Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:30 AM EDT

PDB ID	:	3TNQ
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.; Taylor, S.S.
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:

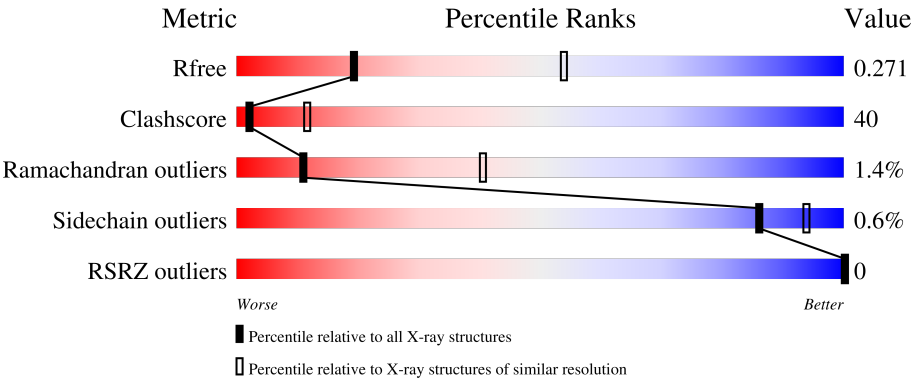
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	47% 46% • 5%
2	A	416	25% 38% • 35%

2 Entry composition (i)

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			

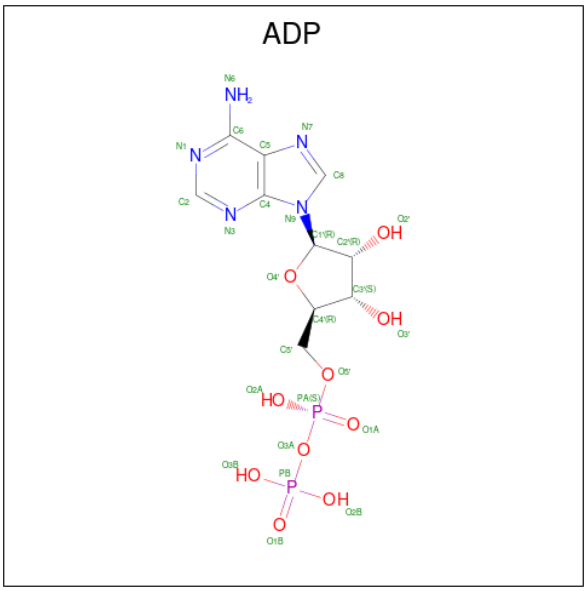
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	LYS	ARG	ENGINEERED MUTATION	UNP P31324

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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.

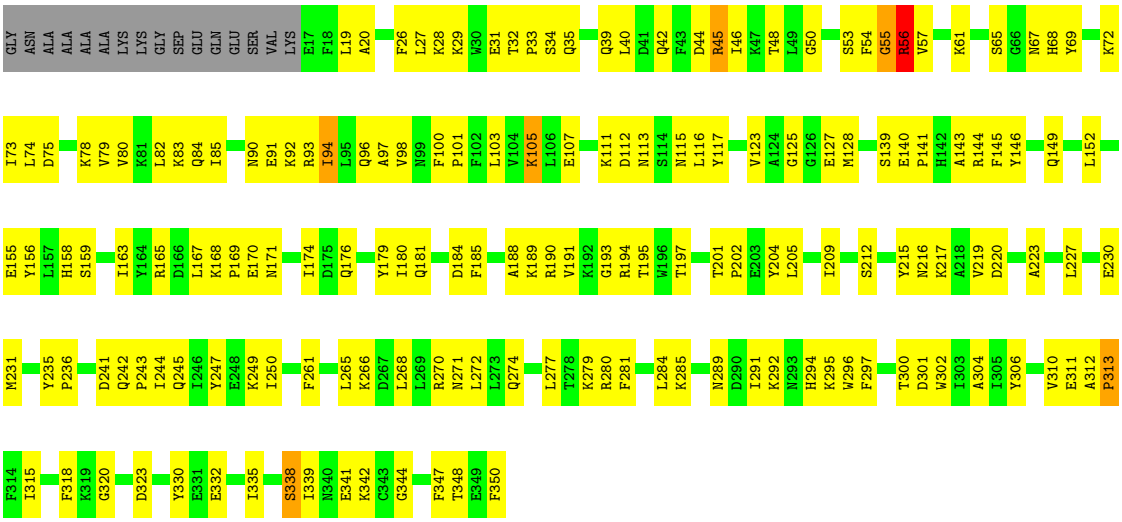
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total	O	0	0
			11	11		
5	A	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

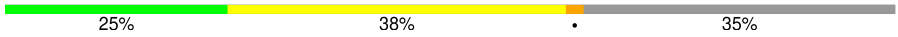
• Molecule 1: Protein kinase, cAMP-dependent, catalytic, alpha

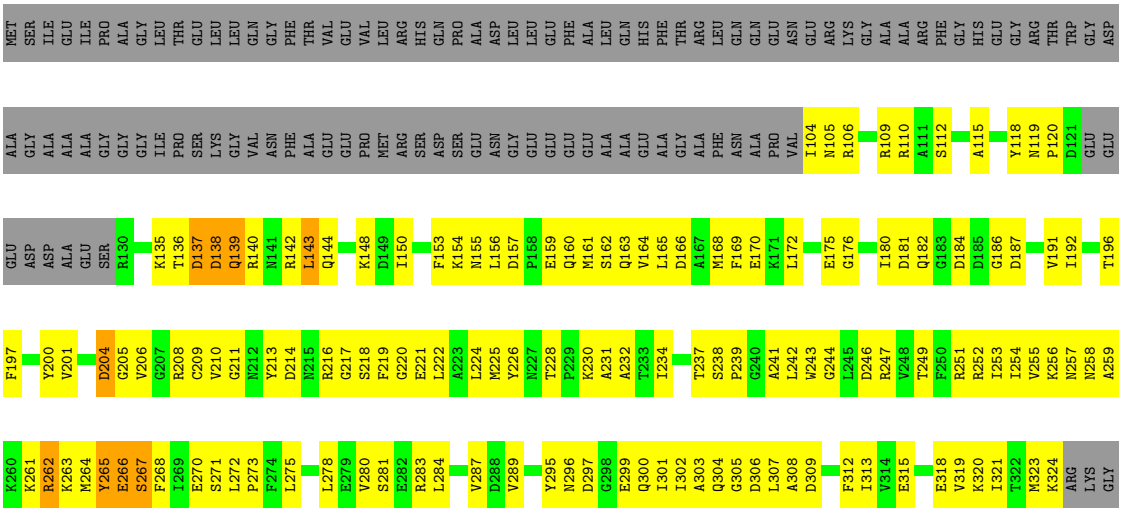
Chain B:

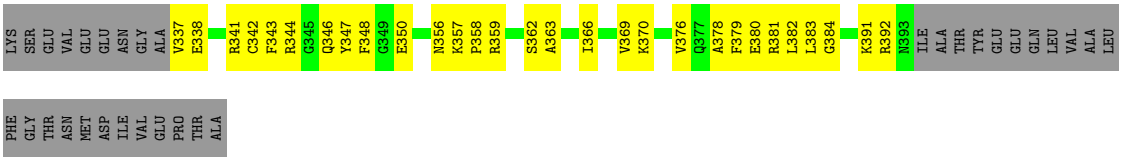


• Molecule 2: cAMP-dependent protein kinase type II-beta regulatory subunit

Chain A:






LYS SER GLU VAL GLU GLU ASN GLY ALA V337 E338 R341 C342 F343 R344 G345 Q346 Y347 F348 G349 E350 N356 K357 P358 R359 S362 A363 I366 V369 K370 V376 Q377 A378 F379 E380 R381 L382 L383 G384 K391 R392 N393 ILE ALA THR TYR GLU GLU GLN LEU VAL ALA LEU
PHE GLY THR ASN MET ASP ILE VAL GLU PRO THR ALA

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.14%)	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)	0.28 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ADP, MG

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	0.46	0/2802	0.70	6/3772 (0.2%)
2	A	0.47	0/2157	0.76	4/2897 (0.1%)
All	All	0.46	0/4959	0.73	10/6669 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	A	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	55	GLY	N-CA-C	-7.34	94.75	113.10
1	B	55	GLY	C-N-CA	6.39	137.67	121.70
2	A	266	GLU	N-CA-C	6.06	127.36	111.00
2	A	155	ASN	N-CA-C	5.77	126.59	111.00
1	B	313	PRO	C-N-CA	5.41	135.22	121.70
1	B	35	GLN	N-CA-C	5.34	125.43	111.00
2	A	137	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	105	LYS	CD-CE-NZ	-5.19	99.75	111.70
2	A	204	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	56	ARG	N-CA-C	5.05	124.65	111.00

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 (i)

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	181	0
2	A	2136	0	2138	220	2
3	B	2	0	0	0	0
4	B	27	0	12	5	0
5	A	2	0	0	0	0
5	B	11	0	0	10	0
All	All	4943	0	4890	393	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 40.

All (393) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CD	2.21	0.94
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:324:LYS:HZ2	2:A:337:VAL:N	1.70	0.90
2:A:238:SER:HB2	2:A:239:PRO:CD	2.02	0.90
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:56:ARG:NH2	1:B:335:ILE:HA	2.01	0.73
1:B:34:SER:H	1:B:96:GLN:CD	1.91	0.73
2:A:320:LYS:HE3	2:A:338:GLU:OE1	1.88	0.73
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
2:A:159:GLU:N	2:A:159:GLU:OE2	2.23	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
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
2:A:104:ILE:CG2	2:A:105:ASN:N	2.53	0.71
1:B:318:PHE:CE1	1:B:323:ASP:HB3	2.25	0.71
1:B:31:GLU:CG	5:B:360:HOH:O	2.39	0.71
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
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:128:MET:HE1	1:B:227:LEU:HD11	1.73	0.70
2:A:241:ALA:C	2:A:242:LEU:HD12	2.12	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:104:ILE:HG22	2:A:105:ASN:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLY:O	1:B:56:ARG:HA	1.94	0.68
1:B:105:LYS:HZ1	1:B:107:GLU:CD	1.95	0.68
1:B:19:LEU:C	1:B:19:LEU:HD23	2.15	0.68
2:A:187:ASP:CG	2:A:247:ARG:NH2	2.48	0.67
2:A:257:ASN:OD1	2:A:261:LYS:CD	2.42	0.67
2:A:263:LYS:HD3	2:A:266:GLU:CD	2.14	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:320:LYS:HD2	2:A:366:ILE:HD11	1.77	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:32:THR:OG1	5:B:360:HOH:O	2.13	0.65
1:B:193:GLY:O	1:B:194:ARG:HG2	1.95	0.65
1:B:33:PRO:C	1:B:96:GLN:HE22	1.99	0.65
2:A:263:LYS:HD3	2:A:266:GLU:OE2	1.97	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:187:ASP:CG	2:A:247:ARG:HH22	2.03	0.62
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
2:A:197:PHE:HZ	2:A:242:LEU:HD11	1.63	0.62
2:A:264:MET:C	2:A:266:GLU:H	2.02	0.62
2:A:266:GLU:C	2:A:268:PHE:N	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:320:LYS:HE3	2:A:338:GLU:CD	2.21	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
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
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
1:B:105:LYS:HZ2	1:B:107:GLU:CD	2.05	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
2:A:175:GLU:HG3	2:A:237:THR:C	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:ASP:O	2:A:139:GLN:C	2.45	0.55
2:A:295:TYR:HB2	2:A:369:VAL:HG22	1.88	0.55
2:A:268:PHE:N	2:A:268:PHE:HD2	2.04	0.55
2:A:118:TYR:OH	2:A:256:LYS:HG3	2.07	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:34:SER:N	1:B:96:GLN:CD	2.57	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
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
2:A:238:SER:CB	2:A:239:PRO:CD	2.67	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
2:A:315:GLU:CD	2:A:370:LYS:HE3	2.30	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:302:ILE:HG13	2:A:363:ALA:HB3	1.93	0.51
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:65:SER:C	1:B:67:ASN:H	2.13	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
1:B:318:PHE:CZ	1:B:320:GLY:C	2.85	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
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: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
2:A:143:LEU:HD11	2:A:243:TRP:CG	2.48	0.48
2:A:264:MET:C	2:A:266:GLU:N	2.65	0.48
2:A:210:VAL:CG1	2:A:211:GLY:N	2.75	0.48
2:A:216:ARG:HG2	2:A:217:GLY:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:148:LYS:O	2:A:154:LYS:HA	2.13	0.48
2:A:172:LEU:C	2:A:172:LEU:HD12	2.34	0.48
2:A:144:GLN:HE22	2:A:161:MET:HG2	1.78	0.47
1:B:339:ILE:C	5:B:357:HOH:O	2.52	0.47
2:A:175:GLU:HG3	2:A:238:SER:HA	1.95	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:306:TYR:CD1	1:B:306:TYR:C	2.88	0.47
1:B:32:THR:CB	5:B:360:HOH:O	2.57	0.47
1:B:289:ASN:C	1:B:291:ILE:N	2.65	0.47
2:A:266:GLU:C	2:A:268:PHE:H	2.17	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
1:B:146:TYR:CD2	1:B:180:ILE:HD11	2.51	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
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:128:MET:HE2	1:B:169:PRO:HA	1.96	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
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
4:B:400:ADP:HO3'	4:B:400:ADP:HO2'	1.48	0.45
2:A:159:GLU:CD	2:A:159:GLU:H	2.19	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:262:ARG:CA	2:A:265:TYR:CD2	2.91	0.45
2:A:356:ASN:O	2:A:357:LYS:C	2.55	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: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
2:A:144:GLN:O	2:A:148:LYS:HG3	2.18	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
1:B:19:LEU:C	1:B:19:LEU:CD2	2.83	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:127:GLU:OE2	4:B:400:ADP:O3'	2.35	0.44
1:B:341:GLU:O	1:B:342:LYS:HD3	2.17	0.44
1:B:54:PHE:HB3	1:B:78:LYS:HG2	1.98	0.44
1:B:90:ASN:O	1:B:91:GLU:C	2.56	0.44
1:B:143:ALA:O	1:B:231:MET:HE3	2.18	0.44
2:A:136:THR:O	2:A:137:ASP:C	2.56	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
1:B:92:LYS:NZ	1:B:350:PHE:O	2.49	0.43
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:193:GLY:C	1:B:194:ARG:HG2	2.38	0.43
2:A:303:ALA:O	2:A:359:ARG:CB	2.67	0.43
2:A:303:ALA:HB3	2:A:306:ASP:CG	2.39	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
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:204:TYR:OH	1:B:230:GLU:OE2	2.24	0.43
1:B:201:THR:O	1:B:202:PRO:C	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:105:ASN:OD1	2:A:105:ASN:C	2.59	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:263:LYS:CD	2:A:266:GLU:CD	2.84	0.41
2:A:278:LEU:HD21	2:A:383:LEU:HD13	2.03	0.41
2:A:379:PHE:CD2	2:A:379:PHE:C	2.94	0.41
1:B:112:ASP:C	1:B:112:ASP:OD1	2.59	0.41
1:B:168:LYS:HE2	1:B:170:GLU:HB2	2.02	0.41
2:A:312:PHE:O	2:A:347:TYR:HA	2.21	0.41
1:B:82:LEU:O	1:B:83:LYS:C	2.58	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
2:A:296:ASN:O	2:A:297:ASP:C	2.58	0.41
2:A:348:PHE:HA	2:A:350:GLU:OE1	2.21	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:ARG:O	1:B:94:ILE:C	2.59	0.40
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.91	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:268:LEU:HD12	1:B:268:LEU:C	2.39	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 (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	B	329/350 (94%)	282 (86%)	43 (13%)	4 (1%)	13	44
2	A	263/416 (63%)	227 (86%)	32 (12%)	4 (2%)	10	39
All	All	592/766 (77%)	509 (86%)	75 (13%)	8 (1%)	11	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	VAL
1	B	94	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	292/301 (97%)	291 (100%)	1 (0%)	92 96
2	A	228/339 (67%)	226 (99%)	2 (1%)	78 91
All	All	520/640 (81%)	517 (99%)	3 (1%)	86 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	250	ILE
2	A	143	LEU
2	A	262	ARG

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

Mol	Chain	Res	Type
1	B	42	GLN
1	B	77	GLN
2	A	144	GLN
2	A	160	GLN
2	A	300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	TPO	B	197	1	8,10,11	1.10	0	10,14,16	2.98	2 (20%)
2	SEP	A	112	3,2	8,9,10	1.83	3 (37%)	7,12,14	2.34	3 (42%)
1	SEP	B	139	1	8,9,10	1.74	3 (37%)	7,12,14	1.61	1 (14%)
1	SEP	B	338	1	8,9,10	1.71	1 (12%)	7,12,14	1.20	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	TPO	B	197	1	-	1/9/11/13	-
2	SEP	A	112	3,2	-	0/6/8/10	-
1	SEP	B	139	1	-	3/6/8/10	-
1	SEP	B	338	1	-	2/6/8/10	-

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(^{o})	Ideal(^{o})
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
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 monosaccharides 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	24,29,29	0.94	2 (8%)	29,45,45	1.17	2 (6%)

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	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	ADP	PA-O3A	2.40	1.62	1.59
4	B	400	ADP	O4'-C1'	2.02	1.43	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	400	ADP	N3-C2-N1	-3.56	123.84	128.67
4	B	400	ADP	C4-C5-N7	-2.45	106.75	109.34

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.

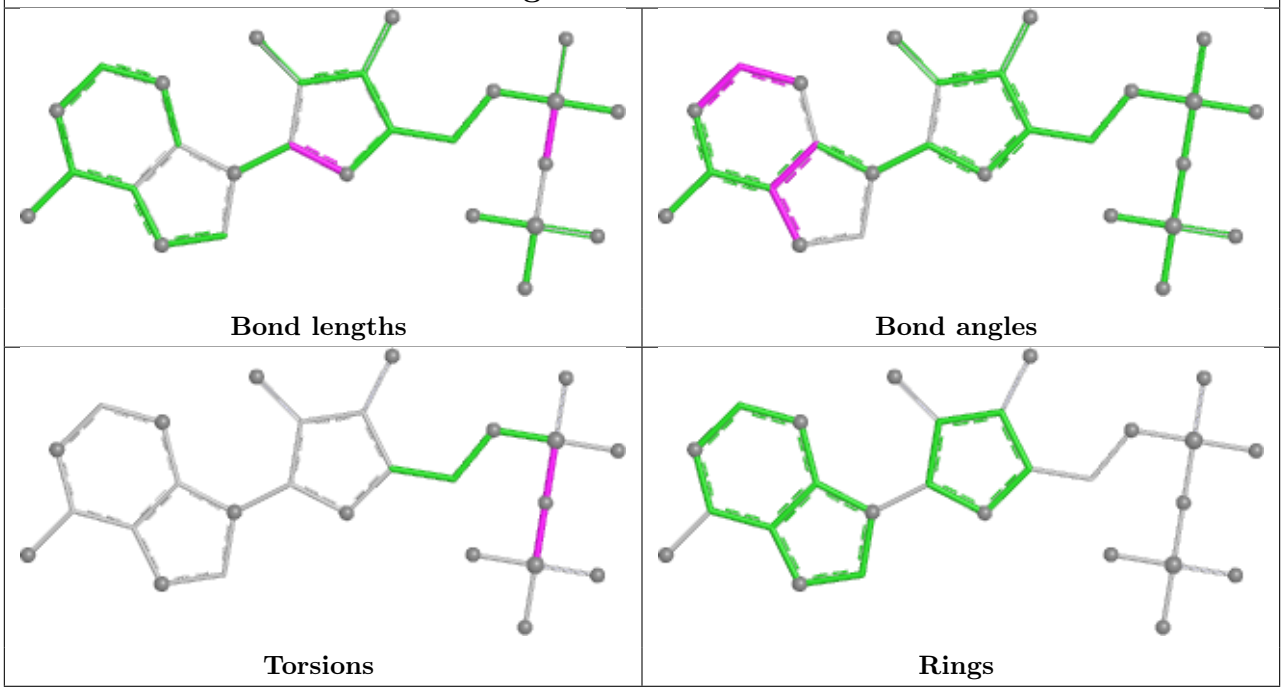
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	400	ADP	5	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 then 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.

Ligand ADP B 400



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, 95^{th} 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%)	-0.50	0	100	100	30, 49, 80, 133	0
2	A	269/416 (64%)	-0.44	0	100	100	32, 57, 81, 107	0
All	All	600/766 (78%)	-0.47	0	100	100	30, 53, 82, 133	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.95	0.11	56,64,68,68	0
1	SEP	B	139	10/11	0.96	0.08	46,53,63,73	0
2	SEP	A	112	10/11	0.96	0.23	32,37,48,55	0
1	TPO	B	197	11/12	0.99	0.18	25,27,33,34	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

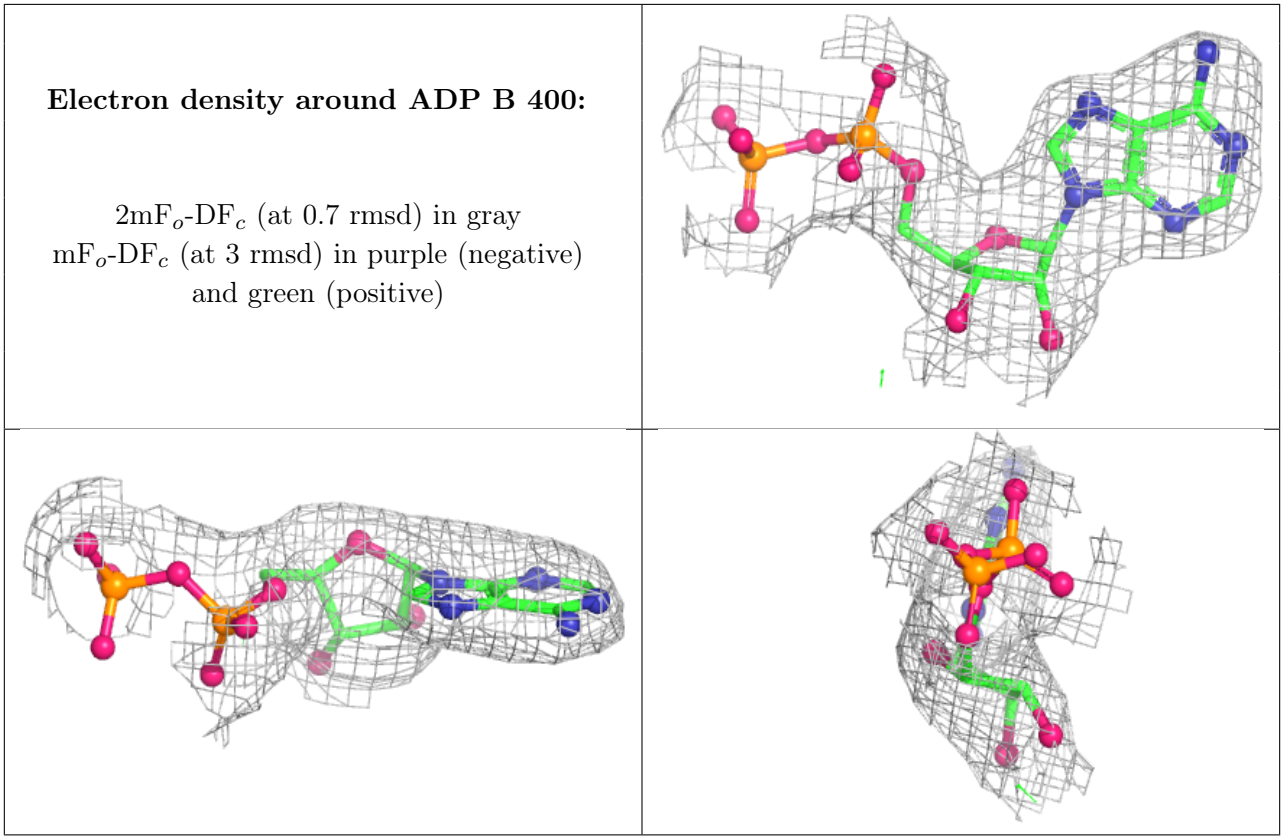
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.92	0.36	39,39,39,39	0
3	MG	B	401	1/1	0.95	0.44	30,30,30,30	0
4	ADP	B	400	27/27	0.95	0.21	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.

Electron density around ADP B 400:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.