



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:00 am BST

PDB ID : 3ULZ
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

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

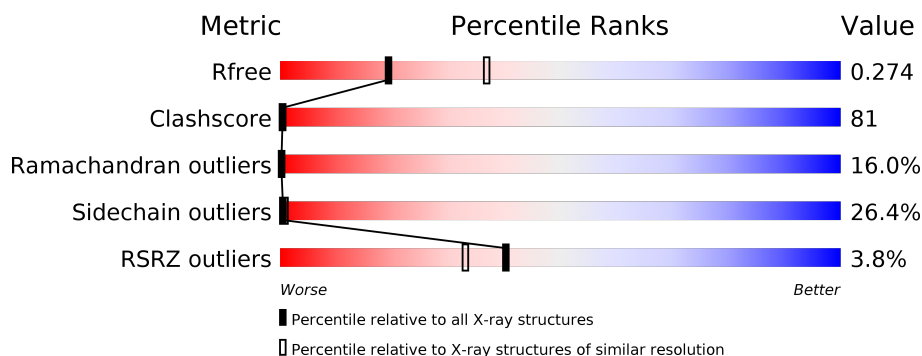
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	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	-
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
1	A	297	Total	C	N	O	P	S	0	0	0
			2366	1477	413	456	6	14			

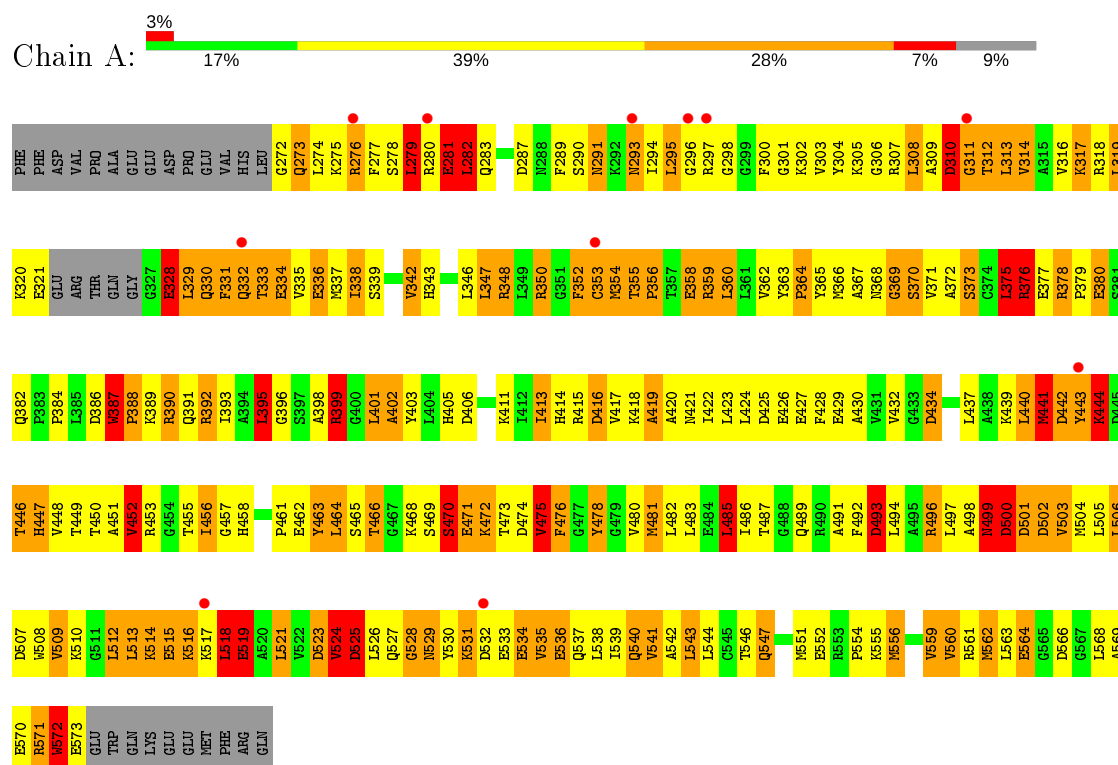
- Molecule 2 is water.

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 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: 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, α , β , γ	70.25Å 75.59Å 71.94Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	41.05 – 2.60 41.05 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.4 (41.05-2.60) 88.3 (41.05-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.224 , 0.279 0.228 , 0.274	Depositor DCC
R_{free} test set	435 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2457	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage'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.*

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: 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	1.47	27/2333 (1.2%)	1.68	46/3130 (1.5%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	GLU	CD-OE2	9.73	1.36	1.25
1	A	478	TYR	CG-CD1	-8.01	1.28	1.39
1	A	564	GLU	CB-CG	6.91	1.65	1.52
1	A	471	GLU	CG-CD	6.73	1.62	1.51
1	A	541	VAL	CA-CB	6.62	1.68	1.54
1	A	564	GLU	CG-CD	6.24	1.61	1.51
1	A	432	VAL	CB-CG1	5.91	1.65	1.52
1	A	419	ALA	CA-CB	-5.85	1.40	1.52
1	A	413	ILE	CA-CB	-5.83	1.41	1.54
1	A	398	ALA	CA-CB	-5.83	1.40	1.52
1	A	342	VAL	CA-CB	-5.82	1.42	1.54
1	A	478	TYR	CA-CB	5.55	1.66	1.53
1	A	478	TYR	CE1-CZ	-5.53	1.31	1.38
1	A	388	PRO	C-O	5.48	1.34	1.23
1	A	403	TYR	CG-CD1	5.44	1.46	1.39
1	A	524	VAL	CB-CG1	-5.44	1.41	1.52
1	A	334	GLU	CG-CD	5.36	1.59	1.51
1	A	559	VAL	CB-CG2	5.31	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	GLU	CD-OE1	5.31	1.31	1.25
1	A	572	TRP	CB-CG	-5.30	1.40	1.50
1	A	536	GLU	CG-CD	5.27	1.59	1.51
1	A	310	ASP	C-N	5.23	1.42	1.33
1	A	403	TYR	CG-CD2	-5.17	1.32	1.39
1	A	475	VAL	CB-CG1	-5.16	1.42	1.52
1	A	509	VAL	CA-CB	5.12	1.65	1.54
1	A	403	TYR	CD1-CE1	5.01	1.46	1.39
1	A	420	ALA	CA-CB	5.01	1.62	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ASP	CB-CA-C	19.09	148.58	110.40
1	A	390	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	A	311	GLY	N-CA-C	-12.19	82.62	113.10
1	A	390	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	568	LEU	CA-CB-CG	8.84	135.62	115.30
1	A	496	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	343	HIS	N-CA-C	-7.71	90.17	111.00
1	A	483	LEU	CB-CG-CD2	7.70	124.09	111.00
1	A	543	LEU	CA-CB-CG	-7.59	97.84	115.30
1	A	493	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	A	310	ASP	O-C-N	-7.53	110.40	123.20
1	A	485	LEU	CA-CB-CG	7.49	132.53	115.30
1	A	525	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	310	ASP	N-CA-C	-7.45	90.89	111.00
1	A	464	LEU	CA-CB-CG	7.05	131.53	115.30
1	A	395	LEU	CA-CB-CG	6.61	130.49	115.30
1	A	310	ASP	CA-C-N	6.47	129.14	116.20
1	A	375	LEU	CB-CG-CD2	6.46	121.99	111.00
1	A	494	LEU	CA-CB-CG	-6.29	100.83	115.30
1	A	310	ASP	C-N-CA	-6.21	109.27	122.30
1	A	560	VAL	CA-CB-CG1	-6.13	101.70	110.90
1	A	485	LEU	CB-CG-CD1	-6.06	100.69	111.00
1	A	521	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	A	313	LEU	CA-CB-CG	-6.00	101.51	115.30
1	A	448	VAL	CB-CA-C	-5.93	100.13	111.40
1	A	319	LEU	CA-CB-CG	5.89	128.84	115.30
1	A	395	LEU	CB-CG-CD2	5.70	120.68	111.00
1	A	512	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	314	VAL	CA-C-N	-5.61	104.86	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ARG	N-CA-C	5.53	125.92	111.00
1	A	485	LEU	CB-CA-C	5.52	120.69	110.20
1	A	282	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	503	VAL	CB-CA-C	-5.47	101.00	111.40
1	A	401	LEU	CA-CB-CG	-5.41	102.86	115.30
1	A	402	ALA	CB-CA-C	5.38	118.17	110.10
1	A	346	LEU	CB-CA-C	-5.38	99.97	110.20
1	A	444	LYS	CD-CE-NZ	5.34	123.99	111.70
1	A	530	TYR	N-CA-C	-5.34	96.59	111.00
1	A	497	LEU	CB-CA-C	5.19	120.06	110.20
1	A	568	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	A	535	VAL	N-CA-C	-5.08	97.29	111.00
1	A	376	ARG	CB-CA-C	-5.05	100.29	110.40
1	A	525	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	543	LEU	CB-CG-CD1	5.03	119.56	111.00
1	A	369	GLY	N-CA-C	5.03	125.67	113.10
1	A	512	LEU	N-CA-C	-5.02	97.45	111.00

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	2361	384	2
2	A	91	0	0	37	1
All	All	2457	0	2361	384	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 81.

All (384) 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:529:ASN:HB2	2:A:618:HOH:O	1.57	1.04
1:A:328:GLU:CD	1:A:329:LEU:H	1.61	1.01
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:329:LEU:C	1:A:331:PHE:H	1.57	0.98
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: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
1:A:306:GLY:O	1:A:313:LEU:HA	1.74	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:HB2	1:A:453:ARG:NH1	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:570:GLU:C	1:A:572:TRP:H	1.78	0.85
1:A:279:LEU:HD12	1:A:279:LEU:C	1.97	0.84
1:A:354:MET:HG2	1:A:355:THR:N	1.92	0.84
1:A:376:ARG:HG3	1:A:376:ARG:HH11	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:329:LEU:C	1:A:331:PHE:N	2.28	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:469:SER:O	1:A:470:SER:HB3	1.82	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: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:CG	1:A:376:ARG:HH11	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
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:347:LEU:CD2	1:A:348:ARG:H	2.03	0.71
1:A:313:LEU:CB	1:A:365:TYR:HB3	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:456:ILE:HG23	1:A:457:GLY:N	2.07	0.70
1:A:529:ASN:O	1:A:529:ASN:OD1	2.09	0.70
1:A:501:ASP:OD2	2:A:633:HOH:O	2.09	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: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: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: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
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:523:ASP:C	1:A:523:ASP:OD2	2.36	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:N	1:A:502:ASP:OD1	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:449:TPO:HG21	1:A:449:TPO:O3P	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:O	1:A:280:ARG:C	2.36	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: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: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:560:VAL:O	1:A:561:ARG:C	2.36	0.61
1:A:348:ARG:HH22	1:A:350:ARG:HE	1.49	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
1:A:289:PHE:O	2:A:617:HOH:O	2.16	0.59
1:A:466:THR:CG2	1:A:466:THR:O	2.51	0.59
1:A:319:LEU:HB2	1:A:359:ARG:O	2.03	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:422:ILE:C	1:A:423:LEU:HD12	2.24	0.58
1:A:353:CYS:HB3	2:A:638:HOH:O	2.03	0.58
1:A:423:LEU:CD1	1:A:423:LEU:N	2.66	0.58
1:A:496:ARG:C	1:A:499:ASN:OD1	2.42	0.58
1:A:296:GLY:N	1:A:303:VAL:CG2	2.67	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:329:LEU:C	1:A:329:LEU:HD12	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:279:LEU:HD12	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:359:ARG:C	1:A:360:LEU:HG	2.24	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:279:LEU:CD1	1:A:279:LEU:C	2.69	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
1:A:570:GLU:C	1:A:572:TRP:N	2.42	0.55
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:556:MET:HE1	1:A:559:VAL:HG11	1.89	0.55
1:A:335:VAL:C	1:A:337:MET:H	2.09	0.55
1:A:387:TRP:NE1	1:A:534:GLU:HB2	2.21	0.55
1:A:455:TPO:O1P	1:A:455:TPO:C	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:331:PHE:O	1:A:332:GLN:C	2.45	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:282:LEU:HD12	1:A:282:LEU:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:C	2:A:621:HOH:O	2.46	0.53
1:A:272:GLY:O	1:A:273:GLN:HB2	2.09	0.53
1:A:303:VAL:CG2	1:A:303:VAL:O	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:352:PHE:C	1:A:352:PHE:CD2	2.78	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:425:ASP:CG	1:A:429:GLU:HB2	2.26	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:318:ARG:HH21	1:A:320:LYS:CE	2.22	0.52
1:A:331:PHE:C	1:A:333:THR:N	2.63	0.52
1:A:347:LEU:HD21	1:A:364:PRO:HD2	1.90	0.52
1:A:419:ALA:C	1:A:421:ASN:H	2.11	0.51
1:A:453:ARG:HH11	1:A:453:ARG:CB	2.19	0.51
1:A:295:LEU:C	1:A:303:VAL:CG2	2.79	0.51
1:A:513:LEU:N	1:A:513:LEU:HD12	2.26	0.51
1:A:313:LEU:HB3	1:A:365:TYR:CG	2.45	0.51
1:A:442:ASP:O	1:A:444:LYS:O	2.28	0.51
1:A:301:GLY:HA3	2:A:659:HOH:O	2.11	0.51
1:A:290:SEP:N	1:A:304:TYR:HE2	2.09	0.51
1:A:331:PHE:O	1:A:334:GLU:N	2.39	0.51
1:A:277:PHE:CE2	1:A:362:VAL:HG21	2.46	0.51
1:A:395:LEU:HA	1:A:563:LEU:HD12	1.93	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:336:GLU:C	2:A:667:HOH:O	2.49	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:513:LEU:O	1:A:514:LYS:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:328:GLU:CG	1:A:329:LEU:N	2.73	0.49
1:A:395:LEU:HD22	1:A:399:ARG:NE	2.27	0.49
1:A:481:MET:HE3	1:A:482:LEU:HD23	1.95	0.49
1:A:487:THR:HB	1:A:489:GLN:CG	2.38	0.49
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: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:395:LEU:HD21	1:A:564:GLU:HG3	1.94	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:523:ASP:OD2	1:A:523:ASP:O	2.31	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:328:GLU:CD	1:A:329:LEU:N	2.46	0.47
1:A:276:ARG:O	1:A:277:PHE:CD1	2.68	0.47
1:A:290:SEP:N	1:A:304:TYR:CE2	2.82	0.47
1:A:307:ARG:C	1:A:308:LEU:O	2.52	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:447:HIS:CD2	1:A:447:HIS:C	2.87	0.47
1:A:328:GLU:O	1:A:330:GLN:N	2.48	0.46
1:A:291:ASN:C	1:A:293:ASN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:313:LEU:C	1:A:365:TYR:HB2	2.36	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:569:ALA:C	1:A:572:TRP:HE1	2.19	0.46
1:A:493:ASP:H	1:A:496:ARG:NH2	2.13	0.46
1:A:489:GLN:NE2	1:A:508:TRP:CH2	2.84	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
1:A:487:THR:CB	1:A:489:GLN:HG2	2.39	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:313:LEU:O	1:A:365:TYR:HB3	2.16	0.45
1:A:366:MET:O	1:A:367:ALA:C	2.54	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:300:PHE:O	1:A:319:LEU:HA	2.17	0.45
1:A:294:ILE:HD12	1:A:302:LYS:HD2	1.97	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:539:ILE:C	1:A:541:VAL:N	2.69	0.45
1:A:515:GLU:HG3	1:A:515:GLU:H	1.61	0.45
1:A:318:ARG:HE	1:A:320:LYS:HE3	1.82	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:CD2	1:A:518:LEU:H	2.30	0.44
1:A:559:VAL:HA	1:A:562:MET:HE2	1.99	0.44
1:A:289:PHE:CD2	1:A:289:PHE:N	2.85	0.44
1:A:514:LYS:O	1:A:516:LYS:CG	2.65	0.44
1:A:282:LEU:CD1	1:A:282:LEU:C	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:LEU:C	1:A:365:TYR:CB	2.86	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:518:LEU:HB2	1:A:519:GLU:HG2	2.00	0.43
1:A:517:LYS:NZ	1:A:519:GLU:OE1	2.43	0.43
1:A:546:THR:O	1:A:547:GLN:C	2.55	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:481:MET:O	1:A:482:LEU:C	2.55	0.43
1:A:519:GLU:H	1:A:519:GLU:HG2	1.34	0.43
1:A:389:LYS:O	1:A:393:ILE:HG13	2.19	0.43
1:A:419:ALA:C	1:A:421:ASN:N	2.66	0.43
1:A:470:SER:C	1:A:472:LYS:N	2.71	0.43
1:A:290:SEP:CA	1:A:304:TYR:CE2	2.89	0.43
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:295:LEU:C	1:A:303:VAL:HG21	2.40	0.42
1:A:280:ARG:C	1:A:282:LEU:H	2.22	0.42
1:A:347:LEU:HD23	2:A:613:HOH:O	2.18	0.42
1:A:561:ARG:HB3	1:A:566:ASP:HB3	2.00	0.42
1:A:470:SER:O	1:A:471:GLU:C	2.56	0.42
1:A:453:ARG:CZ	1:A:453:ARG:HB2	2.49	0.42
1:A:516:LYS:H	1:A:516:LYS:HG3	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:442:ASP:O	1:A:443:TYR:C	2.58	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:540:GLN:O	1:A:544:LEU:HG	2.19	0.41
1:A:521:LEU:C	1:A:521:LEU:HD12	2.40	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:387:TRP:HA	1:A:387:TRP:CE3	2.55	0.41
1:A:329:LEU:C	1:A:329:LEU:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:OE1	1:A:329:LEU:CA	2.68	0.41
1:A:364:PRO:HB2	1:A:366:MET:HE2	2.02	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:HG23	1:A:413:ILE:HD12	1.72	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: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:280:ARG:C	1:A:282:LEU:N	2.74	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:278:SER:HG	1:A:281:GLU:HB3	1.85	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
1:A:535:VAL:O	1:A:536:GLU:C	2.58	0.40
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%)	0 0

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
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

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Mol	Chain	Res	Type
1	A	540	GLN
1	A	499	ASN
1	A	518	LEU
1	A	528	GLY

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	246 / 273 (90%)	181 (74%)	65 (26%)	0 1

All (65) 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	316	VAL
1	A	317	LYS
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	353	CYS
1	A	354	MET
1	A	358	GLU
1	A	359	ARG
1	A	360	LEU
1	A	364	PRO

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Mol	Chain	Res	Type
1	A	368	ASN
1	A	370	SER
1	A	373	SER
1	A	375	LEU
1	A	376	ARG
1	A	377	GLU
1	A	378	ARG
1	A	384	PRO
1	A	387	TRP
1	A	392	ARG
1	A	395	LEU
1	A	416	ASP
1	A	434	ASP
1	A	440	LEU
1	A	441	MET
1	A	444	LYS
1	A	452	VAL
1	A	456	ILE
1	A	463	TYR
1	A	465	SER
1	A	466	THR
1	A	470	SER
1	A	472	LYS
1	A	481	MET
1	A	485	LEU
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	538	LEU
1	A	556	MET
1	A	562	MET
1	A	572	TRP

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Mol	Chain	Res	Type
1	A	573	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	489	GLN
1	A	529	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	450	1	8,10,11	0.63	0	10,14,16	1.17	0
1	TPO	A	449	1	8,10,11	0.49	0	10,14,16	0.74	0
1	SEP	A	290	1	8,9,10	1.10	0	8,12,14	3.68	1 (12%)
1	TPO	A	446	1	8,10,11	1.01	0	10,14,16	1.05	1 (10%)
1	TPO	A	455	1	8,10,11	0.49	0	10,14,16	1.35	2 (20%)
1	TPO	A	312	1	8,10,11	0.49	0	10,14,16	0.74	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	450	1	-	6/9/11/13	-
1	TPO	A	449	1	-	4/9/11/13	-
1	SEP	A	290	1	-	1/5/8/10	-
1	TPO	A	446	1	-	3/9/11/13	-
1	TPO	A	455	1	-	2/9/11/13	-
1	TPO	A	312	1	-	4/9/11/13	-

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	446	TPO	CG2-CB-CA	-2.51	108.22	113.16
1	A	455	TPO	O3P-P-O1P	-2.32	101.60	110.68
1	A	455	TPO	O3P-P-OG1	2.29	116.27	105.99

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 21 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	291/326 (89%)	0.11	11 (3%) 40 33	33, 77, 126, 169	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	3.9
1	A	276	ARG	3.4
1	A	296	GLY	3.2
1	A	297	ARG	3.2
1	A	443	TYR	2.9
1	A	353	CYS	2.5
1	A	532	ASP	2.4
1	A	293	ASN	2.2
1	A	311	GLY	2.2
1	A	517	LYS	2.1
1	A	332	GLN	2.0

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, 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
1	TPO	A	446	11/12	0.69	0.24	73,84,112,116	0
1	TPO	A	312	11/12	0.70	0.22	84,101,140,143	0
1	TPO	A	455	11/12	0.85	0.26	111,123,130,133	0
1	TPO	A	450	11/12	0.86	0.19	81,99,131,131	0
1	TPO	A	449	11/12	0.87	0.13	84,101,140,143	0
1	SEP	A	290	10/11	0.92	0.16	121,130,199,202	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.