



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:31 AM GMT

PDB ID : 4A63
Title : Crystal structure of the p73-ASPP2 complex at 2.6Å 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 wwPDB validation summary 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/ValidationPDFNotes.html>

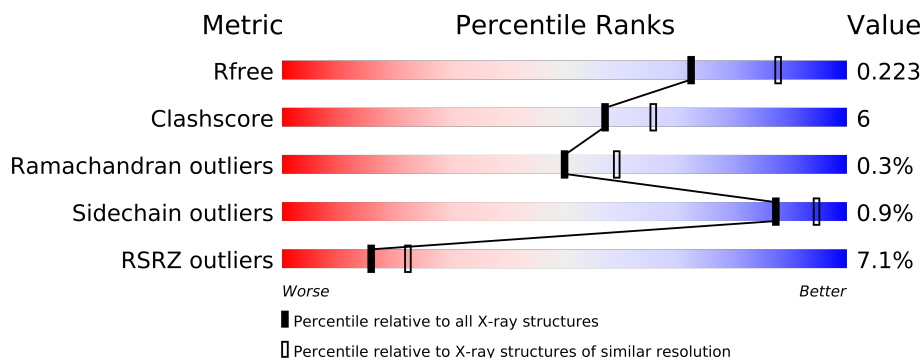
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	208	
1	C	208	
1	E	208	
1	G	208	
1	I	208	
1	K	208	
2	B	239	
2	D	239	
2	F	239	
2	H	239	
2	J	239	
2	L	239	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ZN	G	1	-	X
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 deuterium.

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			

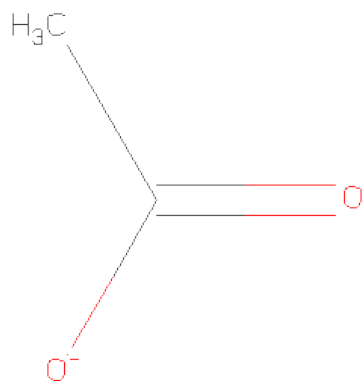
There are 12 discrepancies between the modelled and reference sequences:

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: C₂H₃O₂).



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

- Molecule 5 is water.

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

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

3 Residue-property plots

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.

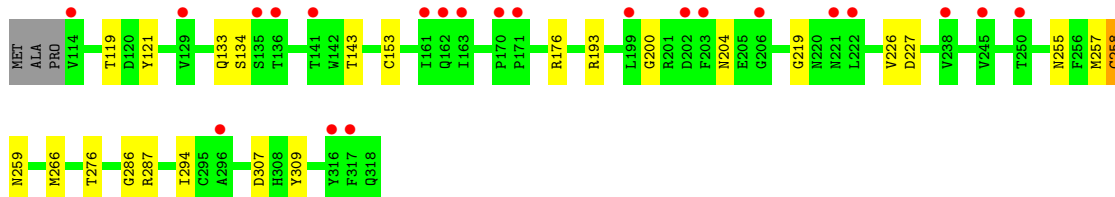
• Molecule 1: TUMOUR PROTEIN 73

Chain A: 



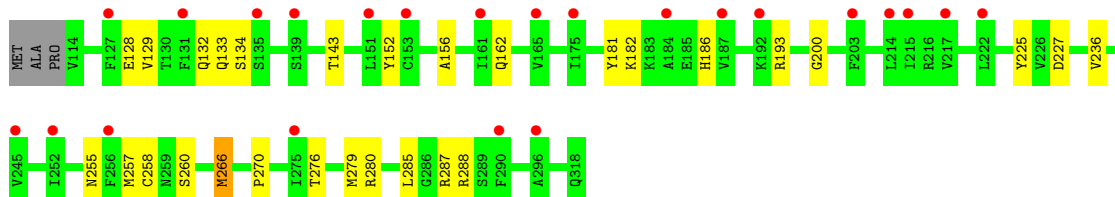
• Molecule 1: TUMOUR PROTEIN 73

Chain C: 



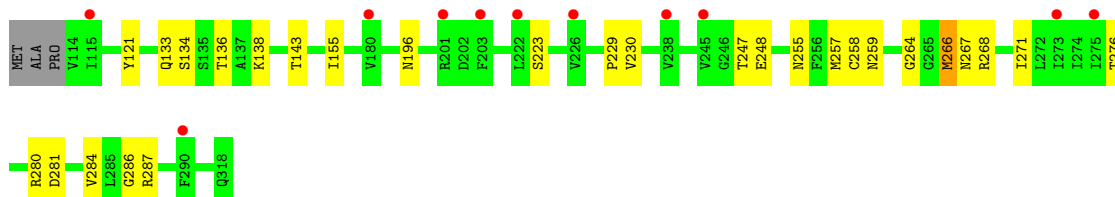
• Molecule 1: TUMOUR PROTEIN 73

Chain E: 



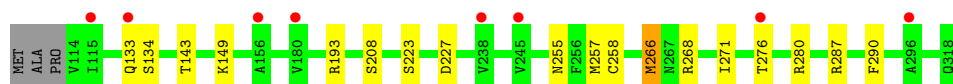
• Molecule 1: TUMOUR PROTEIN 73

Chain G: 



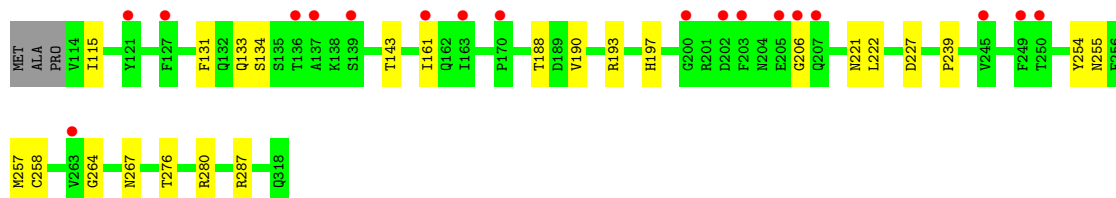
• Molecule 1: TUMOUR PROTEIN 73

Chain I: 



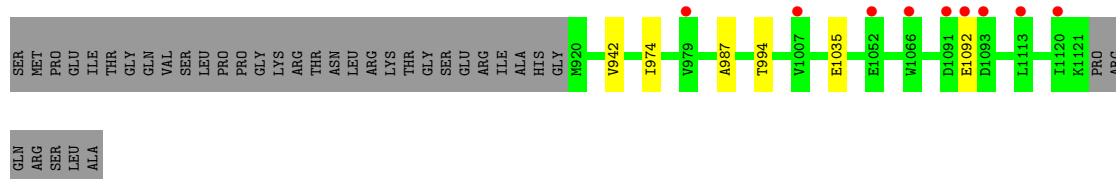
• Molecule 1: TUMOUR PROTEIN 73

Chain K:



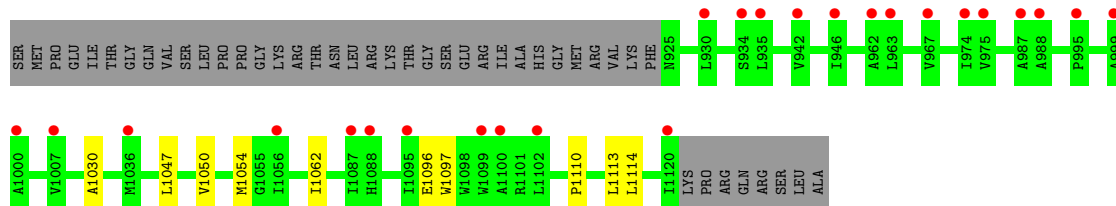
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain B:



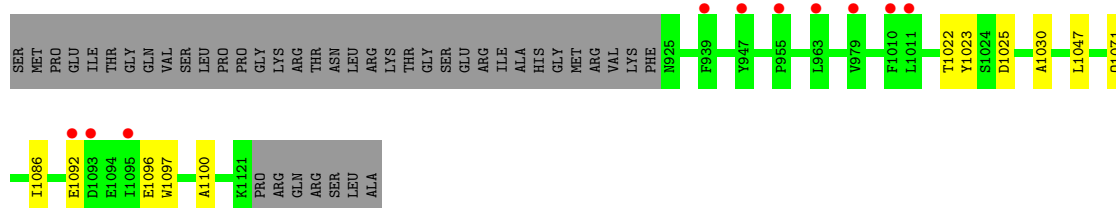
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain D:



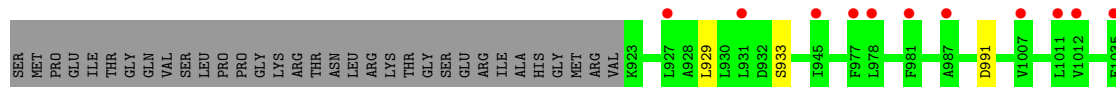
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

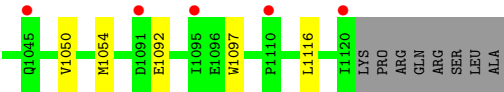
Chain F:



• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

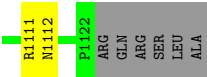
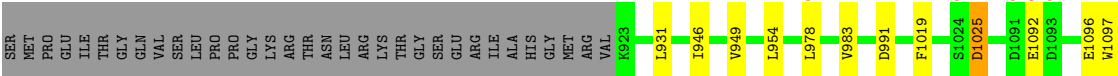
Chain H:





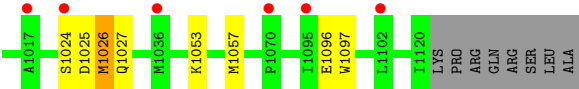
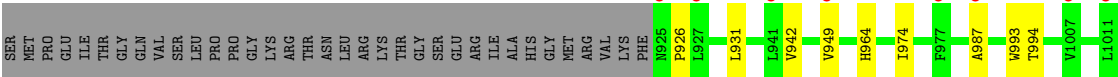
● Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain J:



● Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain L:



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.215 , 0.244 0.225 , 0.223	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)	0.33 , 35.0	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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	38	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	0	1	0
4	G	4	3	0	0	0
4	I	8	6	0	0	0
4	K	8	6	0	1	0
4	L	4	3	0	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	17146	225	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 225 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	Distance(Å)	Clash(Å)
5:C:2062:HOH:O	5:C:2076:HOH:O[2_656]	0.87	1.33

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	38	43
1	C	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	38	43
1	E	203/208 (98%)	200 (98%)	2 (1%)	1 (0%)	38	43
1	G	205/208 (99%)	203 (99%)	1 (0%)	1 (0%)	38	43
1	I	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	38	43
1	K	203/208 (98%)	200 (98%)	2 (1%)	1 (0%)	38	43
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%)	22	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2397/2682 (89%)	2340 (98%)	49 (2%)	8 (0%)	50 59

5 of 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

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	174/183 (95%)	171 (98%)	3 (2%)	73 86
1	C	174/183 (95%)	171 (98%)	3 (2%)	73 86
1	E	167/183 (91%)	166 (99%)	1 (1%)	92 97
1	G	179/183 (98%)	178 (99%)	1 (1%)	92 97
1	I	176/183 (96%)	175 (99%)	1 (1%)	92 97
1	K	174/183 (95%)	173 (99%)	1 (1%)	92 97
2	B	156/205 (76%)	155 (99%)	1 (1%)	92 97
2	D	132/205 (64%)	132 (100%)	0	100 100
2	F	136/205 (66%)	135 (99%)	1 (1%)	91 96
2	H	142/205 (69%)	141 (99%)	1 (1%)	91 96
2	J	157/205 (77%)	154 (98%)	3 (2%)	69 84
2	L	146/205 (71%)	145 (99%)	1 (1%)	91 96
All	All	1913/2328 (82%)	1896 (99%)	17 (1%)	87 94

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	227	ASP

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Mol	Chain	Res	Type
2	F	1092	GLU
2	J	954	LEU
1	C	258	CYS
2	J	1092	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	162	GLN
1	E	267	ASN
1	I	267	ASN
1	C	267	ASN
1	G	267	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	4.15	1 (100%)	0,3,3	0.00	-
4	ACT	C	1320	-	1,3,3	4.22	1 (100%)	0,3,3	0.00	-
4	ACT	C	1321	-	1,3,3	4.31	1 (100%)	0,3,3	0.00	-
4	ACT	G	1319	-	1,3,3	2.37	1 (100%)	0,3,3	0.00	-
4	ACT	I	1319	-	1,3,3	6.10	1 (100%)	0,3,3	0.00	-
4	ACT	I	1320	-	1,3,3	4.48	1 (100%)	0,3,3	0.00	-
4	ACT	K	1319	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
4	ACT	K	1320	-	1,3,3	4.35	1 (100%)	0,3,3	0.00	-
4	ACT	L	1522	-	1,3,3	2.93	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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1319	ACT	CH3-C	6.10	1.57	1.48
4	I	1320	ACT	CH3-C	4.48	1.55	1.48
4	K	1320	ACT	CH3-C	4.35	1.55	1.48
4	C	1321	ACT	CH3-C	4.31	1.54	1.48
4	C	1320	ACT	CH3-C	4.22	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	205/208 (98%)	0.80	9 (4%) 33 42	24, 40, 68, 118	0
1	C	205/208 (98%)	0.99	22 (10%) 6 10	26, 43, 85, 96	0
1	E	205/208 (98%)	0.99	23 (11%) 6 9	34, 52, 83, 102	0
1	G	205/208 (98%)	0.91	11 (5%) 25 33	20, 37, 71, 112	0
1	I	205/208 (98%)	0.82	8 (3%) 37 47	21, 36, 66, 115	0
1	K	205/208 (98%)	0.93	18 (8%) 10 15	23, 41, 75, 104	0
2	B	202/239 (84%)	0.74	9 (4%) 32 41	33, 49, 71, 97	0
2	D	196/239 (82%)	0.93	25 (12%) 4 6	38, 64, 104, 111	0
2	F	197/239 (82%)	0.87	10 (5%) 27 36	35, 61, 99, 114	0
2	H	198/239 (82%)	0.85	16 (8%) 12 17	38, 61, 89, 96	0
2	J	200/239 (83%)	0.69	5 (2%) 54 64	26, 44, 68, 86	0
2	L	196/239 (82%)	0.80	14 (7%) 16 22	32, 56, 102, 111	0
All	All	2419/2682 (90%)	0.86	170 (7%) 16 23	20, 48, 90, 118	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1091	ASP	6.6
1	K	203	PHE	5.4
1	E	245	VAL	5.1
2	F	947	TYR	4.8
1	E	203	PHE	4.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ACT	K	1319	4/4	0.77	16.76	88,89,89,94	0
4	ACT	C	1321	4/4	0.58	13.27	42,50,55,58	0
4	ACT	G	1319	4/4	0.36	9.88	46,46,52,56	0
4	ACT	C	1320	4/4	0.31	6.12	34,35,41,56	0
4	ACT	L	1522	4/4	0.43	4.20	49,50,55,56	0
4	ACT	I	1320	4/4	0.28	3.63	49,50,51,52	0
3	ZN	G	1	1/1	0.21	2.77	37,37,37,37	0
3	ZN	I	1	1/1	0.19	1.65	30,30,30,30	0
3	ZN	K	1	1/1	0.16	1.62	39,39,39,39	0
4	ACT	K	1320	4/4	0.20	1.13	60,64,64,66	0
4	ACT	I	1319	4/4	0.19	0.61	54,54,57,67	0
3	ZN	E	1	1/1	0.17	0.14	45,45,45,45	0
3	ZN	C	1	1/1	0.15	-0.20	44,44,44,44	0
4	ACT	C	1319	4/4	0.17	-0.26	75,77,78,81	0

6.5 Other polymers ⓘ

There are no such residues in this entry.