



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1KWP / pdb_00001kwp
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 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
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

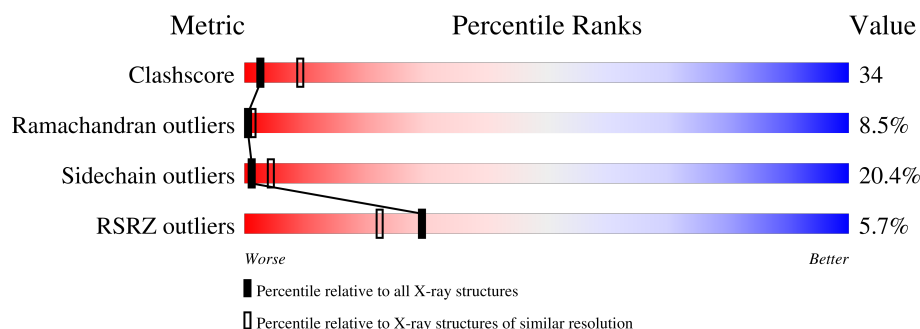
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	400	
1	B	400	

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 (CCD ID: HG) (formula: Hg).

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

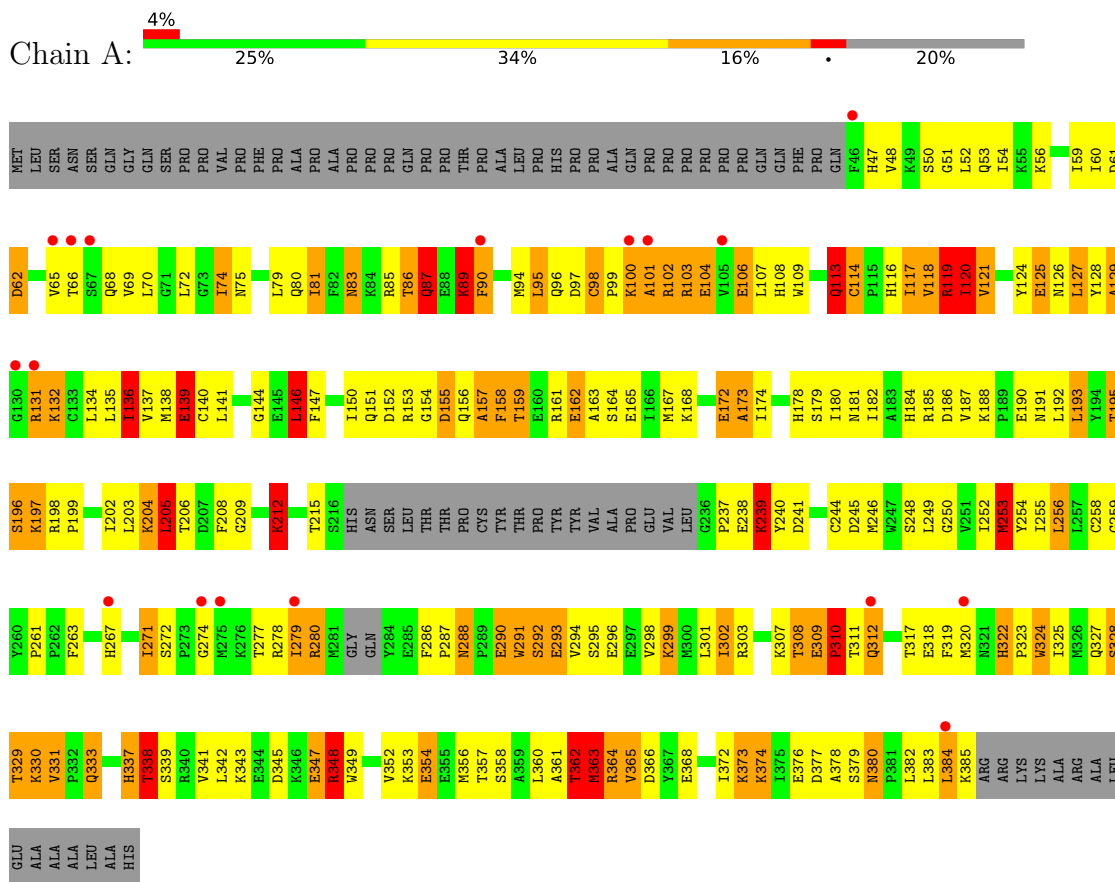
- Molecule 3 is water.

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

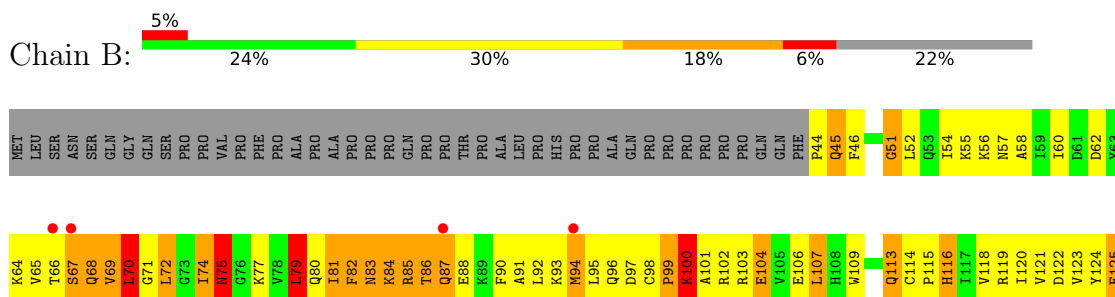
3 Residue-property plots

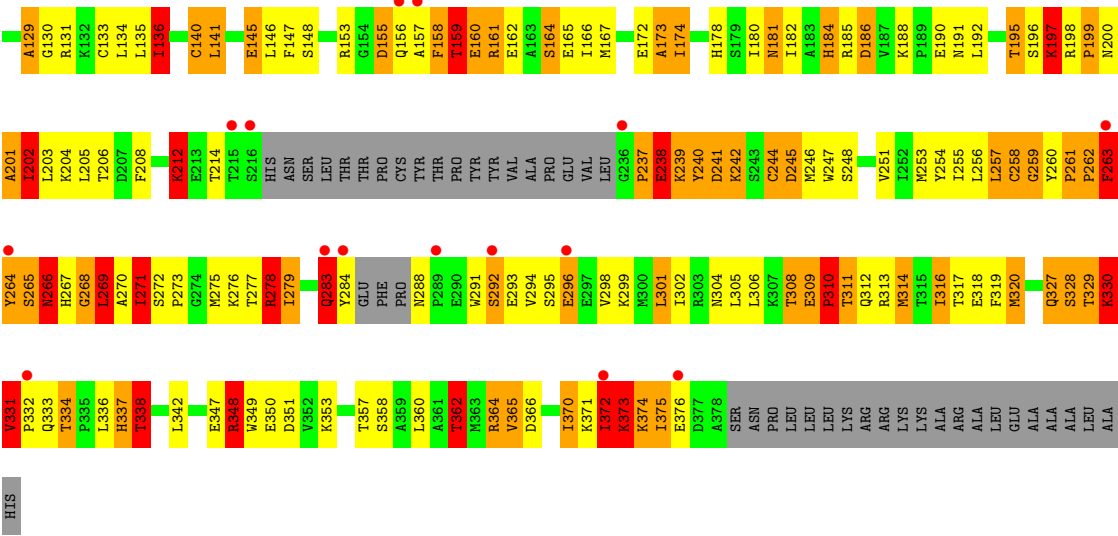
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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 32.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.60-2.80) 99.9 (32.60-2.80)	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 0.242 , (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)	0.38 , 85.5	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	0.81	0/2468	2.23	128/3344 (3.8%)
1	B	0.89	0/2372	2.40	143/3212 (4.5%)
All	All	0.85	0/4840	2.31	271/6556 (4.1%)

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

There are no bond length outliers.

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	CD-NE-CZ	13.39	143.15	124.40
1	B	268	GLY	N-CA-C	12.62	135.74	115.67
1	B	244	CYS	CB-CA-C	11.65	134.15	110.38
1	B	258	CYS	CB-CA-C	11.65	129.45	110.81
1	A	66	THR	CA-C-N	11.37	138.79	122.08
1	A	66	THR	C-N-CA	11.37	138.79	122.08
1	A	278	ARG	NE-CZ-NH2	-10.95	109.35	119.20
1	B	372	ILE	N-CA-CB	-10.50	100.36	112.34
1	B	331	VAL	N-CA-CB	10.38	125.74	111.21
1	B	311	THR	CA-C-N	10.33	137.87	121.44
1	B	311	THR	C-N-CA	10.33	137.87	121.44
1	B	259	GLY	CA-C-O	10.02	129.99	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	LEU	CA-C-N	9.90	130.90	120.00
1	A	70	LEU	C-N-CA	9.90	130.90	120.00
1	A	61	ASP	CA-CB-CG	9.75	122.35	112.60
1	A	196	SER	N-CA-C	9.72	125.60	112.68
1	B	263	PHE	CA-CB-CG	9.60	123.40	113.80
1	B	293	GLU	CB-CG-CD	9.50	128.76	112.60
1	A	106	GLU	CA-C-N	9.06	132.21	120.44
1	A	106	GLU	C-N-CA	9.06	132.21	120.44
1	A	258	CYS	CA-C-O	9.03	132.78	120.13
1	B	258	CYS	O-C-N	-9.00	112.73	122.09
1	B	83	ASN	OD1-CG-ND2	-8.99	113.61	122.60
1	A	62	ASP	CA-CB-CG	8.93	121.53	112.60
1	B	141	LEU	CA-C-O	-8.66	111.19	120.46
1	B	94	MET	O-C-N	-8.59	113.57	123.27
1	B	263	PHE	CA-C-N	8.57	137.91	121.54
1	B	263	PHE	C-N-CA	8.57	137.91	121.54
1	A	126	ASN	CA-CB-CG	8.56	121.16	112.60
1	B	75	ASN	CA-CB-CG	8.35	120.95	112.60
1	A	68	GLN	N-CA-C	-8.27	93.19	110.80
1	B	337	HIS	CA-CB-CG	-8.27	105.53	113.80
1	B	130	GLY	CA-C-O	8.26	127.13	118.95
1	B	348	ARG	N-CA-C	-8.21	102.41	111.36
1	B	370	ILE	N-CA-CB	8.21	119.47	110.53
1	A	103	ARG	CD-NE-CZ	8.14	135.79	124.40
1	A	361	ALA	CA-C-O	-8.07	111.99	120.55
1	B	240	TYR	O-C-N	-7.99	113.84	122.07
1	B	245	ASP	CA-C-O	7.85	129.06	119.79
1	A	212	LYS	CA-CB-CG	7.84	129.78	114.10
1	B	283	GLN	CA-C-O	7.83	131.71	120.51
1	B	57	ASN	OD1-CG-ND2	-7.80	114.80	122.60
1	A	309	GLU	CA-C-N	7.68	129.44	119.84
1	A	309	GLU	C-N-CA	7.68	129.44	119.84
1	A	279	ILE	CA-C-O	7.59	130.27	120.78
1	B	266	ASN	CA-CB-CG	7.58	120.18	112.60
1	B	57	ASN	CA-CB-CG	7.52	120.12	112.60
1	B	212	LYS	CA-C-N	7.43	131.42	120.87
1	B	212	LYS	C-N-CA	7.43	131.42	120.87
1	B	167	MET	CA-C-O	7.41	128.49	119.97
1	A	348	ARG	N-CA-C	-7.39	104.07	113.23
1	B	373	LYS	CA-C-N	7.35	135.58	121.54
1	B	373	LYS	C-N-CA	7.35	135.58	121.54
1	B	259	GLY	N-CA-C	-7.33	105.97	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLY	CA-C-N	7.26	132.98	121.44
1	A	209	GLY	C-N-CA	7.26	132.98	121.44
1	B	293	GLU	CA-CB-CG	7.26	128.61	114.10
1	B	311	THR	O-C-N	-7.24	112.96	122.59
1	B	329	THR	CA-C-N	7.15	135.19	121.54
1	B	329	THR	C-N-CA	7.15	135.19	121.54
1	A	310	PRO	N-CA-C	7.12	127.14	112.47
1	B	259	GLY	O-C-N	-7.12	114.61	122.65
1	A	184	HIS	CA-C-O	7.09	128.00	120.70
1	A	86	THR	N-CA-CB	7.01	122.33	110.49
1	B	44	PRO	N-CA-CB	6.99	110.69	103.00
1	A	363	MET	CA-CB-CG	6.98	128.06	114.10
1	A	131	ARG	CD-NE-CZ	6.95	134.13	124.40
1	A	258	CYS	O-C-N	-6.93	113.11	122.19
1	A	337	HIS	CA-CB-CG	-6.93	106.87	113.80
1	B	96	GLN	CA-C-O	-6.90	112.83	120.69
1	A	329	THR	CA-C-N	6.89	134.71	121.54
1	A	329	THR	C-N-CA	6.89	134.71	121.54
1	A	278	ARG	CA-CB-CG	6.86	127.82	114.10
1	B	365	VAL	O-C-N	-6.83	115.86	123.03
1	B	94	MET	CA-C-N	6.83	133.27	122.62
1	B	94	MET	C-N-CA	6.83	133.27	122.62
1	A	378	ALA	N-CA-C	6.80	120.20	109.39
1	A	101	ALA	N-CA-C	-6.79	104.99	113.55
1	B	242	LYS	CA-CB-CG	6.78	127.66	114.10
1	B	99	PRO	CA-C-O	-6.77	113.62	121.34
1	A	293	GLU	CA-C-N	6.74	134.11	121.97
1	A	293	GLU	C-N-CA	6.74	134.11	121.97
1	A	146	LEU	O-C-N	-6.72	113.65	122.59
1	B	372	ILE	CA-CB-CG2	6.70	121.89	110.50
1	B	245	ASP	N-CA-CB	-6.69	99.99	110.30
1	A	65	VAL	N-CA-C	-6.66	98.68	108.54
1	A	278	ARG	NE-CZ-NH1	6.66	128.16	121.50
1	A	301	LEU	CA-C-N	6.62	128.91	120.56
1	A	301	LEU	C-N-CA	6.62	128.91	120.56
1	A	255	ILE	N-CA-CB	6.61	117.85	110.51
1	A	179	SER	CA-C-O	6.60	127.03	119.18
1	A	288	ASN	O-C-N	6.59	128.90	121.32
1	B	99	PRO	N-CA-C	-6.58	100.87	111.14
1	B	125	GLU	CA-C-O	6.58	128.20	120.70
1	A	278	ARG	CB-CG-CD	6.54	126.35	111.30
1	B	329	THR	O-C-N	-6.52	114.43	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ALA	N-CA-C	-6.51	103.41	112.45
1	A	60	ILE	CB-CA-C	-6.50	100.63	111.29
1	A	294	VAL	CA-C-N	6.50	133.95	121.54
1	A	294	VAL	C-N-CA	6.50	133.95	121.54
1	B	244	CYS	N-CA-C	-6.50	104.05	112.23
1	A	53	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	A	278	ARG	CA-C-O	6.49	127.14	119.28
1	B	62	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	245	ASP	O-C-N	-6.47	113.67	122.33
1	A	86	THR	CA-CB-CG2	6.45	121.46	110.50
1	A	278	ARG	CA-C-N	6.45	133.57	121.97
1	A	278	ARG	C-N-CA	6.45	133.57	121.97
1	A	184	HIS	O-C-N	-6.44	115.13	122.09
1	B	295	SER	N-CA-C	6.44	120.78	112.41
1	B	279	ILE	O-C-N	-6.44	115.20	121.83
1	A	193	LEU	CA-C-O	6.43	127.53	120.71
1	A	205	LEU	N-CA-CB	6.40	121.06	110.63
1	B	83	ASN	CB-CG-ND2	6.38	125.97	116.40
1	B	164	SER	CA-C-O	6.37	127.27	120.70
1	B	195	THR	CB-CA-C	-6.37	100.02	110.85
1	A	181	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	B	319	PHE	N-CA-C	6.33	117.84	111.07
1	B	351	ASP	CA-C-O	-6.32	114.14	120.90
1	B	299	LYS	CA-C-O	-6.30	111.50	120.51
1	B	173	ALA	CA-C-O	6.30	127.64	120.90
1	B	329	THR	CA-C-O	6.28	129.38	122.03
1	A	299	LYS	CA-C-O	-6.27	113.02	120.10
1	A	248	SER	CA-C-O	-6.24	113.94	120.55
1	B	202	ILE	CA-C-O	6.21	128.05	120.84
1	A	363	MET	CA-C-O	6.21	127.13	120.24
1	B	46	PHE	N-CA-C	6.21	120.12	111.74
1	A	184	HIS	CA-C-N	6.17	132.73	123.05
1	A	184	HIS	C-N-CA	6.17	132.73	123.05
1	A	279	ILE	CA-C-N	6.16	133.31	121.54
1	A	279	ILE	C-N-CA	6.16	133.31	121.54
1	B	240	TYR	CA-C-O	6.13	127.25	120.82
1	A	87	GLN	OE1-CD-NE2	6.13	128.73	122.60
1	B	51	GLY	CA-C-O	-6.12	114.62	121.23
1	B	201	ALA	O-C-N	6.08	129.87	123.06
1	B	136	ILE	CB-CG1-CD1	6.08	126.57	113.80
1	B	267	HIS	N-CA-C	-6.08	105.82	113.72
1	B	119	ARG	CA-C-O	6.08	127.98	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	PHE	CA-C-O	6.08	129.20	120.51
1	B	246	MET	CG-SD-CE	-6.02	87.65	100.90
1	B	320	MET	CA-C-O	6.01	126.77	119.49
1	A	364	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	B	278	ARG	CG-CD-NE	5.96	125.10	112.00
1	A	349	TRP	CA-C-N	5.95	128.26	120.28
1	A	349	TRP	C-N-CA	5.95	128.26	120.28
1	B	245	ASP	CB-CG-OD2	-5.93	104.75	118.40
1	A	69	VAL	CA-C-N	5.93	129.04	120.38
1	A	69	VAL	C-N-CA	5.93	129.04	120.38
1	B	312	GLN	N-CA-C	-5.93	104.90	114.09
1	B	140	CYS	O-C-N	-5.93	116.11	123.04
1	B	94	MET	CA-C-O	5.92	126.89	120.43
1	A	348	ARG	NE-CZ-NH2	5.92	124.52	119.20
1	B	372	ILE	CA-C-O	-5.91	116.05	121.72
1	A	158	PHE	CA-C-N	-5.90	114.09	122.94
1	A	158	PHE	C-N-CA	-5.90	114.09	122.94
1	A	286	PHE	CA-C-O	5.90	126.70	120.63
1	A	278	ARG	CG-CD-NE	5.85	124.86	112.00
1	A	81	ILE	O-C-N	-5.84	116.57	123.00
1	A	237	PRO	CA-C-O	-5.83	109.99	120.60
1	B	160	GLU	O-C-N	5.81	128.28	122.12
1	B	366	ASP	CA-C-O	-5.76	114.38	121.06
1	A	354	GLU	CA-CB-CG	5.76	125.61	114.10
1	A	362	THR	CA-CB-OG1	5.75	118.22	109.60
1	B	362	THR	CA-CB-OG1	5.75	118.22	109.60
1	B	122	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	197	LYS	N-CA-CB	5.74	120.19	110.49
1	A	80	GLN	CA-C-O	5.73	126.89	120.70
1	A	89	LYS	O-C-N	-5.72	114.98	122.59
1	B	107	LEU	CA-C-O	5.71	127.35	121.07
1	B	186	ASP	CA-C-O	5.71	126.14	120.32
1	A	308	THR	N-CA-C	-5.70	101.86	110.24
1	B	155	ASP	CA-C-O	-5.70	114.80	120.90
1	A	259	GLY	N-CA-C	-5.70	107.24	115.27
1	B	186	ASP	O-C-N	-5.68	115.16	122.21
1	B	311	THR	N-CA-C	5.67	122.88	110.80
1	A	318	GLU	O-C-N	-5.67	116.20	122.09
1	B	83	ASN	CA-C-N	5.66	128.33	120.29
1	B	83	ASN	C-N-CA	5.66	128.33	120.29
1	B	310	PRO	N-CA-CB	5.66	109.19	103.25
1	B	45	GLN	CA-C-N	5.65	130.15	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	GLN	C-N-CA	5.65	130.15	122.19
1	B	83	ASN	CA-CB-CG	5.65	118.25	112.60
1	B	279	ILE	N-CA-C	5.64	116.41	110.72
1	B	161	ARG	CD-NE-CZ	5.63	132.29	124.40
1	A	347	GLU	CA-C-O	5.63	128.56	120.51
1	A	376	GLU	CA-C-O	5.62	127.45	121.16
1	A	363	MET	O-C-N	-5.61	114.94	122.23
1	B	159	THR	CA-C-N	5.59	128.04	120.38
1	B	159	THR	C-N-CA	5.59	128.04	120.38
1	A	180	ILE	CA-C-N	5.58	130.05	122.07
1	A	180	ILE	C-N-CA	5.58	130.05	122.07
1	A	136	ILE	N-CA-C	5.57	115.81	107.51
1	B	261	PRO	CA-C-O	-5.57	112.49	120.56
1	A	119	ARG	CD-NE-CZ	5.55	132.17	124.40
1	A	302	ILE	N-CA-CB	-5.55	104.05	110.55
1	B	239	LYS	CA-C-N	5.55	127.65	120.44
1	B	239	LYS	C-N-CA	5.55	127.65	120.44
1	A	338	THR	CA-CB-OG1	-5.54	101.30	109.60
1	B	245	ASP	CA-CB-CG	-5.54	107.06	112.60
1	B	304	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	B	100	LYS	N-CA-CB	5.52	119.81	110.49
1	A	140	CYS	N-CA-CB	-5.51	101.06	110.16
1	B	54	ILE	CB-CG1-CD1	5.50	125.36	113.80
1	A	79	LEU	CA-C-O	-5.50	114.73	121.88
1	A	374	LYS	N-CA-CB	5.50	120.96	111.00
1	A	83	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	322	HIS	CA-C-N	5.49	124.68	118.97
1	A	322	HIS	C-N-CA	5.49	124.68	118.97
1	B	301	LEU	CA-C-O	-5.47	115.05	121.07
1	B	84	LYS	CA-C-N	-5.46	114.27	122.24
1	B	84	LYS	C-N-CA	-5.46	114.27	122.24
1	B	116	HIS	CA-CB-CG	-5.46	108.34	113.80
1	B	257	LEU	CA-C-O	5.43	128.28	120.51
1	B	237	PRO	N-CA-CB	5.43	108.95	103.25
1	A	253	MET	CA-CB-CG	5.41	124.92	114.10
1	B	181	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	184	HIS	CG-CD2-NE2	5.38	112.58	107.20
1	A	106	GLU	CB-CG-CD	5.37	121.73	112.60
1	B	278	ARG	CD-NE-CZ	5.37	131.91	124.40
1	B	145	GLU	CB-CG-CD	-5.36	103.48	112.60
1	A	120	ILE	N-CA-CB	5.36	116.56	110.72
1	B	348	ARG	N-CA-CB	5.35	118.07	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	ARG	CG-CD-NE	5.35	123.76	112.00
1	A	286	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	215	THR	N-CA-C	5.34	116.90	107.61
1	A	379	SER	N-CA-C	5.32	118.56	111.75
1	B	263	PHE	O-C-N	-5.31	115.53	122.59
1	A	317	THR	CA-CB-OG1	-5.29	101.67	109.60
1	A	293	GLU	O-C-N	-5.28	115.57	122.59
1	B	91	ALA	CA-C-N	5.28	130.85	122.94
1	B	91	ALA	C-N-CA	5.28	130.85	122.94
1	A	126	ASN	CA-C-N	5.26	130.56	122.77
1	A	126	ASN	C-N-CA	5.26	130.56	122.77
1	A	182	ILE	O-C-N	-5.26	117.66	123.18
1	B	158	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	376	GLU	N-CA-C	5.22	118.00	110.28
1	A	290	GLU	CB-CA-C	-5.21	101.25	109.80
1	A	377	ASP	CB-CA-C	5.21	118.08	110.26
1	A	173	ALA	CA-C-O	5.21	126.29	120.82
1	A	374	LYS	CA-C-O	5.19	126.63	120.66
1	B	265	SER	CB-CA-C	5.18	120.73	110.42
1	B	296	GLU	N-CA-CB	5.18	119.24	110.49
1	A	239	LYS	CA-C-O	-5.17	115.57	121.00
1	B	82	PHE	CA-C-O	-5.17	115.06	121.11
1	A	65	VAL	CB-CA-C	5.16	117.12	111.08
1	B	155	ASP	N-CA-CB	5.14	117.59	109.94
1	A	69	VAL	O-C-N	-5.13	116.16	122.57
1	B	148	SER	N-CA-C	-5.12	104.66	112.04
1	B	241	ASP	CA-C-O	-5.11	115.46	120.82
1	B	314	MET	CA-C-O	-5.10	115.96	121.87
1	B	68	GLN	CA-C-O	-5.08	113.24	120.51
1	A	139	GLU	N-CA-C	-5.08	103.07	110.24
1	A	256	LEU	N-CA-C	5.08	117.48	111.33
1	A	319	PHE	CA-C-O	5.08	126.16	120.82
1	B	309	GLU	CA-C-N	5.08	126.19	119.84
1	B	309	GLU	C-N-CA	5.08	126.19	119.84
1	A	354	GLU	CA-C-N	5.07	127.58	120.28
1	A	354	GLU	C-N-CA	5.07	127.58	120.28
1	B	58	ALA	CA-C-O	5.04	126.89	121.55
1	B	201	ALA	CA-C-O	-5.04	115.31	121.36
1	A	288	ASN	N-CA-CB	5.04	119.34	110.37
1	B	311	THR	CA-C-O	5.04	127.71	120.51
1	B	79	LEU	CA-C-N	5.03	128.49	121.24
1	B	79	LEU	C-N-CA	5.03	128.49	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	TRP	N-CA-CB	-5.02	102.74	110.12
1	B	271	ILE	CB-CG1-CD1	5.02	124.34	113.80
1	B	70	LEU	O-C-N	-5.02	115.92	122.59
1	A	181	ASN	CA-CB-CG	5.01	117.61	112.60
1	A	117	ILE	CA-C-O	-5.01	115.05	120.36
1	B	77	LYS	CA-C-O	-5.01	114.88	120.54
1	A	106	GLU	O-C-N	-5.01	116.81	122.12

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
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	151	0
1	B	2331	0	2173	163	0
2	A	7	0	0	1	0
2	B	7	0	0	5	0
3	A	62	0	0	4	0
3	B	72	0	0	10	1
All	All	4899	0	4480	314	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 34.

All (314) 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:167:MET:HG3	1:A:253:MET:HE3	1.44	1.00
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
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:102:ARG:HH11	1:A:102:ARG:HB2	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:A:167:MET:HE1	1:A:249:LEU:HD22	1.66	0.77
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:B:328:SER:OG	3:B:448:HOH:O	1.98	0.72
1:A:167:MET:HG3	1:A:253:MET:CE	2.17	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:B:258:CYS:SG	3:B:479:HOH:O	2.51	0.67
1:A:97:ASP:O	1:A:98:CYS:HB3	1.94	0.67
1:A:116:HIS:NE2	1:A:172:GLU:HG2	2.10	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:HG3	1:A:119:ARG:HH11	1.59	0.67
1:B:172:GLU:HG3	1:B:320:MET:HE2	1.78	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:MET:HE3	1:B:279:ILE:HD11	1.79	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:HA	1:B:349:TRP:CE3	2.35	0.62
1:B:372:ILE:O	1:B:373:LYS:HB2	1.98	0.62
1:A:165:GLU:HG2	1:A:329:THR:HG22	1.82	0.62
1:B:205:LEU:HD23	1:B:205:LEU:H	1.64	0.62
1:B:261:PRO:O	1:B:263:PHE:CE1	2.53	0.62
1:B:308:THR:HG22	1:B:313:ARG:HA	1.82	0.62
1:A:150:ILE:O	1:A:151:GLN:C	2.44	0.61
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:96:GLN:HG2	3:A:412:HOH:O	2.02	0.59
1:A:348:ARG:O	1:A:352:VAL:HG23	2.03	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: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:B:113:GLN:O	1:B:114:CYS:C	2.47	0.58
1:B:253:MET:HE1	1:B:302:ILE:HG12	1.85	0.58
1:A:274:GLY:O	1:A:277:THR:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:167:MET:CE	1:A:249:LEU:HD22	2.32	0.57
1:B:275:MET:O	1:B:276:LYS:HB2	2.03	0.57
1:A:302:ILE:HG23	1:A:303:ARG:N	2.20	0.57
1:B:75:ASN:HD22	1:B:75:ASN:H	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:302:ILE:HG13	1:B:314:MET:HE1	1.87	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:B:172:GLU:HG3	1:B:320:MET:CE	2.35	0.56
1:A:136:ILE:HD12	1:A:136:ILE:H	1.69	0.56
1:B:212:LYS:HD3	1:B:241:ASP:OD2	2.05	0.56
1:B:349:TRP:HA	1:B:349:TRP:HE3	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
1:B:69:VAL:O	1:B:72:LEU:N	2.28	0.55
1:B:255:ILE:CG1	1:B:261:PRO:HA	2.35	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:A:117:ILE:HG22	1:A:118:VAL:O	2.08	0.54
1:A:287:PRO:O	1:A:288:ASN:C	2.49	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:A:113:GLN:O	1:A:114:CYS:C	2.50	0.54
1:B:259:GLY:HA2	1:B:338:THR:HG23	1.90	0.53
1:A:380:ASN:HD22	1:A:380:ASN:C	2.17	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:HD23	1:A:205:LEU:N	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:HD23	1:B:205:LEU:N	2.24	0.53
1:B:257:LEU:O	1:B:258:CYS:C	2.51	0.53
1:B:331:VAL:HG23	1:B:332:PRO:O	2.09	0.52
1:A:52:LEU:HD12	1:A:109:TRP:CG	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:HB2	1:A:299:LYS:H	1.74	0.52
1:B:283:GLN:O	1:B:288:ASN:N	2.42	0.52
1:A:52:LEU:C	1:A:52:LEU:HD23	2.35	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:B:333:GLN:O	1:B:334:THR:C	2.52	0.52
1:A:108:HIS:HE1	1:A:138:MET:HE3	1.73	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:83:ASN:HD22	1:B:84:LYS:N	2.07	0.51
1:B:348:ARG:HG3	1:B:349:TRP:N	2.25	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
1:B:317:THR:O	1:B:318:GLU:C	2.53	0.51
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:A:244:CYS:HA	1:A:363:MET:HE1	1.94	0.50
1:B:155:ASP:O	1:B:156:GLN:C	2.55	0.50
1:B:94:MET:HG2	1:B:135:LEU:CD2	2.42	0.49
1:B:254:TYR:CG	1:B:262:PRO:HB3	2.47	0.49
1:A:101:ALA:O	1:A:104:GLU:HG3	2.12	0.49
1:B:68:GLN:O	1:B:69:VAL:CB	2.57	0.49
1:B:178:HIS:CE1	1:B:242:LYS:HG2	2.47	0.49
1:A:118:VAL:HG21	1:A:206:THR:HB	1.94	0.49
1:B:75:ASN:H	1:B:75:ASN:ND2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:HIS:HE1	1:A:246:MET:HE1	1.77	0.49
1:A:384:LEU:HD23	1:A:385:LYS:N	2.27	0.49
1:A:155:ASP:O	1:A:156:GLN:C	2.53	0.48
1:A:74:ILE:O	1:A:74:ILE:HD12	2.12	0.48
1:A:108:HIS:CE1	1:A:138:MET:HE3	2.48	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:B:97:ASP:O	1:B:98:CYS:HB3	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:N	1:B:131:ARG:HD3	2.29	0.48
1:B:305:LEU:HB2	1:B:314:MET:HE3	1.95	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:A:186:ASP:HA	1:A:360:LEU:HD13	1.96	0.48
1:A:97:ASP:CG	1:A:102:ARG:HH12	2.21	0.48
1:A:47:HIS:O	1:A:48:VAL:C	2.55	0.48
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:190:GLU:OE1	1:B:353:LYS:HB3	2.14	0.47
1:A:373:LYS:HB3	1:A:373:LYS:HE3	1.70	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:A:117:ILE:O	1:A:118:VAL:C	2.58	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:A:240:TYR:O	1:A:241:ASP:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:HD13	1:B:75:ASN:N	2.30	0.46
1:B:202:ILE:HG12	1:B:203:LEU:N	2.30	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:B:247:TRP:O	1:B:248:SER:C	2.55	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:161:ARG:HD3	1:A:331:VAL:O	2.16	0.46
1:A:178:HIS:CE1	1:A:246:MET:HE1	2.50	0.46
1:B:263:PHE:CD1	1:B:263:PHE:N	2.83	0.45
1:B:185:ARG:HB3	1:B:364:ARG:HD3	1.97	0.45
1:A:212:LYS:NZ	1:A:241:ASP:OD1	2.49	0.45
1:A:253:MET:HE2	1:A:324:TRP:CZ3	2.51	0.45
1:B:147:PHE:CE1	1:B:256:LEU:HD23	2.52	0.45
1:A:104:GLU:HB2	1:A:208:PHE:O	2.17	0.45
1:A:127:LEU:HD12	1:A:131:ARG: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:71:GLY:O	1:B:74:ILE:HD12	2.17	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:A:119:ARG:HB3	1:A:139:GLU:OE2	2.16	0.45
1:A:325:ILE:N	1:A:325:ILE:HD12	2.32	0.45
1:B:82:PHE:HE1	3:B:430:HOH:O	2.00	0.45
1:B:159:THR:HG23	1:B:162:GLU:HG3	1.98	0.45
1:B:305:LEU:CB	1:B:314:MET:HE3	2.46	0.45
1:B:337:HIS:O	1:B:338:THR:C	2.58	0.45
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:238:GLU:O	1:B:239:LYS:C	2.58	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:252:ILE:HG13	1:A:356:MET:HE1	1.99	0.44
1:A:356:MET:O	1:A:357:THR:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG21	1:A:125:GLU:HB2	2.00	0.44
1:A:90:PHE:HE2	1:A:121:VAL:HG11	1.83	0.44
1:A:384:LEU:O	1:A:385:LYS:O	2.35	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:89:LYS:O	1:A:90:PHE:HB2	2.18	0.44
1:A:138:MET:O	1:A:139:GLU:C	2.61	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:B:328:SER:O	1:B:329:THR:C	2.60	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:290:GLU:O	1:A:291:TRP:CB	2.66	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:B:371:LYS:HB2	1:B:371:LYS:HE3	1.80	0.43
1:A:168:LYS:HG3	1:A:320:MET:HE1	2.01	0.43
1:A:358:SER:O	1:A:362:THR:HG23	2.19	0.43
1:B:86:THR:O	1:B:87:GLN:HB3	2.19	0.43
1:B:309:GLU:O	1:B:310:PRO:O	2.37	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:B:263:PHE:CD1	1:B:264:TYR:CE1	3.07	0.42
1:B:75:ASN:HD22	1:B:75:ASN:N	2.16	0.42
1:B:349:TRP:O	1:B:350:GLU:C	2.62	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:67:SER:C	1:B:68:GLN:O	2.63	0.41
1:B:192:LEU:HB3	1:B:203:LEU:HD11	2.02	0.41
1:A:178:HIS:NE2	1:A:245:ASP:OD1	2.46	0.41
1:A:198:ARG:CB	1:A:199:PRO:HD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:237:PRO:O	1:B:238:GLU:C	2.63	0.41
1:B:373:LYS:HD2	1:B:373:LYS:HA	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:B:255:ILE:O	1:B:256:LEU:C	2.64	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:85:ARG:NH1	1:A:85:ARG:HG3	2.35	0.41
1:A:155:ASP:O	1:A:157:ALA:N	2.54	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:153:ARG:O	1:A:154:GLY:C	2.64	0.41
1:B:146:LEU:HG	1:B:147:PHE:N	2.34	0.41
1:A:161:ARG:HA	1:A:331:VAL:HG22	2.02	0.40
1:A:174:ILE:HD11	1:A:187:VAL:HG21	2.02	0.40
1:A:327:GLN:C	1:A:328:SER:O	2.64	0.40
1:B:205:LEU:O	1:B:205:LEU:HG	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:62:ASP:OD1	1:A:124:TYR:OH	2.27	0.40
1:B:240:TYR:CE1	1:B:365:VAL:HG13	2.56	0.40
1:B:327:GLN:HG2	1:B:330:LYS:HE3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:475:HOH:O	3:B:475:HOH:O[2_555]	1.85	0.35

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	313/400 (78%)	245 (78%)	46 (15%)	22 (7%)	1	2
1	B	307/400 (77%)	231 (75%)	45 (15%)	31 (10%)	0	1
All	All	620/800 (78%)	476 (77%)	91 (15%)	53 (8%)	0	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
1	B	375	ILE
1	B	376	GLU
1	A	113	GLN
1	A	155	ASP
1	A	328	SER

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Mol	Chain	Res	Type
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%)	190 (79%)	51 (21%)	1	4
1	B	224/357 (63%)	180 (80%)	44 (20%)	1	5
All	All	465/714 (65%)	370 (80%)	95 (20%)	1	4

All (95) 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	75	ASN
1	A	87	GLN
1	A	95	LEU
1	A	102	ARG
1	A	104	GLU
1	A	106	GLU
1	A	113	GLN
1	A	114	CYS
1	A	119	ARG
1	A	120	ILE
1	A	121	VAL
1	A	125	GLU
1	A	127	LEU
1	A	132	LYS
1	A	136	ILE
1	A	139	GLU
1	A	152	ASP
1	A	159	THR
1	A	172	GLU
1	A	192	LEU
1	A	195	THR
1	A	202	ILE
1	A	205	LEU
1	A	212	LYS
1	A	239	LYS
1	A	253	MET
1	A	271	ILE
1	A	272	SER
1	A	298	VAL
1	A	308	THR
1	A	312	GLN
1	A	330	LYS
1	A	331	VAL
1	A	333	GLN
1	A	338	THR
1	A	339	SER
1	A	343	LYS
1	A	348	ARG

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Mol	Chain	Res	Type
1	A	362	THR
1	A	363	MET
1	A	365	VAL
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	56	LYS
1	B	60	ILE
1	B	72	LEU
1	B	74	ILE
1	B	75	ASN
1	B	79	LEU
1	B	80	GLN
1	B	81	ILE
1	B	85	ARG
1	B	87	GLN
1	B	93	LYS
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	174	ILE
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	301	LEU
1	B	308	THR
1	B	316	ILE

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Mol	Chain	Res	Type
1	B	327	GLN
1	B	330	LYS
1	B	331	VAL
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
1	B	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
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	337	HIS
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	266	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 [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, 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 [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	319/400 (79%)	0.73	17 (5%) 32 24	24, 43, 58, 69	0
1	B	313/400 (78%)	0.69	19 (6%) 27 20	18, 38, 57, 64	0
All	All	632/800 (79%)	0.71	36 (5%) 29 22	18, 41, 58, 69	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ALA	6.7
1	B	264	TYR	4.5
1	A	66	THR	3.8
1	B	216	SER	3.8
1	B	332	PRO	3.1
1	B	215	THR	2.9
1	A	67	SER	2.9
1	B	289	PRO	2.9
1	B	376	GLU	2.8
1	B	87	GLN	2.8
1	A	65	VAL	2.7
1	A	46	PHE	2.7
1	B	296	GLU	2.5
1	B	263	PHE	2.4
1	A	90	PHE	2.3
1	B	67	SER	2.3
1	A	320	MET	2.3
1	B	66	THR	2.3
1	A	279	ILE	2.3
1	A	105	VAL	2.3
1	A	100	LYS	2.3
1	A	274	GLY	2.3
1	A	275	MET	2.2
1	B	292	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	372	ILE	2.2
1	B	94	MET	2.2
1	A	384	LEU	2.2
1	B	156	GLN	2.1
1	A	101	ALA	2.1
1	B	236	GLY	2.1
1	A	267	HIS	2.0
1	A	312	GLN	2.0
1	A	130	GLY	2.0
1	A	131	ARG	2.0
1	B	284	TYR	2.0
1	B	283	GLN	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(Å ²)	Q<0.9
2	HG	B	401	1/1	0.96	0.06	100,100,100,100	0
2	HG	B	403	1/1	0.97	0.04	70,70,70,70	0
2	HG	B	406	1/1	0.97	0.04	67,67,67,67	0
2	HG	A	405	1/1	0.98	0.06	81,81,81,81	0
2	HG	A	401	1/1	0.98	0.05	106,106,106,106	0
2	HG	A	403	1/1	0.98	0.06	78,78,78,78	0
2	HG	A	404	1/1	0.98	0.03	75,75,75,75	0
2	HG	A	402	1/1	0.99	0.05	78,78,78,78	0
2	HG	B	402	1/1	0.99	0.03	60,60,60,60	0
2	HG	A	406	1/1	0.99	0.02	60,60,60,60	0
2	HG	B	404	1/1	0.99	0.03	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	B	405	1/1	0.99	0.05	76,76,76,76	0
2	HG	A	407	1/1	0.99	0.02	56,56,56,56	0
2	HG	B	407	1/1	0.99	0.03	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.