



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:45 PM GMT

PDB ID : 1YIY
Title : Aedes aegypti kynurenine aminotransferase
Authors : Han, Q.; Gao, Y.G.; Robinson, H.; Ding, H.; Wilson, S.; Li, J.
Deposited on : 2005-01-13
Resolution : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

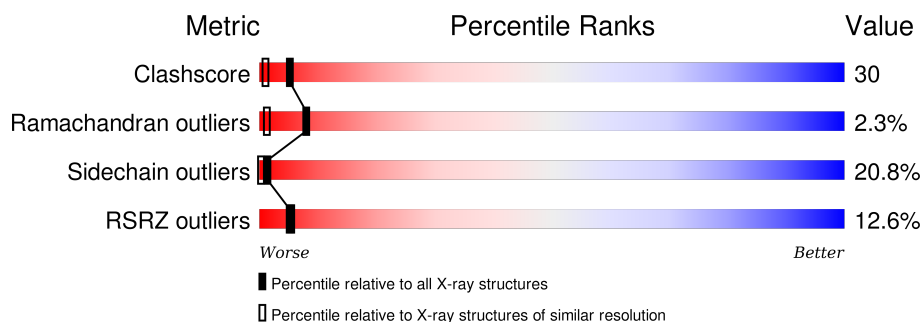
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	429	<div> <div>10%</div> <div>52%</div> <div>35%</div> <div>10%</div> <div>• •</div> </div>
1	B	429	<div> <div>14%</div> <div>49%</div> <div>34%</div> <div>13%</div> <div>• •</div> </div>

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
2	BR	A	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7107 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.

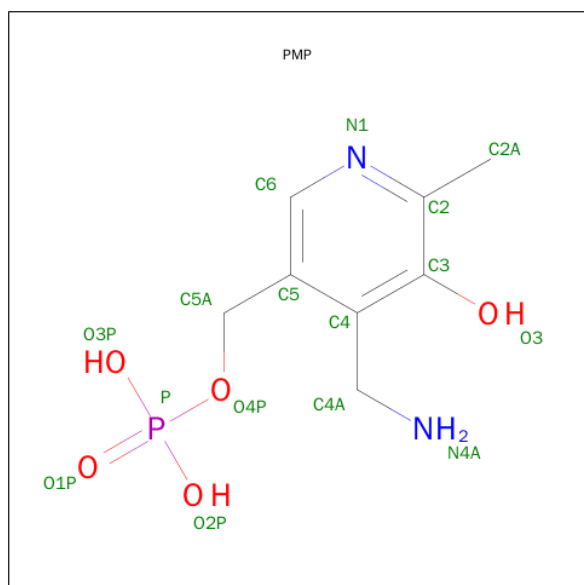
- Molecule 1 is a protein called kynurenine aminotransferase; glutamine transaminase K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3315	2133	549	613	20			
1	B	418	Total	C	N	O	S	0	0	0
			3315	2133	549	613	20			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Br	0	0
			2	2		
2	A	3	Total	Br	0	0
			3	3		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

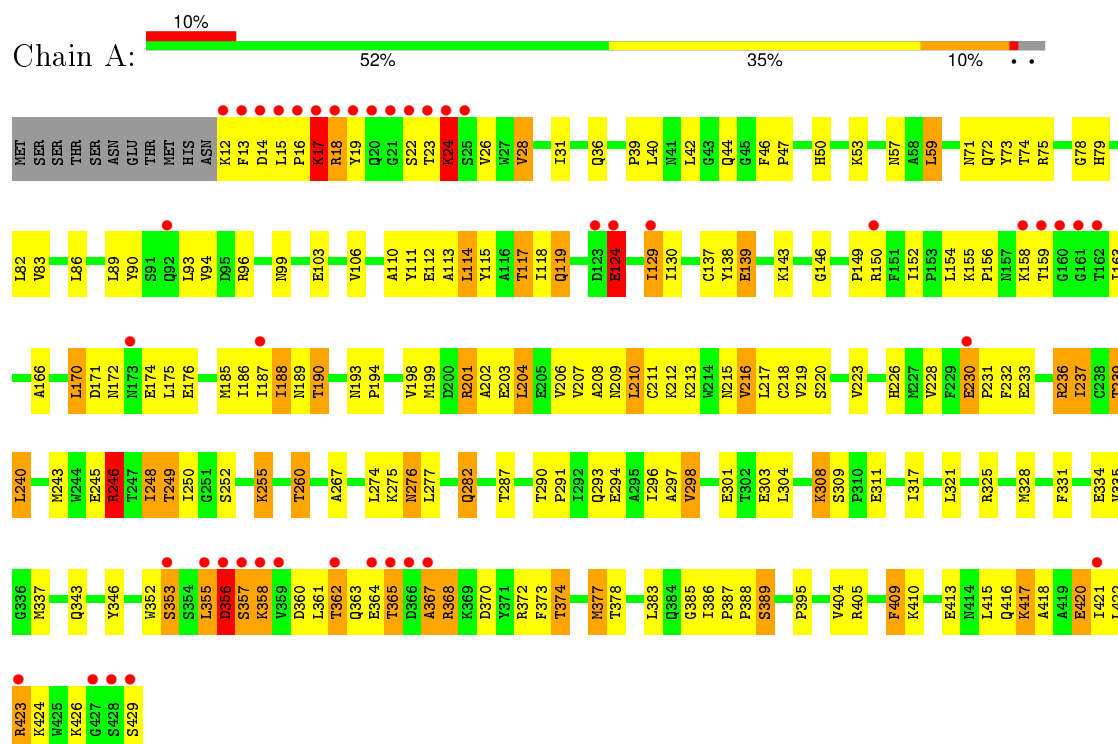
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total	O	0	0
			253	253		
4	B	187	Total	O	0	0
			187	187		

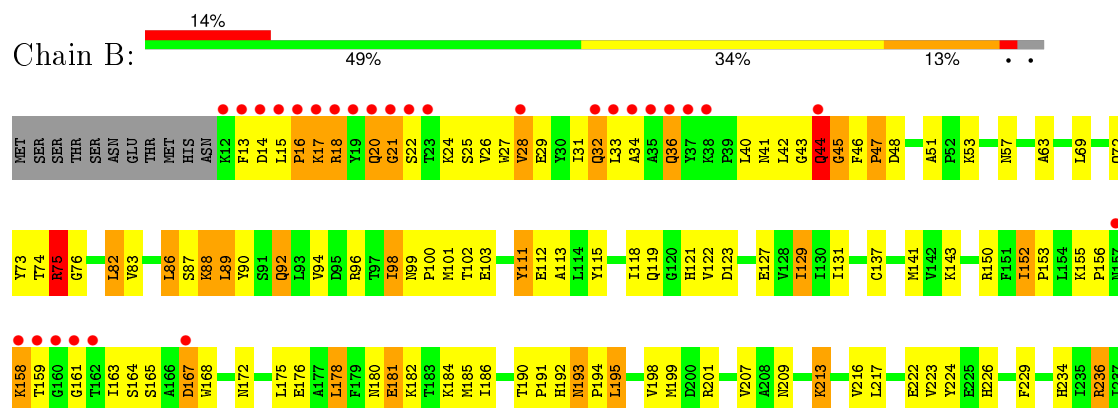
3 Residue-property plots [i](#)

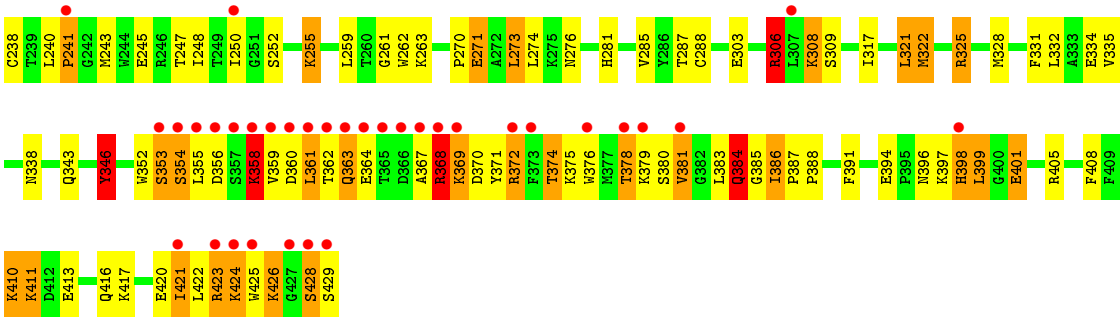
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: kynurenine aminotransferase; glutamine transaminase K



- Molecule 1: kynurenine aminotransferase; glutamine transaminase K





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.36 Å 95.32 Å 167.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 29.71 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (10.00-1.90) 94.6 (29.71-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.98 (at 1.91 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.218 , (Not available) 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 88.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66713 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7107	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, 0.375 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: PMP, BR

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	0.34	0/3403	0.91	4/4618 (0.1%)
1	B	0.36	1/3403 (0.0%)	0.88	6/4618 (0.1%)
All	All	0.35	1/6806 (0.0%)	0.89	10/9236 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LYS	CE-NZ	5.58	1.62	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	B	306	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	246	ARG	CD-NE-CZ	7.90	134.66	123.60
1	B	325	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	374	THR	CA-CB-CG2	-6.45	103.37	112.40
1	A	246	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	B	47	PRO	C-N-CA	5.54	135.56	121.70
1	B	346	TYR	CB-CG-CD1	5.54	124.33	121.00
1	A	325	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	75	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	3315	0	3272	213	0
1	B	3315	0	3272	210	0
2	A	3	0	0	3	0
2	B	2	0	0	1	0
3	A	16	0	11	0	0
3	B	16	0	11	1	0
4	A	253	0	0	50	0
4	B	187	0	0	16	0
All	All	7107	0	6566	403	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 30.

All (403) 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:153:PRO:HG2	1:B:155:LYS:HE2	1.46	0.97
1:B:354:SER:HB3	1:B:361:LEU:HD11	1.50	0.93
1:B:159:THR:HG21	1:B:163:ILE:HD13	1.51	0.92
1:A:248:ILE:HD11	1:A:267:ALA:HB1	1.51	0.91
1:A:176:GLU:HG2	1:A:210:LEU:HD11	1.56	0.85
1:B:248:ILE:HD11	1:B:273:LEU:HB3	1.60	0.84
1:B:383:LEU:HB2	1:B:421:ILE:HD11	1.60	0.84
1:A:139:GLU:HG2	1:A:143:LYS:HD2	1.61	0.82
1:A:71:ASN:HD22	1:B:262:TRP:HE1	1.26	0.82
1:A:117:THR:HA	1:A:277:LEU:HD22	1.60	0.82
1:A:208:ALA:HB1	1:A:243:MET:HE3	1.59	0.81
1:B:24:LYS:HB2	1:B:28:VAL:HG23	1.64	0.80
1:A:130:ILE:HG12	1:A:187:ILE:HD11	1.63	0.80
1:A:113:ALA:O	1:A:117:THR:HG22	1.83	0.78
1:A:187:ILE:HB	4:A:778:HOH:O	1.82	0.78
1:A:364:GLU:HA	4:A:818:HOH:O	1.84	0.78
1:A:96:ARG:HD3	4:A:721:HOH:O	1.84	0.78
1:A:114:LEU:O	1:A:118:ILE:HG13	1.84	0.78
1:A:365:THR:HG22	1:A:372:ARG:NH2	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HB1	4:A:741:HOH:O	1.84	0.77
1:A:413:GLU:O	1:A:417:LYS:HG2	1.85	0.77
1:A:72:GLN:O	1:A:290:THR:HG21	1.86	0.76
1:A:86:LEU:HG	4:A:797:HOH:O	1.85	0.76
1:A:82:LEU:O	1:A:86:LEU:HD23	1.85	0.76
1:A:149:PRO:O	1:A:150:ARG:HD2	1.86	0.76
1:A:335:VAL:HG21	1:A:422:LEU:HD13	1.66	0.76
1:B:118:ILE:O	1:B:122:VAL:HG13	1.85	0.76
1:B:75:ARG:HG3	4:B:658:HOH:O	1.85	0.75
1:B:417:LYS:O	1:B:421:ILE:HG23	1.87	0.75
1:B:198:VAL:HB	4:B:762:HOH:O	1.85	0.74
1:B:411:LYS:HE3	1:B:413:GLU:HG2	1.68	0.74
1:B:172:ASN:O	1:B:176:GLU:HG2	1.86	0.74
1:A:357:SER:HA	1:A:361:LEU:HB2	1.70	0.74
1:A:353:SER:HA	4:A:827:HOH:O	1.87	0.73
1:A:211:CYS:HA	1:A:216:VAL:HG13	1.68	0.73
1:B:27:TRP:O	1:B:31:ILE:HB	1.89	0.73
1:B:24:LYS:HD2	1:B:29:GLU:HB2	1.71	0.72
1:B:180:ASN:ND2	1:B:182:LYS:H	1.87	0.72
1:A:106:VAL:HB	4:A:762:HOH:O	1.88	0.72
1:A:16:PRO:HA	1:B:276:ASN:ND2	2.05	0.71
1:A:223:VAL:HB	4:A:757:HOH:O	1.90	0.71
1:B:127:GLU:OE2	1:B:150:ARG:HD2	1.91	0.71
1:B:180:ASN:HD21	1:B:182:LYS:HB2	1.55	0.71
1:B:90:TYR:O	1:B:94:VAL:HG12	1.92	0.70
1:B:363:GLN:HG2	1:B:372:ARG:HD3	1.72	0.70
1:A:187:ILE:HG13	4:A:758:HOH:O	1.89	0.70
1:A:356:ASP:N	1:A:358:LYS:HD3	2.06	0.70
1:A:187:ILE:HG21	4:A:783:HOH:O	1.90	0.69
1:A:355:LEU:HA	1:A:358:LYS:NZ	2.08	0.69
1:B:369:LYS:O	1:B:372:ARG:HG2	1.91	0.69
4:A:840:HOH:O	1:B:69:LEU:HD12	1.92	0.68
1:B:190:THR:HG22	4:B:747:HOH:O	1.92	0.68
1:A:82:LEU:HG	4:A:800:HOH:O	1.93	0.68
1:A:308:LYS:HG2	4:A:657:HOH:O	1.93	0.68
1:B:223:VAL:HB	1:B:255:LYS:HG3	1.76	0.68
1:A:355:LEU:HB2	1:A:360:ASP:OD2	1.94	0.67
1:A:355:LEU:HB3	1:A:358:LYS:HE2	1.77	0.67
1:B:118:ILE:HG12	1:B:185:MET:HE1	1.77	0.67
1:A:28:VAL:HA	1:B:75:ARG:NH2	2.10	0.67
1:B:167:ASP:HB3	4:B:712:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:SER:HB3	4:A:799:HOH:O	1.96	0.66
1:B:374:THR:HG21	1:B:387:PRO:HD3	1.78	0.66
1:B:192:HIS:HD2	1:B:195:LEU:HB2	1.61	0.66
1:B:308:LYS:H	1:B:308:LYS:HE3	1.60	0.66
1:B:34:ALA:HB1	4:B:706:HOH:O	1.95	0.66
1:A:186:ILE:HG12	1:A:188:ILE:HD12	1.79	0.65
1:B:355:LEU:HB3	1:B:361:LEU:HD12	1.78	0.65
1:B:181:GLU:HA	1:B:181:GLU:OE2	1.95	0.65
1:B:396:ASN:O	1:B:399:LEU:HB2	1.97	0.64
1:B:190:THR:HG21	1:B:199:MET:H	1.62	0.64
1:A:24:LYS:HA	4:A:838:HOH:O	1.97	0.64
1:A:155:LYS:HG3	1:A:156:PRO:HD2	1.78	0.64
1:B:192:HIS:CD2	1:B:195:LEU:HB2	2.32	0.64
1:B:367:ALA:N	1:B:372:ARG:HH22	1.96	0.63
1:B:18:ARG:HH11	1:B:18:ARG:HA	1.64	0.63
1:A:118:ILE:HD12	1:A:119:GLN:N	2.13	0.63
1:B:180:ASN:HD22	1:B:182:LYS:H	1.46	0.63
1:B:335:VAL:HB	1:B:423:ARG:HH12	1.64	0.63
1:A:361:LEU:O	1:A:362:THR:HB	1.99	0.63
1:A:308:LYS:N	1:A:308:LYS:HD3	2.14	0.63
1:B:14:ASP:C	1:B:16:PRO:HD3	2.19	0.63
1:B:168:TRP:CE3	1:B:195:LEU:HD21	2.35	0.62
1:A:260:THR:HG22	1:B:72:GLN:HA	1.80	0.62
1:A:118:ILE:HG12	4:A:756:HOH:O	1.99	0.62
1:B:201:ARG:HH12	1:B:240:LEU:HD22	1.63	0.62
1:B:44:GLN:HE22	1:B:410:LYS:NZ	1.98	0.62
1:A:331:PHE:O	1:A:335:VAL:HG23	1.98	0.62
1:A:423:ARG:HH11	1:A:423:ARG:HA	1.64	0.62
1:A:154:LEU:HD23	1:A:170:LEU:HD13	1.81	0.62
1:A:367:ALA:HB2	4:A:849:HOH:O	2.00	0.62
1:A:421:ILE:HD11	4:A:805:HOH:O	2.00	0.62
1:A:294:GLU:O	1:A:298:VAL:HG13	1.99	0.62
1:B:129:ILE:HG13	1:B:186:ILE:HG13	1.82	0.62
1:A:236:ARG:O	1:A:239:THR:HG22	2.00	0.61
1:A:209:ASN:HB3	1:A:213:LYS:HE2	1.82	0.61
1:B:16:PRO:C	1:B:18:ARG:H	2.04	0.60
1:B:163:ILE:HD12	1:B:167:ASP:OD1	2.01	0.60
1:B:421:ILE:O	1:B:424:LYS:HD3	2.01	0.60
1:B:98:ILE:O	1:B:98:ILE:HG13	2.00	0.60
1:A:78:GLY:HA2	1:A:106:VAL:HG12	1.84	0.60
1:A:199:MET:HG2	1:A:203:GLU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:O	1:B:335:VAL:HG12	2.01	0.60
1:B:222:GLU:OE1	1:B:236:ARG:NH1	2.34	0.60
1:B:355:LEU:CB	1:B:361:LEU:HD12	2.32	0.60
1:A:364:GLU:O	1:A:367:ALA:HB3	2.02	0.59
1:A:17:LYS:HD3	1:B:119:GLN:O	2.02	0.59
1:A:187:ILE:HD13	4:A:783:HOH:O	2.03	0.59
1:A:337:MET:HE3	1:A:352:TRP:HB3	1.84	0.59
1:B:129:ILE:HD11	1:B:152:ILE:HD11	1.85	0.59
1:A:190:THR:CG2	1:A:199:MET:H	2.15	0.59
1:B:361:LEU:HB3	4:B:734:HOH:O	2.02	0.59
1:A:246:ARG:NH1	4:A:618:HOH:O	2.35	0.59
1:B:193:ASN:HD22	1:B:194:PRO:CA	2.16	0.59
1:A:24:LYS:CE	1:A:24:LYS:H	2.16	0.59
1:A:230:GLU:HB2	2:A:602:BR:BR	2.57	0.59
1:A:83:VAL:HG12	4:A:762:HOH:O	2.02	0.58
1:A:130:ILE:HG12	1:A:187:ILE:CD1	2.33	0.58
1:B:193:ASN:HD21	1:B:405:ARG:HH11	1.52	0.58
1:A:99:ASN:HB3	1:A:103:GLU:HG3	1.86	0.58
1:B:261:GLY:HA2	1:B:263:LYS:HE3	1.84	0.58
1:A:115:TYR:O	1:A:119:GLN:HB2	2.03	0.58
1:A:199:MET:HG2	1:A:203:GLU:CB	2.34	0.58
1:B:367:ALA:O	1:B:368:ARG:HG2	2.04	0.57
1:A:352:TRP:CD1	1:A:404:VAL:HG23	2.39	0.57
1:A:418:ALA:O	1:A:421:ILE:HG22	2.04	0.57
1:B:17:LYS:O	1:B:17:LYS:HG3	2.04	0.57
1:A:356:ASP:O	1:A:358:LYS:HG2	2.05	0.57
1:B:226:HIS:HE1	4:B:728:HOH:O	1.87	0.57
1:B:243:MET:O	1:B:247:THR:HG22	2.03	0.57
1:B:308:LYS:H	1:B:308:LYS:CE	2.17	0.57
1:A:17:LYS:HE3	4:A:836:HOH:O	2.04	0.57
1:A:24:LYS:HE3	1:A:24:LYS:H	1.69	0.57
1:B:193:ASN:HD22	1:B:194:PRO:HA	1.70	0.57
1:A:370:ASP:OD1	1:A:389:SER:HB2	2.05	0.57
1:A:71:ASN:ND2	1:B:262:TRP:HE1	1.98	0.57
1:A:199:MET:HB3	1:A:204:LEU:HD13	1.87	0.56
1:B:270:PRO:HG2	1:B:273:LEU:HD22	1.87	0.56
1:B:368:ARG:HD3	1:B:397:LYS:NZ	2.20	0.56
1:B:224:TYR:CE1	1:B:255:LYS:HD3	2.40	0.56
1:A:74:THR:OG1	1:A:79:HIS:HD2	1.88	0.56
1:A:413:GLU:O	1:A:416:GLN:HG2	2.06	0.56
1:A:17:LYS:O	1:A:18:ARG:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:HD3	1:A:308:LYS:H	1.68	0.56
1:B:129:ILE:HG23	1:B:186:ILE:HB	1.87	0.56
1:B:150:ARG:HH11	1:B:150:ARG:HG2	1.69	0.56
1:A:365:THR:HA	1:A:372:ARG:NE	2.20	0.56
1:A:377:MET:HG3	4:A:774:HOH:O	2.06	0.56
1:A:112:GLU:HB2	1:B:285:VAL:HG22	1.89	0.55
1:A:139:GLU:CG	1:A:143:LYS:HD2	2.33	0.55
1:A:15:LEU:HD23	1:A:18:ARG:HA	1.88	0.55
1:A:374:THR:HG23	4:A:774:HOH:O	2.06	0.55
1:B:421:ILE:HA	1:B:424:LYS:HD2	1.88	0.55
1:B:426:LYS:HE2	1:B:428:SER:HA	1.89	0.55
1:A:115:TYR:HA	1:A:118:ILE:HD11	1.89	0.55
1:A:287:THR:HG23	1:B:263:LYS:HD3	1.88	0.55
1:B:152:ILE:HG12	1:B:178:LEU:CD2	2.37	0.55
1:A:215:ASN:HA	1:A:246:ARG:HH21	1.71	0.54
1:B:82:LEU:HD22	1:B:86:LEU:HD22	1.88	0.54
1:A:198:VAL:HG23	4:A:734:HOH:O	2.07	0.54
1:B:32:GLN:NE2	1:B:36:GLN:HE22	2.05	0.54
1:A:223:VAL:HG22	1:A:255:LYS:HB2	1.88	0.54
1:B:378:THR:HB	1:B:384:GLN:OE1	2.08	0.54
1:B:75:ARG:HD3	1:B:76:GLY:N	2.22	0.54
1:A:423:ARG:HH12	1:A:426:LYS:HD3	1.73	0.54
1:B:102:THR:HG23	1:B:103:GLU:HG3	1.90	0.54
1:A:154:LEU:CD2	1:A:170:LEU:HD13	2.37	0.54
1:B:18:ARG:HD2	1:B:143:LYS:HB3	1.89	0.54
1:B:331:PHE:HA	1:B:334:GLU:OE2	2.07	0.54
1:A:362:THR:HG22	4:A:848:HOH:O	2.07	0.54
1:B:335:VAL:HB	1:B:423:ARG:NH1	2.22	0.54
1:A:226:HIS:HE1	4:A:748:HOH:O	1.91	0.54
1:A:356:ASP:H	1:A:358:LYS:HD3	1.71	0.54
1:A:218:CYS:SG	1:A:237:ILE:HD13	2.48	0.54
1:A:39:PRO:HG3	1:A:378:THR:HG23	1.89	0.54
1:A:297:ALA:HA	4:A:800:HOH:O	2.07	0.54
1:B:376:TRP:O	1:B:380:SER:HB2	2.09	0.53
1:A:79:HIS:HE1	1:A:294:GLU:OE1	1.91	0.53
1:B:75:ARG:HH11	1:B:76:GLY:H	1.56	0.53
1:A:90:TYR:HD1	4:A:612:HOH:O	1.92	0.53
1:A:114:LEU:HG	4:A:623:HOH:O	2.09	0.53
1:A:355:LEU:HB3	1:A:358:LYS:HG3	1.89	0.53
1:B:386:ILE:HD11	1:B:405:ARG:NH2	2.23	0.53
1:A:110:ALA:HB2	1:A:252:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:THR:OG1	1:B:199:MET:HG3	2.08	0.53
1:A:118:ILE:HG21	4:A:756:HOH:O	2.07	0.53
1:A:296:ILE:HG22	4:A:800:HOH:O	2.08	0.53
1:B:129:ILE:HD11	1:B:152:ILE:CD1	2.39	0.53
1:B:88:LYS:O	1:B:92:GLN:HG2	2.08	0.53
1:B:75:ARG:HD3	1:B:76:GLY:H	1.73	0.53
1:A:17:LYS:HD2	1:B:122:VAL:O	2.08	0.53
1:A:368:ARG:HD2	4:A:787:HOH:O	2.09	0.52
1:A:365:THR:HG22	1:A:372:ARG:HH21	1.74	0.52
1:B:159:THR:CG2	1:B:163:ILE:HD13	2.34	0.52
1:A:190:THR:OG1	1:A:199:MET:HE3	2.10	0.52
1:B:32:GLN:NE2	1:B:36:GLN:NE2	2.58	0.52
1:A:249:THR:HG23	4:A:769:HOH:O	2.09	0.52
1:B:165:SER:OG	1:B:343:GLN:HG3	2.10	0.52
1:B:44:GLN:HE22	1:B:410:LYS:HZ1	1.58	0.52
1:A:260:THR:CG2	1:B:73:TYR:H	2.23	0.52
1:A:17:LYS:HB2	1:B:123:ASP:HB2	1.91	0.51
1:B:328:MET:HA	1:B:331:PHE:CE1	2.46	0.51
1:B:363:GLN:HG2	1:B:372:ARG:CD	2.39	0.51
1:A:237:ILE:HG13	4:A:770:HOH:O	2.09	0.51
1:B:376:TRP:HA	1:B:379:LYS:HG2	1.92	0.51
1:A:374:THR:HG21	1:A:385:GLY:O	2.11	0.51
1:A:421:ILE:HD13	4:A:785:HOH:O	2.10	0.51
1:B:32:GLN:HG3	1:B:33:LEU:N	2.26	0.51
1:B:121:HIS:O	1:B:184:LYS:HE3	2.10	0.51
1:B:417:LYS:HA	1:B:420:GLU:HG2	1.91	0.51
1:A:386:ILE:HG23	1:A:387:PRO:HD2	1.93	0.51
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.11	0.51
1:B:423:ARG:HD3	1:B:426:LYS:NZ	2.25	0.51
1:B:17:LYS:HZ2	1:B:17:LYS:HB2	1.76	0.51
1:B:164:SER:O	1:B:167:ASP:OD1	2.29	0.51
1:B:367:ALA:HB3	1:B:372:ARG:NH2	2.25	0.51
1:A:59:LEU:HD13	1:B:63:ALA:HB2	1.92	0.51
1:B:113:ALA:HB1	1:B:250:ILE:HD12	1.93	0.50
1:A:409:PHE:O	1:A:410:LYS:HE2	2.11	0.50
1:A:365:THR:HA	1:A:372:ARG:CZ	2.42	0.50
1:B:303:GLU:OE1	1:B:303:GLU:HA	2.11	0.50
1:A:290:THR:OG1	1:A:291:PRO:HD3	2.11	0.50
1:A:78:GLY:HA2	1:A:106:VAL:CG1	2.41	0.50
1:A:129:ILE:HG12	1:A:186:ILE:HG13	1.93	0.50
1:B:378:THR:HG21	1:B:384:GLN:HE22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:GLU:HG3	1:B:421:ILE:N	2.27	0.50
1:A:282:GLN:NE2	1:B:28:VAL:HG21	2.27	0.50
1:B:209:ASN:O	1:B:213:LYS:HG2	2.12	0.50
1:B:369:LYS:HA	1:B:372:ARG:HG2	1.93	0.50
1:B:370:ASP:O	1:B:374:THR:HB	2.11	0.50
1:A:337:MET:CE	1:A:352:TRP:HB3	2.41	0.50
1:A:124:GLU:O	1:A:146:GLY:O	2.30	0.50
1:A:40:LEU:CD1	1:A:417:LYS:HB2	2.41	0.49
1:B:378:THR:HG21	1:B:384:GLN:NE2	2.27	0.49
1:A:117:THR:HB	4:A:847:HOH:O	2.11	0.49
1:B:198:VAL:HG23	4:B:747:HOH:O	2.10	0.49
1:A:201:ARG:HG3	1:A:202:ALA:N	2.27	0.49
1:B:367:ALA:O	1:B:368:ARG:O	2.31	0.49
1:B:354:SER:O	1:B:360:ASP:OD2	2.30	0.49
1:A:138:TYR:HE1	4:A:623:HOH:O	1.96	0.49
1:B:43:GLY:HA2	1:B:386:ILE:HD13	1.94	0.49
1:A:395:PRO:HG2	4:A:798:HOH:O	2.12	0.49
1:B:159:THR:HG22	1:B:163:ILE:HG21	1.95	0.49
1:B:353:SER:O	1:B:353:SER:OG	2.30	0.49
1:B:180:ASN:ND2	1:B:182:LYS:HB2	2.26	0.49
1:B:331:PHE:HB2	1:B:423:ARG:NH2	2.28	0.48
1:B:193:ASN:HD21	1:B:405:ARG:NH1	2.11	0.48
1:A:362:THR:O	1:A:362:THR:HG23	2.12	0.48
1:B:368:ARG:O	1:B:368:ARG:HG2	2.12	0.48
1:A:198:VAL:O	1:A:198:VAL:HG23	2.14	0.48
1:B:16:PRO:C	1:B:18:ARG:N	2.66	0.48
1:B:355:LEU:HA	1:B:358:LYS:O	2.14	0.48
1:B:156:PRO:HB2	1:B:159:THR:CG2	2.43	0.48
1:A:358:LYS:HG2	1:A:358:LYS:H	1.41	0.48
1:B:411:LYS:CE	1:B:413:GLU:HG2	2.42	0.48
1:A:46:PHE:HB2	1:A:47:PRO:HD2	1.95	0.48
1:A:17:LYS:HB2	1:B:123:ASP:CB	2.44	0.48
1:B:352:TRP:O	1:B:356:ASP:OD2	2.31	0.48
1:A:212:LYS:HG3	1:A:243:MET:CE	2.43	0.48
1:A:328:MET:HA	1:A:331:PHE:CE2	2.49	0.48
1:B:192:HIS:HD2	1:B:195:LEU:H	1.61	0.48
1:A:185:MET:HG3	1:A:217:LEU:HB3	1.95	0.48
1:B:226:HIS:HD2	4:B:622:HOH:O	1.97	0.47
1:B:285:VAL:HB	4:B:716:HOH:O	2.13	0.47
1:A:226:HIS:HD2	4:A:801:HOH:O	1.96	0.47
1:A:74:THR:HB	1:A:290:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:ND2	1:A:193:ASN:H	2.11	0.47
1:A:223:VAL:HG22	1:A:255:LYS:CB	2.43	0.47
1:B:335:VAL:O	1:B:335:VAL:HG22	2.14	0.47
1:B:423:ARG:HD3	1:B:426:LYS:HZ2	1.79	0.47
1:B:371:TYR:O	1:B:375:LYS:HG3	2.14	0.47
1:A:74:THR:HG22	1:A:290:THR:HG22	1.97	0.47
1:B:75:ARG:HD2	4:B:713:HOH:O	2.13	0.47
1:A:355:LEU:HG	1:A:355:LEU:H	1.55	0.47
1:A:117:THR:HA	1:A:277:LEU:CD2	2.38	0.47
1:A:16:PRO:HA	1:B:276:ASN:HD22	1.78	0.47
1:B:190:THR:CG2	1:B:199:MET:H	2.25	0.47
1:B:428:SER:O	1:B:429:SER:HB3	2.15	0.47
1:A:194:PRO:HB3	1:A:405:ARG:HD2	1.97	0.47
1:A:373:PHE:CE2	1:A:404:VAL:HG21	2.50	0.47
1:A:150:ARG:HA	1:A:150:ARG:NE	2.28	0.47
1:B:386:ILE:HD11	1:B:405:ARG:HH21	1.79	0.47
1:B:213:LYS:HB3	4:B:727:HOH:O	2.14	0.47
1:B:161:GLY:HA2	1:B:338:ASN:CG	2.34	0.47
1:A:250:ILE:HD11	4:A:847:HOH:O	2.15	0.46
1:A:213:LYS:HB3	4:A:814:HOH:O	2.16	0.46
1:A:190:THR:HG22	4:A:693:HOH:O	2.16	0.46
1:A:190:THR:HG21	1:A:199:MET:H	1.79	0.46
1:A:16:PRO:O	1:A:17:LYS:HB3	2.15	0.46
1:B:362:THR:O	1:B:362:THR:HG23	2.16	0.46
1:B:317:ILE:HG13	1:B:321:LEU:HD22	1.98	0.46
1:A:74:THR:CG2	1:A:290:THR:HG22	2.46	0.46
1:A:423:ARG:NH1	1:A:426:LYS:HD3	2.30	0.46
1:A:220:SER:HB3	1:A:249:THR:HB	1.96	0.46
1:A:50:HIS:HD2	4:B:678:HOH:O	1.99	0.46
1:A:248:ILE:CD1	1:A:277:LEU:HD11	2.45	0.46
1:B:44:GLN:CD	1:B:45:GLY:H	2.20	0.45
1:B:303:GLU:OE1	1:B:306:ARG:HD2	2.16	0.45
1:B:198:VAL:HG12	1:B:343:GLN:HB2	1.97	0.45
1:A:208:ALA:CB	1:A:243:MET:HE3	2.41	0.45
1:A:373:PHE:O	1:A:377:MET:HG2	2.15	0.45
1:A:387:PRO:HA	1:A:388:PRO:HD3	1.80	0.45
1:A:362:THR:HB	4:A:732:HOH:O	2.16	0.45
1:B:381:VAL:HG12	1:B:424:LYS:HE3	1.99	0.45
1:B:417:LYS:O	1:B:420:GLU:HG2	2.16	0.45
1:A:236:ARG:NE	4:A:612:HOH:O	2.50	0.45
1:B:102:THR:OG1	1:B:271:GLU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:OH	1:B:255:LYS:NZ	2.50	0.45
1:B:245:GLU:HB3	2:B:604:BR:BR	2.72	0.45
1:A:118:ILE:HD13	4:A:796:HOH:O	2.16	0.45
1:B:383:LEU:CB	1:B:421:ILE:HD11	2.39	0.45
1:A:355:LEU:HA	1:A:358:LYS:CE	2.47	0.45
1:B:240:LEU:HB3	1:B:241:PRO:HD2	1.99	0.45
1:B:51:ALA:HB3	1:B:259:LEU:HD21	1.99	0.45
1:B:163:ILE:HB	1:B:167:ASP:OD2	2.17	0.45
1:A:89:LEU:O	1:A:93:LEU:HD13	2.16	0.45
1:B:198:VAL:O	1:B:198:VAL:HG13	2.17	0.44
1:B:397:LYS:HD2	4:B:720:HOH:O	2.18	0.44
1:B:369:LYS:HG3	1:B:401:GLU:HG2	1.98	0.44
1:B:346:TYR:HA	1:B:408:PHE:CZ	2.52	0.44
1:A:210:LEU:HD22	4:A:744:HOH:O	2.16	0.44
1:A:365:THR:HG22	1:A:372:ARG:CZ	2.46	0.44
1:A:150:ARG:CZ	1:A:150:ARG:HA	2.47	0.44
1:A:193:ASN:HA	1:A:194:PRO:HA	1.82	0.44
1:A:230:GLU:N	2:A:602:BR:BR	2.91	0.44
1:B:191:PRO:HG2	1:B:224:TYR:O	2.17	0.44
1:B:53:LYS:HE3	1:B:57:ASN:OD1	2.18	0.44
1:A:231:PRO:HG2	1:A:232:PHE:CE1	2.52	0.44
1:A:212:LYS:HG3	1:A:243:MET:HE2	2.00	0.44
1:A:331:PHE:O	1:A:334:GLU:HB3	2.16	0.44
1:A:106:VAL:HG11	1:A:293:GLN:OE1	2.17	0.44
1:A:90:TYR:O	1:A:94:VAL:HG22	2.17	0.44
1:B:112:GLU:OE2	1:B:281:HIS:HD2	2.00	0.44
1:B:89:LEU:O	1:B:92:GLN:HG3	2.18	0.44
1:A:308:LYS:HE2	4:A:657:HOH:O	2.18	0.44
1:B:334:GLU:OE1	1:B:423:ARG:NE	2.51	0.44
1:B:83:VAL:HG13	1:B:100:PRO:O	2.17	0.44
1:B:398:HIS:C	1:B:398:HIS:ND1	2.71	0.44
1:A:219:VAL:HG22	1:A:248:ILE:CG2	2.48	0.43
1:A:282:GLN:HE22	1:B:24:LYS:HA	1.83	0.43
1:A:188:ILE:CD1	1:A:207:VAL:HG11	2.48	0.43
1:A:260:THR:HG22	1:B:72:GLN:CA	2.46	0.43
1:A:228:VAL:HG22	2:A:605:BR:BR	2.73	0.43
1:B:229:PHE:HB3	1:B:322:MET:HE3	2.00	0.43
1:A:208:ALA:O	1:A:243:MET:HE1	2.18	0.43
1:A:356:ASP:OD1	1:A:356:ASP:N	2.50	0.43
1:B:137:CYS:O	1:B:141:MET:HG3	2.17	0.43
1:B:368:ARG:HD3	1:B:397:LYS:HZ3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:SER:HB3	1:B:255:LYS:HG3	2.00	0.43
1:B:159:THR:CG2	1:B:163:ILE:HG21	2.48	0.43
1:A:110:ALA:O	1:A:114:LEU:HD22	2.18	0.43
1:A:417:LYS:HA	1:A:420:GLU:HG3	2.01	0.43
1:B:234:HIS:HD2	4:B:747:HOH:O	2.00	0.43
1:B:131:ILE:HG12	1:B:152:ILE:HD12	2.00	0.43
1:A:223:VAL:HG22	1:A:255:LYS:CG	2.48	0.43
1:A:356:ASP:C	1:A:358:LYS:HG2	2.38	0.43
1:B:129:ILE:HG23	1:B:186:ILE:HA	2.00	0.43
1:A:172:ASN:OD1	1:A:206:VAL:HG11	2.18	0.43
1:B:14:ASP:O	1:B:16:PRO:HD3	2.19	0.43
1:A:282:GLN:NE2	1:B:25:SER:H	2.16	0.43
1:A:166:ALA:HB2	1:A:343:GLN:NE2	2.34	0.43
1:A:231:PRO:CB	4:A:853:HOH:O	2.67	0.42
1:B:20:GLN:HG2	1:B:21:GLY:N	2.33	0.42
1:A:276:ASN:HD22	1:A:276:ASN:N	2.17	0.42
1:B:354:SER:HB3	1:B:361:LEU:CD1	2.37	0.42
1:A:239:THR:HG22	1:A:240:LEU:HD23	2.02	0.42
1:A:215:ASN:OD1	1:A:246:ARG:NH2	2.53	0.42
1:B:376:TRP:CZ3	1:B:425:TRP:HZ2	2.37	0.42
1:A:57:ASN:ND2	4:A:646:HOH:O	2.49	0.42
1:A:248:ILE:CD1	1:A:267:ALA:HB1	2.36	0.42
1:B:421:ILE:O	1:B:425:TRP:HB2	2.20	0.42
1:B:384:GLN:HB3	1:B:385:GLY:H	1.54	0.42
1:B:46:PHE:HB2	1:B:47:PRO:HD2	2.01	0.42
1:B:388:PRO:HA	1:B:391:PHE:HD1	1.84	0.42
1:A:44:GLN:HG3	1:A:410:LYS:NZ	2.35	0.42
1:B:127:GLU:CD	1:B:150:ARG:HD2	2.40	0.42
1:B:111:TYR:HB2	3:B:501:PMP:O3P	2.19	0.42
1:A:40:LEU:HD12	1:A:417:LYS:HB2	2.02	0.41
1:A:297:ALA:O	1:A:301:GLU:HG3	2.20	0.41
1:B:99:ASN:CG	1:B:102:THR:HG22	2.40	0.41
1:B:156:PRO:HB2	1:B:159:THR:OG1	2.20	0.41
1:A:118:ILE:HD12	1:A:119:GLN:H	1.80	0.41
1:B:270:PRO:CG	1:B:273:LEU:HD22	2.50	0.41
1:B:74:THR:O	1:B:287:THR:HG21	2.20	0.41
1:A:111:TYR:CZ	1:A:137:CYS:HB3	2.55	0.41
1:A:171:ASP:HB3	1:A:174:GLU:HB3	2.02	0.41
1:A:277:LEU:N	1:A:277:LEU:HD23	2.34	0.41
1:B:129:ILE:HG23	1:B:186:ILE:CB	2.50	0.41
1:A:199:MET:HG2	1:A:203:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:NZ	1:A:57:ASN:HD21	2.17	0.41
1:B:287:THR:HG22	1:B:288:CYS:H	1.86	0.41
1:B:115:TYR:CZ	1:B:119:GLN:HG3	2.55	0.41
1:B:369:LYS:HA	1:B:372:ARG:HD2	2.02	0.41
1:B:178:LEU:HA	1:B:178:LEU:HD12	1.76	0.41
1:B:238:CYS:CB	1:B:247:THR:HG21	2.50	0.41
1:B:40:LEU:HG	1:B:42:LEU:HD13	2.03	0.40
1:A:364:GLU:CG	1:A:367:ALA:HB3	2.51	0.40
1:A:287:THR:HG23	1:B:263:LYS:CD	2.51	0.40
1:B:386:ILE:HD11	4:B:714:HOH:O	2.21	0.40
1:B:381:VAL:CG1	1:B:424:LYS:HE3	2.51	0.40
1:A:114:LEU:HD13	1:A:250:ILE:HD13	2.03	0.40
1:A:352:TRP:HZ3	1:A:356:ASP:HA	1.87	0.40
1:B:83:VAL:CG1	1:B:100:PRO:HB2	2.51	0.40
1:B:42:LEU:HD22	1:B:383:LEU:HD11	2.04	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	416/429 (97%)	384 (92%)	23 (6%)	9 (2%)	8	1
1	B	416/429 (97%)	378 (91%)	28 (7%)	10 (2%)	7	1
All	All	832/858 (97%)	762 (92%)	51 (6%)	19 (2%)	8	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	14	ASP
1	A	17	LYS

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Mol	Chain	Res	Type
1	A	75	ARG
1	A	356	ASP
1	A	362	THR
1	A	367	ALA
1	B	44	GLN
1	B	384	GLN
1	A	124	GLU
1	B	21	GLY
1	B	36	GLN
1	B	368	ARG
1	A	24	LYS
1	B	158	LYS
1	B	241	PRO
1	B	16	PRO
1	B	28	VAL
1	B	45	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/367 (97%)	283 (80%)	73 (20%)	1	0
1	B	356/367 (97%)	281 (79%)	75 (21%)	1	0
All	All	712/734 (97%)	564 (79%)	148 (21%)	1	0

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	17	LYS
1	A	18	ARG
1	A	19	TYR
1	A	22	SER
1	A	23	THR
1	A	24	LYS

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Mol	Chain	Res	Type
1	A	26	VAL
1	A	28	VAL
1	A	31	ILE
1	A	36	GLN
1	A	42	LEU
1	A	59	LEU
1	A	114	LEU
1	A	117	THR
1	A	119	GLN
1	A	124	GLU
1	A	129	ILE
1	A	139	GLU
1	A	152	ILE
1	A	158	LYS
1	A	159	THR
1	A	163	ILE
1	A	170	LEU
1	A	175	LEU
1	A	188	ILE
1	A	190	THR
1	A	201	ARG
1	A	204	LEU
1	A	210	LEU
1	A	216	VAL
1	A	230	GLU
1	A	233	GLU
1	A	236	ARG
1	A	237	ILE
1	A	239	THR
1	A	240	LEU
1	A	245	GLU
1	A	246	ARG
1	A	248	ILE
1	A	249	THR
1	A	255	LYS
1	A	260	THR
1	A	274	LEU
1	A	275	LYS
1	A	276	ASN
1	A	282	GLN
1	A	298	VAL
1	A	304	LEU

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Mol	Chain	Res	Type
1	A	308	LYS
1	A	309	SER
1	A	311	GLU
1	A	317	ILE
1	A	321	LEU
1	A	346	TYR
1	A	353	SER
1	A	355	LEU
1	A	356	ASP
1	A	357	SER
1	A	358	LYS
1	A	363	GLN
1	A	365	THR
1	A	368	ARG
1	A	377	MET
1	A	383	LEU
1	A	389	SER
1	A	409	PHE
1	A	415	LEU
1	A	417	LYS
1	A	420	GLU
1	A	423	ARG
1	A	424	LYS
1	A	429	SER
1	B	13	PHE
1	B	15	LEU
1	B	17	LYS
1	B	18	ARG
1	B	20	GLN
1	B	22	SER
1	B	26	VAL
1	B	32	GLN
1	B	41	ASN
1	B	44	GLN
1	B	48	ASP
1	B	75	ARG
1	B	82	LEU
1	B	86	LEU
1	B	87	SER
1	B	88	LYS
1	B	89	LEU
1	B	92	GLN

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Mol	Chain	Res	Type
1	B	96	ARG
1	B	98	ILE
1	B	101	MET
1	B	111	TYR
1	B	129	ILE
1	B	152	ILE
1	B	158	LYS
1	B	167	ASP
1	B	175	LEU
1	B	178	LEU
1	B	181	GLU
1	B	193	ASN
1	B	195	LEU
1	B	207	VAL
1	B	213	LYS
1	B	216	VAL
1	B	217	LEU
1	B	236	ARG
1	B	255	LYS
1	B	271	GLU
1	B	273	LEU
1	B	274	LEU
1	B	306	ARG
1	B	308	LYS
1	B	309	SER
1	B	321	LEU
1	B	322	MET
1	B	325	ARG
1	B	346	TYR
1	B	353	SER
1	B	354	SER
1	B	358	LYS
1	B	359	VAL
1	B	361	LEU
1	B	363	GLN
1	B	364	GLU
1	B	368	ARG
1	B	369	LYS
1	B	372	ARG
1	B	374	THR
1	B	378	THR
1	B	381	VAL

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Mol	Chain	Res	Type
1	B	384	GLN
1	B	386	ILE
1	B	394	GLU
1	B	398	HIS
1	B	399	LEU
1	B	401	GLU
1	B	410	LYS
1	B	411	LYS
1	B	416	GLN
1	B	421	ILE
1	B	422	LEU
1	B	423	ARG
1	B	424	LYS
1	B	426	LYS
1	B	428	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	57	ASN
1	A	71	ASN
1	A	79	HIS
1	A	84	GLN
1	A	121	HIS
1	A	157	ASN
1	A	189	ASN
1	A	226	HIS
1	A	276	ASN
1	A	278	GLN
1	A	282	GLN
1	A	363	GLN
1	B	20	GLN
1	B	36	GLN
1	B	41	ASN
1	B	44	GLN
1	B	50	HIS
1	B	172	ASN
1	B	180	ASN
1	B	192	HIS
1	B	193	ASN
1	B	226	HIS

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Mol	Chain	Res	Type
1	B	234	HIS
1	B	278	GLN
1	B	414	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	PMP	A	500	-	16,16,16	1.31	3 (18%)	20,23,23	2.30	7 (35%)
3	PMP	B	501	-	16,16,16	1.25	1 (6%)	20,23,23	1.90	6 (30%)

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	PMP	A	500	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PMP	B	501	-	-	0/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PMP	C3-C2	-2.64	1.38	1.40
3	B	501	PMP	P-O3P	-2.03	1.47	1.54
3	A	500	PMP	P-O3P	-2.01	1.47	1.54
3	A	500	PMP	C2-N1	2.02	1.38	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PMP	O4P-P-O1P	-2.47	100.84	107.14
3	B	501	PMP	O4P-P-O1P	-2.40	101.03	107.14
3	A	500	PMP	C2A-C2-N1	-2.20	113.06	117.95
3	A	500	PMP	C3-C4-C5	-2.01	116.70	118.82
3	B	501	PMP	O3-C3-C2	-2.00	114.18	117.66
3	A	500	PMP	C4-C3-C2	2.43	124.41	120.03
3	B	501	PMP	C4-C3-C2	2.48	124.51	120.03
3	B	501	PMP	C2A-C2-C3	2.82	124.44	121.04
3	A	500	PMP	C4A-C4-C3	2.91	124.78	120.40
3	B	501	PMP	C4A-C4-C3	3.82	126.15	120.40
3	B	501	PMP	O4P-C5A-C5	4.28	116.07	108.99
3	A	500	PMP	O4P-C5A-C5	4.67	116.72	108.99
3	A	500	PMP	C2A-C2-C3	6.28	128.61	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	PMP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	418/429 (97%)	0.80	43 (10%) 9 9	4, 14, 59, 91	0
1	B	418/429 (97%)	1.08	62 (14%) 3 3	4, 17, 63, 91	0
All	All	836/858 (97%)	0.94	105 (12%) 5 5	4, 15, 62, 91	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	THR	17.3
1	B	428	SER	16.5
1	A	359	VAL	14.3
1	A	365	THR	14.3
1	B	355	LEU	13.6
1	A	160	GLY	13.4
1	A	428	SER	13.1
1	B	365	THR	12.7
1	B	23	THR	12.4
1	B	359	VAL	11.9
1	B	429	SER	11.8
1	A	159	THR	11.8
1	A	13	PHE	11.6
1	A	366	ASP	11.0
1	B	16	PRO	10.6
1	A	20	GLN	10.5
1	B	360	ASP	10.0
1	B	361	LEU	9.9
1	A	18	ARG	9.7
1	A	427	GLY	9.3
1	B	14	ASP	9.2
1	B	357	SER	9.0
1	B	13	PHE	8.8
1	A	21	GLY	8.7

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Mol	Chain	Res	Type	RSRZ
1	B	356	ASP	8.5
1	A	12	LYS	8.5
1	A	15	LEU	8.5
1	A	23	THR	8.3
1	B	366	ASP	8.3
1	B	363	GLN	7.9
1	B	161	GLY	7.8
1	A	161	GLY	7.7
1	B	358	LYS	7.7
1	A	16	PRO	7.6
1	B	364	GLU	7.2
1	A	358	LYS	7.2
1	B	18	ARG	6.9
1	B	427	GLY	6.7
1	A	355	LEU	6.7
1	A	19	TYR	6.7
1	B	15	LEU	6.4
1	A	22	SER	6.0
1	B	425	TRP	5.9
1	B	12	LYS	5.7
1	B	22	SER	5.7
1	A	14	ASP	5.5
1	A	429	SER	5.2
1	B	28	VAL	5.0
1	B	367	ALA	4.9
1	B	35	ALA	4.9
1	B	158	LYS	4.9
1	A	158	LYS	4.8
1	B	159	THR	4.6
1	A	162	THR	4.3
1	B	21	GLY	4.2
1	B	37	TYR	4.1
1	A	24	LYS	4.1
1	A	367	ALA	4.0
1	A	362	THR	3.8
1	B	398	HIS	3.8
1	A	353	SER	3.8
1	B	376	TRP	3.8
1	A	25	SER	3.7
1	A	357	SER	3.6
1	B	353	SER	3.6
1	A	356	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	17	LYS	3.6
1	A	230	GLU	3.5
1	B	32	GLN	3.3
1	A	124	GLU	3.3
1	B	44	GLN	3.3
1	B	160	GLY	3.2
1	B	20	GLN	3.2
1	B	354	SER	3.2
1	B	162	THR	3.1
1	A	17	LYS	3.1
1	B	250	ILE	2.8
1	A	123	ASP	2.8
1	B	19	TYR	2.8
1	B	157	ASN	2.7
1	B	381	VAL	2.6
1	B	379	LYS	2.6
1	B	423	ARG	2.6
1	B	34	ALA	2.6
1	A	421	ILE	2.6
1	A	187	ILE	2.6
1	A	364	GLU	2.5
1	B	372	ARG	2.4
1	A	173	ASN	2.4
1	A	150	ARG	2.4
1	A	423	ARG	2.4
1	A	92	GLN	2.3
1	B	241	PRO	2.3
1	B	424	LYS	2.3
1	B	421	ILE	2.2
1	A	129	ILE	2.2
1	B	369	LYS	2.2
1	B	373	PHE	2.2
1	B	368	ARG	2.2
1	B	378	THR	2.2
1	B	33	LEU	2.1
1	B	36	GLN	2.0
1	B	38	LYS	2.0
1	B	307	LEU	2.0
1	B	167	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	PMP	A	500	16/16	0.96	0.15	0.31	3,10,17,25	0
2	BR	B	601	1/1	0.98	0.10	-0.23	33,33,33,33	0
3	PMP	B	501	16/16	0.97	0.13	-0.26	2,10,20,49	0
2	BR	A	602	1/1	0.97	0.11	-0.34	37,37,37,37	0
2	BR	B	604	1/1	0.96	0.13	-	43,43,43,43	0
2	BR	A	605	1/1	0.95	0.08	-	35,35,35,35	1
2	BR	A	603	1/1	0.96	0.11	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.