



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:57 pm BST

PDB ID : 1KWP
Title : Crystal Structure of MAPKAP2
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Deposited on : 2002-01-30
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

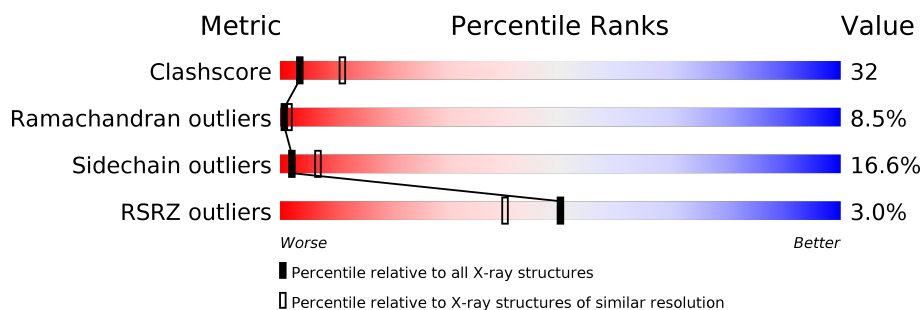
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	400	<div> <div>2%</div> <div>33%</div> <div>31%</div> <div>14%</div> <div>•</div> <div>20%</div> </div>
1	B	400	<div> <div>3%</div> <div>30%</div> <div>33%</div> <div>13%</div> <div>•</div> <div>22%</div> </div>

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
2	HG	B	405	-	-	X	-
2	HG	B	406	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4899 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MAP Kinase Activated Protein Kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2420	1544	419	440	17			
1	B	313	Total	C	N	O	S	0	0	0
			2331	1480	405	428	18			

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	7	Total	Hg	0	0
			7	7		
2	A	7	Total	Hg	0	0
			7	7		

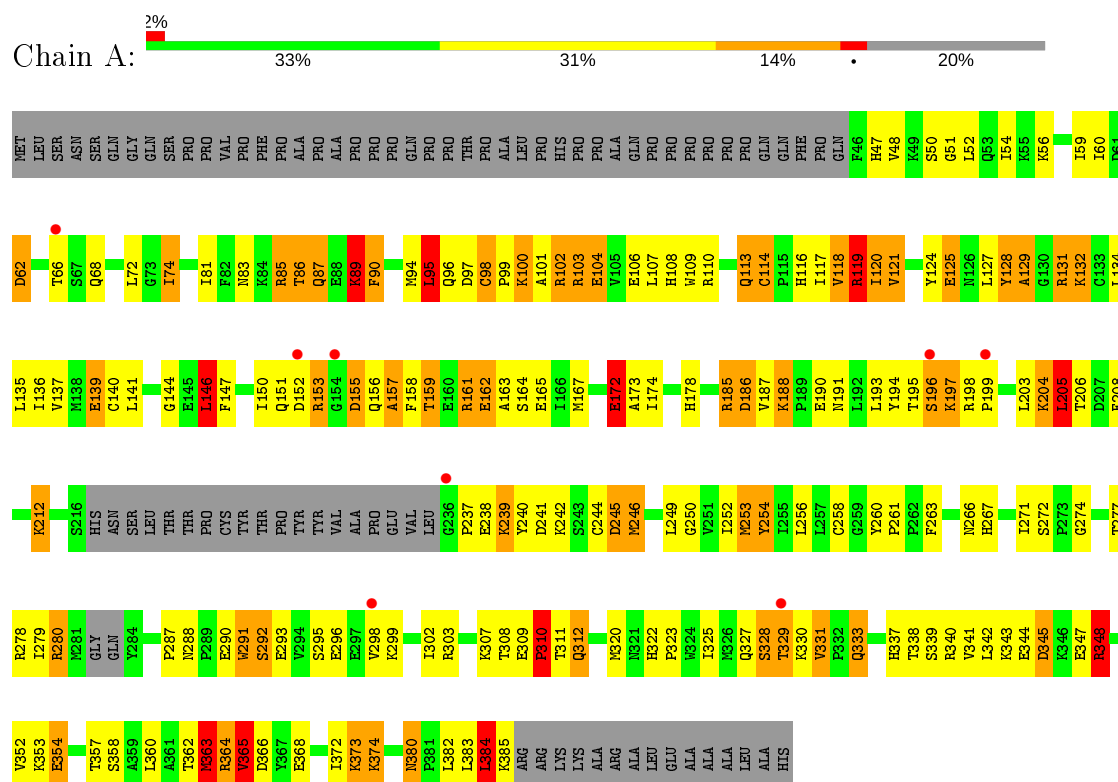
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	72	Total	O	0	0
			72	72		

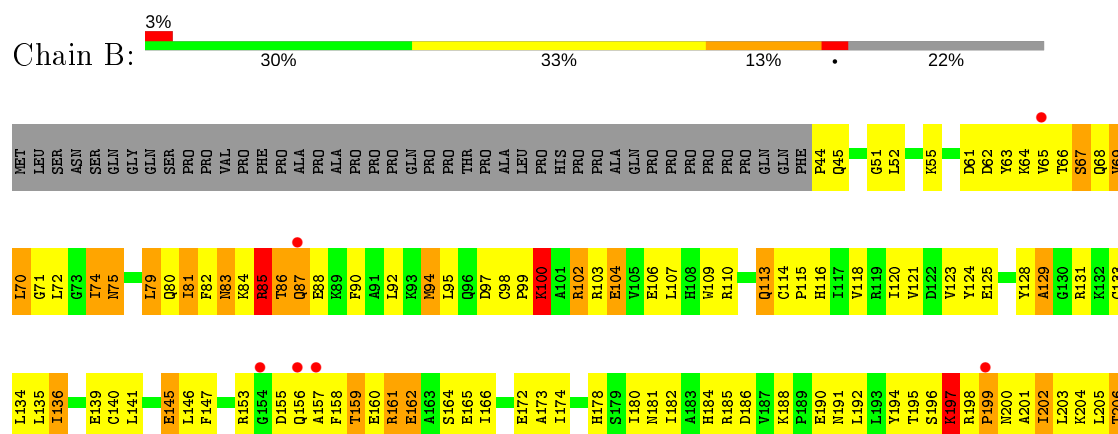
3 Residue-property plots

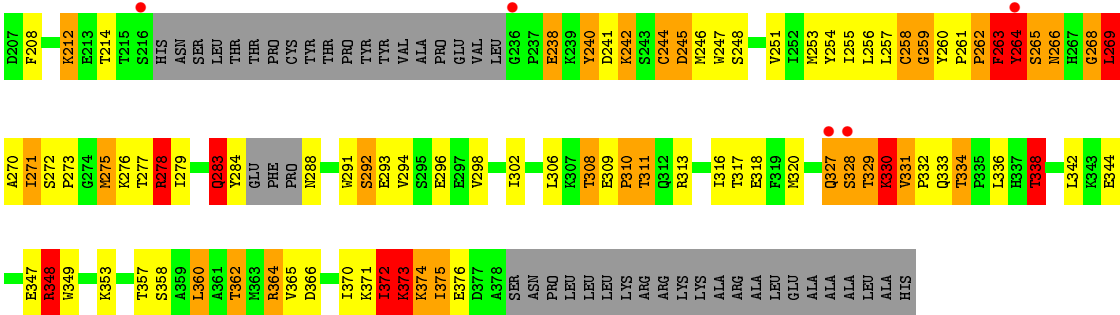
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: MAP Kinase Activated Protein Kinase 2



• Molecule 1: MAP Kinase Activated Protein Kinase 2





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	143.94Å 143.94Å 90.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.60 – 2.80 32.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.60-2.80) 100.0 (32.59-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.81Å)	Xtriage
Refinement program	CNX, REFMAC	Depositor
R, R_{free}	0.233 , 0.245 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 90.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.014 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.005 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$ 0.020 for $-1/3^*h-2/3^*k+4/3^*l, -2/3^*h-1/3^*k-4/3^*l, 1/3^*h-1/3^*k-1/3^*l$ 0.011 for $-h, 2/3^*h+1/3^*k+4/3^*l, 1/3^*h+2/3^*k-1/3^*l$ 0.012 for $1/3^*h+2/3^*k-4/3^*l, -k, -2/3^*h-1/3^*k-1/3^*l$ 0.026 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4899	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: HG

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	0.63	0/2468	1.80	58/3344 (1.7%)
1	B	0.69	1/2372 (0.0%)	1.91	65/3212 (2.0%)
All	All	0.66	1/4840 (0.0%)	1.86	123/6556 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	2
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	CYS	CB-SG	5.79	1.92	1.82

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ARG	NE-CZ-NH2	-21.91	109.35	120.30
1	A	278	ARG	NE-CZ-NH1	15.72	128.16	120.30
1	B	245	ASP	CB-CG-OD2	-15.05	104.75	118.30
1	B	103	ARG	CD-NE-CZ	13.96	143.15	123.60
1	B	244	CYS	CB-CA-C	11.88	134.15	110.40
1	B	63	TYR	CB-CG-CD1	11.19	127.71	121.00
1	A	103	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	62	ASP	CB-CG-OD2	10.31	127.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	B	258	CYS	CB-CA-C	9.53	129.45	110.40
1	A	110	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	A	153	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	B	268	GLY	N-CA-C	9.06	135.74	113.10
1	B	245	ASP	CB-CG-OD1	8.83	126.25	118.30
1	A	103	ARG	CD-NE-CZ	8.71	135.79	123.60
1	A	363	MET	CA-CB-CG	8.69	128.06	113.30
1	A	364	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	B	263	PHE	CB-CG-CD2	8.47	126.73	120.80
1	A	245	ASP	CB-CG-OD2	8.47	125.92	118.30
1	A	348	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	B	145	GLU	OE1-CD-OE2	8.25	133.20	123.30
1	B	246	MET	CG-SD-CE	-7.84	87.65	100.20
1	B	360	LEU	CA-CB-CG	7.79	133.21	115.30
1	A	131	ARG	CD-NE-CZ	7.52	134.13	123.60
1	A	212	LYS	CA-CB-CG	7.44	129.78	113.40
1	A	344	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	B	348	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	348	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	A	103	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	293	GLU	CA-CB-CG	6.92	128.61	113.40
1	A	66	THR	C-N-CA	6.84	138.79	121.70
1	A	253	MET	CA-CB-CG	6.83	124.92	113.30
1	A	161	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	B	63	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	B	278	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	186	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	68	GLN	N-CA-C	-6.60	93.19	111.00
1	A	278	ARG	CA-CB-CG	6.55	127.82	113.40
1	B	61	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	B	161	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	242	LYS	CA-CB-CG	6.48	127.66	113.40
1	B	263	PHE	C-N-CA	6.48	137.91	121.70
1	A	186	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	86	THR	CA-CB-CG2	6.47	121.46	112.40
1	B	331	VAL	N-CA-CB	6.47	125.74	111.50
1	B	311	THR	C-N-CA	6.47	137.87	121.70
1	A	62	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	194	TYR	CB-CG-CD1	6.38	124.83	121.00
1	A	86	THR	N-CA-CB	6.33	122.33	110.30
1	B	278	ARG	CG-CD-NE	6.33	125.10	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	278	ARG	CG-CD-NE	6.22	124.86	111.80
1	B	161	ARG	CD-NE-CZ	6.21	132.29	123.60
1	B	242	LYS	CD-CE-NZ	6.16	125.86	111.70
1	B	258	CYS	O-C-N	-6.16	112.73	123.20
1	B	44	PRO	N-CA-CB	6.15	110.69	103.30
1	B	103	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	119	ARG	CD-NE-CZ	6.12	132.17	123.60
1	A	172	GLU	OE1-CD-OE2	6.11	130.63	123.30
1	B	311	THR	O-C-N	-6.09	112.96	122.70
1	A	258	CYS	CA-C-O	6.04	132.78	120.10
1	A	153	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	128	TYR	CB-CG-CD1	5.94	124.57	121.00
1	A	258	CYS	O-C-N	-5.94	113.11	123.20
1	B	278	ARG	CD-NE-CZ	5.94	131.91	123.60
1	B	139	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	B	245	ASP	N-CA-CB	-5.89	99.99	110.60
1	A	237	PRO	CA-C-N	5.80	129.95	117.20
1	A	85	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	310	PRO	N-CA-C	5.79	127.14	112.10
1	A	374	LYS	N-CA-CB	5.75	120.96	110.60
1	B	62	ASP	OD1-CG-OD2	-5.75	112.37	123.30
1	B	194	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	B	94	MET	O-C-N	-5.71	113.57	122.70
1	B	364	ARG	CG-CD-NE	5.70	123.76	111.80
1	A	278	ARG	CB-CG-CD	5.67	126.35	111.60
1	B	258	CYS	CA-C-N	5.66	127.53	116.20
1	B	344	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	146	LEU	O-C-N	-5.66	113.65	122.70
1	B	245	ASP	O-C-N	-5.65	113.67	122.70
1	B	265	SER	CB-CA-C	5.59	120.73	110.10
1	B	364	ARG	CD-NE-CZ	5.57	131.39	123.60
1	A	354	GLU	CA-CB-CG	5.55	125.61	113.40
1	B	373	LYS	C-N-CA	5.55	135.58	121.70
1	B	240	TYR	O-C-N	-5.54	113.84	122.70
1	B	283	GLN	CA-C-O	5.53	131.71	120.10
1	B	128	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	172	GLU	CG-CD-OE2	-5.51	107.29	118.30
1	A	194	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	162	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	B	372	ILE	CA-CB-CG2	5.49	121.89	110.90
1	A	60	ILE	CB-CA-C	-5.49	100.63	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	MET	CA-CB-CG	5.48	122.61	113.30
1	A	246	MET	CG-SD-CE	-5.46	91.46	100.20
1	A	153	ARG	CD-NE-CZ	5.46	131.25	123.60
1	B	244	CYS	CA-CB-SG	-5.46	104.17	114.00
1	A	196	SER	N-CA-C	5.41	125.60	111.00
1	B	102	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	B	329	THR	C-N-CA	5.40	135.19	121.70
1	B	293	GLU	CB-CG-CD	5.39	128.76	114.20
1	B	110	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	185	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	205	LEU	N-CA-CB	5.33	121.06	110.40
1	B	197	LYS	N-CA-CB	5.33	120.19	110.60
1	A	260	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	140	CYS	N-CA-CB	-5.30	101.06	110.60
1	A	254	TYR	CB-CG-CD1	5.29	124.18	121.00
1	A	384	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	194	TYR	CB-CG-CD1	5.23	124.14	121.00
1	B	259	GLY	CA-C-O	5.22	129.99	120.60
1	A	128	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	264	TYR	CB-CG-CD2	5.20	124.12	121.00
1	A	329	THR	C-N-CA	5.20	134.71	121.70
1	B	85	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	329	THR	O-C-N	-5.17	114.43	122.70
1	A	340	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	100	LYS	N-CA-CB	5.12	119.81	110.60
1	A	364	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	365	VAL	CA-CB-CG2	5.10	118.55	110.90
1	B	206	THR	CA-CB-CG2	-5.08	105.28	112.40
1	B	259	GLY	O-C-N	-5.06	114.61	122.70
1	A	95	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	260	TYR	CB-CG-CD2	5.04	124.02	121.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	LEU	Mainchain
1	A	146	LEU	Mainchain
1	A	162	GLU	Mainchain
1	A	204	LYS	Mainchain
1	A	292	SER	Mainchain
1	A	293	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	366	ASP	Mainchain
1	A	51	GLY	Mainchain
1	B	129	ALA	Mainchain
1	B	262	PRO	Mainchain

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	2420	0	2307	143	0
1	B	2331	0	2173	154	0
2	A	7	0	0	1	0
2	B	7	0	0	5	0
3	A	62	0	0	5	0
3	B	72	0	0	10	1
All	All	4899	0	4480	297	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 32.

All (297) 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:B:244:CYS:SG	2:B:406:HG:HG	0.55	1.33
1:B:140:CYS:SG	2:B:405:HG:HG	1.67	1.12
1:B:140:CYS:HG	2:B:405:HG:HG	1.00	1.01
1:A:104:GLU:HA	1:A:107:LEU:HD12	1.43	0.99
1:A:309:GLU:N	1:A:310:PRO:HD2	1.80	0.96
1:A:114:CYS:SG	2:A:402:HG:HG	1.86	0.92
1:A:302:ILE:HD11	1:A:325:ILE:HD11	1.50	0.92
1:B:129:ALA:HB2	3:B:439:HOH:O	1.72	0.88
1:B:244:CYS:CB	2:B:406:HG:HG	1.81	0.87
1:A:322:HIS:HB3	1:A:325:ILE:HD13	1.56	0.86
1:B:118:VAL:HG21	1:B:206:THR:HB	1.56	0.86
1:A:173:ALA:HB1	1:A:205:LEU:HD21	1.60	0.83
1:A:380:ASN:HD22	1:A:382:LEU:H	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:HIS:HD2	1:B:186:ASP:H	1.26	0.82
1:B:268:GLY:O	1:B:269:LEU:HB2	1.77	0.82
1:A:167:MET:HG3	1:A:253:MET:HE3	1.64	0.80
1:A:102:ARG:HB2	1:A:102:ARG:HH11	1.47	0.79
1:A:309:GLU:H	1:A:310:PRO:HD2	1.43	0.79
1:A:345:ASP:HB3	1:A:348:ARG:HG2	1.65	0.78
1:B:118:VAL:HG22	1:B:141:LEU:HD11	1.67	0.76
1:B:52:LEU:HD13	1:B:109:TRP:CD1	2.21	0.76
1:B:184:HIS:CD2	1:B:186:ASP:H	2.06	0.74
1:A:132:LYS:HG3	3:A:463:HOH:O	1.88	0.73
1:A:271:ILE:HD13	1:A:280:ARG:CB	2.19	0.73
1:A:167:MET:HG3	1:A:253:MET:CE	2.17	0.73
1:B:328:SER:OG	3:B:448:HOH:O	1.98	0.72
1:B:174:ILE:HG22	1:B:316:ILE:HG12	1.71	0.72
1:B:116:HIS:ND1	1:B:202:ILE:HD11	2.07	0.68
1:B:118:VAL:CG2	1:B:206:THR:HB	2.23	0.68
1:A:97:ASP:O	1:A:98:CYS:HB3	1.94	0.67
1:B:258:CYS:SG	3:B:479:HOH:O	2.51	0.67
1:A:116:HIS:NE2	1:A:172:GLU:HG2	2.10	0.67
1:B:275:MET:HE3	1:B:279:ILE:HD11	1.77	0.67
1:A:173:ALA:CB	1:A:205:LEU:HD21	2.25	0.67
1:B:178:HIS:ND1	1:B:242:LYS:HE3	2.10	0.67
1:A:119:ARG:HH11	1:A:119:ARG:HG3	1.59	0.67
1:B:251:VAL:HA	1:B:262:PRO:HG3	1.76	0.66
1:A:380:ASN:ND2	1:A:382:LEU:H	1.95	0.65
1:B:52:LEU:HD11	1:B:123:VAL:HG11	1.77	0.65
1:B:255:ILE:HG12	1:B:261:PRO:HA	1.78	0.65
1:B:188:LYS:NZ	1:B:357:THR:OG1	2.22	0.65
1:A:380:ASN:HD21	1:A:382:LEU:HB2	1.61	0.65
1:B:94:MET:HG2	1:B:135:LEU:HD23	1.77	0.64
1:B:162:GLU:O	1:B:166:ILE:HG13	1.98	0.63
1:B:203:LEU:HD12	1:B:204:LYS:N	2.13	0.63
1:B:133:CYS:SG	2:B:404:HG:HG	2.17	0.63
1:A:309:GLU:N	1:A:310:PRO:CD	2.59	0.62
1:A:161:ARG:NH1	1:A:333:GLN:OE1	2.32	0.62
1:B:349:TRP:CE3	1:B:349:TRP:HA	2.35	0.62
1:B:372:ILE:O	1:B:373:LYS:HB2	1.98	0.62
1:A:167:MET:HE1	1:A:249:LEU:HD22	1.82	0.62
1:A:165:GLU:HG2	1:A:329:THR:HG22	1.82	0.62
1:B:205:LEU:H	1:B:205:LEU:HD23	1.64	0.62
1:B:261:PRO:O	1:B:263:PHE:CE1	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:THR:HG22	1:B:313:ARG:HA	1.82	0.62
1:B:261:PRO:HG2	1:B:263:PHE:CZ	2.36	0.61
1:A:104:GLU:O	1:A:107:LEU:HB2	2.02	0.60
1:A:141:LEU:HD21	1:A:204:LYS:HD2	1.83	0.60
1:B:87:GLN:OE1	1:B:88:GLU:N	2.33	0.60
1:A:240:TYR:CE1	1:A:365:VAL:HG13	2.37	0.60
1:B:268:GLY:O	1:B:269:LEU:CB	2.47	0.60
1:A:99:PRO:O	1:A:100:LYS:HB3	2.01	0.59
1:B:146:LEU:HB3	3:B:472:HOH:O	2.02	0.59
1:A:348:ARG:O	1:A:352:VAL:HG23	2.03	0.59
1:A:96:GLN:HG2	3:A:412:HOH:O	2.02	0.59
1:A:119:ARG:HH11	1:A:119:ARG:CG	2.16	0.59
1:A:302:ILE:HD11	1:A:325:ILE:CD1	2.29	0.59
1:B:203:LEU:HD12	1:B:204:LYS:H	1.68	0.59
1:A:118:VAL:HG23	1:A:205:LEU:O	2.03	0.58
1:A:328:SER:OG	1:A:329:THR:HG23	2.02	0.58
1:A:102:ARG:HH11	1:A:102:ARG:CB	2.15	0.58
1:B:199:PRO:O	1:B:201:ALA:N	2.36	0.58
1:B:275:MET:O	1:B:276:LYS:HB2	2.03	0.58
1:A:203:LEU:HG	3:A:465:HOH:O	2.03	0.58
1:B:165:GLU:CG	3:B:448:HOH:O	2.50	0.58
1:A:94:MET:HG2	1:A:135:LEU:HD23	1.84	0.58
1:B:68:GLN:O	1:B:70:LEU:N	2.37	0.58
1:A:167:MET:CE	1:A:249:LEU:HD22	2.32	0.58
1:A:274:GLY:O	1:A:277:THR:HG22	2.03	0.58
1:B:156:GLN:O	1:B:157:ALA:HB3	2.04	0.58
1:A:83:ASN:O	1:A:87:GLN:HA	2.04	0.57
1:A:302:ILE:HG23	1:A:303:ARG:N	2.20	0.57
1:B:75:ASN:H	1:B:75:ASN:HD22	1.52	0.57
1:B:79:LEU:HD12	1:B:92:LEU:HB3	1.86	0.57
1:A:136:ILE:N	1:A:136:ILE:HD12	2.20	0.56
1:B:263:PHE:CE1	1:B:264:TYR:CE1	2.93	0.56
1:B:52:LEU:HD11	1:B:123:VAL:CG1	2.35	0.56
1:A:150:ILE:O	1:A:151:GLN:C	2.44	0.56
1:A:244:CYS:HA	1:A:363:MET:HE1	1.86	0.56
1:B:172:GLU:HG3	1:B:320:MET:CE	2.35	0.56
1:A:136:ILE:H	1:A:136:ILE:HD12	1.69	0.56
1:B:212:LYS:HD3	1:B:241:ASP:OD2	2.05	0.56
1:B:349:TRP:HE3	1:B:349:TRP:HA	1.71	0.55
1:A:188:LYS:HG3	1:A:190:GLU:OE1	2.05	0.55
1:B:308:THR:CG2	1:B:313:ARG:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:CG1	1:B:261:PRO:HA	2.35	0.55
1:B:69:VAL:O	1:B:72:LEU:N	2.28	0.55
1:B:264:TYR:CD2	1:B:270:ALA:HA	2.42	0.55
1:B:198:ARG:CB	1:B:199:PRO:HD2	2.37	0.55
1:B:253:MET:HE1	1:B:302:ILE:HG12	1.87	0.55
1:A:117:ILE:HG22	1:A:118:VAL:O	2.08	0.54
1:B:165:GLU:HG3	3:B:448:HOH:O	2.07	0.54
1:A:52:LEU:HB2	1:A:109:TRP:CD2	2.42	0.54
1:A:322:HIS:ND1	1:A:323:PRO:HD2	2.23	0.54
1:B:134:LEU:HG	1:B:136:ILE:CD1	2.37	0.54
1:B:259:GLY:HA2	1:B:338:THR:HG23	1.90	0.53
1:B:113:GLN:O	1:B:114:CYS:C	2.47	0.53
1:B:104:GLU:HB2	1:B:208:PHE:O	2.09	0.53
1:B:67:SER:O	1:B:68:GLN:CB	2.56	0.53
1:B:298:VAL:O	1:B:302:ILE:HG22	2.08	0.53
1:A:205:LEU:N	1:A:205:LEU:HD23	2.24	0.53
1:A:320:MET:HA	1:A:325:ILE:HG21	1.91	0.53
1:B:173:ALA:HB1	1:B:205:LEU:HD21	1.89	0.53
1:A:157:ALA:HB3	3:A:436:HOH:O	2.09	0.53
1:B:205:LEU:N	1:B:205:LEU:HD23	2.24	0.53
1:B:331:VAL:HG23	1:B:332:PRO:O	2.09	0.52
1:A:296:GLU:HB2	1:A:299:LYS:H	1.74	0.52
1:A:52:LEU:HD12	1:A:109:TRP:CG	2.44	0.52
1:B:283:GLN:O	1:B:288:ASN:N	2.42	0.52
1:B:180:ILE:HD11	1:B:182:ILE:HD12	1.90	0.52
1:B:191:ASN:O	1:B:205:LEU:HA	2.09	0.52
1:A:196:SER:O	1:A:197:LYS:CB	2.57	0.52
1:A:360:LEU:HB3	1:A:364:ARG:NH2	2.25	0.52
1:A:238:GLU:HG2	1:A:239:LYS:HD2	1.92	0.52
1:B:85:ARG:O	1:B:86:THR:CB	2.57	0.52
1:A:338:THR:O	1:A:342:LEU:HD13	2.10	0.52
1:B:260:TYR:HE1	1:B:348:ARG:HH21	1.57	0.52
1:B:374:LYS:HA	3:B:469:HOH:O	2.10	0.52
1:A:159:THR:HG23	1:A:162:GLU:OE1	2.10	0.51
1:A:302:ILE:HG23	1:A:303:ARG:H	1.75	0.51
1:B:348:ARG:HG3	1:B:349:TRP:N	2.25	0.51
1:B:83:ASN:HD22	1:B:84:LYS:N	2.07	0.51
1:A:205:LEU:HD23	1:A:205:LEU:H	1.75	0.51
1:B:269:LEU:O	1:B:271:ILE:HD13	2.10	0.51
1:A:52:LEU:HD12	1:A:109:TRP:CB	2.41	0.51
1:B:265:SER:O	1:B:266:ASN:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD22	1:A:136:ILE:CD1	2.41	0.50
1:A:239:LYS:HD3	1:A:239:LYS:N	2.26	0.50
1:A:345:ASP:CB	1:A:348:ARG:HG2	2.39	0.50
1:A:161:ARG:O	1:A:165:GLU:HG3	2.11	0.50
1:A:250:GLY:HA3	1:A:307:LYS:HD3	1.94	0.50
1:B:254:TYR:CG	1:B:262:PRO:HB3	2.47	0.49
1:B:94:MET:HG2	1:B:135:LEU:CD2	2.42	0.49
1:A:101:ALA:O	1:A:104:GLU:HG3	2.12	0.49
1:A:287:PRO:O	1:A:288:ASN:C	2.49	0.49
1:B:178:HIS:CE1	1:B:242:LYS:HG2	2.47	0.49
1:B:68:GLN:O	1:B:69:VAL:CB	2.57	0.49
1:A:118:VAL:HG21	1:A:206:THR:HB	1.94	0.49
1:B:97:ASP:O	1:B:98:CYS:HB3	2.12	0.49
1:B:75:ASN:H	1:B:75:ASN:ND2	2.11	0.49
1:A:113:GLN:O	1:A:114:CYS:C	2.50	0.49
1:A:277:THR:HG21	1:A:363:MET:HB3	1.93	0.49
1:B:115:PRO:O	1:B:204:LYS:HE2	2.13	0.49
1:A:128:TYR:O	1:A:129:ALA:HB3	2.13	0.49
1:B:158:PHE:CD2	1:B:336:LEU:HD12	2.48	0.49
1:A:52:LEU:HD21	1:A:54:ILE:HG12	1.94	0.49
1:A:90:PHE:CE2	1:A:121:VAL:HG11	2.48	0.49
1:A:384:LEU:HD23	1:A:385:LYS:N	2.27	0.49
1:A:380:ASN:HD22	1:A:380:ASN:C	2.17	0.48
1:A:116:HIS:CD2	1:A:172:GLU:HG2	2.47	0.48
1:A:144:GLY:O	1:A:193:LEU:HD23	2.13	0.48
1:A:74:ILE:HD12	1:A:74:ILE:O	2.12	0.48
1:B:181:ASN:HB3	1:B:214:THR:O	2.13	0.48
1:B:276:LYS:HE2	3:B:432:HOH:O	2.13	0.48
1:B:372:ILE:O	1:B:373:LYS:CB	2.62	0.48
1:A:337:HIS:O	1:A:341:VAL:HG23	2.12	0.48
1:B:131:ARG:HD3	1:B:131:ARG:N	2.29	0.48
1:B:331:VAL:HB	1:B:332:PRO:HD2	1.94	0.48
1:A:97:ASP:O	1:A:98:CYS:CB	2.61	0.48
1:B:257:LEU:O	1:B:258:CYS:C	2.51	0.48
1:A:186:ASP:HA	1:A:360:LEU:HD13	1.96	0.48
1:A:52:LEU:C	1:A:52:LEU:HD23	2.35	0.47
1:A:327:GLN:O	1:A:330:LYS:HB3	2.14	0.47
1:A:95:LEU:HD22	1:A:136:ILE:HD11	1.97	0.47
1:B:97:ASP:OD2	1:B:102:ARG:NH2	2.46	0.47
1:B:172:GLU:HG3	1:B:320:MET:HE1	1.95	0.47
1:B:190:GLU:OE1	1:B:353:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HE3	1:A:373:LYS:HB3	1.70	0.47
1:B:333:GLN:O	1:B:334:THR:C	2.52	0.47
1:A:52:LEU:HB2	1:A:109:TRP:CE3	2.49	0.47
1:B:134:LEU:HG	1:B:136:ILE:HD11	1.96	0.47
1:B:283:GLN:O	1:B:284:TYR:CB	2.61	0.47
1:B:302:ILE:O	1:B:306:LEU:HG	2.15	0.47
1:B:275:MET:HG2	1:B:278:ARG:HH12	1.79	0.47
1:A:372:ILE:HD12	1:A:373:LYS:O	2.15	0.47
1:B:160:GLU:HG2	1:B:331:VAL:HG21	1.96	0.47
1:A:239:LYS:HD3	1:A:239:LYS:H	1.80	0.46
1:B:275:MET:CE	1:B:279:ILE:HD11	2.45	0.46
1:A:96:GLN:O	1:A:96:GLN:HG3	2.15	0.46
1:A:102:ARG:HH11	1:A:102:ARG:CG	2.28	0.46
1:B:114:CYS:SG	1:B:116:HIS:HB2	2.55	0.46
1:A:322:HIS:CB	1:A:325:ILE:HD13	2.36	0.46
1:B:202:ILE:HG12	1:B:203:LEU:N	2.30	0.46
1:B:74:ILE:HD13	1:B:75:ASN:N	2.30	0.46
1:B:317:THR:O	1:B:318:GLU:C	2.53	0.46
1:B:186:ASP:HA	1:B:360:LEU:HD13	1.97	0.46
1:A:99:PRO:O	1:A:100:LYS:CB	2.64	0.46
1:A:59:ILE:HG13	1:A:124:TYR:CD1	2.51	0.46
1:B:291:TRP:O	1:B:292:SER:O	2.34	0.46
1:A:155:ASP:O	1:A:156:GLN:C	2.53	0.46
1:A:161:ARG:HD3	1:A:331:VAL:O	2.16	0.46
1:A:246:MET:HE1	3:A:453:HOH:O	2.16	0.45
1:B:263:PHE:N	1:B:263:PHE:CD1	2.83	0.45
1:B:185:ARG:HB3	1:B:364:ARG:HD3	1.97	0.45
1:B:147:PHE:CE1	1:B:256:LEU:HD23	2.52	0.45
1:B:155:ASP:O	1:B:156:GLN:C	2.55	0.45
1:A:127:LEU:HD12	1:A:131:ARG:O	2.17	0.45
1:A:104:GLU:HB2	1:A:208:PHE:O	2.17	0.45
1:B:160:GLU:OE2	1:B:332:PRO:HG2	2.16	0.45
1:A:109:TRP:HD1	1:A:120:ILE:CD1	2.30	0.45
1:B:90:PHE:HE2	1:B:121:VAL:HG11	1.82	0.45
1:B:253:MET:O	1:B:256:LEU:HB2	2.15	0.45
1:B:71:GLY:O	1:B:74:ILE:HD12	2.17	0.45
1:A:119:ARG:HB3	1:A:139:GLU:OE2	2.16	0.45
1:A:325:ILE:HD12	1:A:325:ILE:N	2.32	0.45
1:B:159:THR:HG23	1:B:162:GLU:HG3	1.98	0.45
1:B:82:PHE:HE1	3:B:430:HOH:O	2.00	0.45
1:A:212:LYS:NZ	1:A:241:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:OH	1:A:287:PRO:HD3	2.17	0.45
1:B:165:GLU:HG2	3:B:448:HOH:O	2.15	0.45
1:A:108:HIS:HB2	1:A:208:PHE:CG	2.52	0.44
1:B:81:ILE:HD12	1:B:92:LEU:HB2	1.99	0.44
1:B:180:ILE:CD1	1:B:182:ILE:HD12	2.47	0.44
1:A:191:ASN:O	1:A:205:LEU:HA	2.17	0.44
1:A:190:GLU:OE2	1:A:353:LYS:HD2	2.18	0.44
1:A:252:ILE:HG22	1:A:256:LEU:HD12	1.99	0.44
1:A:97:ASP:CG	1:A:102:ARG:HH12	2.21	0.44
1:B:262:PRO:O	1:B:263:PHE:CB	2.65	0.44
1:A:119:ARG:HB2	1:A:119:ARG:NH1	2.33	0.44
1:B:265:SER:O	1:B:266:ASN:HB2	2.18	0.44
1:A:54:ILE:HG21	1:A:125:GLU:HB2	2.00	0.44
1:A:384:LEU:O	1:A:385:LYS:O	2.35	0.44
1:A:90:PHE:HE2	1:A:121:VAL:HG11	1.83	0.44
1:B:99:PRO:O	1:B:100:LYS:CB	2.66	0.44
1:B:358:SER:O	1:B:362:THR:HG23	2.18	0.44
1:A:158:PHE:CE2	1:A:163:ALA:HB2	2.52	0.44
1:A:185:ARG:HD3	1:A:241:ASP:OD2	2.18	0.44
1:A:89:LYS:O	1:A:90:PHE:HB2	2.18	0.44
1:B:278:ARG:CB	1:B:278:ARG:HH11	2.31	0.43
1:B:273:PRO:HB3	1:B:277:THR:HG21	2.01	0.43
1:A:81:ILE:HD11	1:A:137:VAL:HG13	2.00	0.43
1:B:69:VAL:O	1:B:71:GLY:N	2.51	0.43
1:A:167:MET:HG3	1:A:253:MET:HE2	1.99	0.43
1:A:290:GLU:O	1:A:291:TRP:CB	2.66	0.43
1:B:172:GLU:HG3	1:B:320:MET:HE2	1.97	0.43
1:A:141:LEU:HD23	1:A:195:THR:HG23	1.99	0.43
1:A:147:PHE:CZ	1:A:256:LEU:HG	2.54	0.43
1:A:47:HIS:O	1:A:48:VAL:C	2.55	0.43
1:B:371:LYS:HE3	1:B:371:LYS:HB2	1.80	0.43
1:A:358:SER:O	1:A:362:THR:HG23	2.19	0.43
1:B:309:GLU:O	1:B:310:PRO:O	2.37	0.43
1:B:86:THR:O	1:B:87:GLN:HB3	2.19	0.43
1:B:146:LEU:HG	1:B:147:PHE:N	2.34	0.43
1:B:164:SER:OG	1:B:328:SER:HB2	2.19	0.43
1:A:103:ARG:O	1:A:107:LEU:HG	2.18	0.42
1:A:164:SER:HB3	1:A:328:SER:HB2	2.01	0.42
1:B:261:PRO:HG2	1:B:263:PHE:CE2	2.53	0.42
1:A:240:TYR:O	1:A:241:ASP:C	2.53	0.42
1:B:263:PHE:CD1	1:B:264:TYR:CE1	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:N	1:B:75:ASN:HD22	2.16	0.42
1:A:117:ILE:O	1:A:118:VAL:C	2.58	0.42
1:B:66:THR:O	1:B:67:SER:O	2.37	0.42
1:B:97:ASP:OD2	1:B:125:GLU:HG3	2.20	0.42
1:A:198:ARG:CB	1:A:199:PRO:CD	2.98	0.42
1:B:263:PHE:N	1:B:263:PHE:HD1	2.18	0.42
1:A:261:PRO:HB2	1:A:263:PHE:CD2	2.54	0.42
1:A:150:ILE:O	1:A:153:ARG:HG3	2.20	0.41
1:A:303:ARG:O	1:A:307:LYS:HG2	2.20	0.41
1:A:59:ILE:HG13	1:A:124:TYR:CE1	2.55	0.41
1:B:192:LEU:HB3	1:B:203:LEU:HD11	2.02	0.41
1:A:198:ARG:CB	1:A:199:PRO:HD2	2.50	0.41
1:A:178:HIS:NE2	1:A:245:ASP:OD1	2.46	0.41
1:B:247:TRP:O	1:B:248:SER:C	2.55	0.41
1:B:51:GLY:HA2	1:B:109:TRP:CH2	2.56	0.41
1:B:196:SER:O	1:B:197:LYS:CB	2.67	0.41
1:B:373:LYS:HA	1:B:373:LYS:HD2	1.81	0.41
1:B:129:ALA:HB3	1:B:131:ARG:HG2	2.02	0.41
1:B:161:ARG:HA	1:B:331:VAL:HG22	2.02	0.41
1:A:310:PRO:HG2	1:A:312:GLN:HE21	1.85	0.41
1:B:269:LEU:O	1:B:270:ALA:HB3	2.19	0.41
1:B:374:LYS:O	1:B:375:ILE:CB	2.68	0.41
1:A:155:ASP:O	1:A:157:ALA:N	2.54	0.41
1:A:85:ARG:NH1	1:A:85:ARG:HG3	2.35	0.41
1:B:260:TYR:HB3	1:B:261:PRO:HD2	2.01	0.41
1:B:275:MET:HG2	1:B:278:ARG:NH1	2.35	0.41
1:A:174:ILE:HD11	1:A:187:VAL:HG21	2.02	0.40
1:A:161:ARG:HA	1:A:331:VAL:HG22	2.02	0.40
1:B:205:LEU:HG	1:B:205:LEU:O	2.20	0.40
1:A:354:GLU:O	1:A:357:THR:HB	2.22	0.40
1:B:141:LEU:CD2	1:B:195:THR:HG22	2.51	0.40
1:B:55:LYS:HB2	1:B:124:TYR:CD2	2.56	0.40
1:B:72:LEU:O	1:B:75:ASN:ND2	2.52	0.40
1:B:161:ARG:HD3	1:B:329:THR:OG1	2.21	0.40
1:A:242:LYS:O	1:A:246:MET:HE2	2.22	0.40
1:A:62:ASP:OD1	1:A:124:TYR:OH	2.27	0.40
1:B:327:GLN:HG2	1:B:330:LYS:HE3	2.04	0.40
1:B:240:TYR:CE1	1:B:365:VAL:HG13	2.56	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)
3:B:475:HOH:O	3:B:475:HOH:O[2_555]	1.85	0.35

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	313/400 (78%)	245 (78%)	46 (15%)	22 (7%)	1	3
1	B	307/400 (77%)	231 (75%)	45 (15%)	31 (10%)	0	1
All	All	620/800 (78%)	476 (77%)	91 (15%)	53 (8%)	1	1

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LYS
1	A	100	LYS
1	A	197	LYS
1	A	267	HIS
1	A	279	ILE
1	A	280	ARG
1	A	291	TRP
1	A	347	GLU
1	B	86	THR
1	B	100	LYS
1	B	200	ASN
1	B	266	ASN
1	B	269	LEU
1	B	283	GLN
1	B	292	SER
1	B	310	PRO
1	B	311	THR
1	B	347	GLU
1	B	373	LYS
1	B	374	LYS

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Mol	Chain	Res	Type
1	B	375	ILE
1	B	376	GLU
1	A	113	GLN
1	A	155	ASP
1	A	328	SER
1	B	45	GLN
1	B	64	LYS
1	B	65	VAL
1	B	67	SER
1	B	70	LEU
1	B	113	GLN
1	B	197	LYS
1	B	263	PHE
1	B	296	GLU
1	B	330	LYS
1	A	90	PHE
1	A	129	ALA
1	A	311	THR
1	B	69	VAL
1	B	199	PRO
1	B	338	THR
1	A	86	THR
1	A	146	LEU
1	A	157	ALA
1	A	292	SER
1	B	264	TYR
1	A	98	CYS
1	B	153	ARG
1	B	328	SER
1	A	295	SER
1	B	238	GLU
1	A	310	PRO
1	A	118	VAL

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	241/357 (68%)	200 (83%)	41 (17%)	2	6
1	B	224/357 (63%)	188 (84%)	36 (16%)	2	7
All	All	465/714 (65%)	388 (83%)	77 (17%)	2	7

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	56	LYS
1	A	72	LEU
1	A	74	ILE
1	A	87	GLN
1	A	89	LYS
1	A	95	LEU
1	A	102	ARG
1	A	104	GLU
1	A	106	GLU
1	A	114	CYS
1	A	119	ARG
1	A	120	ILE
1	A	121	VAL
1	A	125	GLU
1	A	132	LYS
1	A	139	GLU
1	A	152	ASP
1	A	159	THR
1	A	172	GLU
1	A	188	LYS
1	A	205	LEU
1	A	239	LYS
1	A	266	ASN
1	A	272	SER
1	A	298	VAL
1	A	308	THR
1	A	312	GLN
1	A	331	VAL
1	A	333	GLN
1	A	339	SER
1	A	343	LYS
1	A	348	ARG
1	A	363	MET
1	A	365	VAL

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Mol	Chain	Res	Type
1	A	368	GLU
1	A	373	LYS
1	A	374	LYS
1	A	380	ASN
1	A	383	LEU
1	A	384	LEU
1	B	74	ILE
1	B	75	ASN
1	B	79	LEU
1	B	80	GLN
1	B	81	ILE
1	B	83	ASN
1	B	85	ARG
1	B	87	GLN
1	B	95	LEU
1	B	104	GLU
1	B	106	GLU
1	B	107	LEU
1	B	120	ILE
1	B	136	ILE
1	B	145	GLU
1	B	159	THR
1	B	202	ILE
1	B	212	LYS
1	B	238	GLU
1	B	245	ASP
1	B	263	PHE
1	B	269	LEU
1	B	271	ILE
1	B	272	SER
1	B	278	ARG
1	B	294	VAL
1	B	308	THR
1	B	327	GLN
1	B	330	LYS
1	B	334	THR
1	B	338	THR
1	B	342	LEU
1	B	348	ARG
1	B	362	THR
1	B	370	ILE
1	B	372	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	75	ASN
1	A	80	GLN
1	A	108	HIS
1	A	113	GLN
1	A	156	GLN
1	A	184	HIS
1	A	191	ASN
1	A	266	ASN
1	A	304	ASN
1	A	312	GLN
1	A	380	ASN
1	B	75	ASN
1	B	80	GLN
1	B	83	ASN
1	B	175	GLN
1	B	184	HIS
1	B	191	ASN
1	B	304	ASN

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, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	319/400 (79%)	0.19	8 (2%) 57 47	24, 43, 58, 69	0
1	B	313/400 (78%)	0.07	11 (3%) 44 34	18, 38, 57, 64	0
All	All	632/800 (79%)	0.13	19 (3%) 50 40	18, 41, 58, 69	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ALA	6.9
1	B	236	GLY	4.4
1	A	154	GLY	4.0
1	A	66	THR	3.9
1	A	236	GLY	3.5
1	B	199	PRO	3.1
1	A	196	SER	3.0
1	A	152	ASP	2.9
1	A	199	PRO	2.9
1	A	329	THR	2.8
1	B	65	VAL	2.5
1	B	154	GLY	2.4
1	B	264	TYR	2.4
1	B	327	GLN	2.3
1	B	156	GLN	2.2
1	A	298	VAL	2.2
1	B	216	SER	2.2
1	B	87	GLN	2.1
1	B	328	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	HG	A	403	1/1	0.97	0.04	78,78,78,78	0
2	HG	B	403	1/1	0.97	0.04	70,70,70,70	0
2	HG	B	401	1/1	0.98	0.03	100,100,100,100	0
2	HG	A	405	1/1	0.98	0.03	81,81,81,81	0
2	HG	A	404	1/1	0.98	0.02	75,75,75,75	0
2	HG	A	401	1/1	0.98	0.04	106,106,106,106	0
2	HG	B	405	1/1	0.99	0.05	76,76,76,76	0
2	HG	B	406	1/1	0.99	0.03	67,67,67,67	0
2	HG	B	402	1/1	0.99	0.02	60,60,60,60	0
2	HG	A	402	1/1	0.99	0.03	78,78,78,78	0
2	HG	B	404	1/1	0.99	0.02	66,66,66,66	0
2	HG	A	407	1/1	0.99	0.04	56,56,56,56	0
2	HG	A	406	1/1	1.00	0.03	60,60,60,60	0
2	HG	B	407	1/1	1.00	0.03	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.