:E:31:VAL:HG12	2:E:32:LYS:N	2.34	0.42
1:J:9:ARG:HB2	1:J:77:LEU:O	2.19	0.42
1:D:91:GLU:HA	1:D:92:PRO:HD3	1.88	0.42
3:I:78:ASN:HB2	3:I:101:LEU:HD11	2.00	0.42
3:I:141:ASN:ND2	3:I:145:GLN:O	2.51	0.42
2:B:87:SER:HB2	3:C:132:GLN:OE1	2.20	0.42
1:J:42:GLN:HG2	1:J:77:LEU:HD11	2.02	0.42
1:A:9:ARG:NH1	1:A:9:ARG:HG2	2.35	0.42
3:C:84:VAL:HG22	3:C:128:LEU:HD13	2.02	0.42
3:L:182:ARG:HA	3:L:185:TYR:HD2	1.84	0.42
2:B:86:SER:O	2:B:88:THR:N	2.47	0.42
1:D:37:ARG:HA	1:D:38:PRO:HD3	1.95	0.42
3:F:101:LEU:C	3:F:101:LEU:CD1	2.79	0.42
1:G:1:MET:O	1:G:19:LYS:HA	2.19	0.42
2:E:73:VAL:HG22	2:E:112:CAS:CE2	2.50	0.42
3:F:170:VAL:HG23	3:F:175:TYR:CD1	2.55	0.42
1:J:70:GLN:HG3	4:K:94:PRO:HD3	2.02	0.42
3:F:129:LEU:HD13	3:F:132:GLN:HA	2.02	0.41
1:D:60:CAS:CE1	1:D:60:CAS:HA	2.50	0.41
1:G:80:ARG:HA	1:G:85:PHE:HA	2.02	0.41
1:A:94:SER:OG	2:B:68:HIS:ND1	2.46	0.41
3:C:161:ARG:O	3:C:161:ARG:HG3	2.21	0.41
2:E:33:ARG:HH11	2:E:33:ARG:HG3	1.86	0.41
1:G:80:ARG:HB2	1:G:85:PHE:CE1	2.56	0.41
4:H:72:LYS:HG3	4:H:99:ILE:HD11	2.03	0.41
3:I:70:GLU:OE2	3:I:113:ARG:HD3	2.19	0.41
3:C:165:VAL:O	3:C:169:LEU:HG	2.20	0.41
1:A:19:LYS:HB3	8:A:211:HOH:O	2.19	0.41
1:G:27:LEU:HD22	1:G:57:LEU:HD11	2.02	0.41
3:F:181:VAL:HG12	3:F:183:SER:N	2.36	0.41
3:F:65:SER:HG	3:F:88:TRP:HE1	1.67	0.41
3:F:98:TYR:CD2	3:F:117:TRP:CZ3	3.09	0.41
1:G:44:LEU:HA	1:G:76:GLY:O	2.20	0.41
1:A:86:GLU:HG3	1:A:87:ALA:O	2.21	0.41
2:E:98:GLU:H	2:E:98:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:THR:HG23	1:D:59:GLU:OE1	2.20	0.41
3:F:145:GLN:HA	3:F:146:PRO:HD3	1.98	0.41
4:K:37:LEU:HD22	4:K:43:LYS:HG3	2.03	0.41
3:L:200:ARG:HG2	3:L:200:ARG:HH11	1.86	0.41
2:E:33:ARG:HD3	2:E:37:LEU:CD1	2.51	0.40
3:I:63:LEU:HD23	3:I:63:LEU:HA	1.86	0.40
3:C:102:PRO:HB2	3:C:105:THR:CG2	2.51	0.40
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.95	0.40
1:J:31:VAL:HG13	1:J:35:LEU:HD12	2.02	0.40
4:K:103:LEU:HB3	3:L:162:CYS:SG	2.61	0.40
3:C:181:VAL:HG23	3:C:181:VAL:H	1.59	0.40
1:G:103:MET:CE	4:H:101:LEU:HG	2.52	0.40
4:H:98:GLU:CD	4:H:98:GLU:H	2.25	0.40
1:D:11:LYS:HD3	1:D:91:GLU:CB	2.51	0.40
3:F:84:VAL:HB	3:F:101:LEU:HD11	2.04	0.40

All (3) 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)
1:A:60:CAS:CE1	1:A:65:GLN:CB[8_555]	1.87	0.33
1:A:55:LYS:NZ	8:A:214:HOH:O[8_555]	2.11	0.09
3:I:94:GLU:OE2	3:I:125:HIS:NE2[5_655]	2.15	0.05

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	96/104 (92%)	90 (94%)	5 (5%)	1 (1%)	15 27
1	D	91/104 (88%)	84 (92%)	4 (4%)	3 (3%)	4 5
1	G	99/104 (95%)	90 (91%)	8 (8%)	1 (1%)	15 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	99/104 (95%)	93 (94%)	6 (6%)	0	100	100
2	B	83/97 (86%)	80 (96%)	3 (4%)	0	100	100
2	E	83/97 (86%)	79 (95%)	4 (5%)	0	100	100
3	C	130/162 (80%)	121 (93%)	8 (6%)	1 (1%)	19	34
3	F	138/162 (85%)	128 (93%)	9 (6%)	1 (1%)	22	39
3	I	141/162 (87%)	133 (94%)	7 (5%)	1 (1%)	22	39
3	L	141/162 (87%)	134 (95%)	6 (4%)	1 (1%)	22	39
4	H	81/97 (84%)	81 (100%)	0	0	100	100
4	K	79/97 (81%)	79 (100%)	0	0	100	100
All	All	1261/1452 (87%)	1192 (94%)	60 (5%)	9 (1%)	22	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	D	100	PRO
3	F	68	SER
3	I	204	GLU
3	L	179	ASP
3	C	200	ARG
1	D	97	PRO
1	D	99	LEU
1	G	61	GLY

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	85/90 (94%)	84 (99%)	1 (1%)	71	82
1	D	75/90 (83%)	73 (97%)	2 (3%)	44	65
1	G	88/90 (98%)	85 (97%)	3 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	86/90 (96%)	83 (96%)	3 (4%)	36 56
2	B	75/85 (88%)	72 (96%)	3 (4%)	31 51
2	E	74/85 (87%)	69 (93%)	5 (7%)	16 28
3	C	116/147 (79%)	112 (97%)	4 (3%)	37 58
3	F	122/147 (83%)	115 (94%)	7 (6%)	20 36
3	I	129/147 (88%)	128 (99%)	1 (1%)	81 88
3	L	130/147 (88%)	128 (98%)	2 (2%)	65 78
4	H	73/86 (85%)	68 (93%)	5 (7%)	16 28
4	K	77/86 (90%)	72 (94%)	5 (6%)	17 30
All	All	1130/1290 (88%)	1089 (96%)	41 (4%)	35 55

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
2	B	35	HIS
2	B	67	SER
2	B	86	SER
3	C	80	SER
3	C	85	LEU
3	C	148	PHE
3	C	185	TYR
1	D	27	LEU
1	D	79	PHE
2	E	33	ARG
2	E	35	HIS
2	E	63	ARG
2	E	78	THR
2	E	82	ARG
3	F	65	SER
3	F	80	SER
3	F	111	SER
3	F	115	HIS
3	F	148	PHE
3	F	150	ASN
3	F	183	SER
1	G	3	VAL
1	G	36	LYS
1	G	95	SER

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Mol	Chain	Res	Type
4	H	17	MET
4	H	35	HIS
4	H	68	HIS
4	H	82	ARG
4	H	111	ASP
3	I	183	SER
1	J	11	LYS
1	J	66	THR
1	J	95	SER
4	K	17	MET
4	K	61	ASN
4	K	78	THR
4	K	80	LYS
4	K	86	SER
3	L	96	GLN
3	L	111	SER

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	141	ASN
2	E	27	HIS
1	J	42	GLN
4	K	85	ASN
3	L	174	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

14 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	G	89	1	5,8,9	1.24	0	1,9,11	0.10	0
1	CAS	A	89	1	5,8,9	1.17	0	1,9,11	0.10	0
1	CAS	J	89	1	5,8,9	1.19	0	1,9,11	0.23	0
1	CAS	D	89	1	5,8,9	1.29	0	1,9,11	0.73	0
2	CAS	B	112	2	4,9,9	1.08	0	1,11,11	1.88	0
3	CAS	L	77	3	5,8,9	1.15	0	1,9,11	0.48	0
1	CAS	J	60	1	5,8,9	0.98	0	1,9,11	0.96	0
3	CAS	I	77	3	5,8,9	1.09	0	1,9,11	0.63	0
1	CAS	G	60	1	5,8,9	0.98	0	1,9,11	1.28	0
3	CAS	F	77	3	5,8,9	0.98	0	1,9,11	0.04	0
2	CAS	E	112	2	4,9,9	0.91	0	1,11,11	3.63	1 (100%)
1	CAS	D	60	1	5,8,9	1.06	0	1,9,11	1.60	0
3	CAS	C	77	3	5,8,9	1.13	0	1,9,11	0.11	0
1	CAS	A	60	1	5,8,9	1.60	1 (20%)	1,9,11	1.29	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	G	89	1	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-
2	CAS	B	112	2	-	0/2/9/9	-
3	CAS	L	77	3	-	0/0/7/9	-
1	CAS	J	60	1	-	0/0/7/9	-
3	CAS	I	77	3	-	0/0/7/9	-
1	CAS	G	60	1	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
2	CAS	E	112	2	-	0/2/9/9	-
1	CAS	D	60	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
1	CAS	A	60	1	-	0/0/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	CAS	AS-CE1	3.03	2.04	1.96

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	112	CAS	CA-CB-SG	-3.63	99.16	114.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	112	CAS	2	0
3	L	77	CAS	1	0
1	J	60	CAS	1	0
3	F	77	CAS	1	0
2	E	112	CAS	3	0
1	D	60	CAS	1	0
1	A	60	CAS	0	1

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	$\#\|Z\| > 2$
7	IPA	L	303	-	3,3,3	0.72	0	3,3,3	0.18	0
7	IPA	I	303	-	3,3,3	0.59	0	3,3,3	0.77	0
5	ACT	F	301	-	1,3,3	9.96	1 (100%)	0,3,3	0.00	-
6	F4K	I	302	-	14,14,14	2.35	3 (21%)	17,18,18	1.15	1 (5%)
6	F4K	L	301	-	14,14,14	2.22	3 (21%)	17,18,18	0.71	0
5	ACT	L	302	-	1,3,3	6.49	1 (100%)	0,3,3	0.00	-
5	ACT	I	301	-	1,3,3	9.19	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
6	F4K	I	302	-	-	4/6/6/6	0/2/2/2
6	F4K	L	301	-	-	0/6/6/6	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	301	ACT	CH3-C	9.96	1.61	1.48
5	I	301	ACT	CH3-C	9.19	1.60	1.48
6	I	302	F4K	C06-N09	-6.85	1.34	1.45
6	L	301	F4K	C06-N09	-6.63	1.34	1.45
5	L	302	ACT	CH3-C	6.49	1.57	1.48
6	I	302	F4K	C10-N09	-3.81	1.33	1.39
6	L	301	F4K	C13-N09	-3.45	1.34	1.39
6	I	302	F4K	C13-N09	-3.23	1.34	1.39
6	L	301	F4K	C10-N09	-3.18	1.34	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	302	F4K	C08-C03-C04	2.30	121.78	118.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	302	F4K	C05-C06-N09-C10
6	I	302	F4K	C05-C06-N09-C13
6	I	302	F4K	C07-C06-N09-C10
6	I	302	F4K	C07-C06-N09-C13

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	303	IPA	2	0
6	I	302	F4K	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	100/104 (96%)	-0.34	0 100 100	32, 40, 82, 105	0
1	D	95/104 (91%)	-0.12	2 (2%) 63 72	37, 62, 102, 137	0
1	G	101/104 (97%)	-0.34	3 (2%) 50 59	32, 50, 80, 101	0
1	J	101/104 (97%)	-0.52	0 100 100	30, 36, 67, 105	0
2	B	86/97 (88%)	-0.37	1 (1%) 79 85	34, 45, 90, 107	0
2	E	86/97 (88%)	-0.02	1 (1%) 79 85	37, 55, 87, 125	0
3	C	134/162 (82%)	-0.27	1 (0%) 87 91	39, 62, 90, 113	0
3	F	140/162 (86%)	0.05	5 (3%) 42 51	40, 68, 107, 127	0
3	I	143/162 (88%)	-0.39	1 (0%) 87 91	35, 48, 83, 108	0
3	L	143/162 (88%)	-0.46	0 100 100	30, 41, 79, 120	0
4	H	85/97 (87%)	-0.18	4 (4%) 31 37	36, 55, 96, 114	0
4	K	85/97 (87%)	-0.40	0 100 100	30, 41, 75, 109	0
All	All	1299/1452 (89%)	-0.28	18 (1%) 75 82	30, 50, 92, 137	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	202	THR	4.0
3	F	143	ASP	3.9
3	F	66	VAL	3.5
1	G	102	VAL	3.4
3	C	66	VAL	3.1
4	H	88	THR	3.0
1	G	1	MET	3.0
1	D	38	PRO	2.9
2	B	57	THR	2.9
4	H	87	SER	2.8
1	D	40	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	63	LEU	2.2
3	F	142	VAL	2.2
2	E	85	ASN	2.2
4	H	46	LEU	2.1
3	I	186	GLU	2.1
1	G	80	ARG	2.0
4	H	85	ASN	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
3	CAS	F	77	9/10	0.87	0.17	58,77,109,118	0
1	CAS	A	60	9/10	0.91	0.19	31,39,155,157	0
1	CAS	J	60	9/10	0.93	0.18	28,32,87,89	9
1	CAS	D	89	9/10	0.94	0.13	66,87,142,143	0
1	CAS	D	60	9/10	0.94	0.12	32,36,102,106	0
1	CAS	A	89	9/10	0.94	0.15	40,47,98,119	0
3	CAS	C	77	9/10	0.96	0.15	44,63,97,106	0
2	CAS	B	112	10/10	0.96	0.14	41,54,82,99	0
2	CAS	E	112	10/10	0.97	0.13	47,61,93,96	0
1	CAS	G	89	9/10	0.97	0.12	38,42,92,97	0
3	CAS	I	77	9/10	0.97	0.10	31,42,76,77	0
1	CAS	J	89	9/10	0.97	0.11	29,33,79,82	0
1	CAS	G	60	9/10	0.98	0.10	42,52,79,90	0
3	CAS	L	77	9/10	0.98	0.15	29,30,79,82	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
5	ACT	F	301	4/4	0.91	0.14	37,51,59,62	0
5	ACT	L	302	4/4	0.94	0.21	52,70,71,72	0
5	ACT	I	301	4/4	0.95	0.14	41,46,58,59	0
6	F4K	I	302	13/13	0.95	0.29	36,55,61,64	0
7	IPA	I	303	4/4	0.95	0.17	33,39,41,42	0
7	IPA	L	303	4/4	0.96	0.15	32,41,43,44	0
6	F4K	L	301	13/13	0.97	0.17	33,41,47,47	0

6.5 Other polymers

There are no such residues in this entry.