



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:11 PM UTC

PDB ID : 9V16 / pdb_00009v16
Title : Crystal structure of E. coli glycogen phosphorylase N185A/R267E mutant in complex with AMP
Authors : Takai, M.; Shobu, K.; Fukuda, Y.; Inoue, T.
Deposited on : 2025-05-19
Resolution : 3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

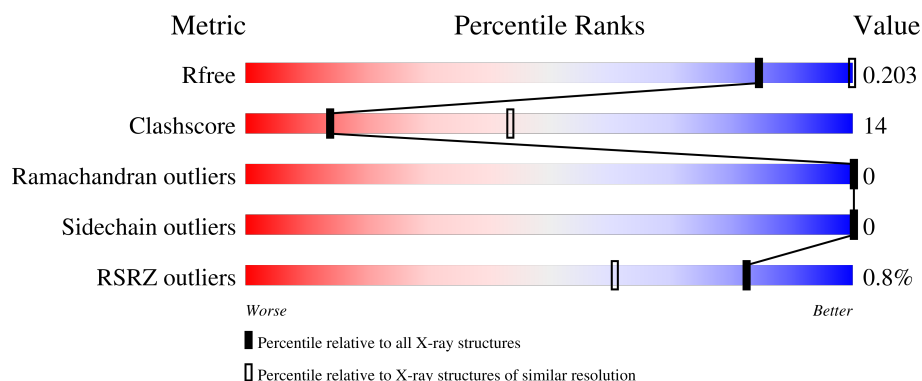
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	817	<div> <div>%</div> <div>67% 31% .</div> </div>
1	B	817	<div> <div>64% 32% .</div> </div>
1	C	817	<div> <div>%</div> <div>67% 29% .</div> </div>
1	D	817	<div> <div>%</div> <div>67% 30% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25769 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 Glycogen phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	P	S	0	0	0
			6478	4114	1121	1219	1	23			
1	B	791	Total	C	N	O	P	S	0	0	0
			6397	4058	1110	1205	1	23			
1	C	792	Total	C	N	O	P	S	0	0	0
			6405	4064	1111	1206	1	23			
1	D	791	Total	C	N	O	P	S	0	0	0
			6397	4058	1110	1205	1	23			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P0AC86
A	0	GLY	-	expression tag	UNP P0AC86
A	185	ALA	ASN	engineered mutation	UNP P0AC86
A	267	GLU	ARG	engineered mutation	UNP P0AC86
B	-1	MET	-	initiating methionine	UNP P0AC86
B	0	GLY	-	expression tag	UNP P0AC86
B	185	ALA	ASN	engineered mutation	UNP P0AC86
B	267	GLU	ARG	engineered mutation	UNP P0AC86
C	-1	MET	-	initiating methionine	UNP P0AC86
C	0	GLY	-	expression tag	UNP P0AC86
C	185	ALA	ASN	engineered mutation	UNP P0AC86
C	267	GLU	ARG	engineered mutation	UNP P0AC86
D	-1	MET	-	initiating methionine	UNP P0AC86
D	0	GLY	-	expression tag	UNP P0AC86
D	185	ALA	ASN	engineered mutation	UNP P0AC86
D	267	GLU	ARG	engineered mutation	UNP P0AC86

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).

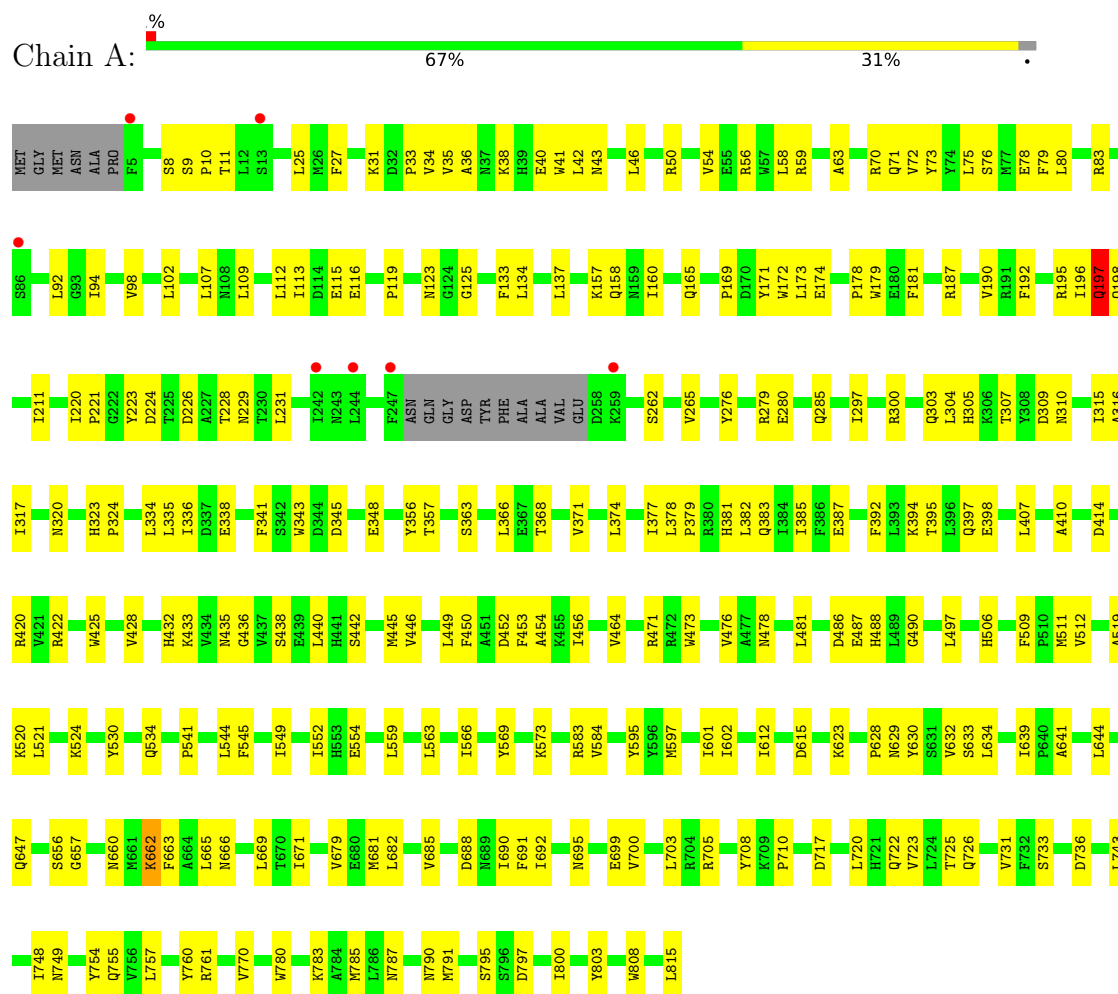


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

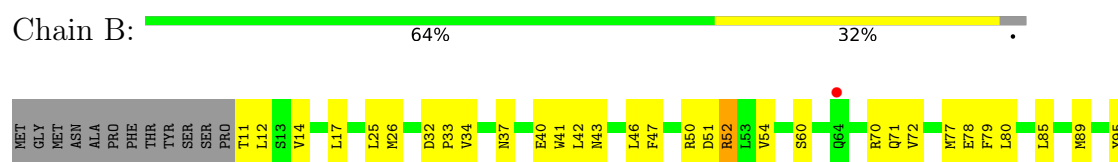
3 Residue-property plots

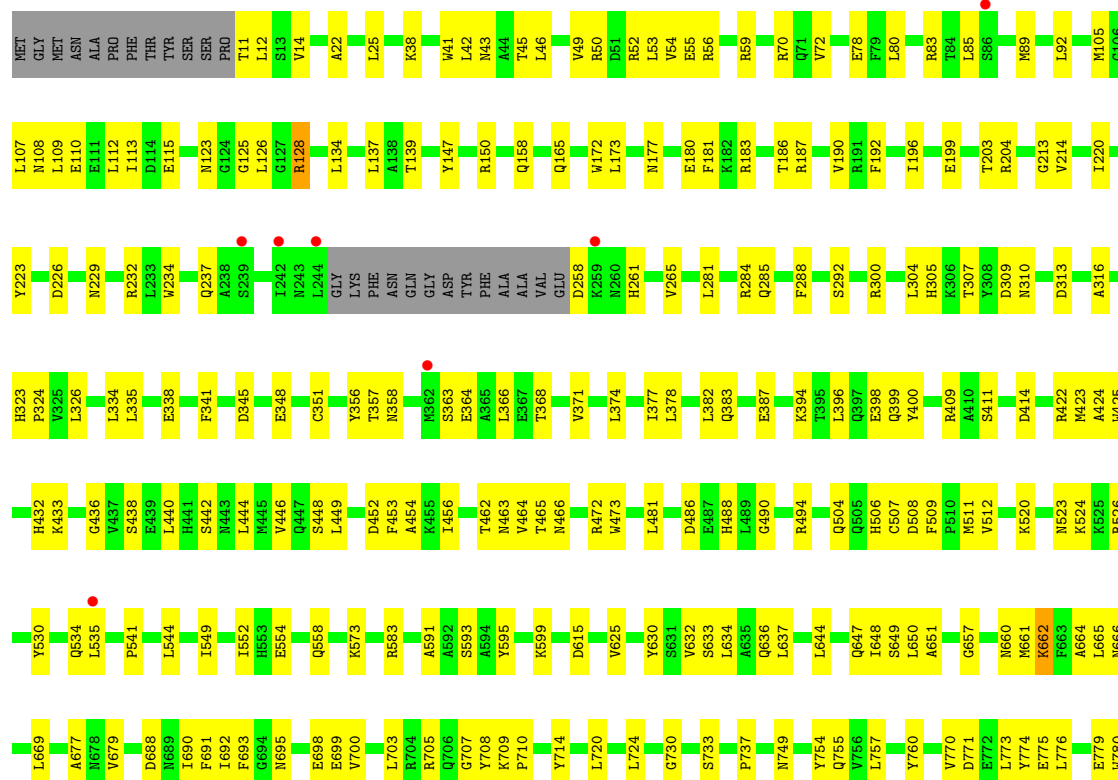
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

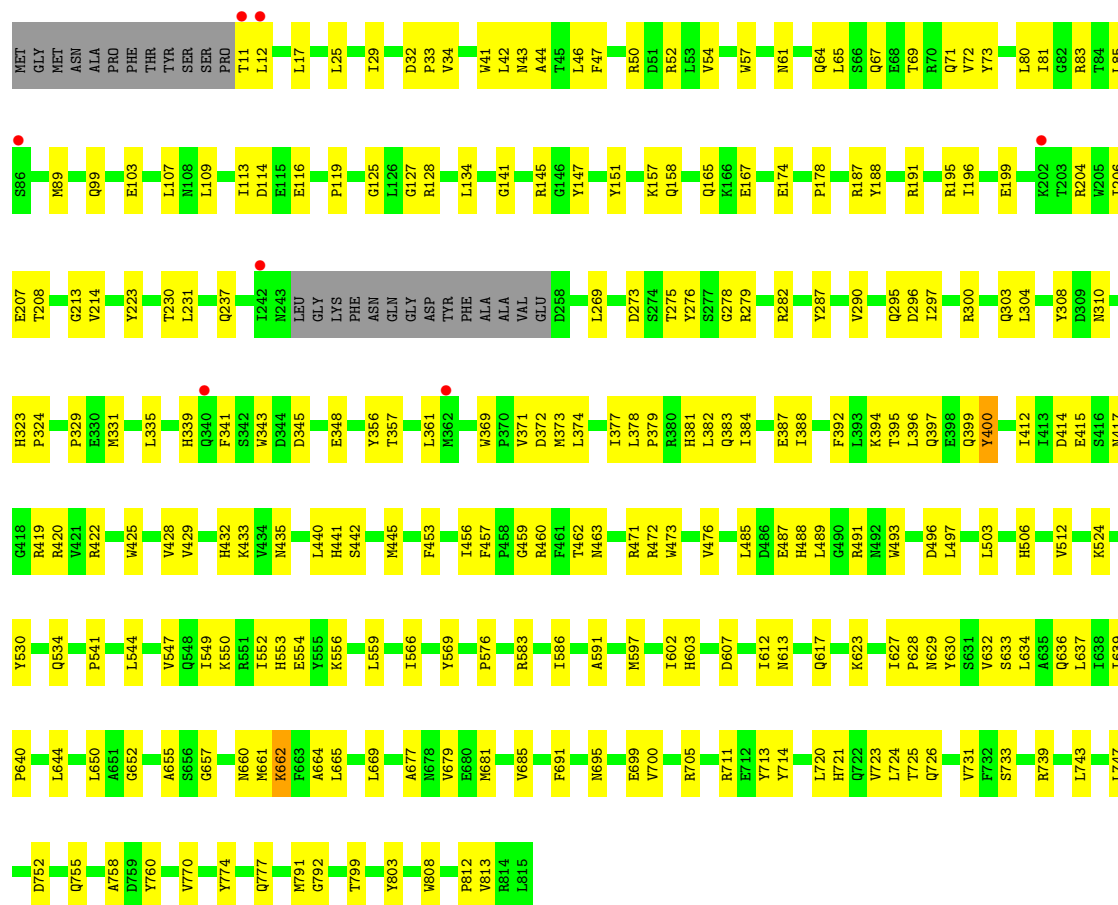
• Molecule 1: Glycogen phosphorylase



• Molecule 1: Glycogen phosphorylase







4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.60Å 185.60Å 451.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.45 49.45 – 3.45	Depositor EDS
% Data completeness (in resolution range)	94.6 (49.45-3.45) 94.5 (49.45-3.45)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.192 , 0.235 (Not available) , 0.203	Depositor DCC
R_{free} test set	4977 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25769	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, AMP

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	0.50	0/6598	0.78	3/8947 (0.0%)
1	B	0.49	0/6513	0.78	0/8832
1	C	0.53	0/6521	0.85	1/8843 (0.0%)
1	D	0.49	0/6513	0.77	0/8832
All	All	0.50	0/26145	0.80	4/35454 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLN	CA-CB-CG	7.37	128.84	114.10
1	A	224	ASP	CA-C-N	5.43	131.92	121.54
1	A	224	ASP	C-N-CA	5.43	131.92	121.54
1	C	801	LYS	CA-CB-CG	5.07	124.24	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	GLN	Peptide
1	B	52	ARG	Sidechain
1	C	128	ARG	Sidechain
1	D	400	TYR	Peptide
1	D	491	ARG	Peptide

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	6478	0	6339	186	0
1	B	6397	0	6261	204	1
1	C	6405	0	6272	180	1
1	D	6397	0	6261	170	0
2	A	23	0	12	3	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	3	0
All	All	25769	0	25181	731	1

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 14.

All (731) 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:C:139:THR:HG22	1:C:223:TYR:H	1.12	1.10
1:B:17:LEU:HD21	1:B:52:ARG:HH12	1.25	1.01
1:D:206:ILE:HD12	1:D:207:GLU:HG3	1.44	1.00
1:D:196:ILE:HD11	1:D:379:PRO:HB2	1.43	0.98
1:B:657:GLY:H	1:B:677:ALA:HB2	1.36	0.89
1:A:56:ARG:HD3	1:A:226:ASP:HA	1.53	0.88
1:C:80:LEU:HD22	1:C:632:VAL:HG23	1.56	0.87
1:C:414:ASP:HB2	1:C:422:ARG:HH11	1.45	0.81
1:B:134:LEU:HD11	1:B:231:LEU:HD13	1.63	0.80
1:D:657:GLY:H	1:D:677:ALA:HB2	1.46	0.80
1:A:506:HIS:HB3	1:A:512:VAL:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ASN:HB3	1:B:699:GLU:HB2	1.66	0.77
1:B:506:HIS:HB3	1:B:512:VAL:HG21	1.66	0.77
1:D:552:ILE:HB	1:D:591:ALA:HB2	1.67	0.77
1:D:695:ASN:HB3	1:D:699:GLU:HB2	1.65	0.77
1:C:535:LEU:HD13	1:C:625:VAL:HG13	1.66	0.76
1:B:776:LEU:HB3	1:B:779:GLU:HB3	1.68	0.76
1:A:394:LYS:O	1:A:398:GLU:HG3	1.86	0.75
1:D:440:LEU:HD22	1:D:679:VAL:HG21	1.69	0.74
1:A:187:ARG:HH22	1:B:174:GLU:HG2	1.52	0.74
1:C:56:ARG:NH2	1:C:92:LEU:HA	2.03	0.74
1:B:662:LLP:NZ	1:B:662:LLP:O3	2.18	0.73
1:C:647:GLN:CD	1:C:660:ASN:HB3	2.12	0.73
1:C:80:LEU:HD22	1:C:632:VAL:CG2	2.18	0.73
1:A:552:ILE:HG13	1:A:602:ILE:HD11	1.70	0.73
1:C:53:LEU:HD23	1:C:92:LEU:HD21	1.70	0.73
1:A:414:ASP:HB2	1:A:422:ARG:HE	1.53	0.73
1:B:196:ILE:HD11	1:B:379:PRO:HB2	1.71	0.72
1:A:488:HIS:CD2	1:A:512:VAL:HG22	2.25	0.72
1:A:38:LYS:HD3	1:A:115:GLU:OE1	1.88	0.72
1:A:43:ASN:HA	1:A:46:LEU:HD12	1.71	0.71
1:B:557:ARG:HH12	1:B:759:ASP:HB2	1.55	0.71
1:C:304:LEU:HB3	1:C:305:HIS:CD2	2.25	0.71
1:A:158:GLN:HG3	1:A:165:GLN:HG3	1.73	0.71
1:B:471:ARG:HG3	1:B:471:ARG:HH11	1.55	0.71
1:D:11:THR:HG22	1:D:12:LEU:H	1.53	0.71
1:B:488:HIS:CD2	1:B:512:VAL:HG22	2.26	0.70
1:D:597:MET:HE1	1:D:743:LEU:HA	1.74	0.70
1:A:80:LEU:HD22	1:A:632:VAL:CG2	2.21	0.70
1:A:425:TRP:CD1	1:A:453:PHE:HZ	2.10	0.69
1:C:363:SER:HB3	1:C:449:LEU:HD13	1.74	0.69
1:D:524:LYS:HE2	1:D:541:PRO:O	1.92	0.69
1:B:726:GLN:HB3	1:B:731:VAL:CG1	2.23	0.69
1:C:139:THR:HG22	1:C:223:TYR:N	1.98	0.69
1:C:38:LYS:HD3	1:C:115:GLU:OE1	1.93	0.69
1:C:688:ASP:O	1:C:783:LYS:NZ	2.26	0.69
1:C:554:GLU:HG3	1:C:595:TYR:OH	1.93	0.69
1:B:17:LEU:HD21	1:B:52:ARG:NH1	2.04	0.68
1:B:726:GLN:HB3	1:B:731:VAL:HG11	1.74	0.68
1:D:134:LEU:HD11	1:D:231:LEU:HD13	1.75	0.68
1:A:647:GLN:CD	1:A:660:ASN:HB3	2.18	0.68
1:D:471:ARG:O	1:D:476:VAL:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:HIS:CD2	1:D:512:VAL:HG22	2.29	0.68
1:A:50:ARG:NH1	1:A:178:PRO:O	2.28	0.67
1:D:331:MET:HE3	1:D:335:LEU:HD11	1.76	0.67
1:D:550:LYS:HE3	1:D:556:LYS:HD2	1.76	0.67
1:C:506:HIS:HB3	1:C:512:VAL:HG21	1.77	0.67
1:B:396:LEU:HD22	1:B:406:LEU:HD21	1.76	0.67
1:B:524:LYS:HE2	1:B:541:PRO:O	1.95	0.67
1:D:25:LEU:HD23	1:D:33:PRO:HG3	1.77	0.67
1:A:304:LEU:HB3	1:A:305:HIS:CD2	2.30	0.67
1:D:377:ILE:HG22	1:D:378:LEU:HG	1.77	0.67
1:C:549:ILE:HD12	1:C:630:TYR:HE1	1.60	0.67
1:C:438:SER:HA	1:C:465:THR:HG23	1.77	0.66
1:C:776:LEU:HB2	1:C:779:GLU:HB2	1.77	0.66
1:C:720:LEU:HD21	1:C:757:LEU:HD22	1.77	0.66
1:C:411:SER:O	1:C:422:ARG:NH2	2.28	0.66
1:D:195:ARG:NE	1:D:207:GLU:OE2	2.29	0.66
1:A:524:LYS:HE2	1:A:541:PRO:O	1.97	0.65
1:B:504:GLN:HA	1:B:507:CYS:SG	2.36	0.65
1:D:506:HIS:HB3	1:D:512:VAL:HG21	1.79	0.65
1:B:80:LEU:HB2	1:B:127:GLY:HA3	1.78	0.65
1:B:511:MET:HE2	1:B:511:MET:HA	1.78	0.65
1:C:139:THR:CG2	1:C:223:TYR:H	2.01	0.65
1:A:125:GLY:HA2	1:A:662:LLP:H5'2	1.78	0.65
1:B:334:LEU:HD23	1:B:338:GLU:HG3	1.78	0.65
1:C:43:ASN:HA	1:C:46:LEU:HD12	1.78	0.65
1:D:329:PRO:HB2	1:D:381:HIS:HD2	1.62	0.65
1:D:569:TYR:CD2	1:D:612:ILE:HG12	2.32	0.64
1:A:80:LEU:HD22	1:A:632:VAL:HG23	1.78	0.64
1:C:42:LEU:HB2	1:C:112:LEU:HD22	1.78	0.64
1:A:383:GLN:O	1:A:387:GLU:HG3	1.98	0.64
1:A:554:GLU:HG3	1:A:595:TYR:OH	1.97	0.64
1:B:411:SER:O	1:B:422:ARG:NH2	2.27	0.64
1:A:377:ILE:HG22	1:A:378:LEU:HG	1.80	0.64
1:A:56:ARG:NH2	1:A:92:LEU:HA	2.13	0.63
1:B:271:PRO:HG3	1:B:281:LEU:HD23	1.78	0.63
1:B:557:ARG:HH21	1:B:650:LEU:HA	1.61	0.63
1:D:713:TYR:CE2	1:D:758:ALA:HA	2.33	0.63
1:A:425:TRP:CD1	1:A:453:PHE:CZ	2.87	0.63
1:D:80:LEU:HD22	1:D:632:VAL:CG2	2.28	0.63
1:D:559:LEU:HD11	1:D:743:LEU:HD21	1.81	0.63
1:D:191:ARG:HD3	1:D:208:THR:OG1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:O	1:A:113:ILE:HG13	2.00	0.62
1:A:300:ARG:HD2	2:A:901:AMP:H5'1	1.80	0.62
1:B:298:LEU:HD21	1:B:331:MET:HE1	1.82	0.62
1:C:549:ILE:HD12	1:C:630:TYR:CE1	2.34	0.62
1:A:345:ASP:O	1:A:348:GLU:HB3	2.00	0.62
1:C:22:ALA:HB2	1:C:105:MET:HE1	1.82	0.62
1:A:440:LEU:HD22	1:A:679:VAL:HG21	1.82	0.61
1:D:43:ASN:HA	1:D:46:LEU:HD12	1.82	0.61
1:D:714:TYR:O	1:D:721:HIS:HB2	2.00	0.61
1:B:196:ILE:CD1	1:B:379:PRO:HB2	2.29	0.61
1:B:11:THR:HG22	1:B:12:LEU:HD12	1.82	0.61
1:A:221:PRO:HA	1:A:228:THR:HG22	1.83	0.61
1:A:368:THR:HG22	1:A:422:ARG:HA	1.83	0.61
1:A:597:MET:HA	1:A:597:MET:HE2	1.83	0.61
1:A:438:SER:HB3	1:A:656:SER:HB2	1.82	0.61
1:B:595:TYR:HD1	1:B:598:ALA:H	1.48	0.61
1:A:559:LEU:HB2	1:A:601:ILE:HD13	1.83	0.60
1:D:726:GLN:HB3	1:D:731:VAL:CG1	2.31	0.60
1:B:714:TYR:CZ	1:B:721:HIS:CD2	2.88	0.60
1:B:147:TYR:HE1	1:B:232:ARG:HD2	1.66	0.60
1:B:363:SER:HB3	1:B:449:LEU:HG	1.83	0.60
1:B:331:MET:HE3	1:B:335:LEU:HD11	1.83	0.60
1:D:472:ARG:HD3	1:D:636:GLN:OE1	2.02	0.60
1:A:223:TYR:HB2	1:A:471:ARG:HD2	1.82	0.60
1:A:300:ARG:HH11	2:A:901:AMP:H5'1	1.66	0.60
1:B:544:LEU:HB3	1:B:583:ARG:HG3	1.83	0.60
1:C:488:HIS:CD2	1:C:512:VAL:HG22	2.36	0.60
1:C:436:GLY:HA3	1:C:442:SER:OG	2.01	0.60
1:D:488:HIS:HD2	1:D:512:VAL:HG22	1.64	0.59
1:B:80:LEU:HD22	1:B:632:VAL:CG2	2.32	0.59
1:D:691:PHE:CE2	1:D:770:VAL:HG22	2.37	0.59
1:A:374:LEU:HD23	1:A:382:LEU:HD13	1.84	0.59
1:A:452:ASP:O	1:A:456:ILE:HG13	2.03	0.59
1:B:287:TYR:HA	1:B:290:VAL:HG22	1.84	0.59
1:B:597:MET:HE1	1:B:743:LEU:HA	1.84	0.59
1:B:657:GLY:HA3	1:B:660:ASN:OD1	2.01	0.59
1:B:25:LEU:HD23	1:B:33:PRO:HG3	1.85	0.59
1:B:271:PRO:HD2	1:B:282:ARG:HG2	1.85	0.59
1:C:664:ALA:HB3	1:C:791:MET:HE2	1.85	0.59
1:D:457:PHE:HB3	1:D:460:ARG:HG3	1.84	0.59
1:A:56:ARG:HH22	1:A:92:LEU:HA	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:VAL:HG22	1:D:586:ILE:HB	1.85	0.59
1:D:187:ARG:HA	1:D:213:GLY:O	2.03	0.59
1:C:56:ARG:HD3	1:C:226:ASP:HA	1.84	0.59
1:C:473:TRP:CD2	1:C:662:LLP:HD2	2.39	0.58
1:B:223:TYR:HB2	1:B:471:ARG:HD3	1.84	0.58
1:D:544:LEU:HB3	1:D:583:ARG:HG3	1.85	0.58
1:A:486:ASP:HA	1:A:490:GLY:O	2.03	0.58
1:A:520:LYS:NZ	1:A:666:ASN:O	2.28	0.58
1:B:470:PRO:HD2	1:B:471:ARG:NH1	2.19	0.58
1:B:568:ARG:HH22	1:B:581:VAL:HB	1.68	0.58
1:B:50:ARG:O	1:B:54:VAL:HG23	2.03	0.58
1:C:524:LYS:HE2	1:C:541:PRO:O	2.04	0.58
1:C:158:GLN:HG3	1:C:165:GLN:HG3	1.86	0.57
1:D:412:ILE:HD11	1:D:429:VAL:HG21	1.85	0.57
1:C:364:GLU:CD	1:C:364:GLU:H	2.12	0.57
1:D:343:TRP:NE1	1:D:387:GLU:OE1	2.37	0.57
1:A:509:PHE:C	1:A:511:MET:H	2.12	0.57
1:A:720:LEU:HD21	1:A:757:LEU:HD22	1.86	0.57
1:B:80:LEU:HD22	1:B:632:VAL:HG21	1.86	0.57
1:B:714:TYR:O	1:B:721:HIS:HB2	2.04	0.57
1:C:414:ASP:HB2	1:C:422:ARG:NH1	2.16	0.57
1:B:468:VAL:HG11	1:B:662:LLP:HG2	1.86	0.57
1:C:41:TRP:CD2	1:C:107:LEU:HD11	2.40	0.57
1:C:323:HIS:HB2	1:C:324:PRO:HD3	1.87	0.56
1:C:509:PHE:HB2	1:C:512:VAL:HG23	1.88	0.56
1:B:43:ASN:HA	1:B:46:LEU:HD12	1.86	0.56
1:C:83:ARG:HG3	1:C:633:SER:OG	2.04	0.56
1:C:593:SER:HA	1:C:599:LYS:HD2	1.87	0.56
1:C:56:ARG:HH22	1:C:92:LEU:HA	1.68	0.56
1:C:199:GLU:OE1	1:C:204:ARG:HD2	2.05	0.56
1:A:569:TYR:CD2	1:A:612:ILE:HG12	2.40	0.56
1:D:392:PHE:O	1:D:395:THR:HB	2.06	0.56
1:A:357:THR:HA	1:A:435:ASN:HB3	1.88	0.56
1:B:46:LEU:HD23	1:B:85:LEU:HD13	1.88	0.56
1:C:126:LEU:HD23	1:C:126:LEU:O	2.06	0.56
1:B:601:ILE:O	1:B:605:ILE:HG13	2.05	0.56
1:A:195:ARG:NH1	1:A:197:GLN:HG2	2.21	0.56
1:B:171:TYR:O	1:B:174:GLU:HB2	2.04	0.56
1:C:265:VAL:HG13	1:C:285:GLN:HA	1.88	0.56
1:B:211:ILE:HD13	1:B:262:SER:HB2	1.87	0.55
1:D:329:PRO:HB2	1:D:381:HIS:CD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:THR:HB	1:C:14:VAL:HG23	1.87	0.55
1:A:497:LEU:HD21	1:A:665:LEU:HD11	1.87	0.55
1:A:80:LEU:HD22	1:A:632:VAL:HG21	1.88	0.55
1:A:722:GLN:O	1:A:725:THR:HB	2.07	0.55
1:B:491:ARG:HH11	1:B:491:ARG:HB3	1.72	0.55
1:B:580:TRP:O	1:B:582:PRO:HD3	2.06	0.55
1:C:573:LYS:HD3	1:C:615:ASP:OD2	2.06	0.55
1:D:80:LEU:HD22	1:D:632:VAL:HG23	1.88	0.55
1:D:83:ARG:NH2	1:D:114:ASP:HA	2.22	0.55
1:D:145:ARG:NH1	2:D:901:AMP:O1P	2.30	0.55
1:C:509:PHE:C	1:C:511:MET:H	2.14	0.55
1:A:54:VAL:O	1:A:58:LEU:HG	2.06	0.55
1:B:273:ASP:HB2	1:B:279:ARG:CG	2.37	0.55
1:C:425:TRP:CD1	1:C:453:PHE:HZ	2.25	0.55
1:C:647:GLN:OE1	1:C:660:ASN:HB3	2.07	0.55
1:B:125:GLY:HA2	1:B:662:LLP:H5'2	1.88	0.55
1:B:187:ARG:HA	1:B:213:GLY:O	2.05	0.55
1:C:396:LEU:HD21	1:C:456:ILE:HD13	1.89	0.55
1:D:57:TRP:HE1	1:D:230:THR:CG2	2.20	0.55
1:D:223:TYR:HB2	1:D:471:ARG:HD3	1.88	0.54
1:D:11:THR:HG22	1:D:12:LEU:N	2.22	0.54
1:A:549:ILE:HD12	1:A:630:TYR:HE1	1.71	0.54
1:C:554:GLU:HB2	1:C:754:TYR:CD2	2.42	0.54
1:D:69:THR:HG21	1:D:813:VAL:HG22	1.89	0.54
1:C:109:LEU:O	1:C:113:ILE:HG13	2.08	0.54
1:D:473:TRP:CD2	1:D:662:LLP:HD2	2.42	0.54
1:B:203:THR:HG21	1:B:383:GLN:HE22	1.73	0.54
1:C:334:LEU:HD23	1:C:338:GLU:HG3	1.88	0.54
1:C:481:LEU:HD12	1:C:481:LEU:O	2.06	0.54
1:B:394:LYS:HA	1:B:397:GLN:HB2	1.89	0.54
1:D:276:TYR:CE2	1:D:373:MET:HE2	2.43	0.54
1:D:279:ARG:HG2	1:D:369:TRP:HZ3	1.73	0.54
1:C:440:LEU:O	1:C:444:LEU:HG	2.07	0.54
1:A:363:SER:O	1:A:366:LEU:HB2	2.09	0.53
1:B:25:LEU:O	1:B:25:LEU:HG	2.07	0.53
1:B:158:GLN:NE2	1:B:590:LYS:HA	2.24	0.53
1:A:46:LEU:HD22	1:A:179:TRP:NE1	2.24	0.53
1:B:534:GLN:O	1:B:535:LEU:HD23	2.08	0.53
1:B:793:TYR:HE1	1:B:798:ARG:HD3	1.74	0.53
1:D:287:TYR:HA	1:D:290:VAL:HG22	1.91	0.53
1:B:441:HIS:C	1:B:441:HIS:CD2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:HH22	1:B:174:GLU:CG	2.20	0.53
1:C:552:ILE:HB	1:C:591:ALA:HB2	1.90	0.53
1:C:657:GLY:HA3	1:C:660:ASN:HD21	1.74	0.53
1:A:75:LEU:O	1:A:320:ASN:HB2	2.09	0.53
1:A:195:ARG:HH12	1:A:197:GLN:HG2	1.74	0.53
1:A:307:THR:HG23	1:A:309:ASP:H	1.74	0.53
1:B:481:LEU:O	1:B:485:LEU:HG	2.08	0.53
1:D:125:GLY:HA2	1:D:662:LLP:H5'2	1.91	0.53
1:C:448:SER:OG	1:C:449:LEU:N	2.41	0.53
1:D:64:GLN:HG2	1:D:813:VAL:HG21	1.91	0.53
1:A:371:VAL:HG13	1:A:382:LEU:HD21	1.90	0.52
1:D:32:ASP:OD1	1:D:34:VAL:HG23	2.09	0.52
1:A:688:ASP:O	1:A:783:LYS:NZ	2.38	0.52
1:B:569:TYR:CD2	1:B:612:ILE:HG12	2.43	0.52
1:C:695:ASN:HB3	1:C:699:GLU:HB2	1.91	0.52
1:B:47:PHE:CE2	1:B:178:PRO:HB3	2.44	0.52
1:B:489:LEU:HD11	1:B:503:LEU:HB2	1.91	0.52
1:D:83:ARG:HG3	1:D:633:SER:OG	2.09	0.52
1:A:690:ILE:HG23	1:A:692:ILE:HG12	1.91	0.52
1:B:155:MET:HG2	1:B:156:PHE:CD1	2.44	0.52
1:D:530:TYR:CZ	1:D:534:GLN:HG3	2.45	0.52
1:B:657:GLY:N	1:B:677:ALA:HB2	2.15	0.52
1:C:356:TYR:CD1	1:C:357:THR:N	2.78	0.52
1:D:485:LEU:O	1:D:489:LEU:HB2	2.10	0.52
1:C:733:SER:O	1:C:733:SER:OG	2.24	0.51
1:B:273:ASP:HB2	1:B:279:ARG:HG2	1.91	0.51
1:B:557:ARG:NH2	1:B:650:LEU:HA	2.24	0.51
1:D:664:ALA:HB3	1:D:791:MET:HE2	1.90	0.51
1:B:450:PHE:O	1:B:453:PHE:N	2.41	0.51
1:C:552:ILE:HD13	1:C:558:GLN:NE2	2.25	0.51
1:D:425:TRP:O	1:D:429:VAL:HG23	2.10	0.51
1:D:473:TRP:CE2	1:D:662:LLP:HD2	2.45	0.51
1:C:472:ARG:HD3	1:C:636:GLN:OE1	2.11	0.51
1:A:72:VAL:HG21	1:A:808:TRP:CD2	2.46	0.51
1:A:554:GLU:HB2	1:A:754:TYR:CD2	2.46	0.51
1:B:549:ILE:HD12	1:B:630:TYR:HE1	1.76	0.51
1:C:368:THR:HG22	1:C:422:ARG:HA	1.92	0.51
1:C:394:LYS:O	1:C:398:GLU:HG3	2.10	0.51
1:D:41:TRP:CD2	1:D:107:LEU:HD11	2.46	0.51
1:A:304:LEU:HB3	1:A:305:HIS:HD2	1.76	0.51
1:B:535:LEU:O	1:B:537:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:LEU:O	1:B:746:SER:OG	2.22	0.51
1:B:488:HIS:HD2	1:B:512:VAL:HG22	1.71	0.51
1:D:399:GLN:C	1:D:400:TYR:HD1	2.19	0.51
1:A:669:LEU:HD12	1:A:780:TRP:CE2	2.47	0.50
1:B:720:LEU:HB2	1:B:760:TYR:CE2	2.46	0.50
1:A:685:VAL:HG12	1:A:790:ASN:HB2	1.91	0.50
1:B:793:TYR:CE1	1:B:798:ARG:HD3	2.46	0.50
1:D:552:ILE:HG13	1:D:602:ILE:HD11	1.93	0.50
1:A:76:SER:HB3	1:A:79:PHE:CE1	2.46	0.50
1:A:102:LEU:HD22	1:A:107:LEU:HD12	1.94	0.50
1:D:493:TRP:HA	1:D:496:ASP:O	2.12	0.50
1:B:191:ARG:HD3	1:B:208:THR:OG1	2.12	0.50
1:A:31:LYS:HD3	1:B:183:ARG:NH1	2.27	0.50
1:A:573:LYS:HD3	1:A:615:ASP:OD2	2.12	0.50
1:B:11:THR:N	1:B:14:VAL:HB	2.27	0.50
1:C:544:LEU:HD12	1:C:774:TYR:CG	2.47	0.50
1:D:188:TYR:HB3	1:D:295:GLN:OE1	2.12	0.50
1:A:157:LYS:HG3	1:A:629:ASN:ND2	2.27	0.50
1:A:473:TRP:CD2	1:A:662:LLP:HD2	2.46	0.50
1:B:561:ASN:O	1:B:565:VAL:HG23	2.12	0.50
1:A:119:PRO:HA	1:A:172:TRP:CE3	2.46	0.50
1:B:89:MET:HE3	1:B:95:TYR:CD2	2.46	0.50
1:B:713:TYR:CE2	1:B:758:ALA:HA	2.47	0.50
1:C:304:LEU:HB3	1:C:305:HIS:HD2	1.75	0.50
1:A:190:VAL:HG12	1:A:192:PHE:CE1	2.47	0.50
1:C:187:ARG:HH22	1:D:174:GLU:HG2	1.77	0.50
1:C:326:LEU:HG	1:C:423:MET:HE1	1.94	0.50
1:C:720:LEU:HB2	1:C:760:TYR:CE2	2.47	0.50
1:A:323:HIS:HB2	1:A:324:PRO:HD3	1.93	0.50
1:C:583:ARG:NH2	1:C:771:ASP:OD1	2.38	0.50
1:C:714:TYR:CD1	1:C:724:LEU:HD12	2.46	0.50
1:D:361:LEU:HD13	1:D:652:GLY:O	2.12	0.50
1:C:72:VAL:HG21	1:C:808:TRP:CD2	2.47	0.49
1:C:371:VAL:HG13	1:C:382:LEU:HD21	1.94	0.49
1:C:703:LEU:O	1:C:703:LEU:HD23	2.11	0.49
1:D:394:LYS:HA	1:D:397:GLN:HB2	1.92	0.49
1:C:707:GLY:O	1:C:709:LYS:HG3	2.12	0.49
1:A:549:ILE:HD12	1:A:630:TYR:CE1	2.47	0.49
1:C:356:TYR:CZ	1:C:358:ASN:HB2	2.47	0.49
1:D:25:LEU:O	1:D:25:LEU:HG	2.13	0.49
1:B:273:ASP:HB3	1:B:282:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:CYS:O	1:C:432:HIS:HB3	2.13	0.49
1:A:83:ARG:HG3	1:A:633:SER:OG	2.12	0.49
1:C:377:ILE:HG22	1:C:378:LEU:HG	1.95	0.49
1:D:50:ARG:O	1:D:54:VAL:HG23	2.11	0.49
1:A:125:GLY:CA	1:A:662:LLP:H5'2	2.42	0.49
1:C:504:GLN:HA	1:C:507:CYS:SG	2.52	0.49
1:C:700:VAL:HG13	1:C:755:GLN:NE2	2.27	0.49
1:D:695:ASN:HB3	1:D:699:GLU:CB	2.39	0.49
1:A:94:ILE:O	1:A:98:VAL:HG23	2.12	0.49
1:A:414:ASP:HB2	1:A:422:ARG:NE	2.25	0.49
1:B:371:VAL:HG23	1:B:419:ARG:O	2.13	0.49
1:C:695:ASN:HB3	1:C:699:GLU:CB	2.41	0.49
1:D:196:ILE:CD1	1:D:379:PRO:HB2	2.29	0.49
1:D:607:ASP:OD2	1:D:739:ARG:NH1	2.46	0.49
1:A:559:LEU:HD11	1:A:743:LEU:HD21	1.94	0.49
1:A:584:VAL:HG22	1:A:623:LYS:HB2	1.94	0.49
1:C:300:ARG:NH1	2:C:901:AMP:O3P	2.46	0.49
1:D:726:GLN:HB3	1:D:731:VAL:HG11	1.93	0.49
1:A:691:PHE:CE2	1:A:770:VAL:HG22	2.47	0.49
1:B:77:MET:HE3	1:B:151:TYR:OH	2.13	0.49
1:C:190:VAL:HG12	1:C:192:PHE:CE1	2.48	0.49
1:A:27:PHE:HB3	1:B:51:ASP:OD1	2.13	0.49
1:C:345:ASP:O	1:C:348:GLU:HB3	2.13	0.49
1:D:371:VAL:HG23	1:D:419:ARG:O	2.13	0.49
1:D:549:ILE:HD12	1:D:630:TYR:HE1	1.78	0.49
1:A:530:TYR:CE1	1:A:534:GLN:HG3	2.48	0.48
1:A:665:LEU:HD22	1:A:791:MET:HB3	1.95	0.48
1:A:787:ASN:O	1:A:791:MET:HG2	2.12	0.48
1:B:281:LEU:HA	1:B:284:ARG:HD2	1.93	0.48
1:B:432:HIS:CD2	1:B:433:LYS:HG2	2.49	0.48
1:C:466:ASN:O	1:C:661:MET:HE1	2.13	0.48
1:B:442:SER:CB	1:B:463:ASN:HB2	2.43	0.48
1:B:491:ARG:HB3	1:B:491:ARG:NH1	2.27	0.48
1:D:733:SER:O	1:D:733:SER:OG	2.31	0.48
1:A:46:LEU:HD22	1:A:179:TRP:HE1	1.78	0.48
1:A:169:PRO:HG2	1:A:171:TYR:CZ	2.48	0.48
1:B:197:GLN:HB2	1:B:206:ILE:HD11	1.95	0.48
1:B:396:LEU:HD21	1:B:456:ILE:HD13	1.95	0.48
1:D:147:TYR:OH	1:D:296:ASP:OD2	2.29	0.48
1:C:669:LEU:HD12	1:C:780:TRP:CZ2	2.49	0.48
1:A:34:VAL:HG12	1:A:35:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:VAL:HG21	1:A:450:PHE:CE1	2.48	0.48
1:C:234:TRP:CE2	1:C:292:SER:HB3	2.49	0.48
1:D:72:VAL:HG21	1:D:808:TRP:CD2	2.48	0.48
1:D:576:PRO:HG3	1:D:617:GLN:HE21	1.78	0.48
1:B:384:ILE:O	1:B:388:ILE:HG13	2.14	0.48
1:C:440:LEU:HD22	1:C:679:VAL:HG21	1.94	0.48
1:D:497:LEU:HD23	1:D:792:GLY:HA2	1.95	0.48
1:B:198:GLN:OE1	1:B:203:THR:HG23	2.14	0.48
1:C:220:ILE:HB	1:C:229:ASN:O	2.14	0.48
1:C:432:HIS:ND1	1:C:433:LYS:HG2	2.29	0.48
1:D:29:ILE:HD12	1:D:44:ALA:HB2	1.94	0.48
1:D:569:TYR:HD2	1:D:612:ILE:HG12	1.75	0.48
1:A:392:PHE:O	1:A:395:THR:HB	2.14	0.48
1:B:71:GLN:HE22	1:B:300:ARG:NH2	2.11	0.48
1:D:713:TYR:CD2	1:D:758:ALA:HA	2.48	0.48
1:A:63:ALA:HB2	1:A:815:LEU:HD23	1.96	0.48
1:A:78:GLU:OE2	1:A:123:ASN:HB3	2.14	0.48
1:B:25:LEU:CD2	1:B:33:PRO:HG3	2.44	0.48
1:D:42:LEU:HD21	1:D:116:GLU:HB2	1.94	0.48
1:D:429:VAL:C	1:D:460:ARG:HH12	2.21	0.48
1:A:41:TRP:CE3	1:A:107:LEU:HD11	2.49	0.47
1:A:700:VAL:HG13	1:A:755:GLN:NE2	2.29	0.47
1:B:37:ASN:ND2	1:B:40:GLU:CD	2.72	0.47
1:B:644:LEU:HD12	1:B:669:LEU:O	2.14	0.47
1:C:399:GLN:C	1:C:400:TYR:HD1	2.21	0.47
1:C:511:MET:HA	1:C:511:MET:HE2	1.96	0.47
1:A:644:LEU:HD12	1:A:669:LEU:O	2.14	0.47
1:A:681:MET:O	1:A:685:VAL:HG22	2.15	0.47
1:C:786:LEU:HD23	1:C:786:LEU:HA	1.66	0.47
1:D:109:LEU:O	1:D:113:ILE:HG13	2.15	0.47
1:D:442:SER:O	1:D:445:MET:HB2	2.14	0.47
1:B:158:GLN:HG3	1:B:165:GLN:HG3	1.96	0.47
1:B:473:TRP:CD2	1:B:662:LLP:HD2	2.50	0.47
1:C:509:PHE:C	1:C:511:MET:N	2.70	0.47
1:C:530:TYR:CE1	1:C:534:GLN:HG3	2.49	0.47
1:D:700:VAL:HG22	1:D:755:GLN:OE1	2.14	0.47
1:B:552:ILE:HD11	1:B:589:GLY:HA3	1.97	0.47
1:B:795:SER:O	1:B:798:ARG:N	2.45	0.47
1:D:335:LEU:HD22	1:D:341:PHE:CE2	2.50	0.47
1:D:432:HIS:CD2	1:D:433:LYS:HG2	2.50	0.47
1:A:392:PHE:HE2	1:A:410:ALA:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASP:OD2	1:C:261:HIS:ND1	2.46	0.47
1:C:334:LEU:O	1:C:338:GLU:HB2	2.14	0.47
1:C:787:ASN:O	1:C:791:MET:HG2	2.14	0.47
1:A:749:ASN:O	1:D:725:THR:HG23	2.15	0.47
1:B:109:LEU:O	1:B:113:ILE:HG13	2.15	0.47
1:B:126:LEU:HD22	1:B:320:ASN:ND2	2.29	0.47
1:B:259:LYS:O	1:B:263:GLU:HG2	2.14	0.47
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.69	0.47
1:B:392:PHE:CZ	1:B:396:LEU:HD11	2.50	0.47
1:C:128:ARG:HD2	1:C:128:ARG:HA	1.65	0.47
1:D:487:GLU:OE1	1:D:488:HIS:HE1	1.98	0.47
1:D:644:LEU:HD12	1:D:669:LEU:O	2.14	0.47
1:D:774:TYR:O	1:D:777:GLN:NE2	2.47	0.47
1:A:265:VAL:HG13	1:A:285:GLN:HA	1.97	0.47
1:B:134:LEU:CD1	1:B:231:LEU:HD13	2.37	0.47
1:B:383:GLN:O	1:B:387:GLU:HG3	2.15	0.47
1:D:799:THR:HG22	1:D:803:TYR:HE2	1.79	0.47
1:A:726:GLN:HB3	1:A:731:VAL:HB	1.97	0.47
1:B:552:ILE:HB	1:B:591:ALA:HB2	1.97	0.47
1:C:446:VAL:HG13	1:C:454:ALA:CB	2.44	0.47
1:A:446:VAL:HG13	1:A:454:ALA:HB1	1.97	0.47
1:A:521:LEU:O	1:A:521:LEU:HG	2.13	0.47
1:B:576:PRO:HG3	1:B:617:GLN:NE2	2.30	0.47
1:C:50:ARG:O	1:C:54:VAL:HG23	2.14	0.47
1:D:128:ARG:HA	1:D:128:ARG:HD2	1.74	0.47
1:A:442:SER:O	1:A:446:VAL:HG23	2.15	0.46
1:B:473:TRP:CE2	1:B:662:LLP:HD2	2.49	0.46
1:C:25:LEU:HG	1:C:25:LEU:O	2.14	0.46
1:C:637:LEU:HD12	1:C:637:LEU:O	2.14	0.46
1:D:67:GLN:OE1	1:D:813:VAL:HG13	2.15	0.46
1:A:25:LEU:HG	1:A:25:LEU:O	2.16	0.46
1:A:720:LEU:HB2	1:A:760:TYR:CE2	2.49	0.46
1:B:691:PHE:CE2	1:B:770:VAL:HG22	2.51	0.46
1:B:693:PHE:CE2	1:B:763:TYR:HB2	2.50	0.46
1:B:705:ARG:HE	1:B:705:ARG:HB2	1.44	0.46
1:D:637:LEU:O	1:D:637:LEU:HD12	2.15	0.46
1:A:315:ILE:O	1:A:315:ILE:HG13	2.15	0.46
1:B:595:TYR:CD1	1:B:598:ALA:HB2	2.50	0.46
1:C:183:ARG:HD3	1:C:183:ARG:N	2.30	0.46
1:C:183:ARG:HB2	1:C:186:THR:OG1	2.14	0.46
1:A:699:GLU:O	1:A:703:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TRP:CZ3	1:C:173:LEU:HD21	2.49	0.46
1:D:47:PHE:CE2	1:D:178:PRO:HB3	2.50	0.46
1:D:214:VAL:HG21	1:D:237:GLN:CD	2.40	0.46
1:B:549:ILE:HG22	1:B:588:GLY:HA3	1.97	0.46
1:C:366:LEU:HD23	1:C:366:LEU:HA	1.74	0.46
1:C:383:GLN:O	1:C:387:GLU:HG3	2.15	0.46
1:D:384:ILE:O	1:D:388:ILE:HG13	2.16	0.46
1:A:432:HIS:CD2	1:A:433:LYS:HG2	2.51	0.46
1:A:639:ILE:HG23	1:A:663:PHE:CD1	2.51	0.46
1:C:648:ILE:HG22	1:C:693:PHE:HZ	1.81	0.46
1:C:108:ASN:HD21	1:C:110:GLU:HG2	1.80	0.46
1:C:363:SER:O	1:C:366:LEU:HB2	2.15	0.46
1:C:648:ILE:HG22	1:C:693:PHE:CZ	2.51	0.46
1:D:639:ILE:HB	1:D:640:PRO:HD3	1.97	0.46
1:D:799:THR:HG22	1:D:803:TYR:CE2	2.50	0.46
1:A:174:GLU:CG	1:B:187:ARG:HH22	2.28	0.46
1:C:265:VAL:HG11	1:C:288:PHE:HB2	1.97	0.46
1:C:366:LEU:HD22	1:C:424:ALA:HB2	1.97	0.46
1:B:374:LEU:HD23	1:B:382:LEU:HD13	1.98	0.46
1:B:549:ILE:HB	1:B:630:TYR:CE1	2.51	0.46
1:D:300:ARG:NH1	2:D:901:AMP:H5'1	2.31	0.46
1:D:462:THR:OG1	1:D:463:ASN:N	2.49	0.46
1:B:441:HIS:ND1	1:B:655:ALA:HB1	2.31	0.46
1:C:196:ILE:CG2	1:C:203:THR:HG23	2.47	0.46
1:C:698:GLU:H	1:C:698:GLU:HG3	1.51	0.46
1:D:489:LEU:HD11	1:D:503:LEU:HB2	1.97	0.46
1:A:397:GLN:OE1	1:A:407:LEU:HD11	2.15	0.45
1:B:422:ARG:O	1:B:425:TRP:HB2	2.17	0.45
1:D:720:LEU:HB2	1:D:760:TYR:CE2	2.52	0.45
1:A:25:LEU:HD23	1:A:33:PRO:HG3	1.98	0.45
1:B:576:PRO:HG3	1:B:617:GLN:HE21	1.81	0.45
1:B:583:ARG:NH1	1:B:767:GLN:OE1	2.45	0.45
1:D:726:GLN:HB3	1:D:731:VAL:HG12	1.99	0.45
1:A:334:LEU:HD23	1:A:338:GLU:HG3	1.98	0.45
1:B:279:ARG:HH22	1:B:370:PRO:CD	2.29	0.45
1:B:695:ASN:HB3	1:B:699:GLU:CB	2.42	0.45
1:C:335:LEU:HB3	1:C:341:PHE:CD2	2.51	0.45
1:C:520:LYS:NZ	1:C:666:ASN:O	2.49	0.45
1:D:71:GLN:HE22	1:D:300:ARG:HH22	1.64	0.45
1:D:157:LYS:HG3	1:D:629:ASN:ND2	2.32	0.45
1:A:196:ILE:HD11	1:A:379:PRO:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ASP:HB2	1:B:279:ARG:HG3	1.99	0.45
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.62	0.45
1:C:45:THR:O	1:C:49:VAL:HG23	2.17	0.45
1:D:73:TYR:CE2	1:D:297:ILE:HG23	2.52	0.45
1:A:42:LEU:HB2	1:A:112:LEU:HD22	1.99	0.45
1:A:442:SER:HA	1:A:445:MET:HE2	1.98	0.45
1:B:41:TRP:CD2	1:B:107:LEU:HD11	2.52	0.45
1:D:345:ASP:O	1:D:348:GLU:HB3	2.17	0.45
1:D:549:ILE:HD12	1:D:630:TYR:CE1	2.51	0.45
1:B:549:ILE:HA	1:B:588:GLY:O	2.16	0.45
1:C:364:GLU:OE1	1:C:364:GLU:N	2.41	0.45
1:C:795:SER:OG	1:C:797:ASP:HB2	2.17	0.45
1:D:80:LEU:HD22	1:D:632:VAL:HG21	1.99	0.45
1:D:414:ASP:HB2	1:D:422:ARG:NH1	2.32	0.45
1:A:8:SER:O	1:A:9:SER:C	2.60	0.45
1:A:280:GLU:HG3	1:A:377:ILE:HD11	1.99	0.45
1:C:258:ASP:HA	1:C:261:HIS:HB3	1.98	0.45
1:D:335:LEU:O	1:D:341:PHE:HB2	2.17	0.45
1:A:59:ARG:HD2	1:A:226:ASP:OD2	2.17	0.45
1:D:705:ARG:HE	1:D:705:ARG:HB2	1.48	0.45
1:A:481:LEU:HD12	1:A:481:LEU:O	2.17	0.45
1:B:60:SER:OG	1:B:226:ASP:O	2.35	0.45
1:B:328:ILE:HD13	1:B:430:VAL:HB	1.99	0.45
1:D:681:MET:O	1:D:685:VAL:HG22	2.17	0.45
1:A:42:LEU:HD21	1:A:116:GLU:HB2	1.99	0.44
1:B:72:VAL:O	1:B:144:GLY:HA2	2.17	0.44
1:C:773:LEU:HD11	1:C:783:LYS:HD2	1.99	0.44
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.69	0.44
1:A:487:GLU:OE1	1:A:488:HIS:CE1	2.70	0.44
1:C:128:ARG:HE	1:C:473:TRP:HZ2	1.65	0.44
1:A:169:PRO:HG2	1:A:171:TYR:CE2	2.52	0.44
1:B:472:ARG:HD3	1:B:636:GLN:OE1	2.18	0.44
1:B:544:LEU:HD23	1:B:545:PHE:N	2.32	0.44
1:C:691:PHE:CE2	1:C:770:VAL:HG22	2.52	0.44
1:D:310:ASN:OD1	1:D:310:ASN:N	2.50	0.44
1:D:613:ASN:O	1:D:623:LYS:NZ	2.50	0.44
1:A:335:LEU:HB3	1:A:341:PHE:CD2	2.52	0.44
1:B:71:GLN:HE22	1:B:300:ARG:HH21	1.65	0.44
1:B:294:ILE:HD12	1:B:294:ILE:HG23	1.78	0.44
1:C:363:SER:HB3	1:C:449:LEU:CD1	2.46	0.44
1:A:80:LEU:CD2	1:A:632:VAL:HG23	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:SER:OG	1:A:797:ASP:HB2	2.17	0.44
1:B:167:GLU:OE1	1:B:167:GLU:N	2.51	0.44
1:B:183:ARG:HB2	1:B:215:ALA:HB3	2.00	0.44
1:B:552:ILE:HG13	1:B:602:ILE:HD11	2.00	0.44
1:D:371:VAL:HG13	1:D:382:LEU:HD11	2.00	0.44
1:D:657:GLY:HA3	1:D:660:ASN:OD1	2.17	0.44
1:B:220:ILE:HD13	1:B:220:ILE:HA	1.63	0.44
1:B:457:PHE:HB3	1:B:460:ARG:HG3	1.99	0.44
1:B:671:ILE:HG23	1:B:671:ILE:O	2.18	0.44
1:D:425:TRP:CD1	1:D:453:PHE:HZ	2.36	0.44
1:A:717:ASP:CG	1:A:761:ARG:HH21	2.26	0.44
1:C:150:ARG:NH2	1:C:173:LEU:HD13	2.32	0.44
1:A:506:HIS:CB	1:A:512:VAL:HG21	2.41	0.44
1:A:509:PHE:HB2	1:A:512:VAL:HG23	2.00	0.44
1:A:545:PHE:HD2	1:A:641:ALA:O	2.00	0.44
1:A:634:LEU:HA	1:A:634:LEU:HD23	1.64	0.44
1:B:787:ASN:O	1:B:791:MET:HG2	2.17	0.44
1:C:281:LEU:HA	1:C:284:ARG:HD2	2.00	0.44
1:C:422:ARG:HH21	1:C:425:TRP:CD1	2.36	0.44
1:D:273:ASP:HB3	1:D:282:ARG:HG3	2.00	0.44
1:D:372:ASP:OD1	1:D:372:ASP:N	2.40	0.44
1:D:603:HIS:CE1	1:D:739:ARG:HH11	2.36	0.44
1:D:603:HIS:CE1	1:D:739:ARG:NH1	2.86	0.44
1:A:310:ASN:OD1	1:A:310:ASN:N	2.50	0.44
1:B:70:ARG:HD3	1:B:809:HIS:O	2.18	0.44
1:B:471:ARG:HG3	1:B:471:ARG:NH1	2.23	0.44
1:C:690:ILE:HG23	1:C:692:ILE:HG12	1.99	0.44
1:A:71:GLN:HE22	1:A:300:ARG:NH2	2.16	0.43
1:B:539:VAL:HB	1:B:584:VAL:HG21	2.00	0.43
1:B:713:TYR:CD2	1:B:758:ALA:HA	2.53	0.43
1:B:742:ASP:OD1	1:B:742:ASP:N	2.51	0.43
1:B:776:LEU:O	1:B:779:GLU:N	2.37	0.43
1:D:644:LEU:HD12	1:D:644:LEU:HA	1.78	0.43
1:B:695:ASN:HB2	1:B:700:VAL:HG23	1.99	0.43
1:C:494:ARG:HG3	1:C:494:ARG:HH11	1.83	0.43
1:D:303:GLN:HG3	2:D:901:AMP:O3'	2.18	0.43
1:D:374:LEU:HD23	1:D:382:LEU:HD13	2.00	0.43
1:A:394:LYS:HA	1:A:394:LYS:HD3	1.73	0.43
1:A:481:LEU:HB2	1:A:519:ALA:HB1	2.00	0.43
1:C:730:GLY:HA3	1:C:737:PRO:HB3	1.99	0.43
1:D:714:TYR:HD1	1:D:724:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:NH2	1:A:316:ALA:HB2	2.33	0.43
1:A:363:SER:HB3	1:A:449:LEU:HD13	1.99	0.43
1:A:733:SER:OG	1:A:736:ASP:O	2.36	0.43
1:B:147:TYR:CE1	1:B:232:ARG:HD2	2.49	0.43
1:B:329:PRO:HB2	1:B:381:HIS:HD2	1.83	0.43
1:B:485:LEU:O	1:B:489:LEU:HB2	2.18	0.43
1:C:634:LEU:HD23	1:C:634:LEU:HA	1.59	0.43
1:D:417:ASN:HD22	1:D:420:ARG:HD2	1.84	0.43
1:A:276:TYR:O	1:A:280:GLU:HB2	2.18	0.43
1:A:315:ILE:HD12	1:A:317:ILE:HD11	2.00	0.43
1:A:464:VAL:HG11	1:A:803:TYR:CE2	2.53	0.43
1:A:471:ARG:O	1:A:476:VAL:HG23	2.18	0.43
1:A:544:LEU:HD22	1:A:583:ARG:HG3	2.00	0.43
1:C:649:SER:O	1:C:650:LEU:C	2.61	0.43
1:D:80:LEU:H	1:D:127:GLY:C	2.25	0.43
1:D:747:LEU:HA	1:D:752:ASP:HB2	2.00	0.43
1:B:279:ARG:HH22	1:B:370:PRO:HD3	1.84	0.43
1:B:558:GLN:O	1:B:562:VAL:HG23	2.18	0.43
1:B:17:LEU:HD13	1:B:98:VAL:HG22	2.00	0.43
1:B:214:VAL:HG21	1:B:237:GLN:CD	2.43	0.43
1:C:374:LEU:HD23	1:C:382:LEU:HD13	2.00	0.43
1:C:665:LEU:CD2	1:C:791:MET:HB3	2.48	0.43
1:D:428:VAL:O	1:D:460:ARG:NH1	2.49	0.43
1:B:70:ARG:NH2	1:B:316:ALA:HB2	2.34	0.43
1:B:78:GLU:OE1	1:B:123:ASN:N	2.34	0.43
1:A:509:PHE:C	1:A:511:MET:N	2.75	0.43
1:A:682:LEU:HD13	1:A:690:ILE:HG21	2.01	0.43
1:B:99:GLN:O	1:B:103:GLU:HG3	2.18	0.43
1:B:305:HIS:O	1:B:307:THR:N	2.51	0.43
1:B:568:ARG:O	1:B:572:ILE:HG13	2.18	0.43
1:B:568:ARG:NH2	1:B:581:VAL:HB	2.32	0.43
1:C:85:LEU:HG	1:C:89:MET:HE2	2.01	0.43
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.70	0.43
1:C:147:TYR:CE1	1:C:232:ARG:HD2	2.54	0.43
1:C:177:ASN:ND2	1:C:180:GLU:HG3	2.34	0.43
1:C:307:THR:HG23	1:C:309:ASP:H	1.84	0.43
1:D:128:ARG:HG2	1:D:662:LLP:C4'	2.49	0.43
1:D:199:GLU:OE1	1:D:204:ARG:HD3	2.18	0.43
1:A:10:PRO:O	1:A:11:THR:C	2.62	0.42
1:A:334:LEU:O	1:A:338:GLU:HB2	2.19	0.42
1:D:356:TYR:O	1:D:435:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LEU:HD21	1:D:456:ILE:HD13	2.00	0.42
1:D:755:GLN:HB3	1:D:758:ALA:HB3	2.00	0.42
1:A:73:TYR:CE2	1:A:297:ILE:HG23	2.54	0.42
1:A:381:HIS:O	1:A:385:ILE:HG13	2.19	0.42
1:B:557:ARG:HD2	1:B:560:MET:HE2	2.01	0.42
1:B:681:MET:O	1:B:685:VAL:HG22	2.19	0.42
1:D:471:ARG:HG3	1:D:471:ARG:HH11	1.83	0.42
1:D:566:ILE:HG22	1:D:723:VAL:HG22	2.01	0.42
1:D:711:ARG:O	1:D:714:TYR:HB3	2.18	0.42
1:C:187:ARG:HA	1:C:213:GLY:O	2.18	0.42
1:D:11:THR:CG2	1:D:12:LEU:H	2.18	0.42
1:D:141:GLY:O	1:D:812:PRO:HA	2.19	0.42
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.92	0.42
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.84	0.42
1:C:462:THR:OG1	1:C:463:ASN:N	2.51	0.42
1:C:486:ASP:HA	1:C:490:GLY:O	2.19	0.42
1:D:275:THR:HG1	1:D:278:GLY:H	1.63	0.42
1:A:71:GLN:HE22	1:A:300:ARG:HH22	1.66	0.42
1:A:336:ILE:HD11	1:A:343:TRP:HA	2.01	0.42
1:A:566:ILE:HG22	1:A:723:VAL:HG22	2.01	0.42
1:A:705:ARG:HE	1:A:705:ARG:HB2	1.32	0.42
1:C:708:TYR:CZ	1:C:710:PRO:HB3	2.55	0.42
1:D:81:ILE:HG13	1:D:119:PRO:HG2	2.01	0.42
1:D:99:GLN:O	1:D:103:GLU:HG3	2.19	0.42
1:D:151:TYR:CZ	1:D:269:LEU:HD13	2.55	0.42
1:A:279:ARG:HH22	1:A:420:ARG:HH22	1.68	0.42
1:B:188:TYR:OH	1:B:296:ASP:HA	2.19	0.42
1:B:436:GLY:HA3	1:B:442:SER:OG	2.20	0.42
1:B:597:MET:O	1:B:601:ILE:HG13	2.20	0.42
1:C:644:LEU:HD12	1:C:669:LEU:O	2.19	0.42
1:D:308:TYR:CE2	1:D:339:HIS:CD2	3.07	0.42
1:B:520:LYS:NZ	1:B:666:ASN:O	2.28	0.42
1:C:464:VAL:HG11	1:C:803:TYR:CE2	2.54	0.42
1:C:508:ASP:O	1:C:509:PHE:C	2.62	0.42
1:A:36:ALA:HA	1:A:40:GLU:OE1	2.19	0.42
1:D:650:LEU:HD12	1:D:650:LEU:HA	1.76	0.42
1:B:197:GLN:HG2	1:B:198:GLN:H	1.84	0.42
1:C:705:ARG:HE	1:C:705:ARG:HB2	1.29	0.42
1:D:661:MET:O	1:D:665:LEU:HB2	2.20	0.42
1:B:323:HIS:HB2	1:B:324:PRO:HD3	2.01	0.42
1:C:356:TYR:HD1	1:C:357:THR:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LYS:HA	1:C:394:LYS:HD3	1.56	0.42
1:C:650:LEU:O	1:C:651:ALA:C	2.63	0.42
1:A:160:ILE:HG12	1:A:628:PRO:HB3	2.01	0.41
1:A:717:ASP:OD1	1:A:761:ARG:NH2	2.48	0.41
1:C:59:ARG:HG2	1:C:815:LEU:HD11	2.02	0.41
1:B:482:SER:HG	1:B:493:TRP:HH2	1.64	0.41
1:C:78:GLU:OE2	1:C:123:ASN:HB3	2.20	0.41
1:C:452:ASP:O	1:C:456:ILE:HG13	2.19	0.41
1:C:771:ASP:O	1:C:775:GLU:HG3	2.20	0.41
1:A:211:ILE:HG12	1:A:262:SER:HB3	2.01	0.41
1:A:220:ILE:HD13	1:A:220:ILE:HA	1.77	0.41
1:A:708:TYR:CE1	1:A:710:PRO:HA	2.55	0.41
1:B:32:ASP:OD1	1:B:34:VAL:HG23	2.19	0.41
1:B:163:GLY:O	1:B:603:HIS:HA	2.20	0.41
1:B:366:LEU:HD22	1:B:424:ALA:HB2	2.02	0.41
1:B:417:ASN:HD22	1:B:417:ASN:HA	1.70	0.41
1:C:70:ARG:NH1	1:C:313:ASP:O	2.40	0.41
1:C:300:ARG:HH11	1:C:300:ARG:HD2	1.73	0.41
1:C:669:LEU:HD12	1:C:780:TRP:CE2	2.55	0.41
1:D:85:LEU:HG	1:D:89:MET:HE2	2.01	0.41
1:D:158:GLN:HG3	1:D:165:GLN:HG3	2.01	0.41
1:D:304:LEU:HA	1:D:304:LEU:HD12	1.81	0.41
1:A:695:ASN:HB3	1:A:699:GLU:HB2	2.02	0.41
1:B:80:LEU:HD22	1:B:632:VAL:HG23	2.02	0.41
1:C:137:LEU:HB3	1:C:229:ASN:ND2	2.35	0.41
1:C:305:HIS:O	1:C:307:THR:N	2.54	0.41
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.82	0.41
1:C:714:TYR:HD1	1:C:724:LEU:HD12	1.84	0.41
1:D:323:HIS:HB2	1:D:324:PRO:HD3	2.02	0.41
1:A:436:GLY:HA3	1:A:442:SER:OG	2.21	0.41
1:B:471:ARG:O	1:B:476:VAL:HG23	2.21	0.41
1:B:527:LEU:HD21	1:B:586:ILE:HD13	2.03	0.41
1:C:409:ARG:O	1:C:422:ARG:NH2	2.53	0.41
1:C:669:LEU:HD23	1:C:669:LEU:HA	1.86	0.41
1:A:27:PHE:HB3	1:B:51:ASP:CG	2.45	0.41
1:A:58:LEU:HD11	1:B:26:MET:HE3	2.03	0.41
1:B:559:LEU:HB2	1:B:601:ILE:HD13	2.03	0.41
1:C:304:LEU:HA	1:C:304:LEU:HD12	1.68	0.41
1:D:17:LEU:HD21	1:D:52:ARG:HH21	1.85	0.41
1:D:61:ASN:O	1:D:65:LEU:HG	2.20	0.41
1:D:167:GLU:N	1:D:167:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:HB3	1:A:229:ASN:ND2	2.36	0.41
1:A:464:VAL:HG11	1:A:803:TYR:CD2	2.55	0.41
1:B:42:LEU:HD21	1:B:116:GLU:HB2	2.01	0.41
1:B:119:PRO:HA	1:B:172:TRP:CE3	2.56	0.41
1:B:160:ILE:HG12	1:B:628:PRO:HB3	2.03	0.41
1:B:276:TYR:CZ	1:B:373:MET:HE2	2.55	0.41
1:D:662:LLP:NZ	1:D:662:LLP:O3	2.47	0.41
1:A:356:TYR:CD1	1:A:357:THR:N	2.88	0.41
1:B:155:MET:HG2	1:B:156:PHE:HD1	1.84	0.41
1:C:214:VAL:HG21	1:C:237:GLN:CD	2.45	0.41
1:C:749:ASN:OD1	1:C:749:ASN:N	2.53	0.41
1:D:46:LEU:HD23	1:D:85:LEU:HD13	2.03	0.41
1:D:356:TYR:CD1	1:D:357:THR:N	2.88	0.41
1:D:634:LEU:HA	1:D:634:LEU:HD23	1.86	0.41
1:A:134:LEU:HD11	1:A:231:LEU:HD13	2.03	0.41
1:C:147:TYR:HE1	1:C:232:ARG:HD2	1.86	0.41
1:D:223:TYR:HB2	1:D:471:ARG:CD	2.49	0.41
1:D:415:GLU:OE1	1:D:415:GLU:HA	2.20	0.41
1:D:553:HIS:ND1	1:D:554:GLU:N	2.69	0.41
1:D:627:ILE:HA	1:D:628:PRO:HD3	1.93	0.41
1:A:50:ARG:NE	1:A:181:PHE:CZ	2.89	0.41
1:A:198:GLN:OE1	1:A:198:GLN:HA	2.20	0.41
1:A:363:SER:HB3	1:A:449:LEU:CD1	2.51	0.41
1:A:657:GLY:HA3	1:A:660:ASN:HD21	1.85	0.41
1:A:671:ILE:HG23	1:A:671:ILE:O	2.21	0.41
1:B:195:ARG:NH2	1:B:207:GLU:OE2	2.53	0.41
1:B:337:ASP:CG	1:B:380:ARG:HH21	2.29	0.41
1:B:470:PRO:HG3	1:B:497:LEU:HD22	2.03	0.41
1:C:52:ARG:HA	1:C:55:GLU:HG3	2.03	0.41
1:C:70:ARG:NH2	1:C:316:ALA:HB2	2.36	0.41
1:C:125:GLY:HA2	1:C:662:LLP:H5'2	2.03	0.41
1:C:310:ASN:OD1	1:C:310:ASN:N	2.54	0.41
1:D:433:LYS:NZ	1:D:459:GLY:O	2.41	0.41
1:A:559:LEU:HB2	1:A:601:ILE:CD1	2.49	0.40
1:A:563:LEU:HD23	1:A:563:LEU:HA	1.85	0.40
1:B:223:TYR:HB2	1:B:471:ARG:CD	2.49	0.40
1:C:50:ARG:NE	1:C:181:PHE:CZ	2.89	0.40
1:D:383:GLN:O	1:D:387:GLU:HG3	2.22	0.40
1:A:446:VAL:HG13	1:A:454:ALA:CB	2.51	0.40
1:B:612:ILE:HD12	1:B:624:VAL:HG21	2.03	0.40
1:C:665:LEU:HD22	1:C:791:MET:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:HIS:CD2	1:D:655:ALA:HB1	2.55	0.40
1:A:190:VAL:HG12	1:A:192:PHE:HE1	1.84	0.40
1:B:644:LEU:HD12	1:B:644:LEU:HA	1.80	0.40
1:C:11:THR:O	1:C:12:LEU:C	2.64	0.40
1:C:442:SER:CB	1:C:463:ASN:HB2	2.51	0.40
1:A:50:ARG:HD2	1:A:181:PHE:CE1	2.56	0.40
1:A:478:ASN:ND2	1:A:481:LEU:HB3	2.36	0.40
1:A:487:GLU:OE1	1:A:488:HIS:HE1	2.03	0.40
1:A:506:HIS:O	1:A:785:MET:HE1	2.22	0.40
1:B:158:GLN:HE22	1:B:590:LYS:HA	1.85	0.40
1:B:595:TYR:CD1	1:B:598:ALA:CB	3.04	0.40
1:C:134:LEU:HD23	1:C:134:LEU:HA	1.87	0.40
1:C:657:GLY:O	1:C:677:ALA:HB2	2.22	0.40
1:A:133:PHE:HB3	1:A:800:ILE:HD11	2.02	0.40
1:A:303:GLN:HB2	2:A:901:AMP:O3'	2.21	0.40
1:A:748:ILE:HD13	1:A:748:ILE:HG21	1.88	0.40
1:B:79:PHE:O	1:B:121:LEU:HB2	2.22	0.40
1:B:109:LEU:O	1:B:110:GLU:C	2.63	0.40
1:B:143:PRO:HD2	1:B:810:ILE:HD12	2.03	0.40
1:B:464:VAL:HG12	1:B:799:THR:HG23	2.03	0.40
1:B:584:VAL:HG22	1:B:623:LYS:HB2	2.04	0.40
1:C:523:ASN:O	1:C:526:ARG:HB3	2.22	0.40
1:D:457:PHE:HB3	1:D:460:ARG:CG	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:ARG:NH2	1:C:223:TYR:O[4_544]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	796/817 (97%)	739 (93%)	57 (7%)	0	100	100
1	B	786/817 (96%)	714 (91%)	72 (9%)	0	100	100
1	C	787/817 (96%)	724 (92%)	63 (8%)	0	100	100
1	D	786/817 (96%)	728 (93%)	58 (7%)	0	100	100
All	All	3155/3268 (96%)	2905 (92%)	250 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	697/708 (98%)	697 (100%)	0	100	100
1	B	688/708 (97%)	688 (100%)	0	100	100
1	C	689/708 (97%)	689 (100%)	0	100	100
1	D	688/708 (97%)	688 (100%)	0	100	100
All	All	2762/2832 (98%)	2762 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	71	GLN
1	A	87	ASN
1	A	123	ASN
1	A	159	ASN
1	A	197	GLN
1	A	229	ASN
1	A	305	HIS
1	A	339	HIS
1	A	432	HIS

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Mol	Chain	Res	Type
1	A	488	HIS
1	A	534	GLN
1	A	787	ASN
1	B	71	GLN
1	B	123	ASN
1	B	352	GLN
1	B	383	GLN
1	B	447	GLN
1	B	561	ASN
1	B	600	HIS
1	B	689	ASN
1	C	71	GLN
1	C	99	GLN
1	C	177	ASN
1	C	229	ASN
1	C	285	GLN
1	C	352	GLN
1	C	504	GLN
1	C	523	ASN
1	C	548	GLN
1	C	561	ASN
1	C	660	ASN
1	C	684	HIS
1	C	790	ASN
1	D	19	HIS
1	D	177	ASN
1	D	285	GLN
1	D	305	HIS
1	D	417	ASN
1	D	463	ASN
1	D	488	HIS
1	D	517	HIS
1	D	540	ASN
1	D	603	HIS
1	D	777	GLN
1	D	787	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	D	662	1	23,24,25	2.51	7 (30%)	25,32,34	1.47	5 (20%)
1	LLP	B	662	1	23,24,25	2.53	7 (30%)	25,32,34	1.51	4 (16%)
1	LLP	C	662	1	23,24,25	2.67	6 (26%)	25,32,34	1.47	4 (16%)
1	LLP	A	662	1	23,24,25	2.53	8 (34%)	25,32,34	1.64	7 (28%)

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	LLP	D	662	1	-	5/16/17/19	0/1/1/1
1	LLP	B	662	1	-	5/16/17/19	0/1/1/1
1	LLP	C	662	1	-	5/16/17/19	0/1/1/1
1	LLP	A	662	1	-	6/16/17/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	662	LLP	C4-C4'	7.85	1.63	1.46
1	D	662	LLP	C4-C4'	7.50	1.62	1.46
1	A	662	LLP	C4-C4'	7.47	1.62	1.46
1	B	662	LLP	C4-C4'	6.97	1.61	1.46
1	C	662	LLP	C4-C5	-5.61	1.34	1.42
1	C	662	LLP	C4'-NZ	5.28	1.44	1.27
1	D	662	LLP	C4'-NZ	5.20	1.44	1.27
1	A	662	LLP	C4'-NZ	5.20	1.44	1.27
1	B	662	LLP	C4'-NZ	5.13	1.44	1.27
1	B	662	LLP	C4-C5	-4.06	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	662	LLP	C4-C5	-3.78	1.36	1.42
1	A	662	LLP	C4-C5	-3.72	1.36	1.42
1	B	662	LLP	C6-N1	3.35	1.41	1.34
1	D	662	LLP	C6-N1	3.30	1.41	1.34
1	B	662	LLP	C2'-C2	3.26	1.55	1.50
1	C	662	LLP	C2'-C2	3.23	1.55	1.50
1	D	662	LLP	C2'-C2	3.19	1.55	1.50
1	A	662	LLP	C6-N1	2.95	1.40	1.34
1	B	662	LLP	C4-C3	-2.95	1.36	1.41
1	A	662	LLP	C2'-C2	2.89	1.55	1.50
1	A	662	LLP	C4-C3	-2.73	1.36	1.41
1	C	662	LLP	C6-N1	2.54	1.39	1.34
1	C	662	LLP	C4-C3	-2.50	1.37	1.41
1	D	662	LLP	C5'-C5	2.39	1.57	1.50
1	D	662	LLP	C4-C3	-2.38	1.37	1.41
1	B	662	LLP	C5'-C5	2.23	1.56	1.50
1	A	662	LLP	C5'-C5	2.22	1.56	1.50
1	A	662	LLP	P-OP4	-2.05	1.53	1.60

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	LLP	C2'-C2-C3	-4.36	115.70	120.80
1	C	662	LLP	CE-NZ-C4'	-3.28	108.22	118.72
1	D	662	LLP	C4-C3-C2	3.18	121.93	120.14
1	B	662	LLP	C4-C4'-NZ	-3.11	109.69	124.04
1	A	662	LLP	C4-C4'-NZ	-3.08	109.81	124.04
1	C	662	LLP	C4-C3-C2	3.05	121.86	120.14
1	C	662	LLP	OP4-C5'-C5	-2.96	103.80	109.36
1	A	662	LLP	C2'-C2-N1	2.94	123.17	117.64
1	B	662	LLP	C4-C3-C2	2.85	121.75	120.14
1	D	662	LLP	C4-C4'-NZ	-2.69	111.62	124.04
1	B	662	LLP	CE-NZ-C4'	-2.54	110.60	118.72
1	C	662	LLP	C5-C4-C4'	-2.27	117.97	121.47
1	D	662	LLP	C2'-C2-N1	2.24	121.86	117.64
1	A	662	LLP	C5-C6-N1	-2.21	120.23	123.83
1	D	662	LLP	C3-C4-C5	2.21	120.05	118.28
1	D	662	LLP	CE-NZ-C4'	-2.19	111.70	118.72
1	A	662	LLP	CE-NZ-C4'	-2.15	111.83	118.72
1	A	662	LLP	C4-C3-C2	2.14	121.35	120.14
1	B	662	LLP	C3-C4-C5	2.02	119.90	118.28
1	A	662	LLP	OP4-C5'-C5	-2.00	105.60	109.36

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	662	LLP	C5'-OP4-P-OP2
1	C	662	LLP	C5'-OP4-P-OP3
1	B	662	LLP	C4-C4'-NZ-CE
1	D	662	LLP	C4-C4'-NZ-CE
1	A	662	LLP	C4-C4'-NZ-CE
1	C	662	LLP	CE-CD-CG-CB
1	D	662	LLP	CE-CD-CG-CB
1	A	662	LLP	CE-CD-CG-CB
1	C	662	LLP	C5'-OP4-P-OP1
1	C	662	LLP	C4-C4'-NZ-CE
1	A	662	LLP	C5'-OP4-P-OP3
1	D	662	LLP	C5'-OP4-P-OP3
1	D	662	LLP	CD-CE-NZ-C4'
1	A	662	LLP	CD-CE-NZ-C4'
1	B	662	LLP	CD-CE-NZ-C4'
1	A	662	LLP	C5'-OP4-P-OP1
1	B	662	LLP	C5'-OP4-P-OP3
1	A	662	LLP	C3-C4-C4'-NZ
1	B	662	LLP	CG-CD-CE-NZ
1	B	662	LLP	C4-C5-C5'-OP4
1	D	662	LLP	C3-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	662	LLP	5	0
1	B	662	LLP	5	0
1	C	662	LLP	2	0
1	A	662	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
2	AMP	C	901	-	25,25,25	1.61	4 (16%)	37,38,38	2.03	8 (21%)
2	AMP	D	901	-	25,25,25	1.56	3 (12%)	37,38,38	2.18	8 (21%)
2	AMP	A	901	-	25,25,25	1.53	4 (16%)	37,38,38	1.93	9 (24%)
2	AMP	B	901	-	25,25,25	1.65	4 (16%)	37,38,38	1.80	9 (24%)

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
2	AMP	C	901	-	-	6/10/26/26	0/3/3/3
2	AMP	D	901	-	-	8/10/26/26	0/3/3/3
2	AMP	A	901	-	-	4/10/26/26	0/3/3/3
2	AMP	B	901	-	-	4/10/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	AMP	C5-C4	5.96	1.49	1.39
2	C	901	AMP	C5-C4	5.52	1.48	1.39
2	A	901	AMP	C5-C4	5.51	1.48	1.39
2	D	901	AMP	C5-C4	5.38	1.48	1.39
2	D	901	AMP	C5-C6	3.44	1.50	1.41
2	B	901	AMP	C8-N7	2.81	1.37	1.31
2	C	901	AMP	C5-N7	-2.80	1.34	1.39
2	D	901	AMP	C8-N7	2.75	1.37	1.31
2	A	901	AMP	C5-C6	2.74	1.48	1.41
2	A	901	AMP	C8-N7	2.73	1.36	1.31
2	B	901	AMP	C5-N7	-2.67	1.34	1.39
2	C	901	AMP	C5-C6	2.53	1.48	1.41
2	B	901	AMP	C5-C6	2.46	1.47	1.41
2	C	901	AMP	C8-N7	2.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	AMP	C5-N7	-2.18	1.35	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	AMP	C5-C4-N3	-7.49	116.40	126.72
2	C	901	AMP	C5-C4-N3	-6.27	118.08	126.72
2	A	901	AMP	C5-C4-N3	-6.12	118.29	126.72
2	B	901	AMP	C5-C4-N3	-5.61	119.00	126.72
2	D	901	AMP	N3-C4-N9	5.54	136.58	127.17
2	C	901	AMP	N3-C4-N9	5.17	135.95	127.17
2	A	901	AMP	N3-C4-N9	5.00	135.68	127.17
2	C	901	AMP	O2P-P-O5'	-4.69	94.44	106.67
2	B	901	AMP	N3-C4-N9	4.54	134.88	127.17
2	D	901	AMP	C4-C5-N7	-4.32	105.64	110.58
2	D	901	AMP	C2-N3-C4	4.25	122.20	111.83
2	C	901	AMP	C2-N3-C4	3.71	120.88	111.83
2	A	901	AMP	C2-N3-C4	3.47	120.31	111.83
2	B	901	AMP	C2-N3-C4	3.28	119.85	111.83
2	C	901	AMP	N3-C2-N1	-3.14	123.82	128.58
2	D	901	AMP	C5-N7-C8	3.08	108.28	103.45
2	A	901	AMP	C4-C5-N7	-3.04	107.10	110.58
2	B	901	AMP	N3-C2-N1	-3.02	124.02	128.58
2	A	901	AMP	N3-C2-N1	-2.89	124.20	128.58
2	D	901	AMP	N3-C2-N1	-2.78	124.37	128.58
2	D	901	AMP	O5'-P-O1P	-2.48	99.73	106.44
2	B	901	AMP	C4-C5-N7	-2.45	107.78	110.58
2	A	901	AMP	O5'-P-O1P	-2.41	99.93	106.44
2	A	901	AMP	C5-N7-C8	2.38	107.19	103.45
2	B	901	AMP	O2P-P-O5'	-2.35	100.55	106.67
2	B	901	AMP	O3P-P-O2P	2.31	116.47	107.80
2	B	901	AMP	N6-C6-N1	2.22	123.32	118.38
2	C	901	AMP	N6-C6-N1	2.22	123.32	118.38
2	C	901	AMP	C4-C5-N7	-2.19	108.07	110.58
2	A	901	AMP	C2-N1-C6	2.14	122.25	118.73
2	B	901	AMP	C2-N1-C6	2.10	122.18	118.73
2	A	901	AMP	C1'-N9-C8	-2.06	122.53	127.09
2	C	901	AMP	C5-C6-N6	-2.04	118.23	123.29
2	D	901	AMP	C6-C5-N7	2.04	136.02	132.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	AMP	C5'-O5'-P-O1P
2	C	901	AMP	C5'-O5'-P-O2P
2	C	901	AMP	C5'-O5'-P-O3P
2	C	901	AMP	O4'-C1'-N9-C8
2	C	901	AMP	O4'-C1'-N9-C4
2	D	901	AMP	C5'-O5'-P-O1P
2	D	901	AMP	C5'-O5'-P-O3P
2	D	901	AMP	O4'-C1'-N9-C8
2	D	901	AMP	O4'-C1'-N9-C4
2	D	901	AMP	C3'-C4'-C5'-O5'
2	B	901	AMP	O4'-C1'-N9-C4
2	D	901	AMP	C4'-C5'-O5'-P
2	D	901	AMP	O4'-C4'-C5'-O5'
2	B	901	AMP	O4'-C4'-C5'-O5'
2	B	901	AMP	C3'-C4'-C5'-O5'
2	C	901	AMP	C3'-C4'-C5'-O5'
2	B	901	AMP	O4'-C1'-N9-C8
2	A	901	AMP	C4'-C5'-O5'-P
2	A	901	AMP	O4'-C1'-N9-C4
2	A	901	AMP	O4'-C1'-N9-C8
2	A	901	AMP	C5'-O5'-P-O1P
2	D	901	AMP	C5'-O5'-P-O2P

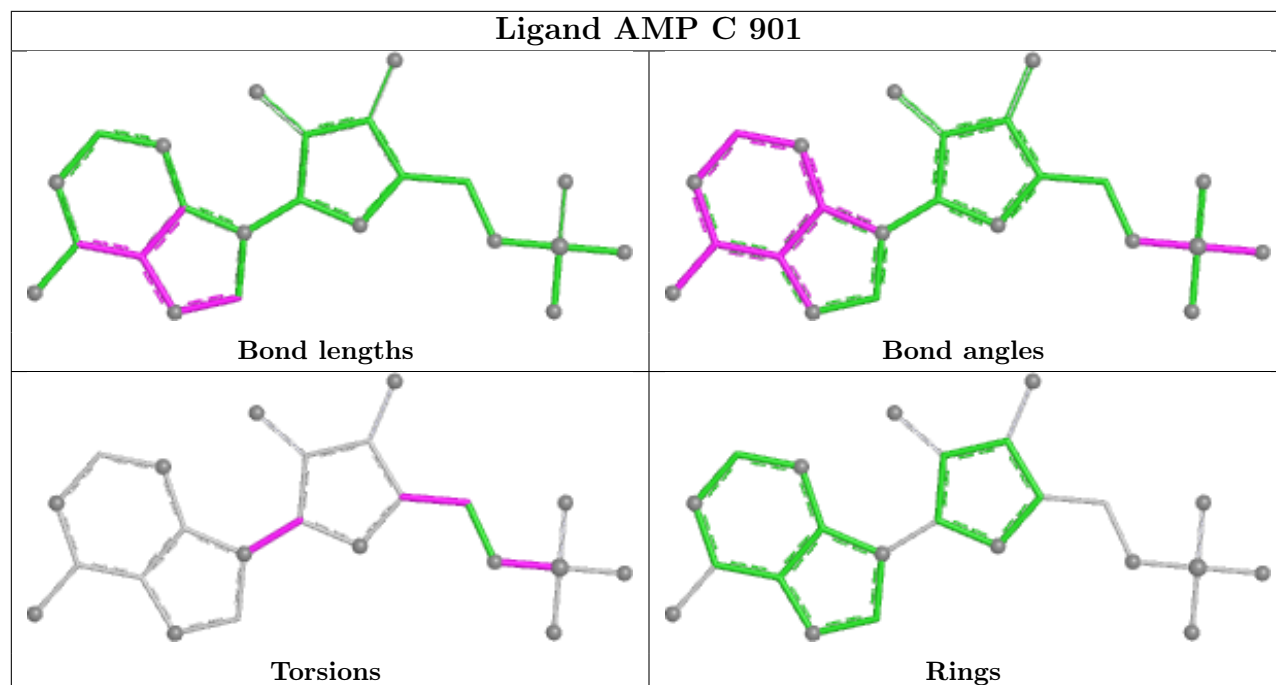
There are no ring outliers.

3 monomers are involved in 7 short contacts:

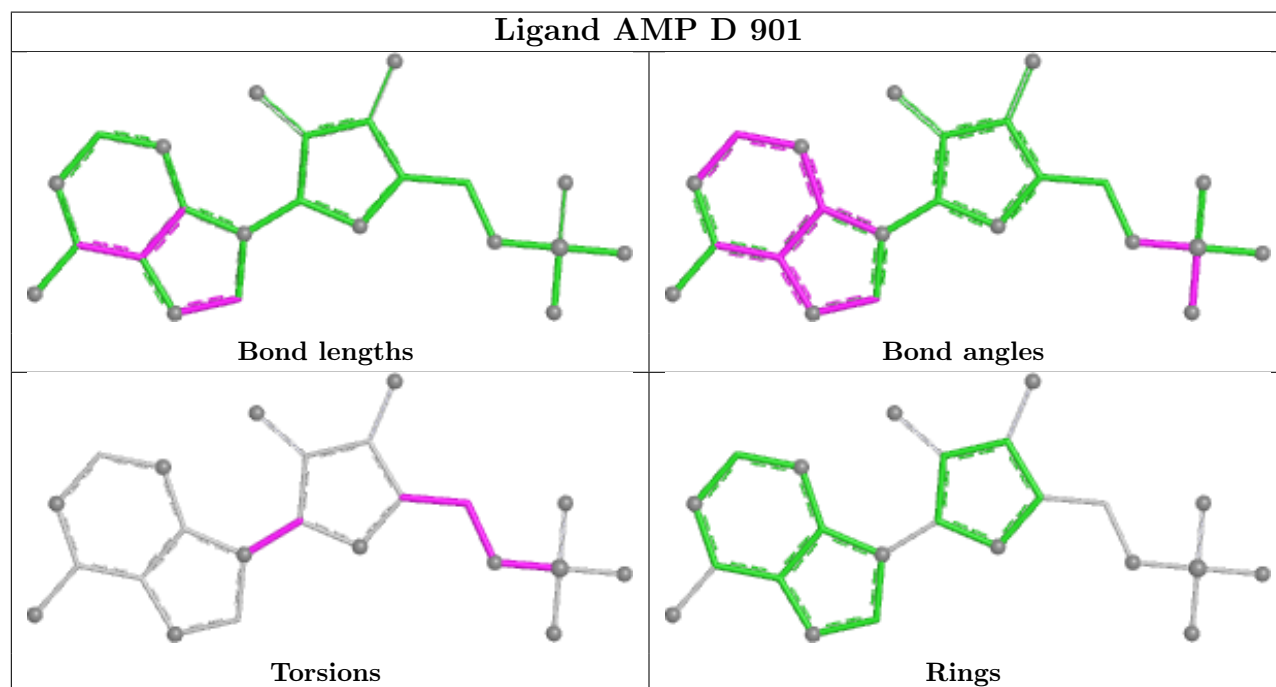
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	AMP	1	0
2	D	901	AMP	3	0
2	A	901	AMP	3	0

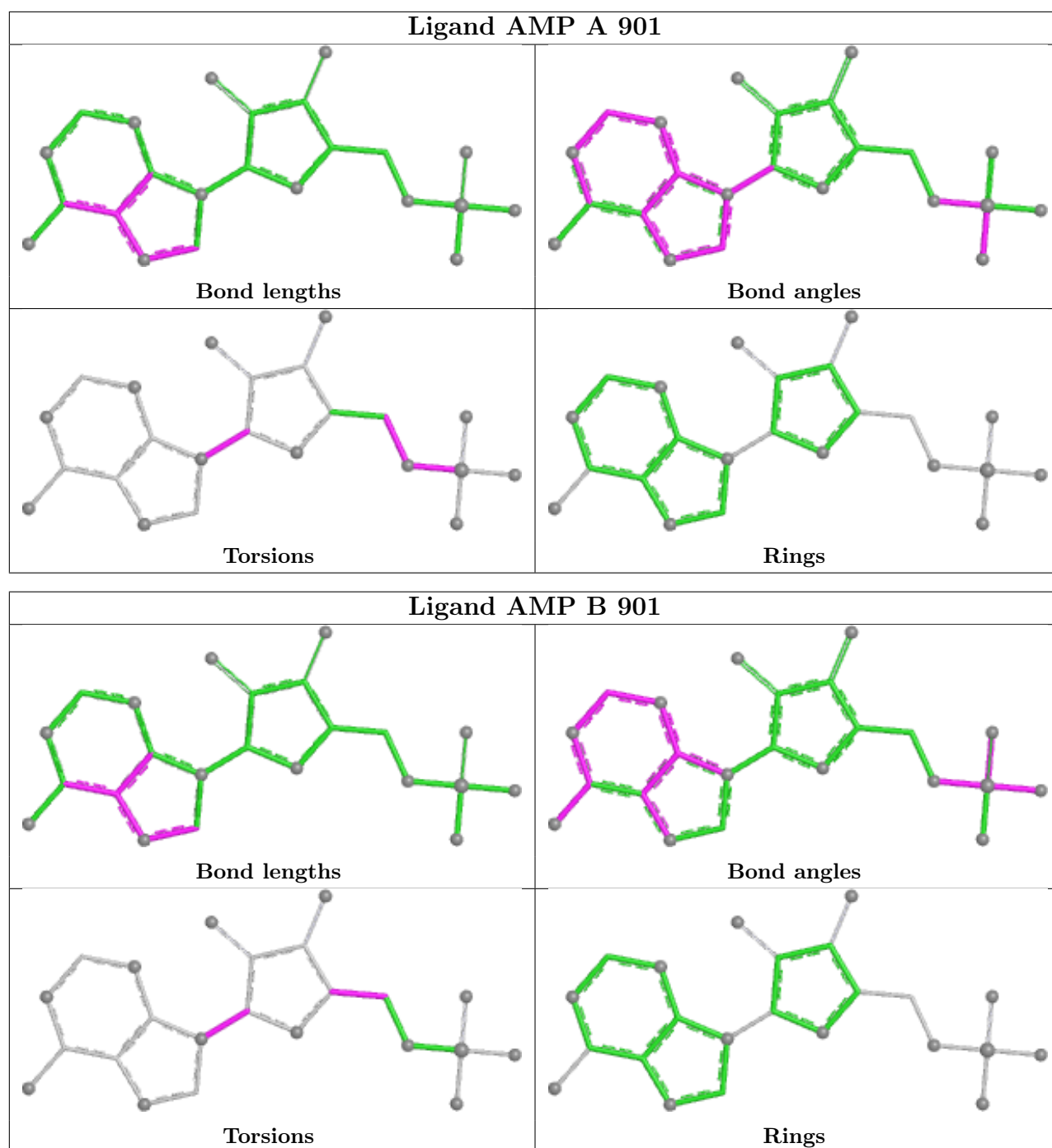
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AMP C 901



Ligand AMP D 901





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	800/817 (97%)	-0.29	7 (0%) 81 58	86, 111, 138, 182	0
1	B	790/817 (96%)	-0.34	3 (0%) 88 73	80, 105, 135, 164	0
1	C	791/817 (96%)	-0.31	8 (1%) 79 56	76, 102, 129, 170	0
1	D	790/817 (96%)	-0.27	7 (0%) 81 58	83, 110, 134, 167	0
All	All	3171/3268 (97%)	-0.30	25 (0%) 82 61	76, 107, 134, 182	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ILE	3.9
1	A	13	SER	3.6
1	A	5	PHE	3.5
1	A	244	LEU	3.5
1	C	815	LEU	3.5
1	A	259	LYS	3.4
1	C	244	LEU	3.3
1	C	242	ILE	3.2
1	C	239	SER	3.2
1	C	362	MET	3.1
1	D	202	LYS	3.1
1	B	242	ILE	2.9
1	C	259	LYS	2.9
1	A	247	PHE	2.8
1	D	242	ILE	2.7
1	D	12	LEU	2.6
1	C	535	LEU	2.3
1	D	340	GLN	2.3
1	B	64	GLN	2.3
1	C	86	SER	2.1
1	B	509	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	11	THR	2.1
1	A	86	SER	2.0
1	D	86	SER	2.0
1	D	362	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	A	662	24/25	0.97	0.09	93,102,113,118	0
1	LLP	C	662	24/25	0.97	0.07	83,95,113,122	0
1	LLP	D	662	24/25	0.97	0.08	81,102,108,117	0
1	LLP	B	662	24/25	0.98	0.08	84,92,105,111	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

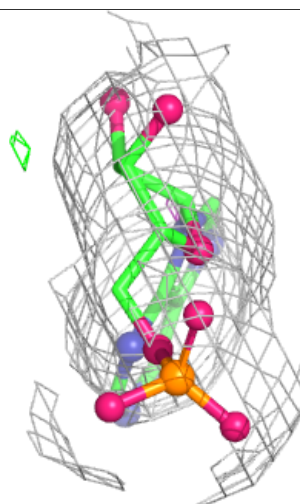
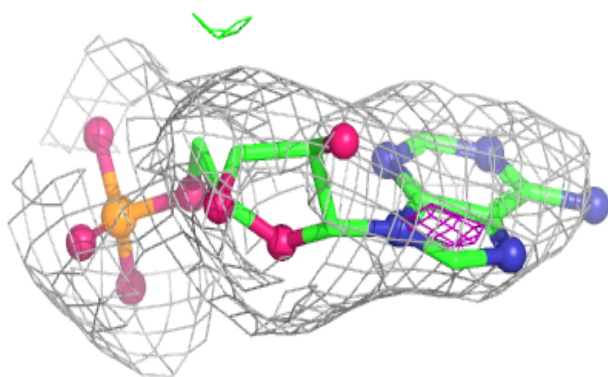
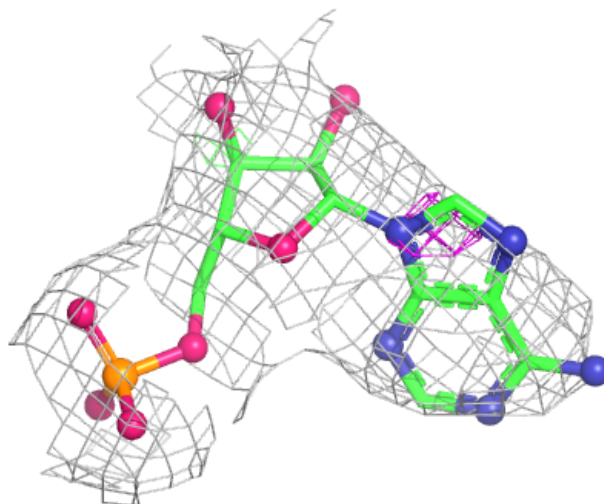
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AMP	A	901	23/23	0.93	0.08	106,128,137,141	0
2	AMP	B	901	23/23	0.93	0.10	90,114,122,135	0
2	AMP	D	901	23/23	0.93	0.09	108,129,131,136	0
2	AMP	C	901	23/23	0.94	0.10	84,113,127,133	0

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

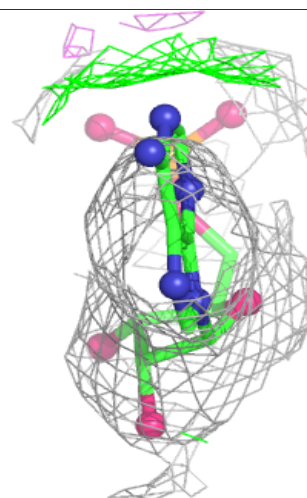
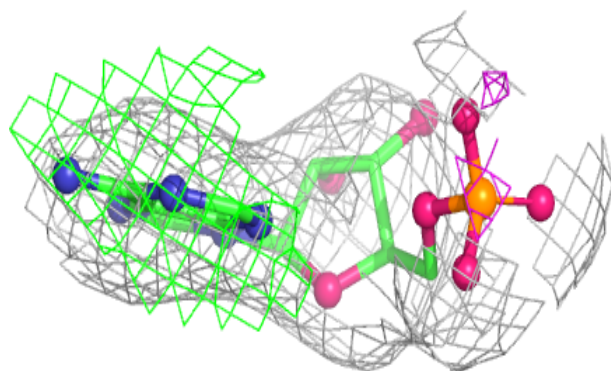
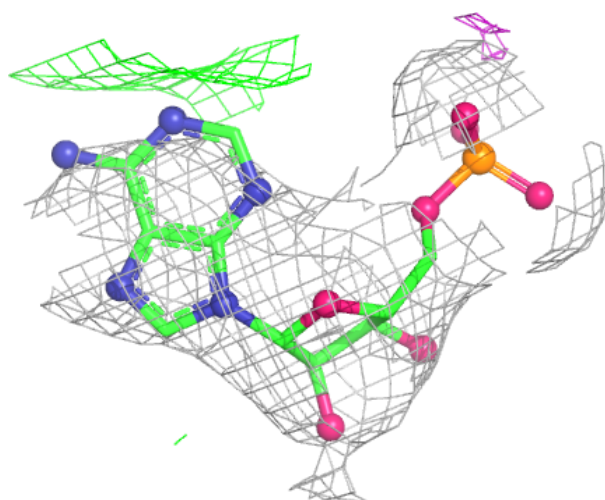
Electron density around AMP A 901:

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



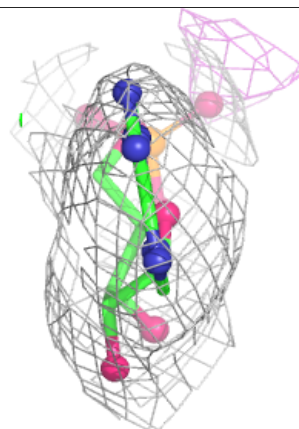
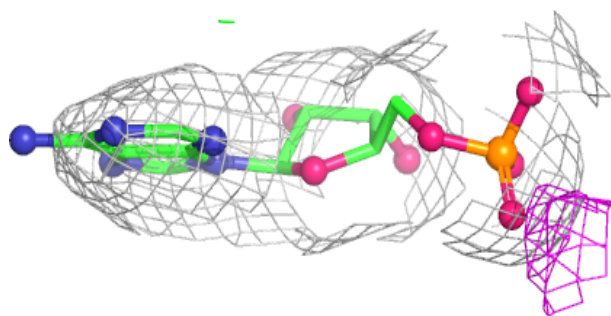
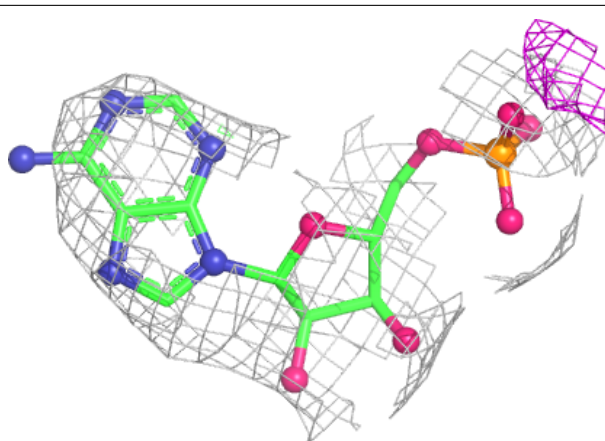
Electron density around AMP B 901:

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



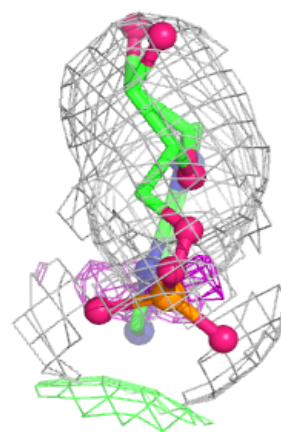
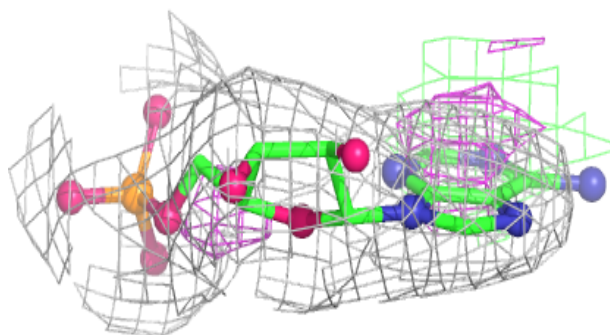
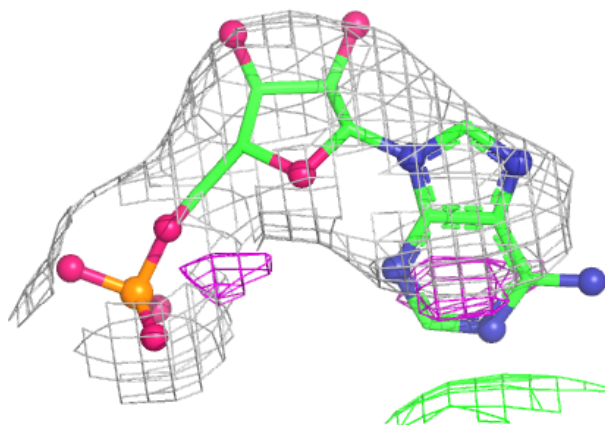
Electron density around AMP D 901:

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



Electron density around AMP C 901:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.