



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:46 AM UTC

PDB ID : 3TNQ / pdb_00003tnq
Title : Structure and Allostery of the PKA RIIB Tetrameric Holoenzyme
Authors : Zhang, P.; Smith-Nguyen, E.V.; Keshwani, M.M.; Deal, M.S.; Kornev, A.P.;
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Deposited on : 2011-09-01
Resolution : 3.10 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

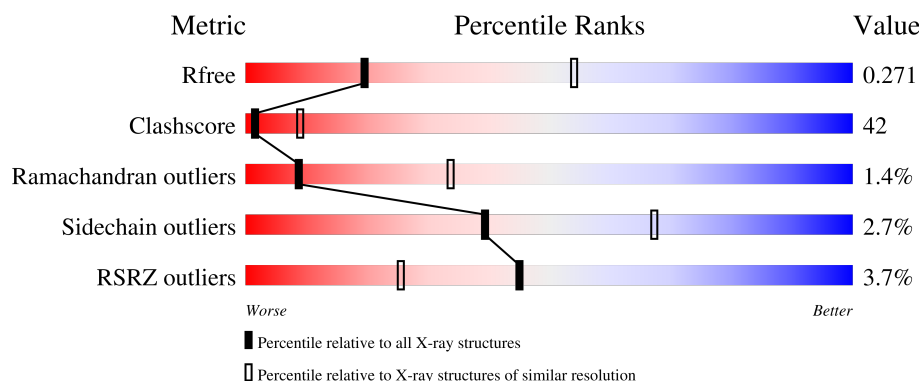
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	B	350	
2	A	416	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4943 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 Protein kinase, cAMP-dependent, catalytic, alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	334	Total	C	N	O	P	S	0	0	0
			2765	1789	462	503	3	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	42	GLN	HIS	conflict	UNP A1L1M0
B	124	ALA	PRO	conflict	UNP A1L1M0

- Molecule 2 is a protein called cAMP-dependent protein kinase type II-beta regulatory subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	270	Total	C	N	O	P	S	0	0	0
			2136	1344	374	402	1	15			

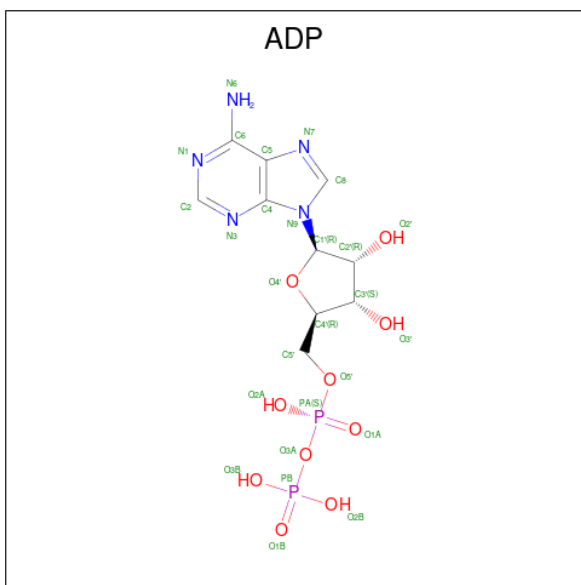
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	LYS	ARG	engineered mutation	UNP P31324

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		

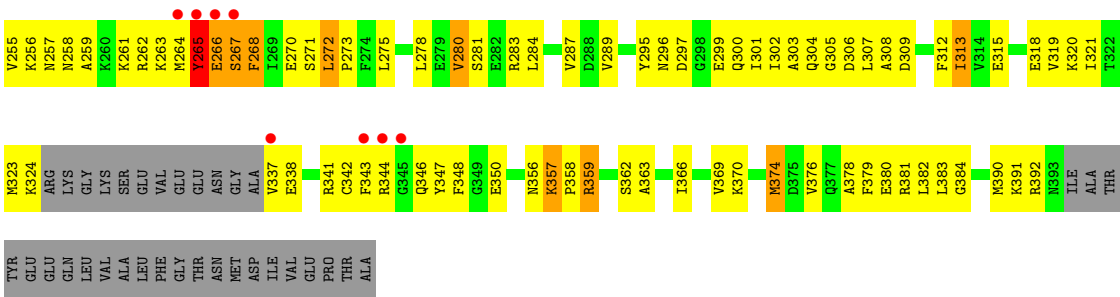
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	11	Total O 11 11	0	0
5	A	2	Total O 2 2	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.82Å 212.75Å 61.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 3.10 38.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	84.8 (38.84-3.10) 84.8 (38.84-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.231 , 0.275 0.227 , 0.271	Depositor DCC
R_{free} test set	831 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4943	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: SEP, TPO, MG, ADP

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	B	0.58	0/2802	1.05	15/3772 (0.4%)
2	A	0.59	1/2157 (0.0%)	1.16	18/2897 (0.6%)
All	All	0.59	1/4959 (0.0%)	1.10	33/6669 (0.5%)

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	B	0	1
2	A	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	209	CYS	CA-C	6.60	1.61	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ARG	N-CA-C	11.74	124.65	110.91
2	A	155	ASN	N-CA-C	10.77	126.59	113.12
2	A	266	GLU	N-CA-C	10.72	127.36	112.45
1	B	55	GLY	CA-C-N	9.76	137.67	122.93
1	B	55	GLY	C-N-CA	9.76	137.67	122.93
2	A	265	TYR	N-CA-C	-8.78	101.66	112.38
2	A	357	LYS	CA-C-N	8.61	130.60	119.84
2	A	357	LYS	C-N-CA	8.61	130.60	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	185	ASP	N-CA-C	8.51	120.74	110.19
1	B	96	GLN	N-CA-C	-8.45	103.11	113.50
1	B	313	PRO	CA-C-N	7.67	135.22	122.33
1	B	313	PRO	C-N-CA	7.67	135.22	122.33
2	A	209	CYS	N-CA-C	-7.43	99.29	110.28
1	B	35	GLN	N-CA-C	6.87	125.43	110.80
2	A	187	ASP	N-CA-C	-6.72	102.39	112.54
1	B	217	LYS	N-CA-C	6.64	119.53	111.82
1	B	183	THR	N-CA-C	6.43	121.66	113.55
1	B	55	GLY	N-CA-C	-6.40	94.75	113.30
2	A	106	ARG	N-CA-C	-6.37	105.47	113.18
2	A	136	THR	N-CA-C	6.33	120.20	110.20
1	B	236	PRO	CA-C-N	6.28	125.85	119.19
1	B	236	PRO	C-N-CA	6.28	125.85	119.19
2	A	133	HIS	CA-C-N	6.25	126.74	119.99
2	A	133	HIS	C-N-CA	6.25	126.74	119.99
2	A	119	ASN	CA-C-N	6.18	125.88	119.82
2	A	119	ASN	C-N-CA	6.18	125.88	119.82
2	A	359	ARG	N-CA-C	5.87	123.30	110.80
2	A	157	ASP	CA-C-N	5.86	127.17	119.84
2	A	157	ASP	C-N-CA	5.86	127.17	119.84
1	B	66	GLY	N-CA-C	-5.81	107.92	115.59
1	B	92	LYS	N-CA-C	5.73	117.33	111.14
2	A	280	VAL	N-CA-C	5.69	115.89	110.42
1	B	19	LEU	N-CA-C	5.17	119.89	111.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	265	TYR	Peptide
1	B	56	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2765	0	2740	196	0
2	A	2136	0	2138	231	2
3	B	2	0	0	0	0
4	B	27	0	12	3	0
5	A	2	0	0	0	0
5	B	11	0	0	10	0
All	All	4943	0	4890	417	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 42.

All (417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PRO:HA	1:B:96:GLN:NE2	1.40	1.35
2:A:266:GLU:OE2	2:A:287:VAL:HG21	1.19	1.32
2:A:204:ASP:CB	2:A:205:GLY:HA3	1.69	1.20
2:A:266:GLU:OE2	2:A:287:VAL:CG2	1.93	1.16
2:A:191:VAL:HG12	2:A:218:SER:HB3	1.16	1.16
2:A:262:ARG:HG3	2:A:263:LYS:H	1.07	1.15
1:B:54:PHE:CD2	1:B:75:ASP:HB2	1.82	1.15
2:A:204:ASP:HB2	2:A:205:GLY:HA3	1.18	1.13
1:B:33:PRO:CA	1:B:96:GLN:HE22	1.63	1.11
2:A:263:LYS:HD2	2:A:266:GLU:HG3	1.13	1.10
1:B:54:PHE:HD2	1:B:75:ASP:HB2	1.05	1.09
2:A:191:VAL:HG12	2:A:218:SER:CB	1.83	1.09
2:A:267:SER:O	2:A:271:SER:HB3	1.52	1.08
2:A:238:SER:HB2	2:A:239:PRO:HD2	1.36	1.05
1:B:33:PRO:CA	1:B:96:GLN:NE2	2.18	1.04
2:A:263:LYS:CD	2:A:266:GLU:HG3	1.89	1.02
1:B:105:LYS:NZ	1:B:107:GLU:CD	2.21	0.99
1:B:78:LYS:HE3	1:B:78:LYS:HA	1.46	0.98
1:B:33:PRO:HA	1:B:96:GLN:HE22	0.90	0.97
1:B:32:THR:HG23	5:B:360:HOH:O	1.62	0.97
2:A:175:GLU:HG3	2:A:237:THR:O	1.66	0.96
1:B:105:LYS:NZ	1:B:107:GLU:OE1	2.02	0.93
2:A:200:TYR:HB2	2:A:208:ARG:O	1.69	0.93
2:A:262:ARG:HA	2:A:265:TYR:CD2	2.05	0.91
1:B:163:ILE:HD11	1:B:165:ARG:HD3	1.51	0.91
1:B:56:ARG:HH22	1:B:335:ILE:HA	1.33	0.90
1:B:163:ILE:CD1	1:B:165:ARG:HD3	2.02	0.90
2:A:238:SER:HB2	2:A:239:PRO:CD	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:238:SER:CB	2:A:239:PRO:HD2	2.02	0.89
2:A:265:TYR:O	2:A:268:PHE:HB2	1.71	0.88
2:A:262:ARG:HG3	2:A:263:LYS:N	1.81	0.88
2:A:156:LEU:HD22	2:A:254:ILE:CD1	2.04	0.87
2:A:324:LYS:HZ2	2:A:337:VAL:N	1.72	0.87
2:A:204:ASP:CB	2:A:205:GLY:CA	2.51	0.87
2:A:192:ILE:HA	2:A:242:LEU:HG	1.55	0.87
1:B:32:THR:CG2	5:B:360:HOH:O	2.20	0.86
1:B:34:SER:N	1:B:96:GLN:OE1	2.09	0.85
1:B:45:ARG:HH11	1:B:335:ILE:H	1.25	0.85
1:B:61:LYS:HD3	1:B:68:HIS:CE1	2.12	0.85
2:A:206:VAL:HB	2:A:208:ARG:HE	1.42	0.84
2:A:156:LEU:CD2	2:A:254:ILE:HD12	2.07	0.84
2:A:265:TYR:O	2:A:268:PHE:CG	2.31	0.84
2:A:157:ASP:OD2	2:A:160:GLN:HG3	1.79	0.83
2:A:257:ASN:OD1	2:A:261:LYS:HD2	1.77	0.82
2:A:262:ARG:HA	2:A:265:TYR:CE2	2.14	0.82
2:A:263:LYS:HD2	2:A:266:GLU:CG	2.05	0.81
1:B:54:PHE:HD2	1:B:75:ASP:CB	1.92	0.80
2:A:295:TYR:HB2	2:A:369:VAL:CG2	2.11	0.80
2:A:266:GLU:O	2:A:270:GLU:HG2	1.81	0.79
1:B:34:SER:H	1:B:96:GLN:CD	1.91	0.79
2:A:204:ASP:HB3	2:A:205:GLY:HA3	1.63	0.78
2:A:315:GLU:OE1	2:A:370:LYS:HG2	1.84	0.78
2:A:265:TYR:O	2:A:268:PHE:CB	2.31	0.77
2:A:156:LEU:HD22	2:A:254:ILE:HD12	1.66	0.76
1:B:184:ASP:OD1	4:B:400:ADP:O2B	2.02	0.76
1:B:78:LYS:HD2	1:B:78:LYS:N	2.00	0.76
1:B:71:MET:HE3	1:B:117:TYR:CD1	2.21	0.75
2:A:160:GLN:HG2	2:A:257:ASN:ND2	2.00	0.75
2:A:204:ASP:HB2	2:A:205:GLY:CA	2.10	0.75
1:B:34:SER:H	1:B:96:GLN:NE2	1.85	0.74
2:A:241:ALA:C	2:A:242:LEU:HD12	2.12	0.74
2:A:241:ALA:O	2:A:242:LEU:HD12	1.87	0.74
2:A:187:ASP:OD1	2:A:247:ARG:NH2	2.21	0.74
1:B:318:PHE:CZ	1:B:320:GLY:O	2.40	0.74
1:B:245:GLN:O	1:B:249:LYS:HG3	1.88	0.74
1:B:71:MET:HE3	1:B:117:TYR:HD1	1.51	0.74
1:B:105:LYS:HZ1	1:B:107:GLU:CD	1.94	0.74
1:B:56:ARG:NH2	1:B:335:ILE:HA	2.01	0.73
2:A:320:LYS:HE3	2:A:338:GLU:OE1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLU:HG3	5:B:360:HOH:O	1.88	0.73
1:B:34:SER:N	1:B:96:GLN:HE22	1.87	0.73
1:B:48:THR:HG22	1:B:330:TYR:HD1	1.53	0.72
1:B:27:LEU:HD21	1:B:190:ARG:HH22	1.53	0.72
2:A:261:LYS:O	2:A:265:TYR:CE2	2.43	0.72
1:B:19:LEU:C	1:B:19:LEU:HD23	2.15	0.72
2:A:159:GLU:N	2:A:159:GLU:OE2	2.23	0.72
2:A:187:ASP:CG	2:A:247:ARG:NH2	2.48	0.72
2:A:169:PHE:CZ	2:A:244:GLY:HA3	2.25	0.72
1:B:53:SER:O	5:B:354:HOH:O	2.06	0.72
2:A:156:LEU:CD2	2:A:254:ILE:CD1	2.67	0.72
2:A:263:LYS:HD3	2:A:266:GLU:CD	2.14	0.72
1:B:44:ASP:HB2	1:B:61:LYS:HB3	1.71	0.72
2:A:197:PHE:CZ	2:A:242:LEU:HD11	2.25	0.71
1:B:156:TYR:O	1:B:159:SER:OG	2.08	0.71
1:B:318:PHE:CE1	1:B:323:ASP:HB3	2.25	0.71
2:A:104:ILE:CG2	2:A:105:ASN:N	2.53	0.71
1:B:31:GLU:CG	5:B:360:HOH:O	2.39	0.71
1:B:128:MET:HE1	1:B:227:LEU:HD11	1.73	0.70
2:A:262:ARG:O	2:A:265:TYR:N	2.21	0.70
2:A:263:LYS:CD	2:A:266:GLU:CG	2.66	0.70
2:A:272:LEU:HB2	2:A:275:LEU:HD12	1.73	0.70
1:B:33:PRO:C	1:B:96:GLN:HE22	1.99	0.70
2:A:206:VAL:HB	2:A:208:ARG:NE	2.05	0.70
2:A:222:LEU:HD21	2:A:226:TYR:CE2	2.27	0.70
1:B:56:ARG:NH2	1:B:335:ILE:HG12	2.05	0.70
1:B:216:ASN:O	1:B:219:VAL:HG22	1.91	0.70
2:A:187:ASP:OD1	2:A:247:ARG:NH1	2.24	0.69
2:A:210:VAL:HG12	2:A:211:GLY:N	2.06	0.69
1:B:261:PHE:CD1	1:B:265:LEU:HD23	2.28	0.69
1:B:265:LEU:HD13	1:B:296:TRP:CE2	2.27	0.69
1:B:54:PHE:O	1:B:74:LEU:HA	1.93	0.69
1:B:163:ILE:HD12	1:B:165:ARG:CG	2.23	0.69
2:A:374:MET:HE3	2:A:374:MET:HA	1.74	0.69
2:A:104:ILE:HG22	2:A:105:ASN:N	2.09	0.68
1:B:50:GLY:O	1:B:56:ARG:HA	1.94	0.68
2:A:257:ASN:OD1	2:A:261:LYS:CD	2.42	0.67
2:A:187:ASP:CG	2:A:247:ARG:HH22	2.03	0.67
1:B:82:LEU:O	1:B:84:GLN:HG2	1.95	0.66
2:A:206:VAL:CB	2:A:208:ARG:HE	2.07	0.66
2:A:266:GLU:C	2:A:268:PHE:N	2.50	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:320:LYS:HD2	2:A:366:ILE:HD11	1.77	0.66
2:A:264:MET:C	2:A:266:GLU:H	2.02	0.66
1:B:61:LYS:HD3	1:B:68:HIS:HE1	1.61	0.66
2:A:136:THR:OG1	2:A:139:GLN:HG3	1.96	0.66
2:A:295:TYR:HB2	2:A:369:VAL:HG23	1.78	0.66
2:A:222:LEU:HD23	2:A:222:LEU:O	1.95	0.66
1:B:274:GLN:HG2	1:B:279:LYS:HB2	1.77	0.66
1:B:193:GLY:O	1:B:194:ARG:HG2	1.95	0.65
2:A:320:LYS:HE3	2:A:338:GLU:CD	2.21	0.65
2:A:263:LYS:HD3	2:A:266:GLU:OE2	1.97	0.65
1:B:32:THR:OG1	5:B:360:HOH:O	2.13	0.65
2:A:270:GLU:HB3	2:A:283:ARG:HD3	1.79	0.65
1:B:341:GLU:OE2	1:B:344:GLY:HA3	1.96	0.65
2:A:206:VAL:CG2	2:A:208:ARG:HH21	2.10	0.65
1:B:230:GLU:HA	1:B:235:TYR:O	1.97	0.64
1:B:26:PHE:HE1	1:B:190:ARG:NH1	1.95	0.64
2:A:159:GLU:HA	2:A:162:SER:HB3	1.79	0.63
1:B:34:SER:N	1:B:96:GLN:NE2	2.45	0.63
1:B:209:ILE:HG12	1:B:215:TYR:CE2	2.33	0.63
2:A:160:GLN:HE21	2:A:257:ASN:HB3	1.63	0.63
2:A:144:GLN:HE21	2:A:148:LYS:HD2	1.64	0.63
2:A:343:PHE:CG	2:A:344:ARG:N	2.66	0.63
1:B:78:LYS:HE3	1:B:78:LYS:CA	2.25	0.63
2:A:160:GLN:O	2:A:164:VAL:HG23	1.99	0.63
2:A:306:ASP:O	2:A:359:ARG:HG2	1.99	0.62
2:A:249:THR:O	2:A:253:ILE:HD13	2.00	0.62
1:B:292:LYS:HA	1:B:302:TRP:CZ2	2.35	0.62
1:B:105:LYS:HZ2	1:B:107:GLU:CD	2.07	0.62
2:A:197:PHE:HZ	2:A:242:LEU:HD11	1.63	0.62
2:A:180:ILE:HG12	2:A:230:LYS:HG3	1.82	0.61
2:A:197:PHE:HB2	2:A:213:TYR:HB2	1.82	0.61
2:A:172:LEU:HA	2:A:241:ALA:HA	1.82	0.61
2:A:175:GLU:HG3	2:A:237:THR:C	2.25	0.61
1:B:268:LEU:O	1:B:268:LEU:HD12	2.00	0.61
1:B:50:GLY:HA2	1:B:330:TYR:CE1	2.36	0.61
2:A:304:GLN:NE2	2:A:323:MET:HG3	2.15	0.61
2:A:343:PHE:CD2	2:A:344:ARG:N	2.69	0.60
1:B:271:ASN:HB3	1:B:281:PHE:CD1	2.35	0.60
2:A:272:LEU:CB	2:A:275:LEU:HD12	2.31	0.60
1:B:74:LEU:HB2	1:B:116:LEU:HB2	1.82	0.60
1:B:170:GLU:HG2	2:A:109:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ALA:HB1	1:B:231:MET:HE3	1.84	0.60
2:A:138:ASP:O	2:A:139:GLN:C	2.45	0.60
2:A:343:PHE:CE2	2:A:344:ARG:HB3	2.37	0.60
1:B:27:LEU:CD2	1:B:190:ARG:HH22	2.13	0.60
2:A:104:ILE:CG2	2:A:105:ASN:H	2.14	0.60
1:B:163:ILE:HD12	1:B:165:ARG:HD3	1.82	0.59
1:B:301:ASP:HB3	1:B:304:ALA:HB3	1.85	0.59
2:A:220:GLY:HA3	2:A:230:LYS:HE3	1.84	0.59
2:A:164:VAL:O	2:A:168:MET:HG3	2.02	0.58
2:A:200:TYR:HB3	2:A:209:CYS:HA	1.85	0.58
1:B:274:GLN:CG	1:B:279:LYS:HB2	2.32	0.58
1:B:34:SER:N	1:B:96:GLN:CD	2.57	0.58
2:A:206:VAL:HG21	2:A:208:ARG:HH21	1.69	0.58
2:A:305:GLY:H	2:A:359:ARG:HB2	1.69	0.58
1:B:339:ILE:HG22	5:B:357:HOH:O	2.02	0.58
2:A:187:ASP:O	2:A:246:ASP:HA	2.04	0.58
2:A:319:VAL:HG12	2:A:320:LYS:N	2.19	0.58
1:B:45:ARG:NH1	1:B:335:ILE:H	1.98	0.58
1:B:128:MET:HE2	1:B:169:PRO:HA	1.84	0.57
2:A:315:GLU:OE1	2:A:370:LYS:CG	2.51	0.57
1:B:54:PHE:CD2	1:B:75:ASP:CB	2.72	0.57
2:A:315:GLU:CD	2:A:370:LYS:HE3	2.30	0.57
1:B:163:ILE:CD1	1:B:165:ARG:CD	2.80	0.57
2:A:181:ASP:O	2:A:184:ASP:HB2	2.04	0.57
2:A:222:LEU:HD21	2:A:226:TYR:CZ	2.39	0.57
2:A:318:GLU:HG3	2:A:366:ILE:HB	1.86	0.57
2:A:191:VAL:CG1	2:A:218:SER:HB3	2.11	0.57
1:B:78:LYS:N	1:B:78:LYS:CD	2.68	0.56
1:B:103:LEU:HD22	1:B:185:PHE:HZ	1.69	0.56
1:B:65:SER:OG	1:B:67:ASN:HB2	2.03	0.56
1:B:100:PHE:CD1	1:B:101:PRO:HD2	2.40	0.56
2:A:187:ASP:OD1	2:A:247:ARG:CZ	2.53	0.56
2:A:307:LEU:HD22	2:A:309:ASP:OD2	2.05	0.56
1:B:40:LEU:HD21	1:B:45:ARG:HD2	1.88	0.56
1:B:272:LEU:HD23	1:B:281:PHE:HB2	1.87	0.56
2:A:309:ASP:O	2:A:376:VAL:HG23	2.05	0.56
2:A:268:PHE:N	2:A:268:PHE:CD2	2.74	0.56
1:B:277:LEU:HB2	2:A:289:VAL:CG1	2.36	0.56
2:A:315:GLU:OE1	2:A:370:LYS:CD	2.54	0.56
2:A:204:ASP:HB3	2:A:205:GLY:CA	2.28	0.55
2:A:295:TYR:HB2	2:A:369:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:268:PHE:N	2:A:268:PHE:HD2	2.04	0.55
1:B:318:PHE:CZ	1:B:320:GLY:C	2.85	0.55
2:A:118:TYR:OH	2:A:256:LYS:HG3	2.07	0.55
1:B:65:SER:C	1:B:67:ASN:H	2.13	0.55
1:B:31:GLU:HG3	1:B:32:THR:HG23	1.90	0.55
2:A:175:GLU:CG	2:A:237:THR:O	2.48	0.55
1:B:40:LEU:O	1:B:40:LEU:HD23	2.06	0.54
1:B:46:ILE:HD11	1:B:61:LYS:HB2	1.88	0.54
1:B:55:GLY:O	1:B:73:ILE:O	2.25	0.54
1:B:26:PHE:CE1	1:B:190:ARG:NH1	2.74	0.54
1:B:50:GLY:O	1:B:57:VAL:N	2.40	0.54
2:A:159:GLU:O	2:A:163:GLN:HG3	2.07	0.54
1:B:266:LYS:O	1:B:270:ARG:HG3	2.07	0.54
2:A:187:ASP:O	2:A:247:ARG:N	2.41	0.54
1:B:94:ILE:O	1:B:98:VAL:HG13	2.07	0.54
2:A:150:ILE:HB	2:A:153:PHE:HD1	1.73	0.54
2:A:378:ALA:HA	2:A:381:ARG:CZ	2.38	0.54
1:B:19:LEU:HD23	1:B:20:ALA:N	2.23	0.54
1:B:285:LYS:HD2	2:A:384:GLY:CA	2.38	0.54
2:A:104:ILE:HG23	2:A:105:ASN:H	1.73	0.53
1:B:115:ASN:HB2	1:B:117:TYR:CZ	2.43	0.53
2:A:172:LEU:C	2:A:172:LEU:HD12	2.34	0.53
1:B:44:ASP:N	1:B:61:LYS:O	2.39	0.53
1:B:163:ILE:HD12	1:B:165:ARG:CD	2.38	0.52
1:B:339:ILE:C	5:B:357:HOH:O	2.52	0.52
2:A:238:SER:CB	2:A:239:PRO:CD	2.67	0.52
2:A:266:GLU:C	2:A:268:PHE:H	2.17	0.52
1:B:125:GLY:HA3	1:B:174:ILE:O	2.09	0.52
2:A:143:LEU:CD1	2:A:243:TRP:CD1	2.92	0.52
2:A:156:LEU:HD22	2:A:254:ILE:HD11	1.86	0.52
2:A:206:VAL:CG1	2:A:208:ARG:HE	2.23	0.52
1:B:289:ASN:C	1:B:291:ILE:N	2.65	0.52
1:B:306:TYR:CD1	1:B:306:TYR:C	2.88	0.52
2:A:140:ARG:NH2	2:A:165:LEU:HD12	2.24	0.52
1:B:29:LYS:HB3	1:B:97:ALA:HA	1.92	0.51
2:A:156:LEU:HD21	2:A:254:ILE:HD12	1.90	0.51
1:B:75:ASP:HB3	1:B:78:LYS:HG2	1.92	0.51
1:B:210:ILE:HG23	2:A:225:MET:HE1	1.91	0.51
1:B:212:SER:OG	2:A:251:ARG:NH1	2.43	0.51
2:A:296:ASN:HB3	2:A:299:GLU:OE2	2.10	0.51
2:A:302:ILE:HG13	2:A:363:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLU:HB2	1:B:141:PRO:HD3	1.92	0.51
1:B:152:LEU:O	1:B:155:GLU:HB3	2.11	0.51
2:A:191:VAL:HG12	2:A:218:SER:HB2	1.85	0.51
1:B:144:ARG:HG3	1:B:296:TRP:CZ3	2.45	0.51
1:B:48:THR:HB	1:B:332:GLU:OE2	2.11	0.50
1:B:145:PHE:O	1:B:149:GLN:NE2	2.42	0.50
2:A:301:ILE:HB	2:A:363:ALA:HB3	1.93	0.50
1:B:271:ASN:HB3	1:B:281:PHE:CG	2.46	0.50
1:B:167:LEU:HD21	1:B:227:LEU:HD22	1.94	0.50
2:A:135:LYS:HE3	2:A:243:TRP:CH2	2.46	0.50
2:A:138:ASP:OD2	2:A:142:ARG:NH2	2.45	0.50
1:B:113:ASN:HA	1:B:341:GLU:HA	1.94	0.50
1:B:48:THR:HG22	1:B:330:TYR:CD1	2.40	0.50
1:B:189:LYS:HE2	1:B:195:THR:OG1	2.11	0.50
2:A:318:GLU:HB2	2:A:342:CYS:O	2.11	0.50
2:A:347:TYR:HD1	2:A:350:GLU:OE1	1.94	0.49
2:A:300:GLN:NE2	2:A:303:ALA:HA	2.27	0.49
2:A:163:GLN:O	2:A:166:ASP:HB2	2.12	0.49
2:A:356:ASN:O	2:A:357:LYS:C	2.55	0.49
2:A:159:GLU:CD	2:A:159:GLU:H	2.19	0.49
1:B:344:GLY:O	1:B:348:THR:HG23	2.13	0.49
2:A:186:GLY:O	2:A:187:ASP:OD1	2.30	0.49
2:A:196:THR:HG22	2:A:214:ASP:HA	1.94	0.49
2:A:341:ARG:O	2:A:341:ARG:HG3	2.13	0.49
2:A:143:LEU:HD11	2:A:243:TRP:CD1	2.47	0.49
1:B:34:SER:HB3	1:B:96:GLN:OE1	2.12	0.48
1:B:171:ASN:ND2	1:B:184:ASP:HB3	2.27	0.48
1:B:90:ASN:O	1:B:91:GLU:C	2.56	0.48
1:B:235:TYR:HB2	1:B:236:PRO:HD2	1.95	0.48
1:B:163:ILE:O	1:B:188:ALA:HA	2.12	0.48
2:A:252:ARG:HG2	2:A:256:LYS:HD2	1.95	0.48
2:A:315:GLU:HB3	2:A:370:LYS:HG2	1.96	0.48
1:B:158:HIS:HB3	1:B:217:LYS:HD3	1.96	0.48
2:A:159:GLU:HG2	2:A:160:GLN:H	1.78	0.48
2:A:216:ARG:HG2	2:A:217:GLY:N	2.28	0.48
2:A:300:GLN:HE21	2:A:303:ALA:HA	1.78	0.48
1:B:48:THR:CG2	1:B:330:TYR:HD1	2.23	0.48
1:B:193:GLY:C	1:B:194:ARG:HG2	2.38	0.48
2:A:143:LEU:HD11	2:A:243:TRP:CG	2.48	0.48
1:B:19:LEU:C	1:B:19:LEU:CD2	2.83	0.48
2:A:210:VAL:CG1	2:A:211:GLY:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:216:ARG:HG2	2:A:217:GLY:H	1.78	0.48
2:A:303:ALA:HB3	2:A:306:ASP:CG	2.39	0.48
2:A:148:LYS:O	2:A:154:LYS:HA	2.13	0.48
1:B:201:THR:O	1:B:202:PRO:C	2.57	0.47
2:A:144:GLN:HE22	2:A:161:MET:HG2	1.78	0.47
2:A:175:GLU:HG3	2:A:238:SER:HA	1.95	0.47
1:B:268:LEU:HD12	1:B:268:LEU:C	2.39	0.47
1:B:78:LYS:CA	1:B:78:LYS:CE	2.91	0.47
2:A:263:LYS:HE2	2:A:284:LEU:HD21	1.96	0.47
1:B:50:GLY:HA2	1:B:330:TYR:HE1	1.79	0.47
1:B:32:THR:CB	5:B:360:HOH:O	2.57	0.47
1:B:204:TYR:OH	1:B:230:GLU:OE2	2.24	0.47
2:A:347:TYR:O	2:A:348:PHE:HB3	2.15	0.47
1:B:338:SEP:HA	1:B:338:SEP:O3P	2.15	0.47
2:A:262:ARG:O	2:A:265:TYR:CD2	2.67	0.47
1:B:72:LYS:HE3	4:B:400:ADP:O1A	2.14	0.47
1:B:123:VAL:HG12	1:B:174:ILE:O	2.14	0.47
2:A:262:ARG:CG	2:A:263:LYS:N	2.65	0.47
1:B:69:TYR:CE2	1:B:107:GLU:HG3	2.49	0.46
1:B:310:VAL:HG12	1:B:311:GLU:N	2.30	0.46
2:A:105:ASN:C	2:A:105:ASN:OD1	2.59	0.46
1:B:48:THR:OG1	1:B:332:GLU:OE1	2.33	0.46
1:B:146:TYR:CD2	1:B:180:ILE:HD11	2.51	0.46
2:A:263:LYS:HB3	2:A:264:MET:HE2	1.98	0.46
2:A:136:THR:O	2:A:137:ASP:C	2.56	0.46
2:A:181:ASP:HB2	2:A:184:ASP:HB2	1.97	0.46
2:A:301:ILE:HD12	2:A:319:VAL:HG13	1.98	0.46
2:A:379:PHE:CD2	2:A:379:PHE:C	2.94	0.46
1:B:53:SER:HA	1:B:54:PHE:HA	1.73	0.46
2:A:140:ARG:NH1	2:A:166:ASP:OD1	2.49	0.46
1:B:82:LEU:O	1:B:83:LYS:C	2.58	0.46
2:A:347:TYR:CD1	2:A:350:GLU:OE1	2.69	0.46
1:B:265:LEU:HD13	1:B:296:TRP:CZ2	2.51	0.45
2:A:263:LYS:CD	2:A:266:GLU:CD	2.84	0.45
1:B:180:ILE:HG22	1:B:181:GLN:N	2.32	0.45
2:A:170:GLU:HB2	2:A:243:TRP:CZ3	2.52	0.45
1:B:93:ARG:O	1:B:94:ILE:C	2.59	0.45
1:B:112:ASP:C	1:B:112:ASP:OD1	2.59	0.45
1:B:294:HIS:ND1	1:B:295:LYS:N	2.65	0.45
2:A:378:ALA:HA	2:A:381:ARG:NH2	2.31	0.45
1:B:19:LEU:HD23	1:B:20:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:PHE:O	1:B:300:THR:HB	2.17	0.45
2:A:201:VAL:HG22	2:A:232:ALA:HA	1.99	0.45
2:A:206:VAL:HG12	2:A:208:ARG:HG2	1.97	0.45
2:A:246:ASP:OD1	2:A:247:ARG:N	2.50	0.45
2:A:347:TYR:CD2	2:A:347:TYR:N	2.85	0.45
1:B:78:LYS:HD2	1:B:78:LYS:H	1.80	0.45
2:A:262:ARG:CA	2:A:265:TYR:CD2	2.91	0.45
1:B:80:VAL:HG22	1:B:85:ILE:HD11	1.99	0.44
1:B:163:ILE:CD1	1:B:165:ARG:CG	2.93	0.44
2:A:119:ASN:HA	2:A:120:PRO:HD3	1.68	0.44
2:A:342:CYS:HA	2:A:346:GLN:OE1	2.17	0.44
1:B:65:SER:C	1:B:67:ASN:N	2.75	0.44
1:B:103:LEU:HD22	1:B:185:PHE:CZ	2.51	0.44
1:B:163:ILE:HD12	1:B:165:ARG:HG2	1.99	0.44
1:B:86:GLU:O	1:B:87:HIS:C	2.57	0.44
1:B:92:LYS:NZ	1:B:350:PHE:O	2.49	0.44
2:A:144:GLN:O	2:A:148:LYS:HG3	2.18	0.44
2:A:296:ASN:O	2:A:297:ASP:C	2.58	0.44
1:B:116:LEU:HD11	1:B:347:PHE:CD1	2.53	0.44
1:B:168:LYS:HE3	2:A:110:ARG:O	2.17	0.44
2:A:120:PRO:HG2	2:A:259:ALA:HB2	1.98	0.44
2:A:280:VAL:HG13	2:A:281:SER:N	2.32	0.44
2:A:380:GLU:HA	2:A:384:GLY:O	2.17	0.44
1:B:54:PHE:O	1:B:75:ASP:N	2.44	0.44
1:B:221:TRP:O	1:B:222:TRP:C	2.60	0.44
1:B:341:GLU:O	1:B:342:LYS:HD3	2.17	0.44
1:B:342:LYS:O	1:B:343:CYS:C	2.61	0.44
1:B:54:PHE:HB3	1:B:78:LYS:HG2	1.98	0.44
1:B:78:LYS:O	1:B:79:VAL:C	2.60	0.44
2:A:219:PHE:CE1	2:A:234:ILE:HD13	2.52	0.44
2:A:321:ILE:HA	2:A:362:SER:O	2.18	0.44
2:A:261:LYS:O	2:A:265:TYR:CZ	2.71	0.44
2:A:263:LYS:HA	2:A:264:MET:HA	1.78	0.44
2:A:272:LEU:HA	2:A:273:PRO:HD3	1.82	0.44
2:A:357:LYS:HA	2:A:358:PRO:HD3	1.66	0.43
2:A:315:GLU:N	2:A:370:LYS:O	2.43	0.43
1:B:198:LEU:HD23	1:B:198:LEU:C	2.43	0.43
2:A:145:GLU:O	2:A:145:GLU:CD	2.61	0.43
2:A:303:ALA:O	2:A:359:ARG:CB	2.67	0.43
1:B:220:ASP:O	1:B:223:ALA:HB3	2.18	0.43
2:A:220:GLY:CA	2:A:230:LYS:HE3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:258:ASN:O	2:A:262:ARG:N	2.52	0.43
1:B:100:PHE:CG	1:B:101:PRO:HD2	2.53	0.43
1:B:146:TYR:O	1:B:147:ALA:C	2.61	0.43
1:B:289:ASN:O	1:B:290:ASP:C	2.62	0.43
2:A:222:LEU:HD23	2:A:222:LEU:C	2.43	0.43
2:A:266:GLU:OE2	2:A:287:VAL:HG22	2.03	0.43
1:B:19:LEU:HD23	1:B:20:ALA:CA	2.49	0.42
1:B:31:GLU:HG2	5:B:360:HOH:O	2.12	0.42
1:B:145:PHE:HZ	1:B:179:TYR:CZ	2.36	0.42
1:B:163:ILE:HG13	1:B:165:ARG:HG3	2.01	0.42
1:B:241:ASP:OD1	1:B:242:GLN:N	2.53	0.42
1:B:176:GLN:O	1:B:315:ILE:HG23	2.20	0.42
2:A:196:THR:C	2:A:197:PHE:CD1	2.98	0.42
1:B:54:PHE:HB3	1:B:75:ASP:HB3	2.00	0.42
2:A:319:VAL:CG1	2:A:320:LYS:N	2.83	0.42
1:B:72:LYS:NZ	4:B:400:ADP:O1A	2.50	0.42
1:B:305:ILE:O	1:B:306:TYR:C	2.63	0.42
2:A:182:GLN:HG3	2:A:231:ALA:O	2.19	0.42
1:B:274:GLN:HB3	1:B:280:ARG:HB2	2.02	0.42
2:A:160:GLN:NE2	2:A:257:ASN:HB3	2.32	0.42
2:A:308:ALA:HB2	2:A:359:ARG:HD3	2.00	0.42
1:B:189:LYS:HE3	1:B:191:VAL:HG22	2.01	0.42
2:A:104:ILE:HG22	2:A:106:ARG:N	2.34	0.41
2:A:120:PRO:HG3	2:A:255:VAL:HG12	2.02	0.41
2:A:156:LEU:CD2	2:A:254:ILE:HD11	2.48	0.41
1:B:111:LYS:NZ	1:B:348:THR:HA	2.35	0.41
2:A:270:GLU:HB3	2:A:283:ARG:CD	2.48	0.41
2:A:221:GLU:O	2:A:224:LEU:HB2	2.20	0.41
2:A:272:LEU:HD11	2:A:313:ILE:HD11	2.03	0.41
1:B:312:ALA:HA	1:B:313:PRO:HD3	1.94	0.41
2:A:169:PHE:CD1	2:A:169:PHE:C	2.99	0.41
2:A:278:LEU:HD21	2:A:383:LEU:HD13	2.03	0.41
1:B:168:LYS:HE2	1:B:170:GLU:HB2	2.02	0.41
2:A:264:MET:C	2:A:266:GLU:N	2.65	0.41
2:A:312:PHE:O	2:A:347:TYR:HA	2.21	0.41
1:B:169:PRO:HD2	2:A:110:ARG:NH2	2.35	0.41
2:A:115:ALA:HB2	2:A:225:MET:O	2.21	0.41
2:A:304:GLN:NE2	2:A:323:MET:CG	2.83	0.41
1:B:158:HIS:CE1	1:B:217:LYS:HB3	2.56	0.41
1:B:284:LEU:HD23	2:A:382:LEU:HD23	2.02	0.41
2:A:222:LEU:HD22	2:A:228:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:348:PHE:HA	2:A:350:GLU:OE1	2.21	0.41
2:A:390:MET:HE2	2:A:390:MET:HB3	1.85	0.41
2:A:304:GLN:HE22	2:A:323:MET:CG	2.34	0.41
1:B:274:GLN:HG2	1:B:279:LYS:CB	2.47	0.40
1:B:298:ALA:C	1:B:300:THR:H	2.29	0.40
2:A:175:GLU:HG2	2:A:176:GLY:N	2.36	0.40
1:B:205:LEU:HD12	1:B:247:TYR:CE1	2.56	0.40
1:B:243:PRO:HB2	2:A:222:LEU:HD11	2.01	0.40
1:B:244:ILE:HD13	2:A:221:GLU:OE2	2.21	0.40
2:A:303:ALA:O	2:A:359:ARG:HB2	2.22	0.40
1:B:39:GLN:O	1:B:42:GLN:HG3	2.22	0.40
1:B:261:PHE:O	1:B:262:SER:C	2.65	0.40
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.91	0.40
2:A:116:GLU:CD	2:A:116:GLU:H	2.30	0.40
2:A:144:GLN:NE2	2:A:161:MET:HE3	2.37	0.40
2:A:280:VAL:O	2:A:284:LEU:HG	2.22	0.40
1:B:26:PHE:HD2	1:B:97:ALA:O	2.05	0.40
1:B:224:LEU:O	1:B:225:GLY:C	2.64	0.40
2:A:227:ASN:OD1	2:A:227:ASN:C	2.64	0.40
2:A:320:LYS:HB2	2:A:366:ILE:CD1	2.52	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)
2:A:391:LYS:CE	2:A:391:LYS:NZ[4_555]	1.53	0.67
2:A:391:LYS:CE	2:A:391:LYS:CE[4_555]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/350 (94%)	282 (86%)	43 (13%)	4 (1%)	10	37
2	A	263/416 (63%)	227 (86%)	32 (12%)	4 (2%)	8	32
All	All	592/766 (77%)	509 (86%)	75 (13%)	8 (1%)	9	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	VAL
1	B	94	ILE
2	A	267	SER
1	B	45	ARG
1	B	28	LYS
2	A	138	ASP
2	A	139	GLN
2	A	392	ARG

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	B	292/301 (97%)	287 (98%)	5 (2%)	53	74
2	A	228/339 (67%)	219 (96%)	9 (4%)	28	60
All	All	520/640 (81%)	506 (97%)	14 (3%)	39	67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	VAL
1	B	98	VAL
1	B	228	ILE
1	B	250	ILE
1	B	329	ASP
2	A	131	ILE
2	A	143	LEU
2	A	228	THR

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Mol	Chain	Res	Type
2	A	233	THR
2	A	234	ILE
2	A	268	PHE
2	A	272	LEU
2	A	313	ILE
2	A	374	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	77	GLN
2	A	119	ASN
2	A	144	GLN
2	A	160	GLN
2	A	163	GLN
2	A	188	ASN
2	A	300	GLN
2	A	377	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	B	338	1	8,9,10	1.71	1 (12%)	7,12,14	1.20	1 (14%)
2	SEP	A	112	3,2	8,9,10	1.83	3 (37%)	7,12,14	2.34	3 (42%)
1	TPO	B	197	1	8,10,11	1.10	0	10,14,16	2.98	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	B	139	1	8,9,10	1.74	3 (37%)	7,12,14	1.61	1 (14%)

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	B	338	1	-	2/6/8/10	-
2	SEP	A	112	3,2	-	0/6/8/10	-
1	TPO	B	197	1	-	1/9/11/13	-
1	SEP	B	139	1	-	3/6/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	112	SEP	P-O1P	3.93	1.62	1.50
1	B	139	SEP	P-O1P	3.63	1.61	1.50
1	B	338	SEP	P-O1P	3.59	1.61	1.50
2	A	112	SEP	P-O2P	2.08	1.62	1.54
1	B	139	SEP	P-O2P	2.04	1.62	1.54
2	A	112	SEP	P-O3P	2.03	1.62	1.54
1	B	139	SEP	P-O3P	2.01	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	TPO	P-OG1-CB	-8.84	99.31	123.33
2	A	112	SEP	OG-CB-CA	4.23	112.26	108.14
1	B	139	SEP	OG-CB-CA	3.79	111.83	108.14
2	A	112	SEP	O3P-P-OG	3.36	115.43	106.67
1	B	338	SEP	OG-P-O1P	2.46	113.10	106.44
2	A	112	SEP	O3P-P-O1P	-2.18	102.35	110.83
1	B	197	TPO	O2P-P-OG1	2.09	113.98	105.85

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	139	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	B	139	SEP	CB-OG-P-O1P
1	B	338	SEP	N-CA-CB-OG
1	B	338	SEP	CA-CB-OG-P
1	B	139	SEP	CB-OG-P-O2P
1	B	197	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	338	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
4	ADP	B	400	3	28,29,29	1.43	5 (17%)	43,45,45	1.76	9 (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
4	ADP	B	400	3	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	ADP	C5-C4	4.55	1.47	1.39
4	B	400	ADP	C5-N7	-2.61	1.34	1.39
4	B	400	ADP	PA-O3A	2.40	1.62	1.59
4	B	400	ADP	C5-C6	2.38	1.47	1.41
4	B	400	ADP	C8-N7	2.33	1.36	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	ADP	C5-C4-N3	-5.48	119.17	126.72
4	B	400	ADP	N3-C4-N9	4.28	134.45	127.17
4	B	400	ADP	C4-C5-N7	-3.35	106.75	110.58
4	B	400	ADP	C2-N3-C4	3.33	119.97	111.83
4	B	400	ADP	N3-C2-N1	-3.14	123.84	128.58
4	B	400	ADP	C2'-C1'-N9	-2.77	106.42	113.30
4	B	400	ADP	C5-N7-C8	2.45	107.29	103.45
4	B	400	ADP	C4-N9-C8	2.39	108.25	105.74
4	B	400	ADP	C2-N1-C6	2.26	122.44	118.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	400	ADP	PA-O3A-PB-O1B
4	B	400	ADP	PB-O3A-PA-O1A

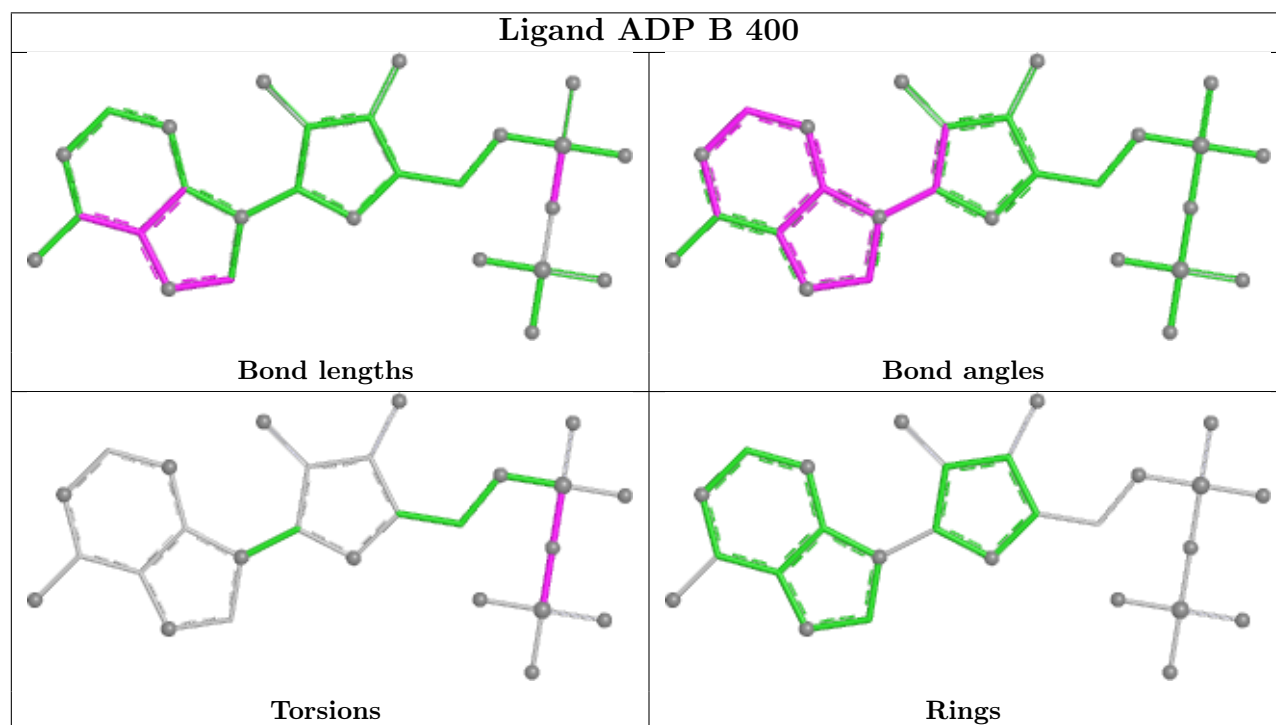
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	400	ADP	3	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

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	B	331/350 (94%)	-0.02	12 (3%)	46 26	30, 49, 80, 133	0
2	A	269/416 (64%)	0.17	10 (3%)	45 25	32, 57, 81, 107	0
All	All	600/766 (78%)	0.07	22 (3%)	45 25	30, 53, 82, 133	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	GLY	4.8
2	A	266	GLU	4.7
1	B	55	GLY	4.6
2	A	343	PHE	4.3
2	A	238	SER	3.3
2	A	264	MET	3.3
2	A	267	SER	3.2
1	B	18	PHE	3.0
1	B	41	ASP	2.9
2	A	265	TYR	2.9
2	A	137	ASP	2.7
1	B	17	GLU	2.6
1	B	56	ARG	2.4
1	B	54	PHE	2.4
2	A	345	GLY	2.3
1	B	58	MET	2.3
1	B	253	GLY	2.2
1	B	241	ASP	2.2
2	A	337	VAL	2.2
1	B	73	ILE	2.1
1	B	120	MET	2.1
2	A	344	ARG	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, 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	SEP	B	338	10/11	0.93	0.08	56,64,68,68	0
1	SEP	B	139	10/11	0.94	0.06	46,53,63,73	0
2	SEP	A	112	10/11	0.96	0.08	32,37,48,55	0
1	TPO	B	197	11/12	0.99	0.07	25,27,33,34	0

6.3 Carbohydrates [i](#)

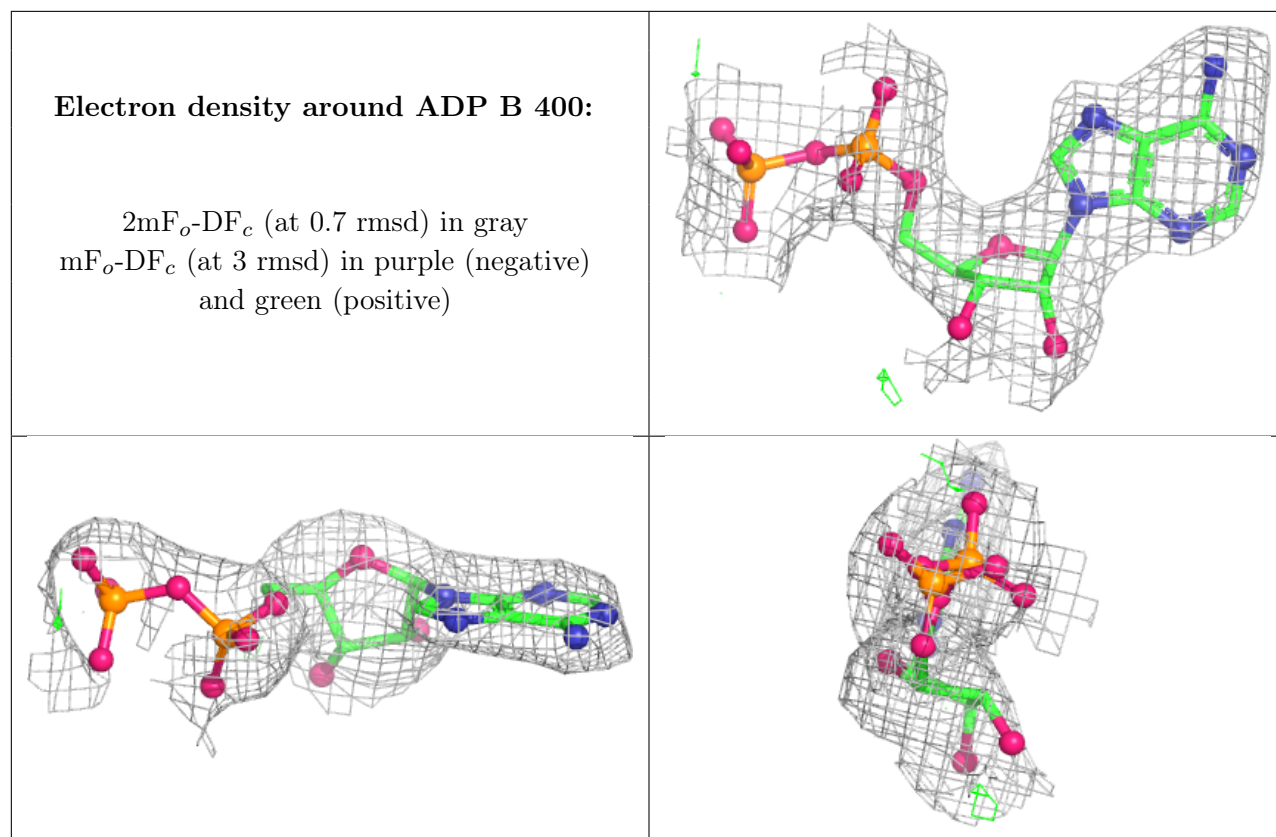
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	402	1/1	0.84	0.20	39,39,39,39	0
3	MG	B	401	1/1	0.95	0.12	30,30,30,30	0
4	ADP	B	400	27/27	0.97	0.08	33,44,48,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.