Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:56 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/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:

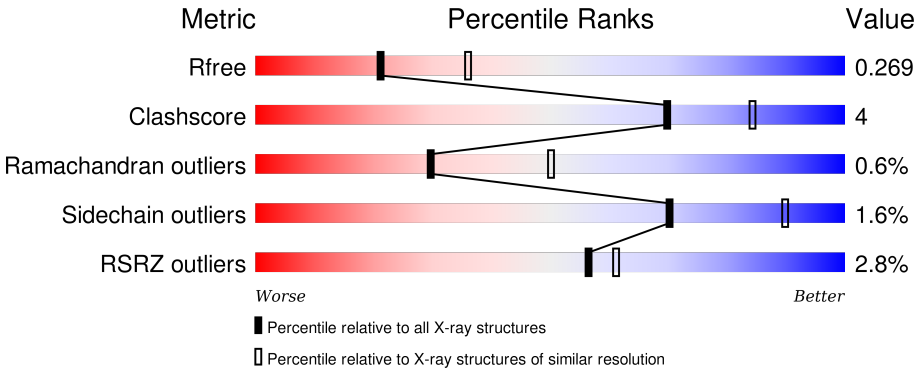
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 88% 10% •
1	D	104	4% 77% 16% • 5%
1	G	104	6% 88% 12% •
1	J	104	% 80% 18% ••
2	B	97	2% 76% 13% 10%

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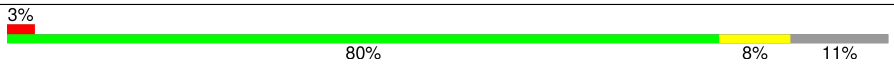
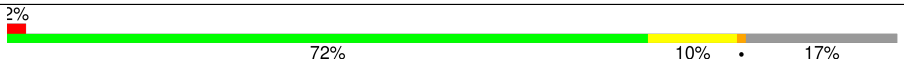
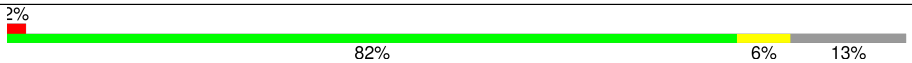
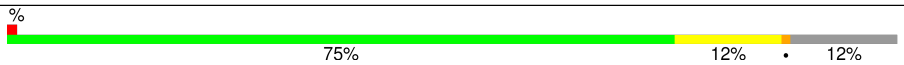
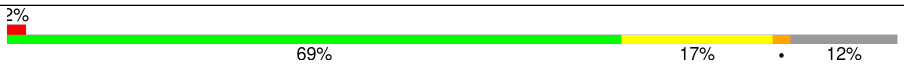
Mol	Chain	Length	Quality of chain
2	E	97	
2	H	97	
2	K	97	
3	C	163	
3	F	163	
3	I	163	
3	L	163	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	F	1207	-	-	-	X
4	ACT	I	1207	-	-	-	X
5	V6F	C	1201	-	-	-	X
7	GOL	J	1104	-	-	-	X

2 Entry composition

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

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

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

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

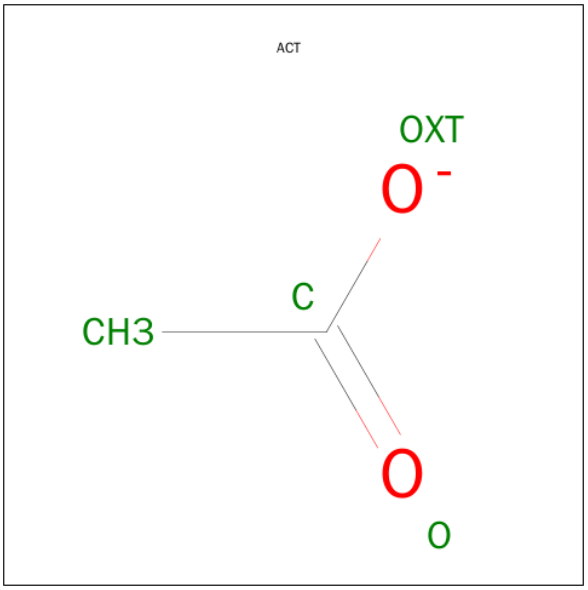
- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR.

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

There are 12 discrepancies between the modelled and reference sequences:

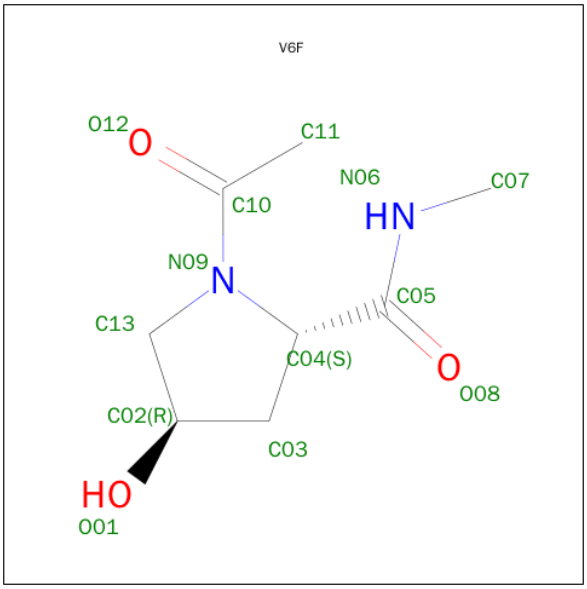
Chain	Residue	Modelled	Actual	Comment	Reference
C	51	GLY	-	EXPRESSION TAG	UNP P40337
C	52	SER	-	EXPRESSION TAG	UNP P40337
C	53	HIS	-	EXPRESSION TAG	UNP P40337
F	51	GLY	-	EXPRESSION TAG	UNP P40337
F	52	SER	-	EXPRESSION TAG	UNP P40337
F	53	HIS	-	EXPRESSION TAG	UNP P40337
I	51	GLY	-	EXPRESSION TAG	UNP P40337
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: $C_2H_3O_2$).



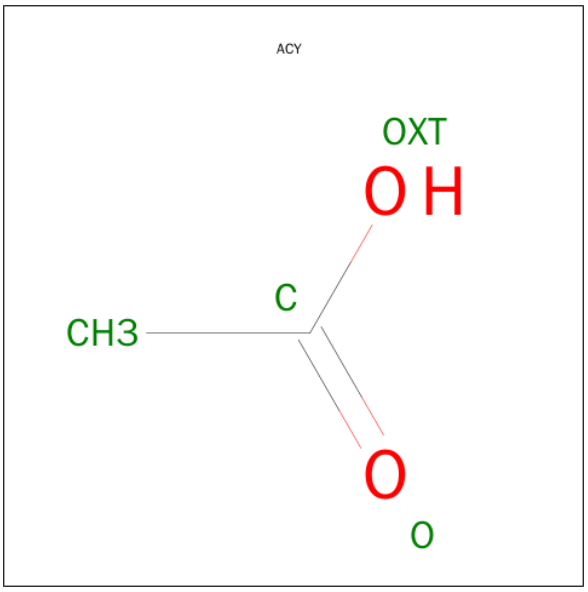
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0

- Molecule 5 is (4R)-1-ACETYL-4-HYDROXY-N-METHYL-L-PROLINAMIDE (three-letter code: V6F) (formula: $C_8H_{14}N_2O_3$).



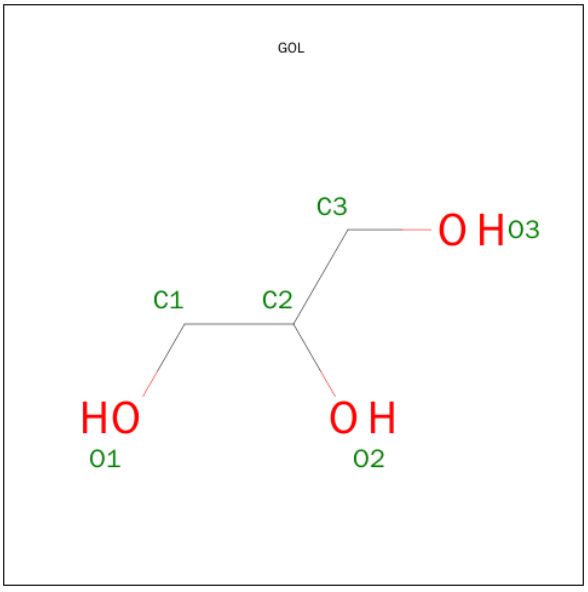
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 13 8 2 3	0	0
5	F	1	Total C N O 13 8 2 3	0	0
5	I	1	Total C N O 13 8 2 3	0	0
5	L	1	Total C N O 13 8 2 3	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- 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 6 3 3	0	0

- Molecule 8 is water.

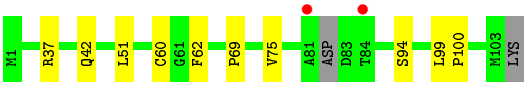
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	38	Total O 38 38	0	0
8	B	10	Total O 10 10	0	0
8	C	23	Total O 23 23	0	0
8	D	21	Total O 21 21	0	0
8	E	11	Total O 11 11	0	0
8	F	11	Total O 11 11	0	0
8	G	27	Total O 27 27	0	0
8	H	26	Total O 26 26	0	0
8	I	25	Total O 25 25	0	0
8	J	42	Total O 42 42	0	0
8	K	21	Total O 21 21	0	0
8	L	34	Total O 34 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

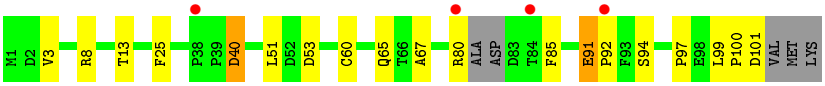
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain A:



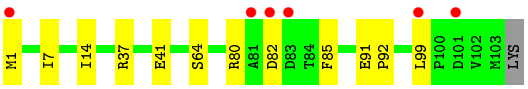
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain D:



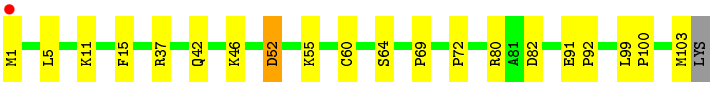
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain G:



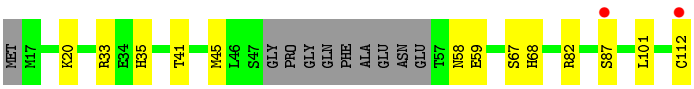
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

Chain J:



• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain B:

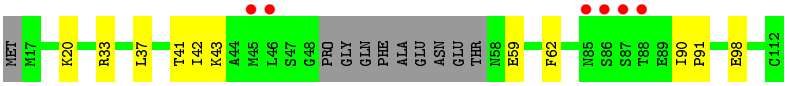


• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain E:

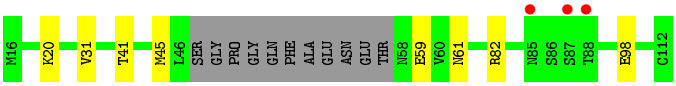
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain H:



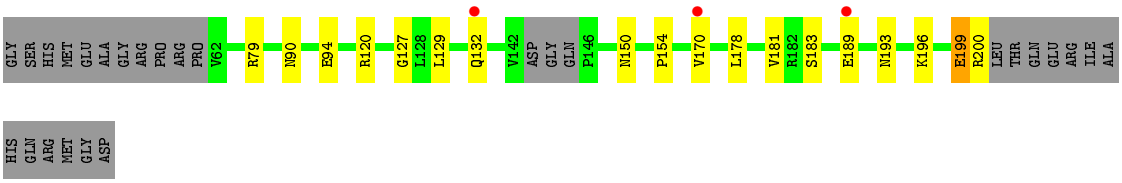
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain K:



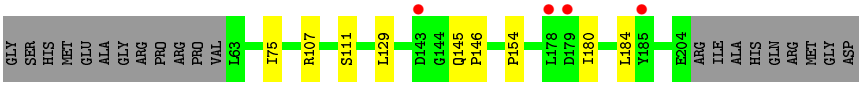
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain C:



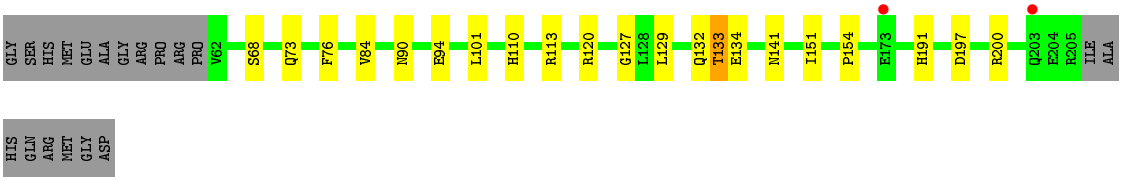
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain F:



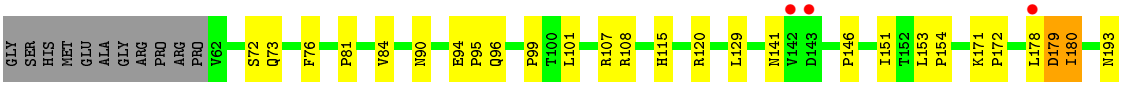
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

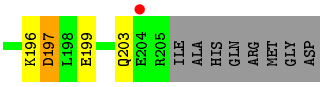
Chain I:



• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain L:




K196
D197
L198
E199
Q203
E204
R205
ILE
ALA
HIS
GLN
ARG
MET
GLY
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.40Å 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
$< I/\sigma(I) >$ [1]	4.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.220 , 0.264 0.219 , 0.269	Depositor DCC
R_{free} test set	2009 reflections (3.67%)	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	10 of 113400 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10786	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.42 % 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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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(^{o})	Ideal(^{o})
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

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
8:J:2002:HOH:O	2:K:82:ARG:NE	2.36	0.57
3:C:181:VAL:HG12	3:C:183:SER:H	1.70	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:197:ASP:OD1	3:I:200:ARG:NH1	2.39	0.55
3:I:129:LEU:HG	3:I:154:PRO:HB3	1.88	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
1:J:5:LEU:O	7:J:1104:GOL:O2	2.27	0.52
3:C:193:ASN:HD22	3:C:196:LYS:H	1.58	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

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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:L:73:GLN:H	3:L:141:ASN:HD21	1.64	0.45
3:C:79:ARG:HD2	3:C:150:ASN:ND2	2.32	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
3:I:68:SER:HB2	3:I:113:ARG:HH12	1.85	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
1:D:51:LEU:HD22	1:D:60:CAS:SG	2.60	0.42
1:J:69:PRO:HG2	2:K:82:ARG:HG2	2.02	0.42
1:A:62:PHE:CZ	1:A:75:VAL:HG22	2.55	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:G:99:LEU:HG	2:H:98:GLU:HG3	2.03	0.41
1:D:80:ARG:HB2	1:D:85:PHE:CE1	2.56	0.41
1:D:8:ARG:HG2	1:D:13:THR:HG23	2.03	0.41
3:C:90:ASN:ND2	3:C:94:GLU:HB2	2.35	0.41
1:J:91:GLU:HA	1:J:92:PRO:HD3	1.92	0.41
2:E:46:LEU:HD12	2:E:46:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:91:GLU:HA	1:G:92:PRO:HD3	1.96	0.40
2:E:93:PHE:HA	2:E:94:PRO:HD3	1.81	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
1:G:7:ILE:HB	1:G:14:ILE:HB	2.03	0.40
3:C:129:LEU:HG	3:C:154:PRO:HB3	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%)	8 13
1	G	99/104 (95%)	95 (96%)	3 (3%)	1 (1%)	19 34
1	J	99/104 (95%)	94 (95%)	4 (4%)	1 (1%)	19 34
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%)	9 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1272/1456 (87%)	1213 (95%)	52 (4%)	7 (1%)	30 50

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

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%)	29 52
1	G	89/90 (99%)	89 (100%)	0	100 100
1	J	86/90 (96%)	84 (98%)	2 (2%)	58 83
2	B	76/86 (88%)	73 (96%)	3 (4%)	39 66
2	E	74/86 (86%)	72 (97%)	2 (3%)	52 79
2	H	74/86 (86%)	74 (100%)	0	100 100
2	K	76/86 (88%)	75 (99%)	1 (1%)	76 92
3	C	114/148 (77%)	113 (99%)	1 (1%)	84 95
3	F	115/148 (78%)	114 (99%)	1 (1%)	84 95
3	I	127/148 (86%)	124 (98%)	3 (2%)	57 82
3	L	132/148 (89%)	131 (99%)	1 (1%)	86 96
All	All	1126/1296 (87%)	1108 (98%)	18 (2%)	70 90

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

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	1.02	0	2,9,11	1.59	1 (50%)
1	CAS	A	89	1	5,8,9	1.05	0	2,9,11	1.47	0
3	CAS	C	77	3	5,8,9	1.07	0	2,9,11	1.49	0
1	CAS	D	60	1	5,8,9	1.04	0	2,9,11	1.63	1 (50%)
1	CAS	D	89	1	5,8,9	1.05	0	2,9,11	1.56	0
3	CAS	F	77	3	5,8,9	1.08	0	2,9,11	1.46	0
1	CAS	G	60	1	5,8,9	1.07	0	2,9,11	1.59	1 (50%)
1	CAS	G	89	1	5,8,9	1.11	0	2,9,11	1.27	0
3	CAS	I	77	3	5,8,9	1.05	0	2,9,11	1.56	0
1	CAS	J	60	1	5,8,9	1.02	0	2,9,11	1.64	1 (50%)
1	CAS	J	89	1	5,8,9	1.09	0	2,9,11	1.47	0
3	CAS	L	77	3	5,8,9	1.07	0	2,9,11	1.44	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	0/0/0/0
1	CAS	A	89	1	-	0/0/7/9	0/0/0/0
3	CAS	C	77	3	-	0/0/7/9	0/0/0/0
1	CAS	D	60	1	-	0/0/7/9	0/0/0/0
1	CAS	D	89	1	-	0/0/7/9	0/0/0/0
3	CAS	F	77	3	-	0/0/7/9	0/0/0/0
1	CAS	G	60	1	-	0/0/7/9	0/0/0/0
1	CAS	G	89	1	-	0/0/7/9	0/0/0/0
3	CAS	I	77	3	-	0/0/7/9	0/0/0/0
1	CAS	J	60	1	-	0/0/7/9	0/0/0/0
1	CAS	J	89	1	-	0/0/7/9	0/0/0/0
3	CAS	L	77	3	-	0/0/7/9	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	60	CAS	O-C-CA	-2.18	119.81	125.49
1	A	60	CAS	O-C-CA	-2.10	120.03	125.49
1	J	60	CAS	O-C-CA	-2.09	120.04	125.49
1	G	60	CAS	O-C-CA	-2.08	120.07	125.49

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	$\#\|Z\| > 2$
4	ACT	A	1104	-	1,3,3	1.16	0	0,3,3	0.00	-
4	ACT	B	1113	-	1,3,3	0.93	0	0,3,3	0.00	-
5	V6F	C	1201	-	13,13,13	2.09	2 (15%)	18,18,18	1.26	1 (5%)
4	ACT	C	1202	-	1,3,3	1.22	0	0,3,3	0.00	-
5	V6F	F	1205	-	13,13,13	2.08	2 (15%)	18,18,18	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ACY	F	1206	-	1,3,3	1.21	0	0,3,3	0.00	-
4	ACT	F	1207	-	1,3,3	1.25	0	0,3,3	0.00	-
5	V6F	I	1206	-	13,13,13	2.06	2 (15%)	18,18,18	1.22	1 (5%)
4	ACT	I	1207	-	1,3,3	1.19	0	0,3,3	0.00	-
7	GOL	J	1104	-	5,5,5	0.39	0	5,5,5	0.22	0
5	V6F	L	1206	-	13,13,13	2.05	2 (15%)	18,18,18	1.26	1 (5%)
4	ACT	L	1207	-	1,3,3	1.18	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
4	ACT	A	1104	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1113	-	-	0/0/0/0	0/0/0/0
5	V6F	C	1201	-	-	0/10/22/22	0/1/1/1
4	ACT	C	1202	-	-	0/0/0/0	0/0/0/0
5	V6F	F	1205	-	-	0/10/22/22	0/1/1/1
6	ACY	F	1206	-	-	0/0/0/0	0/0/0/0
4	ACT	F	1207	-	-	0/0/0/0	0/0/0/0
5	V6F	I	1206	-	-	0/10/22/22	0/1/1/1
4	ACT	I	1207	-	-	0/0/0/0	0/0/0/0
7	GOL	J	1104	-	-	0/4/4/4	0/0/0/0
5	V6F	L	1206	-	-	0/10/22/22	0/1/1/1
4	ACT	L	1207	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1206	V6F	C10-N09	3.89	1.41	1.35
5	L	1206	V6F	C10-N09	3.98	1.41	1.35
5	F	1205	V6F	C10-N09	4.05	1.41	1.35
5	C	1201	V6F	C10-N09	4.22	1.41	1.35
5	L	1206	V6F	C05-N06	5.89	1.41	1.33
5	C	1201	V6F	C05-N06	5.97	1.41	1.33
5	F	1205	V6F	C05-N06	5.97	1.41	1.33
5	I	1206	V6F	C05-N06	6.03	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1206	V6F	C07-N06-C05	-2.73	117.29	122.23
5	I	1206	V6F	C07-N06-C05	-2.70	117.33	122.23
5	C	1201	V6F	C07-N06-C05	-2.70	117.34	122.23
5	F	1205	V6F	C07-N06-C05	-2.55	117.61	122.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1205	V6F	1	0
7	J	1104	GOL	2	0
5	L	1206	V6F	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%)	-0.22	2 (2%) 68 72	15, 29, 64, 71	0
1	D	97/104 (93%)	0.05	4 (4%) 41 46	20, 45, 76, 87	0
1	G	101/104 (97%)	-0.02	6 (5%) 26 29	19, 38, 63, 86	0
1	J	101/104 (97%)	-0.29	1 (0%) 84 86	12, 24, 50, 62	0
2	B	87/97 (89%)	-0.10	2 (2%) 64 67	18, 33, 61, 85	0
2	E	87/97 (89%)	0.07	0 100 100	19, 40, 69, 82	0
2	H	87/97 (89%)	0.09	6 (6%) 20 22	21, 38, 90, 103	0
2	K	86/97 (88%)	-0.15	3 (3%) 48 53	15, 30, 70, 85	0
3	C	135/163 (82%)	-0.06	3 (2%) 65 69	23, 43, 71, 80	0
3	F	141/163 (86%)	0.02	4 (2%) 56 61	21, 42, 73, 98	0
3	I	143/163 (87%)	-0.18	2 (1%) 78 80	18, 36, 63, 93	0
3	L	143/163 (87%)	-0.11	4 (2%) 56 61	13, 29, 71, 84	0
All	All	1308/1456 (89%)	-0.08	37 (2%) 56 61	12, 36, 70, 103	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	87	SER	5.3
2	K	88	THR	3.8
2	K	87	SER	3.6
2	H	46	LEU	3.4
3	F	143	ASP	3.2
3	L	143	ASP	3.1
1	G	82	ASP	3.1
2	H	88	THR	3.1
1	G	1	MET	3.0
1	G	81	ALA	2.9
3	L	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	87	SER	2.8
1	G	83	ASP	2.8
1	D	84	THR	2.7
3	I	203	GLN	2.7
3	F	178	LEU	2.7
2	H	85	ASN	2.6
1	A	81	ALA	2.6
1	G	101	ASP	2.5
3	C	189	GLU	2.5
1	D	38	PRO	2.5
3	F	185	TYR	2.5
3	I	173	GLU	2.5
3	F	179	ASP	2.5
1	D	80	ARG	2.4
3	L	204	GLU	2.4
3	C	170	VAL	2.4
2	K	85	ASN	2.4
2	H	86	SER	2.4
2	B	112	CYS	2.3
2	H	45	MET	2.3
1	A	84	THR	2.3
1	J	1	MET	2.1
3	C	132	GLN	2.1
3	L	142	VAL	2.1
1	G	99	LEU	2.1
1	D	92	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
1	CAS	A	60	9/10	0.94	0.13	-	15,22,41,86	0
1	CAS	G	89	9/10	0.93	0.15	-	17,30,96,159	0
1	CAS	A	89	9/10	0.95	0.15	-	30,31,125,125	0
3	CAS	I	77	9/10	0.98	0.10	-	16,17,66,76	0
3	CAS	F	77	9/10	0.97	0.10	-	26,35,73,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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	C	77	9/10	0.97	0.11	-	25,28,73,103	0
1	CAS	J	89	9/10	0.96	0.11	-	15,20,68,80	0
1	CAS	D	89	9/10	0.86	0.15	-	33,52,89,149	0
3	CAS	L	77	9/10	0.98	0.09	-	12,20,54,76	0
1	CAS	J	60	9/10	0.96	0.12	-	20,26,82,83	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	ACT	F	1207	4/4	0.86	0.24	7.04	53,56,58,61	0
7	GOL	J	1104	6/6	0.81	0.33	5.98	50,53,54,54	0
4	ACT	I	1207	4/4	0.94	0.20	3.16	63,66,66,67	0
5	V6F	C	1201	13/13	0.92	0.21	2.66	35,41,46,48	0
4	ACT	C	1202	4/4	0.89	0.18	1.94	46,50,52,53	0
4	ACT	L	1207	4/4	0.91	0.20	1.85	53,54,57,58	0
5	V6F	I	1206	13/13	0.95	0.16	1.36	19,29,39,40	0
4	ACT	A	1104	4/4	0.95	0.14	0.81	52,53,54,56	0
5	V6F	F	1205	13/13	0.94	0.16	0.44	36,41,48,51	0
4	ACT	B	1113	4/4	0.96	0.15	0.04	49,50,50,51	0
6	ACY	F	1206	4/4	0.90	0.17	-0.02	60,61,62,62	0
5	V6F	L	1206	13/13	0.96	0.13	-0.32	15,27,32,34	0

6.5 Other polymers (i)

There are no such residues in this entry.