



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 1BX6 / pdb_00001bx6
Title : CRYSTAL STRUCTURE OF THE POTENT NATURAL PRODUCT INHIBITOR BALANOL IN COMPLEX WITH THE CATALYTIC SUBUNIT OF CAMP-DEPENDENT PROTEIN KINASE
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Deposited on : 1998-10-13
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

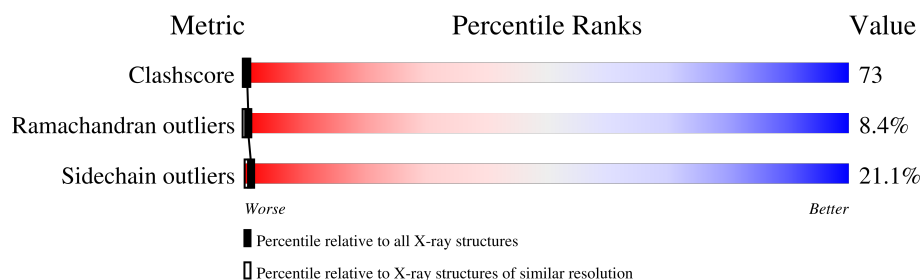
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	19% 53% 22% . .

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	338	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3146 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.

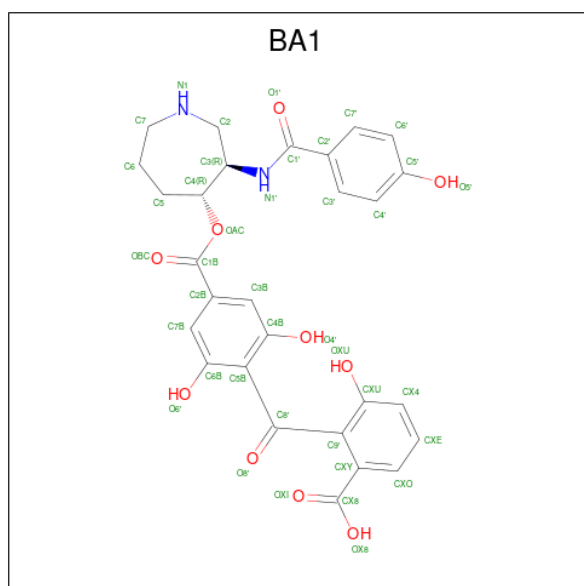
- Molecule 1 is a protein called CAMP-DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	339	2801	1813	469	509	2	8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SEP	SER	conflict	UNP P05132
A	197	TPO	THR	modified residue	UNP P05132
A	338	SEP	SER	modified residue	UNP P05132

- Molecule 2 is BALANOL (CCD ID: BA1) (formula: $C_{28}H_{26}N_2O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	40	28	2	10	0	0

- Molecule 3 is water.

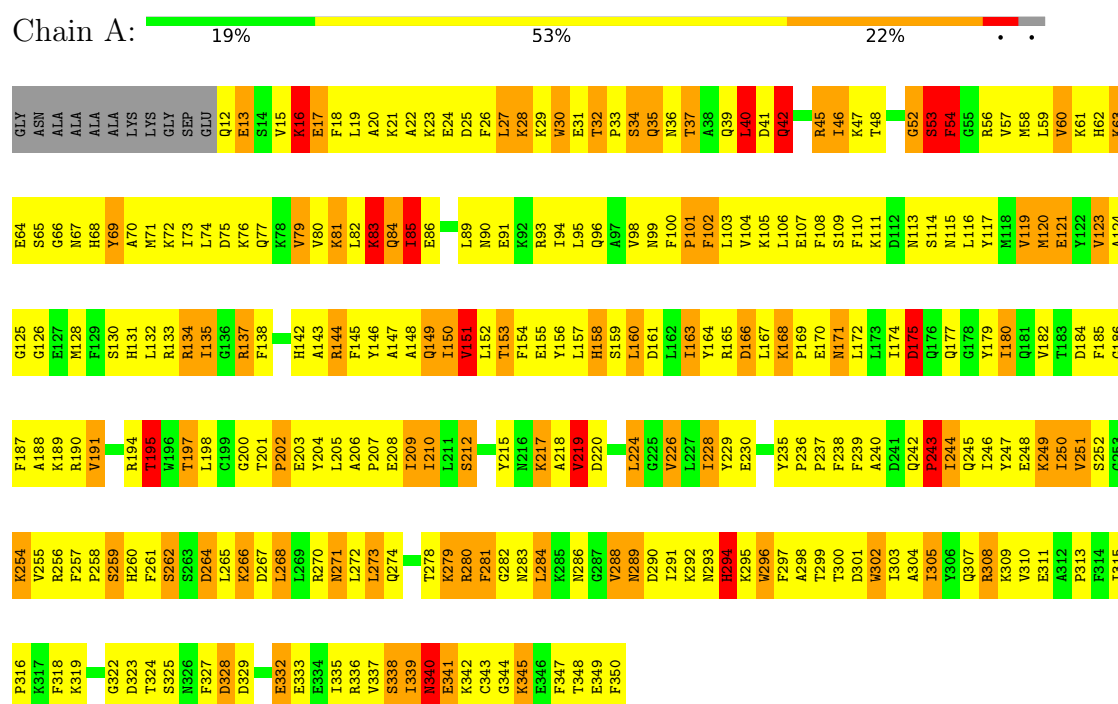
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	305	Total 305	O 305	0	0

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. 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. 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.

Note EDS was not executed.

• Molecule 1: CAMP-DEPENDENT PROTEIN KINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.19Å 73.18Å 99.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	84.0 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	TNT 5E, X-PLOR	Depositor
R, R_{free}	0.202 , 0.340	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3146	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO, BA1

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	1.54	18/2849 (0.6%)	1.55	25/3836 (0.7%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	LYS	C-N	-7.33	1.25	1.34
1	A	84	GLN	N-CA	-7.07	1.38	1.46
1	A	85	ILE	N-CA	-6.45	1.39	1.46
1	A	102	PHE	CA-C	-6.45	1.44	1.52
1	A	52	GLY	CA-C	-6.35	1.44	1.51
1	A	209	ILE	CA-CB	-6.25	1.46	1.54
1	A	182	VAL	CA-C	-6.15	1.45	1.52
1	A	32	THR	N-CA	-6.03	1.40	1.46
1	A	42	GLN	CA-C	-5.90	1.45	1.52
1	A	244	ILE	N-CA	-5.78	1.39	1.46
1	A	69	TYR	CA-C	-5.59	1.45	1.52
1	A	121	GLU	N-CA	-5.57	1.39	1.46
1	A	271	ASN	N-CA	-5.55	1.39	1.46
1	A	195	THR	CA-C	-5.36	1.46	1.52
1	A	243	PRO	C-N	-5.35	1.27	1.33
1	A	224	LEU	C-N	-5.28	1.27	1.33
1	A	46	ILE	CA-CB	-5.23	1.49	1.55
1	A	94	ILE	CA-CB	-5.13	1.48	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	GLU	N-CA-C	-12.81	97.34	113.23
1	A	46	ILE	N-CA-C	9.29	120.49	111.67
1	A	84	GLN	CA-C-O	7.24	126.53	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	N-CA-C	-6.62	103.75	110.97
1	A	294	HIS	CB-CA-C	-6.44	97.60	110.42
1	A	98	VAL	CB-CA-C	-6.43	100.75	111.29
1	A	94	ILE	CB-CA-C	-6.33	103.60	111.70
1	A	64	GLU	N-CA-CB	6.16	119.47	110.47
1	A	166	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	42	GLN	N-CA-C	-6.02	103.68	113.19
1	A	54	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	63	LYS	CA-C-N	-5.84	111.64	122.09
1	A	63	LYS	C-N-CA	-5.84	111.64	122.09
1	A	328	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	151	VAL	N-CA-CB	-5.50	104.85	110.62
1	A	144	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	32	THR	C-N-CD	-5.45	102.67	125.00
1	A	340	ASN	N-CA-CB	5.34	119.52	110.49
1	A	30	TRP	N-CA-C	-5.29	107.84	114.56
1	A	171	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	271	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	289	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	41	ASP	N-CA-C	5.17	121.81	110.80
1	A	102	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	41	ASP	N-CA-CB	5.02	118.97	110.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2801	0	2782	409	0
2	A	40	0	23	8	0
3	A	305	0	0	51	0
All	All	3146	0	2805	412	0

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 73.

All (412) 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:69:TYR:HE2	1:A:107:GLU:HG3	1.27	0.96
1:A:100:PHE:HE2	1:A:153:THR:HA	1.35	0.92
1:A:33:PRO:HB3	1:A:96:GLN:NE2	1.85	0.92
1:A:113:ASN:HB3	1:A:341:GLU:HA	1.52	0.90
1:A:304:ALA:HA	1:A:309:LYS:HD3	1.51	0.90
1:A:13:GLU:HA	1:A:16:LYS:HE2	1.55	0.89
1:A:62:HIS:HD2	1:A:65:SER:HB2	1.39	0.88
1:A:115:ASN:HB2	1:A:117:TYR:CE1	2.09	0.86
1:A:100:PHE:CE2	1:A:153:THR:HA	2.12	0.85
1:A:189:LYS:HG2	1:A:191:VAL:HG13	1.57	0.84
1:A:69:TYR:CE2	1:A:107:GLU:HG3	2.13	0.83
1:A:258:PRO:HG2	1:A:261:PHE:CE1	2.15	0.82
1:A:339:ILE:C	3:A:655:HOH:O	2.22	0.81
1:A:71:MET:HB2	1:A:119:VAL:HG22	1.61	0.81
1:A:134:ARG:HH11	1:A:134:ARG:HB3	1.46	0.80
1:A:158:HIS:CD2	1:A:217:LYS:HB2	2.17	0.80
1:A:93:ARG:HD3	3:A:474:HOH:O	1.83	0.79
1:A:91:GLU:O	1:A:95:LEU:HB2	1.83	0.79
1:A:149:GLN:HE22	1:A:179:TYR:HD2	1.31	0.78
1:A:288:VAL:HG13	1:A:292:LYS:HD2	1.66	0.78
1:A:316:PRO:HG2	1:A:318:PHE:HZ	1.50	0.77
1:A:86:GLU:HB3	3:A:545:HOH:O	1.85	0.77
1:A:57:VAL:HG23	2:A:351:BA1:OBC	1.85	0.77
1:A:304:ALA:HA	1:A:309:LYS:CD	2.15	0.77
1:A:209:ILE:HG12	1:A:215:TYR:CD2	2.20	0.77
1:A:12:GLN:O	1:A:16:LYS:HD3	1.85	0.76
1:A:13:GLU:HA	1:A:16:LYS:CE	2.15	0.76
1:A:128:MET:HE2	1:A:169:PRO:HB3	1.67	0.76
1:A:267:ASP:O	1:A:270:ARG:HB2	1.85	0.76
1:A:28:LYS:HG2	3:A:629:HOH:O	1.84	0.76
1:A:45:ARG:HD2	1:A:335:ILE:HD13	1.68	0.76
1:A:250:ILE:HD13	3:A:480:HOH:O	1.86	0.75
1:A:19:LEU:HA	1:A:22:ALA:HB3	1.67	0.75
1:A:65:SER:O	1:A:67:ASN:N	2.18	0.75
1:A:303:ILE:HG22	1:A:307:GLN:NE2	2.02	0.75
1:A:62:HIS:CD2	1:A:65:SER:HB2	2.20	0.75
1:A:206:ALA:CB	1:A:219:VAL:HG22	2.17	0.74
1:A:304:ALA:CA	1:A:309:LYS:HD3	2.16	0.74
1:A:125:GLY:HA2	1:A:318:PHE:CE1	2.23	0.74
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HG	3:A:429:HOH:O	1.88	0.73
1:A:229:TYR:CD1	1:A:237:PRO:HD3	2.22	0.72
1:A:45:ARG:HB3	1:A:58:MET:HE1	1.69	0.72
1:A:105:LYS:HD3	1:A:121:GLU:OE1	1.90	0.71
1:A:150:ILE:CD1	1:A:180:ILE:HD11	2.20	0.71
1:A:293:ASN:O	1:A:294:HIS:O	2.09	0.71
1:A:293:ASN:O	1:A:294:HIS:C	2.35	0.69
1:A:25:ASP:HB3	3:A:382:HOH:O	1.92	0.69
1:A:338:SEP:O1P	1:A:340:ASN:ND2	2.25	0.69
1:A:33:PRO:HB3	1:A:96:GLN:HE22	1.56	0.69
1:A:13:GLU:HB3	3:A:370:HOH:O	1.90	0.69
1:A:144:ARG:NH2	3:A:585:HOH:O	2.25	0.69
1:A:24:GLU:O	1:A:25:ASP:C	2.33	0.69
1:A:226:VAL:HB	1:A:237:PRO:HG2	1.73	0.68
1:A:281:PHE:C	1:A:283:ASN:H	2.02	0.68
1:A:189:LYS:NZ	1:A:197:TPO:O2P	2.24	0.68
1:A:288:VAL:HG13	1:A:292:LYS:CD	2.23	0.68
1:A:125:GLY:HA3	1:A:174:ILE:O	1.94	0.68
1:A:134:ARG:HH11	1:A:134:ARG:CB	2.06	0.68
1:A:288:VAL:CG1	1:A:292:LYS:HD2	2.24	0.67
1:A:40:LEU:HD23	1:A:117:TYR:CE2	2.29	0.67
1:A:208:GLU:HG2	3:A:485:HOH:O	1.94	0.67
1:A:189:LYS:HG2	1:A:191:VAL:CG1	2.24	0.67
1:A:105:LYS:HD3	1:A:121:GLU:CD	2.19	0.67
1:A:30:TRP:CZ3	1:A:93:ARG:HG2	2.30	0.67
1:A:206:ALA:HB1	1:A:208:GLU:OE1	1.95	0.67
1:A:100:PHE:CG	1:A:101:PRO:HD2	2.30	0.67
1:A:86:GLU:HB2	3:A:639:HOH:O	1.94	0.67
1:A:206:ALA:HB3	1:A:219:VAL:HG22	1.75	0.67
1:A:16:LYS:O	1:A:17:GLU:C	2.39	0.66
1:A:73:ILE:HG23	1:A:117:TYR:CD2	2.30	0.66
1:A:73:ILE:HG23	1:A:117:TYR:CE2	2.31	0.66
1:A:158:HIS:HD2	1:A:217:LYS:HB2	1.60	0.66
1:A:333:GLU:HB3	3:A:541:HOH:O	1.96	0.66
1:A:99:ASN:ND2	3:A:525:HOH:O	2.29	0.65
1:A:175:ASP:OD2	1:A:179:TYR:HB2	1.96	0.65
1:A:207:PRO:HA	1:A:210:ILE:HD12	1.76	0.65
1:A:283:ASN:HA	3:A:594:HOH:O	1.96	0.65
1:A:295:LYS:O	1:A:298:ALA:N	2.29	0.65
1:A:36:ASN:ND2	3:A:391:HOH:O	2.28	0.65
1:A:246:ILE:O	1:A:250:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ASN:O	1:A:293:ASN:ND2	2.29	0.65
1:A:110:PHE:CE1	1:A:117:TYR:CG	2.86	0.64
1:A:45:ARG:NH1	1:A:45:ARG:HG3	2.12	0.64
1:A:113:ASN:CB	1:A:341:GLU:HA	2.26	0.64
1:A:336:ARG:NH1	3:A:536:HOH:O	2.29	0.64
1:A:39:GLN:O	1:A:40:LEU:C	2.41	0.63
1:A:195:THR:HG22	3:A:477:HOH:O	1.98	0.63
1:A:150:ILE:HD13	1:A:180:ILE:HD11	1.78	0.63
1:A:154:PHE:CE2	1:A:220:ASP:HB3	2.33	0.63
1:A:45:ARG:HD2	1:A:335:ILE:CD1	2.28	0.63
1:A:82:LEU:O	1:A:83:LYS:C	2.37	0.63
1:A:235:TYR:HB2	1:A:236:PRO:CD	2.28	0.63
1:A:268:LEU:HD12	1:A:268:LEU:O	1.99	0.63
1:A:19:LEU:O	1:A:20:ALA:C	2.41	0.63
1:A:270:ARG:HD3	3:A:506:HOH:O	1.97	0.63
1:A:76:LYS:HG2	1:A:116:LEU:CD2	2.29	0.63
1:A:108:PHE:HD2	1:A:119:VAL:CG1	2.11	0.63
1:A:62:HIS:HD2	1:A:65:SER:CB	2.11	0.62
1:A:208:GLU:CD	1:A:280:ARG:HH22	2.06	0.62
1:A:348:THR:N	3:A:542:HOH:O	2.31	0.62
1:A:13:GLU:CA	1:A:16:LYS:HE2	2.29	0.62
1:A:146:TYR:O	1:A:149:GLN:N	2.32	0.62
1:A:95:LEU:HB3	1:A:106:LEU:HD12	1.81	0.62
1:A:224:LEU:HD12	1:A:224:LEU:O	1.99	0.62
1:A:76:LYS:HG2	1:A:116:LEU:HD21	1.82	0.62
1:A:341:GLU:OE2	1:A:344:GLY:HA3	1.99	0.62
1:A:137:ARG:O	1:A:137:ARG:NE	2.29	0.62
1:A:342:LYS:O	1:A:343:CYS:C	2.42	0.62
1:A:19:LEU:O	1:A:22:ALA:N	2.32	0.62
1:A:316:PRO:HB2	1:A:318:PHE:CZ	2.34	0.62
1:A:76:LYS:O	1:A:79:VAL:HB	1.99	0.62
1:A:224:LEU:O	1:A:228:ILE:HG13	2.00	0.62
1:A:58:MET:O	1:A:60:VAL:HG13	2.00	0.62
1:A:115:ASN:HB2	1:A:117:TYR:CZ	2.35	0.62
1:A:35:GLN:HG3	3:A:544:HOH:O	2.00	0.61
1:A:100:PHE:CD1	1:A:101:PRO:HD2	2.35	0.61
1:A:235:TYR:HB2	1:A:236:PRO:HD2	1.81	0.61
1:A:298:ALA:HB3	3:A:438:HOH:O	2.00	0.61
1:A:75:ASP:O	1:A:76:LYS:C	2.43	0.61
1:A:295:LYS:O	1:A:297:PHE:N	2.34	0.60
1:A:349:GLU:HG2	3:A:644:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:HB3	3:A:479:HOH:O	2.01	0.60
1:A:125:GLY:HA2	1:A:318:PHE:HE1	1.65	0.60
1:A:230:GLU:HA	1:A:235:TYR:O	2.01	0.60
1:A:286:ASN:ND2	1:A:289:ASN:HD22	1.98	0.60
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.66	0.60
1:A:249:LYS:O	1:A:250:ILE:C	2.41	0.60
1:A:345:LYS:HE2	3:A:543:HOH:O	2.00	0.60
1:A:135:ILE:HG21	1:A:138:PHE:HE1	1.65	0.60
1:A:147:ALA:O	1:A:148:ALA:C	2.41	0.60
1:A:15:VAL:O	1:A:18:PHE:HB3	2.01	0.60
1:A:304:ALA:CB	1:A:309:LYS:HD3	2.31	0.60
1:A:316:PRO:HG2	1:A:318:PHE:CZ	2.36	0.60
1:A:154:PHE:CD2	1:A:220:ASP:HB3	2.37	0.60
1:A:261:PHE:HB3	1:A:266:LYS:HG3	1.83	0.59
1:A:279:LYS:HD3	1:A:279:LYS:N	2.16	0.59
1:A:124:ALA:HB1	3:A:424:HOH:O	2.02	0.59
1:A:90:ASN:ND2	3:A:359:HOH:O	2.34	0.59
1:A:168:LYS:HB2	1:A:169:PRO:HD2	1.84	0.59
1:A:15:VAL:HG13	1:A:16:LYS:N	2.17	0.58
1:A:144:ARG:HG3	1:A:296:TRP:CZ3	2.39	0.58
1:A:175:ASP:OD1	1:A:177:GLN:N	2.25	0.58
1:A:113:ASN:HB3	1:A:341:GLU:CA	2.30	0.58
1:A:100:PHE:HA	3:A:524:HOH:O	2.03	0.58
1:A:32:THR:N	1:A:33:PRO:HD3	2.18	0.58
1:A:131:HIS:HA	1:A:134:ARG:HH12	1.69	0.58
1:A:206:ALA:O	1:A:210:ILE:HD12	2.03	0.58
1:A:16:LYS:HG3	1:A:17:GLU:H	1.68	0.58
1:A:281:PHE:O	1:A:283:ASN:N	2.37	0.58
1:A:164:TYR:HE1	1:A:166:ASP:C	2.12	0.58
1:A:172:LEU:CD2	1:A:180:ILE:HD12	2.33	0.58
1:A:134:ARG:HB3	1:A:134:ARG:NH1	2.18	0.57
1:A:16:LYS:CG	1:A:17:GLU:H	2.16	0.57
1:A:45:ARG:CD	1:A:335:ILE:HD13	2.32	0.57
1:A:83:LYS:HG2	1:A:85:ILE:HG22	1.86	0.57
1:A:133:ARG:NH2	1:A:230:GLU:OE2	2.38	0.57
1:A:150:ILE:HD11	1:A:180:ILE:HD11	1.86	0.57
1:A:71:MET:HB2	1:A:119:VAL:CG2	2.33	0.57
1:A:279:LYS:C	1:A:284:LEU:HD21	2.30	0.57
1:A:335:ILE:N	1:A:335:ILE:HD12	2.20	0.57
1:A:59:LEU:HD11	1:A:68:HIS:HB3	1.86	0.56
1:A:187:PHE:N	1:A:187:PHE:CD1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HB2	1:A:219:VAL:HG22	1.86	0.56
1:A:340:ASN:O	1:A:342:LYS:HD3	2.05	0.56
1:A:19:LEU:HA	1:A:22:ALA:CB	2.34	0.56
1:A:194:ARG:HG2	3:A:476:HOH:O	2.05	0.56
1:A:242:GLN:O	1:A:245:GLN:N	2.38	0.56
1:A:80:VAL:C	1:A:82:LEU:H	2.14	0.56
1:A:205:LEU:C	1:A:206:ALA:O	2.47	0.56
1:A:39:GLN:N	1:A:42:GLN:OE1	2.25	0.56
1:A:143:ALA:O	1:A:144:ARG:C	2.48	0.56
1:A:235:TYR:CD1	1:A:235:TYR:N	2.73	0.56
1:A:75:ASP:O	1:A:79:VAL:HG23	2.05	0.56
1:A:133:ARG:HA	3:A:429:HOH:O	2.04	0.56
1:A:54:PHE:CD2	1:A:79:VAL:HG22	2.41	0.55
1:A:187:PHE:N	1:A:187:PHE:HD1	2.03	0.55
1:A:237:PRO:HB2	1:A:238:PHE:CD1	2.41	0.55
1:A:86:GLU:HA	3:A:405:HOH:O	2.07	0.55
1:A:111:LYS:NZ	1:A:347:PHE:O	2.35	0.55
1:A:336:ARG:O	1:A:336:ARG:HG3	2.07	0.55
1:A:19:LEU:O	1:A:22:ALA:HB3	2.06	0.55
1:A:56:ARG:NH2	1:A:333:GLU:OE1	2.40	0.55
1:A:212:SER:HA	3:A:478:HOH:O	2.06	0.55
1:A:267:ASP:HA	1:A:270:ARG:HH11	1.72	0.54
1:A:46:ILE:HD11	1:A:61:LYS:HB2	1.89	0.54
1:A:311:GLU:HG2	3:A:468:HOH:O	2.08	0.54
1:A:258:PRO:HB2	1:A:260:HIS:CE1	2.43	0.54
1:A:100:PHE:HE2	1:A:153:THR:CA	2.14	0.53
1:A:13:GLU:HB2	3:A:549:HOH:O	2.08	0.53
1:A:125:GLY:HA2	1:A:318:PHE:CZ	2.43	0.53
1:A:110:PHE:CE1	1:A:117:TYR:HB2	2.43	0.53
1:A:348:THR:HG22	3:A:555:HOH:O	2.09	0.53
2:A:351:BA1:H62	3:A:356:HOH:O	2.08	0.53
1:A:13:GLU:HA	1:A:16:LYS:HD3	1.90	0.53
1:A:31:GLU:C	1:A:33:PRO:HD3	2.34	0.53
1:A:247:TYR:O	1:A:251:VAL:HB	2.09	0.52
1:A:160:LEU:CD1	1:A:160:LEU:N	2.71	0.52
1:A:265:LEU:HB2	1:A:296:TRP:HE1	1.72	0.52
1:A:47:LYS:HD3	1:A:324:THR:HG21	1.91	0.52
1:A:204:TYR:OH	1:A:230:GLU:OE1	2.26	0.52
1:A:261:PHE:O	1:A:266:LYS:HD2	2.09	0.52
1:A:101:PRO:HD3	3:A:524:HOH:O	2.10	0.52
1:A:150:ILE:HD11	1:A:180:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HG23	1:A:154:PHE:CE1	2.44	0.52
1:A:168:LYS:HB2	1:A:169:PRO:CD	2.40	0.52
1:A:194:ARG:NE	3:A:476:HOH:O	2.36	0.52
1:A:13:GLU:HG3	1:A:16:LYS:HE2	1.91	0.52
1:A:261:PHE:O	1:A:262:SER:C	2.48	0.52
1:A:111:LYS:HE2	1:A:350:PHE:O	2.10	0.52
1:A:131:HIS:O	1:A:132:LEU:C	2.46	0.52
1:A:292:LYS:NZ	3:A:615:HOH:O	2.18	0.52
1:A:301:ASP:O	1:A:303:ILE:N	2.43	0.52
1:A:74:LEU:HD21	2:A:351:BA1:OXU	2.10	0.52
1:A:163:ILE:HG12	1:A:165:ARG:HG3	1.91	0.52
1:A:316:PRO:CG	1:A:318:PHE:CZ	2.93	0.52
1:A:261:PHE:C	1:A:262:SER:O	2.53	0.51
1:A:52:GLY:O	1:A:54:PHE:N	2.43	0.51
1:A:13:GLU:HA	1:A:16:LYS:CD	2.40	0.51
1:A:242:GLN:NE2	1:A:243:PRO:HD2	2.25	0.51
1:A:40:LEU:CD2	1:A:117:TYR:CE2	2.93	0.51
1:A:146:TYR:O	1:A:147:ALA:C	2.54	0.51
1:A:103:LEU:HD22	1:A:185:PHE:CZ	2.40	0.51
1:A:303:ILE:O	1:A:307:GLN:NE2	2.39	0.51
1:A:135:ILE:HD12	1:A:135:ILE:O	2.11	0.51
1:A:156:TYR:CD1	1:A:156:TYR:C	2.89	0.51
1:A:83:LYS:HG2	1:A:85:ILE:CG2	2.41	0.51
1:A:164:TYR:HE1	1:A:166:ASP:O	1.93	0.51
1:A:71:MET:SD	1:A:73:ILE:HD11	2.50	0.50
1:A:100:PHE:O	1:A:102:PHE:N	2.44	0.50
1:A:131:HIS:HA	1:A:134:ARG:NH1	2.26	0.50
1:A:69:TYR:HE2	1:A:107:GLU:CG	2.11	0.50
1:A:79:VAL:HG12	1:A:80:VAL:N	2.27	0.50
1:A:150:ILE:HD13	1:A:150:ILE:N	2.26	0.50
1:A:341:GLU:CD	1:A:344:GLY:HA3	2.37	0.50
1:A:265:LEU:HB2	1:A:296:TRP:NE1	2.26	0.50
1:A:324:THR:O	1:A:324:THR:HG22	2.11	0.50
1:A:189:LYS:HD3	1:A:195:THR:HG21	1.94	0.50
1:A:264:ASP:HB2	1:A:296:TRP:HD1	1.76	0.50
1:A:350:PHE:CD1	1:A:350:PHE:C	2.90	0.50
1:A:79:VAL:O	1:A:82:LEU:N	2.45	0.50
1:A:123:VAL:HG22	1:A:123:VAL:O	2.12	0.50
1:A:145:PHE:CE2	1:A:313:PRO:HD2	2.47	0.50
1:A:207:PRO:O	1:A:208:GLU:C	2.51	0.50
1:A:200:GLY:HA3	1:A:205:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:CG1	1:A:70:ALA:HB1	2.41	0.49
1:A:39:GLN:O	1:A:42:GLN:HG3	2.11	0.49
1:A:322:GLY:O	1:A:323:ASP:C	2.55	0.49
1:A:131:HIS:O	1:A:135:ILE:HG22	2.13	0.49
1:A:73:ILE:CG2	1:A:117:TYR:CE2	2.95	0.49
1:A:15:VAL:HG13	1:A:16:LYS:H	1.77	0.49
1:A:151:VAL:O	1:A:152:LEU:C	2.52	0.49
1:A:161:ASP:HB3	1:A:191:VAL:O	2.12	0.49
1:A:281:PHE:CE2	1:A:290:ASP:HB3	2.48	0.49
1:A:17:GLU:O	1:A:18:PHE:C	2.55	0.49
1:A:198:LEU:C	1:A:198:LEU:HD23	2.38	0.49
1:A:37:THR:HG22	1:A:109:SER:H	1.77	0.49
1:A:145:PHE:CD2	1:A:313:PRO:HD2	2.48	0.49
1:A:209:ILE:O	1:A:210:ILE:C	2.54	0.49
1:A:142:HIS:CD2	1:A:313:PRO:HG2	2.49	0.48
1:A:156:TYR:O	1:A:159:SER:HB3	2.13	0.48
1:A:189:LYS:HD3	1:A:191:VAL:HG11	1.94	0.48
1:A:106:LEU:C	1:A:106:LEU:HD23	2.38	0.48
1:A:229:TYR:CD1	1:A:229:TYR:C	2.90	0.48
1:A:307:GLN:C	1:A:308:ARG:HG3	2.38	0.48
1:A:108:PHE:HD2	1:A:119:VAL:HG12	1.76	0.48
1:A:271:ASN:HB3	1:A:281:PHE:CD1	2.48	0.48
1:A:279:LYS:O	1:A:284:LEU:HD21	2.12	0.48
1:A:154:PHE:HZ	1:A:167:LEU:HD13	1.78	0.48
1:A:25:ASP:O	1:A:26:PHE:C	2.56	0.48
1:A:85:ILE:HG23	1:A:86:GLU:H	1.79	0.48
1:A:201:THR:O	1:A:202:PRO:C	2.57	0.48
1:A:273:LEU:N	1:A:273:LEU:CD1	2.77	0.48
1:A:34:SER:HB3	3:A:576:HOH:O	2.15	0.47
1:A:205:LEU:O	1:A:206:ALA:C	2.57	0.47
1:A:272:LEU:C	1:A:274:GLN:H	2.21	0.47
1:A:288:VAL:CG1	1:A:289:ASN:N	2.75	0.47
1:A:301:ASP:O	1:A:302:TRP:C	2.57	0.47
1:A:316:PRO:CB	1:A:318:PHE:CZ	2.98	0.47
1:A:145:PHE:CD2	1:A:313:PRO:CD	2.97	0.47
1:A:21:LYS:HG2	3:A:546:HOH:O	2.13	0.47
1:A:27:LEU:O	1:A:28:LYS:C	2.55	0.47
1:A:80:VAL:C	1:A:82:LEU:N	2.72	0.47
1:A:164:TYR:CE1	1:A:166:ASP:C	2.92	0.47
1:A:288:VAL:HG12	1:A:289:ASN:N	2.30	0.47
1:A:16:LYS:O	1:A:19:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ALA:HB1	1:A:305:ILE:CD1	2.45	0.47
1:A:106:LEU:HD23	1:A:107:GLU:N	2.30	0.47
1:A:286:ASN:ND2	1:A:286:ASN:O	2.48	0.47
1:A:257:PHE:HD1	3:A:491:HOH:O	1.98	0.47
1:A:301:ASP:O	1:A:304:ALA:N	2.42	0.47
1:A:30:TRP:CE3	1:A:93:ARG:HG2	2.50	0.46
1:A:172:LEU:HD23	1:A:180:ILE:HD12	1.96	0.46
1:A:316:PRO:HB2	1:A:318:PHE:CE1	2.51	0.46
1:A:36:ASN:O	1:A:37:THR:HB	2.15	0.46
1:A:100:PHE:CD1	1:A:101:PRO:CD	2.97	0.46
1:A:261:PHE:O	1:A:262:SER:O	2.33	0.46
1:A:274:GLN:HG2	1:A:280:ARG:N	2.30	0.46
1:A:71:MET:HG3	1:A:119:VAL:HG23	1.98	0.46
1:A:81:LYS:O	1:A:82:LEU:HG	2.15	0.46
2:A:351:BA1:H51	2:A:351:BA1:H21	1.38	0.46
1:A:158:HIS:CE1	1:A:220:ASP:OD2	2.68	0.46
1:A:295:LYS:C	1:A:297:PHE:N	2.74	0.46
1:A:337:VAL:O	1:A:338:SEP:O	2.34	0.46
1:A:21:LYS:HE2	3:A:546:HOH:O	2.16	0.46
1:A:17:GLU:O	1:A:20:ALA:HB3	2.16	0.46
1:A:262:SER:O	1:A:266:LYS:HD2	2.15	0.46
1:A:151:VAL:HG12	1:A:152:LEU:N	2.30	0.45
1:A:40:LEU:C	1:A:40:LEU:CD1	2.90	0.45
1:A:63:LYS:HG2	3:A:635:HOH:O	2.15	0.45
1:A:90:ASN:O	1:A:93:ARG:N	2.49	0.45
1:A:272:LEU:O	1:A:274:GLN:N	2.48	0.45
1:A:168:LYS:O	1:A:172:LEU:HD12	2.16	0.45
1:A:218:ALA:HB1	1:A:280:ARG:NH1	2.32	0.45
1:A:45:ARG:HH11	1:A:45:ARG:CG	2.30	0.45
1:A:80:VAL:HG23	1:A:347:PHE:CZ	2.51	0.45
1:A:65:SER:C	1:A:67:ASN:H	2.22	0.45
1:A:338:SEP:OG	1:A:339:ILE:N	2.50	0.45
1:A:345:LYS:HD2	1:A:345:LYS:HA	1.73	0.45
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.73	0.45
1:A:328:ASP:OD1	1:A:329:ASP:N	2.49	0.45
1:A:15:VAL:CG1	1:A:16:LYS:N	2.80	0.44
1:A:150:ILE:HD11	1:A:172:LEU:HD21	2.00	0.44
1:A:131:HIS:HD2	1:A:174:ILE:HD12	1.82	0.44
1:A:45:ARG:HB3	1:A:58:MET:CE	2.44	0.44
1:A:205:LEU:O	1:A:206:ALA:O	2.35	0.44
1:A:145:PHE:O	1:A:148:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LEU:HD12	1:A:268:LEU:C	2.39	0.44
1:A:168:LYS:HD2	1:A:170:GLU:CD	2.42	0.44
1:A:21:LYS:O	1:A:22:ALA:C	2.60	0.44
1:A:248:GLU:O	1:A:252:SER:HB3	2.18	0.44
1:A:332:GLU:H	1:A:332:GLU:HG2	1.33	0.43
1:A:95:LEU:HD12	1:A:95:LEU:HA	1.70	0.43
1:A:168:LYS:HG3	1:A:171:ASN:OD1	2.18	0.43
1:A:12:GLN:HB3	3:A:374:HOH:O	2.16	0.43
1:A:267:ASP:HA	1:A:270:ARG:NH1	2.32	0.43
1:A:76:LYS:HG2	1:A:116:LEU:HD22	1.99	0.43
1:A:194:ARG:HA	1:A:215:TYR:O	2.18	0.43
1:A:15:VAL:CG1	1:A:16:LYS:H	2.31	0.43
1:A:110:PHE:CE1	1:A:117:TYR:CB	3.01	0.43
1:A:164:TYR:O	1:A:165:ARG:HB2	2.18	0.43
1:A:16:LYS:O	1:A:18:PHE:N	2.52	0.43
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.84	0.43
1:A:108:PHE:CD2	1:A:119:VAL:CG1	2.98	0.43
1:A:158:HIS:ND1	1:A:158:HIS:N	2.66	0.43
1:A:165:ARG:HH12	1:A:197:TPO:P	2.42	0.43
1:A:310:VAL:HG12	1:A:311:GLU:N	2.34	0.43
1:A:339:ILE:HD13	1:A:339:ILE:HG21	1.74	0.43
1:A:40:LEU:C	1:A:40:LEU:HD13	2.44	0.43
1:A:108:PHE:CD2	1:A:119:VAL:HG12	2.54	0.43
1:A:132:LEU:C	3:A:429:HOH:O	2.62	0.43
1:A:72:LYS:HB2	1:A:120:MET:HE2	2.01	0.43
1:A:85:ILE:HG23	1:A:86:GLU:HG2	2.01	0.43
1:A:110:PHE:CD1	1:A:110:PHE:C	2.97	0.42
1:A:145:PHE:O	1:A:149:GLN:HG2	2.19	0.42
1:A:108:PHE:HD2	1:A:119:VAL:HG11	1.84	0.42
1:A:240:ALA:HB3	1:A:246:ILE:HG12	2.01	0.42
1:A:337:VAL:O	1:A:338:SEP:C	2.68	0.42
1:A:209:ILE:HG12	1:A:215:TYR:CE2	2.53	0.42
1:A:251:VAL:CG1	1:A:252:SER:N	2.79	0.42
1:A:251:VAL:HG12	1:A:252:SER:N	2.34	0.42
1:A:28:LYS:C	1:A:30:TRP:H	2.26	0.42
1:A:126:GLY:HA2	1:A:327:PHE:CZ	2.54	0.42
1:A:174:ILE:O	1:A:175:ASP:C	2.60	0.42
1:A:254:LYS:O	1:A:254:LYS:HD3	2.19	0.42
1:A:53:SER:OG	2:A:351:BA1:OX8	2.37	0.42
1:A:152:LEU:O	1:A:155:GLU:HB3	2.19	0.42
1:A:52:GLY:HA3	2:A:351:BA1:C4B	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:O	1:A:93:ARG:HB3	2.20	0.42
1:A:240:ALA:HB3	1:A:246:ILE:CG1	2.50	0.42
1:A:272:LEU:C	1:A:274:GLN:N	2.77	0.42
1:A:146:TYR:HD1	1:A:146:TYR:HA	1.73	0.42
1:A:89:LEU:O	1:A:90:ASN:C	2.63	0.42
1:A:135:ILE:CG2	1:A:138:PHE:HE1	2.30	0.42
1:A:79:VAL:HB	1:A:80:VAL:H	1.48	0.42
1:A:280:ARG:O	1:A:283:ASN:HB3	2.20	0.41
1:A:242:GLN:C	1:A:244:ILE:N	2.77	0.41
1:A:286:ASN:HB3	1:A:290:ASP:OD1	2.20	0.41
1:A:242:GLN:O	1:A:244:ILE:N	2.53	0.41
1:A:271:ASN:O	1:A:274:GLN:CB	2.69	0.41
1:A:323:ASP:HB3	3:A:473:HOH:O	2.20	0.41
1:A:77:GLN:O	1:A:81:LYS:HB2	2.20	0.41
1:A:258:PRO:HB2	1:A:260:HIS:ND1	2.35	0.41
1:A:274:GLN:HB3	1:A:280:ARG:HA	2.02	0.41
1:A:335:ILE:HD12	1:A:335:ILE:H	1.85	0.41
1:A:79:VAL:CG1	1:A:80:VAL:N	2.79	0.41
1:A:120:MET:H	1:A:120:MET:HG2	1.73	0.41
1:A:160:LEU:N	1:A:160:LEU:HD13	2.36	0.41
1:A:79:VAL:C	1:A:81:LYS:N	2.77	0.41
1:A:149:GLN:O	1:A:153:THR:OG1	2.37	0.41
1:A:23:LYS:NZ	3:A:447:HOH:O	2.32	0.41
1:A:23:LYS:HG2	1:A:27:LEU:HD11	2.02	0.41
1:A:58:MET:HE3	1:A:58:MET:HB3	1.62	0.41
1:A:83:LYS:HD2	3:A:609:HOH:O	2.21	0.41
1:A:83:LYS:HE2	3:A:638:HOH:O	2.20	0.41
1:A:100:PHE:C	1:A:102:PHE:N	2.79	0.41
1:A:184:ASP:OD2	2:A:351:BA1:H7B	2.20	0.41
1:A:319:LYS:HG3	1:A:323:ASP:OD2	2.21	0.41
1:A:291:ILE:O	1:A:292:LYS:C	2.64	0.41
1:A:40:LEU:HD13	1:A:40:LEU:O	2.21	0.40
1:A:130:SER:O	1:A:134:ARG:N	2.46	0.40
1:A:146:TYR:CD1	1:A:180:ILE:CG2	3.03	0.40
1:A:242:GLN:HA	1:A:243:PRO:HD3	1.99	0.40
1:A:259:SER:HB3	3:A:653:HOH:O	2.20	0.40
2:A:351:BA1:OXI	2:A:351:BA1:C8'	2.69	0.40
1:A:250:ILE:HG23	3:A:480:HOH:O	2.19	0.40
1:A:304:ALA:HB1	1:A:309:LYS:HD3	2.03	0.40
1:A:350:PHE:O	1:A:350:PHE:HD1	2.04	0.40
1:A:18:PHE:CD2	1:A:19:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ILE:C	1:A:212:SER:H	2.30	0.40
1:A:85:ILE:HG23	1:A:86:GLU:N	2.36	0.40
1:A:189:LYS:CG	1:A:191:VAL:CG1	2.97	0.40

There are no symmetry-related clashes.

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	335/350 (96%)	236 (70%)	71 (21%)	28 (8%)	0 0

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	66	GLY
1	A	79	VAL
1	A	294	HIS
1	A	296	TRP
1	A	302	TRP
1	A	17	GLU
1	A	35	GLN
1	A	53	SER
1	A	83	LYS
1	A	175	ASP
1	A	188	ALA
1	A	203	GLU
1	A	219	VAL
1	A	282	GLY
1	A	341	GLU
1	A	40	LEU
1	A	202	PRO

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Mol	Chain	Res	Type
1	A	29	LYS
1	A	262	SER
1	A	284	LEU
1	A	37	THR
1	A	101	PRO
1	A	281	PHE
1	A	81	LYS
1	A	243	PRO
1	A	186	GLY
1	A	210	ILE

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	298/302 (99%)	235 (79%)	63 (21%)	1 0

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

Mol	Chain	Res	Type
1	A	16	LYS
1	A	27	LEU
1	A	28	LYS
1	A	34	SER
1	A	40	LEU
1	A	42	GLN
1	A	45	ARG
1	A	48	THR
1	A	53	SER
1	A	54	PHE
1	A	60	VAL
1	A	83	LYS
1	A	84	GLN
1	A	85	ILE
1	A	104	VAL
1	A	114	SER

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Mol	Chain	Res	Type
1	A	119	VAL
1	A	120	MET
1	A	123	VAL
1	A	134	ARG
1	A	135	ILE
1	A	137	ARG
1	A	149	GLN
1	A	150	ILE
1	A	151	VAL
1	A	153	THR
1	A	158	HIS
1	A	160	LEU
1	A	163	ILE
1	A	175	ASP
1	A	180	ILE
1	A	190	ARG
1	A	191	VAL
1	A	195	THR
1	A	212	SER
1	A	217	LYS
1	A	219	VAL
1	A	226	VAL
1	A	228	ILE
1	A	249	LYS
1	A	250	ILE
1	A	251	VAL
1	A	254	LYS
1	A	255	VAL
1	A	256	ARG
1	A	259	SER
1	A	266	LYS
1	A	268	LEU
1	A	273	LEU
1	A	278	THR
1	A	279	LYS
1	A	280	ARG
1	A	288	VAL
1	A	299	THR
1	A	300	THR
1	A	305	ILE
1	A	308	ARG
1	A	315	ILE

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Mol	Chain	Res	Type
1	A	325	SER
1	A	332	GLU
1	A	339	ILE
1	A	340	ASN
1	A	345	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	149	GLN
1	A	176	GLN
1	A	177	GLN
1	A	242	GLN
1	A	283	ASN
1	A	286	ASN
1	A	289	ASN
1	A	293	ASN
1	A	326	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	A	338	1	8,9,10	1.27	1 (12%)	7,12,14	0.73	0
1	TPO	A	197	1	8,10,11	1.52	1 (12%)	10,14,16	1.51	2 (20%)

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	SEP	A	338	1	-	2/6/8/10	-
1	TPO	A	197	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	TPO	P-OG1	-2.57	1.55	1.59
1	A	338	SEP	P-O2P	-2.08	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TPO	P-OG1-CB	-3.05	115.05	123.33
1	A	197	TPO	O2P-P-OG1	2.19	114.37	105.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	N-CA-CB-OG
1	A	338	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	SEP	4	0
1	A	197	TPO	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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
2	BA1	A	351	-	43,43,43	1.67	9 (20%)	54,61,61	2.34	20 (37%)

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
2	BA1	A	351	-	-	9/28/40/40	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	351	BA1	OAC-C1B	4.42	1.43	1.34
2	A	351	BA1	C7'-C6'	3.94	1.45	1.38
2	A	351	BA1	O5'-C5'	3.44	1.44	1.37
2	A	351	BA1	C7-N1	-3.04	1.40	1.47
2	A	351	BA1	C9'-CXU	-2.90	1.36	1.41
2	A	351	BA1	C5B-C8'	-2.77	1.45	1.50
2	A	351	BA1	C2B-C1B	-2.68	1.44	1.50
2	A	351	BA1	C5B-C4B	-2.42	1.37	1.41
2	A	351	BA1	CXE-CXO	2.19	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	351	BA1	C2'-C1'-N1'	6.18	128.49	117.04
2	A	351	BA1	C3-N1'-C1'	-5.46	113.01	122.94
2	A	351	BA1	CXY-C9'-CXU	5.26	123.28	118.42
2	A	351	BA1	C6-C5-C4	4.35	127.81	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	351	BA1	CXE-CX4-CXU	-3.80	115.36	120.05
2	A	351	BA1	OXU-CXU-C9'	-3.74	114.22	121.14
2	A	351	BA1	C6B-C5B-C4B	3.64	121.26	117.36
2	A	351	BA1	C2-C3-N1'	-3.50	103.05	109.55
2	A	351	BA1	O1'-C1'-C2'	-3.31	114.34	120.90
2	A	351	BA1	OAC-C1B-C2B	3.15	116.97	111.90
2	A	351	BA1	C9'-C8'-C5B	3.02	127.37	121.38
2	A	351	BA1	OX8-CX8-OXI	-2.94	117.03	123.35
2	A	351	BA1	O1'-C1'-N1'	-2.87	117.01	122.47
2	A	351	BA1	CXO-CXY-C9'	-2.65	116.43	120.16
2	A	351	BA1	C3'-C4'-C5'	2.53	122.55	119.88
2	A	351	BA1	O8'-C8'-C5B	-2.44	115.55	119.76
2	A	351	BA1	OAC-C4-C3	2.43	111.84	107.16
2	A	351	BA1	CXU-C9'-C8'	-2.36	114.72	120.03
2	A	351	BA1	C3B-C2B-C1B	-2.24	115.72	120.09
2	A	351	BA1	C2B-C7B-C6B	-2.11	118.24	120.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	351	BA1	C5-C4-OAC-C1B
2	A	351	BA1	OAC-C1B-C2B-C3B
2	A	351	BA1	OAC-C1B-C2B-C7B
2	A	351	BA1	OBC-C1B-C2B-C3B
2	A	351	BA1	OBC-C1B-C2B-C7B
2	A	351	BA1	C3-C4-OAC-C1B
2	A	351	BA1	OBC-C1B-OAC-C4
2	A	351	BA1	C2B-C1B-OAC-C4
2	A	351	BA1	C4-C3-N1'-C1'

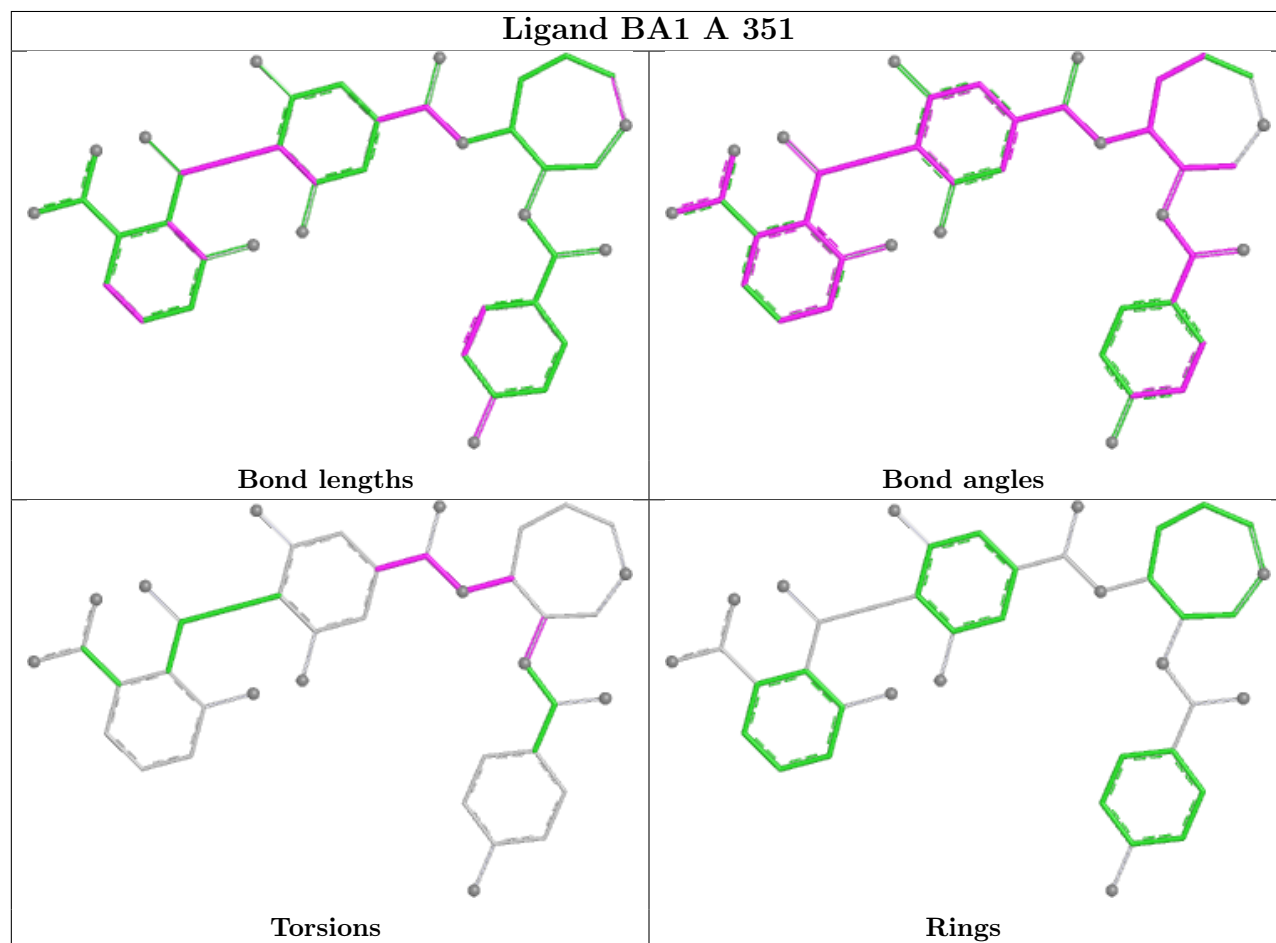
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	351	BA1	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.