Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:42 PM GMT

PDB ID	:	4A63
Title	:	Crystal structure of the p73-ASPP2 complex at 2.6A resolution
Authors	:	Canning, P.; Sharpe, T.; Krojer, T.; Savitsky, P.; Cooper, C.D.O.; Salah, E.; Keates, T.; Muniz, J.; Vollmar, M.; Von Delft, F.; Weigelt, J.; Arrowsmith, C.; Bountra, C.; Edwards, A.; Bullock, A.N.
Deposited on	:	2011-10-31
Resolution	:	2.27 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:

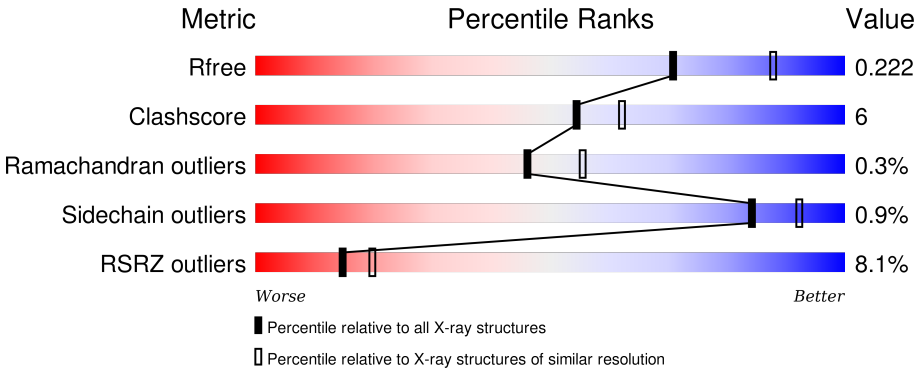
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.27 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	208	3% 91% 7%
1	C	208	10% 87% 11%
1	E	208	10% 85% 13%
1	G	208	6% 85% 13%
1	I	208	4% 90% 8%

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Mol	Chain	Length	Quality of chain
1	K	208	9% 87% 12%
2	B	239	5% 82% 15%
2	D	239	13% 78% 18%
2	F	239	8% 78% 5% 18%
2	H	239	8% 79% 17%
2	J	239	3% 78% 5% 16%
2	L	239	7% 75% 7% 18%

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	C	1320	-	-	-	X
4	ACT	C	1321	-	-	-	X
4	ACT	G	1319	-	-	-	X
4	ACT	I	1320	-	-	-	X
4	ACT	K	1319	-	-	-	X
4	ACT	L	1522	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19119 atoms, of which 27 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 TUMOUR PROTEIN 73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1592	1002	280	299	11			
1	C	205	Total	C	N	O	S	0	0	0
			1586	1000	278	297	11			
1	E	205	Total	C	N	O	S	0	0	0
			1558	983	272	292	11			
1	G	205	Total	C	N	O	S	0	2	0
			1608	1011	285	299	13			
1	I	205	Total	C	N	O	S	0	0	0
			1593	1001	282	299	11			
1	K	205	Total	C	N	O	S	0	0	0
			1588	1000	281	296	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	MET	-	EXPRESSION TAG	UNP O15350
A	312	ALA	-	EXPRESSION TAG	UNP O15350
A	313	GLU	-	EXPRESSION TAG	UNP O15350
A	314	ASN	-	EXPRESSION TAG	UNP O15350
A	315	LEU	-	EXPRESSION TAG	UNP O15350
A	316	TYR	-	EXPRESSION TAG	UNP O15350
A	317	PHE	-	EXPRESSION TAG	UNP O15350
A	318	GLN	-	EXPRESSION TAG	UNP O15350
C	111	MET	-	EXPRESSION TAG	UNP O15350
C	312	ALA	-	EXPRESSION TAG	UNP O15350
C	313	GLU	-	EXPRESSION TAG	UNP O15350
C	314	ASN	-	EXPRESSION TAG	UNP O15350
C	315	LEU	-	EXPRESSION TAG	UNP O15350
C	316	TYR	-	EXPRESSION TAG	UNP O15350
C	317	PHE	-	EXPRESSION TAG	UNP O15350
C	318	GLN	-	EXPRESSION TAG	UNP O15350
E	111	MET	-	EXPRESSION TAG	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
E	312	ALA	-	EXPRESSION TAG	UNP O15350
E	313	GLU	-	EXPRESSION TAG	UNP O15350
E	314	ASN	-	EXPRESSION TAG	UNP O15350
E	315	LEU	-	EXPRESSION TAG	UNP O15350
E	316	TYR	-	EXPRESSION TAG	UNP O15350
E	317	PHE	-	EXPRESSION TAG	UNP O15350
E	318	GLN	-	EXPRESSION TAG	UNP O15350
G	111	MET	-	EXPRESSION TAG	UNP O15350
G	312	ALA	-	EXPRESSION TAG	UNP O15350
G	313	GLU	-	EXPRESSION TAG	UNP O15350
G	314	ASN	-	EXPRESSION TAG	UNP O15350
G	315	LEU	-	EXPRESSION TAG	UNP O15350
G	316	TYR	-	EXPRESSION TAG	UNP O15350
G	317	PHE	-	EXPRESSION TAG	UNP O15350
G	318	GLN	-	EXPRESSION TAG	UNP O15350
I	111	MET	-	EXPRESSION TAG	UNP O15350
I	312	ALA	-	EXPRESSION TAG	UNP O15350
I	313	GLU	-	EXPRESSION TAG	UNP O15350
I	314	ASN	-	EXPRESSION TAG	UNP O15350
I	315	LEU	-	EXPRESSION TAG	UNP O15350
I	316	TYR	-	EXPRESSION TAG	UNP O15350
I	317	PHE	-	EXPRESSION TAG	UNP O15350
I	318	GLN	-	EXPRESSION TAG	UNP O15350
K	111	MET	-	EXPRESSION TAG	UNP O15350
K	312	ALA	-	EXPRESSION TAG	UNP O15350
K	313	GLU	-	EXPRESSION TAG	UNP O15350
K	314	ASN	-	EXPRESSION TAG	UNP O15350
K	315	LEU	-	EXPRESSION TAG	UNP O15350
K	316	TYR	-	EXPRESSION TAG	UNP O15350
K	317	PHE	-	EXPRESSION TAG	UNP O15350
K	318	GLN	-	EXPRESSION TAG	UNP O15350

- Molecule 2 is a protein called APOPTOSIS STIMULATING OF P53 PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	202	Total	C	N	O	S	0	0	0
			1538	973	249	303	13			
2	D	196	Total	C	N	O	S	0	0	0
			1411	892	238	267	14			
2	F	197	Total	C	N	O	S	0	0	0
			1436	905	234	284	13			
2	H	198	Total	C	N	O	S	0	0	0
			1467	936	237	281	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	200	Total	C	N	O	S	0	0	0
			1531	974	250	294	13			
2	L	196	Total	C	N	O	S	0	0	0
			1472	933	240	286	13			

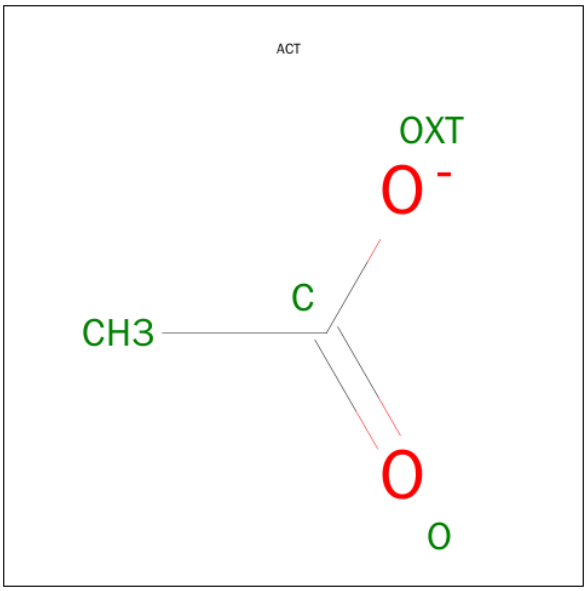
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	890	SER	-	EXPRESSION TAG	UNP Q13625
B	891	MET	-	EXPRESSION TAG	UNP Q13625
D	890	SER	-	EXPRESSION TAG	UNP Q13625
D	891	MET	-	EXPRESSION TAG	UNP Q13625
F	890	SER	-	EXPRESSION TAG	UNP Q13625
F	891	MET	-	EXPRESSION TAG	UNP Q13625
H	890	SER	-	EXPRESSION TAG	UNP Q13625
H	891	MET	-	EXPRESSION TAG	UNP Q13625
J	890	SER	-	EXPRESSION TAG	UNP Q13625
J	891	MET	-	EXPRESSION TAG	UNP Q13625
L	890	SER	-	EXPRESSION TAG	UNP Q13625
L	891	MET	-	EXPRESSION TAG	UNP Q13625

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C H O 7 2 3 2	0	0
4	C	1	Total C H O 7 2 3 2	0	0
4	C	1	Total C H O 7 2 3 2	0	0
4	G	1	Total C H O 7 2 3 2	0	0
4	I	1	Total C H O 7 2 3 2	0	0
4	I	1	Total C H O 7 2 3 2	0	0
4	K	1	Total C H O 7 2 3 2	0	0
4	K	1	Total C H O 7 2 3 2	0	0
4	L	1	Total C H O 7 2 3 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	28	Total O 28 28	0	0
5	C	102	Total O 102 102	0	0
5	D	8	Total O 8 8	0	0

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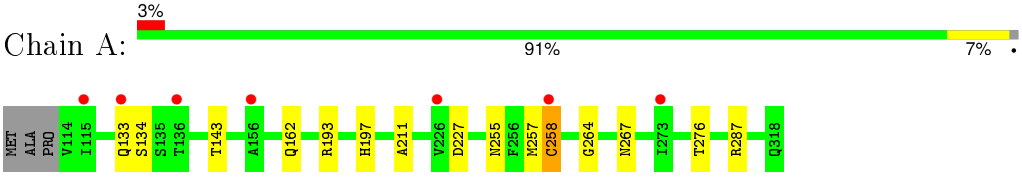
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	64	Total O 64 64	0	0
5	F	12	Total O 12 12	0	0
5	G	128	Total O 128 128	0	0
5	H	12	Total O 12 12	0	0
5	I	137	Total O 137 137	0	0
5	J	52	Total O 52 52	0	0
5	K	98	Total O 98 98	0	0
5	L	30	Total O 30 30	0	0

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.

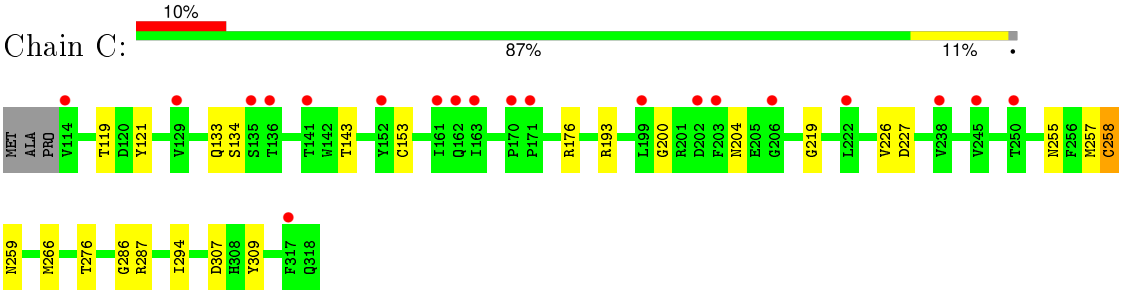
- Molecule 1: TUMOUR PROTEIN 73

Chain A:



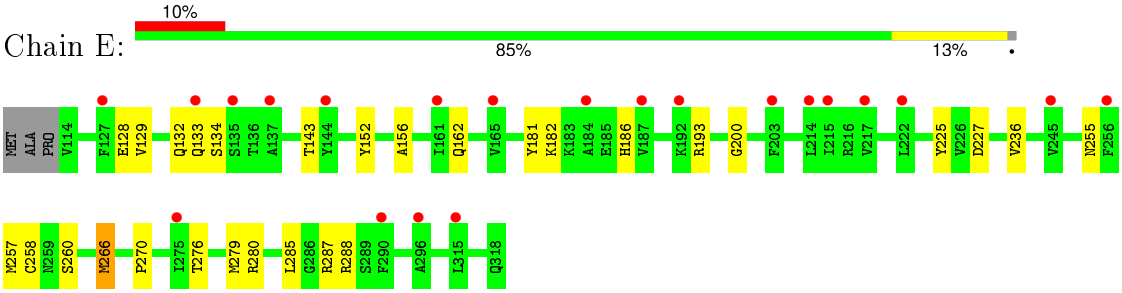
- Molecule 1: TUMOUR PROTEIN 73

Chain C:



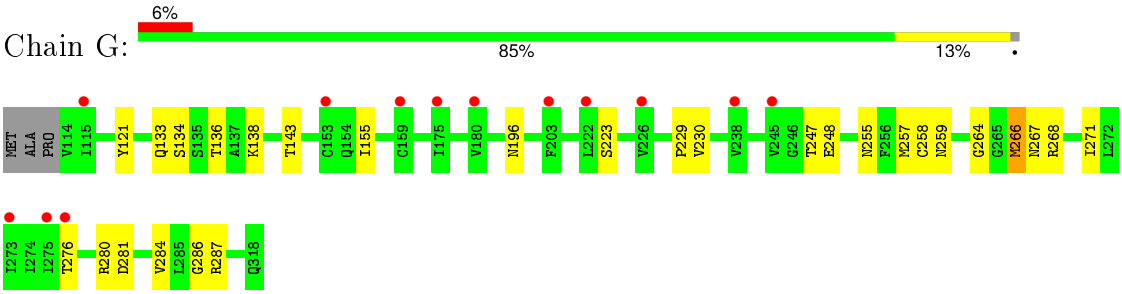
- Molecule 1: TUMOUR PROTEIN 73

Chain E:



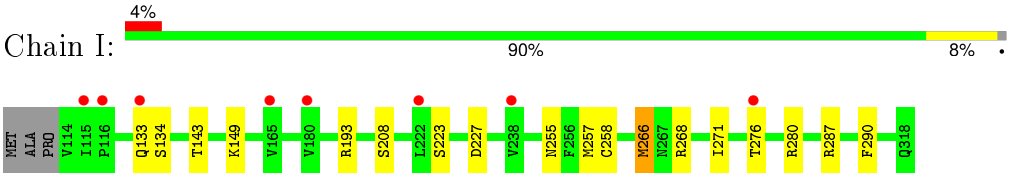
- Molecule 1: TUMOUR PROTEIN 73

Chain G:



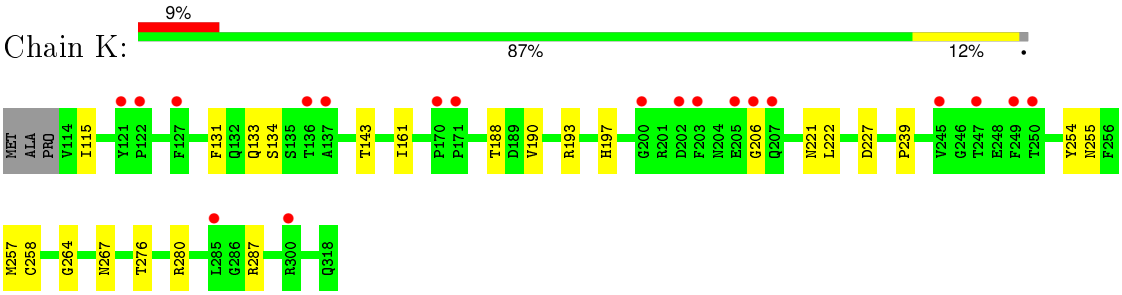
• Molecule 1: TUMOUR PROTEIN 73

Chain I:



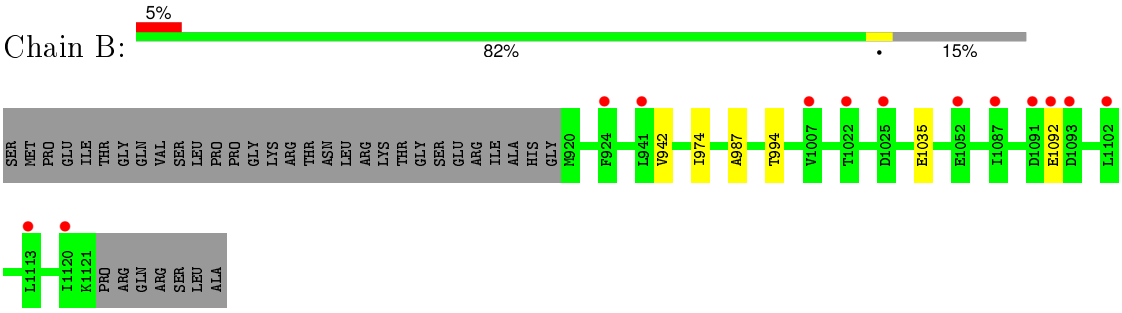
• Molecule 1: TUMOUR PROTEIN 73

Chain K:



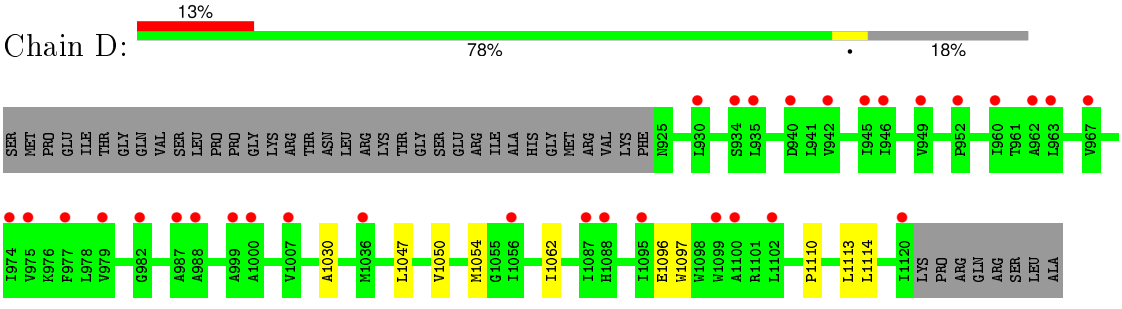
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain B:



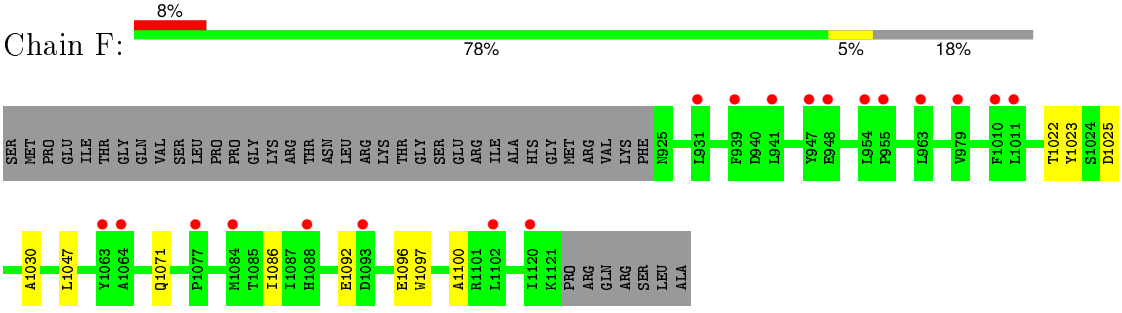
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain D:



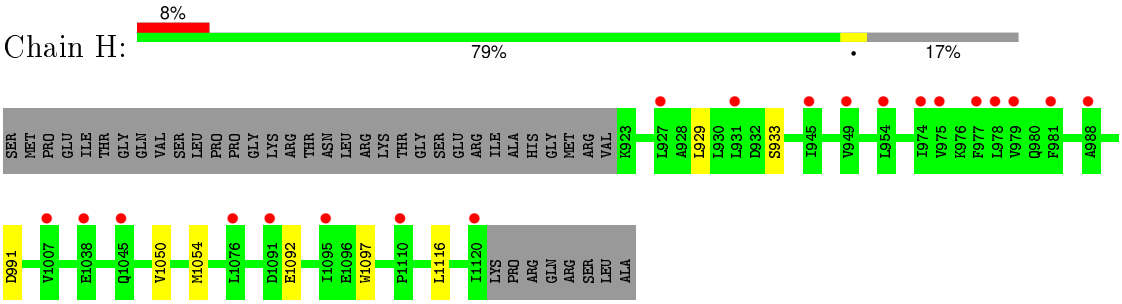
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain F:



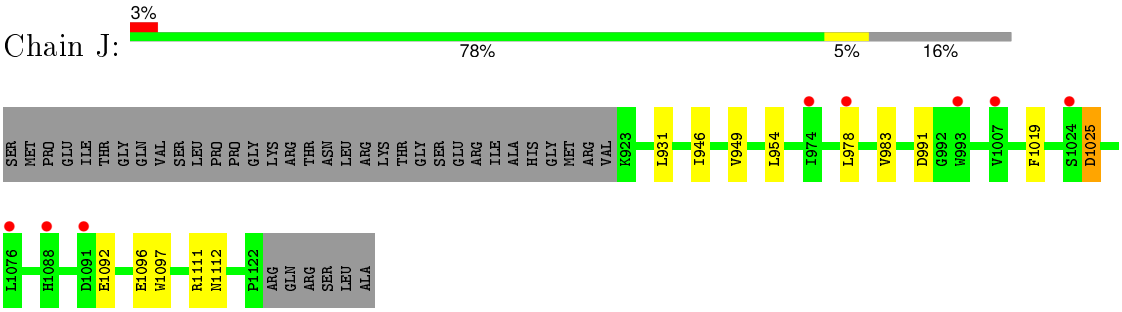
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain H:



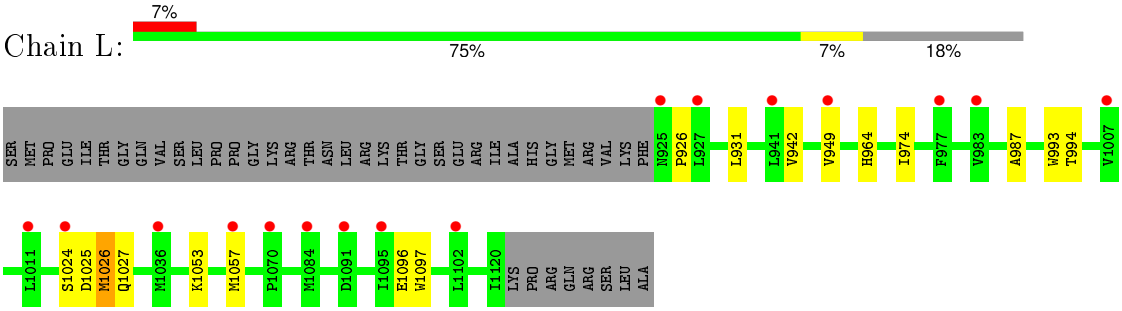
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain J:



• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	132.81Å 170.10Å 177.56Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	85.05 – 2.27 85.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.1 (85.05-2.27) 97.3 (85.05-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.215 , 0.244 0.225 , 0.222	Depositor DCC
R_{free} test set	5537 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	45.4	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.7	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 111026 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19119	wwPDB-VP
Average B, all atoms (Å^2)	51.0	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 46.98 % 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 1.0594e-04.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: ZN, 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	0.54	0/1633	0.68	0/2226
1	C	0.51	1/1627 (0.1%)	0.67	0/2217
1	E	0.49	0/1599	0.68	1/2186 (0.0%)
1	G	0.56	1/1655 (0.1%)	0.68	0/2255
1	I	0.55	1/1634 (0.1%)	0.69	0/2227
1	K	0.52	0/1629	0.67	0/2220
2	B	0.52	0/1574	0.64	0/2149
2	D	0.48	0/1443	0.62	0/1977
2	F	0.46	0/1469	0.63	0/2014
2	H	0.46	0/1503	0.61	0/2057
2	J	0.52	0/1568	0.67	2/2140 (0.1%)
2	L	0.52	0/1506	0.65	0/2059
All	All	0.51	3/18840 (0.0%)	0.66	3/25727 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	266	MET	SD-CE	-5.93	1.44	1.77
1	C	266	MET	SD-CE	-5.82	1.45	1.77
1	I	266	MET	SD-CE	-5.71	1.45	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1025	ASP	CB-CG-OD2	6.75	124.38	118.30
1	E	266	MET	CB-CG-SD	-6.57	92.68	112.40
2	J	1025	ASP	CB-CG-OD1	-6.52	112.43	118.30

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	1592	0	1536	20	0
1	C	1586	0	1535	32	0
1	E	1558	0	1478	39	0
1	G	1608	0	1568	39	0
1	I	1593	0	1541	27	0
1	K	1588	0	1537	37	0
2	B	1538	0	1390	3	0
2	D	1411	0	1254	6	0
2	F	1436	0	1249	7	0
2	H	1467	0	1311	5	0
2	J	1531	0	1415	10	0
2	L	1472	0	1332	8	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	C	12	9	9	1	0
4	G	4	3	3	1	0
4	I	8	6	6	0	0
4	K	8	6	6	1	0
4	L	4	3	3	0	0
5	B	28	0	0	0	0
5	C	102	0	0	15	1
5	D	8	0	0	1	0
5	E	64	0	0	21	0
5	F	12	0	0	1	0
5	G	128	0	0	18	0
5	H	12	0	0	1	0
5	I	137	0	0	13	0
5	J	52	0	0	1	0
5	K	98	0	0	12	0
5	L	30	0	0	1	0
All	All	19092	27	17173	226	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:ARG:CD	5:E:2007:HOH:O	1.72	1.32
1:I:149:LYS:HB2	5:I:2026:HOH:O	1.15	1.31
1:I:290:PHE:CD2	5:I:2115:HOH:O	1.78	1.30
5:I:2098:HOH:O	2:J:1097:TRP:CZ2	1.84	1.29
1:K:280:ARG:HB2	5:K:2035:HOH:O	1.13	1.29
1:E:276:THR:CG2	1:E:287:ARG:HG3	1.65	1.27
1:K:221:ASN:HA	5:K:2070:HOH:O	1.33	1.26
1:I:276:THR:CG2	1:I:287:ARG:HG3	1.64	1.25
1:C:307:ASP:HB3	5:C:2090:HOH:O	1.37	1.24
1:A:276:THR:CG2	1:A:287:ARG:HG3	1.69	1.22
1:K:276:THR:CG2	1:K:287:ARG:HG3	1.70	1.21
5:E:2049:HOH:O	1:K:280:ARG:NH2	1.69	1.20
1:C:307:ASP:CB	5:C:2090:HOH:O	1.89	1.17
1:E:270:PRO:HG2	5:E:2024:HOH:O	0.99	1.16
1:C:121:TYR:HB3	5:C:2011:HOH:O	1.46	1.16
1:E:276:THR:HG22	1:E:287:ARG:CG	1.76	1.15
1:G:276:THR:CG2	1:G:287:ARG:HG3	1.77	1.15
1:K:239:PRO:HG2	5:K:2082:HOH:O	1.42	1.14
1:G:136:THR:HG23	5:G:2110:HOH:O	1.48	1.14
1:A:276:THR:HG22	1:A:287:ARG:CG	1.79	1.12
1:K:276:THR:HG22	1:K:287:ARG:CG	1.79	1.12
1:I:276:THR:HG22	1:I:287:ARG:CG	1.78	1.11
1:I:290:PHE:CE2	5:I:2115:HOH:O	1.96	1.10
1:C:307:ASP:CG	5:C:2090:HOH:O	1.87	1.09
1:G:281:ASP:HB3	5:I:2060:HOH:O	1.55	1.05
1:G:276:THR:HG22	1:G:287:ARG:CG	1.86	1.04
1:G:259:ASN:ND2	5:G:2036:HOH:O	1.91	1.00
1:E:288:ARG:HD3	5:E:2007:HOH:O	1.44	0.99
1:G:286:GLY:C	5:G:2101:HOH:O	1.99	0.99
1:K:206:GLY:O	5:K:2062:HOH:O	1.80	0.99
1:E:288:ARG:NE	5:E:2007:HOH:O	1.82	0.98
1:G:255:ASN:HB3	1:G:257:MET:HE1	1.43	0.98
1:C:226:VAL:HG11	5:C:2042:HOH:O	1.63	0.98
1:E:236:VAL:HG23	5:E:2032:HOH:O	1.63	0.96
1:G:121:TYR:O	5:G:2010:HOH:O	1.72	0.95
1:E:280:ARG:O	5:E:2049:HOH:O	1.84	0.94
1:E:225:TYR:CE1	5:E:2032:HOH:O	2.21	0.92
1:C:121:TYR:CD2	5:C:2011:HOH:O	2.23	0.92
1:G:276:THR:HG22	1:G:287:ARG:HG3	0.93	0.91
1:I:268:ARG:HG3	5:I:2098:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ARG:NH1	5:C:2042:HOH:O	2.03	0.90
1:K:276:THR:HG21	1:K:287:ARG:NH1	1.89	0.88
1:E:225:TYR:CD1	5:E:2032:HOH:O	2.27	0.85
1:I:255:ASN:HB2	1:I:257:MET:CE	2.07	0.84
1:A:276:THR:HG21	1:A:287:ARG:NH1	1.93	0.83
1:E:276:THR:HG21	1:E:287:ARG:NH1	1.92	0.83
1:C:121:TYR:CB	5:C:2011:HOH:O	2.12	0.83
1:G:284:VAL:CG1	5:G:2101:HOH:O	2.26	0.83
1:G:230:VAL:HG23	5:G:2090:HOH:O	1.79	0.82
1:G:276:THR:HG21	1:G:287:ARG:NH1	1.94	0.82
1:G:229:PRO:HG2	5:G:2090:HOH:O	1.78	0.82
1:I:255:ASN:CB	1:I:257:MET:CE	2.58	0.82
1:G:230:VAL:N	5:G:2088:HOH:O	2.04	0.82
1:I:276:THR:HG21	1:I:287:ARG:NH1	1.95	0.81
1:A:276:THR:HG22	1:A:287:ARG:HG3	0.84	0.81
1:C:276:THR:HG22	1:C:287:ARG:HG3	1.61	0.80
1:K:190:VAL:O	5:K:2051:HOH:O	1.97	0.80
1:G:138:LYS:CB	5:G:2109:HOH:O	2.30	0.79
1:A:255:ASN:CB	1:A:257:MET:CE	2.61	0.78
1:K:276:THR:HG22	1:K:287:ARG:HG3	0.86	0.78
1:E:276:THR:HG22	1:E:287:ARG:HG3	0.81	0.77
1:K:222:LEU:HD12	5:K:2082:HOH:O	1.83	0.77
1:E:276:THR:HG21	1:E:287:ARG:HH11	1.49	0.77
1:K:276:THR:HG21	1:K:287:ARG:HH11	1.47	0.77
1:I:290:PHE:HD2	5:I:2115:HOH:O	1.33	0.76
1:K:280:ARG:CB	5:K:2035:HOH:O	1.89	0.76
1:E:129:VAL:HG23	5:E:2009:HOH:O	1.86	0.76
1:G:259:ASN:O	5:G:2094:HOH:O	2.03	0.76
1:G:286:GLY:O	5:G:2101:HOH:O	1.99	0.76
1:K:254:TYR:O	5:K:2032:HOH:O	1.96	0.76
1:I:276:THR:HG22	1:I:287:ARG:HG3	0.84	0.75
1:A:255:ASN:HB2	1:A:257:MET:CE	2.17	0.74
1:A:276:THR:HG21	1:A:287:ARG:HH11	1.51	0.73
1:K:255:ASN:HB2	1:K:257:MET:CE	2.18	0.73
1:E:152:TYR:CD2	5:E:2055:HOH:O	2.42	0.73
1:C:287:ARG:N	5:C:2011:HOH:O	2.21	0.73
1:A:255:ASN:HB3	1:A:257:MET:CE	2.19	0.73
1:G:276:THR:HG21	1:G:287:ARG:HH11	1.52	0.72
1:E:193:ARG:HG3	1:E:258:CYS:SG	2.29	0.72
1:K:239:PRO:CG	5:K:2082:HOH:O	2.17	0.72
1:C:255:ASN:HB2	1:C:257:MET:CE	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:TYR:O	5:C:2093:HOH:O	2.07	0.71
1:K:255:ASN:CB	1:K:257:MET:CE	2.69	0.69
1:C:255:ASN:CB	1:C:257:MET:CE	2.70	0.69
1:I:276:THR:HG21	1:I:287:ARG:HH11	1.55	0.69
1:G:255:ASN:CB	1:G:257:MET:HE1	2.21	0.68
1:A:255:ASN:HB3	1:A:257:MET:HE2	1.75	0.68
1:A:193:ARG:HD3	1:A:211:ALA:O	1.92	0.68
1:I:255:ASN:HB3	1:I:257:MET:CE	2.23	0.67
2:L:1026:MET:HG2	5:L:2006:HOH:O	1.93	0.67
1:G:255:ASN:HB3	1:G:257:MET:CE	2.20	0.67
1:E:182:LYS:HB3	5:E:2024:HOH:O	1.96	0.65
1:I:255:ASN:HB3	1:I:257:MET:HE2	1.79	0.65
1:C:121:TYR:O	5:C:2011:HOH:O	2.15	0.65
1:K:255:ASN:CB	1:K:257:MET:HE1	2.28	0.64
1:A:264:GLY:H	1:A:267:ASN:HD22	1.44	0.64
1:E:128:GLU:C	5:E:2009:HOH:O	2.35	0.64
1:I:149:LYS:CB	5:I:2026:HOH:O	1.94	0.63
1:E:287:ARG:O	5:E:2007:HOH:O	2.15	0.63
1:G:255:ASN:CB	1:G:257:MET:CE	2.76	0.62
1:G:266:MET:HE2	1:G:271:ILE:HG21	1.81	0.62
1:I:266:MET:HE2	1:I:271:ILE:HG21	1.81	0.61
1:I:255:ASN:CB	1:I:257:MET:HE2	2.30	0.61
1:E:260:SER:HA	1:E:266:MET:SD	2.42	0.59
1:I:193:ARG:HG3	1:I:258:CYS:SG	2.42	0.59
1:K:222:LEU:CD1	5:K:2082:HOH:O	2.46	0.59
1:K:255:ASN:HB2	1:K:257:MET:HE1	1.85	0.59
1:C:121:TYR:HD2	5:C:2011:HOH:O	1.73	0.58
1:E:288:ARG:HG2	5:E:2007:HOH:O	2.01	0.58
2:D:1110:PRO:HG2	2:D:1113:LEU:HD22	1.86	0.57
1:E:280:ARG:HA	5:E:2049:HOH:O	2.04	0.57
1:E:193:ARG:NE	1:E:257:MET:HB3	2.19	0.57
2:J:991:ASP:HB3	5:J:2016:HOH:O	2.04	0.57
2:F:1022:THR:HG21	5:F:2002:HOH:O	2.05	0.57
1:A:255:ASN:CB	1:A:257:MET:HE2	2.33	0.56
1:E:132:GLN:H	1:E:162:GLN:HE22	1.52	0.56
1:I:255:ASN:CB	1:I:257:MET:HE1	2.34	0.56
1:I:276:THR:CG2	1:I:287:ARG:CG	2.59	0.56
1:K:255:ASN:HB3	1:K:257:MET:CE	2.34	0.56
1:C:255:ASN:HB3	1:C:257:MET:CE	2.34	0.56
1:G:247:THR:HG22	1:G:248:GLU:H	1.71	0.56
1:I:290:PHE:HB3	5:I:2022:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:ASN:HB3	1:E:257:MET:CE	2.36	0.55
1:K:161:ILE:HD12	1:K:254:TYR:CD2	2.42	0.55
1:K:264:GLY:H	1:K:267:ASN:HD22	1.54	0.55
2:L:1053:LYS:O	2:L:1057:MET:HG2	2.07	0.55
1:E:156:ALA:HA	1:E:257:MET:CE	2.37	0.55
1:C:255:ASN:HB2	1:C:257:MET:HE3	1.88	0.54
1:E:276:THR:CG2	1:E:287:ARG:CG	2.59	0.54
1:C:193:ARG:NE	1:C:257:MET:HB3	2.23	0.54
1:C:255:ASN:HB3	1:C:257:MET:HE1	1.89	0.53
1:I:255:ASN:HB2	1:I:257:MET:HE3	1.89	0.53
1:C:255:ASN:CB	1:C:257:MET:HE3	2.37	0.53
1:C:193:ARG:HG3	1:C:258:CYS:SG	2.48	0.53
1:E:156:ALA:HA	1:E:257:MET:HE2	1.89	0.53
1:K:287:ARG:HE	4:K:1319:ACT:C	2.22	0.52
1:G:284:VAL:HG12	5:G:2101:HOH:O	1.98	0.52
1:E:225:TYR:CZ	5:E:2032:HOH:O	2.54	0.52
1:K:193:ARG:HG2	1:K:258:CYS:SG	2.51	0.51
2:D:1050:VAL:HG13	5:D:2007:HOH:O	2.09	0.51
2:J:1025:ASP:OD1	2:J:1025:ASP:O	2.29	0.51
4:C:1320:ACT:OXT	1:I:287:ARG:NE	2.36	0.51
1:K:255:ASN:HB3	1:K:257:MET:HE1	1.92	0.51
2:L:1096:GLU:HG2	2:L:1097:TRP:CD1	2.46	0.50
1:A:255:ASN:CB	1:A:257:MET:HE1	2.38	0.50
2:H:1050:VAL:O	2:H:1054:MET:HB2	2.12	0.50
2:L:1025:ASP:C	2:L:1027:GLN:H	2.15	0.50
1:E:200:GLY:HA2	2:F:1023:TYR:O	2.11	0.50
1:A:193:ARG:HG3	1:A:258:CYS:SG	2.51	0.49
2:H:1054:MET:HG3	2:H:1116:LEU:HD13	1.93	0.49
1:G:264:GLY:H	1:G:267:ASN:HD22	1.58	0.49
1:E:270:PRO:CG	5:E:2024:HOH:O	1.85	0.49
1:C:255:ASN:CB	1:C:257:MET:HE1	2.42	0.49
1:G:155:ILE:CG2	5:G:2032:HOH:O	2.61	0.49
1:C:286:GLY:HA2	5:C:2011:HOH:O	2.11	0.49
1:G:268:ARG:HD2	2:H:1097:TRP:CD2	2.48	0.49
2:B:942:VAL:HG11	2:B:974:ILE:HG23	1.94	0.48
1:E:152:TYR:CE2	5:E:2055:HOH:O	2.63	0.48
1:A:255:ASN:HB3	1:A:257:MET:HE1	1.95	0.48
1:K:239:PRO:CD	5:K:2082:HOH:O	2.56	0.48
2:L:964:HIS:HE1	2:L:993:TRP:O	1.97	0.48
2:D:1096:GLU:HG3	2:D:1097:TRP:CD1	2.50	0.47
1:K:131:PHE:CE2	1:K:161:ILE:HG12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:CG1	5:C:2042:HOH:O	2.41	0.47
1:C:119:THR:HG21	5:I:2025:HOH:O	2.14	0.47
1:K:276:THR:CG2	1:K:287:ARG:CG	2.63	0.47
1:G:255:ASN:HB2	1:G:257:MET:CE	2.45	0.46
1:G:247:THR:HG22	1:G:248:GLU:N	2.31	0.46
1:C:134:SER:HB2	1:C:143:THR:HA	1.98	0.46
1:K:239:PRO:HD2	5:K:2082:HOH:O	2.15	0.46
1:E:288:ARG:CG	5:E:2007:HOH:O	2.30	0.46
1:C:200:GLY:O	1:C:204:ASN:ND2	2.48	0.46
1:G:280:ARG:NH2	1:I:223:SER:OG	2.48	0.46
1:K:134:SER:HB2	1:K:143:THR:HA	1.98	0.46
1:G:286:GLY:CA	5:G:2101:HOH:O	2.58	0.45
5:I:2096:HOH:O	2:J:1096:GLU:HG2	2.15	0.45
2:F:1096:GLU:HG2	2:F:1097:TRP:CD1	2.51	0.45
1:I:134:SER:HB2	1:I:143:THR:HA	1.98	0.45
1:K:193:ARG:HH21	1:K:197:HIS:HB3	1.81	0.45
1:E:225:TYR:CG	5:E:2032:HOH:O	2.63	0.45
1:G:136:THR:CG2	5:G:2110:HOH:O	2.31	0.45
1:C:193:ARG:HE	1:C:257:MET:HB3	1.80	0.45
2:D:1050:VAL:O	2:D:1054:MET:HB2	2.15	0.45
2:H:991:ASP:HB3	5:H:2001:HOH:O	2.16	0.45
2:L:942:VAL:HG11	2:L:974:ILE:HG23	1.99	0.45
2:J:978:LEU:O	2:J:983:VAL:HB	2.18	0.44
1:A:276:THR:CG2	1:A:287:ARG:CG	2.62	0.44
2:F:1025:ASP:OD1	2:F:1025:ASP:O	2.36	0.44
1:K:264:GLY:H	1:K:267:ASN:ND2	2.15	0.44
1:G:223:SER:OG	1:I:280:ARG:NH2	2.50	0.44
1:A:134:SER:HB2	1:A:143:THR:HA	2.00	0.44
1:A:264:GLY:H	1:A:267:ASN:ND2	2.14	0.43
1:C:286:GLY:C	5:C:2011:HOH:O	2.52	0.43
1:A:255:ASN:HB2	1:A:257:MET:HE3	1.95	0.43
1:E:279:MET:SD	1:E:285:LEU:HD11	2.58	0.43
1:K:193:ARG:NH2	1:K:197:HIS:HB3	2.33	0.43
2:J:946:ILE:O	2:J:949:VAL:HG22	2.18	0.43
2:L:926:PRO:HB2	2:L:949:VAL:HG12	2.00	0.43
1:E:186:HIS:NE2	2:F:1071:GLN:O	2.51	0.43
1:G:134:SER:HB2	1:G:143:THR:HA	2.01	0.43
2:D:1062:ILE:HD13	2:D:1114:LEU:HD13	2.01	0.43
1:G:284:VAL:HG13	5:G:2101:HOH:O	2.05	0.42
1:G:155:ILE:HG23	5:G:2032:HOH:O	2.17	0.42
2:J:1019:PHE:HB2	2:J:1112:ASN:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:SER:HB2	1:E:143:THR:HA	1.99	0.42
1:G:121:TYR:HB2	4:G:1319:ACT:H2	2.01	0.42
1:C:119:THR:CG2	5:I:2025:HOH:O	2.66	0.42
1:G:196:ASN:ND2	5:G:2066:HOH:O	2.43	0.42
2:L:987:ALA:O	2:L:994:THR:HA	2.20	0.42
1:K:255:ASN:HB2	1:K:257:MET:HE3	2.00	0.42
1:C:259:ASN:HA	1:C:294:ILE:HB	2.02	0.42
1:E:181:TYR:OH	1:E:266:MET:HA	2.19	0.42
2:J:1025:ASP:C	2:J:1025:ASP:OD1	2.59	0.42
2:H:929:LEU:O	2:H:933:SER:HB2	2.20	0.42
2:B:987:ALA:O	2:B:994:THR:HA	2.20	0.41
1:A:193:ARG:HE	1:A:197:HIS:HB3	1.84	0.41
2:J:1096:GLU:HA	2:J:1111:ARG:HG2	2.02	0.41
2:F:1030:ALA:HB2	2:F:1047:LEU:HB3	2.02	0.41
2:B:1035:GLU:HG2	1:C:219:GLY:HA2	2.03	0.41
1:G:280:ARG:HG2	1:I:208:SER:HB2	2.03	0.41
5:I:2098:HOH:O	2:J:1097:TRP:CE2	2.46	0.40
2:F:1086:ILE:HD13	2:F:1100:ALA:HB2	2.03	0.40
2:D:1030:ALA:HB2	2:D:1047:LEU:HB3	2.04	0.40
1:K:161:ILE:HD12	1:K:254:TYR:HD2	1.83	0.40
1:E:255:ASN:HB3	1:E:257:MET:HE3	2.02	0.40
1:K:115:ILE:HD11	1:K:188:THR:HG22	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2062:HOH:O	5:C:2076:HOH:O[2_656]	0.87	1.33

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	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	34	39
1	C	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	34	39
1	E	203/208 (98%)	200 (98%)	2 (1%)	1 (0%)	34	39
1	G	205/208 (99%)	203 (99%)	1 (0%)	1 (0%)	34	39
1	I	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	34	39
1	K	203/208 (98%)	200 (98%)	2 (1%)	1 (0%)	34	39
2	B	200/239 (84%)	193 (96%)	7 (4%)	0	100	100
2	D	194/239 (81%)	187 (96%)	7 (4%)	0	100	100
2	F	195/239 (82%)	189 (97%)	6 (3%)	0	100	100
2	H	196/239 (82%)	189 (96%)	7 (4%)	0	100	100
2	J	198/239 (83%)	190 (96%)	8 (4%)	0	100	100
2	L	194/239 (81%)	186 (96%)	6 (3%)	2 (1%)	19	20
All	All	2397/2682 (89%)	2340 (98%)	49 (2%)	8 (0%)	46	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	I	133	GLN
2	L	1026	MET
1	E	133	GLN
1	G	133	GLN
1	K	133	GLN
2	L	1024	SER
1	C	133	GLN

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	174/183 (95%)	171 (98%)	3 (2%)	68	82
1	C	174/183 (95%)	171 (98%)	3 (2%)	68	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	167/183 (91%)	166 (99%)	1 (1%)	90 95
1	G	179/183 (98%)	178 (99%)	1 (1%)	90 95
1	I	176/183 (96%)	175 (99%)	1 (1%)	90 95
1	K	174/183 (95%)	173 (99%)	1 (1%)	90 95
2	B	156/205 (76%)	155 (99%)	1 (1%)	90 95
2	D	132/205 (64%)	132 (100%)	0	100 100
2	F	136/205 (66%)	135 (99%)	1 (1%)	88 94
2	H	142/205 (69%)	141 (99%)	1 (1%)	88 94
2	J	157/205 (77%)	154 (98%)	3 (2%)	65 79
2	L	146/205 (71%)	145 (99%)	1 (1%)	88 94
All	All	1913/2328 (82%)	1896 (99%)	17 (1%)	84 92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	227	ASP
1	A	258	CYS
2	B	1092	GLU
1	C	153	CYS
1	C	227	ASP
1	C	258	CYS
1	E	227	ASP
2	F	1092	GLU
1	G	258	CYS
2	H	1092	GLU
1	I	227	ASP
2	J	931	LEU
2	J	954	LEU
2	J	1092	GLU
1	K	227	ASP
2	L	931	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN

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Mol	Chain	Res	Type
1	A	267	ASN
1	C	224	GLN
1	C	267	ASN
1	E	162	GLN
1	E	267	ASN
1	G	207	GLN
1	G	267	ASN
1	I	267	ASN
1	K	267	ASN
2	L	964	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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	C	1319	-	1,3,3	4.25	1 (100%)	0,3,3	0.00	-
4	ACT	C	1320	-	1,3,3	4.32	1 (100%)	0,3,3	0.00	-
4	ACT	C	1321	-	1,3,3	4.42	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	G	1319	-	1,3,3	2.44	1 (100%)	0,3,3	0.00	-
4	ACT	I	1319	-	1,3,3	6.25	1 (100%)	0,3,3	0.00	-
4	ACT	I	1320	-	1,3,3	4.59	1 (100%)	0,3,3	0.00	-
4	ACT	K	1319	-	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
4	ACT	K	1320	-	1,3,3	4.46	1 (100%)	0,3,3	0.00	-
4	ACT	L	1522	-	1,3,3	3.01	1 (100%)	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACT	C	1319	-	-	0/0/0/0	0/0/0/0
4	ACT	C	1320	-	-	0/0/0/0	0/0/0/0
4	ACT	C	1321	-	-	0/0/0/0	0/0/0/0
4	ACT	G	1319	-	-	0/0/0/0	0/0/0/0
4	ACT	I	1319	-	-	0/0/0/0	0/0/0/0
4	ACT	I	1320	-	-	0/0/0/0	0/0/0/0
4	ACT	K	1319	-	-	0/0/0/0	0/0/0/0
4	ACT	K	1320	-	-	0/0/0/0	0/0/0/0
4	ACT	L	1522	-	-	0/0/0/0	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1319	ACT	CH3-C	2.44	1.52	1.48
4	K	1319	ACT	CH3-C	2.61	1.52	1.48
4	L	1522	ACT	CH3-C	3.01	1.53	1.48
4	C	1319	ACT	CH3-C	4.25	1.54	1.48
4	C	1320	ACT	CH3-C	4.32	1.54	1.48
4	C	1321	ACT	CH3-C	4.42	1.54	1.48
4	K	1320	ACT	CH3-C	4.46	1.55	1.48
4	I	1320	ACT	CH3-C	4.59	1.55	1.48
4	I	1319	ACT	CH3-C	6.25	1.57	1.48

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
4	C	1320	ACT	1	0
4	G	1319	ACT	1	0
4	K	1319	ACT	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

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	205/208 (98%)	0.87	7 (3%) 49 57	24, 40, 68, 118	0
1	C	205/208 (98%)	1.05	20 (9%) 10 13	26, 43, 85, 96	0
1	E	205/208 (98%)	1.02	21 (10%) 9 12	34, 52, 83, 102	0
1	G	205/208 (98%)	0.99	13 (6%) 23 30	20, 37, 71, 112	0
1	I	205/208 (98%)	0.93	8 (3%) 43 51	21, 36, 66, 115	0
1	K	205/208 (98%)	0.99	19 (9%) 11 15	23, 41, 75, 104	0
2	B	202/239 (84%)	0.82	13 (6%) 23 29	33, 49, 71, 97	0
2	D	196/239 (82%)	1.16	32 (16%) 2 4	38, 64, 104, 111	0
2	F	197/239 (82%)	0.97	19 (9%) 10 14	35, 61, 99, 114	0
2	H	198/239 (82%)	0.96	20 (10%) 9 12	38, 61, 89, 96	0
2	J	200/239 (83%)	0.79	8 (4%) 42 49	26, 44, 68, 86	0
2	L	196/239 (82%)	0.97	16 (8%) 14 19	32, 56, 102, 111	0
All	All	2419/2682 (90%)	0.96	196 (8%) 15 20	20, 48, 90, 118	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1091	ASP	5.3
1	K	203	PHE	5.3
2	F	947	TYR	5.2
1	E	245	VAL	4.8
2	D	942	VAL	4.8
2	H	981	PHE	4.7
2	L	927	LEU	4.4
2	D	935	LEU	4.3
2	L	941	LEU	4.3
2	D	974	ILE	4.2
1	C	222	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	136	THR	3.9
1	C	245	VAL	3.9
2	H	945	ILE	3.9
1	A	136	THR	3.8
2	L	949	VAL	3.8
2	D	1088	HIS	3.8
1	E	161	ILE	3.7
2	H	1091	ASP	3.7
2	B	1120	ILE	3.7
1	E	127	PHE	3.7
1	C	135	SER	3.6
2	L	1095	ILE	3.6
1	K	245	VAL	3.6
2	L	977	PHE	3.6
1	K	206	GLY	3.6
2	F	939	PHE	3.5
2	B	1093	ASP	3.5
2	D	962	ALA	3.5
1	E	203	PHE	3.5
2	D	975	VAL	3.4
2	H	931	LEU	3.3
1	C	203	PHE	3.3
2	D	946	ILE	3.3
2	D	1095	ILE	3.3
2	D	963	LEU	3.2
2	D	1007	VAL	3.2
2	H	978	LEU	3.2
2	H	927	LEU	3.2
2	F	979	VAL	3.2
1	E	135	SER	3.1
1	K	200	GLY	3.1
1	C	161	ILE	3.1
2	H	977	PHE	3.1
1	C	199	LEU	3.1
2	D	1056	ILE	3.0
1	K	249	PHE	3.0
2	H	1095	ILE	3.0
2	D	1087	ILE	3.0
2	H	1120	ILE	3.0
1	K	205	GLU	3.0
1	K	170	PRO	3.0
1	E	184	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	977	PHE	3.0
2	L	925	ASN	2.9
2	D	1102	LEU	2.9
2	F	963	LEU	2.9
2	D	1120	ILE	2.9
2	F	955	PRO	2.9
2	D	934	SER	2.9
1	G	222	LEU	2.9
2	F	1102	LEU	2.9
1	C	114	VAL	2.8
2	B	1092	GLU	2.8
2	D	979	VAL	2.8
1	K	136	THR	2.8
2	J	1091	ASP	2.8
2	L	1007	VAL	2.8
2	D	1099	TRP	2.8
2	D	1100	ALA	2.8
2	D	967	VAL	2.8
1	A	258	CYS	2.8
2	D	930	LEU	2.7
2	F	1120	ILE	2.7
1	E	214	LEU	2.7
1	K	202	ASP	2.7
2	B	1113	LEU	2.7
2	D	999	ALA	2.7
1	C	202	ASP	2.7
2	L	1102	LEU	2.7
1	I	115	ILE	2.7
2	F	1063	TYR	2.6
2	L	1091	ASP	2.6
1	E	187	VAL	2.6
1	E	165	VAL	2.6
2	H	1007	VAL	2.6
1	G	115	ILE	2.6
1	C	206	GLY	2.6
1	G	226	VAL	2.6
2	F	954	LEU	2.6
2	D	949	VAL	2.6
1	E	222	LEU	2.6
1	I	276	THR	2.6
1	A	115	ILE	2.6
2	H	954	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	171	PRO	2.5
2	D	945	ILE	2.5
1	I	238	VAL	2.5
2	D	988	ALA	2.5
1	E	275	ILE	2.5
1	C	317	PHE	2.5
2	F	1064	ALA	2.4
1	C	141	THR	2.4
1	G	238	VAL	2.4
1	G	245	VAL	2.4
1	G	273	ILE	2.4
2	B	1007	VAL	2.4
1	C	162	GLN	2.4
2	D	982	GLY	2.4
1	E	290	PHE	2.4
1	K	137	ALA	2.4
1	C	163	ILE	2.4
1	C	238	VAL	2.4
2	J	1024	SER	2.4
2	D	987	ALA	2.4
1	G	275	ILE	2.3
1	C	250	THR	2.3
2	D	1000	ALA	2.3
2	F	931	LEU	2.3
2	L	1011	LEU	2.3
1	E	133	GLN	2.3
1	C	129	VAL	2.3
1	I	180	VAL	2.3
2	H	1045	GLN	2.3
2	H	1076	LEU	2.3
2	L	1036	MET	2.3
2	H	1038	GLU	2.3
2	L	983	VAL	2.3
2	F	1010	PHE	2.3
2	J	1076	LEU	2.3
1	K	171	PRO	2.2
1	A	226	VAL	2.2
2	L	1024	SER	2.2
1	K	127	PHE	2.2
1	K	207	GLN	2.2
1	C	170	PRO	2.2
2	B	1025	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	974	ILE	2.2
1	I	133	GLN	2.2
1	K	121	TYR	2.2
2	B	1052	GLU	2.2
2	J	978	LEU	2.2
1	E	192	LYS	2.2
1	G	203	PHE	2.2
1	A	133	GLN	2.2
2	B	941	LEU	2.2
2	F	941	LEU	2.2
2	F	1011	LEU	2.2
1	G	276	THR	2.1
1	I	165	VAL	2.1
1	I	116	PRO	2.1
1	E	315	LEU	2.1
1	K	285	LEU	2.1
2	F	948	GLU	2.1
2	H	988	ALA	2.1
1	G	153	CYS	2.1
1	G	159[A]	CYS	2.1
2	J	974	ILE	2.1
2	H	979	VAL	2.1
2	J	993	TRP	2.1
2	B	1102	LEU	2.1
2	L	1084	MET	2.1
1	E	215	ILE	2.1
1	G	175	ILE	2.1
2	H	1110	PRO	2.1
2	H	949	VAL	2.1
2	H	975	VAL	2.1
2	J	1007	VAL	2.1
1	I	222	LEU	2.1
2	B	1022	THR	2.1
1	A	273	ILE	2.1
1	K	122	PRO	2.1
2	D	952	PRO	2.1
2	D	960	ILE	2.1
2	F	1093	ASP	2.1
2	L	1070	PRO	2.1
1	E	144	TYR	2.1
2	J	1088	HIS	2.1
1	K	247	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	924	PHE	2.0
1	A	156	ALA	2.0
1	K	300	ARG	2.0
1	K	250	THR	2.0
1	E	256	PHE	2.0
1	E	296	ALA	2.0
2	D	1036	MET	2.0
2	F	1084	MET	2.0
2	L	1057	MET	2.0
2	B	1087	ILE	2.0
1	E	217	VAL	2.0
1	G	180	VAL	2.0
2	D	940	ASP	2.0
1	E	137	ALA	2.0
2	F	1088	HIS	2.0
1	C	152	TYR	2.0
2	F	1077	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	K	1319	4/4	0.93	0.72	16.27	88,89,89,94	0
4	ACT	C	1321	4/4	0.87	0.54	13.06	42,50,55,58	0
4	ACT	G	1319	4/4	0.92	0.32	6.74	46,46,52,56	0
4	ACT	C	1320	4/4	0.96	0.33	6.19	34,35,41,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACT	I	1320	4/4	0.88	0.27	3.04	49,50,51,52	0
4	ACT	L	1522	4/4	0.91	0.36	2.89	49,50,55,56	0
3	ZN	G	1	1/1	1.00	0.22	1.61	37,37,37,37	0
3	ZN	K	1	1/1	0.99	0.18	1.55	39,39,39,39	0
3	ZN	I	1	1/1	1.00	0.20	1.32	30,30,30,30	0
4	ACT	K	1320	4/4	0.89	0.21	1.05	60,64,64,66	0
4	ACT	I	1319	4/4	0.93	0.20	0.69	54,54,57,67	0
3	ZN	E	1	1/1	0.99	0.17	-0.32	45,45,45,45	0
3	ZN	C	1	1/1	0.99	0.16	-0.40	44,44,44,44	0
4	ACT	C	1319	4/4	0.90	0.19	-	75,77,78,81	0

6.5 Other polymers (i)

There are no such residues in this entry.