



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:49 PM UTC

PDB ID : 4A63 / pdb_00004a63
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

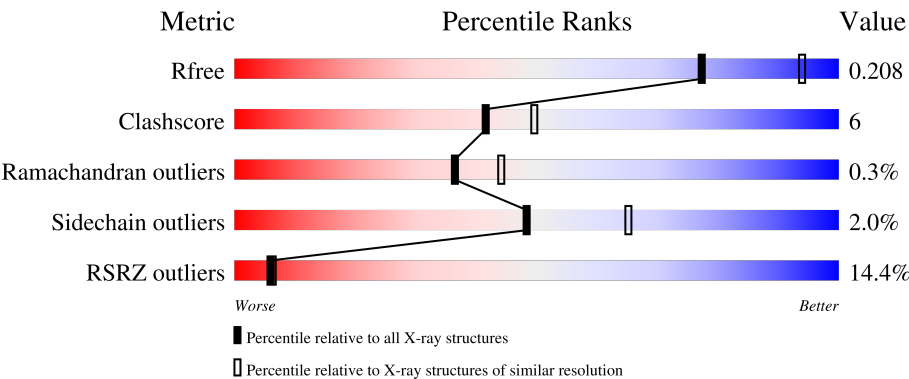
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	208	6% 90% 8% ..
1	C	208	12% 88% 10% ..
1	E	208	11% 84% 14% ..
1	G	208	5% 83% 14% ..
1	I	208	7% 88% 9% ..

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Mol	Chain	Length	Quality of chain
1	K	208	8% 86% 12%
2	B	239	7% 80% 5% 15%
2	D	239	30% 77% 5% 18%
2	F	239	23% 76% 6% 18%
2	H	239	22% 77% 6% 17%
2	J	239	3% 76% 7% 16%
2	L	239	19% 72% 9% 18%

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			

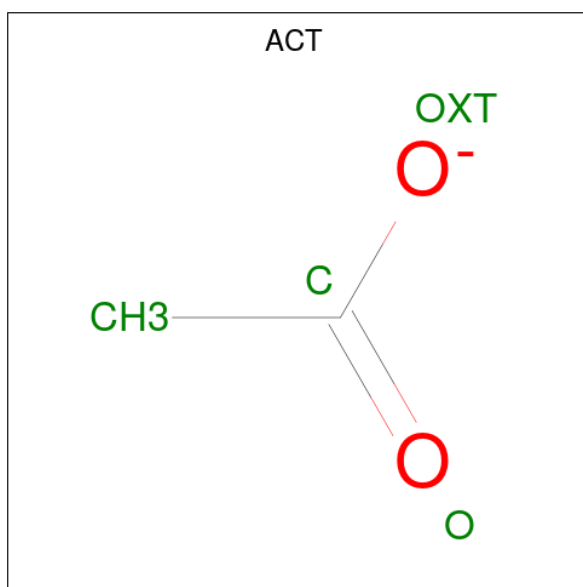
There are 12 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ACETATE ION (CCD ID: 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 [i](#)

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

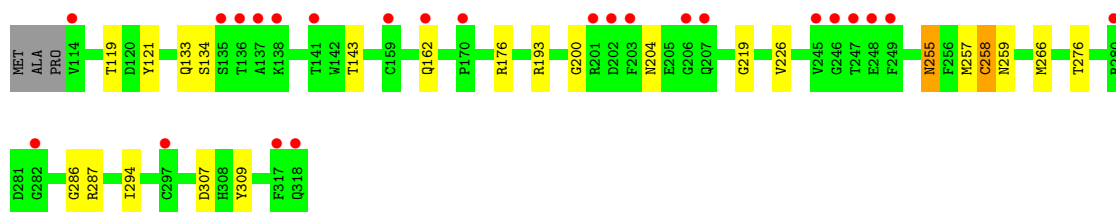
• Molecule 1: TUMOUR PROTEIN 73

Chain A: 



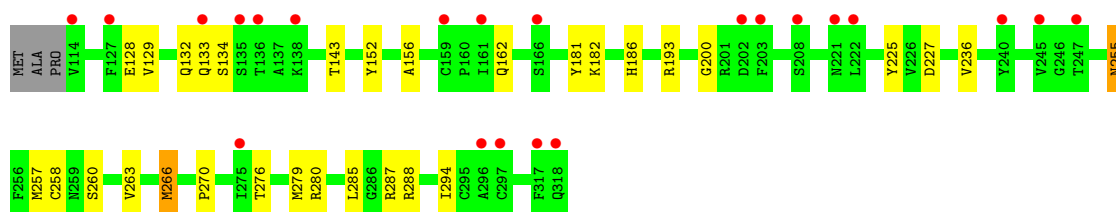
• Molecule 1: TUMOUR PROTEIN 73

Chain C: 



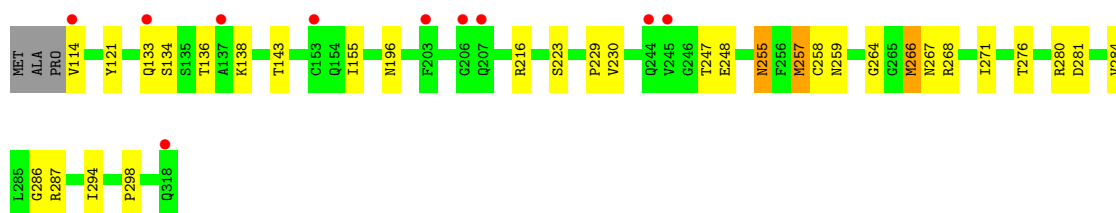
• Molecule 1: TUMOUR PROTEIN 73

Chain E: 



• Molecule 1: TUMOUR PROTEIN 73

Chain G: 



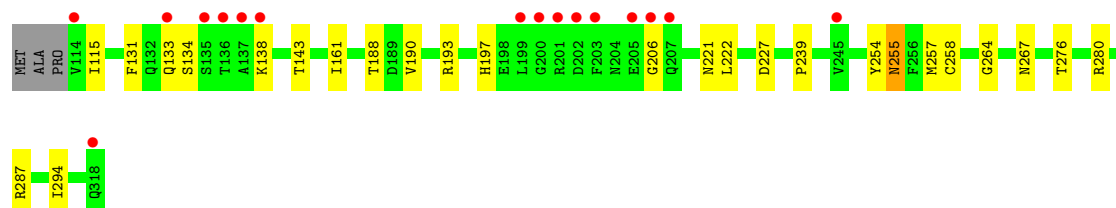
- Molecule 1: TUMOUR PROTEIN 73

Chain I: 



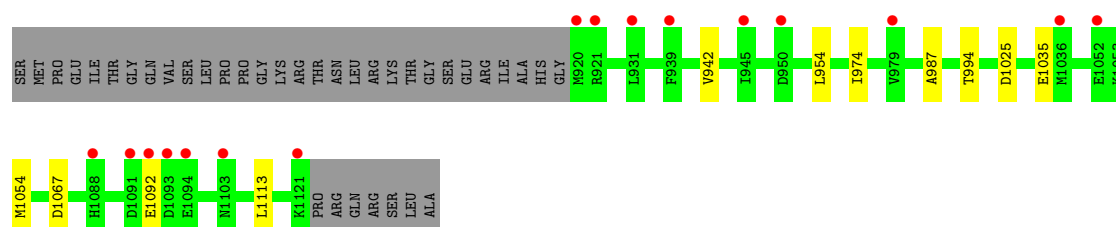
- Molecule 1: TUMOUR PROTEIN 73

Chain K: 



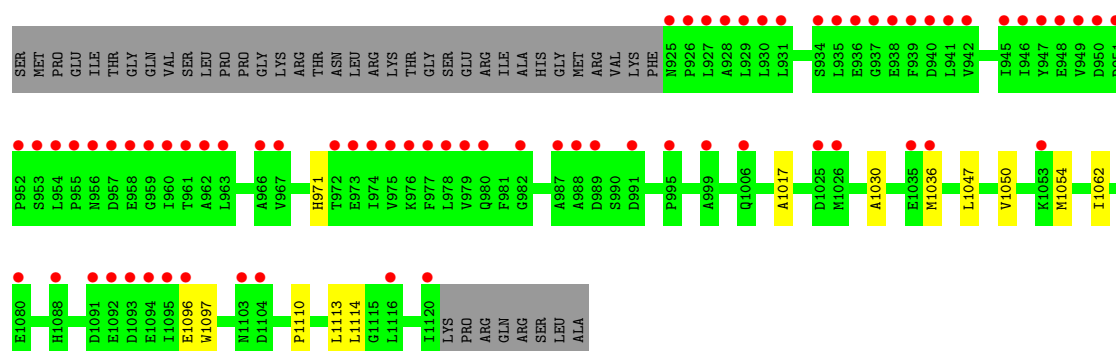
- Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain B: 



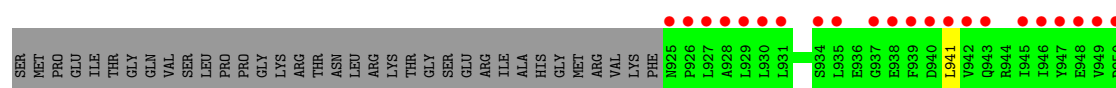
- Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

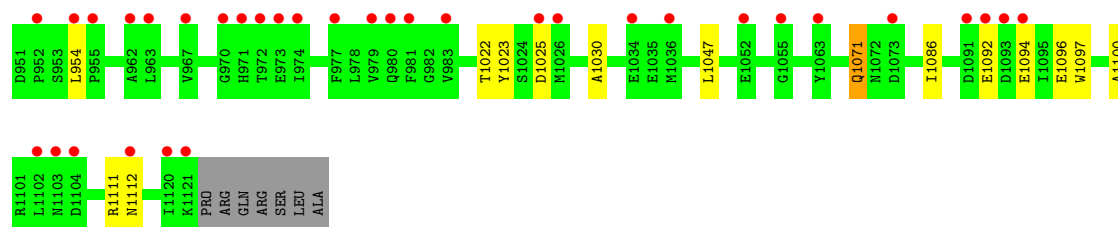
Chain D: 



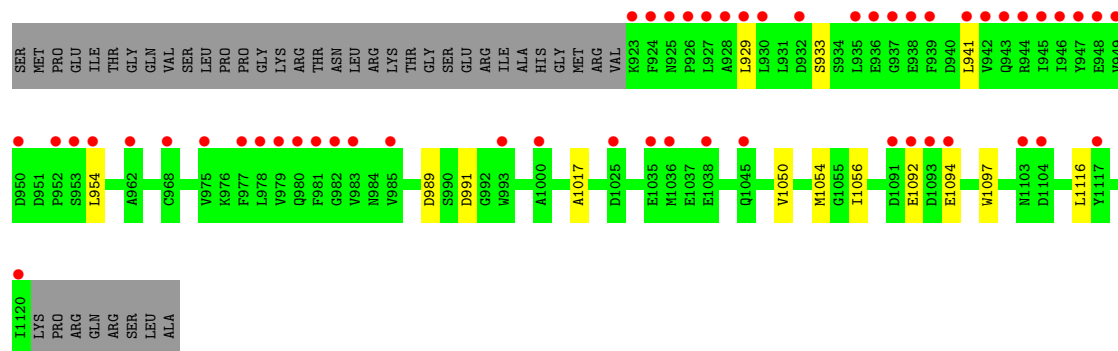
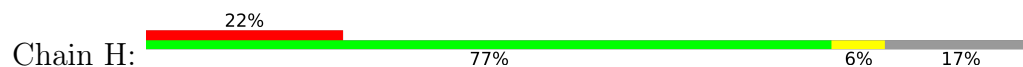
- Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2

Chain F: 

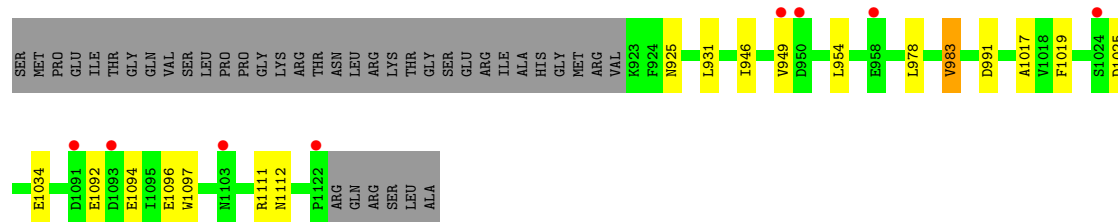
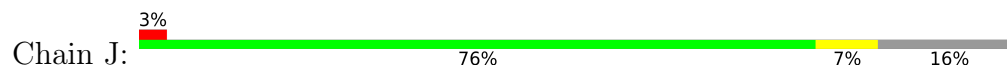




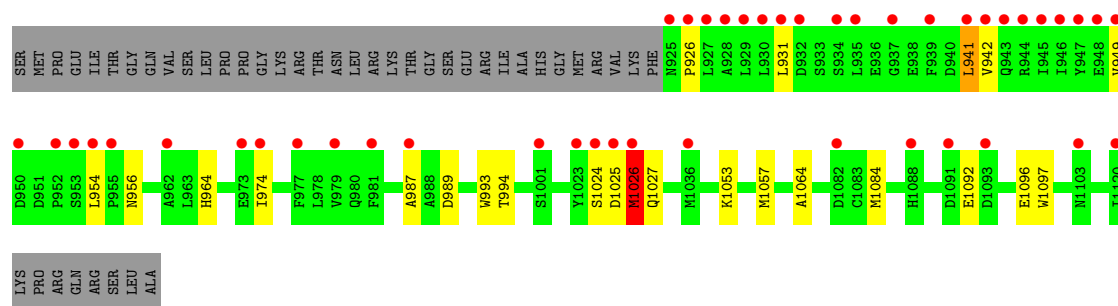
• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2



• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2



• Molecule 2: APOPTOSIS STIMULATING OF P53 PROTEIN 2



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
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.215 , 0.244 (Not available) , 0.208	Depositor DCC
R_{free} test set	5537 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	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: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.92	1/1633 (0.1%)	1.20	2/2226 (0.1%)
1	C	0.91	1/1627 (0.1%)	1.22	1/2217 (0.0%)
1	E	0.84	0/1599	1.23	2/2186 (0.1%)
1	G	1.00	2/1655 (0.1%)	1.23	3/2255 (0.1%)
1	I	0.96	1/1634 (0.1%)	1.23	4/2227 (0.2%)
1	K	0.89	0/1629	1.20	1/2220 (0.0%)
2	B	0.89	0/1574	1.29	4/2149 (0.2%)
2	D	0.86	0/1443	1.33	4/1977 (0.2%)
2	F	0.84	0/1469	1.34	5/2014 (0.2%)
2	H	0.82	0/1503	1.29	6/2057 (0.3%)
2	J	0.89	0/1568	1.29	7/2140 (0.3%)
2	L	0.90	0/1506	1.36	6/2059 (0.3%)
All	All	0.90	5/18840 (0.0%)	1.27	45/25727 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	266	MET	SD-CE	-13.96	1.44	1.79
1	C	266	MET	SD-CE	-13.72	1.45	1.79
1	I	266	MET	SD-CE	-13.48	1.45	1.79
1	A	266	MET	SD-CE	-10.93	1.52	1.79
1	G	257	MET	SD-CE	-7.05	1.61	1.79

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	255	ASN	CA-CB-CG	8.45	121.05	112.60
1	K	255	ASN	CA-CB-CG	7.96	120.56	112.60
1	E	255	ASN	CA-CB-CG	7.95	120.55	112.60
1	A	255	ASN	CA-CB-CG	7.91	120.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	989	ASP	CA-CB-CG	7.68	120.28	112.60
1	I	255	ASN	CA-CB-CG	7.45	120.05	112.60
2	F	1112	ASN	CA-CB-CG	6.75	119.35	112.60
1	E	266	MET	CB-CG-SD	-6.67	92.68	112.70
2	H	1056	ILE	N-CA-C	-6.54	106.46	111.62
2	J	1094	GLU	CA-C-N	6.39	129.22	120.46
2	J	1094	GLU	C-N-CA	6.39	129.22	120.46
2	H	989	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	255	ASN	CA-CB-CG	6.16	118.76	112.60
2	J	1017	ALA	CA-C-N	5.91	128.22	120.60
2	J	1017	ALA	C-N-CA	5.91	128.22	120.60
2	L	956	ASN	CA-CB-CG	5.90	118.50	112.60
2	L	1026	MET	CA-C-N	5.58	129.48	121.50
2	L	1026	MET	C-N-CA	5.58	129.48	121.50
2	F	1111	ARG	CA-C-N	5.53	127.69	120.28
2	F	1111	ARG	C-N-CA	5.53	127.69	120.28
1	G	298	PRO	CA-C-N	5.45	126.03	119.98
1	G	298	PRO	C-N-CA	5.45	126.03	119.98
1	A	259	ASN	CA-CB-CG	5.40	118.00	112.60
2	J	925	ASN	CA-CB-CG	5.39	117.99	112.60
2	H	1094	GLU	CA-C-N	5.29	127.70	120.46
2	H	1094	GLU	C-N-CA	5.29	127.70	120.46
1	I	136	THR	CA-C-N	5.29	128.59	120.82
1	I	136	THR	C-N-CA	5.29	128.59	120.82
1	I	227	ASP	CA-CB-CG	5.23	117.83	112.60
2	H	1017	ALA	CA-C-N	5.19	127.09	120.56
2	H	1017	ALA	C-N-CA	5.19	127.09	120.56
2	F	1094	GLU	CA-C-N	5.14	128.59	120.47
2	F	1094	GLU	C-N-CA	5.14	128.59	120.47
2	D	1017	ALA	CA-C-N	5.13	127.02	120.56
2	D	1017	ALA	C-N-CA	5.13	127.02	120.56
2	B	1067	ASP	CA-CB-CG	5.13	117.73	112.60
2	D	971	HIS	CA-C-N	5.10	127.37	120.38
2	D	971	HIS	C-N-CA	5.10	127.37	120.38
2	J	1034	GLU	CA-C-N	5.10	127.12	120.28
2	J	1034	GLU	C-N-CA	5.10	127.12	120.28
2	L	941	LEU	CA-C-N	5.10	127.18	120.60
2	L	941	LEU	C-N-CA	5.10	127.18	120.60
2	B	1025	ASP	N-CA-C	-5.03	102.62	110.42
2	B	1025	ASP	CA-C-N	-5.02	114.91	122.24
2	B	1025	ASP	C-N-CA	-5.02	114.91	122.24

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	19	0
1	C	1586	0	1535	31	0
1	E	1558	0	1478	39	0
1	G	1608	0	1568	41	0
1	I	1593	0	1541	27	0
1	K	1588	0	1537	36	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	9	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	17	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:C:307:ASP:CG	5:C:2090:HOH:O	1.87	1.13
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:G:281:ASP:HB3	5:I:2060:HOH:O	1.55	1.05
1:G:286:GLY:C	5:G:2101:HOH:O	1.99	1.04
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:229:PRO:HG2	5:G:2090:HOH:O	1.78	0.82
1:G:276:THR:HG21	1:G:287:ARG:NH1	1.94	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:C:255:ASN:HB3	1:C:257:MET:HE1	1.65	0.79
1:G:138:LYS:CB	5:G:2109:HOH:O	2.30	0.79
1:I:255:ASN:HB3	1:I:257:MET:HE1	1.63	0.78
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:A:255:ASN:HB3	1:A:257:MET:HE1	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ASN:HB3	1:G:257:MET:HE2	1.71	0.73
1:E:193:ARG:HG3	1:E:258:CYS:SG	2.29	0.72
1:G:276:THR:HG21	1:G:287:ARG:HH11	1.52	0.72
1:K:239:PRO:CG	5:K:2082:HOH:O	2.17	0.72
1:A:255:ASN:HB3	1:A:257:MET:CE	2.19	0.72
1:G:255:ASN:HB3	1:G:257:MET:CE	2.20	0.72
1:C:255:ASN:HB2	1:C:257:MET:CE	2.20	0.71
1:K:255:ASN:HB3	1:K:257:MET:HE1	1.71	0.71
1:C:309:TYR:O	5:C:2093:HOH:O	2.07	0.71
1:I:255:ASN:CB	1:I:257:MET:HE1	2.21	0.70
1:K:255:ASN:CB	1:K:257:MET:CE	2.69	0.69
1:C:255:ASN:CB	1:C:257:MET:HE1	2.22	0.69
1:I:266:MET:HE2	1:I:271:ILE:HG21	1.75	0.69
1:G:255:ASN:CB	1:G:257:MET:HE2	2.22	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:E:128:GLU:C	5:E:2009:HOH:O	2.35	0.68
1:A:193:ARG:HD3	1:A:211:ALA:O	1.92	0.68
2:L:1026:MET:HG2	5:L:2006:HOH:O	1.93	0.67
1:K:255:ASN:CB	1:K:257:MET:HE1	2.27	0.65
1:E:182:LYS:HB3	5:E:2024:HOH:O	1.96	0.65
1:C:121:TYR:O	5:C:2011:HOH:O	2.15	0.65
1:G:266:MET:HE2	1:G:271:ILE:HG21	1.79	0.65
1:A:264:GLY:H	1:A:267:ASN:HD22	1.44	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:I:255:ASN:HB3	1:I:257:MET:CE	2.23	0.63
1:G:255:ASN:CB	1:G:257:MET:CE	2.76	0.63
1:A:255:ASN:CB	1:A:257:MET:HE1	2.28	0.62
1:K:255:ASN:HB2	1:K:257:MET:HE3	1.83	0.60
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: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
1:I:255:ASN:HB2	1:I:257:MET:HE3	1.86	0.57
2:D:1110:PRO:HG2	2:D:1113:LEU:HD22	1.86	0.57
1:E:193:ARG:NE	1:E:257:MET:HB3	2.19	0.57
1:E:280:ARG:HA	5:E:2049:HOH:O	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLN:H	1:E:162:GLN:HE22	1.52	0.56
1:I:276:THR:CG2	1:I:287:ARG:CG	2.59	0.56
1:G:247:THR:HG22	1:G:248:GLU:H	1.71	0.56
1:K:255:ASN:HB3	1:K:257:MET:CE	2.34	0.55
1:E:255:ASN:HB3	1:E:257:MET:CE	2.36	0.55
1:I:290:PHE:HB3	5:I:2022:HOH:O	2.06	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
2:L:1025:ASP:C	2:L:1027:GLN:H	2.15	0.54
1:G:216:ARG:HD2	1:G:257:MET:HE3	1.89	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:E:156:ALA:HA	1:E:257:MET:HE1	1.90	0.53
1:C:193:ARG:HG3	1:C:258:CYS:SG	2.48	0.53
1:K:287:ARG:HE	4:K:1319:ACT:C	2.22	0.52
1:E:225:TYR:CZ	5:E:2032:HOH:O	2.54	0.52
1:G:284:VAL:HG12	5:G:2101:HOH:O	1.98	0.52
2:D:1050:VAL:HG13	5:D:2007:HOH:O	2.09	0.51
1:K:193:ARG:HG2	1:K:258:CYS:SG	2.51	0.51
2:J:1025:ASP:O	2:J:1025:ASP:OD1	2.29	0.51
4:C:1320:ACT:OXT	1:I:287:ARG:NE	2.36	0.51
2:L:1096:GLU:HG2	2:L:1097:TRP:CD1	2.46	0.50
1:A:255:ASN:HB2	1:A:257:MET:HE3	1.93	0.50
1:E:200:GLY:HA2	2:F:1023:TYR:O	2.11	0.50
2:H:1050:VAL:O	2:H:1054:MET:HB2	2.12	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: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:K:239:PRO:CD	5:K:2082:HOH:O	2.56	0.48
1:C:286:GLY:C	5:C:2011:HOH:O	2.52	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:119:THR:HG21	5:I:2025:HOH:O	2.14	0.47
1:C:226:VAL:CG1	5:C:2042:HOH:O	2.41	0.47
1:K:276:THR:CG2	1:K:287:ARG:CG	2.63	0.47
1:C:134:SER:HB2	1:C:143:THR:HA	1.98	0.46
1:C:255:ASN:HB3	1:C:257:MET:CE	2.34	0.46
1:G:247:THR:HG22	1:G:248:GLU:N	2.31	0.46
1:G:255:ASN:HB2	1:G:257:MET:CE	2.45	0.46
2:J:1025:ASP:OD1	2:J:1025:ASP:C	2.59	0.46
1:K:239:PRO:HD2	5:K:2082:HOH:O	2.15	0.46
1:C:200:GLY:O	1:C:204:ASN:ND2	2.48	0.46
1:E:288:ARG:CG	5:E:2007:HOH:O	2.30	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
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
5:I:2096:HOH:O	2:J:1096:GLU:HG2	2.15	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: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
1:G:136:THR:CG2	5:G:2110:HOH:O	2.31	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:O	2:F:1025:ASP:OD1	2.36	0.44
1:G:223:SER:OG	1:I:280:ARG:NH2	2.50	0.44
1:K:264:GLY:H	1:K:267:ASN:ND2	2.15	0.44
1:A:134:SER:HB2	1:A:143:THR:HA	2.00	0.44
1:G:255:ASN:HB2	1:G:257:MET:HE2	1.98	0.44
1:A:255:ASN:CB	1:A:257:MET:HE2	2.45	0.44
1:E:255:ASN:HB3	1:E:257:MET:HE3	1.99	0.44
1:A:264:GLY:H	1:A:267:ASN:ND2	2.14	0.43
1:E:279:MET:SD	1:E:285:LEU:HD11	2.58	0.43
1:I:266:MET:HE2	1:I:271:ILE:CG2	2.47	0.43
1:C:255:ASN:HB2	1:C:257:MET:HE3	1.98	0.43
2:J:946:ILE:O	2:J:949:VAL:HG22	2.18	0.43
1:K:193:ARG:NH2	1:K:197:HIS:HB3	2.33	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
2:D:1062:ILE:HD13	2:D:1114:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:SER:HB2	1:G:143:THR:HA	2.01	0.43
1:E:134:SER:HB2	1:E:143:THR:HA	1.99	0.42
1:G:155:ILE:HG23	5:G:2032:HOH:O	2.17	0.42
1:G:284:VAL:HG13	5:G:2101:HOH:O	2.05	0.42
2:J:1019:PHE:HB2	2:J:1112:ASN:HA	1.99	0.42
1:C:119:THR:CG2	5:I:2025:HOH:O	2.66	0.42
1:G:121:TYR:HB2	4:G:1319:ACT:H2	2.01	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: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: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:F:1030:ALA:HB2	2:F:1047:LEU:HB3	2.02	0.41
2:J:1096:GLU:HA	2:J:1111:ARG:HG2	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
2:F:1086:ILE:HD13	2:F:1100:ALA:HB2	2.03	0.40
5:I:2098:HOH:O	2:J:1097:TRP:CE2	2.46	0.40
2:D:1030:ALA:HB2	2:D:1047:LEU:HB3	2.04	0.40
2:L:1064:ALA:HB2	2:L:1084:MET:HE1	2.04	0.40
1:G:255:ASN:HB3	1:G:257:MET:HE1	1.98	0.40
1:K:115:ILE:HD11	1:K:188:THR:HG22	2.04	0.40
1:K:161:ILE:HD12	1:K:254:TYR:HD2	1.83	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 ⓘ

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%)	24	29
1	C	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	24	29
1	E	203/208 (98%)	200 (98%)	2 (1%)	1 (0%)	24	29
1	G	205/208 (99%)	203 (99%)	1 (0%)	1 (0%)	24	29
1	I	203/208 (98%)	201 (99%)	1 (0%)	1 (0%)	24	29
1	K	203/208 (98%)	200 (98%)	2 (1%)	1 (0%)	24	29
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%)	12	13
All	All	2397/2682 (89%)	2340 (98%)	49 (2%)	8 (0%)	36	44

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 ⓘ

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%)	170 (98%)	4 (2%)	44	60
1	C	174/183 (95%)	172 (99%)	2 (1%)	65	79
1	E	167/183 (91%)	164 (98%)	3 (2%)	51	68
1	G	179/183 (98%)	176 (98%)	3 (2%)	53	70
1	I	176/183 (96%)	172 (98%)	4 (2%)	44	60
1	K	174/183 (95%)	171 (98%)	3 (2%)	53	70
2	B	156/205 (76%)	152 (97%)	4 (3%)	40	56
2	D	132/205 (64%)	131 (99%)	1 (1%)	73	84
2	F	136/205 (66%)	132 (97%)	4 (3%)	37	52
2	H	142/205 (69%)	139 (98%)	3 (2%)	47	63
2	J	157/205 (77%)	153 (98%)	4 (2%)	42	58
2	L	146/205 (71%)	142 (97%)	4 (3%)	39	55
All	All	1913/2328 (82%)	1874 (98%)	39 (2%)	48	65

All (39) 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
1	A	294	ILE
2	B	954	LEU
2	B	1054	MET
2	B	1092	GLU
2	B	1113	LEU
1	C	162	GLN
1	C	258	CYS
2	D	1036	MET
1	E	227	ASP
1	E	263	VAL
1	E	294	ILE
2	F	941	LEU
2	F	954	LEU
2	F	1071	GLN
2	F	1092	GLU
1	G	114	VAL
1	G	258	CYS
1	G	294	ILE
2	H	941	LEU

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Mol	Chain	Res	Type
2	H	954	LEU
2	H	1092	GLU
1	I	227	ASP
1	I	263	VAL
1	I	294	ILE
1	I	297	CYS
2	J	931	LEU
2	J	954	LEU
2	J	983	VAL
2	J	1092	GLU
1	K	138	LYS
1	K	227	ASP
1	K	294	ILE
2	L	931	LEU
2	L	941	LEU
2	L	954	LEU
2	L	1092	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	162	GLN
1	A	196	ASN
1	A	234	GLN
1	A	267	ASN
1	A	318	GLN
2	B	925	ASN
2	B	980	GLN
2	B	1027	GLN
2	B	1042	GLN
2	B	1058	ASN
1	C	154	GLN
1	C	224	GLN
1	C	234	GLN
1	C	267	ASN
1	C	308	HIS
2	D	965	ASN
2	D	1071	GLN
1	E	162	GLN
1	E	267	ASN
2	F	1058	ASN

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Mol	Chain	Res	Type
1	G	125	HIS
1	G	154	GLN
1	G	207	GLN
1	G	224	GLN
1	G	267	ASN
1	G	318	GLN
2	H	965	ASN
2	H	1042	GLN
2	H	1071	GLN
1	I	154	GLN
1	I	196	ASN
1	I	318	GLN
2	J	925	ASN
2	J	965	ASN
1	K	154	GLN
1	K	267	ASN
2	L	964	HIS
2	L	980	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	K	1319	-	3,3,3	0.99	0	3,3,3	0.89	0
4	ACT	K	1320	-	3,3,3	1.20	0	3,3,3	1.14	0
4	ACT	L	1522	-	3,3,3	0.99	0	3,3,3	0.95	0
4	ACT	C	1321	-	3,3,3	0.97	0	3,3,3	1.09	0
4	ACT	I	1320	-	3,3,3	0.99	0	3,3,3	1.32	0
4	ACT	C	1319	-	3,3,3	1.13	0	3,3,3	0.82	0
4	ACT	C	1320	-	3,3,3	1.25	0	3,3,3	0.88	0
4	ACT	G	1319	-	3,3,3	0.79	0	3,3,3	1.04	0
4	ACT	I	1319	-	3,3,3	1.38	1 (33%)	3,3,3	0.99	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1319	ACT	CH3-C	2.12	1.57	1.49

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	K	1319	ACT	1	0
4	C	1320	ACT	1	0
4	G	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, 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%)	0.40	12 (5%)	28 29	24, 40, 68, 118	0
1	C	205/208 (98%)	0.71	24 (11%)	9 10	26, 43, 85, 96	0
1	E	205/208 (98%)	1.00	22 (10%)	11 12	34, 52, 83, 102	0
1	G	205/208 (98%)	0.36	10 (4%)	35 36	20, 37, 71, 112	2 (0%)
1	I	205/208 (98%)	0.30	15 (7%)	21 22	21, 36, 66, 115	0
1	K	205/208 (98%)	0.56	16 (7%)	19 20	23, 41, 75, 104	0
2	B	202/239 (84%)	0.78	16 (7%)	18 19	33, 49, 71, 97	0
2	D	196/239 (82%)	1.69	71 (36%)	1 1	38, 64, 104, 111	0
2	F	197/239 (82%)	1.60	56 (28%)	1 1	35, 61, 99, 114	0
2	H	198/239 (82%)	1.45	53 (26%)	1 1	38, 61, 89, 96	0
2	J	200/239 (83%)	0.40	8 (4%)	42 44	26, 44, 68, 86	0
2	L	196/239 (82%)	1.37	45 (22%)	2 2	32, 56, 102, 111	0
All	All	2419/2682 (90%)	0.88	348 (14%)	6 6	20, 48, 90, 118	2 (0%)

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	1024	SER	6.8
2	F	1121	LYS	6.5
2	F	947	TYR	6.5
2	F	925	ASN	6.1
2	D	950	ASP	6.0
2	L	925	ASN	5.9
2	D	939	PHE	5.9
1	C	114	VAL	5.8
2	F	939	PHE	5.5
1	C	318	GLN	5.5
2	F	941	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	1120	ILE	5.4
1	K	318	GLN	5.3
1	K	135	SER	5.3
2	F	927	LEU	5.2
2	F	1103	ASN	5.2
1	K	205	GLU	5.0
2	F	943	GLN	5.0
1	I	133	GLN	4.9
2	B	1121	LYS	4.9
2	B	1093	ASP	4.9
2	D	1120	ILE	4.9
2	D	977	PHE	4.9
2	F	940	ASP	4.8
2	D	952	PRO	4.8
2	D	941	LEU	4.8
2	D	928	ALA	4.8
1	E	318	GLN	4.7
2	B	920	MET	4.7
2	F	949	VAL	4.7
1	C	245	VAL	4.6
2	L	1025	ASP	4.6
1	E	245	VAL	4.6
1	C	136	THR	4.6
2	D	1093	ASP	4.5
2	F	1093	ASP	4.5
1	A	114	VAL	4.4
2	F	950	ASP	4.4
2	H	950	ASP	4.4
2	L	946	ILE	4.4
2	L	949	VAL	4.4
2	D	925	ASN	4.4
2	F	974	ILE	4.4
2	L	1093	ASP	4.4
2	F	929	LEU	4.3
2	D	940	ASP	4.3
2	B	1091	ASP	4.2
2	J	1093	ASP	4.2
2	H	946	ILE	4.2
2	H	1091	ASP	4.2
2	L	939	PHE	4.2
1	E	296	ALA	4.2
1	K	200	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	206	GLY	4.1
1	K	114	VAL	4.1
2	H	925	ASN	4.1
2	F	926	PRO	4.1
2	D	937	GLY	4.0
1	A	136	THR	4.0
2	L	947	TYR	4.0
1	A	133	GLN	3.9
2	F	1091	ASP	3.9
2	H	949	VAL	3.9
2	L	927	LEU	3.9
2	L	945	ILE	3.9
2	D	957	ASP	3.8
2	D	1036	MET	3.8
2	D	935	LEU	3.8
2	F	935	LEU	3.8
2	D	946	ILE	3.8
2	L	931	LEU	3.8
2	L	935	LEU	3.8
2	F	946	ILE	3.7
2	L	942	VAL	3.7
2	D	947	TYR	3.7
1	A	137	ALA	3.7
2	H	924	PHE	3.7
2	L	950	ASP	3.7
2	L	928	ALA	3.7
2	H	1035	GLU	3.7
2	D	954	LEU	3.6
2	F	928	ALA	3.6
2	D	958	GLU	3.6
2	H	943	GLN	3.6
2	D	927	LEU	3.6
1	I	245	VAL	3.6
2	F	942	VAL	3.6
1	E	133	GLN	3.6
1	E	275	ILE	3.5
1	C	203	PHE	3.5
1	A	318	GLN	3.5
2	D	976	LYS	3.5
1	I	136	THR	3.5
1	K	136	THR	3.5
2	D	1088	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	201	ARG	3.5
1	G	245	VAL	3.5
2	B	1103	ASN	3.5
2	F	1052	GLU	3.5
1	G	133	GLN	3.5
2	D	938	GLU	3.4
2	D	945	ILE	3.4
2	L	977	PHE	3.4
1	K	245	VAL	3.4
2	D	953	SER	3.4
2	F	945	ILE	3.4
2	D	972	THR	3.4
1	I	114	VAL	3.4
1	I	137	ALA	3.4
2	F	1104	ASP	3.4
1	E	161	ILE	3.3
2	D	926	PRO	3.3
1	K	203	PHE	3.3
2	H	977	PHE	3.3
1	C	247	THR	3.3
2	F	1092	GLU	3.3
2	L	948	GLU	3.3
2	L	952	PRO	3.3
2	D	942	VAL	3.3
2	F	934	SER	3.3
2	F	967	VAL	3.3
2	L	1026	MET	3.2
2	L	1091	ASP	3.2
1	K	138	LYS	3.2
2	L	926	PRO	3.2
2	H	947	TYR	3.2
2	D	962	ALA	3.2
2	J	1103	ASN	3.2
2	H	923	LYS	3.2
2	D	931	LEU	3.2
2	H	980	GLN	3.2
1	A	135	SER	3.2
1	C	137	ALA	3.2
1	C	317	PHE	3.1
2	D	1025	ASP	3.1
2	J	950	ASP	3.1
1	I	318	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	1092	GLU	3.1
2	F	938	GLU	3.1
2	F	948	GLU	3.1
1	E	135	SER	3.1
2	L	981	PHE	3.1
1	I	138	LYS	3.1
1	K	202	ASP	3.1
1	C	135	SER	3.1
2	F	937	GLY	3.1
1	A	245	VAL	3.1
2	D	1026	MET	3.1
2	H	1093	ASP	3.0
2	F	930	LEU	3.0
2	L	954	LEU	3.0
2	H	936	GLU	3.0
2	H	926	PRO	3.0
2	D	979	VAL	3.0
2	F	1112	ASN	3.0
2	J	1091	ASP	3.0
1	E	203	PHE	3.0
2	H	952	PRO	3.0
2	F	931	LEU	3.0
2	L	932	ASP	3.0
2	L	973	GLU	2.9
2	H	939	PHE	2.9
2	H	941	LEU	2.9
2	L	941	LEU	2.9
2	D	980	GLN	2.9
2	F	963	LEU	2.9
2	H	981	PHE	2.9
2	F	972	THR	2.9
2	H	927	LEU	2.8
2	H	962	ALA	2.8
2	D	973	GLU	2.8
2	F	1034	GLU	2.8
2	D	982	GLY	2.8
2	D	955	PRO	2.8
2	H	930	LEU	2.8
2	F	970	GLY	2.8
2	D	1006	GLN	2.8
2	F	955	PRO	2.8
2	F	1063	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	114	VAL	2.8
2	D	949	VAL	2.8
1	C	159	CYS	2.8
2	F	981	PHE	2.8
2	D	975	VAL	2.8
2	H	985	VAL	2.8
2	B	945	ILE	2.7
1	K	133	GLN	2.7
2	F	952	PRO	2.7
1	K	137	ALA	2.7
1	G	203	PHE	2.7
1	E	221	ASN	2.7
2	H	1094	GLU	2.7
2	F	1026	MET	2.7
1	C	280	ARG	2.7
1	G	137	ALA	2.7
1	E	114	VAL	2.7
2	D	961	THR	2.7
2	D	1091	ASP	2.7
2	H	932	ASP	2.7
1	C	138	LYS	2.7
2	D	936	GLU	2.7
2	B	931	LEU	2.7
2	D	1103	ASN	2.7
2	H	1104	ASP	2.7
2	F	1094	GLU	2.7
2	F	979	VAL	2.6
2	H	979	VAL	2.6
2	B	921	ARG	2.6
2	L	955	PRO	2.6
2	F	1036	MET	2.6
1	E	138	LYS	2.6
1	E	247	THR	2.6
2	D	1095	ILE	2.6
2	L	953	SER	2.6
2	L	1120	ILE	2.6
1	I	132	GLN	2.6
2	L	929	LEU	2.6
1	E	159	CYS	2.6
2	D	948	GLU	2.6
2	F	1025	ASP	2.6
2	J	1122	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	134	SER	2.6
2	B	1036	MET	2.6
1	E	136	THR	2.6
2	H	983	VAL	2.6
2	D	929	LEU	2.5
1	K	207	GLN	2.5
1	A	159	CYS	2.5
1	C	202	ASP	2.5
2	H	982	GLY	2.5
1	C	207	GLN	2.5
2	D	960	ILE	2.5
2	H	945	ILE	2.5
2	D	930	LEU	2.5
2	H	935	LEU	2.5
2	L	1103	ASN	2.5
1	G	206	GLY	2.5
1	I	135	SER	2.5
2	B	1052	GLU	2.5
1	E	222	LEU	2.5
2	H	1103	ASN	2.5
1	C	282	GLY	2.5
1	C	249	PHE	2.4
1	G	318	GLN	2.4
2	D	988	ALA	2.4
2	D	1092	GLU	2.4
2	H	993	TRP	2.4
2	F	971	HIS	2.4
2	L	1088	HIS	2.4
1	C	162	GLN	2.4
2	H	1045	GLN	2.4
2	H	938	GLU	2.4
2	F	1120	ILE	2.4
2	H	975	VAL	2.4
2	L	1036	MET	2.4
2	L	930	LEU	2.4
1	E	297	CYS	2.4
1	K	199	LEU	2.4
2	B	1088	HIS	2.4
2	B	950	ASP	2.3
2	D	1104	ASP	2.3
2	D	995	PRO	2.3
1	C	206	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	968	CYS	2.3
2	J	949	VAL	2.3
2	D	1080	GLU	2.3
2	F	980	GLN	2.3
2	L	1023	TYR	2.3
2	F	962	ALA	2.3
1	E	208	SER	2.3
2	D	974	ILE	2.3
2	B	1094	GLU	2.3
2	D	1035	GLU	2.3
2	F	973	GLU	2.3
2	H	1117	TYR	2.3
2	H	928	ALA	2.3
1	A	132	GLN	2.3
2	D	999	ALA	2.3
2	F	977	PHE	2.2
2	D	951	ASP	2.2
2	D	991	ASP	2.2
2	H	1025	ASP	2.2
2	H	944	ARG	2.2
2	F	1055	GLY	2.2
2	D	1096	GLU	2.2
1	E	166	SER	2.2
2	F	954	LEU	2.2
2	H	929	LEU	2.2
2	F	1073	ASP	2.2
2	L	937	GLY	2.2
2	H	1092	GLU	2.2
1	E	240	TYR	2.2
2	D	1116	LEU	2.2
2	F	983	VAL	2.2
1	E	127	PHE	2.2
1	A	138	LYS	2.2
2	H	948	GLU	2.2
2	D	934	SER	2.2
2	H	953	SER	2.2
2	L	1001	SER	2.2
2	D	963	LEU	2.1
2	D	978	LEU	2.1
2	H	954	LEU	2.1
1	E	202	ASP	2.1
2	D	1053	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	937	GLY	2.1
2	L	934	SER	2.1
2	L	987	ALA	2.1
2	D	967	VAL	2.1
1	I	244	GLN	2.1
2	B	939	PHE	2.1
1	C	246	GLY	2.1
2	D	959	GLY	2.1
1	C	141	THR	2.1
2	D	966	ALA	2.1
2	H	1000	ALA	2.1
2	J	1024	SER	2.1
1	C	248	GLU	2.1
2	D	1094	GLU	2.1
2	F	1102	LEU	2.1
2	L	943	GLN	2.1
1	I	206	GLY	2.1
2	L	944	ARG	2.1
1	C	297	CYS	2.1
2	H	1038	GLU	2.1
2	L	974	ILE	2.1
2	H	942	VAL	2.1
1	I	203	PHE	2.1
2	J	958	GLU	2.0
2	L	962	ALA	2.0
1	G	244	GLN	2.0
2	D	956	ASN	2.0
2	D	989	ASP	2.0
1	C	201	ARG	2.0
2	B	979	VAL	2.0
2	L	979	VAL	2.0
1	A	317	PHE	2.0
1	E	317	PHE	2.0
2	H	1036	MET	2.0
1	I	139	SER	2.0
2	D	987	ALA	2.0
1	A	258	CYS	2.0
1	G	153	CYS	2.0
1	G	207	GLN	2.0
1	I	297	CYS	2.0
2	H	978	LEU	2.0
2	L	1082	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	170	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	L	1522	4/4	0.79	0.25	49,50,55,56	0
4	ACT	C	1321	4/4	0.84	0.33	42,50,55,58	0
4	ACT	I	1319	4/4	0.85	0.16	54,54,57,67	0
4	ACT	K	1320	4/4	0.86	0.17	60,64,64,66	0
4	ACT	I	1320	4/4	0.86	0.18	49,50,51,52	0
4	ACT	C	1319	4/4	0.87	0.16	75,77,78,81	0
4	ACT	G	1319	4/4	0.87	0.23	46,46,52,56	0
4	ACT	C	1320	4/4	0.93	0.20	34,35,41,56	0
4	ACT	K	1319	4/4	0.93	0.32	88,89,89,94	0
3	ZN	K	1	1/1	0.99	0.04	39,39,39,39	0
3	ZN	E	1	1/1	0.99	0.03	45,45,45,45	0
3	ZN	G	1	1/1	1.00	0.06	37,37,37,37	0
3	ZN	I	1	1/1	1.00	0.03	30,30,30,30	0
3	ZN	C	1	1/1	1.00	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.