



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:56 pm BST

PDB ID : 4AWJ  
Title : pVHL:EloB:EloC complex, in complex with capped Hydroxyproline  
Authors : Van Molle, I.; Thomann, A.; Buckley, D.L.; So, E.C.; Lang, S.; Crews, C.M.; Ciulli, A.  
Deposited on : 2012-06-04  
Resolution : 2.50 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](mailto: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

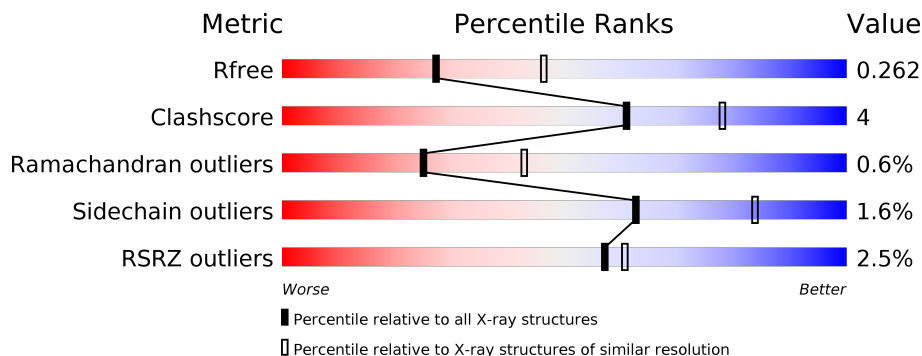
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	104	
1	D	104	
1	G	104	
1	J	104	
2	B	97	
2	E	97	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	H	97	<p>6% 78% 11% 10%</p>
2	K	97	<p>3% 80% 8% 11%</p>
3	C	163	<p>2% 72% 10% 17%</p>
3	F	163	<p>2% 82% 6% 13%</p>
3	I	163	<p>0% 75% 12% 12%</p>
3	L	163	<p>2% 69% 17% 12%</p>

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 10786 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	As	C	N	O				S
1	A	102	Total 799	As 2	C 508	N 135	O 149	S 5	0	0	0
1	D	99	Total 767	As 2	C 486	N 128	O 148	S 3	0	0	0
1	G	103	Total 819	As 2	C 518	N 136	O 158	S 5	0	0	0
1	J	103	Total 809	As 2	C 514	N 136	O 152	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	87	Total 686	C 444	N 109	O 127	S 6	0	0	0
2	E	87	Total 680	C 441	N 106	O 127	S 6	0	0	0
2	H	87	Total 674	C 435	N 107	O 126	S 6	0	0	0
2	K	86	Total 682	C 442	N 107	O 126	S 7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15369
E	16	MET	-	expression tag	UNP Q15369
H	16	MET	-	expression tag	UNP Q15369
K	16	MET	-	expression tag	UNP Q15369

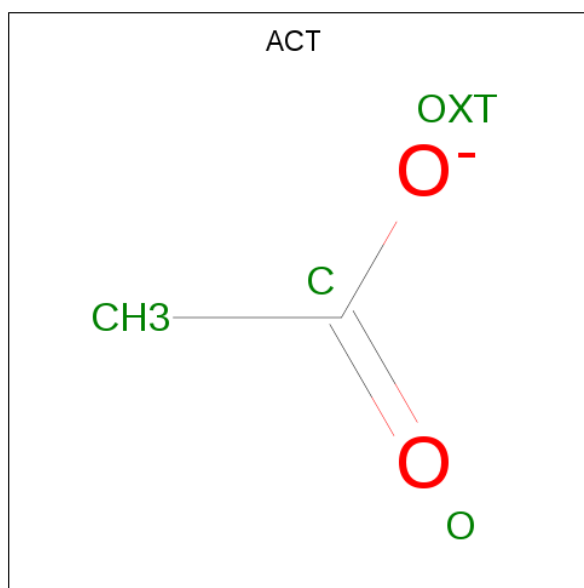
- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	As	C	N	O	S			
3	C	136	1062	1	679	185	195	2	0	0	0
3	F	142	1096	1	704	189	200	2	0	0	0
3	I	144	1147	1	730	204	210	2	0	0	0
3	L	144	1190	1	756	218	213	2	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

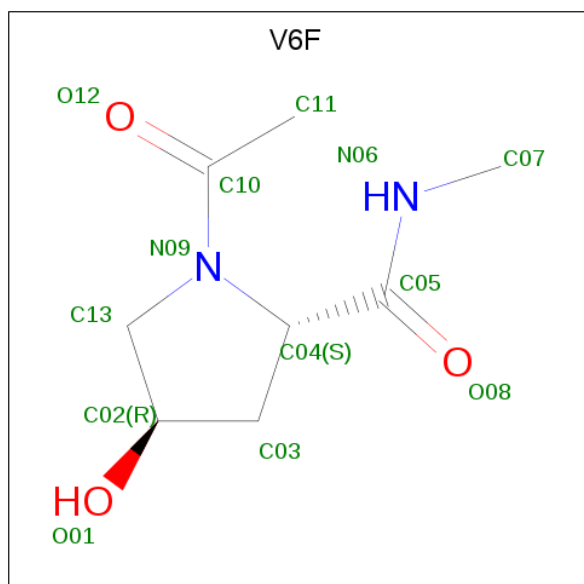
Chain	Residue	Modelled	Actual	Comment	Reference
C	51	GLY	-	expression tag	UNP P40337
C	52	SER	-	expression tag	UNP P40337
C	53	HIS	-	expression tag	UNP P40337
F	51	GLY	-	expression tag	UNP P40337
F	52	SER	-	expression tag	UNP P40337
F	53	HIS	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337
L	51	GLY	-	expression tag	UNP P40337
L	52	SER	-	expression tag	UNP P40337
L	53	HIS	-	expression tag	UNP P40337

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 5 is (4R)-1-acetyl-4-hydroxy-N-methyl-L-prolinamide (three-letter code: V6F) (formula: C<sub>8</sub>H<sub>14</sub>N<sub>2</sub>O<sub>3</sub>).



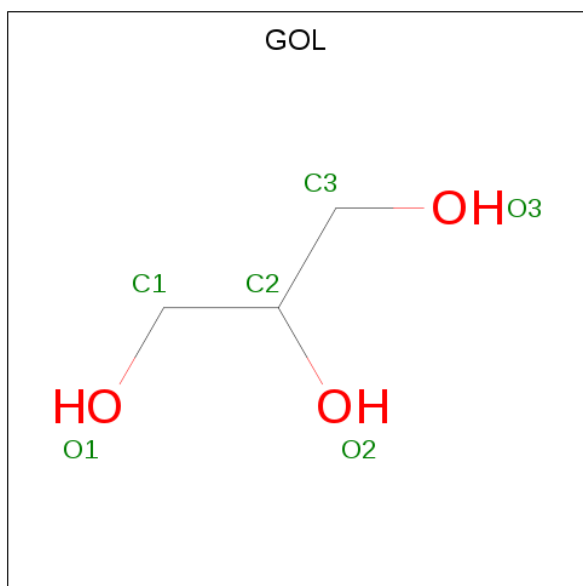
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 13 8 2 3	0	0
5	F	1	Total C N O 13 8 2 3	0	0
5	I	1	Total C N O 13 8 2 3	0	0
5	L	1	Total C N O 13 8 2 3	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

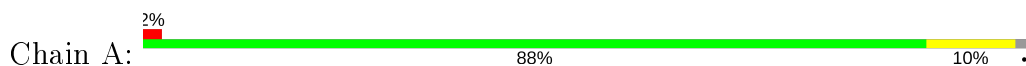
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	A	38	Total 38	O 38	0	0
8	B	10	Total 10	O 10	0	0
8	C	23	Total 23	O 23	0	0
8	D	21	Total 21	O 21	0	0
8	E	11	Total 11	O 11	0	0
8	F	11	Total 11	O 11	0	0
8	G	27	Total 27	O 27	0	0
8	H	26	Total 26	O 26	0	0
8	I	25	Total 25	O 25	0	0
8	J	42	Total 42	O 42	0	0
8	K	21	Total 21	O 21	0	0
8	L	34	Total 34	O 34	0	0



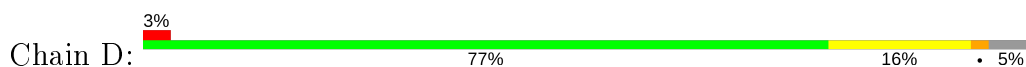
### 3 Residue-property plots [i](#)

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.

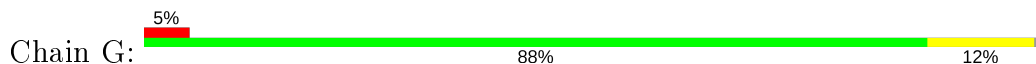
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



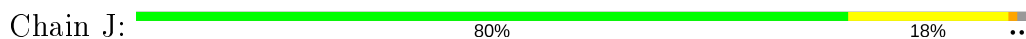
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



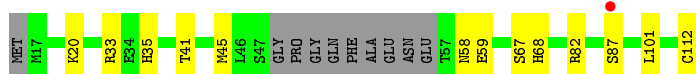
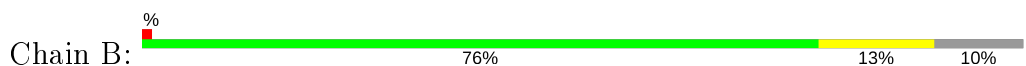
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



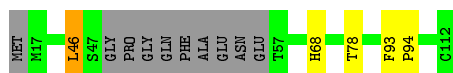
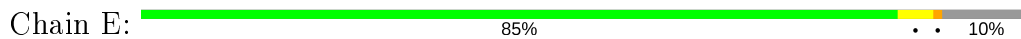
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



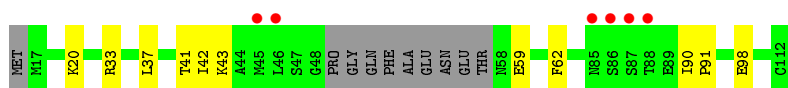
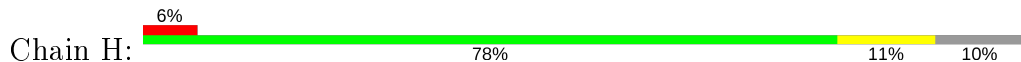
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



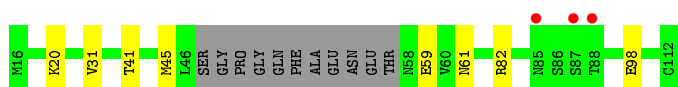
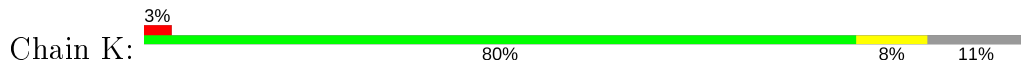
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



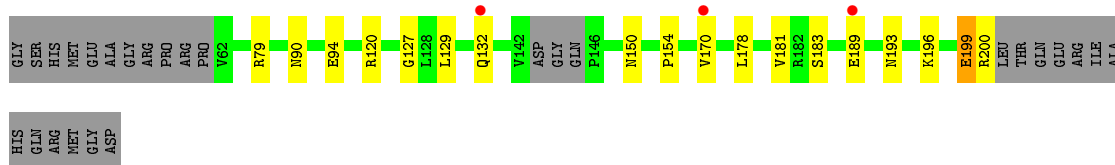
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



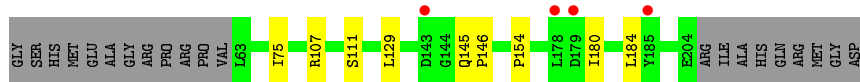
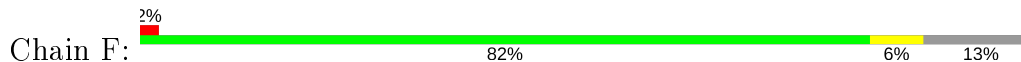
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



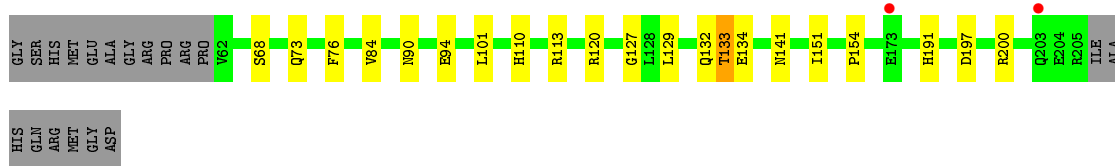
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

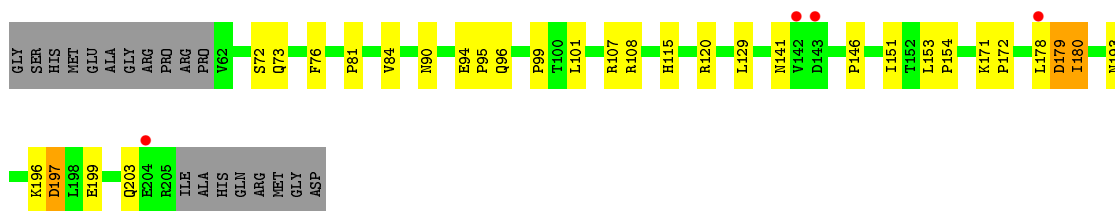


• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.40Å 93.40Å 362.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 2.50 29.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.54-2.50) 100.0 (29.54-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.37 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.220 , 0.264 0.214 , 0.262	Depositor DCC
$R_{free}$ test set	2837 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtrriage
Anisotropy	0.366	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.42 % 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 1.3109e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, GOL, ACY, V6F, 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	0.22	0/794	0.42	0/1069
1	D	0.22	0/761	0.45	1/1027 (0.1%)
1	G	0.22	0/815	0.40	0/1099
1	J	0.22	0/805	0.42	0/1086
2	B	0.21	0/700	0.38	0/945
2	E	0.31	0/694	0.41	0/938
2	H	0.21	0/687	0.40	0/927
2	K	0.22	0/696	0.38	0/939
3	C	0.22	0/1080	0.41	0/1479
3	F	0.20	0/1116	0.40	0/1532
3	I	0.21	0/1166	0.41	0/1595
3	L	0.21	0/1210	0.42	0/1650
All	All	0.22	0/10524	0.41	1/14286 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	PRO	N-CA-CB	5.87	110.34	103.30

There are no chirality outliers.

There are no planarity outliers.

### 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	799	0	787	7	0
1	D	767	0	732	8	0
1	G	819	0	807	6	0
1	J	809	0	799	13	0
2	B	686	0	682	7	0
2	E	680	0	665	3	0
2	H	674	0	669	7	0
2	K	682	0	678	6	0
3	C	1062	0	1004	12	0
3	F	1096	0	1031	5	0
3	I	1147	0	1115	12	0
3	L	1190	0	1172	17	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	F	4	0	3	0	0
4	I	4	0	3	0	0
4	L	4	0	3	0	0
5	C	13	0	14	0	0
5	F	13	0	14	1	0
5	I	13	0	14	0	0
5	L	13	0	14	1	0
6	F	4	0	3	0	0
7	J	6	0	8	2	0
8	A	38	0	0	0	0
8	B	10	0	0	0	0
8	C	23	0	0	0	0
8	D	21	0	0	0	0
8	E	11	0	0	0	0
8	F	11	0	0	0	0
8	G	27	0	0	0	0
8	H	26	0	0	0	0
8	I	25	0	0	0	0
8	J	42	0	0	1	0
8	K	21	0	0	0	0
8	L	34	0	0	0	0
All	All	10786	0	10226	93	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 4.

All (93) 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:I:73:GLN:H	3:I:141:ASN:HD21	1.26	0.82
1:J:72:PRO:HB3	7:J:1104:GOL:H12	1.67	0.76
3:L:90:ASN:HD22	3:L:96:GLN:HE21	1.40	0.68
3:L:72:SER:HA	3:L:141:ASN:HD21	1.62	0.65
3:I:84:VAL:HG11	3:I:151:ILE:HD13	1.82	0.62
1:G:37:ARG:NH1	1:G:41:GLU:OE1	2.35	0.60
2:H:37:LEU:HD22	2:H:43:LYS:HG3	1.84	0.59
2:B:33:ARG:NH2	2:B:58:ASN:OD1	2.37	0.58
1:D:25:PHE:HB2	1:D:53:ASP:HB3	1.86	0.57
3:C:181:VAL:HG12	3:C:183:SER:H	1.70	0.57
8:J:2002:HOH:O	2:K:82:ARG:NE	2.36	0.57
3:L:84:VAL:HG11	3:L:151:ILE:HD13	1.88	0.56
3:C:90:ASN:HD21	3:C:94:GLU:HB2	1.71	0.55
3:I:129:LEU:HG	3:I:154:PRO:HB3	1.88	0.55
3:I:197:ASP:OD1	3:I:200:ARG:NH1	2.39	0.55
3:C:170:VAL:HG21	3:C:178:LEU:HD11	1.87	0.55
3:C:79:ARG:HD2	3:C:150:ASN:HD21	1.71	0.55
3:C:199:GLU:OE1	3:C:200:ARG:N	2.38	0.55
1:J:15:PHE:HB2	2:K:31:VAL:HG12	1.91	0.53
1:A:94:SER:H	2:B:67:SER:HB2	1.73	0.53
1:J:99:LEU:HG	2:K:98:GLU:HG3	1.90	0.53
2:H:42:ILE:HD11	2:H:62:PHE:HZ	1.72	0.53
3:L:193:ASN:HB3	3:L:196:LYS:HB2	1.91	0.52
2:K:20:LYS:HB3	2:K:59:GLU:HG2	1.91	0.52
3:C:193:ASN:HD22	3:C:196:LYS:H	1.58	0.52
1:J:5:LEU:O	7:J:1104:GOL:O2	2.27	0.52
1:A:94:SER:OG	2:B:68:HIS:ND1	2.36	0.52
3:L:76:PHE:HB3	3:L:101:LEU:HD11	1.92	0.51
1:A:37:ARG:O	1:A:42:GLN:NE2	2.42	0.51
3:F:129:LEU:HG	3:F:154:PRO:HB3	1.92	0.50
1:D:3:VAL:HG22	1:D:67:ALA:HB3	1.92	0.50
1:D:40:ASP:N	1:D:40:ASP:OD1	2.44	0.50
3:F:75:ILE:HD13	2:H:41:THR:HG23	1.93	0.50
1:J:37:ARG:O	1:J:42:GLN:NE2	2.45	0.49
1:G:80:ARG:HA	1:G:85:PHE:HA	1.95	0.48
2:B:41:THR:O	2:B:45:MET:HG3	2.13	0.48
2:K:41:THR:HG22	2:K:45:MET:HE2	1.95	0.48
3:L:90:ASN:ND2	3:L:96:GLN:HE21	2.10	0.48
3:I:76:PHE:HB3	3:I:101:LEU:HD11	1.95	0.47
2:B:20:LYS:HB3	2:B:59:GLU:HG2	1.95	0.47
1:J:99:LEU:HD22	1:J:103:MET:HB2	1.95	0.47
1:D:94:SER:OG	2:E:68:HIS:ND1	2.33	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:LYS:HB3	2:H:59:GLU:HG2	1.97	0.47
2:H:90:ILE:HA	2:H:91:PRO:HD3	1.78	0.46
3:L:129:LEU:HG	3:L:154:PRO:HB3	1.98	0.46
3:C:120:ARG:HD3	3:C:127:GLY:HA2	1.98	0.46
3:L:81:PRO:HD2	3:L:153:LEU:HG	1.97	0.46
3:L:108[B]:ARG:HH22	3:L:146:PRO:HG3	1.81	0.45
3:I:73:GLN:H	3:I:141:ASN:ND2	2.04	0.45
1:A:69:PRO:HG2	2:B:82:ARG:HG2	1.98	0.45
3:L:179:ASP:HB3	3:L:180:ILE:H	1.52	0.45
3:C:79:ARG:HD2	3:C:150:ASN:ND2	2.32	0.45
3:L:73:GLN:H	3:L:141:ASN:HD21	1.64	0.45
3:L:115:HIS:ND1	5:L:1206:V6F:O01	2.42	0.44
3:I:73:GLN:HE22	3:I:110:HIS:CD2	2.35	0.44
1:D:91:GLU:HA	1:D:92:PRO:HD3	1.85	0.44
3:I:133:THR:HG22	3:I:134:GLU:H	1.82	0.44
3:I:90:ASN:HD21	3:I:94:GLU:HB2	1.82	0.44
3:I:73:GLN:N	3:I:141:ASN:HD21	2.05	0.44
1:J:52:ASP:HB3	1:J:55:LYS:HG2	2.01	0.43
3:F:111:SER:HA	5:F:1205:V6F:H032	2.00	0.43
2:H:33:ARG:O	2:H:37:LEU:HG	2.18	0.43
3:L:99:PRO:HB2	3:L:107:ARG:NH1	2.33	0.43
3:I:120:ARG:HD3	3:I:127:GLY:HA2	2.01	0.43
3:L:199:GLU:O	3:L:203:GLN:HG2	2.19	0.42
1:J:1:MET:HB3	1:J:64:SER:OG	2.20	0.42
1:A:99:LEU:HD12	1:A:100:PRO:HD2	2.02	0.42
3:F:145:GLN:HA	3:F:146:PRO:HD3	1.88	0.42
3:I:68:SER:HB2	3:I:113:ARG:HH12	1.85	0.42
1:D:51:LEU:HD22	1:D:60:CAS:SG	2.60	0.42
1:A:62:PHE:CZ	1:A:75:VAL:HG22	2.55	0.42
1:J:69:PRO:HG2	2:K:82:ARG:HG2	2.02	0.42
2:B:87:SER:HA	3:C:132:GLN:NE2	2.34	0.42
3:L:94:GLU:HA	3:L:95:PRO:HD3	1.89	0.41
1:G:1:MET:HB3	1:G:64:SER:OG	2.20	0.41
1:A:51:LEU:HD22	1:A:60:CAS:SG	2.60	0.41
3:L:171:LYS:HA	3:L:172:PRO:HD3	1.96	0.41
1:D:8:ARG:HG2	1:D:13:THR:HG23	2.03	0.41
1:D:80:ARG:HB2	1:D:85:PHE:CE1	2.56	0.41
1:G:99:LEU:HG	2:H:98:GLU:HG3	2.03	0.41
3:C:90:ASN:ND2	3:C:94:GLU:HB2	2.35	0.41
2:E:46:LEU:HD12	2:E:46:LEU:HA	1.78	0.41
1:J:91:GLU:HA	1:J:92:PRO:HD3	1.92	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:93:PHE:HA	2:E:94:PRO:HD3	1.81	0.40
1:G:91:GLU:HA	1:G:92:PRO:HD3	1.96	0.40
1:J:99:LEU:HD23	1:J:100:PRO:HD2	2.03	0.40
1:J:11:LYS:HG3	1:J:91:GLU:HG3	2.02	0.40
3:F:180:ILE:HB	3:F:184:LEU:HD12	2.03	0.40
1:J:46:LYS:HD2	1:J:60:CAS:O	2.21	0.40
3:C:189:GLU:HG2	3:C:189:GLU:H	1.72	0.40
3:C:129:LEU:HG	3:C:154:PRO:HB3	2.03	0.40
1:G:7:ILE:HB	1:G:14:ILE:HB	2.03	0.40
3:L:120[B]:ARG:HH22	3:L:197:ASP:CG	2.25	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	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
1	D	93/104 (89%)	87 (94%)	4 (4%)	2 (2%)	6	10
1	G	99/104 (95%)	95 (96%)	3 (3%)	1 (1%)	15	28
1	J	99/104 (95%)	94 (95%)	4 (4%)	1 (1%)	15	28
2	B	83/97 (86%)	81 (98%)	2 (2%)	0	100	100
2	E	83/97 (86%)	81 (98%)	2 (2%)	0	100	100
2	H	83/97 (86%)	80 (96%)	3 (4%)	0	100	100
2	K	82/97 (84%)	81 (99%)	1 (1%)	0	100	100
3	C	131/163 (80%)	124 (95%)	7 (5%)	0	100	100
3	F	139/163 (85%)	131 (94%)	8 (6%)	0	100	100
3	I	141/163 (86%)	133 (94%)	8 (6%)	0	100	100
3	L	143/163 (88%)	133 (93%)	7 (5%)	3 (2%)	7	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1272/1456 (87%)	1213 (95%)	52 (4%)	7 (1%)	25 43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	97	PRO
3	L	178	LEU
3	L	180	ILE
3	L	179	ASP
1	G	82	ASP
1	D	99	LEU
1	J	82	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	84/90 (93%)	84 (100%)	0	100 100
1	D	79/90 (88%)	75 (95%)	4 (5%)	24 45
1	G	89/90 (99%)	89 (100%)	0	100 100
1	J	86/90 (96%)	84 (98%)	2 (2%)	50 76
2	B	76/86 (88%)	73 (96%)	3 (4%)	32 57
2	E	74/86 (86%)	72 (97%)	2 (3%)	44 71
2	H	74/86 (86%)	74 (100%)	0	100 100
2	K	76/86 (88%)	75 (99%)	1 (1%)	69 87
3	C	114/148 (77%)	113 (99%)	1 (1%)	78 92
3	F	115/148 (78%)	114 (99%)	1 (1%)	78 92
3	I	127/148 (86%)	124 (98%)	3 (2%)	49 74
3	L	132/148 (89%)	131 (99%)	1 (1%)	81 93
All	All	1126/1296 (87%)	1108 (98%)	18 (2%)	62 84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	35	HIS
2	B	101	LEU
2	B	112	CYS
3	C	199	GLU
1	D	40	ASP
1	D	65	GLN
1	D	91	GLU
1	D	101	ASP
2	E	46	LEU
2	E	78	THR
3	F	107	ARG
3	I	132	GLN
3	I	133	THR
3	I	191	HIS
1	J	52	ASP
1	J	80	ARG
2	K	61	ASN
3	L	197	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
3	C	132	GLN
3	C	193	ASN
1	D	42	GLN
1	G	42	GLN
1	G	49	GLN
3	I	96	GLN
3	I	110	HIS
3	I	141	ASN
1	J	49	GLN
3	L	96	GLN
3	L	141	ASN
3	L	145	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	A	60	1	5,8,9	1.15	0	1,9,11	0.62	0
1	CAS	G	89	1	5,8,9	1.24	0	1,9,11	0.37	0
1	CAS	A	89	1	5,8,9	1.18	0	1,9,11	0.74	0
3	CAS	I	77	3	5,8,9	1.17	0	1,9,11	0.93	0
3	CAS	F	77	3	5,8,9	1.21	0	1,9,11	0.64	0
1	CAS	G	60	1	5,8,9	1.20	0	1,9,11	0.64	0
1	CAS	D	60	1	5,8,9	1.16	0	1,9,11	0.58	0
3	CAS	C	77	3	5,8,9	1.20	0	1,9,11	0.77	0
1	CAS	J	89	1	5,8,9	1.22	0	1,9,11	0.69	0
1	CAS	D	89	1	5,8,9	1.18	0	1,9,11	1.05	0
3	CAS	L	77	3	5,8,9	1.19	0	1,9,11	0.63	0
1	CAS	J	60	1	5,8,9	1.14	0	1,9,11	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	A	60	1	-	0/0/7/9	-
1	CAS	G	89	1	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
3	CAS	I	77	3	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
1	CAS	G	60	1	-	0/0/7/9	-
1	CAS	D	60	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
1	CAS	J	60	1	-	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.

3 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	V6F	C	1201	-	13,13,13	2.09	2 (15%)	18,18,18	1.30	1 (5%)
5	V6F	I	1206	-	13,13,13	2.05	2 (15%)	18,18,18	1.26	1 (5%)
6	ACY	F	1206	-	1,3,3	1.38	0	0,3,3	0.00	-
4	ACT	F	1207	-	1,3,3	1.42	0	0,3,3	0.00	-
7	GOL	J	1104	-	5,5,5	0.42	0	5,5,5	0.17	0
4	ACT	B	1113	-	1,3,3	1.08	0	0,3,3	0.00	-
4	ACT	A	1104	-	1,3,3	1.32	0	0,3,3	0.00	-
5	V6F	L	1206	-	13,13,13	2.05	2 (15%)	18,18,18	1.29	1 (5%)
4	ACT	C	1202	-	1,3,3	1.39	0	0,3,3	0.00	-
4	ACT	L	1207	-	1,3,3	1.35	0	0,3,3	0.00	-
5	V6F	F	1205	-	13,13,13	2.08	2 (15%)	18,18,18	1.32	1 (5%)
4	ACT	I	1207	-	1,3,3	1.37	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	V6F	C	1201	-	-	0/10/22/22	0/1/1/1
5	V6F	I	1206	-	-	0/10/22/22	0/1/1/1
7	GOL	J	1104	-	-	4/4/4/4	-
5	V6F	F	1205	-	-	0/10/22/22	0/1/1/1
5	V6F	L	1206	-	-	0/10/22/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1206	V6F	C05-N06	5.91	1.41	1.33
5	F	1205	V6F	C05-N06	5.85	1.41	1.33
5	C	1201	V6F	C05-N06	5.85	1.41	1.33
5	L	1206	V6F	C05-N06	5.77	1.41	1.33
5	C	1201	V6F	C10-N09	4.36	1.41	1.35
5	F	1205	V6F	C10-N09	4.18	1.41	1.35
5	L	1206	V6F	C10-N09	4.11	1.41	1.35
5	I	1206	V6F	C10-N09	4.02	1.41	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1206	V6F	C07-N06-C05	-2.85	117.29	122.22
5	I	1206	V6F	C07-N06-C05	-2.82	117.33	122.22
5	C	1201	V6F	C07-N06-C05	-2.82	117.34	122.22
5	F	1205	V6F	C07-N06-C05	-2.66	117.61	122.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	1104	GOL	O1-C1-C2-O2
7	J	1104	GOL	O1-C1-C2-C3
7	J	1104	GOL	C1-C2-C3-O3
7	J	1104	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	1104	GOL	2	0
5	L	1206	V6F	1	0
5	F	1205	V6F	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	100/104 (96%)	-0.29	2 (2%) 65 68	15, 29, 64, 71	0
1	D	97/104 (93%)	-0.02	3 (3%) 49 52	20, 45, 76, 87	0
1	G	101/104 (97%)	-0.08	5 (4%) 28 30	19, 38, 63, 86	0
1	J	101/104 (97%)	-0.34	0 100 100	12, 24, 50, 62	0
2	B	87/97 (89%)	-0.16	1 (1%) 80 82	18, 33, 61, 85	0
2	E	87/97 (89%)	0.03	0 100 100	19, 40, 69, 82	0
2	H	87/97 (89%)	0.07	6 (6%) 16 17	21, 38, 90, 103	0
2	K	86/97 (88%)	-0.21	3 (3%) 44 47	15, 30, 70, 85	0
3	C	135/163 (82%)	-0.11	3 (2%) 62 65	23, 43, 71, 80	0
3	F	141/163 (86%)	-0.02	4 (2%) 53 56	21, 42, 73, 98	0
3	I	143/163 (87%)	-0.23	2 (1%) 75 77	18, 36, 63, 93	0
3	L	143/163 (87%)	-0.15	4 (2%) 53 56	13, 29, 71, 84	0
All	All	1308/1456 (89%)	-0.13	33 (2%) 57 61	12, 36, 70, 103	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	87	SER	5.4
2	K	88	THR	3.9
2	H	46	LEU	3.6
2	K	87	SER	3.3
3	F	143	ASP	3.2
1	G	82	ASP	3.1
1	G	81	ALA	3.0
2	H	88	THR	3.0
3	L	143	ASP	2.8
1	G	83	ASP	2.7
2	H	85	ASN	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	185	TYR	2.7
1	G	1	MET	2.6
3	F	178	LEU	2.6
3	L	178	LEU	2.6
1	D	38	PRO	2.5
3	I	203	GLN	2.5
3	I	173	GLU	2.5
1	D	84	THR	2.4
2	K	85	ASN	2.4
1	A	84	THR	2.4
3	L	204	GLU	2.4
2	H	45	MET	2.3
1	G	101	ASP	2.3
3	C	189	GLU	2.3
1	D	80	ARG	2.2
1	A	81	ALA	2.2
2	B	87	SER	2.2
2	H	86	SER	2.2
3	F	179	ASP	2.1
3	L	142	VAL	2.1
3	C	132	GLN	2.1
3	C	170	VAL	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CAS	D	89	9/10	0.85	0.14	33,52,89,149	0
1	CAS	G	89	9/10	0.93	0.15	17,30,96,159	0
1	CAS	A	60	9/10	0.94	0.13	15,22,41,86	0
1	CAS	A	89	9/10	0.95	0.16	30,31,125,125	0
1	CAS	J	89	9/10	0.96	0.11	15,20,68,80	0
1	CAS	J	60	9/10	0.96	0.12	20,26,82,83	0
3	CAS	C	77	9/10	0.97	0.10	25,28,73,103	0
3	CAS	F	77	9/10	0.97	0.10	26,35,73,83	0
1	CAS	G	60	9/10	0.97	0.11	27,33,62,80	0
1	CAS	D	60	9/10	0.97	0.10	22,25,56,74	0
3	CAS	L	77	9/10	0.98	0.09	12,20,54,76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CAS	I	77	9/10	0.98	0.10	16,17,66,76	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	GOL	J	1104	6/6	0.80	0.36	50,53,54,54	0
4	ACT	F	1207	4/4	0.83	0.27	53,56,58,61	0
4	ACT	C	1202	4/4	0.89	0.18	46,50,52,53	0
6	ACY	F	1206	4/4	0.90	0.18	60,61,62,62	0
4	ACT	L	1207	4/4	0.90	0.19	53,54,57,58	0
5	V6F	C	1201	13/13	0.92	0.20	35,41,46,48	0
4	ACT	I	1207	4/4	0.93	0.20	63,66,66,67	0
5	V6F	F	1205	13/13	0.94	0.16	36,41,48,51	0
5	V6F	I	1206	13/13	0.95	0.16	19,29,39,40	0
4	ACT	A	1104	4/4	0.95	0.14	52,53,54,56	0
4	ACT	B	1113	4/4	0.96	0.15	49,50,50,51	0
5	V6F	L	1206	13/13	0.96	0.13	15,27,32,34	0

### 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.