Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:48 PM GMT

PDB ID	:	4DIN
Title	:	Novel Localization and Quaternary Structure of the PKA RI beta Holoenzyme
Authors	:	Ilouz, R.; Bubis, J.; Wu, J.; Yim, Y.Y.; Deal, M.S.; Kornev, A.P.; Ma, Y.; Blumenthal, D.K.; Taylor, S.S.
Deposited on	:	2012-01-31
Resolution	:	3.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

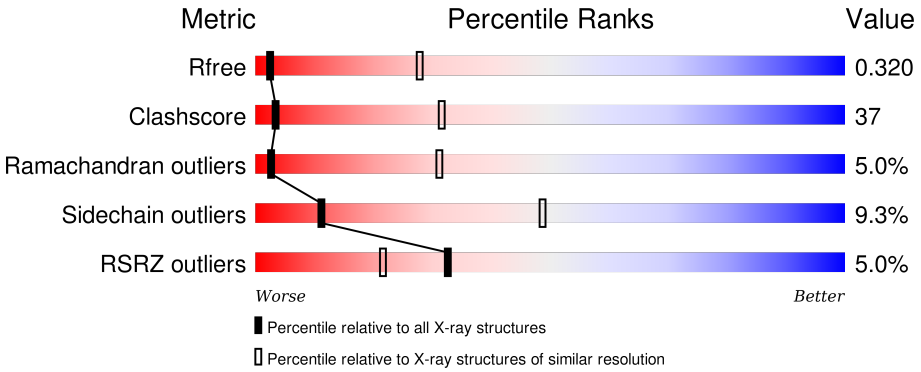
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

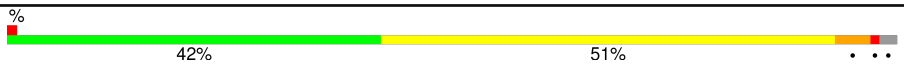
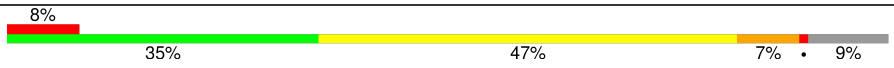
The reported resolution of this entry is 3.70 Å.

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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	350	
2	B	381	

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	TPO	A	197	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5426 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.

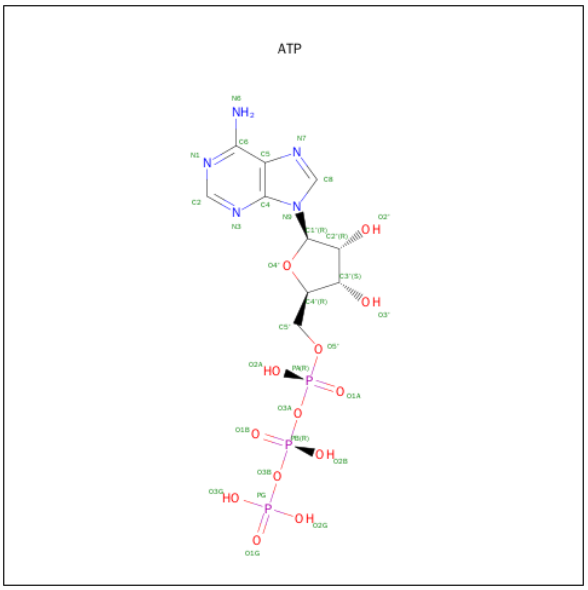
- Molecule 1 is a protein called cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	P	S	0	0	0
			2747	1778	458	501	2	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	345	Total	C	N	O	S	0	0	0
			2646	1674	462	503	7			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

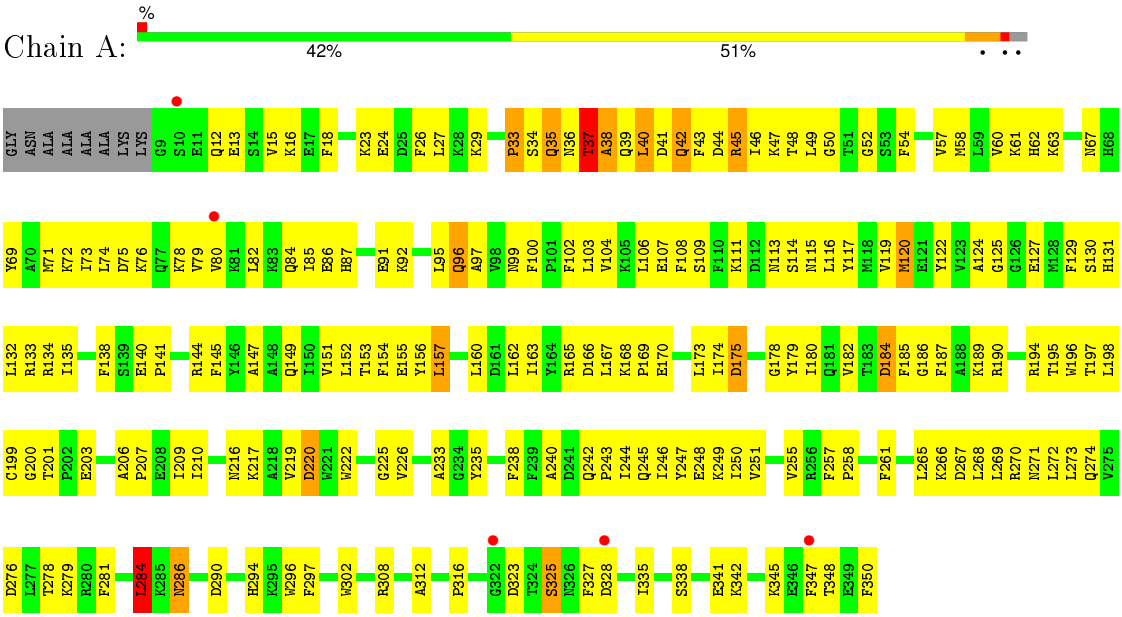
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

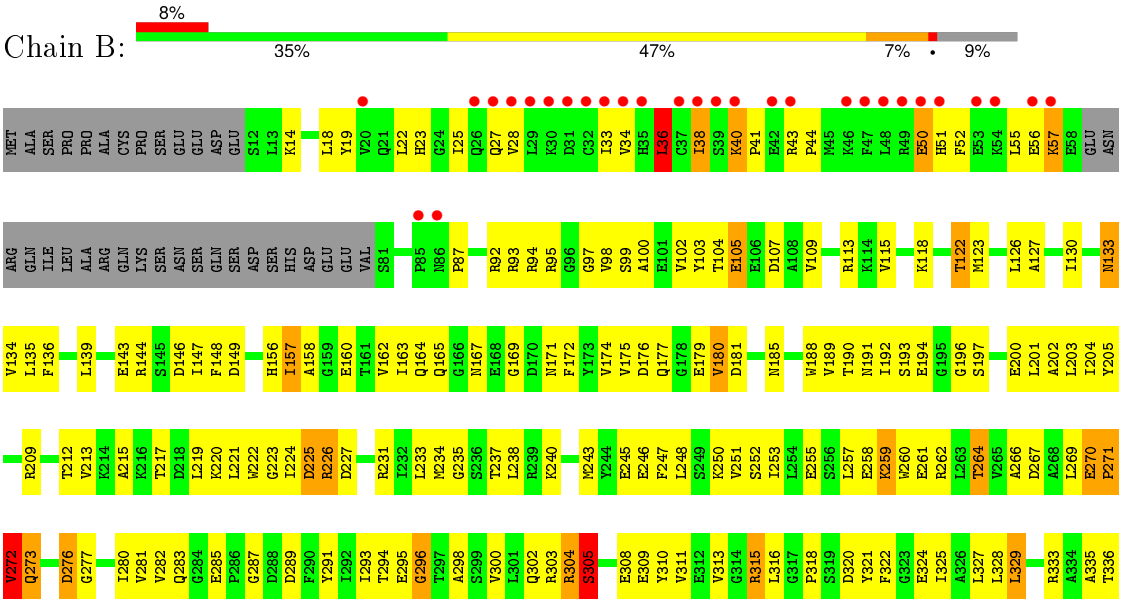
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain A:



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

Chain B:




V337
V338
A339
R340
G341
P342
L343
K344
C345
V346
K347
L348
D349
R350
P351
R352
F353
E354
R355
V356
L357
G358
P359
C360
S361
E362
I363
L364
K365
R366
N367
I368
Q369
R370
Y371
N372
S373
F374
I375
S376
L377
T378
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	172.19Å 172.19Å 146.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.70 49.71 – 3.49	Depositor EDS
% Data completeness (in resolution range)	67.7 (50.00-3.70) 80.6 (49.71-3.49)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.48Å)	Xtriage
Refinement program	CNS 1.3 with DEN refinement	Depositor
R, R_{free}	0.211 , 0.293 0.266 , 0.320	Depositor DCC
R_{free} test set	688 reflections (5.96%)	DCC
Wilson B-factor (Å^2)	89.5	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 169.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 16172 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5426	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, ATP, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/2793	0.48	1/3775 (0.0%)
2	B	0.24	0/2694	0.52	4/3652 (0.1%)
All	All	0.26	0/5487	0.50	5/7427 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	272	VAL	CB-CA-C	7.46	125.57	111.40
2	B	305	SER	CB-CA-C	6.83	123.07	110.10
2	B	273	GLN	N-CA-CB	6.56	122.40	110.60
2	B	44	PRO	N-CA-CB	5.58	109.99	103.30
1	A	37	THR	CB-CA-C	-5.17	97.65	111.60

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	2747	0	2654	193	0
2	B	2646	0	2542	214	0
3	A	31	0	12	2	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5426	0	5208	390	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 37.

All (390) 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)
2:B:272:VAL:O	2:B:273:GLN:HG3	1.57	1.05
1:A:75:ASP:HA	1:A:115:ASN:HB3	1.46	0.97
2:B:298:ALA:HB2	2:B:343:LEU:HD21	1.50	0.93
1:A:284:LEU:H	1:A:284:LEU:HD22	1.34	0.93
1:A:134:ARG:HG2	2:B:92:ARG:HH12	1.31	0.92
2:B:280:ILE:HD13	2:B:337:VAL:HG12	1.54	0.90
2:B:304:ARG:HD3	2:B:304:ARG:H	1.36	0.89
1:A:335:ILE:HD12	1:A:335:ILE:H	1.38	0.86
1:A:35:GLN:HG2	1:A:36:ASN:H	1.40	0.85
2:B:368:ILE:HD12	2:B:368:ILE:H	1.42	0.82
2:B:113:ARG:HD2	2:B:146:ASP:HB3	1.61	0.81
1:A:240:ALA:HB2	1:A:249:LYS:HE3	1.64	0.80
1:A:45:ARG:HA	1:A:60:VAL:HG12	1.65	0.79
2:B:201:LEU:HD12	2:B:204:ILE:HD11	1.65	0.79
2:B:130:ILE:HD13	2:B:136:PHE:HB3	1.63	0.79
2:B:180:VAL:HG12	2:B:215:ALA:HA	1.65	0.78
2:B:237:THR:HA	2:B:240:LYS:HE3	1.66	0.77
2:B:352:ARG:HA	2:B:355:ARG:NH1	2.01	0.75
2:B:172:PHE:HB2	2:B:203:LEU:HG	1.69	0.74
2:B:203:LEU:HD21	2:B:224:ILE:HG23	1.68	0.74
1:A:209:ILE:HD11	1:A:219:VAL:HB	1.69	0.74
1:A:147:ALA:O	1:A:151:VAL:HG23	1.86	0.74
2:B:304:ARG:O	2:B:308:GLU:HB2	1.88	0.73
1:A:80:VAL:HA	1:A:85:ILE:HD11	1.71	0.73
2:B:258:GLU:OE1	2:B:260:TRP:HB2	1.88	0.73
1:A:125:GLY:HA3	1:A:174:ILE:O	1.89	0.72
2:B:294:THR:HG23	2:B:345:CYS:HA	1.70	0.72
1:A:71:MET:HA	1:A:119:VAL:HA	1.70	0.72
1:A:242:GLN:HB2	1:A:245:GLN:HG3	1.72	0.71
1:A:247:TYR:O	1:A:251:VAL:HG23	1.90	0.69
2:B:259:LYS:HA	2:B:262:ARG:NH2	2.07	0.69
2:B:167:ASN:O	2:B:209:ARG:HG2	1.93	0.69
2:B:115:VAL:HA	2:B:149:ASP:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:ALA:HB1	2:B:343:LEU:HD13	1.76	0.68
1:A:206:ALA:H	1:A:209:ILE:HD12	1.57	0.68
2:B:362:GLU:HA	2:B:365:LYS:HB2	1.76	0.68
2:B:258:GLU:HB3	2:B:261:GLU:HG3	1.77	0.67
2:B:271:PRO:O	2:B:345:CYS:O	2.13	0.67
2:B:257:LEU:HD12	2:B:261:GLU:HB3	1.76	0.67
2:B:354:GLU:HG2	2:B:359:PRO:HA	1.75	0.67
1:A:210:ILE:HG21	1:A:247:TYR:HB3	1.78	0.66
2:B:255:GLU:HB2	2:B:370:ARG:NE	2.11	0.66
2:B:221:LEU:HD23	2:B:221:LEU:H	1.60	0.66
2:B:253:ILE:HG12	2:B:253:ILE:O	1.95	0.66
1:A:24:GLU:HA	1:A:27:LEU:HD22	1.77	0.64
2:B:40:LYS:H	2:B:41:PRO:HD2	1.63	0.64
2:B:172:PHE:CZ	2:B:197:SER:HB2	2.32	0.64
1:A:78:LYS:O	1:A:82:LEU:HG	1.96	0.64
2:B:181:ASP:HB3	2:B:188:TRP:HE1	1.62	0.64
2:B:277:GLY:O	2:B:338:VAL:HG23	1.98	0.64
2:B:233:LEU:O	2:B:237:THR:HG23	1.99	0.63
1:A:54:PHE:CE2	1:A:84:GLN:HG3	2.34	0.63
1:A:48:THR:HA	1:A:58:MET:HG2	1.81	0.62
2:B:135:LEU:HD12	2:B:200:GLU:HG2	1.81	0.62
2:B:113:ARG:NH1	2:B:146:ASP:HA	2.14	0.62
1:A:79:VAL:HG12	1:A:85:ILE:HD13	1.82	0.62
1:A:274:GLN:HE21	1:A:274:GLN:HA	1.64	0.62
2:B:234:MET:O	2:B:238:LEU:HG	1.99	0.62
1:A:240:ALA:HB3	1:A:246:ILE:HG13	1.82	0.62
1:A:335:ILE:H	1:A:335:ILE:CD1	2.11	0.61
1:A:57:VAL:HG22	1:A:72:LYS:HB2	1.80	0.61
2:B:205:TYR:HA	2:B:226:ARG:HD3	1.81	0.61
2:B:252:SER:HB2	2:B:374:PHE:HZ	1.64	0.61
1:A:73:ILE:N	1:A:73:ILE:HD12	2.15	0.61
1:A:111:LYS:NZ	1:A:348:THR:HA	2.16	0.61
1:A:165:ARG:NH1	1:A:195:THR:HG21	2.15	0.61
2:B:245:GLU:HA	2:B:248:LEU:HD12	1.82	0.61
1:A:45:ARG:HB2	1:A:45:ARG:HH11	1.65	0.60
1:A:23:LYS:O	1:A:27:LEU:HD13	2.01	0.60
1:A:281:PHE:HA	1:A:284:LEU:HD21	1.84	0.60
1:A:87:HIS:CE1	1:A:197:TPO:HG21	2.37	0.60
1:A:76:LYS:HG3	1:A:115:ASN:HA	1.83	0.60
2:B:368:ILE:CD1	2:B:368:ILE:H	2.13	0.60
2:B:348:LEU:CD2	2:B:352:ARG:HD3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HA	2:B:107:ASP:OD1	2.02	0.59
2:B:356:VAL:O	2:B:357:LEU:HD22	2.02	0.59
1:A:37:THR:O	1:A:38:ALA:HB2	2.03	0.59
1:A:107:GLU:H	1:A:120:MET:HA	1.68	0.59
1:A:39:GLN:HE21	1:A:41:ASP:HB2	1.68	0.59
2:B:253:ILE:HG21	2:B:324:GLU:HB3	1.85	0.59
2:B:310:TYR:HE1	2:B:336:THR:HG1	1.51	0.59
2:B:293:ILE:HD13	2:B:316:LEU:O	2.03	0.58
2:B:227:ASP:O	2:B:231:ARG:HG2	2.03	0.58
1:A:69:TYR:CD2	1:A:107:GLU:HG3	2.38	0.58
1:A:45:ARG:CZ	1:A:335:ILE:HD13	2.33	0.58
1:A:78:LYS:HG2	1:A:82:LEU:HD11	1.86	0.58
2:B:348:LEU:HD21	2:B:352:ARG:HD3	1.84	0.58
1:A:248:GLU:HG2	2:B:134:VAL:HB	1.84	0.58
2:B:258:GLU:HG2	2:B:259:LYS:N	2.18	0.58
2:B:257:LEU:HB3	2:B:262:ARG:HG3	1.86	0.58
2:B:103:TYR:HD2	2:B:107:ASP:HB3	1.69	0.58
1:A:170:GLU:OE2	2:B:95:ARG:HB2	2.04	0.57
1:A:335:ILE:HD12	1:A:335:ILE:N	2.16	0.57
1:A:200:GLY:O	2:B:97:GLY:HA3	2.04	0.57
1:A:216:ASN:O	1:A:219:VAL:HG22	2.05	0.56
2:B:164:GLN:HA	2:B:212:THR:HG23	1.87	0.56
2:B:98:VAL:HG12	2:B:99:SER:N	2.20	0.56
1:A:189:LYS:HE3	1:A:197:TPO:O3P	2.05	0.56
1:A:47:LYS:HD2	1:A:48:THR:N	2.21	0.56
1:A:58:MET:SD	1:A:335:ILE:HD11	2.46	0.56
2:B:352:ARG:HG3	2:B:355:ARG:NH2	2.21	0.56
2:B:174:VAL:O	2:B:221:LEU:HB2	2.06	0.56
1:A:52:GLY:HA3	3:A:400:ATP:PB	2.46	0.56
1:A:243:PRO:HB2	2:B:201:LEU:HD22	1.87	0.56
2:B:339:ALA:HB2	2:B:343:LEU:HD22	1.87	0.56
2:B:189:VAL:HG13	2:B:190:THR:N	2.21	0.56
1:A:135:ILE:HD11	1:A:138:PHE:HE1	1.71	0.56
2:B:98:VAL:HG12	2:B:99:SER:H	1.70	0.55
1:A:135:ILE:HD11	1:A:138:PHE:CE1	2.41	0.55
1:A:86:GLU:CD	1:A:86:GLU:H	2.09	0.55
2:B:295:GLU:HB2	2:B:344:LYS:HB2	1.88	0.55
2:B:158:ALA:HB2	2:B:217:THR:HA	1.89	0.55
1:A:26:PHE:HD2	1:A:27:LEU:HD12	1.70	0.55
2:B:181:ASP:HB3	2:B:188:TRP:NE1	2.21	0.55
1:A:36:ASN:CG	1:A:37:THR:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HB3	1:A:186:GLY:O	2.07	0.55
2:B:162:VAL:HG12	2:B:163:ILE:HG23	1.89	0.55
1:A:33:PRO:HA	1:A:96:GLN:NE2	2.22	0.55
2:B:165:GLN:HE22	2:B:185:ASN:H	1.55	0.55
1:A:35:GLN:HG2	1:A:36:ASN:N	2.18	0.55
2:B:368:ILE:HD12	2:B:368:ILE:N	2.18	0.54
2:B:264:THR:HB	2:B:357:LEU:HD21	1.88	0.54
1:A:131:HIS:O	1:A:135:ILE:HG12	2.08	0.54
1:A:40:LEU:O	1:A:40:LEU:HD12	2.08	0.54
2:B:370:ARG:HG2	2:B:374:PHE:HE1	1.70	0.54
1:A:104:VAL:HG22	1:A:182:VAL:O	2.07	0.54
2:B:367:ASN:C	2:B:367:ASN:HD22	2.11	0.54
1:A:278:THR:HG21	2:B:352:ARG:NE	2.23	0.54
2:B:258:GLU:HG2	2:B:259:LYS:H	1.73	0.53
2:B:252:SER:HA	2:B:255:GLU:HG3	1.89	0.53
2:B:352:ARG:HA	2:B:355:ARG:CZ	2.37	0.53
2:B:118:LYS:NZ	2:B:118:LYS:HB2	2.24	0.53
1:A:258:PRO:HD2	1:A:261:PHE:CD1	2.43	0.53
2:B:180:VAL:HG23	2:B:192:ILE:HG22	1.91	0.53
1:A:45:ARG:HH21	1:A:335:ILE:HB	1.73	0.53
1:A:82:LEU:O	1:A:84:GLN:HG2	2.08	0.53
2:B:353:PHE:O	2:B:356:VAL:HG12	2.08	0.52
2:B:169:GLY:HA2	2:B:209:ARG:CZ	2.39	0.52
1:A:163:ILE:HG12	1:A:165:ARG:CG	2.38	0.52
1:A:169:PRO:HD2	2:B:95:ARG:NH2	2.23	0.52
1:A:265:LEU:O	1:A:268:LEU:HB3	2.09	0.52
2:B:273:GLN:HG2	2:B:344:LYS:HG2	1.90	0.52
2:B:304:ARG:HD3	2:B:304:ARG:N	2.16	0.52
2:B:348:LEU:HD13	2:B:349:ASP:N	2.25	0.52
2:B:176:ASP:HB3	2:B:220:LYS:O	2.09	0.52
1:A:197:TPO:CG2	2:B:102:VAL:HG22	2.40	0.52
2:B:255:GLU:HB2	2:B:370:ARG:CZ	2.40	0.52
2:B:221:LEU:HD23	2:B:221:LEU:N	2.24	0.52
1:A:175:ASP:O	1:A:316:PRO:HG3	2.09	0.52
1:A:54:PHE:HE2	1:A:84:GLN:HG3	1.75	0.52
2:B:248:LEU:HD11	2:B:266:ALA:HB2	1.92	0.52
2:B:174:VAL:HG12	2:B:197:SER:HB3	1.91	0.51
2:B:258:GLU:H	2:B:261:GLU:HB2	1.75	0.51
1:A:26:PHE:CD2	1:A:160:LEU:HD22	2.46	0.51
2:B:189:VAL:HG13	2:B:190:THR:HG22	1.91	0.51
1:A:71:MET:CE	1:A:117:TYR:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:CD	2:B:94:ARG:HH12	2.14	0.51
1:A:268:LEU:HB2	1:A:294:HIS:CE1	2.46	0.51
2:B:36:LEU:HD12	2:B:38:ILE:CB	2.40	0.51
1:A:165:ARG:HH11	1:A:195:THR:HG21	1.75	0.51
1:A:197:TPO:HG21	2:B:102:VAL:HG22	1.91	0.51
1:A:284:LEU:HD23	1:A:290:ASP:OD2	2.11	0.51
2:B:315:ARG:O	2:B:316:LEU:HD23	2.11	0.51
1:A:149:GLN:HE22	1:A:180:ILE:H	1.59	0.51
2:B:246:GLU:O	2:B:250:LYS:HG2	2.10	0.51
2:B:270:GLU:HG2	2:B:347:LYS:O	2.11	0.51
1:A:92:LYS:O	1:A:96:GLN:HG3	2.10	0.51
1:A:133:ARG:HD2	2:B:92:ARG:HB2	1.93	0.50
2:B:365:LYS:C	2:B:367:ASN:H	2.14	0.50
1:A:274:GLN:OE1	1:A:276:ASP:HB3	2.11	0.50
2:B:225:ASP:OD1	2:B:227:ASP:HB3	2.12	0.50
2:B:165:GLN:NE2	2:B:185:ASN:H	2.10	0.50
2:B:276:ASP:HB2	2:B:341:GLY:HA2	1.93	0.50
2:B:304:ARG:O	2:B:308:GLU:CB	2.59	0.50
2:B:350:ARG:HB3	2:B:351:PRO:HD3	1.94	0.50
1:A:274:GLN:NE2	1:A:274:GLN:HA	2.26	0.50
2:B:259:LYS:HG2	2:B:260:TRP:N	2.25	0.50
2:B:291:TYR:CD1	2:B:347:LYS:HB3	2.46	0.50
1:A:153:THR:O	1:A:156:TYR:HB3	2.12	0.50
2:B:205:TYR:CA	2:B:226:ARG:HD3	2.42	0.50
2:B:291:TYR:HB2	2:B:322:PHE:CZ	2.47	0.49
1:A:37:THR:O	1:A:38:ALA:CB	2.58	0.49
1:A:145:PHE:CE1	1:A:312:ALA:HA	2.47	0.49
2:B:157:ILE:O	2:B:160:GLU:HB2	2.12	0.49
1:A:100:PHE:HB3	1:A:103:LEU:HG	1.94	0.49
1:A:71:MET:CA	1:A:119:VAL:HA	2.42	0.49
1:A:113:ASN:HD22	1:A:341:GLU:N	2.10	0.49
1:A:36:ASN:O	1:A:109:SER:O	2.30	0.49
1:A:69:TYR:CE2	1:A:107:GLU:HG3	2.48	0.49
2:B:175:VAL:HA	2:B:221:LEU:HB3	1.93	0.49
1:A:206:ALA:O	1:A:210:ILE:HG13	2.12	0.49
1:A:174:ILE:HG22	1:A:178:GLY:HA2	1.94	0.49
2:B:50:GLU:HG2	2:B:51:HIS:H	1.75	0.49
2:B:280:ILE:HD12	2:B:280:ILE:N	2.27	0.49
1:A:26:PHE:CD2	1:A:27:LEU:HD12	2.48	0.49
2:B:235:GLY:HA2	2:B:238:LEU:HD12	1.93	0.49
1:A:174:ILE:HA	1:A:179:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LYS:O	1:A:348:THR:HG22	2.12	0.49
1:A:36:ASN:CG	1:A:37:THR:N	2.67	0.49
1:A:36:ASN:O	1:A:37:THR:CB	2.61	0.49
1:A:43:PHE:CD1	1:A:62:HIS:HA	2.47	0.49
1:A:269:LEU:O	1:A:273:LEU:HB2	2.13	0.49
2:B:143:GLU:O	2:B:147:ILE:HG13	2.12	0.48
1:A:169:PRO:HD2	2:B:95:ARG:HH21	1.79	0.48
2:B:283:GLN:NE2	2:B:302:GLN:HG3	2.28	0.48
2:B:174:VAL:HG12	2:B:197:SER:CB	2.43	0.48
1:A:162:LEU:HD23	1:A:190:ARG:HA	1.94	0.48
1:A:194:ARG:HG2	1:A:194:ARG:HH11	1.78	0.48
2:B:172:PHE:CB	2:B:203:LEU:HG	2.41	0.48
1:A:127:GLU:OE2	1:A:170:GLU:HA	2.13	0.48
1:A:132:LEU:HD13	1:A:138:PHE:CD2	2.48	0.48
1:A:141:PRO:O	1:A:144:ARG:HB3	2.13	0.48
1:A:225:GLY:HA3	1:A:272:LEU:HD22	1.95	0.48
1:A:152:LEU:O	1:A:155:GLU:HB3	2.14	0.48
1:A:42:GLN:HA	1:A:63:LYS:HD2	1.96	0.48
1:A:338:SEP:OG	1:A:342:LYS:HE2	2.13	0.48
1:A:113:ASN:HD22	1:A:341:GLU:CA	2.27	0.47
2:B:298:ALA:HB1	2:B:338:VAL:O	2.14	0.47
1:A:276:ASP:OD1	1:A:279:LYS:HE2	2.14	0.47
2:B:36:LEU:H	2:B:36:LEU:HD23	1.78	0.47
2:B:133:ASN:HB3	2:B:136:PHE:HD2	1.79	0.47
2:B:172:PHE:O	2:B:223:GLY:HA2	2.14	0.47
1:A:122:TYR:CE2	1:A:124:ALA:HB2	2.49	0.47
1:A:278:THR:HG21	2:B:352:ARG:HE	1.80	0.47
1:A:187:PHE:CG	1:A:199:CYS:HB2	2.49	0.47
2:B:219:LEU:H	2:B:219:LEU:HD23	1.79	0.47
2:B:144:ARG:HG2	2:B:148:PHE:CE1	2.49	0.47
2:B:139:LEU:HD13	2:B:147:ILE:HD12	1.95	0.47
2:B:370:ARG:HB3	2:B:370:ARG:NH1	2.30	0.47
1:A:29:LYS:HE2	1:A:97:ALA:HA	1.96	0.47
2:B:164:GLN:HG3	2:B:165:GLN:N	2.28	0.46
2:B:325:ILE:HG22	2:B:329:LEU:HD21	1.98	0.46
2:B:179:GLU:O	2:B:219:LEU:HD22	2.16	0.46
2:B:179:GLU:HG2	2:B:193:SER:HA	1.97	0.46
1:A:272:LEU:C	1:A:272:LEU:HD23	2.36	0.46
1:A:270:ARG:HH11	1:A:270:ARG:HG3	1.81	0.46
1:A:163:ILE:HG12	1:A:165:ARG:HG3	1.97	0.46
2:B:281:VAL:O	2:B:336:THR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:O	1:A:103:LEU:HD23	2.15	0.46
1:A:238:PHE:CG	1:A:250:ILE:HG12	2.50	0.46
1:A:45:ARG:NH2	1:A:335:ILE:HB	2.31	0.46
2:B:375:ILE:HG12	2:B:376:SER:N	2.31	0.46
1:A:154:PHE:CZ	1:A:167:LEU:HD22	2.51	0.46
2:B:130:ILE:HD13	2:B:136:PHE:CB	2.41	0.46
1:A:175:ASP:OD2	1:A:179:TYR:HB2	2.15	0.46
2:B:118:LYS:HZ2	2:B:118:LYS:HB2	1.81	0.46
2:B:248:LEU:CD1	2:B:266:ALA:HB2	2.44	0.46
2:B:189:VAL:HG13	2:B:190:THR:H	1.81	0.46
1:A:61:LYS:O	1:A:62:HIS:C	2.54	0.46
2:B:270:GLU:O	2:B:346:VAL:HA	2.16	0.46
2:B:100:ALA:HB2	2:B:205:TYR:HB3	1.98	0.46
2:B:283:GLN:HB2	2:B:335:ALA:C	2.35	0.46
2:B:300:VAL:HB	2:B:313:VAL:HG23	1.97	0.46
2:B:339:ALA:CB	2:B:343:LEU:HD22	2.47	0.45
2:B:172:PHE:CE2	2:B:197:SER:HB2	2.51	0.45
1:A:258:PRO:HG2	1:A:261:PHE:CE2	2.51	0.45
1:A:198:LEU:CD2	2:B:204:ILE:HB	2.47	0.45
2:B:328:LEU:C	2:B:350:ARG:HD2	2.35	0.45
1:A:163:ILE:HD12	1:A:217:LYS:HA	1.97	0.45
2:B:293:ILE:HG22	2:B:318:PRO:HA	1.98	0.45
1:A:149:GLN:NE2	1:A:180:ILE:HB	2.31	0.45
1:A:267:ASP:HA	1:A:270:ARG:HG3	1.98	0.45
1:A:206:ALA:N	1:A:209:ILE:HD12	2.27	0.45
2:B:359:PRO:O	2:B:363:ILE:HD13	2.15	0.45
1:A:140:GLU:HB3	1:A:141:PRO:HD3	1.99	0.45
2:B:19:TYR:CB	2:B:22:LEU:HD12	2.46	0.45
1:A:37:THR:HG21	1:A:108:PHE:HB3	1.97	0.45
1:A:92:LYS:HB2	1:A:350:PHE:CE2	2.52	0.45
2:B:127:ALA:HA	2:B:148:PHE:HZ	1.82	0.45
1:A:203:GLU:O	1:A:226:VAL:HG11	2.17	0.45
2:B:348:LEU:HD11	2:B:353:PHE:HB2	1.99	0.45
2:B:303:ARG:HA	2:B:309:GLU:O	2.17	0.45
1:A:168:LYS:HD3	1:A:201:THR:HG21	1.99	0.45
2:B:329:LEU:HD23	2:B:329:LEU:N	2.32	0.45
2:B:163:ILE:HD11	2:B:213:VAL:HG23	1.99	0.45
1:A:196:TRP:O	1:A:197:TPO:C	2.64	0.45
2:B:217:THR:O	2:B:219:LEU:N	2.49	0.45
1:A:173:LEU:HD12	1:A:173:LEU:N	2.31	0.45
1:A:74:LEU:O	1:A:116:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:GLU:O	2:B:109:VAL:HG23	2.17	0.44
2:B:271:PRO:HA	2:B:346:VAL:HG12	1.99	0.44
2:B:376:SER:C	2:B:377:LEU:HD22	2.38	0.44
2:B:133:ASN:HD22	2:B:133:ASN:HA	1.58	0.44
2:B:359:PRO:HB2	2:B:362:GLU:OE1	2.17	0.44
1:A:45:ARG:NH2	1:A:335:ILE:N	2.65	0.44
1:A:106:LEU:HD13	1:A:120:MET:HG2	1.99	0.44
2:B:177:GLN:O	2:B:219:LEU:HB2	2.17	0.44
2:B:349:ASP:HB2	2:B:351:PRO:HD2	1.98	0.44
2:B:172:PHE:HZ	2:B:197:SER:HB2	1.80	0.44
1:A:87:HIS:HE1	1:A:197:TPO:HG21	1.81	0.44
2:B:251:VAL:HG13	2:B:324:GLU:OE2	2.18	0.44
1:A:207:PRO:HD3	1:A:222:TRP:CE2	2.52	0.44
2:B:372:ASN:O	2:B:375:ILE:HD13	2.17	0.44
2:B:175:VAL:HG12	2:B:194:GLU:HA	2.00	0.44
1:A:71:MET:SD	1:A:73:ILE:HD11	2.58	0.44
1:A:73:ILE:N	1:A:73:ILE:CD1	2.80	0.44
2:B:372:ASN:HA	2:B:375:ILE:HD11	1.99	0.44
1:A:244:ILE:HD11	2:B:134:VAL:CG1	2.48	0.44
1:A:132:LEU:HD13	1:A:138:PHE:CE2	2.53	0.44
2:B:273:GLN:HB2	2:B:273:GLN:HE21	1.63	0.44
1:A:265:LEU:HD13	1:A:296:TRP:CE2	2.53	0.44
2:B:356:VAL:HG13	2:B:357:LEU:HD23	2.01	0.43
1:A:347:PHE:O	1:A:350:PHE:HB3	2.18	0.43
1:A:80:VAL:HG23	1:A:347:PHE:CZ	2.53	0.43
2:B:202:ALA:O	2:B:226:ARG:HG3	2.19	0.43
1:A:163:ILE:O	1:A:163:ILE:HG23	2.18	0.43
1:A:95:LEU:HD21	1:A:185:PHE:CD1	2.54	0.43
1:A:179:TYR:OH	1:A:308:ARG:HA	2.18	0.43
1:A:272:LEU:C	1:A:274:GLN:H	2.21	0.43
1:A:184:ASP:HB2	3:A:400:ATP:O1A	2.18	0.43
2:B:302:GLN:O	2:B:311:VAL:HG22	2.18	0.43
2:B:321:TYR:O	2:B:322:PHE:HB3	2.18	0.43
2:B:325:ILE:O	2:B:329:LEU:HD23	2.18	0.43
1:A:144:ARG:NH1	1:A:296:TRP:O	2.50	0.43
2:B:122:THR:O	2:B:126:LEU:HG	2.18	0.43
1:A:251:VAL:HG12	1:A:251:VAL:O	2.19	0.43
2:B:252:SER:HB2	2:B:374:PHE:CZ	2.49	0.43
2:B:118:LYS:HD3	2:B:222:TRP:CZ3	2.53	0.43
2:B:118:LYS:HZ3	2:B:123:MET:HG2	1.83	0.43
1:A:261:PHE:CG	1:A:265:LEU:HD23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:LEU:HD13	2:B:349:ASP:O	2.19	0.43
1:A:206:ALA:HB3	1:A:209:ILE:CD1	2.48	0.43
2:B:280:ILE:HD13	2:B:337:VAL:CG1	2.37	0.42
1:A:140:GLU:OE2	1:A:265:LEU:HD22	2.18	0.42
2:B:294:THR:O	2:B:295:GLU:HG3	2.19	0.42
2:B:203:LEU:HD21	2:B:224:ILE:O	2.19	0.42
1:A:140:GLU:CB	1:A:141:PRO:HD3	2.49	0.42
2:B:282:VAL:O	2:B:285:GLU:HB2	2.18	0.42
2:B:104:THR:H	2:B:107:ASP:CG	2.22	0.42
2:B:315:ARG:HH11	2:B:315:ARG:HG2	1.84	0.42
1:A:327:PHE:HB3	1:A:328:ASP:H	1.61	0.42
2:B:368:ILE:O	2:B:372:ASN:HB2	2.19	0.42
2:B:353:PHE:CE2	2:B:360:CYS:HB2	2.55	0.42
1:A:69:TYR:HB3	1:A:119:VAL:HG23	2.01	0.42
1:A:133:ARG:HD2	2:B:92:ARG:CB	2.50	0.42
1:A:35:GLN:O	1:A:36:ASN:C	2.58	0.42
1:A:179:TYR:HB3	1:A:180:ILE:H	1.72	0.42
2:B:296:GLY:HA3	2:B:342:PRO:O	2.19	0.42
2:B:289:ASP:OD1	2:B:349:ASP:HB3	2.18	0.42
1:A:78:LYS:HG2	1:A:82:LEU:CD1	2.48	0.42
1:A:39:GLN:HG2	1:A:42:GLN:OE1	2.20	0.42
2:B:247:PHE:O	2:B:250:LYS:HB2	2.20	0.42
2:B:285:GLU:O	2:B:333:ARG:HG2	2.20	0.42
1:A:129:PHE:O	1:A:133:ARG:HG3	2.19	0.42
2:B:262:ARG:NH1	2:B:262:ARG:HB2	2.35	0.42
1:A:15:VAL:O	1:A:18:PHE:HB3	2.19	0.42
1:A:48:THR:HG22	1:A:50:GLY:H	1.85	0.42
2:B:303:ARG:HB2	2:B:310:TYR:CG	2.55	0.42
2:B:303:ARG:HB2	2:B:310:TYR:CD2	2.55	0.42
1:A:154:PHE:HD1	1:A:157:LEU:HD12	1.85	0.42
2:B:136:PHE:HA	2:B:139:LEU:CD1	2.50	0.41
2:B:180:VAL:HG23	2:B:192:ILE:CG2	2.50	0.41
1:A:238:PHE:CE1	1:A:250:ILE:HA	2.55	0.41
1:A:15:VAL:HG13	1:A:16:LYS:N	2.35	0.41
1:A:286:ASN:HB2	1:A:290:ASP:OD2	2.20	0.41
2:B:329:LEU:HA	2:B:350:ARG:NH1	2.36	0.41
1:A:49:LEU:HB2	1:A:57:VAL:O	2.21	0.41
1:A:104:VAL:HG23	1:A:104:VAL:O	2.20	0.41
2:B:287:GLY:HA2	2:B:333:ARG:CZ	2.51	0.41
1:A:233:ALA:HB1	1:A:235:TYR:CE1	2.56	0.41
2:B:304:ARG:O	2:B:308:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:VAL:HB	2:B:196:GLY:H	1.84	0.41
1:A:71:MET:HG3	1:A:73:ILE:HD11	2.02	0.41
2:B:276:ASP:CB	2:B:341:GLY:HA2	2.51	0.41
1:A:152:LEU:HD21	1:A:302:TRP:CE3	2.55	0.41
2:B:364:LEU:O	2:B:364:LEU:HD12	2.21	0.41
2:B:217:THR:O	2:B:219:LEU:HD23	2.21	0.41
1:A:34:SER:OG	1:A:35:GLN:N	2.52	0.41
2:B:130:ILE:O	2:B:133:ASN:HB2	2.21	0.41
1:A:261:PHE:HB3	1:A:266:LYS:HG2	2.02	0.41
1:A:323:ASP:OD2	1:A:325:SER:HB2	2.21	0.41
2:B:362:GLU:H	2:B:362:GLU:CD	2.14	0.41
2:B:130:ILE:C	2:B:130:ILE:HD12	2.41	0.40
2:B:269:LEU:CD2	2:B:348:LEU:HB2	2.51	0.40
1:A:257:PHE:HA	1:A:258:PRO:HD3	1.95	0.40
1:A:91:GLU:HG2	1:A:185:PHE:O	2.21	0.40
2:B:57:LYS:NZ	2:B:57:LYS:HB2	2.36	0.40
1:A:76:LYS:HB2	1:A:114:SER:O	2.20	0.40
1:A:284:LEU:N	1:A:284:LEU:HD13	2.36	0.40
1:A:197:TPO:OG1	2:B:102:VAL:HG22	2.21	0.40
1:A:39:GLN:HG2	1:A:42:GLN:CD	2.41	0.40
1:A:140:GLU:N	1:A:141:PRO:CD	2.84	0.40
2:B:283:GLN:HB2	2:B:335:ALA:HA	2.03	0.40
1:A:162:LEU:CD2	1:A:190:ARG:HD2	2.51	0.40
2:B:156:HIS:ND1	2:B:162:VAL:HG22	2.36	0.40
2:B:163:ILE:HD13	2:B:209:ARG:CD	2.52	0.40
1:A:217:LYS:O	1:A:220:ASP:HB2	2.21	0.40
1:A:168:LYS:HE2	1:A:201:THR:HG21	2.04	0.40
2:B:354:GLU:CG	2:B:359:PRO:HA	2.47	0.40
1:A:222:TRP:HZ2	1:A:250:ILE:HG23	1.86	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	338/350 (97%)	266 (79%)	61 (18%)	11 (3%)	5 44
2	B	341/381 (90%)	252 (74%)	66 (19%)	23 (7%)	1 24
All	All	679/731 (93%)	518 (76%)	127 (19%)	34 (5%)	3 31

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ALA
1	A	46	ILE
1	A	166	ASP
2	B	23	HIS
2	B	28	VAL
2	B	38	ILE
2	B	43	ARG
2	B	271	PRO
2	B	272	VAL
2	B	356	VAL
1	A	12	GLN
1	A	175	ASP
1	A	184	ASP
2	B	14	LYS
2	B	27	GLN
2	B	33	ILE
2	B	36	LEU
2	B	50	GLU
2	B	276	ASP
1	A	284	LEU
2	B	296	GLY
2	B	353	PHE
1	A	33	PRO
1	A	67	ASN
2	B	305	SER
2	B	329	LEU
1	A	35	GLN
1	A	255	VAL
2	B	18	LEU
2	B	40	LYS
2	B	87	PRO
2	B	367	ASN
2	B	25	ILE
2	B	34	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	280/303 (92%)	263 (94%)	17 (6%)	23 65
2	B	268/334 (80%)	234 (87%)	34 (13%)	5 32
All	All	548/637 (86%)	497 (91%)	51 (9%)	11 49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	37	THR
1	A	40	LEU
1	A	42	GLN
1	A	44	ASP
1	A	45	ARG
1	A	96	GLN
1	A	99	ASN
1	A	120	MET
1	A	130	SER
1	A	157	LEU
1	A	220	ASP
1	A	271	ASN
1	A	284	LEU
1	A	286	ASN
1	A	297	PHE
1	A	325	SER
2	B	36	LEU
2	B	52	PHE
2	B	55	LEU
2	B	56	GLU
2	B	57	LYS
2	B	93	ARG
2	B	105	GLU
2	B	122	THR
2	B	133	ASN
2	B	157	ILE

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Mol	Chain	Res	Type
2	B	171	ASN
2	B	180	VAL
2	B	191	ASN
2	B	225	ASP
2	B	226	ARG
2	B	243	MET
2	B	259	LYS
2	B	264	THR
2	B	267	ASP
2	B	270	GLU
2	B	272	VAL
2	B	304	ARG
2	B	305	SER
2	B	315	ARG
2	B	320	ASP
2	B	327	LEU
2	B	340	ARG
2	B	343	LEU
2	B	347	LYS
2	B	362	GLU
2	B	367	ASN
2	B	369	GLN
2	B	372	ASN
2	B	375	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	39	GLN
1	A	42	GLN
1	A	67	ASN
1	A	87	HIS
1	A	90	ASN
1	A	96	GLN
1	A	99	ASN
1	A	113	ASN
1	A	149	GLN
1	A	242	GLN
1	A	271	ASN
1	A	307	GLN
2	B	21	GLN

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Mol	Chain	Res	Type
2	B	133	ASN
2	B	142	ASN
2	B	164	GLN
2	B	165	GLN
2	B	185	ASN
2	B	273	GLN
2	B	302	GLN
2	B	367	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	TPO	A	197	1	8,10,11	0.63	0	7,14,16	1.25	0
1	SEP	A	338	1	8,9,10	0.66	0	8,12,14	1.75	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	197	1	-	0/8/11/13	0/0/0/0
1	SEP	A	338	1	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SEP	OG-CB-CA	4.25	111.90	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	197	TPO	7	0
1	A	338	SEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
3	ATP	A	400	4	24,33,33	0.68	0	31,52,52	1.89	3 (9%)

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
3	ATP	A	400	4	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	ATP	PA-O3A-PB	-7.05	112.92	132.73
3	A	400	ATP	PB-O3B-PG	-6.22	111.80	132.67
3	A	400	ATP	O3A-PA-O5'	2.46	109.47	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	400	ATP	2	0

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	A	340/350 (97%)	0.04	5 (1%) 76 62	84, 145, 188, 212	0
2	B	345/381 (90%)	0.29	29 (8%) 14 9	79, 159, 245, 276	0
All	All	685/731 (93%)	0.17	34 (4%) 32 21	79, 151, 233, 276	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	56	GLU	7.4
2	B	47	PHE	6.9
2	B	29	LEU	6.3
2	B	31	ASP	5.5
2	B	50	GLU	5.2
2	B	32	CYS	4.9
2	B	26	GLN	4.8
2	B	42	GLU	3.9
2	B	39	SER	3.8
2	B	51	HIS	3.8
2	B	86	ASN	3.6
1	A	10	SER	3.5
2	B	35	HIS	3.5
2	B	49	ARG	3.4
2	B	34	VAL	3.2
2	B	53	GLU	3.1
2	B	54	LYS	3.1
2	B	48	LEU	3.0
2	B	57	LYS	3.0
2	B	28	VAL	2.9
2	B	40	LYS	2.8
2	B	38	ILE	2.5
2	B	85	PRO	2.4
1	A	328	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	33	ILE	2.3
2	B	30	LYS	2.3
2	B	46	LYS	2.3
1	A	347	PHE	2.3
2	B	43	ARG	2.2
1	A	80	VAL	2.2
2	B	27	GLN	2.2
2	B	20	VAL	2.1
1	A	322	GLY	2.1
2	B	37	CYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	SEP	A	338	10/11	0.86	0.11	-	110,165,173,176	0
1	TPO	A	197	11/12	0.92	0.20	-	98,114,158,165	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	ATP	A	400	31/31	0.87	0.25	-0.52	212,212,212,212	0
4	MG	A	402	1/1	0.93	0.20	-1.31	131,131,131,131	0
4	MG	A	401	1/1	0.96	0.26	-	141,141,141,141	0

6.5 Other polymers (i)

There are no such residues in this entry.