Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 09:59 PM EDT

PDB ID	:	6GMX
Title	:	pVHL:EloB:EloC in complex with 6-chlorothiochroman-4-one
Authors	:	Van Molle, I.; Lucas, X.; Ciulli, A.
Deposited on	:	2018-05-28
Resolution	:	2.53 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

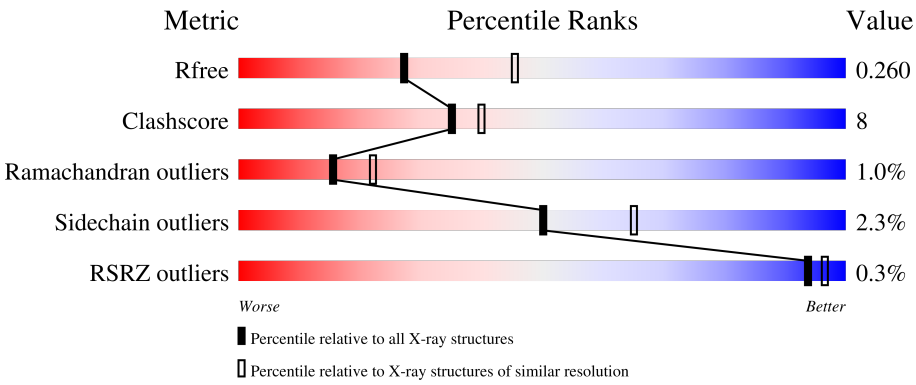
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	76% 20% • •
1	G	104	87% 11% • •
1	J	104	88% 11% • •
2	B	97	80% 7% • 10%
2	H	97	% 70% 18% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	97	72% 13% • 11%
3	C	162	70% 13% • 15%
3	F	162	2% 69% 17% •• 12%
3	I	162	70% 19% • 11%
3	L	162	75% 10% • 11%
4	D	104	75% 14% •• 8%
5	E	97	72% 15% • 10%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10861 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
			Total	As	C	N	O	S			
1	A	103	806	2	512	136	152	4	0	0	0
1	G	103	808	2	512	135	154	5	0	0	0
1	J	103	809	2	514	136	152	5	0	0	0

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	87	679	440	107	126	6	0	0	0
2	H	85	672	436	109	122	5	0	0	0
2	K	86	698	450	111	130	7	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	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
			Total	As	C	N	O	S			
3	C	138	1100	1	702	198	197	2	0	1	0
3	F	142	1143	1	728	208	204	2	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
3	I	144	1153	1	736	207	207	2	0	0	0
3	L	144	1175	1	746	214	212	2	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
4	D	96	738	1	473	123	138	3	0	0	0

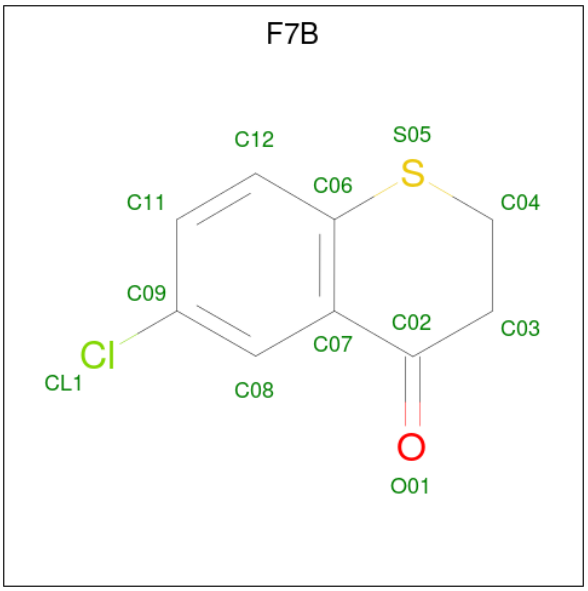
- Molecule 5 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
5	E	87	677	1	437	107	126	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

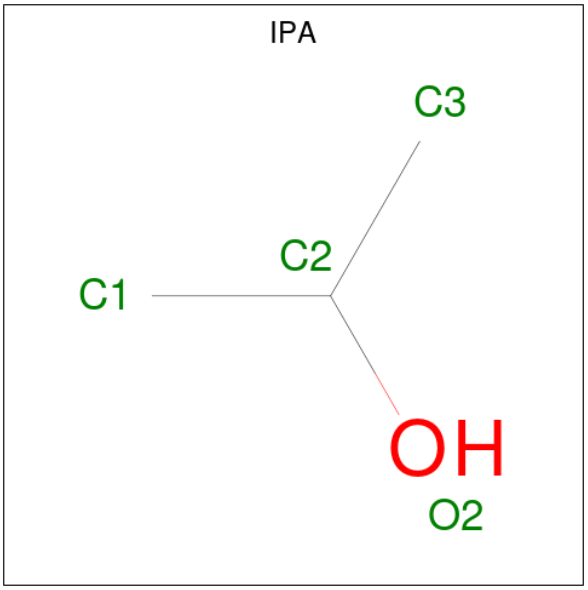
Chain	Residue	Modelled	Actual	Comment	Reference
E	16	MET	-	initiating methionine	UNP Q15369
E	112	CAS	-	expression tag	UNP Q15369

- Molecule 6 is 6-chloranyl-2,3-dihydrothiochromen-4-one (three-letter code: F7B) (formula: C_9H_7ClOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	O	S		
6	B	1	12	9	1	1	1	0	0
			Total	C	Cl	O	S		
6	K	1	12	9	1	1	1	0	0

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



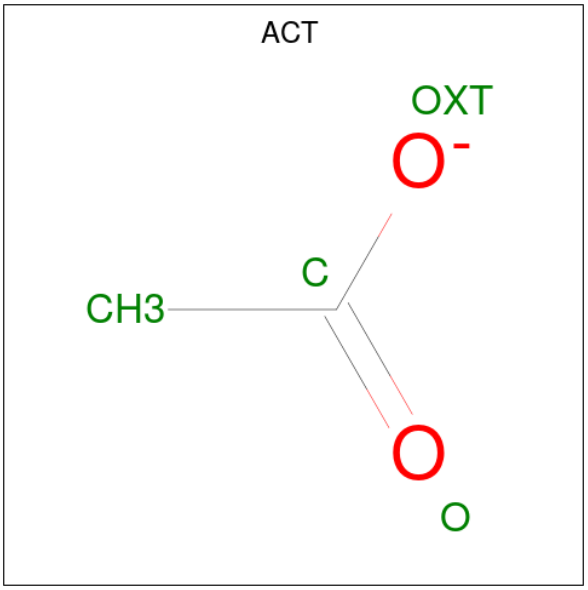
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	C	1	4	3	1		0	0
			Total	C	O			
7	F	1	4	3	1		0	0

Continued on next page...

Continued from previous page...

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	49	Total O 49 49	0	0
9	B	25	Total O 25 25	0	0
9	C	21	Total O 21 21	0	0
9	D	18	Total O 18 18	0	0
9	E	17	Total O 17 17	0	0

Continued on next page...

Continued from previous page...

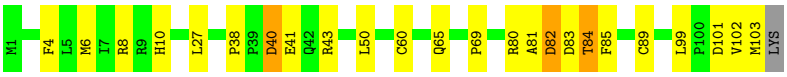
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	F	25	25	25	0	0
			Total	O		
9	G	19	19	19	0	0
			Total	O		
9	H	20	20	20	0	0
			Total	O		
9	I	38	38	38	0	0
			Total	O		
9	J	44	44	44	0	0
			Total	O		
9	K	27	27	27	0	0
			Total	O		
9	L	52	52	52	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

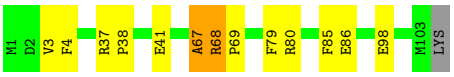
- Molecule 1: Elongin-B

Chain A:



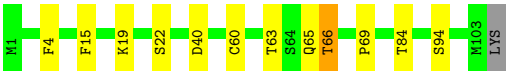
- Molecule 1: Elongin-B

Chain G:



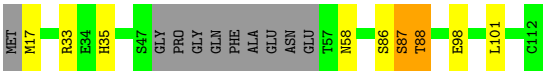
- Molecule 1: Elongin-B

Chain J:



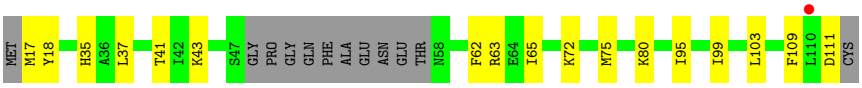
- Molecule 2: Elongin-C

Chain B:



- Molecule 2: Elongin-C

Chain H:



- Molecule 2: Elongin-C

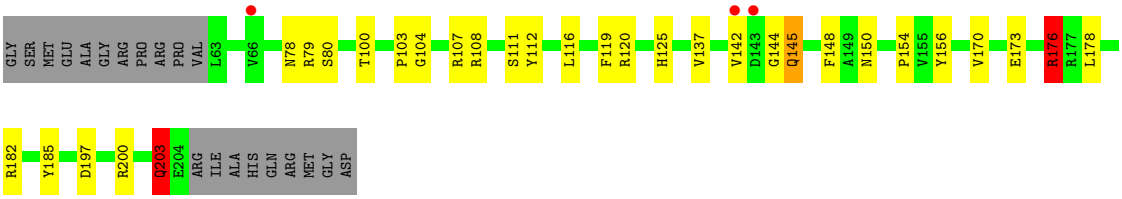
Chain K:

• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C:

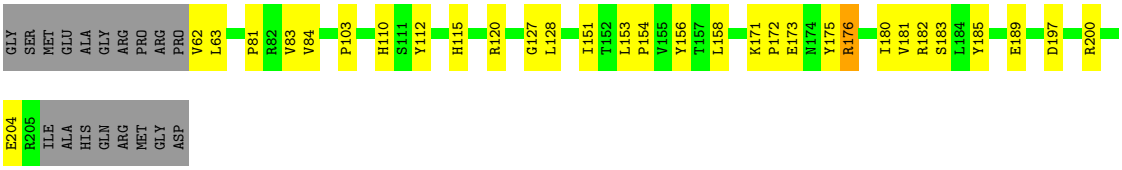
• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:



• Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain I:



• Molecule 3: von Hippel-Lindau disease tumor suppressor

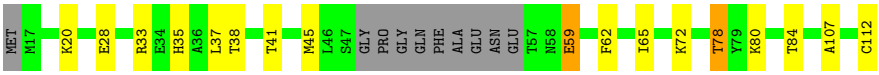
Chain L:

• Molecule 4: Elongin-B

Chain D:

• Molecule 5: Elongin-C

Chain E:


MET
M17
K20
E28
R33
E34
H35
A36
L37
T38
T41
M45
L46
S47
GLY
PRO
GLY
GLN
PHE
ALA
GLU
ASN
GLU
T57
N58
E59
F62
I65
K72
T78
Y79
K80
T84
A107
C112

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	94.00Å 94.00Å 365.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.00 – 2.53 94.00 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (94.00-2.53) 100.0 (94.00-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.10 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.188 , 0.361 0.189 , 0.260	Depositor DCC
R_{free} test set	2823 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10861	wwPDB-VP
Average B, all atoms (Å^2)	55.0	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 29.48 % 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 1.5374e-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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, ACT, F7B, IPA

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	0.57	0/802	0.75	1/1083 (0.1%)
1	G	0.56	1/804 (0.1%)	0.75	1/1086 (0.1%)
1	J	0.57	0/805	0.75	0/1086
2	B	0.57	0/693	0.75	1/937 (0.1%)
2	H	0.50	0/686	0.66	1/927 (0.1%)
2	K	0.53	0/712	0.64	0/959
3	C	0.59	0/1118	0.78	2/1528 (0.1%)
3	F	0.64	1/1163 (0.1%)	0.92	7/1591 (0.4%)
3	I	0.56	0/1173	0.79	1/1604 (0.1%)
3	L	0.58	0/1195	0.82	4/1631 (0.2%)
4	D	0.54	0/743	0.70	0/1005
5	E	0.47	0/681	0.62	0/923
All	All	0.56	2/10575 (0.0%)	0.76	18/14360 (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	A	0	2
3	C	0	2
3	L	0	1
4	D	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	67	ALA	C-N	6.39	1.48	1.34
3	F	173	GLU	CB-CG	6.25	1.64	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	186	GLU	CA-CB-CG	10.31	136.09	113.40
3	F	145	GLN	N-CA-CB	-8.59	95.14	110.60
3	L	186	GLU	N-CA-CB	-8.38	95.52	110.60
2	B	101	LEU	CA-CB-CG	-8.24	96.36	115.30
3	F	176	ARG	NE-CZ-NH1	7.51	124.06	120.30
3	I	176	ARG	NE-CZ-NH1	-6.84	116.88	120.30
2	H	80	LYS	CD-CE-NZ	6.76	127.24	111.70
3	F	144	GLY	C-N-CA	6.46	137.84	121.70
3	C	69	ARG	NE-CZ-NH1	-6.42	117.09	120.30
3	C	199	GLU	CA-CB-CG	6.12	126.87	113.40
1	G	68	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	F	145	GLN	CA-CB-CG	6.07	126.75	113.40
3	F	176	ARG	CA-CB-CG	-5.83	100.57	113.40
3	F	176	ARG	CB-CA-C	-5.44	99.52	110.40
1	A	65	GLN	CA-CB-CG	-5.29	101.76	113.40
3	L	144	GLY	C-N-CA	5.21	134.73	121.70
3	F	176	ARG	NE-CZ-NH2	-5.19	117.71	120.30
3	L	153	LEU	CB-CG-CD1	-5.06	102.40	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ASP	Peptide
1	A	82	ASP	Peptide
3	C	191	HIS	Sidechain
3	C	64	ARG	Sidechain
4	D	60	CAS	Mainchain
3	L	204	GLU	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	806	0	792	15	0
1	G	808	0	791	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	809	0	800	7	0
2	B	679	0	671	5	0
2	H	672	0	675	12	0
2	K	698	0	697	10	0
3	C	1100	0	1056	16	0
3	F	1143	0	1111	24	0
3	I	1153	0	1127	28	0
3	L	1175	0	1149	25	0
4	D	738	0	726	20	0
5	E	677	0	650	10	0
6	B	12	0	0	0	0
6	K	12	0	0	0	0
7	C	4	0	8	0	0
7	F	4	0	8	1	0
7	I	4	0	8	0	0
7	L	4	0	8	0	0
8	F	4	0	3	0	0
8	L	4	0	3	0	0
9	A	49	0	0	0	0
9	B	25	0	0	0	0
9	C	21	0	0	1	0
9	D	18	0	0	4	0
9	E	17	0	0	2	0
9	F	25	0	0	0	0
9	G	19	0	0	0	0
9	H	20	0	0	0	0
9	I	38	0	0	1	0
9	J	44	0	0	1	0
9	K	27	0	0	2	0
9	L	52	0	0	0	0
All	All	10861	0	10283	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (170) 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)
3:F:100:THR:O	3:F:107:ARG:NH2	1.68	1.27
4:D:99:LEU:HD22	4:D:100:PRO:CD	1.64	1.26
3:I:180:ILE:HG13	3:I:185:TYR:CE1	1.78	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:ARG:CZ	4:D:39:PRO:HG2	1.79	1.12
3:I:180:ILE:HG13	3:I:185:TYR:HE1	0.98	1.11
3:I:176:ARG:HH12	3:I:185:TYR:HB3	1.21	1.03
3:F:200:ARG:O	3:F:203:GLN:HB2	1.58	1.02
4:D:99:LEU:HD22	4:D:100:PRO:HD2	1.06	1.01
4:D:99:LEU:CD2	4:D:100:PRO:HD2	1.94	0.97
3:F:176:ARG:NH1	3:F:185:TYR:HB3	1.81	0.95
3:L:176:ARG:NH1	3:L:185:TYR:HB3	1.83	0.92
3:F:108:ARG:HH11	2:H:41:THR:HG22	1.31	0.92
3:L:176:ARG:CZ	3:L:185:TYR:HB3	2.02	0.90
3:L:176:ARG:NH2	3:L:185:TYR:HB3	1.86	0.89
3:F:142:VAL:O	3:F:145:GLN:HG3	1.74	0.88
3:F:203:GLN:NE2	3:F:203:GLN:HA	1.89	0.87
3:L:176:ARG:HH22	3:L:185:TYR:CB	1.88	0.86
3:F:120[B]:ARG:NH2	3:F:197:ASP:OD2	2.09	0.85
1:J:63:THR:HG22	1:J:65:GLN:H	1.42	0.84
4:D:29:ARG:NE	4:D:39:PRO:HG2	1.93	0.83
3:L:176:ARG:HH12	3:L:185:TYR:HB3	1.45	0.82
4:D:29:ARG:NH2	4:D:39:PRO:HG2	1.95	0.81
1:A:38:PRO:HG2	1:A:41:GLU:HG3	1.61	0.80
1:G:3:VAL:HG22	1:G:67:ALA:HB3	1.69	0.75
3:L:176:ARG:NH2	3:L:185:TYR:CB	2.47	0.75
4:D:99:LEU:CD2	4:D:100:PRO:CD	2.58	0.73
4:D:99:LEU:CD1	9:D:218:HOH:O	2.36	0.72
3:I:180:ILE:CG1	3:I:185:TYR:HE1	1.91	0.72
2:B:33:ARG:NH1	2:B:58:ASN:OD1	2.19	0.72
3:L:176:ARG:HH22	3:L:185:TYR:HB3	1.49	0.72
3:L:181:VAL:HG12	3:L:183:SER:H	1.54	0.71
3:C:99:PRO:O	3:C:107:ARG:NH2	2.24	0.71
3:F:104:GLY:HA3	2:H:63:ARG:HD2	1.73	0.70
2:K:63:ARG:NH2	9:K:301:HOH:O	2.15	0.70
3:C:132:GLN:NE2	9:C:401:HOH:O	2.25	0.69
4:D:99:LEU:HD12	9:D:218:HOH:O	1.93	0.69
3:F:176:ARG:HH12	3:F:185:TYR:HB3	1.57	0.69
3:L:176:ARG:NH2	3:L:185:TYR:CG	2.61	0.68
4:D:3:VAL:HG22	4:D:67:ALA:HB3	1.76	0.66
3:I:182:ARG:O	3:I:185:TYR:HB2	1.97	0.65
3:L:178:LEU:O	3:L:179:ASP:HB2	1.97	0.64
3:F:79:ARG:HD2	3:F:150:ASN:HB3	1.79	0.64
4:D:99:LEU:HD22	4:D:100:PRO:HD3	1.75	0.64
2:K:64[B]:GLU:HG2	2:K:65:ILE:HG13	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:LYS:HB3	5:E:59:GLU:HB3	1.81	0.62
2:K:16:MET:SD	2:K:32:LYS:HD3	2.39	0.62
4:D:56:THR:OG1	4:D:59:GLU:HG3	2.00	0.62
3:F:142:VAL:O	3:F:145:GLN:CG	2.47	0.62
3:F:120[B]:ARG:NH1	3:F:125:HIS:O	2.32	0.61
1:J:63:THR:H	1:J:66:THR:HG22	1.65	0.61
1:J:19:LYS:O	1:J:22:SER:HB3	2.01	0.60
4:D:23:THR:OG1	4:D:26:GLU:HG3	2.03	0.59
3:L:170:VAL:HG21	3:L:178:LEU:HD21	1.84	0.59
2:B:86:SER:O	2:B:88:THR:N	2.34	0.58
3:C:120[A]:ARG:HD3	3:C:127:GLY:HA2	1.85	0.58
3:F:142:VAL:O	3:F:145:GLN:HB2	2.03	0.58
3:I:175:TYR:HD2	3:I:189:GLU:HG3	1.69	0.58
3:C:73:GLN:H	3:C:141:ASN:HD21	1.50	0.58
3:I:176:ARG:NH1	3:I:185:TYR:HB3	2.04	0.58
1:G:4:PHE:CE1	1:G:69:PRO:HG3	2.39	0.57
3:L:181:VAL:HG12	3:L:183:SER:N	2.20	0.57
5:E:33:ARG:O	5:E:37:LEU:HG	2.04	0.57
3:L:204:GLU:N	3:L:204:GLU:OE2	2.37	0.57
3:F:182:ARG:HA	3:F:185:TYR:CD2	2.39	0.56
3:L:179:ASP:O	3:L:180:ILE:HG12	2.05	0.56
4:D:25:PHE:HB2	4:D:53:ASP:HB3	1.88	0.56
3:I:180:ILE:HG13	3:I:185:TYR:CD1	2.38	0.55
2:H:41:THR:HG21	2:H:109:PHE:O	2.06	0.55
1:A:99:LEU:HD13	2:B:98:GLU:HA	1.88	0.55
1:G:3:VAL:HG22	1:G:67:ALA:CB	2.38	0.54
3:I:182:ARG:HA	3:I:185:TYR:CD2	2.42	0.54
4:D:65:GLN:OE1	9:D:201:HOH:O	2.18	0.54
1:G:68:ARG:HH11	1:G:68:ARG:HG3	1.73	0.54
2:H:103:LEU:HD21	3:I:158:LEU:HD11	1.89	0.54
4:D:99:LEU:HD11	9:D:218:HOH:O	2.02	0.53
3:L:73:GLN:OE1	3:L:108:ARG:NH1	2.42	0.53
2:H:37:LEU:HD22	2:H:43:LYS:HG3	1.90	0.52
1:G:37:ARG:NH2	1:G:80:ARG:O	2.42	0.52
3:L:182:ARG:O	3:L:185:TYR:HB2	2.08	0.52
1:J:94:SER:OG	2:K:68:HIS:ND1	2.29	0.52
3:C:120[B]:ARG:NH2	3:C:197:ASP:OD2	2.37	0.52
3:L:176:ARG:HH22	3:L:185:TYR:CA	2.23	0.52
2:H:17:MET:HG3	2:H:18:TYR:CD1	2.46	0.51
1:A:83:ASP:O	1:A:84:THR:HG22	2.10	0.51
3:F:154:PRO:HG2	3:F:156:TYR:CE1	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:SER:O	2:B:88:THR:HG23	2.10	0.51
3:C:130:VAL:O	3:C:132:GLN:O	2.29	0.51
2:B:87:SER:OG	3:C:132:GLN:CD	2.49	0.51
1:A:80:ARG:NH1	1:A:82:ASP:O	2.43	0.50
3:I:120:ARG:HD3	3:I:127:GLY:HA2	1.92	0.50
3:I:176:ARG:HH12	3:I:185:TYR:CB	2.09	0.49
1:A:43:ARG:HG3	1:A:85:PHE:CE1	2.48	0.49
3:F:176:ARG:CZ	3:F:185:TYR:HB3	2.42	0.48
3:F:182:ARG:O	3:F:185:TYR:HB2	2.14	0.48
1:J:4:PHE:CE2	1:J:69:PRO:HG3	2.48	0.48
3:L:175:TYR:O	3:L:185:TYR:CE1	2.67	0.48
3:I:62:VAL:HG13	3:I:63:LEU:H	1.79	0.48
5:E:38:THR:HG23	5:E:80:LYS:NZ	2.29	0.48
3:L:112:TYR:HB2	3:L:115:HIS:CE1	2.49	0.48
5:E:41:THR:O	5:E:45:MET:HG3	2.13	0.48
5:E:78:THR:HG22	9:E:212:HOH:O	2.14	0.47
2:H:62:PHE:HB3	2:H:65:ILE:HD12	1.96	0.47
3:I:171:LYS:HB3	3:I:173:GLU:OE2	2.14	0.47
1:A:4:PHE:CE1	1:A:69:PRO:HG3	2.50	0.47
1:G:3:VAL:CG2	1:G:67:ALA:HB3	2.42	0.47
3:I:110:HIS:HB3	9:I:424:HOH:O	2.13	0.47
2:K:72:LYS:HG3	2:K:99:ILE:CD1	2.44	0.47
3:C:153:LEU:HD23	3:C:153:LEU:HA	1.80	0.46
5:E:80:LYS:O	5:E:84:THR:HG23	2.14	0.46
3:I:176:ARG:NH2	3:I:189:GLU:OE1	2.49	0.46
3:I:175:TYR:CD2	3:I:189:GLU:HG3	2.48	0.46
1:J:15:PHE:HE1	2:K:29:PHE:HD2	1.64	0.46
3:L:176:ARG:NH2	3:L:185:TYR:CD1	2.84	0.46
1:G:38:PRO:HD2	1:G:41:GLU:OE2	2.15	0.45
1:G:80:ARG:HA	1:G:85:PHE:HA	1.98	0.45
3:I:154:PRO:HG2	3:I:156:TYR:CE1	2.51	0.45
1:G:79:PHE:O	1:G:86:GLU:HG2	2.15	0.45
2:H:95:ILE:HD13	2:H:103:LEU:HD23	1.97	0.45
3:I:200:ARG:HG2	3:I:204:GLU:OE2	2.16	0.45
3:C:181:VAL:HG22	3:C:183:SER:H	1.81	0.45
1:A:43:ARG:HB3	1:A:50:LEU:HD11	1.97	0.45
3:F:170:VAL:HG21	3:F:178:LEU:HD11	1.99	0.45
3:L:120[B]:ARG:HD3	3:L:127:GLY:HA2	1.99	0.45
1:J:60:CAS:CE1	1:J:60:CAS:HA	2.46	0.45
3:I:84:VAL:HG11	3:I:151:ILE:HD13	1.99	0.45
3:I:181:VAL:HG12	3:I:183:SER:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:PRO:HA	3:I:175:TYR:CD1	2.52	0.44
1:A:80:ARG:HB2	1:A:85:PHE:CE1	2.53	0.44
3:C:84:VAL:HG22	3:C:128:LEU:HD13	2.00	0.44
3:C:199:GLU:O	3:C:200:ARG:HB3	2.18	0.44
4:D:3:VAL:HG22	4:D:67:ALA:CB	2.45	0.44
1:A:103:MET:HE2	3:C:169:LEU:HB2	1.99	0.44
1:A:102:VAL:HG13	3:C:170:VAL:HG13	1.99	0.43
5:E:107:ALA:HA	5:E:112:CAS:CE2	2.49	0.43
3:I:83:VAL:HG22	3:I:103:PRO:HD3	2.00	0.43
3:C:69:ARG:HH11	3:C:69:ARG:HD2	1.69	0.43
3:F:119:PHE:O	3:F:120[B]:ARG:HD3	2.19	0.43
2:K:35:HIS:HE1	9:K:318:HOH:O	2.01	0.43
3:I:197:ASP:OD2	3:I:200:ARG:NH1	2.40	0.43
1:A:102:VAL:CG1	3:C:170:VAL:HG13	2.48	0.43
1:A:6:MET:CE	1:A:8:ARG:HD2	2.49	0.43
3:I:112:TYR:HB2	3:I:115:HIS:CD2	2.53	0.43
3:C:74:VAL:CG2	3:C:109:ILE:HB	2.50	0.42
3:F:112:TYR:CE1	7:F:301:IPA:H31	2.55	0.42
2:H:72:LYS:HA	2:H:75:MET:HE2	2.00	0.42
4:D:55:LYS:HG3	4:D:60:CAS:CE2	2.50	0.42
5:E:62:PHE:CD1	5:E:65:ILE:HD12	2.54	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.53	0.42
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.49	0.42
4:D:3:VAL:CG2	4:D:67:ALA:HB3	2.48	0.42
3:F:108:ARG:NH1	2:H:41:THR:HG22	2.13	0.42
3:F:142:VAL:O	3:F:145:GLN:CB	2.67	0.42
2:H:72:LYS:HG3	2:H:99:ILE:CD1	2.50	0.42
5:E:72:LYS:HE3	9:E:205:HOH:O	2.20	0.42
3:I:81:PRO:HD2	3:I:153:LEU:HG	2.02	0.42
2:K:37:LEU:HD22	2:K:43:LYS:HG3	2.02	0.41
5:E:20:LYS:HD3	5:E:28:GLU:HB3	2.02	0.41
9:J:221:HOH:O	2:K:78:THR:HG21	2.21	0.41
3:L:112:TYR:HB2	3:L:115:HIS:NE2	2.35	0.41
3:I:112:TYR:HB2	3:I:115:HIS:NE2	2.35	0.41
2:K:109:PHE:CD2	2:K:110:LEU:HD13	2.56	0.41
1:A:6:MET:HE3	1:A:8:ARG:HD2	2.03	0.41
3:F:116:LEU:HD22	3:F:137:VAL:HG22	2.02	0.41
3:L:81:PRO:HD2	3:L:153:LEU:HG	2.01	0.41
3:L:179:ASP:HB3	3:L:180:ILE:H	1.67	0.41
4:D:100:PRO:HB2	4:D:101:ASP:H	1.67	0.41
3:F:78:ASN:ND2	3:F:103:PRO:HA	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:112:TYR:HB2	3:L:115:HIS:CD2	2.56	0.40
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.81	0.40
2:H:72:LYS:HG3	2:H:99:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	99/104 (95%)	91 (92%)	6 (6%)	2 (2%)	7 8
1	G	99/104 (95%)	93 (94%)	5 (5%)	1 (1%)	15 22
1	J	99/104 (95%)	93 (94%)	5 (5%)	1 (1%)	15 22
2	B	83/97 (86%)	79 (95%)	2 (2%)	2 (2%)	6 5
2	H	81/97 (84%)	80 (99%)	1 (1%)	0	100 100
2	K	83/97 (86%)	83 (100%)	0	0	100 100
3	C	134/162 (83%)	127 (95%)	7 (5%)	0	100 100
3	F	140/162 (86%)	134 (96%)	5 (4%)	1 (1%)	22 30
3	I	141/162 (87%)	135 (96%)	6 (4%)	0	100 100
3	L	142/162 (88%)	133 (94%)	6 (4%)	3 (2%)	7 7
4	D	91/104 (88%)	85 (93%)	3 (3%)	3 (3%)	4 2
5	E	83/97 (86%)	79 (95%)	4 (5%)	0	100 100
All	All	1275/1452 (88%)	1212 (95%)	50 (4%)	13 (1%)	15 22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	87	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	88	THR
3	L	179	ASP
3	L	180	ILE
1	A	81	ALA
4	D	100	PRO
3	F	203	GLN
3	L	143	ASP
1	A	84	THR
1	J	84	THR
4	D	97	PRO
4	D	99	LEU
1	G	98	GLU

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%)	82 (96%)	3 (4%)	36	49
1	G	86/90 (96%)	86 (100%)	0	100	100
1	J	86/90 (96%)	84 (98%)	2 (2%)	50	65
2	B	75/86 (87%)	73 (97%)	2 (3%)	44	59
2	H	75/86 (87%)	73 (97%)	2 (3%)	44	59
2	K	79/86 (92%)	75 (95%)	4 (5%)	24	32
3	C	118/147 (80%)	116 (98%)	2 (2%)	60	75
3	F	125/147 (85%)	120 (96%)	5 (4%)	31	43
3	I	127/147 (86%)	127 (100%)	0	100	100
3	L	130/147 (88%)	129 (99%)	1 (1%)	81	88
4	D	78/91 (86%)	76 (97%)	2 (3%)	46	61
5	E	72/85 (85%)	69 (96%)	3 (4%)	30	40
All	All	1136/1292 (88%)	1110 (98%)	26 (2%)	50	65

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

Mol	Chain	Res	Type
1	A	10	HIS
1	A	27	LEU
1	A	40	ASP
2	B	17	MET
2	B	35	HIS
3	C	148	PHE
3	C	200	ARG
4	D	19	LYS
4	D	99	LEU
5	E	35	HIS
5	E	59	GLU
5	E	78	THR
3	F	80	SER
3	F	111	SER
3	F	148	PHE
3	F	176	ARG
3	F	203	GLN
2	H	35	HIS
2	H	111	ASP
1	J	40	ASP
1	J	66	THR
2	K	35	HIS
2	K	61	ASN
2	K	78	THR
2	K	110	LEU
3	L	186	GLU

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

Mol	Chain	Res	Type
3	F	150	ASN
3	F	203	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	1.12	0	1,9,11	0.83	0
3	CAS	C	77	3	5,8,9	1.14	0	1,9,11	1.76	0
1	CAS	A	89	1	5,8,9	1.35	0	1,9,11	2.58	1 (100%)
1	CAS	G	60	1	5,8,9	1.23	0	1,9,11	1.96	0
1	CAS	J	89	1	5,8,9	1.33	0	1,9,11	1.23	0
1	CAS	A	60	1	5,8,9	2.75	1 (20%)	1,9,11	2.64	1 (100%)
1	CAS	J	60	1	5,8,9	0.95	0	1,9,11	1.30	0
5	CAS	E	112	5	6,9,9	1.04	0	5,11,11	1.06	0
3	CAS	I	77	3	5,8,9	1.07	0	1,9,11	1.82	0
3	CAS	L	77	3	5,8,9	1.04	0	1,9,11	1.20	0
4	CAS	D	60	4	5,8,9	1.13	0	1,9,11	1.69	0
3	CAS	F	77	3	5,8,9	1.09	0	1,9,11	1.92	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	-
3	CAS	C	77	3	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
1	CAS	G	60	1	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-
1	CAS	A	60	1	-	0/0/7/9	-
1	CAS	J	60	1	-	0/0/7/9	-
5	CAS	E	112	5	-	2/6/9/9	-
3	CAS	I	77	3	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
4	CAS	D	60	4	-	0/0/7/9	-
3	CAS	F	77	3	-	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	5.72	2.11	1.96

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	60	CAS	CA-CB-SG	-2.64	103.33	114.43
1	A	89	CAS	CA-CB-SG	-2.58	103.58	114.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	112	CAS	N-CA-CB-SG
5	E	112	CAS	C-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	60	CAS	1	0
5	E	112	CAS	1	0
4	D	60	CAS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	I	301	-	3,3,3	0.54	0	3,3,3	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ACT	L	302	-	3,3,3	1.92	1 (33%)	3,3,3	1.37	0
7	IPA	F	301	-	3,3,3	0.47	0	3,3,3	0.72	0
7	IPA	L	301	-	3,3,3	0.60	0	3,3,3	0.38	0
7	IPA	C	301	-	3,3,3	0.66	0	3,3,3	0.65	0
8	ACT	F	302	-	3,3,3	1.68	1 (33%)	3,3,3	1.38	0
6	F7B	B	201	-	13,13,13	1.00	0	18,18,18	2.06	5 (27%)
6	F7B	K	201	-	13,13,13	0.85	0	18,18,18	2.05	4 (22%)

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	F7B	B	201	-	-	-	0/2/2/2
6	F7B	K	201	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	302	ACT	CH3-C	2.71	1.60	1.49
8	F	302	ACT	CH3-C	2.34	1.58	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	201	F7B	C03-C02-C07	5.39	124.65	117.50
6	K	201	F7B	C03-C02-C07	4.86	123.94	117.50
6	B	201	F7B	O01-C02-C07	-4.14	116.90	121.71
6	K	201	F7B	C04-S05-C06	4.11	113.65	101.27
6	K	201	F7B	O01-C02-C07	-4.00	117.07	121.71
6	B	201	F7B	C04-S05-C06	3.07	110.50	101.27
6	B	201	F7B	C07-C06-S05	-2.47	117.95	122.80
6	B	201	F7B	C12-C06-C07	2.46	122.26	119.14
6	K	201	F7B	C04-C03-C02	2.32	118.41	113.09

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
7	F	301	IPA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	101/104 (97%)	-0.19	0	100	100	32, 43, 88, 107	0
1	G	101/104 (97%)	-0.20	0	100	100	34, 57, 85, 98	0
1	J	101/104 (97%)	-0.30	0	100	100	31, 42, 69, 83	0
2	B	87/97 (89%)	-0.27	0	100	100	32, 44, 88, 103	0
2	H	85/97 (87%)	-0.07	1 (1%)	79	84	38, 54, 94, 120	0
2	K	86/97 (88%)	-0.17	0	100	100	32, 44, 78, 132	0
3	C	137/162 (84%)	-0.22	0	100	100	35, 53, 86, 110	0
3	F	141/162 (87%)	-0.09	3 (2%)	63	70	38, 58, 93, 131	0
3	I	143/162 (88%)	-0.22	0	100	100	33, 50, 82, 113	0
3	L	143/162 (88%)	-0.27	0	100	100	31, 42, 81, 95	0
4	D	95/104 (91%)	-0.04	0	100	100	35, 62, 96, 113	0
5	E	86/97 (88%)	-0.08	0	100	100	38, 55, 88, 117	0
All	All	1306/1452 (89%)	-0.18	4 (0%)	94	96	31, 51, 88, 132	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	110	LEU	2.4
3	F	142	VAL	2.1
3	F	66	VAL	2.0
3	F	143	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CAS	A	60	9/10	0.87	0.19	30,30,92,100	9
1	CAS	A	89	9/10	0.90	0.15	42,55,93,97	9
3	CAS	F	77	9/10	0.91	0.15	32,48,97,99	9
4	CAS	D	60	9/10	0.92	0.17	34,41,120,124	9
1	CAS	J	60	9/10	0.93	0.19	30,39,115,116	9
5	CAS	E	112	10/10	0.93	0.28	46,63,100,103	10
1	CAS	G	89	9/10	0.95	0.11	37,40,131,133	9
1	CAS	J	89	9/10	0.95	0.12	30,40,102,106	9
3	CAS	I	77	9/10	0.95	0.17	33,38,97,101	0
1	CAS	G	60	9/10	0.96	0.17	29,41,105,105	9
3	CAS	L	77	9/10	0.96	0.15	29,35,97,99	0
3	CAS	C	77	9/10	0.96	0.14	33,40,103,105	9

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	F7B	K	201	12/12	0.80	0.27	71,92,98,104	12
6	F7B	B	201	12/12	0.83	0.26	62,82,88,96	12
8	ACT	L	302	4/4	0.88	0.14	64,66,75,76	0
7	IPA	L	301	4/4	0.89	0.18	44,46,54,56	0
7	IPA	F	301	4/4	0.92	0.24	57,57,65,69	0
7	IPA	C	301	4/4	0.93	0.20	43,50,60,68	0
7	IPA	I	301	4/4	0.93	0.14	51,62,65,67	0
8	ACT	F	302	4/4	0.94	0.13	57,59,61,63	0

6.5 Other polymers (i)

There are no such residues in this entry.