



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:57 pm GMT

PDB ID : 2Q2Z
Title : Crystal Structure of KSP in Complex with Inhibitor 22
Authors : Yan, Y.
Deposited on : 2007-05-29
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

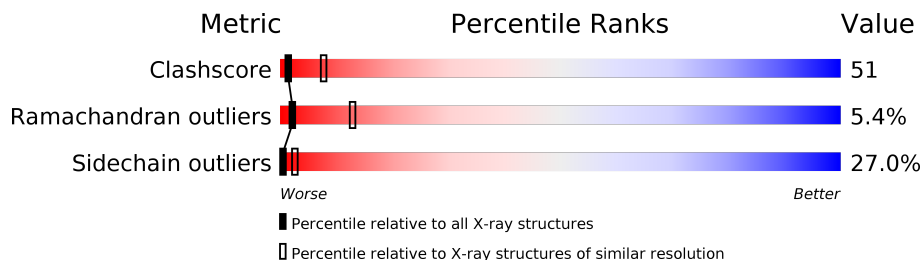
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	

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
3	ADP	A	601	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5466 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 Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			
1	B	330	Total	C	N	O	S	0	0	0
			2594	1624	452	508	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

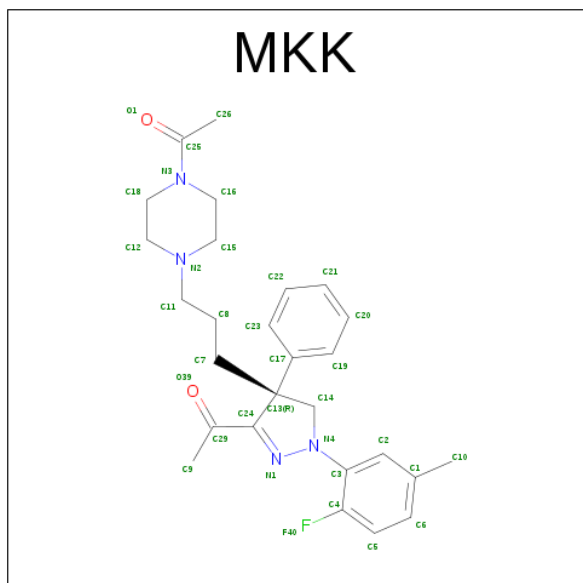
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is 1-[(4R)-4-[3-(4-ACETYLPYPERAZIN-1-YL)PROPYL]-1-(2-FLUORO-5-METHYLPHENYL)-4-PHENYL-4,5-DIHYDRO-1H-PYRAZOL-3-YL]ETHANONE (three-letter code: MKK) (formula: C₂₇H₃₃FN₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			34	27	1	4	2		
4	B	1	Total	C	F	N	O	0	0
			34	27	1	4	2		

- Molecule 5 is water.

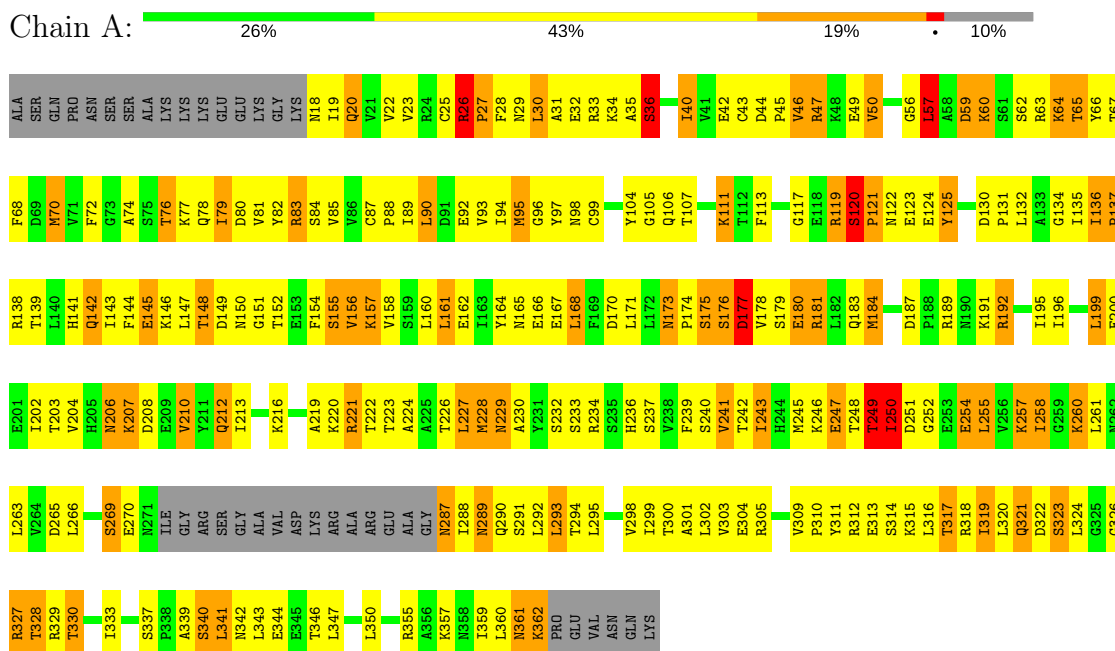
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	88	Total	O	0	0
			88	88		
5	B	66	Total	O	0	0
			66	66		

3 Residue-property plots

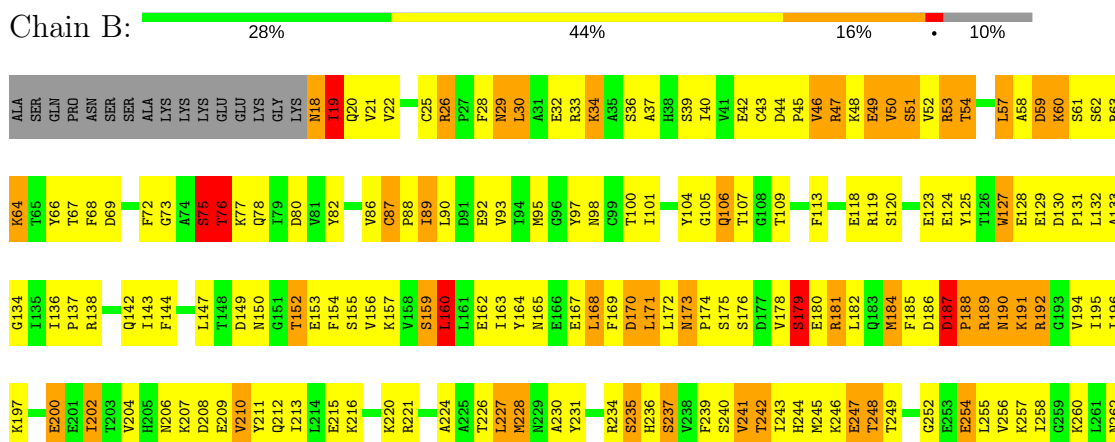
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

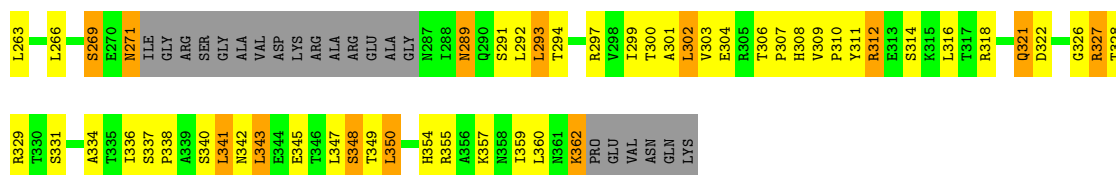
Note EDS was not executed.

• Molecule 1: Kinesin-like protein KIF11



• Molecule 1: Kinesin-like protein KIF11





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.20Å 79.45Å 160.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.60 – 3.00	Depositor
% Data completeness (in resolution range)	92.8 (35.60-3.00)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	BUSTER-TNT 1.9.2	Depositor
R, R_{free}	0.188 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5466	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MKK, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/2632	0.84	4/3559 (0.1%)
1	B	0.63	0/2632	0.87	3/3559 (0.1%)
All	All	0.63	0/5264	0.85	7/7118 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASP	C-N-CD	-9.79	99.07	120.60
1	A	26	ARG	C-N-CD	-6.79	105.67	120.60
1	B	170	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	120	SER	C-N-CD	-6.04	107.30	120.60
1	A	26	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	26	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	B	160	LEU	CA-CB-CG	-5.25	103.23	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2594	0	2618	287	0
1	B	2594	0	2618	255	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	11	2	0
3	B	27	0	12	3	0
4	A	34	0	33	3	0
4	B	34	0	33	5	0
5	A	88	0	0	4	0
5	B	66	0	0	1	0
All	All	5466	0	5325	543	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 51.

All (543) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:HB2	1:A:200:GLU:HG3	1.23	1.11
1:B:89:ILE:HD12	1:B:101:ILE:HD11	1.18	1.10
1:B:190:ASN:HB2	1:B:192:ARG:HH12	1.16	1.07
1:A:157:LYS:HD2	1:A:203:THR:HG23	1.38	1.05
1:B:192:ARG:HB3	1:B:192:ARG:HH11	1.23	1.02
1:B:18:ASN:HB2	1:B:360:LEU:HD23	1.42	1.01
1:A:168:LEU:HD21	1:A:184:MET:HG3	1.43	1.00
1:A:184:MET:HE1	1:A:318:ARG:HE	1.28	0.99
1:A:161:LEU:HD11	1:A:196:ILE:HD13	1.43	0.98
1:B:184:MET:HE1	1:B:318:ARG:HE	1.26	0.98
1:B:78:GLN:HB2	1:B:138:ARG:HH21	1.28	0.96
1:A:229:ASN:N	1:A:229:ASN:HD22	1.55	0.95
1:A:136:ILE:HG13	1:A:263:LEU:HD12	1.48	0.95
1:A:136:ILE:HG22	1:A:137:PRO:HD3	1.45	0.95
1:B:89:ILE:HD12	1:B:101:ILE:CD1	1.97	0.95
1:A:341:LEU:H	1:A:341:LEU:HD12	1.32	0.94
1:B:162:GLU:HG2	1:B:237:SER:HA	1.51	0.93
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.50	0.92
1:A:144:PHE:HZ	1:A:204:VAL:HG12	1.35	0.90
1:A:184:MET:HE1	1:A:318:ARG:NE	1.87	0.90
1:A:70:MET:HE1	1:A:84:SER:HB3	1.54	0.90
1:B:336:ILE:HG21	1:B:350:LEU:HD11	1.55	0.89
1:A:339:ALA:HB1	1:A:341:LEU:HD13	1.56	0.88
1:A:298:VAL:HG21	1:A:317:THR:HG21	1.55	0.88
1:B:293:LEU:HB3	1:B:297:ARG:NH1	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:H	1:A:229:ASN:HD22	1.20	0.87
1:A:311:TYR:CD1	1:A:321:GLN:HB2	2.10	0.87
1:A:245:MET:HE3	1:A:257:LYS:HB3	1.57	0.86
1:B:78:GLN:HB2	1:B:138:ARG:NH2	1.90	0.86
1:A:111:LYS:HG3	3:A:601:ADP:O2B	1.75	0.86
1:A:157:LYS:CD	1:A:203:THR:HG23	2.05	0.85
1:A:173:ASN:HB2	1:A:200:GLU:CG	2.05	0.85
1:B:163:ILE:HG12	1:B:168:LEU:HD23	1.56	0.84
1:A:298:VAL:HG21	1:A:317:THR:CG2	2.08	0.84
1:B:242:THR:HG23	1:B:260:LYS:HB2	1.57	0.83
1:B:190:ASN:HB2	1:B:192:ARG:NH1	1.93	0.83
1:A:147:LEU:HB2	1:A:154:PHE:CE2	2.14	0.81
1:B:248:THR:HG23	1:B:254:GLU:HG2	1.62	0.81
1:A:144:PHE:CZ	1:A:204:VAL:HG12	2.14	0.81
1:B:72:PHE:HD1	1:B:76:THR:HG21	1.44	0.81
1:B:43:CYS:O	1:B:45:PRO:HD3	1.81	0.81
1:A:70:MET:CE	1:A:84:SER:HB3	2.10	0.80
1:B:246:LYS:HD3	1:B:254:GLU:OE1	1.82	0.80
1:B:289:ASN:O	1:B:293:LEU:HD13	1.82	0.80
1:A:27:PRO:HB3	1:A:74:ALA:HB1	1.64	0.80
1:A:105:GLY:C	1:A:269:SER:HB3	2.02	0.79
1:B:47:ARG:HG2	1:B:49:GLU:OE1	1.83	0.78
1:B:190:ASN:CB	1:B:192:ARG:HH12	1.97	0.77
1:A:191:LYS:HA	5:A:682:HOH:O	1.84	0.77
1:A:156:VAL:HG13	1:A:243:ILE:HG23	1.67	0.77
1:A:26:ARG:HH11	1:A:26:ARG:HG3	1.50	0.77
1:B:120:SER:HA	1:B:132:LEU:HD12	1.66	0.77
1:A:247:GLU:HB3	1:A:255:LEU:HB2	1.67	0.76
1:B:194:VAL:O	1:B:195:ILE:HD13	1.85	0.76
1:A:44:ASP:OD1	1:A:46:VAL:HG13	1.84	0.76
1:B:262:ASN:O	1:B:263:LEU:HD23	1.85	0.76
1:A:173:ASN:ND2	1:A:175:SER:H	1.83	0.76
1:A:161:LEU:HD11	1:A:196:ILE:CD1	2.16	0.76
1:B:192:ARG:HB3	1:B:192:ARG:NH1	2.00	0.76
1:B:301:ALA:CB	1:B:309:VAL:HG22	2.16	0.76
1:B:104:TYR:CE1	1:B:349:THR:HG23	2.20	0.76
1:B:105:GLY:O	1:B:269:SER:HB3	1.85	0.75
1:A:130:ASP:OD2	1:A:131:PRO:HD2	1.86	0.75
1:A:362:LYS:O	1:A:362:LYS:HE3	1.84	0.75
1:B:299:ILE:HG23	1:B:359:ILE:HD11	1.69	0.75
1:A:173:ASN:CB	1:A:200:GLU:HG3	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ILE:HG22	1:A:199:LEU:HB2	1.69	0.75
1:A:245:MET:CE	1:A:257:LYS:HB3	2.16	0.75
1:B:167:GLU:OE2	1:B:181:ARG:HD3	1.87	0.74
1:A:196:ILE:HD11	1:A:319:ILE:HD13	1.68	0.74
1:A:136:ILE:CG1	1:A:263:LEU:HD12	2.18	0.74
1:A:229:ASN:N	1:A:229:ASN:ND2	2.30	0.74
1:A:158:VAL:HG12	1:A:241:VAL:HB	1.68	0.74
1:A:90:LEU:O	1:A:94:ILE:HG13	1.87	0.74
1:B:104:TYR:HE1	1:B:349:THR:HG23	1.51	0.74
1:A:56:GLY:HA3	5:A:638:HOH:O	1.88	0.73
1:B:248:THR:CG2	1:B:254:GLU:HG2	2.18	0.73
1:A:141:HIS:CD2	1:A:207:LYS:HD3	2.24	0.73
1:B:181:ARG:HH11	1:B:181:ARG:HG2	1.53	0.73
1:A:339:ALA:HB1	1:A:341:LEU:CD1	2.18	0.73
1:A:168:LEU:CD2	1:A:184:MET:HG3	2.17	0.72
1:B:173:ASN:HD21	1:B:175:SER:HB2	1.55	0.72
1:B:48:LYS:HD3	1:B:69:ASP:O	1.89	0.72
1:B:184:MET:CE	1:B:194:VAL:HG21	2.19	0.72
1:A:162:GLU:HG2	1:A:237:SER:HA	1.72	0.71
1:A:42:GLU:HG3	1:A:63:ARG:HH12	1.55	0.71
1:B:172:LEU:O	1:B:174:PRO:HD3	1.90	0.71
1:B:164:TYR:CE1	1:B:228:MET:HG2	2.24	0.71
1:A:25:CYS:HB2	1:A:43:CYS:SG	2.31	0.71
1:A:299:ILE:HD13	1:A:359:ILE:HD11	1.73	0.70
1:A:165:ASN:O	1:A:165:ASN:ND2	2.22	0.70
1:A:247:GLU:OE2	1:A:255:LEU:HG	1.91	0.70
1:A:82:TYR:CE2	1:A:138:ARG:HB2	2.26	0.70
1:A:341:LEU:HD12	1:A:341:LEU:N	2.04	0.70
1:A:60:LYS:NZ	1:A:60:LYS:HB3	2.05	0.70
1:A:289:ASN:O	1:A:293:LEU:HD22	1.91	0.70
1:A:49:GLU:HB2	1:A:66:TYR:O	1.90	0.70
1:B:19:ILE:HD12	1:B:359:ILE:CG2	2.20	0.70
1:A:229:ASN:H	1:A:229:ASN:ND2	1.89	0.70
1:A:246:LYS:HA	1:A:255:LEU:O	1.92	0.69
1:A:294:THR:O	1:A:298:VAL:HG23	1.92	0.69
1:B:184:MET:HE1	1:B:318:ARG:NE	2.02	0.69
1:B:306:THR:HG23	1:B:307:PRO:HD2	1.72	0.69
1:B:67:THR:O	1:B:357:LYS:NZ	2.25	0.69
1:B:184:MET:CE	1:B:318:ARG:HE	2.04	0.68
1:A:289:ASN:HB3	1:A:292:LEU:HB3	1.75	0.68
1:A:92:GLU:OE2	1:A:329:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:ND2	1:B:175:SER:H	1.91	0.68
1:B:106:GLN:NE2	1:B:345:GLU:HB2	2.08	0.68
1:B:75:SER:HB2	5:B:632:HOH:O	1.92	0.68
1:A:339:ALA:HB3	1:A:342:ASN:ND2	2.08	0.68
1:B:170:ASP:OD2	1:B:173:ASN:HB2	1.93	0.68
1:A:22:VAL:HG12	1:A:70:MET:CB	2.23	0.67
1:B:98:ASN:O	1:B:328:THR:HG23	1.93	0.67
1:B:248:THR:HG23	1:B:254:GLU:CG	2.24	0.67
1:A:78:GLN:NE2	1:A:132:LEU:O	2.26	0.67
1:B:143:ILE:HG21	1:B:156:VAL:HG21	1.76	0.67
1:A:26:ARG:CG	1:A:26:ARG:HH11	2.07	0.67
1:B:192:ARG:HG2	1:B:192:ARG:O	1.93	0.66
1:A:301:ALA:CB	1:A:309:VAL:HG22	2.25	0.66
1:A:43:CYS:O	1:A:45:PRO:HD3	1.96	0.66
1:B:291:SER:HB3	1:B:316:LEU:HB3	1.77	0.66
1:B:196:ILE:HD12	1:B:196:ILE:N	2.11	0.66
1:B:153:GLU:OE2	1:B:153:GLU:HA	1.96	0.66
1:A:158:VAL:HA	1:A:240:SER:O	1.96	0.66
1:A:79:ILE:HD13	1:A:138:ARG:NH1	2.10	0.66
1:B:54:THR:HG21	1:B:64:LYS:HG3	1.77	0.66
1:B:30:LEU:O	1:B:34:LYS:HB2	1.96	0.65
1:A:300:THR:O	1:A:304:GLU:HG3	1.96	0.65
1:A:125:TYR:HA	5:A:683:HOH:O	1.96	0.65
1:B:184:MET:HE3	1:B:194:VAL:HG21	1.78	0.65
1:A:311:TYR:CE1	1:A:321:GLN:HB2	2.30	0.65
1:A:25:CYS:CB	1:A:43:CYS:SG	2.85	0.65
1:A:250:ILE:HD13	1:A:250:ILE:H	1.61	0.65
1:B:326:GLY:O	1:B:362:LYS:N	2.25	0.65
1:B:75:SER:O	1:B:77:LYS:HE2	1.96	0.65
1:A:148:THR:HG22	1:A:149:ASP:N	2.10	0.65
1:B:318:ARG:O	1:B:321:GLN:HG2	1.97	0.65
1:A:136:ILE:HG22	1:A:137:PRO:CD	2.24	0.64
1:A:92:GLU:HG2	1:A:97:TYR:CD2	2.32	0.64
1:A:295:LEU:CD1	1:A:324:LEU:HD11	2.27	0.64
1:B:153:GLU:HB3	1:B:246:LYS:HB3	1.79	0.64
1:B:301:ALA:HB3	1:B:309:VAL:HG22	1.78	0.64
1:A:242:THR:OG1	1:A:260:LYS:HD2	1.97	0.64
1:A:98:ASN:CB	1:A:328:THR:HG23	2.28	0.64
1:A:136:ILE:HG13	1:A:263:LEU:CD1	2.25	0.64
1:A:29:ASN:OD1	1:A:31:ALA:HB3	1.97	0.64
1:B:42:GLU:O	1:B:50:VAL:HA	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:CD1	1:B:340:SER:HA	2.29	0.63
1:A:158:VAL:HG12	1:A:241:VAL:HA	1.79	0.63
1:A:177:ASP:OD1	1:A:178:VAL:N	2.30	0.63
1:A:341:LEU:CD1	1:A:341:LEU:H	2.06	0.63
1:B:154:PHE:HA	1:B:244:HIS:O	1.97	0.63
1:B:105:GLY:C	1:B:269:SER:HB3	2.18	0.63
1:B:301:ALA:HB1	1:B:309:VAL:HG22	1.79	0.63
1:A:94:ILE:HG21	1:A:147:LEU:HD21	1.81	0.63
1:A:298:VAL:CG2	1:A:317:THR:HG21	2.27	0.63
1:A:170:ASP:O	1:A:220:LYS:NZ	2.31	0.62
1:B:204:VAL:HG22	1:B:213:ILE:CD1	2.29	0.62
1:A:173:ASN:O	1:A:220:LYS:HE3	1.99	0.62
1:B:78:GLN:CB	1:B:138:ARG:HH21	2.09	0.62
1:A:34:LYS:HG2	1:A:35:ALA:N	2.14	0.62
1:A:92:GLU:HA	1:A:95:MET:CE	2.30	0.62
1:A:56:GLY:O	1:A:57:LEU:HB2	1.99	0.61
1:A:161:LEU:CD1	1:A:196:ILE:HD13	2.25	0.61
1:B:300:THR:HG23	1:B:304:GLU:OE1	2.00	0.61
1:A:255:LEU:HD12	1:A:257:LYS:HD3	1.82	0.61
1:A:136:ILE:CD1	1:A:263:LEU:HD12	2.30	0.61
1:A:30:LEU:HA	1:A:33:ARG:HB2	1.81	0.61
1:A:362:LYS:HE3	1:A:362:LYS:C	2.20	0.61
1:B:187:ASP:OD2	1:B:188:PRO:HD2	2.00	0.61
1:A:293:LEU:N	1:A:293:LEU:HD13	2.16	0.61
1:B:136:ILE:HG12	1:B:263:LEU:HD12	1.82	0.61
1:A:89:ILE:HG23	1:A:99:CYS:SG	2.40	0.61
1:B:227:LEU:H	1:B:227:LEU:HD23	1.65	0.61
1:B:184:MET:HE2	1:B:318:ARG:HH21	1.66	0.60
1:A:171:LEU:HD11	1:A:221:ARG:HA	1.83	0.60
1:A:184:MET:CE	1:A:318:ARG:HE	2.10	0.60
1:A:230:ALA:O	1:A:234:ARG:HG3	2.01	0.60
1:B:341:LEU:O	1:B:341:LEU:HG	2.00	0.60
1:A:161:LEU:HD13	1:A:319:ILE:HD12	1.84	0.60
1:A:136:ILE:CG2	1:A:137:PRO:HD3	2.24	0.60
1:A:247:GLU:HG2	1:A:248:THR:H	1.67	0.60
1:A:204:VAL:HG22	1:A:213:ILE:CD1	2.32	0.60
1:B:184:MET:HE2	1:B:318:ARG:NH2	2.17	0.60
1:B:124:GLU:HG2	1:B:125:TYR:CD1	2.37	0.59
1:A:176:SER:OG	1:A:180:GLU:HG3	2.01	0.59
1:B:191:LYS:HA	1:B:191:LYS:NZ	2.16	0.59
1:B:312:ARG:HA	1:B:318:ARG:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:O	1:A:208:ASP:N	2.36	0.59
1:B:212:GLN:HG2	1:B:216:LYS:HZ3	1.68	0.59
1:A:68:PHE:HA	1:A:357:LYS:HE3	1.84	0.59
1:B:89:ILE:CD1	1:B:101:ILE:HD11	2.12	0.59
1:B:336:ILE:HG21	1:B:350:LEU:CD1	2.28	0.58
1:A:82:TYR:HE2	1:A:138:ARG:HB2	1.67	0.58
1:B:82:TYR:CE2	1:B:86:VAL:HG11	2.38	0.58
1:B:87:CYS:HB3	1:B:88:PRO:HD3	1.85	0.58
1:A:89:ILE:HG23	1:A:99:CYS:CB	2.34	0.58
1:B:245:MET:HB2	1:B:257:LYS:HB2	1.86	0.58
1:A:144:PHE:O	1:A:146:LYS:N	2.36	0.58
1:A:250:ILE:HD13	1:A:250:ILE:N	2.19	0.58
1:B:184:MET:HE2	1:B:194:VAL:HG21	1.85	0.58
1:A:250:ILE:CD1	1:A:250:ILE:H	2.16	0.58
1:B:162:GLU:CD	1:B:171:LEU:HD23	2.24	0.57
1:B:52:VAL:HG11	1:B:347:LEU:CD2	2.34	0.57
1:A:150:ASN:O	1:A:152:THR:N	2.35	0.57
1:A:156:VAL:HA	1:A:242:THR:O	2.04	0.57
1:A:93:VAL:HG23	1:A:99:CYS:SG	2.45	0.57
1:A:93:VAL:HG21	1:A:261:LEU:HB2	1.87	0.57
1:B:134:GLY:O	1:B:137:PRO:HG2	2.04	0.57
1:A:85:VAL:O	1:A:89:ILE:HD12	2.04	0.57
1:A:187:ASP:HA	1:A:195:ILE:HD12	1.87	0.57
1:A:295:LEU:HD11	1:A:324:LEU:HD11	1.86	0.57
1:B:327:ARG:HA	1:B:362:LYS:HA	1.85	0.57
1:B:143:ILE:CD1	1:B:243:ILE:HD11	2.35	0.57
1:A:301:ALA:HB1	1:A:309:VAL:HG22	1.87	0.57
1:B:322:ASP:OD1	1:B:328:THR:OG1	2.22	0.57
1:B:178:VAL:O	1:B:180:GLU:N	2.38	0.56
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.69	0.56
1:A:221:ARG:O	1:A:224:ALA:HB3	2.04	0.56
1:B:302:LEU:HD13	1:B:309:VAL:HG21	1.86	0.56
1:B:72:PHE:CD1	1:B:76:THR:HG21	2.33	0.56
1:B:89:ILE:HG12	1:B:329:ARG:NH1	2.20	0.56
1:A:204:VAL:CG2	1:A:213:ILE:HD13	2.36	0.56
1:B:100:THR:OG1	1:B:262:ASN:HB2	2.05	0.56
1:B:159:SER:O	1:B:239:PHE:HA	2.04	0.56
1:B:28:PHE:HA	1:B:32:GLU:OE2	2.05	0.56
1:B:28:PHE:CE1	1:B:37:ALA:HB1	2.40	0.56
1:B:157:LYS:HA	1:B:202:ILE:O	2.06	0.56
1:A:122:ASN:O	1:A:123:GLU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:CG1	1:A:243:ILE:HG23	2.34	0.55
1:A:22:VAL:HG12	1:A:70:MET:HB2	1.87	0.55
1:A:346:THR:HG22	1:A:350:LEU:HD12	1.89	0.55
1:A:92:GLU:HG3	1:A:95:MET:HE3	1.87	0.55
1:A:301:ALA:HB3	1:A:309:VAL:HG22	1.87	0.55
1:B:160:LEU:HD12	1:B:160:LEU:C	2.22	0.55
1:A:327:ARG:HA	1:A:362:LYS:O	2.05	0.55
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.70	0.55
1:A:162:GLU:HA	1:A:236:HIS:O	2.05	0.55
1:A:29:ASN:C	1:A:31:ALA:H	2.10	0.55
1:A:299:ILE:HD13	1:A:359:ILE:CD1	2.36	0.55
1:B:271:ASN:HD22	1:B:271:ASN:C	2.08	0.55
1:B:184:MET:CG	1:B:318:ARG:HH21	2.19	0.55
1:B:66:TYR:HB2	1:B:68:PHE:HE1	1.71	0.54
1:A:158:VAL:CG1	1:A:241:VAL:HB	2.37	0.54
1:B:227:LEU:N	1:B:227:LEU:HD23	2.22	0.54
1:B:19:ILE:HD12	1:B:359:ILE:HG21	1.87	0.54
1:A:104:TYR:HB2	1:A:266:LEU:HD12	1.90	0.54
1:A:254:GLU:OE2	1:A:254:GLU:O	2.26	0.54
1:A:98:ASN:HB2	1:A:328:THR:HG23	1.88	0.54
1:A:142:GLN:HA	1:A:142:GLN:OE1	2.07	0.54
1:A:156:VAL:HG12	1:A:242:THR:O	2.08	0.54
1:A:204:VAL:O	1:A:204:VAL:HG12	2.08	0.54
1:B:63:ARG:HG2	1:B:63:ARG:NH1	2.23	0.54
1:A:158:VAL:HG12	1:A:241:VAL:CB	2.36	0.53
1:A:196:ILE:O	1:A:196:ILE:HG22	2.07	0.53
1:A:26:ARG:CG	1:A:26:ARG:NH1	2.66	0.53
1:B:52:VAL:CG1	1:B:343:LEU:HD21	2.38	0.53
1:B:211:TYR:O	1:B:215:GLU:HG3	2.07	0.53
1:B:29:ASN:O	1:B:33:ARG:HG2	2.08	0.53
1:B:306:THR:HG22	1:B:308:HIS:H	1.72	0.53
1:B:89:ILE:HD12	1:B:101:ILE:CG1	2.38	0.53
1:A:124:GLU:HB3	1:A:125:TYR:CD1	2.42	0.53
1:B:191:LYS:HZ2	1:B:191:LYS:HA	1.73	0.53
1:A:294:THR:OG1	1:A:314:SER:HB3	2.09	0.53
1:A:44:ASP:OD2	1:A:47:ARG:HG3	2.09	0.53
1:B:20:GLN:NE2	1:B:331:SER:OG	2.42	0.52
1:B:25:CYS:HB2	1:B:43:CYS:SG	2.50	0.52
1:A:196:ILE:HD11	1:A:319:ILE:CD1	2.39	0.52
1:A:221:ARG:O	1:A:224:ALA:N	2.40	0.52
1:A:136:ILE:HD11	1:A:239:PHE:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLN:HA	1:B:215:GLU:HG3	1.92	0.52
1:B:306:THR:HG23	1:B:307:PRO:CD	2.40	0.52
1:B:133:ALA:HB2	4:B:605:MKK:H20	1.92	0.52
1:A:92:GLU:HA	1:A:95:MET:HE2	1.91	0.52
1:A:219:ALA:O	1:A:222:THR:HB	2.10	0.52
1:A:96:GLY:O	1:A:258:ILE:O	2.28	0.52
1:A:147:LEU:HB2	1:A:154:PHE:HE2	1.72	0.51
1:A:298:VAL:HG21	1:A:317:THR:HG22	1.88	0.51
1:A:76:THR:HG22	1:A:80:ASP:HB2	1.93	0.51
1:B:113:PHE:CD1	1:B:118:GLU:HG3	2.44	0.51
1:B:142:GLN:HA	1:B:142:GLN:HE21	1.75	0.51
1:B:26:ARG:O	1:B:338:PRO:HG3	2.10	0.51
1:B:52:VAL:HG11	1:B:347:LEU:HD23	1.92	0.51
1:B:93:VAL:HA	1:B:97:TYR:O	2.10	0.51
1:B:227:LEU:N	1:B:227:LEU:CD2	2.72	0.51
1:B:106:GLN:HE21	1:B:345:GLU:HB2	1.73	0.51
1:B:354:HIS:CE1	1:B:357:LYS:NZ	2.79	0.51
1:A:30:LEU:O	1:A:30:LEU:HG	2.10	0.51
1:A:89:ILE:CG2	1:A:99:CYS:CB	2.89	0.51
1:A:90:LEU:HD21	1:A:143:ILE:HG13	1.92	0.51
1:A:117:GLY:HA3	1:A:134:GLY:H	1.75	0.51
1:A:144:PHE:C	1:A:146:LYS:H	2.14	0.51
1:A:141:HIS:HD2	1:A:207:LYS:HD3	1.74	0.51
1:A:27:PRO:CB	1:A:74:ALA:HB1	2.38	0.51
1:B:26:ARG:CB	3:B:602:ADP:N7	2.74	0.51
1:A:144:PHE:O	1:A:148:THR:HB	2.11	0.51
1:A:196:ILE:HG21	1:A:199:LEU:HG	1.93	0.51
1:A:343:LEU:HD11	1:A:347:LEU:HD11	1.93	0.50
1:A:40:ILE:HG21	1:A:340:SER:HB3	1.93	0.50
1:A:90:LEU:O	1:A:90:LEU:HD12	2.12	0.50
1:B:187:ASP:O	1:B:189:ARG:N	2.45	0.50
1:B:184:MET:CE	1:B:318:ARG:NE	2.71	0.50
1:B:26:ARG:HG3	1:B:26:ARG:O	2.11	0.50
1:B:194:VAL:HG13	1:B:195:ILE:N	2.27	0.50
1:A:255:LEU:HD12	1:A:257:LYS:CD	2.41	0.49
1:B:28:PHE:HB3	1:B:32:GLU:HB2	1.93	0.49
1:B:44:ASP:OD1	1:B:46:VAL:HG23	2.12	0.49
1:A:294:THR:CB	1:A:314:SER:HB3	2.43	0.49
1:A:343:LEU:HD12	1:A:347:LEU:HG	1.94	0.49
1:A:249:THR:C	1:A:251:ASP:H	2.15	0.49
1:A:322:ASP:O	1:A:326:GLY:HA3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASN:HD22	1:B:173:ASN:C	2.14	0.49
1:B:40:ILE:HD11	1:B:340:SER:HA	1.94	0.49
1:B:47:ARG:HG3	1:B:47:ARG:O	2.12	0.49
1:B:26:ARG:NH2	1:B:32:GLU:OE2	2.45	0.49
1:A:29:ASN:O	1:A:31:ALA:N	2.45	0.49
1:B:152:THR:HG23	1:B:247:GLU:HG2	1.94	0.49
1:B:173:ASN:HD22	1:B:175:SER:H	1.59	0.49
1:B:185:PHE:O	1:B:195:ILE:N	2.37	0.49
1:A:89:ILE:CG2	1:A:99:CYS:HB3	2.43	0.49
1:A:288:ILE:HG13	1:A:288:ILE:O	2.12	0.49
1:B:248:THR:HG22	1:B:252:GLY:O	2.13	0.49
1:A:22:VAL:HG23	1:A:333:ILE:HA	1.95	0.49
1:B:191:LYS:CA	1:B:191:LYS:NZ	2.76	0.49
1:A:113:PHE:O	1:A:117:GLY:HA2	2.13	0.48
1:B:120:SER:CA	1:B:132:LEU:HD12	2.41	0.48
1:B:169:PHE:HZ	1:B:181:ARG:NH1	2.11	0.48
1:B:54:THR:HA	1:B:343:LEU:HD11	1.95	0.48
1:A:20:GLN:OE1	1:A:329:ARG:NH2	2.41	0.48
1:A:327:ARG:O	1:A:362:LYS:HA	2.13	0.48
1:B:106:GLN:HE21	1:B:345:GLU:CB	2.27	0.48
4:B:605:MKK:H182	4:B:605:MKK:H262	1.62	0.48
1:A:34:LYS:C	1:A:36:SER:H	2.16	0.48
1:A:64:LYS:HG2	1:A:66:TYR:OH	2.13	0.48
1:A:92:GLU:O	1:A:95:MET:HG3	2.14	0.48
1:A:309:VAL:HG12	1:A:311:TYR:CD2	2.49	0.48
1:B:133:ALA:HB2	4:B:605:MKK:C20	2.44	0.48
1:A:44:ASP:OD2	1:A:47:ARG:HD3	2.13	0.48
1:A:22:VAL:HG12	1:A:70:MET:HB3	1.93	0.48
1:B:113:PHE:CE1	1:B:118:GLU:HG3	2.48	0.48
1:B:212:GLN:CG	1:B:216:LYS:NZ	2.77	0.48
1:A:96:GLY:HA2	1:A:258:ILE:O	2.14	0.48
1:A:237:SER:OG	1:A:265:ASP:HB3	2.13	0.47
1:A:247:GLU:CB	1:A:255:LEU:HB2	2.40	0.47
1:B:181:ARG:HH11	1:B:181:ARG:CG	2.21	0.47
1:B:77:LYS:O	1:B:80:ASP:HB2	2.14	0.47
1:B:26:ARG:O	1:B:338:PRO:HD3	2.15	0.47
1:A:89:ILE:HG23	1:A:99:CYS:HB3	1.97	0.47
1:B:47:ARG:HG2	1:B:49:GLU:CD	2.33	0.47
1:A:210:VAL:O	1:A:213:ILE:HB	2.14	0.47
1:B:216:LYS:O	1:B:220:LYS:HB2	2.14	0.47
1:B:289:ASN:HB3	1:B:292:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HG12	1:A:241:VAL:CA	2.44	0.47
1:A:196:ILE:CG2	1:A:199:LEU:HB2	2.44	0.47
1:B:33:ARG:HA	1:B:37:ALA:HB2	1.97	0.47
1:B:26:ARG:HB2	3:B:602:ADP:N7	2.30	0.47
1:B:147:LEU:CD2	1:B:150:ASN:ND2	2.78	0.47
1:B:57:LEU:HD13	1:B:59:ASP:HB2	1.97	0.47
1:B:57:LEU:HD12	1:B:60:LYS:H	1.80	0.47
1:A:164:TYR:O	1:A:165:ASN:HB3	2.14	0.47
1:A:26:ARG:HD3	3:A:601:ADP:C8	2.50	0.47
1:A:36:SER:OG	1:A:36:SER:O	2.29	0.47
1:B:63:ARG:HG2	1:B:63:ARG:HH11	1.78	0.47
1:A:105:GLY:O	1:A:111:LYS:HD3	2.15	0.46
1:A:70:MET:HE1	1:A:72:PHE:HZ	1.78	0.46
1:A:78:GLN:HG3	1:A:132:LEU:O	2.15	0.46
1:B:47:ARG:HH11	1:B:47:ARG:CG	2.27	0.46
1:B:87:CYS:HB3	1:B:88:PRO:CD	2.44	0.46
1:A:147:LEU:CB	1:A:154:PHE:CE2	2.95	0.46
1:A:224:ALA:HB1	1:A:228:MET:HE1	1.97	0.46
1:A:27:PRO:HB3	1:A:74:ALA:CB	2.42	0.46
1:B:142:GLN:HA	1:B:142:GLN:NE2	2.30	0.46
1:B:231:TYR:O	1:B:235:SER:OG	2.30	0.46
1:B:306:THR:HA	1:B:307:PRO:HD3	1.73	0.46
1:B:181:ARG:CG	1:B:181:ARG:NH1	2.76	0.46
1:B:164:TYR:CD1	1:B:228:MET:HG2	2.51	0.46
1:B:26:ARG:HB3	3:B:602:ADP:N7	2.30	0.46
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.79	0.46
1:A:92:GLU:HA	1:A:95:MET:HG3	1.96	0.46
1:B:206:ASN:C	1:B:208:ASP:H	2.18	0.46
1:B:221:ARG:O	1:B:224:ALA:HB3	2.15	0.46
1:A:154:PHE:HD1	1:A:155:SER:N	2.14	0.46
1:A:174:PRO:HD2	5:A:633:HOH:O	2.15	0.46
1:B:82:TYR:CE2	1:B:86:VAL:CG1	2.98	0.46
1:A:119:ARG:NH1	1:A:119:ARG:HG3	2.31	0.46
1:A:121:PRO:C	1:A:123:GLU:H	2.19	0.46
1:A:206:ASN:C	1:A:208:ASP:H	2.19	0.46
1:A:82:TYR:CE2	1:A:138:ARG:CB	2.98	0.46
1:B:129:GLU:O	1:B:131:PRO:HD3	2.15	0.46
1:B:188:PRO:HD2	1:B:189:ARG:H	1.81	0.46
1:B:343:LEU:HD22	1:B:347:LEU:HG	1.96	0.46
1:B:47:ARG:CZ	1:B:47:ARG:HB2	2.45	0.46
1:B:89:ILE:O	1:B:93:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HG3	1:A:119:ARG:HH11	1.81	0.46
1:A:147:LEU:HB2	1:A:154:PHE:CD2	2.51	0.46
1:B:345:GLU:HA	1:B:348:SER:HB2	1.98	0.45
1:B:52:VAL:O	1:B:63:ARG:HA	2.15	0.45
1:A:173:ASN:ND2	1:A:173:ASN:C	2.69	0.45
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.97	0.45
1:A:125:TYR:N	1:A:125:TYR:CD1	2.83	0.45
1:B:104:TYR:O	1:B:334:ALA:HA	2.17	0.45
1:B:173:ASN:C	1:B:173:ASN:ND2	2.70	0.45
1:A:247:GLU:HG2	1:A:248:THR:N	2.30	0.45
1:B:212:GLN:O	1:B:212:GLN:HG2	2.15	0.45
1:A:136:ILE:HG21	4:A:604:MKK:H5	1.98	0.45
1:B:341:LEU:CD2	1:B:342:ASN:ND2	2.79	0.45
1:B:169:PHE:CZ	1:B:181:ARG:NH1	2.85	0.45
1:A:299:ILE:CD1	1:A:359:ILE:HD11	2.45	0.45
1:A:82:TYR:OH	1:A:139:THR:HA	2.17	0.45
1:B:202:ILE:CD1	1:B:202:ILE:N	2.79	0.45
1:B:47:ARG:NH1	1:B:47:ARG:CG	2.80	0.45
1:B:230:ALA:O	1:B:234:ARG:HB2	2.17	0.44
1:A:192:ARG:O	1:A:321:GLN:NE2	2.51	0.44
1:A:28:PHE:CD2	1:A:32:GLU:HB2	2.52	0.44
1:A:81:VAL:O	1:A:85:VAL:HG13	2.17	0.44
1:A:145:GLU:O	1:A:145:GLU:HG3	2.17	0.44
1:A:303:VAL:C	1:A:305:ARG:H	2.21	0.44
1:A:92:GLU:HA	1:A:95:MET:HE3	2.00	0.44
1:A:98:ASN:C	1:A:328:THR:HG23	2.38	0.44
1:B:181:ARG:HG2	1:B:181:ARG:NH1	2.26	0.44
1:B:309:VAL:O	1:B:311:TYR:N	2.42	0.44
1:B:51:SER:HB3	1:B:63:ARG:HE	1.81	0.44
1:A:136:ILE:HD11	1:A:263:LEU:HB2	1.98	0.44
1:A:99:CYS:O	1:A:261:LEU:HA	2.17	0.44
1:A:78:GLN:HG3	1:A:132:LEU:C	2.37	0.44
1:B:186:ASP:HB3	1:B:191:LYS:HE3	1.99	0.44
1:B:294:THR:OG1	1:B:314:SER:HB3	2.17	0.44
1:B:18:ASN:HB2	1:B:360:LEU:HA	1.99	0.44
1:B:28:PHE:CZ	1:B:37:ALA:HB1	2.52	0.44
1:A:154:PHE:C	1:A:154:PHE:CD1	2.91	0.44
1:A:207:LYS:O	1:A:207:LYS:HG2	2.17	0.44
1:A:57:LEU:C	1:A:59:ASP:H	2.21	0.44
1:B:127:TRP:CD1	1:B:211:TYR:HB2	2.52	0.44
1:B:162:GLU:HG2	1:B:237:SER:CA	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG11	1:A:350:LEU:HD21	1.99	0.44
1:A:23:VAL:HG21	1:A:68:PHE:CE1	2.53	0.44
1:A:147:LEU:CB	1:A:154:PHE:CD2	3.01	0.44
1:A:156:VAL:HG12	1:A:243:ILE:HA	1.99	0.44
1:B:155:SER:O	1:B:243:ILE:HA	2.18	0.44
1:B:184:MET:CE	1:B:318:ARG:HH21	2.28	0.44
1:B:63:ARG:CG	1:B:63:ARG:HH11	2.28	0.44
1:A:323:SER:CB	1:A:330:THR:HG21	2.48	0.43
1:B:119:ARG:HD2	4:B:605:MKK:C20	2.47	0.43
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.79	0.43
1:A:289:ASN:HB3	1:A:292:LEU:CB	2.47	0.43
1:A:28:PHE:HD2	1:A:32:GLU:HB2	1.81	0.43
1:A:70:MET:HE3	1:A:84:SER:HB3	1.98	0.43
1:B:136:ILE:CG1	1:B:263:LEU:HD12	2.46	0.43
1:A:120:SER:HA	1:A:121:PRO:HD3	1.38	0.43
1:B:196:ILE:N	1:B:196:ILE:CD1	2.80	0.43
1:B:29:ASN:HB2	1:B:30:LEU:H	1.61	0.43
1:B:47:ARG:HG2	1:B:49:GLU:CG	2.48	0.43
1:A:107:THR:OG1	1:A:270:GLU:OE1	2.36	0.43
1:B:178:VAL:C	1:B:180:GLU:H	2.21	0.43
1:B:210:VAL:HG22	1:B:211:TYR:N	2.32	0.43
1:B:354:HIS:CE1	1:B:357:LYS:HZ1	2.37	0.43
1:B:25:CYS:CB	1:B:43:CYS:SG	3.07	0.43
1:B:53:ARG:HG3	1:B:63:ARG:NH1	2.32	0.43
1:B:106:GLN:HG2	1:B:107:THR:N	2.33	0.43
1:B:119:ARG:HA	1:B:119:ARG:HD2	1.76	0.43
1:B:165:ASN:O	1:B:165:ASN:ND2	2.51	0.43
1:A:224:ALA:HB1	1:A:228:MET:CE	2.49	0.43
1:A:292:LEU:HD12	1:A:292:LEU:HA	1.64	0.43
1:B:204:VAL:HG22	1:B:213:ILE:HD13	2.01	0.43
1:B:241:VAL:O	1:B:241:VAL:HG22	2.19	0.43
1:A:117:GLY:HA3	1:A:134:GLY:N	2.33	0.43
1:B:212:GLN:HG2	1:B:216:LYS:NZ	2.31	0.43
1:B:302:LEU:CD1	1:B:309:VAL:HG21	2.48	0.43
1:A:94:ILE:O	1:A:94:ILE:HG22	2.19	0.43
1:B:73:GLY:O	1:B:76:THR:OG1	2.37	0.43
1:A:227:LEU:HB3	1:A:228:MET:HG3	2.00	0.43
1:A:248:THR:HG22	1:A:248:THR:O	2.18	0.43
1:A:323:SER:HB3	1:A:330:THR:HG21	2.01	0.43
1:A:361:ASN:HB2	1:A:362:LYS:H	1.58	0.43
1:A:65:THR:O	1:A:65:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:HA	1:B:131:PRO:HD2	1.54	0.43
1:A:207:LYS:HB3	1:A:207:LYS:HE3	1.86	0.43
1:A:29:ASN:C	1:A:31:ALA:N	2.73	0.43
1:B:144:PHE:HZ	1:B:204:VAL:O	2.02	0.43
1:A:295:LEU:CD1	1:A:324:LEU:CD1	2.96	0.42
1:B:19:ILE:HD12	1:B:359:ILE:HG22	2.00	0.42
1:B:341:LEU:C	1:B:341:LEU:HD23	2.39	0.42
1:A:165:ASN:O	1:A:166:GLU:HB2	2.19	0.42
1:A:250:ILE:N	1:A:250:ILE:CD1	2.81	0.42
1:B:194:VAL:CG1	1:B:195:ILE:N	2.81	0.42
1:B:341:LEU:HD21	1:B:342:ASN:ND2	2.34	0.42
1:A:79:ILE:HD13	1:A:138:ARG:HH11	1.81	0.42
1:B:120:SER:HA	1:B:132:LEU:CD1	2.45	0.42
1:A:119:ARG:HA	1:A:119:ARG:HD2	1.63	0.42
1:A:166:GLU:OE1	1:A:291:SER:OG	2.35	0.42
1:B:210:VAL:O	1:B:213:ILE:N	2.49	0.42
1:B:92:GLU:CD	1:B:329:ARG:HD2	2.39	0.42
1:A:287:ASN:HA	1:A:287:ASN:HD22	1.62	0.42
1:B:143:ILE:HD11	1:B:243:ILE:HD11	2.00	0.42
1:A:316:LEU:O	1:A:320:LEU:N	2.51	0.42
1:A:204:VAL:CG2	1:A:213:ILE:CD1	2.95	0.42
1:A:156:VAL:CG1	1:A:243:ILE:HA	2.50	0.42
1:B:228:MET:HE2	1:B:228:MET:N	2.35	0.42
1:A:119:ARG:HD3	4:A:604:MKK:C20	2.50	0.42
1:B:163:ILE:HB	1:B:236:HIS:HB2	2.02	0.42
1:B:57:LEU:HB2	1:B:58:ALA:H	1.72	0.42
1:B:57:LEU:HD13	1:B:59:ASP:H	1.85	0.42
1:B:240:SER:OG	1:B:262:ASN:ND2	2.53	0.41
1:B:46:VAL:C	1:B:48:LYS:H	2.23	0.41
1:A:120:SER:N	1:A:130:ASP:OD1	2.25	0.41
1:B:147:LEU:HD22	1:B:150:ASN:ND2	2.35	0.41
1:A:136:ILE:CD1	1:A:263:LEU:CD1	2.98	0.41
1:A:34:LYS:CG	1:A:35:ALA:N	2.83	0.41
1:B:162:GLU:HA	1:B:236:HIS:O	2.20	0.41
1:B:248:THR:HG22	1:B:252:GLY:C	2.41	0.41
1:B:303:VAL:HG21	1:B:355:ARG:O	2.20	0.41
1:A:164:TYR:O	1:A:165:ASN:CB	2.67	0.41
1:A:299:ILE:HA	1:A:302:LEU:HD12	2.01	0.41
1:A:70:MET:CE	1:A:72:PHE:HZ	2.33	0.41
1:A:206:ASN:C	1:A:208:ASP:N	2.74	0.41
1:A:309:VAL:HG13	1:A:310:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG23	1:B:179:SER:N	2.36	0.41
1:B:200:GLU:OE2	1:B:200:GLU:HA	2.12	0.41
1:A:44:ASP:C	1:A:44:ASP:OD1	2.58	0.41
1:B:247:GLU:O	1:B:255:LEU:HG	2.20	0.41
1:B:119:ARG:CD	4:B:605:MKK:C20	2.98	0.41
1:A:83:ARG:NH1	1:A:83:ARG:HG2	2.35	0.41
1:B:164:TYR:O	1:B:165:ASN:HB3	2.20	0.41
1:B:72:PHE:HB3	1:B:76:THR:OG1	2.21	0.41
1:A:212:GLN:HG2	1:A:213:ILE:N	2.35	0.41
1:A:119:ARG:CD	4:A:604:MKK:C20	2.99	0.41
1:B:164:TYR:CD1	1:B:164:TYR:C	2.95	0.41
1:A:290:GLN:HA	1:A:290:GLN:OE1	2.20	0.41
1:A:74:ALA:C	1:A:76:THR:H	2.24	0.41
1:B:191:LYS:HZ3	1:B:191:LYS:CB	2.33	0.41
1:A:77:LYS:O	1:A:80:ASP:N	2.53	0.40
1:B:106:GLN:O	1:B:109:THR:HG23	2.21	0.40
1:A:167:GLU:HG2	1:A:181:ARG:CZ	2.51	0.40
1:A:18:ASN:CB	1:A:360:LEU:HA	2.51	0.40
1:A:44:ASP:CG	1:A:47:ARG:HG3	2.41	0.40
1:B:29:ASN:O	1:B:33:ARG:HD3	2.21	0.40
1:A:311:TYR:O	1:A:313:GLU:N	2.55	0.40
1:B:184:MET:HG3	1:B:318:ARG:HH21	1.84	0.40
1:A:254:GLU:H	1:A:254:GLU:HG3	1.66	0.40
1:A:309:VAL:CG1	1:A:311:TYR:CE2	3.05	0.40
1:B:21:VAL:C	1:B:22:VAL:HG13	2.41	0.40
1:B:52:VAL:HG11	1:B:347:LEU:HD21	2.02	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	326/367 (89%)	261 (80%)	44 (14%)	21 (6%)	1	8
1	B	326/367 (89%)	266 (82%)	46 (14%)	14 (4%)	3	18
All	All	652/734 (89%)	527 (81%)	90 (14%)	35 (5%)	2	13

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	135	ILE
1	A	145	GLU
1	A	177	ASP
1	A	189	ARG
1	A	312	ARG
1	B	149	ASP
1	B	179	SER
1	A	151	GLY
1	A	207	LYS
1	A	247	GLU
1	A	250	ILE
1	B	19	ILE
1	B	36	SER
1	B	123	GLU
1	B	189	ARG
1	B	249	THR
1	A	106	GLN
1	A	210	VAL
1	B	75	SER
1	B	76	THR
1	B	310	PRO
1	A	27	PRO
1	A	36	SER
1	A	137	PRO
1	A	57	LEU
1	B	46	VAL
1	B	187	ASP
1	B	188	PRO
1	B	266	LEU
1	A	249	THR
1	A	40	ILE
1	A	252	GLY
1	A	88	PRO
1	A	121	PRO

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	293/321 (91%)	208 (71%)	85 (29%)	0	2
1	B	293/321 (91%)	220 (75%)	73 (25%)	1	3
All	All	586/642 (91%)	428 (73%)	158 (27%)	0	2

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	20	GLN
1	A	26	ARG
1	A	36	SER
1	A	46	VAL
1	A	47	ARG
1	A	50	VAL
1	A	57	LEU
1	A	59	ASP
1	A	60	LYS
1	A	62	SER
1	A	64	LYS
1	A	65	THR
1	A	67	THR
1	A	70	MET
1	A	76	THR
1	A	79	ILE
1	A	83	ARG
1	A	87	CYS
1	A	90	LEU
1	A	95	MET
1	A	111	LYS
1	A	119	ARG
1	A	120	SER
1	A	125	TYR
1	A	136	ILE
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	148	THR
1	A	155	SER
1	A	156	VAL
1	A	157	LYS
1	A	160	LEU
1	A	161	LEU
1	A	168	LEU
1	A	173	ASN
1	A	175	SER
1	A	176	SER
1	A	177	ASP
1	A	179	SER
1	A	180	GLU
1	A	181	ARG
1	A	183	GLN
1	A	184	MET
1	A	192	ARG
1	A	199	LEU
1	A	202	ILE
1	A	206	ASN
1	A	212	GLN
1	A	216	LYS
1	A	221	ARG
1	A	223	THR
1	A	226	THR
1	A	227	LEU
1	A	228	MET
1	A	229	ASN
1	A	232	SER
1	A	233	SER
1	A	241	VAL
1	A	243	ILE
1	A	249	THR
1	A	250	ILE
1	A	254	GLU
1	A	255	LEU
1	A	257	LYS
1	A	258	ILE
1	A	260	LYS
1	A	269	SER
1	A	287	ASN
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	293	LEU
1	A	315	LYS
1	A	317	THR
1	A	319	ILE
1	A	321	GLN
1	A	323	SER
1	A	327	ARG
1	A	328	THR
1	A	330	THR
1	A	337	SER
1	A	340	SER
1	A	341	LEU
1	A	344	GLU
1	A	355	ARG
1	A	361	ASN
1	A	362	LYS
1	B	18	ASN
1	B	19	ILE
1	B	26	ARG
1	B	29	ASN
1	B	30	LEU
1	B	34	LYS
1	B	39	SER
1	B	47	ARG
1	B	49	GLU
1	B	50	VAL
1	B	51	SER
1	B	53	ARG
1	B	54	THR
1	B	57	LEU
1	B	59	ASP
1	B	60	LYS
1	B	61	SER
1	B	62	SER
1	B	64	LYS
1	B	75	SER
1	B	76	THR
1	B	87	CYS
1	B	89	ILE
1	B	90	LEU
1	B	95	MET
1	B	106	GLN

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Mol	Chain	Res	Type
1	B	127	TRP
1	B	128	GLU
1	B	152	THR
1	B	159	SER
1	B	160	LEU
1	B	168	LEU
1	B	171	LEU
1	B	173	ASN
1	B	176	SER
1	B	179	SER
1	B	181	ARG
1	B	184	MET
1	B	190	ASN
1	B	191	LYS
1	B	192	ARG
1	B	197	LYS
1	B	200	GLU
1	B	202	ILE
1	B	207	LYS
1	B	209	GLU
1	B	210	VAL
1	B	226	THR
1	B	227	LEU
1	B	228	MET
1	B	235	SER
1	B	237	SER
1	B	241	VAL
1	B	242	THR
1	B	247	GLU
1	B	248	THR
1	B	254	GLU
1	B	256	VAL
1	B	258	ILE
1	B	269	SER
1	B	271	ASN
1	B	289	ASN
1	B	293	LEU
1	B	302	LEU
1	B	312	ARG
1	B	321	GLN
1	B	327	ARG
1	B	337	SER

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Mol	Chain	Res	Type
1	B	341	LEU
1	B	343	LEU
1	B	348	SER
1	B	350	LEU
1	B	362	LYS

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	38	HIS
1	A	106	GLN
1	A	141	HIS
1	A	173	ASN
1	A	183	GLN
1	A	206	ASN
1	A	229	ASN
1	A	262	ASN
1	A	287	ASN
1	A	289	ASN
1	A	321	GLN
1	A	342	ASN
1	B	20	GLN
1	B	106	GLN
1	B	122	ASN
1	B	142	GLN
1	B	165	ASN
1	B	173	ASN
1	B	205	HIS
1	B	212	GLN
1	B	262	ASN
1	B	271	ASN
1	B	287	ASN
1	B	289	ASN
1	B	290	GLN
1	B	354	HIS

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ADP	A	601	2	25,29,29	2.26	8 (32%)	24,45,45	3.32	6 (25%)
4	MKK	A	604	-	33,37,37	3.15	20 (60%)	39,53,53	3.37	22 (56%)
3	ADP	B	602	2	25,29,29	2.01	5 (20%)	24,45,45	2.52	7 (29%)
4	MKK	B	605	-	33,37,37	2.70	14 (42%)	39,53,53	2.74	15 (38%)

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	ADP	A	601	2	1/1/6/6	0/12/32/32	0/3/3/3
4	MKK	A	604	-	-	0/25/50/50	0/4/4/4
3	ADP	B	602	2	-	0/12/32/32	0/3/3/3
4	MKK	B	605	-	-	0/25/50/50	0/4/4/4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	MKK	N4-N1	-4.58	1.25	1.37
4	A	604	MKK	N4-N1	-3.07	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	PB-O3A	-3.07	1.55	1.60
3	A	601	ADP	C8-N7	-2.99	1.29	1.34
4	A	604	MKK	F40-C4	-2.94	1.28	1.35
3	B	602	ADP	C8-N7	-2.31	1.30	1.34
4	A	604	MKK	C3-C4	-2.28	1.36	1.40
3	A	601	ADP	C5-C4	-2.21	1.35	1.40
3	A	601	ADP	PB-O2B	-2.15	1.46	1.54
3	A	601	ADP	C4-N3	-2.05	1.32	1.35
4	A	604	MKK	C18-C12	2.00	1.59	1.51
4	A	604	MKK	C7-C13	2.01	1.57	1.55
4	A	604	MKK	C18-N3	2.03	1.50	1.47
3	A	601	ADP	C5'-C4'	2.10	1.58	1.51
3	A	601	ADP	C3'-C4'	2.24	1.58	1.53
4	B	605	MKK	C13-C17	2.24	1.57	1.53
4	A	604	MKK	C12-N2	2.25	1.53	1.47
3	B	602	ADP	C2'-C1'	2.28	1.57	1.53
3	A	601	ADP	O2'-C2'	2.32	1.48	1.43
3	B	602	ADP	PA-O1A	2.48	1.60	1.50
4	A	604	MKK	C11-N2	2.71	1.53	1.47
4	B	605	MKK	C22-C23	2.77	1.44	1.38
4	B	605	MKK	C19-C17	2.79	1.43	1.39
4	B	605	MKK	C22-C21	2.85	1.45	1.38
4	A	604	MKK	C2-C1	3.02	1.44	1.39
4	B	605	MKK	C23-C17	3.10	1.44	1.39
4	B	605	MKK	C6-C1	3.12	1.47	1.38
4	A	604	MKK	C22-C23	3.39	1.45	1.38
4	A	604	MKK	C6-C5	3.55	1.45	1.38
4	A	604	MKK	C19-C17	3.57	1.45	1.39
4	A	604	MKK	C22-C21	3.60	1.46	1.38
4	A	604	MKK	C9-C29	3.61	1.57	1.50
4	B	605	MKK	C9-C29	3.62	1.57	1.50
4	B	605	MKK	C5-C4	3.72	1.45	1.37
4	A	604	MKK	C20-C19	3.92	1.46	1.38
4	A	604	MKK	C25-N3	4.09	1.48	1.35
4	B	605	MKK	C21-C20	4.68	1.49	1.38
4	B	605	MKK	C2-C1	4.84	1.47	1.39
4	A	604	MKK	C16-N3	4.91	1.55	1.47
4	B	605	MKK	C20-C19	4.97	1.48	1.38
4	B	605	MKK	C6-C5	5.33	1.48	1.38
4	A	604	MKK	C21-C20	5.68	1.51	1.38
4	B	605	MKK	C2-C3	5.90	1.49	1.39
4	A	604	MKK	C23-C17	6.06	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	O4'-C1'	7.31	1.51	1.41
4	A	604	MKK	C2-C3	7.80	1.52	1.39
3	A	601	ADP	O4'-C1'	8.77	1.53	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	ADP	C4'-O4'-C1'	-14.23	94.62	109.77
4	B	605	MKK	C26-C25-N3	-9.43	106.43	118.30
4	A	604	MKK	C9-C29-C24	-9.21	112.80	119.00
3	B	602	ADP	C4'-O4'-C1'	-7.95	101.31	109.77
4	A	604	MKK	C21-C22-C23	-6.78	110.88	120.21
4	A	604	MKK	C14-C13-C17	-5.41	101.47	111.76
3	B	602	ADP	O3B-PB-O1B	-5.35	89.56	110.50
4	A	604	MKK	C6-C5-C4	-4.90	113.79	119.01
4	B	605	MKK	C9-C29-C24	-4.81	115.76	119.00
4	A	604	MKK	C18-C12-N2	-4.71	101.11	110.63
4	A	604	MKK	C14-N4-N1	-4.37	103.41	111.79
4	A	604	MKK	C20-C19-C17	-4.29	116.13	120.77
4	B	605	MKK	C6-C5-C4	-4.22	114.52	119.01
4	B	605	MKK	C14-N4-N1	-3.91	104.30	111.79
3	B	602	ADP	O2'-C2'-C3'	-3.89	99.38	111.83
4	B	605	MKK	C12-C18-N3	-3.72	101.96	110.44
3	A	601	ADP	O3'-C3'-C2'	-3.48	100.67	111.83
4	B	605	MKK	C18-C12-N2	-3.34	103.87	110.63
4	A	604	MKK	F40-C4-C5	-3.10	111.58	118.49
4	A	604	MKK	C12-C18-N3	-2.98	103.66	110.44
4	B	605	MKK	C15-C16-N3	-2.96	103.70	110.44
3	A	601	ADP	O5'-PA-O1A	-2.91	97.51	109.25
4	B	605	MKK	C18-N3-C25	-2.77	115.51	122.96
3	B	602	ADP	O3'-C3'-C2'	-2.60	103.50	111.83
4	A	604	MKK	C8-C11-N2	-2.42	107.85	113.90
4	A	604	MKK	C18-N3-C25	-2.30	116.78	122.96
4	B	605	MKK	C8-C11-N2	-2.18	108.45	113.90
3	A	601	ADP	O3B-PB-O2B	2.05	115.88	107.61
4	B	605	MKK	O39-C29-C24	2.12	121.90	118.63
4	A	604	MKK	F40-C4-C3	2.16	120.36	118.40
4	B	605	MKK	C16-N3-C25	2.22	128.93	122.96
3	A	601	ADP	C5-C6-N6	2.30	125.16	120.47
3	B	602	ADP	O4'-C4'-C3'	2.55	110.23	105.17
4	A	604	MKK	C5-C4-C3	2.58	128.04	123.05
4	A	604	MKK	C5-C6-C1	2.84	125.15	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	605	MKK	C2-C3-C4	2.85	119.16	116.46
4	A	604	MKK	C23-C17-C19	2.96	122.43	117.94
4	A	604	MKK	C12-N2-C15	2.98	115.61	108.87
4	A	604	MKK	C16-N3-C25	3.01	131.03	122.96
3	B	602	ADP	O3B-PB-O2B	3.14	120.27	107.61
3	B	602	ADP	O3'-C3'-C4'	3.23	120.52	111.09
3	A	601	ADP	C2'-C3'-C4'	3.26	108.96	102.62
4	B	605	MKK	C22-C23-C17	3.48	124.52	120.77
4	B	605	MKK	C12-N2-C15	3.90	117.70	108.87
4	A	604	MKK	C22-C23-C17	3.95	125.03	120.77
4	A	604	MKK	C22-C21-C20	4.04	126.61	119.89
4	A	604	MKK	O1-C25-N3	4.26	126.71	121.02
4	A	604	MKK	C10-C1-C2	4.83	128.04	120.94
4	A	604	MKK	O39-C29-C24	5.11	126.51	118.63
4	B	605	MKK	O1-C25-N3	5.42	128.26	121.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	ADP	C1'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ADP	2	0
4	A	604	MKK	3	0
3	B	602	ADP	3	0
4	B	605	MKK	5	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.