



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:34 AM UTC

PDB ID : 3ULZ / pdb\_00003ulz  
Title : Crystal structure of apo BAK1  
Authors : Lou, Z.Y.; Yan, L.M.; Ma, Y.Y.  
Deposited on : 2011-11-11  
Resolution : 2.60 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](mailto: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>.

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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)  
Xtrriage (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

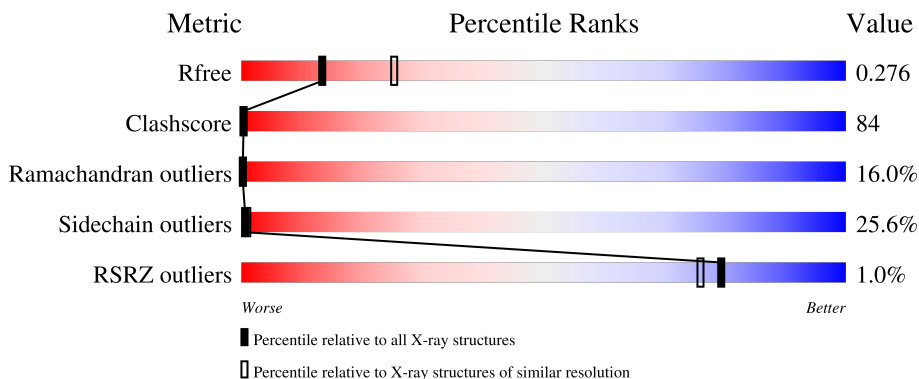
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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	326	

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
1	SEP	A	290	-	-	X	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
1	TPO	A	449	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2457 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 BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	297	2366	1477	413	456	6	14	0	0	0

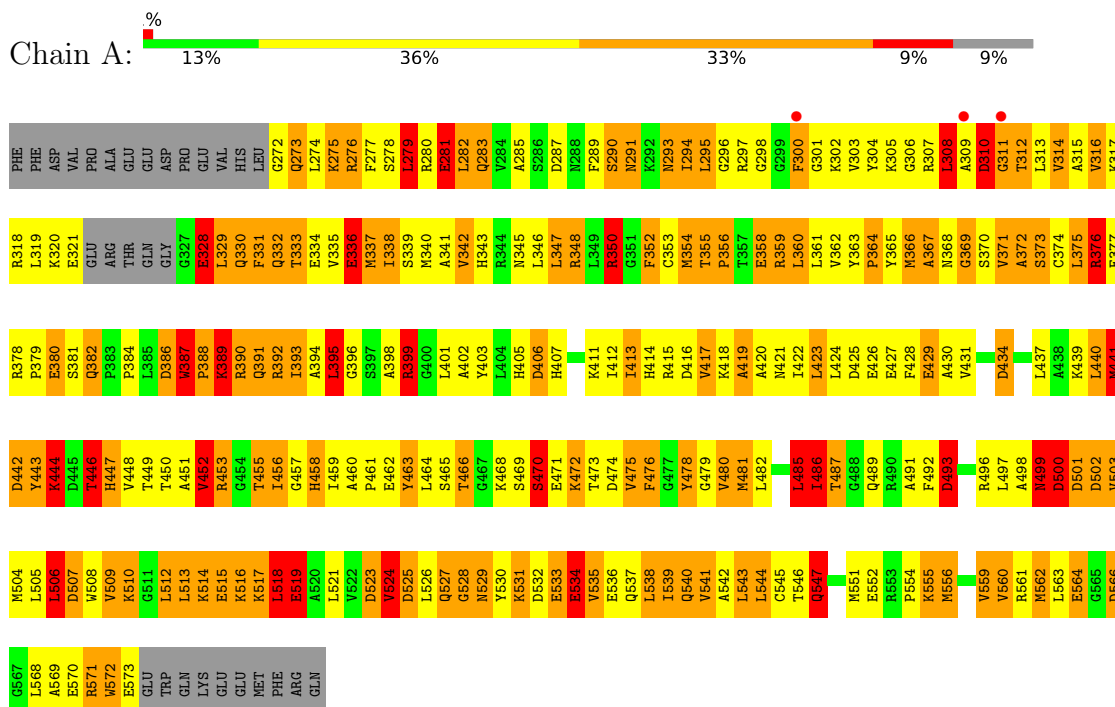
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		

### 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: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.25Å 75.59Å 71.94Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	41.05 – 2.60 41.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (41.05-2.60) 88.8 (41.05-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.224 , 0.279 0.230 , 0.276	Depositor DCC
$R_{free}$ test set	435 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.1	Xtrriage
Anisotropy	0.739	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 80.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.83	43/2333 (1.8%)	2.03	83/3130 (2.7%)

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	7

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	VAL	CA-CB	11.84	1.68	1.54
1	A	413	ILE	CA-CB	-10.88	1.41	1.54
1	A	342	VAL	CA-CB	-9.72	1.42	1.54
1	A	509	VAL	CA-CB	9.26	1.65	1.54
1	A	403	TYR	CA-C	-9.11	1.41	1.52
1	A	398	ALA	CA-CB	-8.48	1.40	1.53
1	A	478	TYR	CA-CB	8.11	1.66	1.53
1	A	388	PRO	C-O	7.88	1.34	1.24
1	A	539	ILE	CA-CB	7.86	1.64	1.54
1	A	419	ALA	CA-CB	-7.84	1.40	1.53
1	A	413	ILE	CA-C	-7.35	1.43	1.52
1	A	412	ILE	CA-C	-7.24	1.43	1.52
1	A	316	VAL	CA-CB	-7.10	1.45	1.54
1	A	530	TYR	CA-C	-7.10	1.44	1.52
1	A	372	ALA	CA-C	-6.95	1.44	1.52
1	A	417	VAL	CA-CB	6.94	1.61	1.53
1	A	480	VAL	CA-CB	6.65	1.62	1.54
1	A	342	VAL	C-O	-6.63	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	493	ASP	N-CA	6.62	1.54	1.46
1	A	479	GLY	CA-C	6.57	1.59	1.52
1	A	497	LEU	CA-C	6.51	1.61	1.52
1	A	310	ASP	C-N	6.50	1.42	1.33
1	A	559	VAL	CA-C	6.49	1.60	1.52
1	A	564	GLU	CD-OE2	5.79	1.36	1.25
1	A	559	VAL	C-O	5.76	1.30	1.24
1	A	367	ALA	CA-CB	-5.66	1.44	1.53
1	A	315	ALA	CA-CB	-5.65	1.46	1.53
1	A	328	GLU	CA-C	5.62	1.60	1.52
1	A	392	ARG	C-O	5.58	1.31	1.24
1	A	429	GLU	CA-C	-5.57	1.45	1.52
1	A	559	VAL	CA-CB	5.56	1.60	1.54
1	A	403	TYR	C-O	-5.54	1.17	1.24
1	A	345	ASN	N-CA	-5.53	1.39	1.46
1	A	538	LEU	CA-C	5.47	1.60	1.52
1	A	314	VAL	CA-CB	-5.47	1.47	1.54
1	A	420	ALA	CA-CB	5.38	1.62	1.53
1	A	386	ASP	CA-C	-5.29	1.46	1.53
1	A	388	PRO	CA-C	5.29	1.59	1.52
1	A	394	ALA	CA-C	5.25	1.59	1.52
1	A	343	HIS	CA-C	-5.18	1.46	1.52
1	A	506	LEU	CA-C	-5.13	1.45	1.52
1	A	391	GLN	C-O	5.05	1.29	1.24
1	A	478	TYR	CG-CD1	-5.05	1.28	1.39

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ASP	CB-CA-C	19.18	148.58	110.42
1	A	343	HIS	N-CA-C	-11.82	90.17	108.14
1	A	463	TYR	N-CA-C	-11.59	98.17	111.03
1	A	311	GLY	N-CA-C	-10.58	82.62	113.30
1	A	310	ASP	N-CA-C	-9.35	90.89	110.80
1	A	310	ASP	O-C-N	-9.16	110.40	122.59
1	A	407	HIS	N-CA-C	-9.09	98.81	112.54
1	A	507	ASP	N-CA-C	-8.78	100.89	111.69
1	A	336	GLU	N-CA-C	-8.60	102.92	113.15
1	A	458	HIS	N-CA-C	8.55	123.76	113.16
1	A	517	LYS	N-CA-C	8.39	122.84	107.99
1	A	392	ARG	N-CA-C	8.32	122.54	112.38
1	A	285	ALA	N-CA-C	-8.30	102.71	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	TYR	N-CA-C	-8.23	96.59	108.60
1	A	420	ALA	N-CA-C	-8.20	103.17	113.01
1	A	382	GLN	CA-C-N	8.11	128.73	120.38
1	A	382	GLN	C-N-CA	8.11	128.73	120.38
1	A	545	CYS	N-CA-C	7.89	122.67	112.89
1	A	509	VAL	N-CA-C	-7.82	103.18	110.53
1	A	572	TRP	N-CA-C	7.74	119.90	108.14
1	A	493	ASP	N-CA-C	7.66	121.21	108.73
1	A	431	VAL	N-CA-C	7.63	118.85	106.72
1	A	283	GLN	N-CA-C	-7.61	101.98	111.11
1	A	341	ALA	N-CA-C	7.43	119.58	107.32
1	A	399	ARG	N-CA-C	7.10	125.92	110.80
1	A	393	ILE	N-CA-C	-7.03	102.43	112.35
1	A	406	ASP	N-CA-C	6.95	123.28	114.31
1	A	275	LYS	N-CA-C	6.93	121.27	107.62
1	A	310	ASP	CA-C-N	-6.91	109.27	121.70
1	A	310	ASP	C-N-CA	-6.91	109.27	121.70
1	A	350	ARG	N-CA-C	-6.79	103.34	111.69
1	A	560	VAL	CA-C-N	-6.75	111.43	120.54
1	A	560	VAL	C-N-CA	-6.75	111.43	120.54
1	A	300	PHE	N-CA-C	-6.69	102.25	110.61
1	A	346	LEU	CB-CA-C	-6.60	99.97	110.14
1	A	395	LEU	N-CA-C	6.54	118.06	111.07
1	A	459	ILE	CA-C-N	6.42	129.32	120.39
1	A	459	ILE	C-N-CA	6.42	129.32	120.39
1	A	376	ARG	CB-CA-C	-6.41	100.29	110.86
1	A	512	LEU	N-CA-C	-6.27	97.45	110.80
1	A	371	VAL	N-CA-C	-6.15	103.40	111.09
1	A	559	VAL	CB-CA-C	6.10	119.44	111.81
1	A	337	MET	N-CA-C	6.05	117.96	111.36
1	A	390	ARG	NE-CZ-NH2	-6.05	113.76	119.20
1	A	448	VAL	CB-CA-C	-5.93	100.13	111.40
1	A	390	ARG	N-CA-C	-5.90	104.76	111.14
1	A	555	LYS	N-CA-C	-5.81	102.86	110.53
1	A	535	VAL	N-CA-C	-5.79	97.29	109.34
1	A	566	ASP	N-CA-C	5.78	123.11	110.80
1	A	486	ILE	N-CA-C	5.76	117.19	110.62
1	A	412	ILE	O-C-N	5.66	129.31	123.20
1	A	374	CYS	N-CA-C	5.63	119.24	112.38
1	A	294	ILE	N-CA-C	5.57	115.58	108.12
1	A	543	LEU	N-CA-C	5.56	117.34	111.28
1	A	314	VAL	CA-C-N	-5.55	115.04	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	VAL	C-N-CA	-5.55	115.04	122.42
1	A	527	GLN	N-CA-C	5.53	122.58	110.80
1	A	510	LYS	CA-CB-CG	-5.53	103.04	114.10
1	A	568	LEU	CA-CB-CG	5.52	135.62	116.30
1	A	485	LEU	CB-CA-C	5.46	120.69	110.70
1	A	366	MET	N-CA-C	5.42	117.52	107.99
1	A	497	LEU	CB-CA-C	5.42	120.06	110.85
1	A	328	GLU	N-CA-C	5.39	122.28	110.80
1	A	500	ASP	CA-C-N	-5.33	113.31	123.32
1	A	500	ASP	C-N-CA	-5.33	113.31	123.32
1	A	423	LEU	N-CA-C	5.28	118.25	110.59
1	A	487	THR	CB-CA-C	-5.28	101.16	109.34
1	A	543	LEU	CA-CB-CG	-5.28	97.84	116.30
1	A	369	GLY	N-CA-C	5.27	125.67	113.18
1	A	480	VAL	CB-CA-C	-5.23	105.17	112.02
1	A	503	VAL	N-CA-C	-5.23	104.72	112.04
1	A	394	ALA	CA-C-N	5.17	127.16	120.44
1	A	394	ALA	C-N-CA	5.17	127.16	120.44
1	A	407	HIS	CA-C-O	5.17	124.88	119.51
1	A	480	VAL	N-CA-CB	5.12	117.13	110.57
1	A	560	VAL	CA-CB-CG1	-5.12	101.70	110.40
1	A	389	LYS	N-CA-C	-5.10	105.72	111.28
1	A	547	GLN	CB-CG-CD	-5.08	103.97	112.60
1	A	460	ALA	CA-C-N	-5.06	113.43	119.05
1	A	460	ALA	C-N-CA	-5.06	113.43	119.05
1	A	544	LEU	N-CA-C	-5.05	105.78	111.28
1	A	444	LYS	CA-C-N	-5.01	112.68	121.70
1	A	444	LYS	C-N-CA	-5.01	112.68	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	GLY	Mainchain
1	A	312	TPO	Mainchain
1	A	314	VAL	Mainchain
1	A	441	MET	Peptide
1	A	446	TPO	Mainchain
1	A	500	ASP	Peptide
1	A	534	GLU	Peptide

## 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	2366	0	2363	395	2
2	A	91	0	0	38	1
All	All	2457	0	2363	395	2

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 84.

All (395) 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:A:526:LEU:O	1:A:529:ASN:HB3	1.37	1.23
1:A:509:VAL:O	1:A:512:LEU:HB2	1.39	1.15
1:A:379:PRO:O	2:A:634:HOH:O	1.64	1.14
1:A:379:PRO:HG2	1:A:382:GLN:HG3	1.18	1.12
1:A:289:PHE:HB2	2:A:647:HOH:O	1.48	1.10
1:A:425:ASP:OD1	1:A:429:GLU:HB2	1.51	1.08
1:A:302:LYS:N	2:A:659:HOH:O	1.86	1.06
1:A:328:GLU:CD	1:A:329:LEU:H	1.61	1.05
1:A:529:ASN:HB2	2:A:618:HOH:O	1.57	1.04
1:A:329:LEU:C	1:A:331:PHE:H	1.57	1.03
1:A:318:ARG:HB3	2:A:659:HOH:O	1.61	1.00
1:A:506:LEU:O	1:A:510:LYS:HG3	1.61	0.99
1:A:347:LEU:HD13	1:A:363:TYR:CD1	1.98	0.98
1:A:280:ARG:HA	1:A:283:GLN:HG3	1.45	0.98
1:A:298:GLY:H	1:A:302:LYS:HA	1.33	0.93
1:A:331:PHE:O	1:A:333:THR:N	2.02	0.92
1:A:387:TRP:HB3	1:A:388:PRO:HD3	1.52	0.92
1:A:310:ASP:OD1	1:A:312:TPO:O1P	1.87	0.91
1:A:570:GLU:O	1:A:572:TRP:N	2.02	0.91
1:A:570:GLU:C	1:A:572:TRP:H	1.78	0.90
1:A:279:LEU:C	1:A:279:LEU:HD12	1.97	0.89
1:A:297:ARG:HA	1:A:302:LYS:HG2	1.54	0.89
1:A:482:LEU:O	1:A:486:ILE:HG13	1.73	0.88
1:A:354:MET:HG2	1:A:355:THR:H	1.37	0.88
1:A:387:TRP:HE1	1:A:534:GLU:CB	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:GLY:O	1:A:313:LEU:HA	1.74	0.87
1:A:329:LEU:C	1:A:331:PHE:N	2.28	0.87
1:A:279:LEU:O	1:A:282:LEU:N	2.05	0.87
1:A:290:SEP:HA	1:A:304:TYR:HE2	1.39	0.87
1:A:496:ARG:HB3	2:A:633:HOH:O	1.73	0.87
1:A:531:LYS:HD3	1:A:532:ASP:N	1.89	0.86
1:A:453:ARG:NH1	1:A:453:ARG:HB2	1.91	0.86
1:A:487:THR:HB	1:A:489:GLN:HG2	1.57	0.86
1:A:510:LYS:O	1:A:513:LEU:HD13	1.75	0.86
1:A:302:LYS:HE2	2:A:666:HOH:O	1.75	0.85
1:A:283:GLN:HA	1:A:289:PHE:CE2	2.11	0.85
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.42	0.84
1:A:387:TRP:HB3	1:A:388:PRO:CD	2.08	0.84
1:A:290:SEP:HA	1:A:304:TYR:CE2	2.12	0.84
1:A:354:MET:HG2	1:A:355:THR:N	1.92	0.83
1:A:378:ARG:NH1	2:A:670:HOH:O	2.13	0.81
1:A:379:PRO:CG	1:A:382:GLN:HG3	2.08	0.81
1:A:328:GLU:OE1	1:A:329:LEU:N	2.13	0.81
1:A:453:ARG:HB2	1:A:453:ARG:HH11	1.46	0.80
1:A:319:LEU:HB3	1:A:358:GLU:HG3	1.62	0.80
1:A:300:PHE:HB2	2:A:629:HOH:O	1.80	0.80
1:A:302:LYS:N	2:A:641:HOH:O	2.14	0.79
1:A:276:ARG:HA	1:A:352:PHE:CE2	2.17	0.79
1:A:462:GLU:O	1:A:466:THR:HB	1.82	0.78
1:A:293:ASN:ND2	1:A:305:LYS:O	2.14	0.78
1:A:387:TRP:O	1:A:390:ARG:N	2.17	0.77
1:A:296:GLY:O	1:A:303:VAL:HG22	1.85	0.77
1:A:450:TPO:O3P	1:A:451:ALA:N	2.16	0.77
1:A:556:MET:O	1:A:559:VAL:HB	1.83	0.77
1:A:405:HIS:O	1:A:411:LYS:NZ	2.17	0.76
1:A:526:LEU:O	1:A:529:ASN:CB	2.27	0.75
1:A:274:LEU:N	2:A:664:HOH:O	1.76	0.75
1:A:328:GLU:CG	1:A:329:LEU:H	2.00	0.75
1:A:379:PRO:HG2	1:A:382:GLN:CG	2.11	0.74
1:A:469:SER:O	1:A:470:SER:HB3	1.82	0.74
1:A:512:LEU:HB3	1:A:513:LEU:HD12	1.67	0.74
1:A:276:ARG:HA	1:A:352:PHE:HE2	1.52	0.73
1:A:449:TPO:CG2	1:A:468:LYS:HG2	2.18	0.73
1:A:376:ARG:HH11	1:A:376:ARG:CG	2.01	0.72
1:A:500:ASP:HB3	2:A:636:HOH:O	1.87	0.72
1:A:514:LYS:H	1:A:514:LYS:HD2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HB2	1:A:365:TYR:HB3	1.70	0.72
1:A:449:TPO:HG22	1:A:468:LYS:HG2	1.71	0.72
1:A:298:GLY:HA3	2:A:641:HOH:O	1.89	0.72
1:A:313:LEU:CB	1:A:365:TYR:HB3	2.20	0.71
1:A:347:LEU:CD2	1:A:348:ARG:H	2.03	0.71
1:A:378:ARG:HG3	2:A:612:HOH:O	1.90	0.71
1:A:319:LEU:HD12	1:A:359:ARG:HB2	1.72	0.71
1:A:360:LEU:HD12	2:A:638:HOH:O	1.90	0.71
1:A:569:ALA:HA	1:A:572:TRP:HE1	1.56	0.71
1:A:382:GLN:HB2	2:A:634:HOH:O	1.89	0.71
1:A:303:VAL:HG23	1:A:303:VAL:O	1.89	0.71
1:A:387:TRP:HE1	1:A:534:GLU:HB3	1.53	0.71
1:A:415:ARG:HB2	1:A:437:LEU:O	1.92	0.70
1:A:387:TRP:HZ2	1:A:534:GLU:O	1.73	0.70
1:A:353:CYS:HB3	1:A:360:LEU:HD12	1.73	0.70
1:A:529:ASN:OD1	1:A:529:ASN:O	2.09	0.70
1:A:501:ASP:OD2	2:A:633:HOH:O	2.09	0.69
1:A:456:ILE:HG23	1:A:457:GLY:N	2.07	0.69
1:A:317:LYS:O	1:A:360:LEU:HB3	1.91	0.69
1:A:401:LEU:HB3	1:A:556:MET:HG3	1.74	0.69
1:A:554:PRO:HB2	1:A:559:VAL:HG23	1.75	0.69
1:A:329:LEU:O	1:A:331:PHE:N	2.25	0.69
1:A:523:ASP:OD2	1:A:523:ASP:C	2.36	0.69
1:A:304:TYR:CE1	2:A:666:HOH:O	2.46	0.68
1:A:350:ARG:HB2	1:A:362:VAL:HG12	1.74	0.68
1:A:280:ARG:HA	1:A:283:GLN:CG	2.22	0.68
1:A:334:GLU:HA	1:A:337:MET:HB2	1.76	0.68
1:A:279:LEU:O	1:A:280:ARG:C	2.36	0.68
1:A:280:ARG:CA	1:A:283:GLN:HG3	2.23	0.68
1:A:294:ILE:HD11	1:A:304:TYR:CZ	2.29	0.68
1:A:318:ARG:HA	1:A:360:LEU:HD23	1.75	0.67
1:A:275:LYS:HB3	1:A:277:PHE:CE1	2.29	0.67
1:A:370:SER:HG	1:A:373:SER:H	1.41	0.67
1:A:300:PHE:CB	2:A:629:HOH:O	2.40	0.67
1:A:506:LEU:O	1:A:510:LYS:CG	2.41	0.67
1:A:466:THR:HG23	1:A:466:THR:O	1.95	0.67
1:A:469:SER:O	1:A:470:SER:CB	2.41	0.67
1:A:302:LYS:CE	2:A:666:HOH:O	2.35	0.66
1:A:560:VAL:O	1:A:561:ARG:C	2.36	0.66
1:A:569:ALA:O	1:A:572:TRP:NE1	2.29	0.65
1:A:331:PHE:CE2	1:A:359:ARG:HB3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:SEP:CA	1:A:304:TYR:HE2	2.07	0.64
1:A:378:ARG:HD2	1:A:382:GLN:O	1.98	0.64
1:A:350:ARG:HB2	1:A:362:VAL:CG1	2.28	0.64
1:A:492:PHE:HA	1:A:503:VAL:O	1.98	0.64
1:A:496:ARG:O	1:A:499:ASN:OD1	2.16	0.64
1:A:502:ASP:OD1	1:A:502:ASP:N	2.31	0.64
1:A:312:TPO:O3P	1:A:312:TPO:HG21	1.98	0.63
1:A:378:ARG:HG2	1:A:382:GLN:HB2	1.80	0.63
1:A:318:ARG:HH21	1:A:320:LYS:HE3	1.63	0.63
1:A:319:LEU:HD22	1:A:358:GLU:OE2	1.97	0.63
1:A:475:VAL:O	1:A:478:TYR:N	2.32	0.63
1:A:336:GLU:HB2	2:A:667:HOH:O	1.97	0.63
1:A:371:VAL:CG2	1:A:422:ILE:HB	2.29	0.63
1:A:422:ILE:C	1:A:423:LEU:HD12	2.24	0.63
1:A:449:TPO:HG21	1:A:449:TPO:O3P	1.98	0.63
1:A:360:LEU:N	2:A:638:HOH:O	1.93	0.62
1:A:388:PRO:HA	1:A:391:GLN:HB2	1.79	0.62
1:A:513:LEU:HD12	1:A:513:LEU:H	1.64	0.62
1:A:376:ARG:CG	1:A:376:ARG:NH1	2.60	0.62
1:A:496:ARG:C	1:A:499:ASN:OD1	2.42	0.62
1:A:415:ARG:NH1	1:A:437:LEU:O	2.32	0.62
1:A:276:ARG:O	1:A:276:ARG:HG3	1.99	0.62
1:A:513:LEU:O	1:A:514:LYS:O	2.18	0.62
1:A:387:TRP:HE1	1:A:534:GLU:HB2	1.63	0.62
1:A:534:GLU:HA	1:A:537:GLN:OE1	2.00	0.61
1:A:329:LEU:C	1:A:329:LEU:HD12	2.25	0.61
1:A:425:ASP:CG	1:A:429:GLU:HB2	2.26	0.61
1:A:554:PRO:HB2	1:A:559:VAL:CG2	2.30	0.61
1:A:572:TRP:N	1:A:572:TRP:CD1	2.67	0.61
1:A:348:ARG:HH22	1:A:350:ARG:HE	1.49	0.61
1:A:359:ARG:C	1:A:360:LEU:HG	2.24	0.61
1:A:456:ILE:CG2	1:A:457:GLY:N	2.63	0.61
1:A:279:LEU:HA	1:A:282:LEU:HG	1.84	0.60
1:A:307:ARG:O	1:A:308:LEU:O	2.19	0.60
1:A:347:LEU:CD2	1:A:364:PRO:HD2	2.30	0.60
1:A:423:LEU:HD12	1:A:423:LEU:N	2.16	0.60
1:A:462:GLU:OE2	1:A:473:THR:HG22	2.01	0.60
1:A:489:GLN:HB3	1:A:496:ARG:NH1	2.17	0.60
1:A:446:TPO:O1P	1:A:447:HIS:ND1	2.33	0.60
1:A:461:PRO:O	1:A:464:LEU:HG	2.01	0.60
1:A:332:GLN:O	1:A:336:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:O	2:A:617:HOH:O	2.16	0.59
1:A:466:THR:O	1:A:466:THR:CG2	2.51	0.59
1:A:319:LEU:HB2	1:A:359:ARG:O	2.03	0.59
1:A:331:PHE:O	1:A:332:GLN:C	2.45	0.59
1:A:461:PRO:HA	1:A:464:LEU:HG	1.85	0.59
1:A:514:LYS:O	1:A:516:LYS:HG3	2.03	0.59
1:A:313:LEU:CB	1:A:365:TYR:CB	2.81	0.59
1:A:331:PHE:CZ	1:A:359:ARG:HB3	2.38	0.59
1:A:570:GLU:C	1:A:572:TRP:N	2.42	0.59
1:A:353:CYS:HB3	2:A:638:HOH:O	2.03	0.58
1:A:423:LEU:N	1:A:423:LEU:CD1	2.66	0.58
1:A:335:VAL:C	1:A:337:MET:H	2.09	0.58
1:A:282:LEU:HD12	1:A:282:LEU:C	2.28	0.58
1:A:321:GLU:C	2:A:621:HOH:O	2.46	0.58
1:A:296:GLY:N	1:A:303:VAL:CG2	2.67	0.57
1:A:352:PHE:C	1:A:352:PHE:CD2	2.78	0.57
1:A:371:VAL:HG23	1:A:422:ILE:O	2.04	0.57
1:A:513:LEU:H	1:A:513:LEU:CD1	2.17	0.57
1:A:338:ILE:CD1	1:A:348:ARG:HG2	2.34	0.57
1:A:396:GLY:O	1:A:399:ARG:HB2	2.03	0.57
1:A:277:PHE:HE2	1:A:362:VAL:HG21	1.70	0.57
1:A:482:LEU:HB2	1:A:542:ALA:HB2	1.86	0.57
1:A:447:HIS:HB2	1:A:468:LYS:HB3	1.87	0.57
1:A:569:ALA:O	1:A:572:TRP:CD1	2.57	0.57
1:A:370:SER:HG	1:A:373:SER:N	2.03	0.57
1:A:371:VAL:HG23	1:A:422:ILE:HB	1.86	0.57
1:A:505:LEU:HD12	1:A:505:LEU:O	2.05	0.57
1:A:279:LEU:HD12	1:A:279:LEU:O	2.05	0.56
1:A:347:LEU:HD23	1:A:348:ARG:H	1.70	0.56
1:A:523:ASP:O	1:A:525:ASP:N	2.38	0.56
1:A:321:GLU:N	1:A:321:GLU:OE1	2.37	0.56
1:A:331:PHE:C	1:A:333:THR:N	2.63	0.56
1:A:392:ARG:NH1	1:A:429:GLU:OE1	2.39	0.56
1:A:475:VAL:O	1:A:478:TYR:HB3	2.05	0.56
1:A:295:LEU:C	1:A:303:VAL:CG2	2.79	0.56
1:A:419:ALA:C	1:A:421:ASN:H	2.11	0.56
1:A:313:LEU:HB3	1:A:365:TYR:CB	2.35	0.56
1:A:447:HIS:ND1	1:A:468:LYS:HD3	2.21	0.56
1:A:509:VAL:CG1	1:A:512:LEU:HD12	2.34	0.56
1:A:301:GLY:O	1:A:302:LYS:HG3	2.06	0.56
1:A:496:ARG:HA	1:A:499:ASN:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:HD22	1:A:348:ARG:H	1.69	0.55
1:A:289:PHE:O	1:A:290:SEP:O	2.25	0.55
1:A:304:TYR:HE1	2:A:666:HOH:O	1.86	0.55
1:A:387:TRP:NE1	1:A:534:GLU:CB	2.65	0.55
1:A:295:LEU:HD21	1:A:305:LYS:HD3	1.89	0.55
1:A:336:GLU:C	2:A:667:HOH:O	2.49	0.55
1:A:387:TRP:NE1	1:A:534:GLU:HB2	2.21	0.55
1:A:513:LEU:O	1:A:514:LYS:C	2.50	0.55
1:A:455:TPO:C	1:A:455:TPO:O1P	2.54	0.55
1:A:555:LYS:O	1:A:559:VAL:HG23	2.07	0.55
1:A:294:ILE:CD1	1:A:304:TYR:CZ	2.90	0.54
1:A:347:LEU:HD22	1:A:363:TYR:HD1	1.72	0.54
1:A:370:SER:OG	1:A:372:ALA:N	2.40	0.54
1:A:569:ALA:CA	1:A:572:TRP:HE1	2.21	0.54
1:A:298:GLY:N	1:A:302:LYS:HA	2.14	0.54
1:A:447:HIS:HE2	1:A:449:TPO:P	2.30	0.54
1:A:279:LEU:HG	1:A:280:ARG:N	2.23	0.53
1:A:279:LEU:HD11	1:A:283:GLN:HG2	1.90	0.53
1:A:272:GLY:O	1:A:273:GLN:HB2	2.09	0.53
1:A:303:VAL:O	1:A:303:VAL:CG2	2.56	0.53
1:A:509:VAL:HG13	1:A:512:LEU:HD12	1.89	0.53
1:A:572:TRP:N	1:A:572:TRP:HD1	2.06	0.53
1:A:489:GLN:HB3	1:A:496:ARG:HH12	1.74	0.53
1:A:537:GLN:O	1:A:541:VAL:HG23	2.09	0.53
1:A:293:ASN:HB3	1:A:304:TYR:CD2	2.45	0.52
1:A:491:ALA:HA	1:A:505:LEU:HB3	1.92	0.52
1:A:531:LYS:HB3	1:A:534:GLU:HG3	1.92	0.52
1:A:347:LEU:CD1	1:A:363:TYR:CD1	2.84	0.52
1:A:294:ILE:HG22	1:A:296:GLY:H	1.74	0.52
1:A:415:ARG:HH11	1:A:439:LYS:HG2	1.75	0.52
1:A:293:ASN:HB3	1:A:304:TYR:HD2	1.75	0.52
1:A:347:LEU:HD11	1:A:363:TYR:HB3	1.92	0.52
1:A:278:SER:OG	1:A:281:GLU:HB3	2.09	0.52
1:A:328:GLU:OE1	1:A:329:LEU:HA	2.10	0.52
1:A:382:GLN:O	2:A:670:HOH:O	2.19	0.52
1:A:307:ARG:C	1:A:308:LEU:O	2.52	0.52
1:A:318:ARG:HH21	1:A:320:LYS:CE	2.22	0.52
1:A:347:LEU:HD21	1:A:364:PRO:HD2	1.90	0.52
1:A:453:ARG:HH11	1:A:453:ARG:CB	2.19	0.51
1:A:447:HIS:C	1:A:447:HIS:CD2	2.87	0.51
1:A:513:LEU:HD12	1:A:513:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HB3	1:A:365:TYR:CG	2.45	0.51
1:A:291:ASN:C	1:A:293:ASN:H	2.19	0.51
1:A:442:ASP:O	1:A:444:LYS:O	2.28	0.51
1:A:328:GLU:CD	1:A:329:LEU:N	2.46	0.51
1:A:277:PHE:CE2	1:A:362:VAL:HG21	2.46	0.51
1:A:290:SEP:N	1:A:304:TYR:HE2	2.09	0.51
1:A:301:GLY:HA3	2:A:659:HOH:O	2.11	0.51
1:A:331:PHE:O	1:A:334:GLU:N	2.39	0.51
1:A:313:LEU:C	1:A:365:TYR:HB2	2.36	0.51
1:A:395:LEU:HA	1:A:563:LEU:HD12	1.93	0.51
1:A:569:ALA:C	1:A:572:TRP:HE1	2.19	0.51
1:A:481:MET:CE	1:A:482:LEU:HD23	2.40	0.50
1:A:561:ARG:HB3	1:A:566:ASP:CB	2.41	0.50
1:A:347:LEU:HD13	1:A:363:TYR:CG	2.44	0.50
1:A:366:MET:O	1:A:367:ALA:C	2.54	0.50
1:A:418:LYS:O	1:A:421:ASN:N	2.42	0.50
1:A:283:GLN:HG2	1:A:289:PHE:HE2	1.77	0.50
1:A:279:LEU:CG	1:A:280:ARG:N	2.75	0.50
1:A:380:GLU:OE2	2:A:631:HOH:O	2.20	0.50
1:A:426:GLU:HB3	1:A:427:GLU:OE2	2.12	0.50
1:A:524:VAL:O	2:A:607:HOH:O	2.19	0.49
1:A:539:ILE:C	1:A:541:VAL:N	2.69	0.49
1:A:482:LEU:O	1:A:486:ILE:CG1	2.55	0.49
1:A:496:ARG:CA	1:A:499:ASN:OD1	2.59	0.49
1:A:425:ASP:OD1	1:A:429:GLU:CB	2.42	0.49
1:A:571:ARG:O	1:A:572:TRP:HB3	2.13	0.49
1:A:405:HIS:O	1:A:411:LYS:HG2	2.12	0.49
1:A:449:TPO:HG23	1:A:468:LYS:HG2	1.93	0.49
1:A:455:TPO:O1P	1:A:455:TPO:O	2.31	0.49
1:A:282:LEU:C	1:A:282:LEU:CD1	2.86	0.49
1:A:395:LEU:HD22	1:A:399:ARG:NE	2.27	0.49
1:A:487:THR:HB	1:A:489:GLN:CG	2.38	0.49
1:A:313:LEU:C	1:A:365:TYR:CB	2.86	0.48
1:A:347:LEU:HD22	1:A:348:ARG:N	2.29	0.48
1:A:338:ILE:HD12	1:A:348:ARG:HG2	1.96	0.48
1:A:395:LEU:HD21	1:A:564:GLU:HG3	1.94	0.48
1:A:402:ALA:O	1:A:406:ASP:HB2	2.14	0.48
1:A:453:ARG:HD3	2:A:688:HOH:O	2.14	0.48
1:A:276:ARG:CA	1:A:352:PHE:HE2	2.22	0.48
1:A:366:MET:HG3	1:A:423:LEU:HB3	1.95	0.48
1:A:470:SER:C	1:A:472:LYS:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:C	1:A:279:LEU:CD1	2.69	0.48
1:A:523:ASP:OD2	1:A:523:ASP:O	2.31	0.48
1:A:546:THR:O	1:A:547:GLN:C	2.55	0.48
1:A:371:VAL:CG1	1:A:485:LEU:HD23	2.44	0.48
1:A:425:ASP:OD2	1:A:428:PHE:N	2.47	0.48
1:A:458:HIS:CD2	1:A:480:VAL:HB	2.49	0.48
1:A:302:LYS:CD	2:A:666:HOH:O	2.62	0.47
1:A:278:SER:N	1:A:281:GLU:OE1	2.24	0.47
1:A:453:ARG:CD	2:A:688:HOH:O	2.61	0.47
1:A:290:SEP:O	1:A:291:ASN:HB2	2.14	0.47
1:A:276:ARG:O	1:A:277:PHE:CD1	2.68	0.47
1:A:280:ARG:C	1:A:282:LEU:H	2.22	0.47
1:A:290:SEP:N	1:A:304:TYR:CE2	2.82	0.47
1:A:419:ALA:C	1:A:421:ASN:N	2.66	0.47
1:A:531:LYS:HD3	1:A:532:ASP:H	1.77	0.47
1:A:318:ARG:HH21	1:A:320:LYS:NZ	2.13	0.47
1:A:491:ALA:HA	1:A:505:LEU:CB	2.45	0.47
1:A:348:ARG:HH22	1:A:350:ARG:NE	2.10	0.47
1:A:328:GLU:O	1:A:330:GLN:N	2.48	0.46
1:A:301:GLY:O	1:A:302:LYS:CG	2.63	0.46
1:A:415:ARG:CB	1:A:437:LEU:O	2.63	0.46
1:A:297:ARG:HG3	1:A:302:LYS:HD3	1.97	0.46
1:A:386:ASP:O	1:A:387:TRP:O	2.34	0.46
1:A:387:TRP:HZ2	1:A:534:GLU:C	2.23	0.46
1:A:442:ASP:O	1:A:443:TYR:C	2.58	0.46
1:A:481:MET:O	1:A:482:LEU:C	2.55	0.46
1:A:295:LEU:C	1:A:303:VAL:HG21	2.40	0.46
1:A:371:VAL:HG21	1:A:422:ILE:HB	1.95	0.46
1:A:387:TRP:CZ2	1:A:535:VAL:HG22	2.50	0.46
1:A:521:LEU:HD12	1:A:521:LEU:C	2.40	0.46
1:A:307:ARG:HA	1:A:312:TPO:O	2.15	0.46
1:A:388:PRO:HA	1:A:391:GLN:HG3	1.97	0.46
1:A:543:LEU:HA	1:A:543:LEU:HD23	1.14	0.46
1:A:329:LEU:C	1:A:329:LEU:CD1	2.89	0.46
1:A:489:GLN:NE2	1:A:508:TRP:CH2	2.84	0.46
1:A:493:ASP:H	1:A:496:ARG:NH2	2.13	0.46
1:A:372:ALA:O	1:A:375:LEU:N	2.48	0.46
1:A:514:LYS:O	1:A:516:LYS:N	2.49	0.46
1:A:338:ILE:HG23	1:A:339:SER:N	2.31	0.46
1:A:294:ILE:HG22	1:A:296:GLY:N	2.31	0.45
1:A:364:PRO:HB2	1:A:366:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:THR:CB	1:A:489:GLN:HG2	2.39	0.45
1:A:313:LEU:O	1:A:365:TYR:HB3	2.16	0.45
1:A:330:GLN:HA	1:A:333:THR:HG23	1.98	0.45
1:A:348:ARG:O	1:A:364:PRO:HD2	2.16	0.45
1:A:276:ARG:O	1:A:277:PHE:HD1	1.99	0.45
1:A:552:GLU:O	1:A:571:ARG:NH1	2.45	0.45
1:A:294:ILE:HD12	1:A:302:LYS:HD2	1.97	0.45
1:A:300:PHE:O	1:A:319:LEU:HA	2.17	0.45
1:A:447:HIS:NE2	1:A:449:TPO:O1P	2.44	0.45
1:A:533:GLU:O	1:A:537:GLN:OE1	2.34	0.45
1:A:535:VAL:O	1:A:536:GLU:C	2.58	0.45
1:A:515:GLU:H	1:A:515:GLU:HG3	1.61	0.45
1:A:318:ARG:HE	1:A:320:LYS:HE3	1.82	0.45
1:A:559:VAL:HA	1:A:562:MET:HE2	1.99	0.45
1:A:393:ILE:HA	1:A:430:ALA:HB2	1.99	0.44
1:A:347:LEU:CD2	1:A:348:ARG:N	2.75	0.44
1:A:518:LEU:H	1:A:518:LEU:CD2	2.30	0.44
1:A:481:MET:HE3	1:A:482:LEU:HD23	1.99	0.44
1:A:289:PHE:CD2	1:A:289:PHE:N	2.85	0.44
1:A:335:VAL:C	1:A:337:MET:N	2.71	0.44
1:A:514:LYS:O	1:A:516:LYS:CG	2.65	0.44
1:A:347:LEU:CD1	1:A:363:TYR:HB3	2.48	0.44
1:A:371:VAL:HG22	1:A:424:LEU:HD21	2.00	0.44
1:A:440:LEU:N	1:A:440:LEU:HD23	2.32	0.44
1:A:451:ALA:HB3	1:A:453:ARG:NH2	2.32	0.44
1:A:309:ALA:C	1:A:310:ASP:O	2.58	0.44
1:A:280:ARG:C	1:A:282:LEU:N	2.74	0.43
1:A:447:HIS:CE1	1:A:468:LYS:HD3	2.52	0.43
1:A:452:VAL:HG13	1:A:463:TYR:CE2	2.52	0.43
1:A:456:ILE:HG21	1:A:492:PHE:CG	2.52	0.43
1:A:517:LYS:NZ	1:A:519:GLU:OE1	2.43	0.43
1:A:518:LEU:HB2	1:A:519:GLU:HG2	2.00	0.43
1:A:301:GLY:C	1:A:302:LYS:HG3	2.43	0.43
1:A:561:ARG:O	1:A:564:GLU:N	2.51	0.43
1:A:338:ILE:HD11	1:A:348:ARG:HG2	2.00	0.43
1:A:528:GLY:O	1:A:529:ASN:HB2	2.18	0.43
1:A:386:ASP:HA	1:A:526:LEU:CD2	2.49	0.43
1:A:471:GLU:HG2	2:A:614:HOH:O	2.18	0.43
1:A:519:GLU:HG2	1:A:519:GLU:H	1.34	0.43
1:A:389:LYS:O	1:A:393:ILE:HG13	2.19	0.43
1:A:290:SEP:CA	1:A:304:TYR:CE2	2.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HD11	1:A:417:VAL:HG21	2.00	0.42
1:A:476:PHE:CD2	1:A:546:THR:HA	2.55	0.42
1:A:506:LEU:HD12	1:A:510:LYS:HD2	2.02	0.42
1:A:347:LEU:HD23	2:A:613:HOH:O	2.18	0.42
1:A:481:MET:HE3	1:A:482:LEU:N	2.34	0.42
1:A:561:ARG:HB3	1:A:566:ASP:HB3	2.00	0.42
1:A:378:ARG:C	2:A:634:HOH:O	2.62	0.42
1:A:381:SER:O	1:A:382:GLN:C	2.62	0.42
1:A:453:ARG:HB2	1:A:453:ARG:CZ	2.49	0.42
1:A:516:LYS:HG3	1:A:516:LYS:H	1.63	0.42
1:A:294:ILE:HD11	1:A:304:TYR:OH	2.19	0.42
1:A:387:TRP:CB	1:A:388:PRO:CD	2.84	0.42
1:A:509:VAL:HG12	1:A:512:LEU:CD1	2.50	0.41
1:A:531:LYS:CD	1:A:533:GLU:H	2.33	0.41
1:A:307:ARG:O	1:A:308:LEU:C	2.62	0.41
1:A:540:GLN:O	1:A:544:LEU:HG	2.19	0.41
1:A:328:GLU:CG	1:A:329:LEU:N	2.73	0.41
1:A:561:ARG:HB3	1:A:566:ASP:HB2	2.02	0.41
1:A:313:LEU:O	1:A:365:TYR:CB	2.67	0.41
1:A:360:LEU:C	1:A:361:LEU:HG	2.46	0.41
1:A:387:TRP:HA	1:A:387:TRP:CE3	2.55	0.41
1:A:470:SER:C	1:A:472:LYS:H	2.28	0.41
1:A:364:PRO:HB2	1:A:366:MET:HE2	2.03	0.41
1:A:443:TYR:O	1:A:444:LYS:C	2.64	0.41
1:A:328:GLU:OE1	1:A:329:LEU:CA	2.68	0.41
1:A:282:LEU:HD12	1:A:283:GLN:N	2.36	0.41
1:A:355:THR:HA	1:A:356:PRO:HD2	1.87	0.41
1:A:378:ARG:HG2	2:A:634:HOH:O	2.20	0.41
1:A:413:ILE:HD12	1:A:413:ILE:HG23	1.72	0.41
1:A:470:SER:O	1:A:471:GLU:C	2.56	0.41
1:A:294:ILE:CD1	1:A:302:LYS:HD2	2.51	0.40
1:A:332:GLN:CG	1:A:333:THR:N	2.83	0.40
1:A:425:ASP:OD2	1:A:425:ASP:C	2.63	0.40
1:A:540:GLN:OE1	1:A:572:TRP:CZ2	2.74	0.40
1:A:396:GLY:O	1:A:399:ARG:CB	2.69	0.40
1:A:332:GLN:O	1:A:336:GLU:CG	2.69	0.40
1:A:370:SER:OG	1:A:373:SER:N	2.43	0.40
1:A:518:LEU:O	1:A:521:LEU:HG	2.21	0.40
1:A:336:GLU:O	1:A:340:MET:HE3	2.22	0.40
1:A:338:ILE:HG13	1:A:342:VAL:HG22	2.02	0.40
1:A:414:HIS:N	1:A:474:ASP:OD2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ALA:O	1:A:310:ASP:O	2.39	0.40

All (2) 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)
1:A:272:GLY:O	2:A:661:HOH:O[2_554]	1.82	0.38
1:A:307:ARG:NE	1:A:552:GLU:OE1[3_545]	2.12	0.08

## 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	287/326 (88%)	199 (69%)	42 (15%)	46 (16%)	<b>0</b> <b>0</b>

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	279	LEU
1	A	308	LEU
1	A	329	LEU
1	A	331	PHE
1	A	332	GLN
1	A	355	THR
1	A	356	PRO
1	A	380	GLU
1	A	443	TYR
1	A	444	LYS
1	A	447	HIS
1	A	452	VAL
1	A	498	ALA

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Mol	Chain	Res	Type
1	A	513	LEU
1	A	514	LYS
1	A	519	GLU
1	A	523	ASP
1	A	524	VAL
1	A	527	GLN
1	A	310	ASP
1	A	328	GLU
1	A	330	GLN
1	A	369	GLY
1	A	470	SER
1	A	475	VAL
1	A	476	PHE
1	A	515	GLU
1	A	529	ASN
1	A	547	GLN
1	A	551	MET
1	A	571	ARG
1	A	281	GLU
1	A	287	ASP
1	A	387	TRP
1	A	399	ARG
1	A	442	ASP
1	A	434	ASP
1	A	516	LYS
1	A	291	ASN
1	A	416	ASP
1	A	441	MET
1	A	540	GLN
1	A	499	ASN
1	A	518	LEU
1	A	528	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	246/273 (90%)	183 (74%)	63 (26%)	<b>0</b> <b>1</b>

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ARG
1	A	279	LEU
1	A	281	GLU
1	A	282	LEU
1	A	293	ASN
1	A	295	LEU
1	A	308	LEU
1	A	316	VAL
1	A	328	GLU
1	A	333	THR
1	A	336	GLU
1	A	338	ILE
1	A	347	LEU
1	A	348	ARG
1	A	350	ARG
1	A	352	PHE
1	A	354	MET
1	A	358	GLU
1	A	359	ARG
1	A	360	LEU
1	A	364	PRO
1	A	368	ASN
1	A	373	SER
1	A	375	LEU
1	A	376	ARG
1	A	377	GLU
1	A	384	PRO
1	A	387	TRP
1	A	389	LYS
1	A	395	LEU
1	A	434	ASP
1	A	440	LEU
1	A	441	MET
1	A	444	LYS
1	A	452	VAL
1	A	453	ARG
1	A	456	ILE
1	A	465	SER

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Mol	Chain	Res	Type
1	A	466	THR
1	A	470	SER
1	A	472	LYS
1	A	481	MET
1	A	485	LEU
1	A	486	ILE
1	A	493	ASP
1	A	499	ASN
1	A	500	ASP
1	A	501	ASP
1	A	502	ASP
1	A	504	MET
1	A	506	LEU
1	A	507	ASP
1	A	518	LEU
1	A	519	GLU
1	A	524	VAL
1	A	525	ASP
1	A	531	LYS
1	A	533	GLU
1	A	534	GLU
1	A	538	LEU
1	A	556	MET
1	A	562	MET
1	A	573	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	414	HIS
1	A	489	GLN
1	A	527	GLN
1	A	529	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	TPO	A	312	1	8,10,11	0.51	0	10,14,16	0.83	0
1	TPO	A	455	1	8,10,11	0.51	0	10,14,16	1.45	2 (20%)
1	TPO	A	449	1	8,10,11	0.51	0	10,14,16	0.82	0
1	SEP	A	290	1	8,9,10	1.13	0	7,12,14	3.94	1 (14%)
1	TPO	A	446	1	8,10,11	1.07	0	10,14,16	1.09	1 (10%)
1	TPO	A	450	1	8,10,11	0.69	0	10,14,16	1.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	312	1	-	4/9/11/13	-
1	TPO	A	455	1	-	2/9/11/13	-
1	TPO	A	449	1	-	4/9/11/13	-
1	SEP	A	290	1	-	2/6/8/10	-
1	TPO	A	446	1	-	3/9/11/13	-
1	TPO	A	450	1	-	6/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	SEP	OG-CB-CA	10.16	118.03	108.14
1	A	455	TPO	O3P-P-OG1	2.68	116.27	105.85
1	A	446	TPO	CG2-CB-CA	-2.59	108.22	113.26
1	A	455	TPO	O3P-P-O1P	-2.37	101.60	110.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	290	SEP	N-CA-CB-OG
1	A	290	SEP	C-CA-CB-OG
1	A	312	TPO	N-CA-CB-CG2
1	A	312	TPO	N-CA-CB-OG1
1	A	312	TPO	C-CA-CB-CG2
1	A	312	TPO	O-C-CA-CB
1	A	446	TPO	N-CA-CB-CG2
1	A	446	TPO	N-CA-CB-OG1
1	A	446	TPO	C-CA-CB-CG2
1	A	449	TPO	N-CA-CB-CG2
1	A	449	TPO	N-CA-CB-OG1
1	A	449	TPO	C-CA-CB-CG2
1	A	449	TPO	O-C-CA-CB
1	A	450	TPO	N-CA-CB-OG1
1	A	450	TPO	O-C-CA-CB
1	A	450	TPO	CA-CB-OG1-P
1	A	455	TPO	CA-CB-OG1-P
1	A	450	TPO	C-CA-CB-CG2
1	A	450	TPO	N-CA-CB-CG2
1	A	455	TPO	O-C-CA-CB
1	A	450	TPO	CB-OG1-P-O1P

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	312	TPO	3	0
1	A	455	TPO	2	0
1	A	449	TPO	6	0
1	A	290	SEP	8	0
1	A	446	TPO	1	0
1	A	450	TPO	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	291/326 (89%)	0.25	3 (1%) 79 76	33, 77, 126, 169	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	GLY	2.2
1	A	309	ALA	2.1
1	A	300	PHE	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPO	A	446	11/12	0.60	0.17	73,84,112,116	0
1	SEP	A	290	10/11	0.71	0.11	121,130,199,202	0
1	TPO	A	449	11/12	0.73	0.10	84,101,140,143	0
1	TPO	A	312	11/12	0.77	0.14	84,101,140,143	0
1	TPO	A	450	11/12	0.84	0.13	81,99,131,131	0
1	TPO	A	455	11/12	0.86	0.16	111,123,130,133	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.