



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:59 am BST

PDB ID : 1RFU
Title : Crystal structure of pyridoxal kinase complexed with ADP and PLP
Authors : Liang, D.-C.; Jiang, T.; Li, M.-H.
Deposited on : 2003-11-10
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

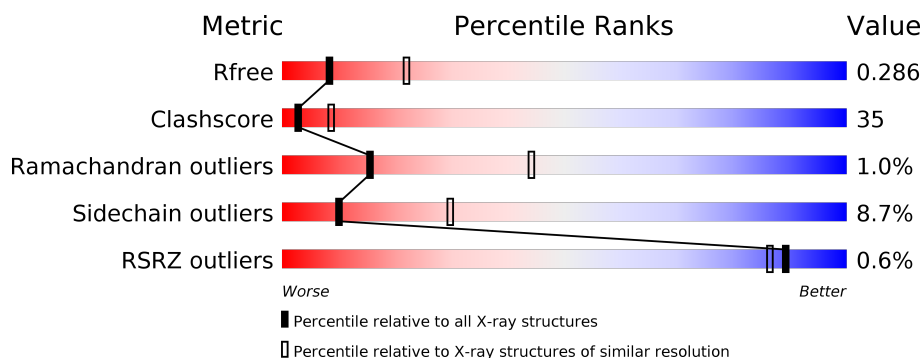
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	312	
1	B	312	
1	C	312	
1	D	312	
1	E	312	
1	F	312	

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Mol	Chain	Length	Quality of chain
1	G	312	<div><div></div><div>42%</div><div>53%</div><div>5%</div></div>
1	H	312	<div>%<div><div></div><div>37%</div><div>58%</div><div>5%</div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20123 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 pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	B	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	C	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	D	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	E	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	F	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	G	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	H	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

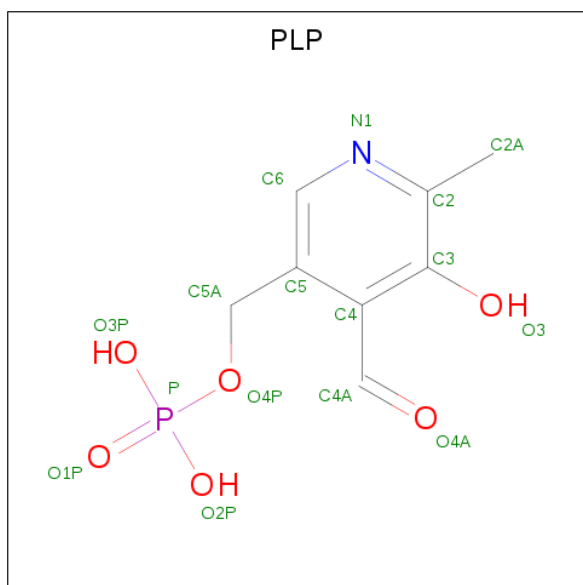
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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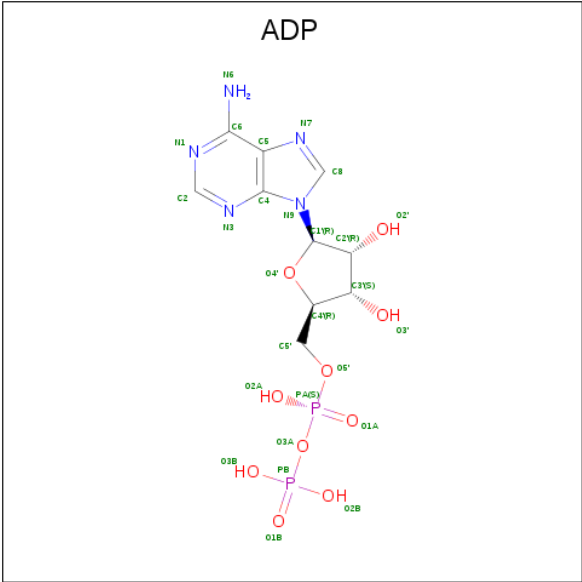
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total	O	0	0
			73	73		
5	B	54	Total	O	0	0
			54	54		
5	C	20	Total	O	0	0
			20	20		
5	D	9	Total	O	0	0
			9	9		

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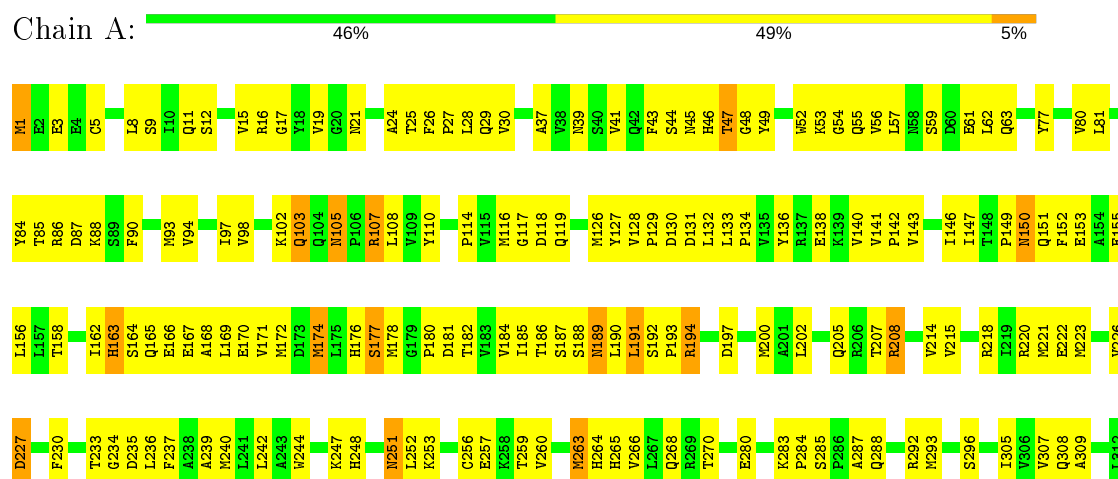
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	41	Total 41	O 41	0	0
5	F	37	Total 37	O 37	0	0
5	G	21	Total 21	O 21	0	0
5	H	12	Total 12	O 12	0	0

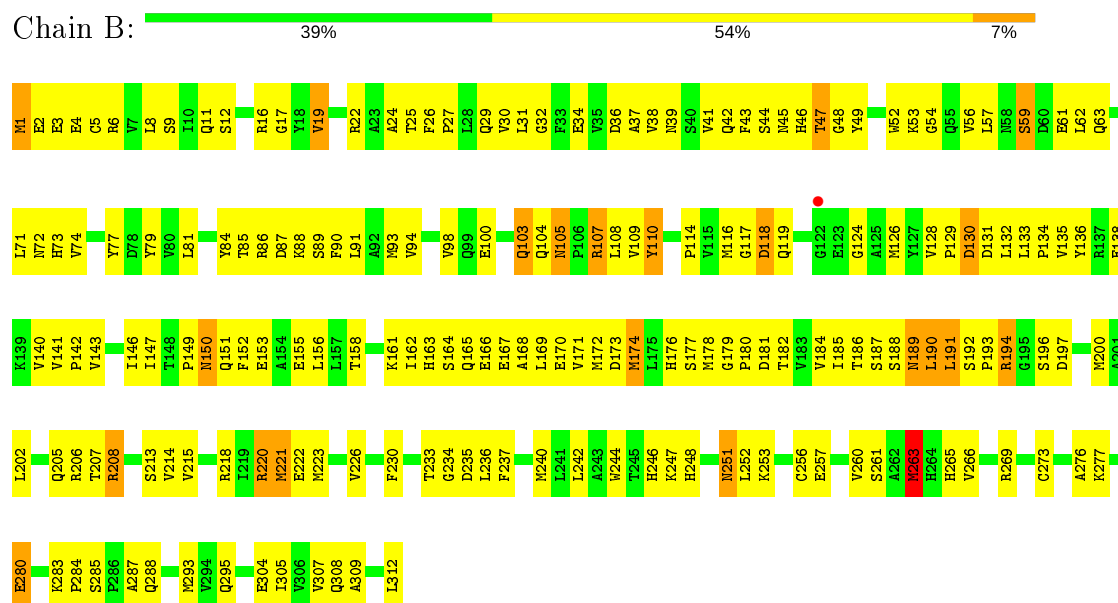
3 Residue-property plots

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.

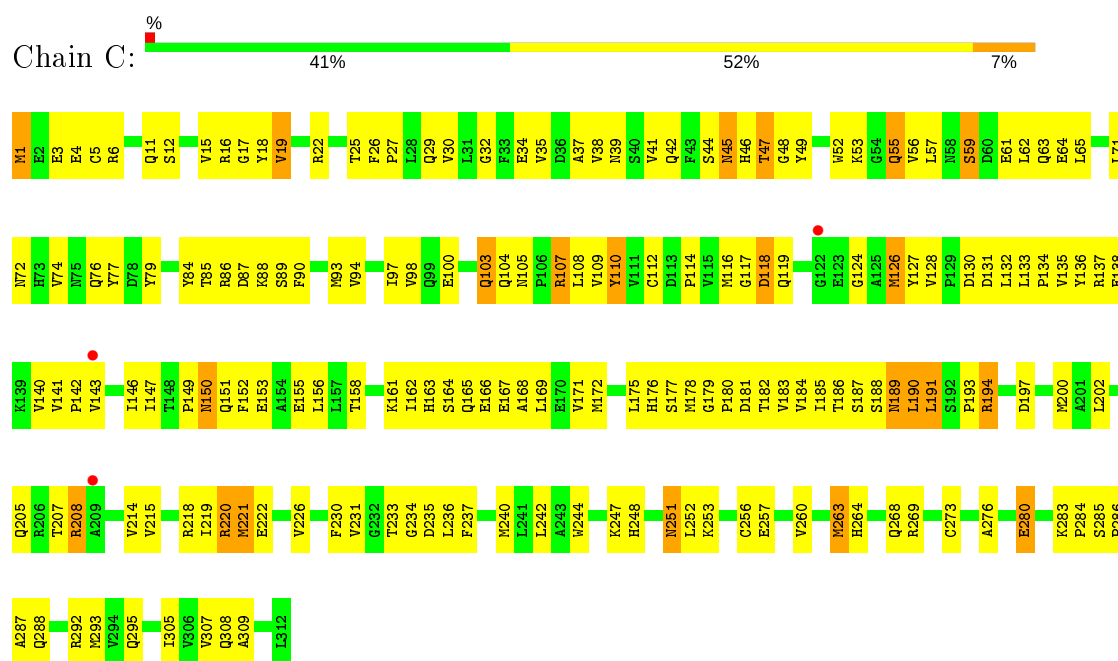
- Molecule 1: pyridoxal kinase



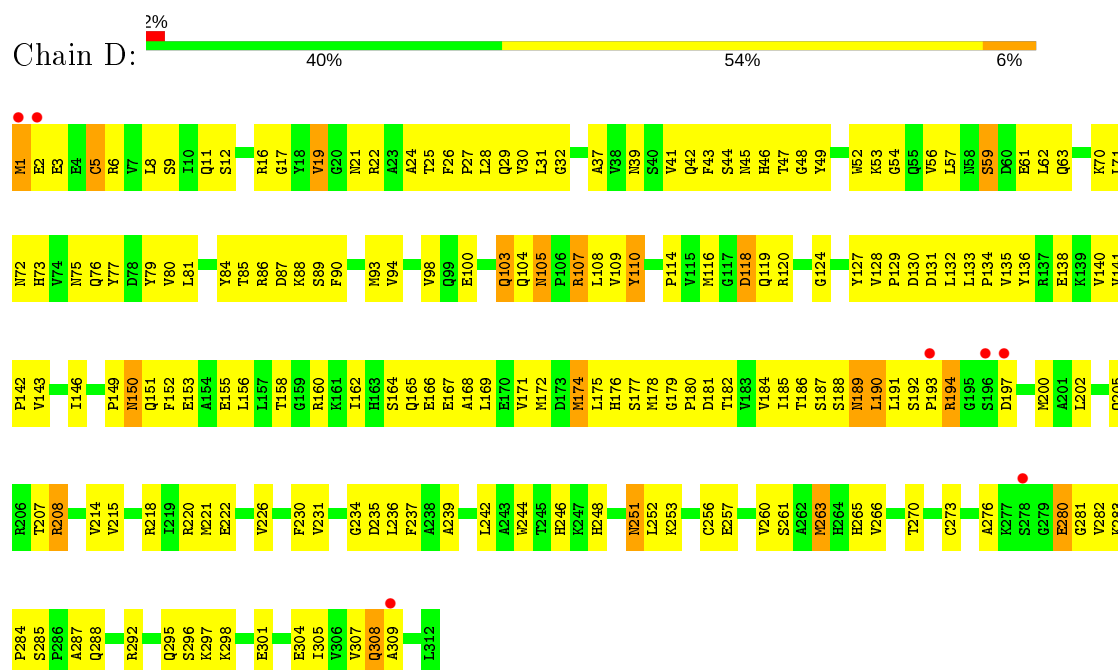
- Molecule 1: pyridoxal kinase



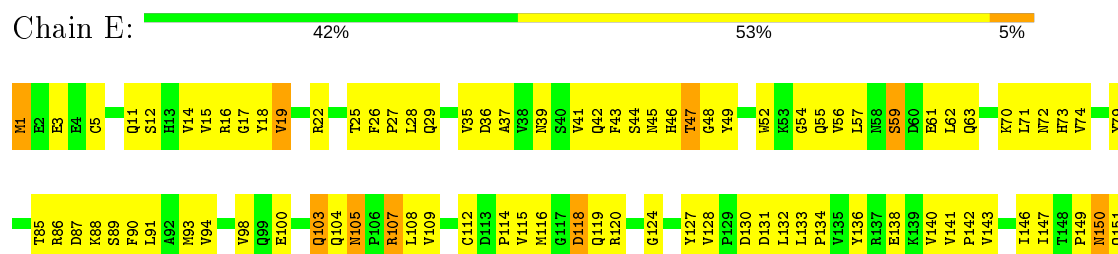
- Molecule 1: pyridoxal kinase



- Molecule 1: pyridoxal kinase



- Molecule 1: pyridoxal kinase



V282	K283	P284	S285	P286	A287	Q288	R292	M293	V294	Q295	S296	K297	I305	V306	V307	Q308	A309	T310	V311	L312																																				
T207	R208	V214	V215	R218	I219	R220	M221	E222	M223	V226	D227	A228	V229	F230	T233	G234	D235	L236	F237	M238	A239	R240	L241	L242	A243	V244	R247	H248	M251	L252	R253	C256	E257	V260	M263	H264	H265	V266	L267	Q268	R269	T270	C273	A276	G279	E280	G281									
I146	I147	T148	P149	M150	Q151	F152	E153	A154	E155	L156	L157	T158	G159	R160	F161	I162	H163	S164	Q165	E166	E167	A168	L169	E170	V171	M172	D173	M174	L175	H176	S177	M178	G179	P180	D181	T182	V183	V184	T185	T186	S187	S188	M189	L190	L191	S192	P193	R194	D197	Y198	L199	M200	A201	L202	Q205	R206
M1	E2	E3	E4	C5	R6	S9	I10	Q11	S12	V15	R16	G17	Y18	V19	G20	N21	R22	T25	F26	P27	L28	Q29	V30	L31	E34	N39	S40	V41	Q42	F43	S44	N45	H46	T47	G48	Y49	S50	H51	M52	K53	G54	Q55	V56	L57	N58	S59	D60	E61	L62	Q63	L69	K70	L71			
N72	H73	Q76	Y79	V80	L81	T85	R86	D87	K88	S89	F90	N93	V94	V98	Q99	E100	Q103	Q104	M105	P106	R107	L108	V109	Y110	V111	C112	D113	P114	V115	M116	C117	D118	Q119	G122	M126	Y127	V128	P129	D130	D131	L132	L133	P134	V135	Y136	R137	E138	V141	P142	V143						

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	109.09 Å 109.09 Å 284.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.5 (20.00-2.80) 56.7 (19.94-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.79 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.238 , 0.286	Depositor DCC
R_{free} test set	3623 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20123	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to $7.5074e-08$. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: ZN, ADP, PLP

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	0.51	0/2484	0.74	1/3367 (0.0%)
1	B	0.54	0/2484	0.79	5/3367 (0.1%)
1	C	0.47	0/2484	0.74	3/3367 (0.1%)
1	D	0.45	0/2484	0.71	1/3367 (0.0%)
1	E	0.54	0/2484	0.76	1/3367 (0.0%)
1	F	0.55	0/2484	0.76	1/3367 (0.0%)
1	G	0.45	0/2484	0.71	1/3367 (0.0%)
1	H	0.44	0/2484	0.71	1/3367 (0.0%)
All	All	0.50	0/19872	0.74	14/26936 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	2
1	H	0	2
All	All	0	5

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	C	220	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	F	178	MET	CG-SD-CE	6.12	110.00	100.20
1	B	221	MET	CG-SD-CE	6.12	109.99	100.20
1	C	126	MET	CG-SD-CE	6.12	109.99	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	MET	CG-SD-CE	6.12	109.99	100.20
1	H	116	MET	CG-SD-CE	6.11	109.98	100.20
1	B	174	MET	CG-SD-CE	6.08	109.94	100.20
1	D	174	MET	CG-SD-CE	6.03	109.84	100.20
1	C	221	MET	CG-SD-CE	6.00	109.81	100.20
1	G	174	MET	CG-SD-CE	6.00	109.80	100.20
1	E	174	MET	CG-SD-CE	5.98	109.77	100.20
1	B	263	MET	CG-SD-CE	5.95	109.72	100.20
1	B	223	MET	CG-SD-CE	5.79	109.47	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	18	TYR	Sidechain
1	F	127	TYR	Sidechain
1	F	18	TYR	Sidechain
1	H	127	TYR	Sidechain
1	H	18	TYR	Sidechain

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	2439	0	2442	176	0
1	B	2439	0	2442	200	0
1	C	2439	0	2442	198	0
1	D	2439	0	2442	182	0
1	E	2439	0	2442	172	0
1	F	2439	0	2442	180	0
1	G	2439	0	2442	163	0
1	H	2439	0	2442	209	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	15	0	7	2	0
3	B	15	0	6	1	0
3	C	15	0	6	1	0
3	D	15	0	7	1	0
3	E	15	0	6	1	0
3	F	15	0	7	2	0
3	G	15	0	6	1	0
3	H	15	0	7	1	0
4	A	27	0	12	3	0
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	2	0
4	G	27	0	12	1	0
4	H	27	0	12	2	0
5	A	73	0	0	4	0
5	B	54	0	0	5	0
5	C	20	0	0	2	0
5	D	9	0	0	2	0
5	E	41	0	0	3	0
5	F	37	0	0	5	0
5	G	21	0	0	2	0
5	H	12	0	0	3	0
All	All	20123	0	19684	1390	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 35.

All (1390) 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:129:PRO:HG3	1:B:191:LEU:HB2	1.22	1.19
1:B:39:ASN:H	1:F:42:GLN:HE22	1.07	0.95
1:A:191:LEU:HB2	1:D:129:PRO:HG3	1.50	0.93
1:H:208:ARG:HH11	1:H:208:ARG:HG3	1.31	0.93
1:A:39:ASN:H	1:E:42:GLN:HE22	1.05	0.92
1:G:150:ASN:HB2	1:G:153:GLU:OE1	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:THR:HG22	1:E:87:ASP:H	1.37	0.89
1:A:208:ARG:HH11	1:A:208:ARG:HG3	1.38	0.89
1:F:150:ASN:HB2	1:F:153:GLU:OE1	1.71	0.89
1:B:85:THR:HG22	1:B:87:ASP:H	1.38	0.88
1:C:4:GLU:OE2	1:H:292:ARG:NH2	2.06	0.88
1:E:150:ASN:HB2	1:E:153:GLU:OE1	1.74	0.88
1:B:236:LEU:HB3	1:B:263:MET:HE1	1.56	0.87
1:H:85:THR:HG22	1:H:87:ASP:H	1.39	0.87
1:C:85:THR:HG22	1:C:87:ASP:H	1.39	0.87
1:F:85:THR:HG22	1:F:87:ASP:H	1.38	0.87
1:D:150:ASN:HB2	1:D:153:GLU:OE1	1.76	0.85
1:C:39:ASN:H	1:H:42:GLN:HE22	1.24	0.85
1:F:103:GLN:N	1:F:103:GLN:HE21	1.73	0.85
1:E:158:THR:HG21	1:E:171:VAL:HG13	1.55	0.85
1:G:85:THR:HG22	1:G:87:ASP:H	1.40	0.85
1:F:119:GLN:HG2	1:F:152:PHE:HB2	1.59	0.84
1:A:129:PRO:N	1:B:191:LEU:HD12	1.93	0.84
1:H:242:LEU:HD23	1:H:242:LEU:O	1.77	0.83
1:C:150:ASN:HB2	1:C:153:GLU:OE1	1.77	0.83
1:F:208:ARG:HH11	1:F:208:ARG:HG3	1.43	0.83
1:C:151:GLN:O	1:C:155:GLU:HG3	1.78	0.83
1:B:103:GLN:HE21	1:B:103:GLN:N	1.76	0.83
1:A:128:VAL:C	1:B:191:LEU:HD12	1.99	0.82
1:C:103:GLN:N	1:C:103:GLN:HE21	1.78	0.82
1:D:85:THR:HG22	1:D:87:ASP:H	1.41	0.82
1:H:47:THR:HG22	1:H:52:TRP:CE2	2.14	0.82
1:G:208:ARG:HG3	1:G:208:ARG:HH11	1.45	0.81
1:A:105:ASN:HD21	1:A:107:ARG:HB2	1.44	0.81
1:E:103:GLN:HE21	1:E:103:GLN:N	1.79	0.81
1:F:158:THR:HG21	1:F:171:VAL:HG13	1.61	0.81
1:H:158:THR:HG21	1:H:171:VAL:HG13	1.63	0.80
1:E:208:ARG:HG3	1:E:208:ARG:HH11	1.46	0.80
1:A:85:THR:HG22	1:A:87:ASP:H	1.44	0.80
1:F:165:GLN:O	1:F:168:ALA:HB3	1.81	0.80
1:G:103:GLN:N	1:G:103:GLN:HE21	1.80	0.80
1:H:165:GLN:HA	1:H:190:LEU:HD21	1.62	0.80
1:H:150:ASN:HB2	1:H:153:GLU:OE1	1.82	0.80
1:A:119:GLN:HB3	1:A:152:PHE:HB2	1.65	0.79
1:B:150:ASN:HB2	1:B:153:GLU:OE1	1.83	0.79
1:G:151:GLN:O	1:G:155:GLU:HG3	1.83	0.79
1:H:165:GLN:O	1:H:168:ALA:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:THR:HB	1:G:215:VAL:HG13	1.66	0.78
1:D:119:GLN:HB3	1:D:152:PHE:HB2	1.66	0.78
1:F:164:SER:OG	1:F:167:GLU:HG2	1.84	0.78
1:H:119:GLN:HB3	1:H:152:PHE:HB2	1.66	0.78
1:B:103:GLN:HE21	1:B:103:GLN:CA	1.96	0.78
1:E:103:GLN:HE21	1:E:103:GLN:CA	1.97	0.78
1:C:39:ASN:H	1:H:42:GLN:NE2	1.82	0.77
1:B:158:THR:HG21	1:B:171:VAL:HG13	1.64	0.77
1:D:158:THR:HG21	1:D:171:VAL:HG13	1.67	0.77
1:G:103:GLN:CA	1:G:103:GLN:HE21	1.97	0.77
1:E:242:LEU:HD23	1:E:242:LEU:O	1.85	0.77
1:G:158:THR:HG21	1:G:171:VAL:HG13	1.65	0.77
1:B:165:GLN:O	1:B:168:ALA:HB3	1.83	0.77
1:F:242:LEU:HD23	1:F:242:LEU:C	2.05	0.77
1:F:242:LEU:HD23	1:F:242:LEU:O	1.83	0.77
1:G:214:VAL:O	1:G:214:VAL:HG23	1.84	0.76
1:A:305:ILE:HD12	1:A:305:ILE:N	1.99	0.76
1:H:103:GLN:N	1:H:103:GLN:HE21	1.83	0.76
1:B:208:ARG:HG3	1:B:208:ARG:HH11	1.50	0.76
1:C:103:GLN:HE21	1:C:103:GLN:CA	1.97	0.76
1:D:165:GLN:HA	1:D:190:LEU:HD21	1.67	0.76
1:F:94:VAL:O	1:F:98:VAL:HG23	1.86	0.76
1:H:270:THR:OG1	5:H:7414:HOH:O	2.04	0.76
1:G:94:VAL:O	1:G:98:VAL:HG23	1.84	0.76
1:E:119:GLN:HB3	1:E:152:PHE:HB2	1.66	0.76
1:A:158:THR:HG21	1:A:171:VAL:HG13	1.69	0.75
1:D:103:GLN:HE21	1:D:103:GLN:N	1.85	0.75
1:D:94:VAL:O	1:D:98:VAL:HG23	1.87	0.75
1:G:25:THR:O	1:G:29:GLN:HG3	1.86	0.75
1:G:236:LEU:HB3	1:G:263:MET:HE1	1.69	0.74
1:H:94:VAL:O	1:H:98:VAL:HG23	1.87	0.74
1:C:94:VAL:O	1:C:98:VAL:HG23	1.88	0.74
1:C:72:ASN:OD1	1:H:49:TYR:HB3	1.87	0.74
1:E:105:ASN:ND2	1:E:107:ARG:H	1.86	0.73
1:H:164:SER:OG	1:H:167:GLU:HG2	1.87	0.73
1:F:108:LEU:HD23	1:F:108:LEU:C	2.08	0.73
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.53	0.73
1:C:242:LEU:HD23	1:C:242:LEU:C	2.08	0.73
1:F:105:ASN:ND2	1:F:107:ARG:H	1.87	0.73
1:A:39:ASN:H	1:E:42:GLN:NE2	1.85	0.73
1:E:165:GLN:O	1:E:168:ALA:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:VAL:O	1:E:98:VAL:HG23	1.88	0.73
1:H:242:LEU:HD23	1:H:242:LEU:C	2.08	0.73
1:C:242:LEU:HD23	1:C:242:LEU:O	1.88	0.72
1:A:165:GLN:O	1:A:168:ALA:HB3	1.89	0.72
1:D:305:ILE:HD12	1:D:305:ILE:N	2.04	0.72
1:B:305:ILE:N	1:B:305:ILE:HD12	2.04	0.72
1:H:208:ARG:NH1	1:H:208:ARG:HG3	2.04	0.72
1:D:214:VAL:O	1:D:214:VAL:HG23	1.88	0.72
1:F:25:THR:O	1:F:29:GLN:HG3	1.88	0.72
1:E:214:VAL:HG23	1:E:214:VAL:O	1.89	0.72
1:C:236:LEU:HB3	1:C:263:MET:HE1	1.72	0.71
1:C:305:ILE:HD12	1:C:305:ILE:N	2.05	0.71
1:E:25:THR:O	1:E:29:GLN:HG3	1.89	0.71
1:B:214:VAL:HG23	1:B:214:VAL:O	1.89	0.71
1:A:151:GLN:O	1:A:155:GLU:HG3	1.90	0.71
3:A:401:PLP:P	4:A:402:ADP:O3B	2.49	0.71
1:D:41:VAL:HG12	1:D:56:VAL:HG13	1.70	0.71
1:C:71:LEU:HD13	1:H:51:HIS:HB3	1.71	0.71
1:B:150:ASN:HB3	1:B:153:GLU:H	1.55	0.71
1:A:129:PRO:CG	1:B:191:LEU:HB2	2.11	0.71
1:F:174:MET:O	1:F:178:MET:HG3	1.91	0.71
1:F:253:LYS:O	1:F:257:GLU:HG3	1.91	0.71
1:B:105:ASN:ND2	1:B:107:ARG:H	1.89	0.71
1:D:242:LEU:HD23	1:D:242:LEU:C	2.11	0.71
1:A:208:ARG:HG2	1:A:214:VAL:HG12	1.73	0.70
1:E:151:GLN:O	1:E:155:GLU:HG3	1.90	0.70
1:G:305:ILE:N	1:G:305:ILE:HD12	2.06	0.70
1:C:165:GLN:O	1:C:168:ALA:HB3	1.90	0.70
1:B:1:MET:HE1	1:B:5:CYS:HB2	1.71	0.70
1:D:105:ASN:ND2	1:D:107:ARG:H	1.88	0.70
1:G:119:GLN:HB3	1:G:152:PHE:HB2	1.72	0.70
1:C:158:THR:HG21	1:C:171:VAL:HG13	1.74	0.70
1:F:47:THR:HG22	1:F:52:TRP:CE2	2.27	0.70
1:D:207:THR:HB	1:D:215:VAL:HG13	1.73	0.70
1:G:26:PHE:HB3	1:G:27:PRO:HD3	1.72	0.70
1:A:129:PRO:HG3	1:B:191:LEU:CB	2.13	0.70
1:A:150:ASN:HB3	1:A:153:GLU:H	1.55	0.70
1:D:39:ASN:H	1:G:42:GLN:HE22	1.40	0.70
1:B:242:LEU:C	1:B:242:LEU:HD23	2.12	0.70
1:E:150:ASN:HB3	1:E:153:GLU:H	1.57	0.70
1:F:103:GLN:CA	1:F:103:GLN:HE21	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLN:HB3	1:B:152:PHE:HB2	1.73	0.69
1:E:242:LEU:C	1:E:242:LEU:HD23	2.13	0.69
1:E:253:LYS:O	1:E:257:GLU:HG3	1.92	0.69
1:C:164:SER:OG	1:C:167:GLU:HG2	1.92	0.69
1:A:214:VAL:O	1:A:214:VAL:HG23	1.91	0.69
1:E:151:GLN:OE1	1:E:188:SER:HB2	1.92	0.69
1:C:207:THR:HB	1:C:215:VAL:HG13	1.74	0.69
1:F:214:VAL:O	1:F:214:VAL:HG23	1.91	0.69
1:A:236:LEU:HB3	1:A:263:MET:HE1	1.75	0.69
1:D:164:SER:OG	1:D:167:GLU:HG2	1.92	0.69
1:F:119:GLN:CG	1:F:152:PHE:HB2	2.23	0.69
1:H:305:ILE:N	1:H:305:ILE:HD12	2.07	0.69
1:D:301:GLU:OE1	1:G:297:LYS:NZ	2.22	0.69
1:H:236:LEU:HB3	1:H:263:MET:HE1	1.75	0.69
1:C:214:VAL:HG23	1:C:214:VAL:O	1.91	0.69
1:E:158:THR:CG2	1:E:171:VAL:HG13	2.23	0.69
1:D:103:GLN:CA	1:D:103:GLN:HE21	2.06	0.68
1:A:165:GLN:HA	1:A:190:LEU:HD21	1.75	0.68
1:G:256:CYS:O	1:G:260:VAL:HG23	1.93	0.68
1:C:208:ARG:HG3	1:C:208:ARG:HH11	1.56	0.68
1:C:119:GLN:HB3	1:C:152:PHE:HB2	1.74	0.68
1:G:165:GLN:O	1:G:168:ALA:HB3	1.93	0.68
1:C:88:LYS:HE3	1:D:280:GLU:OE1	1.94	0.68
1:F:100:GLU:O	1:F:104:GLN:HG3	1.94	0.68
1:F:207:THR:HB	1:F:215:VAL:HG13	1.74	0.68
1:G:219:ILE:HD11	1:G:256:CYS:SG	2.34	0.68
1:A:242:LEU:HD23	1:A:242:LEU:C	2.14	0.67
1:E:108:LEU:C	1:E:108:LEU:HD23	2.13	0.67
1:F:108:LEU:HD23	1:F:109:VAL:N	2.08	0.67
1:H:103:GLN:HE21	1:H:103:GLN:CA	2.06	0.67
1:C:150:ASN:HB3	1:C:153:GLU:H	1.56	0.67
1:A:1:MET:CE	1:A:5:CYS:HB2	2.25	0.67
1:C:4:GLU:CD	1:H:292:ARG:HH22	1.96	0.67
1:D:234:GLY:O	1:D:237:PHE:HB3	1.94	0.67
1:E:207:THR:HB	1:E:215:VAL:HG13	1.74	0.67
1:E:47:THR:HG22	1:E:52:TRP:CE2	2.30	0.67
1:F:150:ASN:HB3	1:F:153:GLU:H	1.59	0.67
1:F:158:THR:CG2	1:F:171:VAL:HG13	2.24	0.67
1:A:208:ARG:NH1	1:A:208:ARG:HG3	2.04	0.67
1:D:165:GLN:O	1:D:168:ALA:HB3	1.93	0.67
1:G:150:ASN:HB3	1:G:153:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:SER:OG	1:G:167:GLU:HG2	1.94	0.67
1:C:256:CYS:O	1:C:260:VAL:HG23	1.95	0.67
1:D:150:ASN:HB3	1:D:153:GLU:H	1.60	0.67
1:E:305:ILE:HD12	1:E:305:ILE:N	2.10	0.67
1:A:170:GLU:O	1:A:174:MET:HG3	1.95	0.67
1:B:149:PRO:HD2	1:B:184:VAL:O	1.94	0.67
1:B:151:GLN:O	1:B:155:GLU:HG3	1.93	0.67
1:D:151:GLN:O	1:D:155:GLU:HG3	1.95	0.67
1:F:119:GLN:HE21	1:F:150:ASN:ND2	1.92	0.67
1:A:207:THR:HB	1:A:215:VAL:HG13	1.77	0.67
1:F:305:ILE:HD12	1:F:305:ILE:N	2.09	0.67
1:G:253:LYS:O	1:G:257:GLU:HG3	1.95	0.67
1:H:207:THR:HB	1:H:215:VAL:HG13	1.77	0.67
1:F:220:ARG:HG2	1:F:221:MET:N	2.10	0.66
1:H:256:CYS:O	1:H:260:VAL:HG23	1.94	0.66
1:H:214:VAL:O	1:H:214:VAL:HG23	1.93	0.66
1:F:150:ASN:O	1:F:151:GLN:C	2.30	0.66
1:C:57:LEU:HD21	1:H:55:GLN:NE2	2.10	0.66
1:H:146:ILE:HG12	1:H:182:THR:HB	1.77	0.66
1:E:220:ARG:HG2	1:E:221:MET:N	2.11	0.66
1:G:151:GLN:OE1	1:G:188:SER:HB2	1.95	0.66
1:G:242:LEU:HD23	1:G:242:LEU:O	1.96	0.66
1:B:220:ARG:HG2	1:B:221:MET:N	2.11	0.66
1:E:285:SER:OG	1:E:288:GLN:HG3	1.96	0.66
1:F:146:ILE:HG12	1:F:182:THR:HB	1.77	0.66
1:H:165:GLN:HA	1:H:190:LEU:CD2	2.26	0.66
1:A:150:ASN:HB2	1:A:153:GLU:OE1	1.95	0.66
1:C:44:SER:OG	1:C:45:ASN:ND2	2.29	0.66
1:D:236:LEU:HB3	1:D:263:MET:HE1	1.77	0.66
1:B:193:PRO:HG2	1:B:220:ARG:NH1	2.11	0.65
1:B:242:LEU:HD23	1:B:242:LEU:O	1.96	0.65
1:B:25:THR:O	1:B:29:GLN:HG3	1.97	0.65
1:C:47:THR:HG22	1:C:52:TRP:CE2	2.31	0.65
1:H:220:ARG:HG2	1:H:221:MET:N	2.09	0.65
1:E:1:MET:HE1	1:E:5:CYS:HB2	1.78	0.65
1:C:220:ARG:HG2	1:C:221:MET:N	2.09	0.65
1:A:103:GLN:HE21	1:A:103:GLN:CA	2.09	0.65
1:G:108:LEU:HD23	1:G:108:LEU:C	2.17	0.65
1:D:1:MET:HE1	1:D:5:CYS:HB2	1.78	0.65
1:E:165:GLN:HA	1:E:190:LEU:HD21	1.76	0.65
1:F:285:SER:OG	1:F:288:GLN:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:HA	1:A:190:LEU:CD2	2.27	0.65
1:A:191:LEU:HB3	1:D:86:ARG:HH21	1.61	0.65
1:G:105:ASN:ND2	1:G:107:ARG:H	1.94	0.65
1:A:105:ASN:ND2	1:A:107:ARG:H	1.93	0.65
1:B:207:THR:HB	1:B:215:VAL:HG13	1.77	0.65
1:D:1:MET:CE	1:D:5:CYS:HB2	2.26	0.65
1:H:41:VAL:HG12	1:H:56:VAL:HG13	1.79	0.65
1:E:150:ASN:O	1:E:151:GLN:C	2.31	0.65
1:B:37:ALA:O	1:F:15:VAL:HA	1.97	0.65
1:A:235:ASP:OD2	3:A:401:PLP:H5A1	1.96	0.64
1:A:41:VAL:HG12	1:A:56:VAL:HG13	1.78	0.64
1:D:248:HIS:HB3	1:D:251:ASN:HB2	1.79	0.64
1:G:207:THR:HB	1:G:215:VAL:CG1	2.27	0.64
1:H:158:THR:CG2	1:H:171:VAL:HG13	2.26	0.64
1:H:193:PRO:HG2	1:H:220:ARG:NH1	2.12	0.64
1:F:105:ASN:HD21	1:F:107:ARG:HB2	1.63	0.64
1:H:151:GLN:O	1:H:155:GLU:HG3	1.98	0.64
1:D:108:LEU:C	1:D:108:LEU:HD23	2.17	0.64
1:B:194:ARG:HG2	1:B:222:GLU:OE1	1.98	0.64
1:D:149:PRO:HG2	1:D:185:ILE:HD13	1.79	0.64
1:D:208:ARG:HH11	1:D:208:ARG:HG3	1.62	0.64
1:E:256:CYS:O	1:E:260:VAL:HG23	1.97	0.64
1:H:172:MET:HA	1:H:175:LEU:HD12	1.80	0.64
1:A:191:LEU:HB3	1:D:86:ARG:NH2	2.12	0.64
1:D:149:PRO:HD2	1:D:184:VAL:O	1.98	0.64
1:D:158:THR:CG2	1:D:171:VAL:HG13	2.27	0.64
1:D:242:LEU:O	1:D:242:LEU:HD23	1.97	0.64
1:H:108:LEU:C	1:H:108:LEU:HD23	2.18	0.64
1:D:49:TYR:OH	1:D:287:ALA:HA	1.98	0.64
1:F:165:GLN:HA	1:F:190:LEU:HD21	1.79	0.64
1:C:57:LEU:HD21	1:H:55:GLN:HE21	1.62	0.64
1:D:105:ASN:HD21	1:D:107:ARG:HB2	1.63	0.64
1:B:34:GLU:OE1	1:F:18:TYR:HE1	1.80	0.64
1:H:253:LYS:O	1:H:257:GLU:HG3	1.99	0.63
1:B:47:THR:HG22	1:B:52:TRP:CE2	2.32	0.63
1:E:176:HIS:HA	1:E:180:PRO:O	1.99	0.63
1:A:285:SER:OG	1:A:288:GLN:HG3	1.98	0.63
1:C:25:THR:O	1:C:29:GLN:HG3	1.97	0.63
1:D:42:GLN:HE22	1:G:39:ASN:H	1.46	0.63
1:D:205:GLN:HB2	1:D:252:LEU:HD22	1.80	0.63
1:B:248:HIS:HB3	1:B:251:ASN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:SER:OG	1:B:288:GLN:HG3	1.99	0.63
1:G:1:MET:HE1	1:G:5:CYS:HB2	1.80	0.63
1:H:105:ASN:ND2	1:H:107:ARG:H	1.96	0.63
1:B:165:GLN:HA	1:B:190:LEU:HD21	1.80	0.63
1:F:236:LEU:HB3	1:F:263:MET:HE1	1.81	0.63
1:C:194:ARG:HG2	1:C:222:GLU:OE1	1.98	0.63
1:B:151:GLN:OE1	1:B:188:SER:HB2	1.98	0.62
1:G:242:LEU:C	1:G:242:LEU:HD23	2.19	0.62
1:B:169:LEU:HD22	1:B:218:ARG:HD2	1.81	0.62
1:D:146:ILE:HG12	1:D:182:THR:HB	1.80	0.62
1:H:47:THR:HG22	1:H:52:TRP:NE1	2.14	0.62
1:F:208:ARG:NH1	1:F:208:ARG:HG3	2.13	0.62
1:H:150:ASN:HB3	1:H:153:GLU:H	1.63	0.62
1:A:253:LYS:O	1:A:257:GLU:HG3	1.98	0.62
1:F:16:ARG:NH1	5:F:5417:HOH:O	2.32	0.62
1:G:1:MET:CE	1:G:5:CYS:HB2	2.30	0.62
1:A:174:MET:O	1:A:177:SER:HB3	1.99	0.62
1:B:226:VAL:HG11	1:B:230:PHE:HZ	1.65	0.62
1:F:172:MET:HA	1:F:175:LEU:HD12	1.82	0.62
1:G:158:THR:CG2	1:G:171:VAL:HG13	2.30	0.62
1:H:142:PRO:HA	1:H:178:MET:O	2.00	0.62
1:A:226:VAL:HG11	1:A:230:PHE:HZ	1.64	0.62
1:A:305:ILE:HD12	1:A:305:ILE:H	1.62	0.62
1:C:88:LYS:HE3	1:D:280:GLU:CD	2.20	0.62
1:F:26:PHE:HB3	1:F:27:PRO:HD3	1.80	0.62
1:G:138:GLU:O	1:G:142:PRO:HG2	1.99	0.62
1:G:176:HIS:HA	1:G:180:PRO:O	1.99	0.62
1:A:158:THR:CG2	1:A:171:VAL:HG13	2.29	0.61
1:B:158:THR:CG2	1:B:171:VAL:HG13	2.29	0.61
1:G:47:THR:HG22	1:G:52:TRP:CE2	2.34	0.61
1:A:94:VAL:O	1:A:98:VAL:HG23	2.00	0.61
1:D:165:GLN:HA	1:D:190:LEU:CD2	2.29	0.61
1:B:4:GLU:OE2	1:F:292:ARG:NH2	2.33	0.61
1:H:26:PHE:HB3	1:H:27:PRO:HD3	1.83	0.61
1:H:292:ARG:N	5:H:7414:HOH:O	2.20	0.61
1:A:220:ARG:HG2	1:A:221:MET:N	2.15	0.61
1:D:26:PHE:HB3	1:D:27:PRO:HD3	1.83	0.61
1:A:193:PRO:HG2	1:A:220:ARG:NH1	2.16	0.61
1:C:26:PHE:HB3	1:C:27:PRO:HD3	1.82	0.61
1:E:105:ASN:HD21	1:E:107:ARG:HB2	1.65	0.61
1:C:71:LEU:HB3	1:H:51:HIS:CG	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:GLN:O	1:F:155:GLU:HG3	2.00	0.61
1:G:285:SER:OG	1:G:288:GLN:HG3	2.00	0.61
1:A:62:LEU:HB2	1:A:90:PHE:CE1	2.36	0.61
1:C:35:VAL:O	1:H:22:ARG:NH2	2.24	0.61
1:B:47:THR:HG22	1:B:52:TRP:NE1	2.16	0.61
1:G:150:ASN:O	1:G:151:GLN:C	2.37	0.61
1:F:119:GLN:HG2	1:F:152:PHE:CB	2.28	0.61
1:B:253:LYS:O	1:B:257:GLU:HG3	2.00	0.61
1:C:285:SER:OG	1:C:288:GLN:HG3	2.00	0.61
1:F:187:SER:OG	4:F:5402:ADP:O2A	2.19	0.61
1:D:283:LYS:HD3	1:D:284:PRO:HD2	1.83	0.60
1:F:41:VAL:HG12	1:F:56:VAL:HG13	1.82	0.60
1:H:187:SER:HA	1:H:200:MET:O	2.00	0.60
1:C:29:GLN:HB3	1:H:26:PHE:CE1	2.37	0.60
1:A:57:LEU:HD21	1:E:55:GLN:NE2	2.16	0.60
1:D:285:SER:OG	1:D:288:GLN:HG3	2.01	0.60
1:D:47:THR:HG22	1:D:52:TRP:CE2	2.36	0.60
1:F:256:CYS:O	1:F:260:VAL:HG23	2.01	0.60
1:C:108:LEU:C	1:C:108:LEU:HD23	2.22	0.60
1:C:39:ASN:N	1:H:42:GLN:HE22	1.95	0.60
1:F:187:SER:HA	1:F:200:MET:O	2.01	0.60
1:B:47:THR:HG22	1:B:52:TRP:CD1	2.37	0.60
1:B:253:LYS:HG3	1:B:309:ALA:HB3	1.82	0.60
1:B:34:GLU:OE1	1:F:18:TYR:CE1	2.54	0.60
1:F:151:GLN:OE1	1:F:188:SER:HB2	2.01	0.60
1:G:220:ARG:HG2	1:G:221:MET:N	2.15	0.60
1:B:176:HIS:HE1	1:B:181:ASP:O	1.84	0.60
1:H:151:GLN:OE1	1:H:188:SER:HB2	2.02	0.60
1:B:116:MET:O	1:B:128:VAL:HG22	2.01	0.60
1:G:273:CYS:O	1:G:276:ALA:HB3	2.02	0.60
1:C:253:LYS:HG3	1:C:309:ALA:HB3	1.84	0.60
1:B:251:ASN:ND2	5:B:1426:HOH:O	2.34	0.59
1:B:57:LEU:HD21	1:F:55:GLN:NE2	2.17	0.59
1:D:218:ARG:HH11	1:D:218:ARG:HG3	1.66	0.59
1:G:208:ARG:HG3	1:G:208:ARG:NH1	2.17	0.59
1:H:226:VAL:HG11	1:H:230:PHE:HZ	1.67	0.59
1:H:234:GLY:O	1:H:237:PHE:HB3	2.02	0.59
1:A:103:GLN:HE21	1:A:103:GLN:N	2.00	0.59
1:B:189:ASN:O	1:B:190:LEU:C	2.40	0.59
1:C:189:ASN:O	1:C:190:LEU:C	2.40	0.59
1:F:47:THR:HG22	1:F:52:TRP:NE1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:PRO:HA	1:G:178:MET:O	2.03	0.59
1:G:150:ASN:HB2	1:G:153:GLU:CD	2.21	0.59
1:G:49:TYR:OH	1:G:287:ALA:HA	2.02	0.59
1:H:116:MET:O	1:H:128:VAL:HG22	2.02	0.59
1:F:136:TYR:O	1:F:141:VAL:HG23	2.02	0.59
1:G:165:GLN:HA	1:G:190:LEU:HD21	1.83	0.59
1:H:176:HIS:HA	1:H:180:PRO:O	2.02	0.59
1:B:150:ASN:O	1:B:151:GLN:C	2.41	0.59
1:B:256:CYS:O	1:B:260:VAL:HG23	2.03	0.59
1:D:218:ARG:NH1	1:D:218:ARG:HG3	2.17	0.59
1:E:150:ASN:HB2	1:E:153:GLU:CD	2.23	0.59
1:C:105:ASN:ND2	1:C:107:ARG:H	2.01	0.59
1:D:142:PRO:HA	1:D:178:MET:O	2.01	0.59
1:A:47:THR:HG22	1:A:52:TRP:CE2	2.38	0.59
1:C:146:ILE:HG12	1:C:182:THR:HB	1.85	0.59
1:D:186:THR:HG22	1:D:237:PHE:CE2	2.38	0.59
1:F:116:MET:O	1:F:128:VAL:HG22	2.02	0.59
1:G:44:SER:OG	1:G:45:ASN:ND2	2.36	0.59
1:A:176:HIS:HE1	1:A:181:ASP:O	1.86	0.59
1:A:186:THR:HG22	1:A:237:PHE:CE2	2.38	0.59
1:B:187:SER:HA	1:B:200:MET:O	2.02	0.59
1:B:1:MET:CE	1:B:5:CYS:HB2	2.33	0.59
1:E:208:ARG:HG3	1:E:208:ARG:NH1	2.18	0.59
1:E:164:SER:OG	1:E:167:GLU:HG2	2.02	0.58
1:F:12:SER:HA	1:F:41:VAL:HG22	1.85	0.58
1:H:248:HIS:HB3	1:H:251:ASN:HB2	1.85	0.58
1:A:116:MET:O	1:A:128:VAL:HG22	2.04	0.58
1:D:226:VAL:HG11	1:D:230:PHE:HZ	1.68	0.58
1:B:42:GLN:HE22	1:F:39:ASN:H	1.49	0.58
1:D:162:ILE:CD1	1:D:171:VAL:HG21	2.33	0.58
1:E:108:LEU:HD23	1:E:109:VAL:N	2.18	0.58
1:A:102:LYS:NZ	1:A:108:LEU:O	2.36	0.58
1:E:202:LEU:HD23	1:E:220:ARG:HA	1.85	0.58
1:G:171:VAL:O	1:G:175:LEU:HG	2.04	0.58
1:B:187:SER:OG	4:B:1402:ADP:O2A	2.20	0.58
1:C:57:LEU:CD2	1:H:55:GLN:NE2	2.67	0.58
1:A:164:SER:OG	1:A:167:GLU:CG	2.51	0.58
1:D:87:ASP:OD2	1:D:89:SER:HB2	2.04	0.58
1:H:105:ASN:HD21	1:H:107:ARG:HB2	1.68	0.58
1:H:171:VAL:O	1:H:175:LEU:HG	2.04	0.58
1:B:218:ARG:NH1	5:B:1443:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:PRO:HG2	1:D:220:ARG:NH1	2.19	0.58
1:D:87:ASP:HB3	1:D:90:PHE:HB2	1.86	0.58
1:F:189:ASN:O	1:F:190:LEU:C	2.42	0.58
1:B:165:GLN:HA	1:B:190:LEU:CD2	2.34	0.58
1:B:234:GLY:O	1:B:237:PHE:HB3	2.03	0.58
1:D:187:SER:HA	1:D:200:MET:O	2.02	0.58
1:G:46:HIS:CE1	1:G:48:GLY:HA3	2.38	0.58
1:A:133:LEU:N	1:A:134:PRO:HD2	2.19	0.58
1:A:251:ASN:ND2	5:A:405:HOH:O	2.35	0.58
1:D:57:LEU:HA	1:D:61:GLU:OE2	2.04	0.58
1:E:171:VAL:O	1:E:175:LEU:HG	2.04	0.58
1:G:136:TYR:O	1:G:141:VAL:HG23	2.03	0.58
1:G:218:ARG:HH11	1:G:218:ARG:HG3	1.69	0.58
1:H:189:ASN:O	1:H:190:LEU:C	2.42	0.58
1:B:133:LEU:N	1:B:134:PRO:HD2	2.19	0.57
1:C:34:GLU:OE1	1:H:18:TYR:OH	2.18	0.57
1:D:133:LEU:N	1:D:134:PRO:HD2	2.19	0.57
1:F:234:GLY:O	1:F:237:PHE:HB3	2.04	0.57
1:G:283:LYS:HD3	1:G:284:PRO:HD2	1.86	0.57
1:A:28:LEU:HD21	1:A:239:ALA:O	2.04	0.57
1:B:94:VAL:O	1:B:98:VAL:HG23	2.05	0.57
1:D:62:LEU:HB2	1:D:90:PHE:CE1	2.40	0.57
1:E:142:PRO:HA	1:E:178:MET:O	2.04	0.57
1:G:172:MET:HG2	1:G:183:VAL:CG1	2.34	0.57
1:A:1:MET:HE1	1:A:5:CYS:HB2	1.85	0.57
1:C:187:SER:HA	1:C:200:MET:O	2.04	0.57
1:C:207:THR:HB	1:C:215:VAL:CG1	2.33	0.57
1:A:189:ASN:O	1:A:190:LEU:C	2.42	0.57
1:E:133:LEU:N	1:E:134:PRO:HD2	2.20	0.57
1:F:193:PRO:HG2	1:F:220:ARG:NH1	2.19	0.57
1:G:133:LEU:HD22	1:G:156:LEU:HG	1.87	0.57
1:E:44:SER:OG	1:E:45:ASN:ND2	2.37	0.57
1:A:25:THR:O	1:A:29:GLN:HG3	2.05	0.57
1:A:205:GLN:HB2	1:A:252:LEU:HD22	1.87	0.57
1:C:226:VAL:HG11	1:C:230:PHE:HZ	1.70	0.57
1:G:202:LEU:HD23	1:G:220:ARG:HA	1.87	0.57
1:B:176:HIS:HA	1:B:180:PRO:O	2.05	0.57
1:D:176:HIS:HA	1:D:180:PRO:O	2.04	0.57
1:E:100:GLU:O	1:E:104:GLN:HG3	2.05	0.57
1:E:207:THR:HB	1:E:215:VAL:CG1	2.34	0.57
1:F:149:PRO:HG2	1:F:185:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:NH1	1:B:208:ARG:HG3	2.19	0.57
1:E:46:HIS:CE1	1:E:48:GLY:HA3	2.40	0.57
1:F:133:LEU:N	1:F:134:PRO:HD2	2.19	0.57
1:D:207:THR:HB	1:D:215:VAL:CG1	2.35	0.57
1:F:150:ASN:HB2	1:F:153:GLU:CD	2.26	0.57
1:H:208:ARG:NH1	5:H:7405:HOH:O	2.37	0.57
1:H:87:ASP:HB3	1:H:90:PHE:HB2	1.87	0.57
1:A:305:ILE:CD1	1:A:305:ILE:N	2.68	0.56
1:G:105:ASN:HD21	1:G:107:ARG:HB2	1.70	0.56
1:B:62:LEU:HB2	1:B:90:PHE:CE1	2.40	0.56
1:C:150:ASN:HB2	1:C:153:GLU:CD	2.25	0.56
1:D:151:GLN:OE1	1:D:188:SER:HB2	2.06	0.56
1:G:41:VAL:HG12	1:G:56:VAL:HG13	1.86	0.56
1:B:213:SER:HA	5:B:1444:HOH:O	2.04	0.56
1:G:172:MET:HG2	1:G:183:VAL:HG12	1.87	0.56
1:B:149:PRO:HG2	1:B:185:ILE:CD1	2.35	0.56
1:D:253:LYS:O	1:D:257:GLU:HG3	2.06	0.56
1:E:47:THR:HG22	1:E:52:TRP:NE1	2.21	0.56
1:A:242:LEU:HD23	1:A:242:LEU:O	2.06	0.56
1:H:63:GLN:OE1	1:H:93:MET:CE	2.54	0.56
1:C:193:PRO:HG2	1:C:220:ARG:NH1	2.21	0.56
1:D:116:MET:O	1:D:128:VAL:HG22	2.06	0.56
1:H:283:LYS:HD3	1:H:284:PRO:HD2	1.86	0.56
1:B:202:LEU:HD23	1:B:220:ARG:HA	1.86	0.56
1:F:62:LEU:HB2	1:F:90:PHE:CE1	2.41	0.56
1:A:108:LEU:C	1:A:108:LEU:HD23	2.26	0.56
1:A:202:LEU:HD23	1:A:220:ARG:HA	1.86	0.56
1:B:142:PRO:HA	1:B:178:MET:O	2.05	0.56
1:B:26:PHE:HB3	1:B:27:PRO:HD3	1.87	0.56
1:C:248:HIS:HB3	1:C:251:ASN:HB2	1.88	0.56
1:C:26:PHE:O	1:C:30:VAL:HG13	2.06	0.56
1:D:220:ARG:HG2	1:D:221:MET:N	2.21	0.56
1:E:187:SER:HA	1:E:200:MET:O	2.05	0.56
1:D:47:THR:HG22	1:D:52:TRP:CD1	2.40	0.56
1:E:26:PHE:HB3	1:E:27:PRO:HD3	1.87	0.56
1:H:57:LEU:HA	1:H:61:GLU:OE2	2.06	0.56
1:A:234:GLY:O	1:A:237:PHE:HB3	2.05	0.56
1:C:117:GLY:HA3	1:C:126:MET:HA	1.87	0.56
1:C:142:PRO:HA	1:C:178:MET:O	2.06	0.56
1:D:85:THR:HG21	1:D:90:PHE:HB3	1.86	0.56
1:F:105:ASN:ND2	1:F:105:ASN:C	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:THR:HG22	1:F:52:TRP:CD1	2.41	0.56
1:G:146:ILE:HG12	1:G:182:THR:HB	1.88	0.56
1:B:141:VAL:N	1:B:142:PRO:CD	2.69	0.55
1:B:6:ARG:HD3	5:F:5417:HOH:O	2.05	0.55
1:D:63:GLN:OE1	1:D:93:MET:CE	2.53	0.55
1:E:116:MET:O	1:E:128:VAL:HG22	2.05	0.55
1:E:47:THR:HG22	1:E:52:TRP:CD1	2.41	0.55
1:D:53:LYS:HE2	1:G:71:LEU:HD11	1.87	0.55
1:H:133:LEU:N	1:H:134:PRO:HD2	2.21	0.55
1:H:150:ASN:O	1:H:151:GLN:C	2.43	0.55
1:H:172:MET:HG2	1:H:183:VAL:CG1	2.36	0.55
1:B:108:LEU:HD23	1:B:108:LEU:C	2.26	0.55
1:C:88:LYS:HG3	1:C:135:VAL:HG21	1.88	0.55
1:C:161:LYS:NZ	5:C:2417:HOH:O	2.38	0.55
1:D:162:ILE:HD11	1:D:171:VAL:HG21	1.88	0.55
1:D:202:LEU:HD23	1:D:220:ARG:HA	1.89	0.55
1:E:166:GLU:O	1:E:167:GLU:C	2.44	0.55
1:E:12:SER:HA	1:E:41:VAL:HG22	1.86	0.55
1:G:189:ASN:O	1:G:190:LEU:C	2.44	0.55
1:H:285:SER:OG	1:H:288:GLN:HG3	2.06	0.55
1:C:100:GLU:O	1:C:104:GLN:HG3	2.06	0.55
1:D:256:CYS:O	1:D:260:VAL:HG23	2.07	0.55
1:E:163:HIS:NE2	1:E:167:GLU:OE1	2.39	0.55
1:A:107:ARG:HH11	1:A:107:ARG:CG	2.17	0.55
1:C:253:LYS:O	1:C:257:GLU:HG3	2.06	0.55
1:F:44:SER:OG	1:F:45:ASN:ND2	2.39	0.55
1:G:214:VAL:CG2	1:G:214:VAL:O	2.54	0.55
1:G:85:THR:HG22	1:G:87:ASP:N	2.18	0.55
1:A:26:PHE:HB3	1:A:27:PRO:HD3	1.89	0.55
1:C:186:THR:HG22	1:C:237:PHE:CE2	2.42	0.55
1:D:214:VAL:O	1:D:214:VAL:CG2	2.54	0.55
1:E:136:TYR:O	1:E:141:VAL:HG23	2.06	0.55
1:E:253:LYS:HG3	1:E:309:ALA:HB3	1.88	0.55
1:B:207:THR:HB	1:B:215:VAL:CG1	2.36	0.55
1:C:138:GLU:O	1:C:142:PRO:HG2	2.07	0.55
1:F:194:ARG:HG2	1:F:222:GLU:OE1	2.07	0.55
1:H:46:HIS:CE1	1:H:48:GLY:HA3	2.42	0.55
1:A:172:MET:CE	1:A:202:LEU:HB3	2.37	0.55
1:B:105:ASN:HD21	1:B:107:ARG:HB2	1.71	0.55
1:C:176:HIS:HA	1:C:180:PRO:O	2.06	0.55
1:E:138:GLU:O	1:E:142:PRO:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLN:HA	1:E:190:LEU:CD2	2.37	0.55
1:F:211:ASP:OD1	1:F:213:SER:OG	2.22	0.55
1:H:100:GLU:O	1:H:104:GLN:HG3	2.07	0.55
1:E:233:THR:HB	4:E:4402:ADP:H5'1	1.88	0.55
1:H:202:LEU:HD23	1:H:220:ARG:HA	1.87	0.55
1:A:141:VAL:N	1:A:142:PRO:CD	2.69	0.55
1:A:149:PRO:HD2	1:A:184:VAL:O	2.07	0.55
1:D:150:ASN:HB2	1:D:153:GLU:CD	2.28	0.55
1:D:59:SER:OG	1:D:89:SER:HB3	2.07	0.55
1:E:28:LEU:HD21	1:E:239:ALA:O	2.07	0.55
1:E:236:LEU:HB3	1:E:263:MET:HE1	1.87	0.55
1:G:218:ARG:NH1	1:G:218:ARG:HG3	2.21	0.55
1:B:169:LEU:CD2	1:B:218:ARG:HD2	2.36	0.55
1:F:283:LYS:HD3	1:F:284:PRO:HD2	1.89	0.55
1:H:150:ASN:HB2	1:H:153:GLU:CD	2.26	0.55
1:H:47:THR:HG22	1:H:52:TRP:CD1	2.42	0.55
1:A:150:ASN:O	1:A:151:GLN:C	2.43	0.54
1:C:165:GLN:HA	1:C:190:LEU:HD21	1.88	0.54
1:C:219:ILE:HD11	1:C:256:CYS:SG	2.47	0.54
1:F:143:VAL:HG22	1:F:143:VAL:O	2.07	0.54
1:D:297:LYS:NZ	1:G:301:GLU:OE1	2.27	0.54
1:B:305:ILE:HD12	1:B:305:ILE:H	1.72	0.54
1:E:283:LYS:HD3	1:E:284:PRO:HD2	1.89	0.54
1:G:253:LYS:HG3	1:G:309:ALA:HB3	1.89	0.54
1:A:136:TYR:O	1:A:141:VAL:HG23	2.08	0.54
1:B:166:GLU:O	1:B:167:GLU:C	2.45	0.54
1:C:158:THR:CG2	1:C:171:VAL:HG13	2.36	0.54
1:C:208:ARG:HG2	1:C:214:VAL:HG12	1.90	0.54
1:F:207:THR:HB	1:F:215:VAL:CG1	2.36	0.54
1:B:164:SER:OG	1:B:167:GLU:HG2	2.08	0.54
1:B:85:THR:HG23	5:B:1411:HOH:O	2.07	0.54
1:E:194:ARG:HG2	1:E:222:GLU:OE1	2.07	0.54
1:F:138:GLU:O	1:F:142:PRO:HG2	2.06	0.54
1:C:37:ALA:O	1:H:15:VAL:HA	2.07	0.54
1:H:25:THR:O	1:H:29:GLN:HG3	2.07	0.54
1:H:235:ASP:OD2	3:H:7401:PLP:H5A1	2.08	0.54
1:A:114:PRO:HG3	1:A:149:PRO:HB3	1.88	0.54
1:A:207:THR:HB	1:A:215:VAL:CG1	2.37	0.54
1:C:162:ILE:CD1	1:C:171:VAL:HG21	2.38	0.54
1:E:49:TYR:OH	1:E:287:ALA:HA	2.07	0.54
1:F:46:HIS:CE1	1:F:48:GLY:HA3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:GLN:OE1	1:F:93:MET:CE	2.54	0.54
1:F:85:THR:HG21	1:F:90:PHE:HB3	1.90	0.54
1:H:47:THR:HG22	1:H:52:TRP:CD2	2.43	0.54
1:A:187:SER:HA	1:A:200:MET:O	2.07	0.54
1:A:24:ALA:O	1:A:27:PRO:HD2	2.08	0.54
1:D:88:LYS:HG3	1:D:135:VAL:HG21	1.88	0.54
1:A:253:LYS:HG3	1:A:309:ALA:HB3	1.88	0.54
1:B:149:PRO:HG2	1:B:185:ILE:HD13	1.90	0.54
1:F:142:PRO:HA	1:F:178:MET:O	2.07	0.54
1:F:16:ARG:HG2	1:F:17:GLY:N	2.23	0.54
1:C:34:GLU:OE1	1:H:18:TYR:CE1	2.60	0.54
1:F:119:GLN:HG2	1:F:152:PHE:H	1.72	0.54
1:B:163:HIS:NE2	1:B:167:GLU:OE1	2.41	0.54
1:D:120:ARG:NH1	5:D:3411:HOH:O	2.41	0.54
1:D:176:HIS:HE1	1:D:181:ASP:O	1.91	0.54
1:D:298:LYS:NZ	1:G:298:LYS:NZ	2.56	0.54
1:E:85:THR:HG21	1:E:90:PHE:HB3	1.89	0.54
1:H:176:HIS:HE1	1:H:181:ASP:O	1.90	0.54
1:B:138:GLU:O	1:B:142:PRO:HG2	2.08	0.53
1:D:150:ASN:O	1:D:151:GLN:C	2.45	0.53
1:H:62:LEU:HB2	1:H:90:PHE:CE1	2.44	0.53
1:H:44:SER:OG	1:H:45:ASN:ND2	2.41	0.53
1:B:283:LYS:HD3	1:B:284:PRO:HD2	1.89	0.53
1:B:1:MET:HE3	1:B:32:GLY:O	2.08	0.53
1:D:208:ARG:HG2	1:D:214:VAL:HG12	1.90	0.53
1:E:133:LEU:HD22	1:E:156:LEU:HG	1.89	0.53
1:F:253:LYS:HG3	1:F:309:ALA:HB3	1.89	0.53
1:G:141:VAL:N	1:G:142:PRO:CD	2.72	0.53
1:H:138:GLU:O	1:H:142:PRO:HG2	2.08	0.53
1:H:172:MET:HG2	1:H:183:VAL:HG12	1.90	0.53
1:A:214:VAL:O	1:A:214:VAL:CG2	2.55	0.53
1:B:114:PRO:HG3	1:B:149:PRO:HB3	1.90	0.53
1:B:186:THR:HG22	1:B:237:PHE:CE2	2.44	0.53
1:C:114:PRO:HG3	1:C:149:PRO:HB3	1.90	0.53
1:C:57:LEU:HA	1:C:61:GLU:OE2	2.08	0.53
1:C:63:GLN:OE1	1:C:93:MET:CE	2.56	0.53
1:D:189:ASN:O	1:D:190:LEU:C	2.47	0.53
1:G:305:ILE:CD1	1:G:305:ILE:N	2.71	0.53
1:C:151:GLN:OE1	1:C:188:SER:HB2	2.09	0.53
1:D:25:THR:O	1:D:29:GLN:HG3	2.07	0.53
1:E:189:ASN:O	1:E:190:LEU:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:THR:HG22	1:F:237:PHE:CE2	2.43	0.53
1:G:307:VAL:HG23	1:G:307:VAL:O	2.08	0.53
1:B:143:VAL:HG22	1:B:143:VAL:O	2.08	0.53
1:C:38:VAL:HG22	1:H:15:VAL:CG2	2.39	0.53
1:C:72:ASN:CG	1:H:49:TYR:HB3	2.29	0.53
1:D:174:MET:O	1:D:177:SER:HB3	2.08	0.53
1:C:1:MET:HE1	1:C:5:CYS:HB2	1.91	0.53
1:C:305:ILE:CD1	1:C:305:ILE:N	2.71	0.53
1:H:171:VAL:HG12	1:H:175:LEU:HD11	1.91	0.53
1:H:193:PRO:HG2	1:H:220:ARG:HH12	1.74	0.53
1:H:63:GLN:OE1	1:H:93:MET:HE2	2.09	0.53
1:A:37:ALA:O	1:E:15:VAL:HA	2.08	0.53
1:F:49:TYR:OH	1:F:287:ALA:HA	2.09	0.53
1:A:176:HIS:HA	1:A:180:PRO:O	2.09	0.53
1:B:248:HIS:HB3	1:B:251:ASN:CB	2.38	0.53
1:C:141:VAL:N	1:C:142:PRO:CD	2.72	0.53
1:C:208:ARG:HG3	1:C:208:ARG:NH1	2.23	0.53
1:C:64:GLU:O	1:H:53:LYS:HB2	2.09	0.53
1:F:176:HIS:HA	1:F:180:PRO:O	2.09	0.53
1:F:214:VAL:CG2	1:F:214:VAL:O	2.56	0.53
1:G:147:ILE:HD11	1:G:183:VAL:HG22	1.91	0.53
1:G:176:HIS:HE1	1:G:181:ASP:O	1.91	0.53
1:G:186:THR:HG22	1:G:237:PHE:CE2	2.44	0.53
1:B:85:THR:HG21	1:B:90:PHE:HB3	1.92	0.52
1:C:103:GLN:N	1:C:103:GLN:NE2	2.53	0.52
1:B:305:ILE:N	1:B:305:ILE:CD1	2.72	0.52
1:D:63:GLN:OE1	1:D:93:MET:HE2	2.08	0.52
1:E:169:LEU:HD22	1:E:218:ARG:HD2	1.91	0.52
1:F:147:ILE:HB	1:F:149:PRO:HD3	1.90	0.52
1:G:187:SER:HA	1:G:200:MET:O	2.09	0.52
1:H:164:SER:OG	1:H:167:GLU:CG	2.57	0.52
1:B:150:ASN:HB2	1:B:153:GLU:CD	2.30	0.52
1:C:103:GLN:CA	1:C:103:GLN:NE2	2.70	0.52
1:C:133:LEU:N	1:C:134:PRO:HD2	2.24	0.52
1:E:105:ASN:C	1:E:105:ASN:HD22	2.12	0.52
1:E:307:VAL:HG23	1:E:307:VAL:O	2.08	0.52
1:E:85:THR:HG22	1:E:86:ARG:N	2.24	0.52
1:G:100:GLU:O	1:G:104:GLN:HG3	2.10	0.52
1:G:169:LEU:HD22	1:G:218:ARG:HD2	1.90	0.52
1:H:219:ILE:HD11	1:H:256:CYS:SG	2.49	0.52
1:B:162:ILE:CD1	1:B:171:VAL:HG21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:OH	1:C:287:ALA:HA	2.08	0.52
1:D:253:LYS:HG3	1:D:309:ALA:HB3	1.91	0.52
1:E:218:ARG:HH11	1:E:218:ARG:HG3	1.72	0.52
1:A:150:ASN:HB2	1:A:153:GLU:CD	2.29	0.52
1:D:248:HIS:HB3	1:D:251:ASN:CB	2.39	0.52
1:E:143:VAL:HG22	1:E:143:VAL:O	2.09	0.52
1:A:176:HIS:CE1	1:A:181:ASP:O	2.63	0.52
1:C:47:THR:HG22	1:C:52:TRP:NE1	2.25	0.52
1:E:186:THR:HG22	1:E:237:PHE:CE2	2.44	0.52
1:A:223:MET:SD	4:A:402:ADP:O2'	2.61	0.52
1:A:52:TRP:CZ2	1:B:196:SER:HB2	2.44	0.52
1:B:214:VAL:CG2	1:B:214:VAL:O	2.57	0.52
1:E:218:ARG:NH1	1:E:218:ARG:HG3	2.24	0.52
1:C:38:VAL:HG23	1:H:15:VAL:HG13	1.92	0.52
1:A:248:HIS:HB3	1:A:251:ASN:HB2	1.92	0.52
1:A:293:MET:O	1:A:296:SER:N	2.38	0.52
1:C:202:LEU:HD23	1:C:220:ARG:HA	1.90	0.52
1:F:165:GLN:HA	1:F:190:LEU:CD2	2.39	0.52
1:G:133:LEU:N	1:G:134:PRO:HD2	2.24	0.52
1:C:105:ASN:HD21	1:C:107:ARG:HB2	1.74	0.52
1:F:202:LEU:HD23	1:F:220:ARG:HA	1.91	0.52
1:A:146:ILE:HG12	1:A:182:THR:HB	1.92	0.52
1:A:218:ARG:NH1	1:A:218:ARG:HG3	2.25	0.52
1:B:158:THR:HB	1:B:174:MET:HE2	1.91	0.52
1:B:41:VAL:HG12	1:B:56:VAL:HG13	1.92	0.52
1:E:16:ARG:HG2	1:E:17:GLY:N	2.25	0.52
1:G:143:VAL:O	1:G:143:VAL:HG22	2.09	0.52
1:G:208:ARG:HG2	1:G:214:VAL:HG12	1.92	0.52
1:A:49:TYR:OH	1:A:287:ALA:HA	2.10	0.51
1:B:236:LEU:HG	1:B:240:MET:CE	2.40	0.51
1:D:100:GLU:O	1:D:104:GLN:HG3	2.10	0.51
1:F:166:GLU:O	1:F:167:GLU:C	2.47	0.51
1:F:297:LYS:O	1:F:301:GLU:HG3	2.10	0.51
1:B:100:GLU:O	1:B:104:GLN:HG3	2.10	0.51
1:B:46:HIS:CE1	1:B:48:GLY:HA3	2.46	0.51
1:B:87:ASP:HB3	1:B:90:PHE:HB2	1.92	0.51
1:D:43:PHE:HA	1:D:54:GLY:HA3	1.92	0.51
1:E:88:LYS:HA	1:E:132:LEU:HD23	1.92	0.51
1:B:26:PHE:O	1:B:30:VAL:HG13	2.10	0.51
1:C:136:TYR:O	1:C:141:VAL:HG23	2.09	0.51
1:C:42:GLN:HE22	1:H:39:ASN:H	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ASP:OD2	3:D:3401:PLP:H5A1	2.10	0.51
1:E:146:ILE:HG12	1:E:182:THR:HB	1.92	0.51
1:F:172:MET:HG2	1:F:183:VAL:CG1	2.41	0.51
1:F:307:VAL:O	1:F:307:VAL:HG23	2.11	0.51
1:H:214:VAL:O	1:H:214:VAL:CG2	2.58	0.51
1:H:218:ARG:HH11	1:H:218:ARG:HG3	1.75	0.51
1:B:136:TYR:O	1:B:141:VAL:HG23	2.11	0.51
1:B:176:HIS:CE1	1:B:181:ASP:O	2.63	0.51
1:D:251:ASN:ND2	5:D:3406:HOH:O	2.42	0.51
1:G:103:GLN:N	1:G:103:GLN:NE2	2.55	0.51
1:G:147:ILE:HB	1:G:149:PRO:HD3	1.92	0.51
1:H:264:HIS:CE1	1:H:268:GLN:HG3	2.45	0.51
1:D:143:VAL:O	1:D:143:VAL:HG22	2.11	0.51
1:F:218:ARG:NH1	1:F:218:ARG:HG3	2.26	0.51
1:H:12:SER:HA	1:H:41:VAL:HG22	1.91	0.51
1:H:194:ARG:HG2	1:H:222:GLU:OE1	2.10	0.51
1:B:103:GLN:NE2	1:B:103:GLN:CA	2.70	0.51
1:E:133:LEU:CD2	1:E:156:LEU:HG	2.40	0.51
1:D:12:SER:HA	1:D:41:VAL:HG22	1.93	0.51
1:E:115:VAL:HA	1:E:153:GLU:OE2	2.11	0.51
1:F:270:THR:HA	1:F:292:ARG:HG3	1.92	0.51
1:H:253:LYS:HG3	1:H:309:ALA:HB3	1.92	0.51
1:G:103:GLN:HA	1:G:103:GLN:HE21	1.74	0.51
1:C:63:GLN:OE1	1:C:93:MET:HE1	2.11	0.50
1:E:141:VAL:N	1:E:142:PRO:CD	2.74	0.50
1:E:305:ILE:CD1	1:E:305:ILE:N	2.74	0.50
1:G:194:ARG:HG2	1:G:222:GLU:OE1	2.11	0.50
1:H:16:ARG:HG2	1:H:17:GLY:N	2.24	0.50
1:A:305:ILE:CD1	1:A:305:ILE:H	2.23	0.50
1:B:117:GLY:HA3	1:B:126:MET:HA	1.93	0.50
1:C:283:LYS:HD3	1:C:284:PRO:HD2	1.93	0.50
1:D:190:LEU:O	1:D:192:SER:N	2.44	0.50
1:D:208:ARG:HG3	1:D:208:ARG:NH1	2.26	0.50
1:H:108:LEU:HD23	1:H:109:VAL:N	2.26	0.50
1:H:85:THR:HG22	1:H:87:ASP:N	2.19	0.50
1:A:149:PRO:HG2	1:A:185:ILE:HD13	1.94	0.50
1:A:270:THR:HA	1:A:292:ARG:HG3	1.93	0.50
1:C:166:GLU:O	1:C:167:GLU:C	2.49	0.50
1:E:166:GLU:O	1:E:168:ALA:N	2.44	0.50
1:F:105:ASN:ND2	1:F:107:ARG:N	2.57	0.50
1:F:208:ARG:HG2	1:F:214:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:SER:HA	1:G:41:VAL:HG22	1.92	0.50
1:B:146:ILE:HG12	1:B:182:THR:HB	1.92	0.50
1:B:19:VAL:O	1:B:22:ARG:HB2	2.11	0.50
1:C:116:MET:O	1:C:128:VAL:HG22	2.12	0.50
1:C:214:VAL:O	1:C:214:VAL:CG2	2.59	0.50
1:D:105:ASN:C	1:D:105:ASN:ND2	2.64	0.50
1:E:172:MET:HA	1:E:175:LEU:HD12	1.92	0.50
1:G:176:HIS:CE1	1:G:181:ASP:O	2.65	0.50
1:G:205:GLN:HB2	1:G:252:LEU:HD22	1.92	0.50
1:H:208:ARG:HG2	1:H:214:VAL:HG12	1.93	0.50
1:A:138:GLU:O	1:A:142:PRO:HG2	2.11	0.50
1:A:1:MET:HE1	1:A:5:CYS:H	1.76	0.50
1:D:176:HIS:CE1	1:D:181:ASP:O	2.64	0.50
1:E:172:MET:HG2	1:E:183:VAL:HG12	1.94	0.50
1:A:166:GLU:O	1:A:169:LEU:N	2.44	0.50
1:D:47:THR:HG22	1:D:52:TRP:NE1	2.27	0.50
1:E:214:VAL:CG2	1:E:214:VAL:O	2.57	0.50
1:A:172:MET:HE1	1:A:202:LEU:HB3	1.92	0.50
1:A:46:HIS:CE1	1:A:48:GLY:HA3	2.47	0.50
1:B:140:VAL:C	1:B:142:PRO:HD2	2.32	0.50
1:E:85:THR:HG22	1:E:87:ASP:N	2.17	0.50
1:A:117:GLY:HA3	1:A:126:MET:HA	1.94	0.50
1:A:142:PRO:HA	1:A:178:MET:O	2.12	0.50
1:C:165:GLN:HA	1:C:190:LEU:CD2	2.41	0.50
1:D:305:ILE:CD1	1:D:305:ILE:N	2.73	0.50
1:C:62:LEU:HB2	1:C:90:PHE:CE1	2.47	0.50
1:D:136:TYR:O	1:D:141:VAL:HG23	2.12	0.50
1:D:141:VAL:N	1:D:142:PRO:CD	2.75	0.50
1:D:187:SER:OG	4:D:3402:ADP:O2A	2.28	0.50
1:E:88:LYS:HA	1:E:132:LEU:CD2	2.42	0.50
1:E:172:MET:HG2	1:E:183:VAL:CG1	2.42	0.50
1:E:193:PRO:HG2	1:E:220:ARG:NH1	2.26	0.50
1:G:248:HIS:HB3	1:G:251:ASN:HB2	1.94	0.50
1:H:147:ILE:HB	1:H:149:PRO:HD3	1.92	0.50
1:H:149:PRO:HG2	1:H:185:ILE:HD13	1.92	0.50
1:H:207:THR:HB	1:H:215:VAL:CG1	2.42	0.50
1:A:256:CYS:O	1:A:260:VAL:HG23	2.11	0.49
1:C:176:HIS:HE1	1:C:181:ASP:O	1.94	0.49
1:E:103:GLN:HE21	1:E:103:GLN:HA	1.77	0.49
1:E:147:ILE:HB	1:E:149:PRO:HD3	1.93	0.49
1:E:62:LEU:HB2	1:E:90:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:LEU:HB2	1:G:90:PHE:CE1	2.47	0.49
1:B:105:ASN:C	1:B:105:ASN:ND2	2.65	0.49
1:C:205:GLN:HB2	1:C:252:LEU:HD22	1.94	0.49
1:C:242:LEU:CD2	1:C:242:LEU:C	2.80	0.49
1:C:65:LEU:O	1:H:44:SER:HB3	2.12	0.49
1:E:105:ASN:C	1:E:105:ASN:ND2	2.63	0.49
1:F:219:ILE:HD11	1:F:256:CYS:SG	2.52	0.49
1:A:150:ASN:HB2	1:A:153:GLU:CG	2.42	0.49
1:C:41:VAL:HG12	1:C:56:VAL:HG13	1.93	0.49
1:C:71:LEU:HB3	1:H:51:HIS:CD2	2.47	0.49
1:D:9:SER:HA	1:D:81:LEU:O	2.12	0.49
1:F:141:VAL:N	1:F:142:PRO:CD	2.75	0.49
1:H:305:ILE:N	1:H:305:ILE:CD1	2.74	0.49
1:H:220:ARG:HB2	1:H:312:LEU:HD11	1.93	0.49
1:A:16:ARG:HG2	1:A:17:GLY:N	2.26	0.49
1:A:63:GLN:OE1	1:A:93:MET:CE	2.61	0.49
1:B:44:SER:OG	1:B:45:ASN:ND2	2.45	0.49
1:E:149:PRO:HD2	1:E:184:VAL:O	2.12	0.49
1:F:63:GLN:OE1	1:F:93:MET:HE2	2.13	0.49
1:H:218:ARG:HG3	1:H:218:ARG:NH1	2.27	0.49
1:C:218:ARG:HH11	1:C:218:ARG:HG3	1.78	0.49
1:E:103:GLN:NE2	1:E:103:GLN:N	2.56	0.49
1:F:72:ASN:O	1:F:73:HIS:HB2	2.12	0.49
1:A:240:MET:CE	1:A:263:MET:SD	3.00	0.49
1:F:1:MET:HE1	1:F:5:CYS:HB2	1.95	0.49
1:G:166:GLU:O	1:G:167:GLU:C	2.51	0.49
1:G:165:GLN:HA	1:G:190:LEU:CD2	2.41	0.49
1:H:307:VAL:O	1:H:307:VAL:HG23	2.13	0.49
1:B:24:ALA:O	1:B:27:PRO:HD2	2.13	0.49
1:B:307:VAL:HG23	1:B:307:VAL:O	2.11	0.49
1:C:87:ASP:HB3	1:C:90:PHE:HB2	1.95	0.49
1:F:16:ARG:HH11	1:F:16:ARG:HG3	1.78	0.49
1:C:38:VAL:HG22	1:H:15:VAL:HG22	1.95	0.49
1:H:292:ARG:NH2	1:H:295:GLN:NE2	2.61	0.49
1:F:105:ASN:HD22	1:F:105:ASN:C	2.13	0.49
1:F:305:ILE:CD1	1:F:305:ILE:N	2.76	0.49
1:H:190:LEU:O	1:H:192:SER:N	2.46	0.49
1:H:1:MET:CE	1:H:5:CYS:HB2	2.42	0.49
1:H:252:LEU:O	1:H:256:CYS:SG	2.70	0.49
1:H:80:VAL:HG23	1:H:108:LEU:HD11	1.95	0.49
1:E:103:GLN:NE2	1:E:103:GLN:CA	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:LEU:C	1:F:242:LEU:CD2	2.77	0.49
1:C:169:LEU:HD22	1:C:218:ARG:HD2	1.95	0.49
1:C:26:PHE:CE1	1:H:29:GLN:HB3	2.48	0.49
1:E:248:HIS:HB3	1:E:251:ASN:HB2	1.95	0.49
1:E:265:HIS:O	1:E:266:VAL:C	2.50	0.49
1:C:133:LEU:HD22	1:C:156:LEU:HG	1.95	0.48
1:F:248:HIS:HB3	1:F:251:ASN:HB2	1.95	0.48
1:A:307:VAL:HG23	1:A:307:VAL:O	2.13	0.48
1:B:172:MET:CE	1:B:202:LEU:HB3	2.43	0.48
1:C:149:PRO:HD2	1:C:184:VAL:O	2.14	0.48
1:C:218:ARG:NH1	1:C:218:ARG:HG3	2.28	0.48
1:E:194:ARG:NH1	5:E:4423:HOH:O	2.46	0.48
1:H:186:THR:HG22	1:H:237:PHE:CE2	2.48	0.48
1:A:244:TRP:HD1	1:A:259:THR:OG1	1.95	0.48
1:C:64:GLU:HG2	1:H:53:LYS:HB3	1.95	0.48
1:E:186:THR:O	1:E:187:SER:HB3	2.13	0.48
1:F:85:THR:HG22	1:F:86:ARG:N	2.28	0.48
1:G:202:LEU:HD21	1:G:220:ARG:HG3	1.95	0.48
1:H:270:THR:HA	1:H:292:ARG:HG3	1.95	0.48
1:H:85:THR:HG21	1:H:90:PHE:HB3	1.95	0.48
1:A:162:ILE:CD1	1:A:171:VAL:HG21	2.43	0.48
1:B:49:TYR:OH	1:B:287:ALA:HA	2.14	0.48
1:C:150:ASN:O	1:C:151:GLN:C	2.49	0.48
1:D:108:LEU:HD23	1:D:109:VAL:N	2.29	0.48
1:H:208:ARG:NH1	1:H:208:ARG:CG	2.68	0.48
1:H:28:LEU:HD21	1:H:239:ALA:O	2.14	0.48
1:H:242:LEU:CD2	1:H:242:LEU:C	2.79	0.48
1:C:110:TYR:C	1:C:110:TYR:CD2	2.85	0.48
1:D:307:VAL:HG23	1:D:307:VAL:O	2.12	0.48
1:E:114:PRO:HG3	1:E:149:PRO:HB3	1.95	0.48
1:E:235:ASP:OD2	3:E:4401:PLP:H5A1	2.14	0.48
1:G:28:LEU:HD21	1:G:239:ALA:O	2.14	0.48
1:G:47:THR:HG22	1:G:52:TRP:NE1	2.26	0.48
1:A:129:PRO:HG3	1:B:191:LEU:O	2.13	0.48
1:B:103:GLN:HA	1:B:103:GLN:HE21	1.78	0.48
1:C:16:ARG:HG2	1:C:17:GLY:N	2.27	0.48
1:C:247:LYS:HG3	1:C:248:HIS:CE1	2.48	0.48
1:F:172:MET:HG2	1:F:183:VAL:HG12	1.96	0.48
1:F:218:ARG:HH11	1:F:218:ARG:HG3	1.76	0.48
1:G:247:LYS:HG3	1:G:248:HIS:CE1	2.49	0.48
1:G:80:VAL:HG23	1:G:108:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HG2	1:B:17:GLY:N	2.29	0.48
1:B:208:ARG:HG2	1:B:214:VAL:HG12	1.96	0.48
1:C:103:GLN:HE21	1:C:103:GLN:HA	1.76	0.48
1:D:140:VAL:O	1:D:143:VAL:HG12	2.14	0.48
1:H:16:ARG:HH11	1:H:16:ARG:HG3	1.78	0.48
1:G:16:ARG:HG2	1:G:17:GLY:N	2.27	0.48
1:A:162:ILE:HD11	1:A:171:VAL:HG21	1.95	0.48
1:B:151:GLN:HB2	1:B:187:SER:O	2.14	0.48
1:C:147:ILE:HB	1:C:149:PRO:HD3	1.96	0.48
1:E:247:LYS:HG3	1:E:248:HIS:CE1	2.49	0.48
1:F:149:PRO:HD2	1:F:184:VAL:O	2.14	0.48
1:F:226:VAL:HG11	1:F:230:PHE:HZ	1.78	0.48
1:H:186:THR:O	1:H:187:SER:HB3	2.14	0.48
1:A:140:VAL:C	1:A:142:PRO:HD2	2.35	0.47
1:B:57:LEU:HA	1:B:61:GLU:OE2	2.14	0.47
1:D:305:ILE:HD12	1:D:305:ILE:H	1.74	0.47
1:E:166:GLU:O	1:E:169:LEU:N	2.47	0.47
1:B:4:GLU:CD	1:F:292:ARG:HH22	2.17	0.47
1:H:205:GLN:HB2	1:H:252:LEU:HD22	1.96	0.47
1:A:218:ARG:HG3	1:A:218:ARG:HH11	1.78	0.47
1:E:169:LEU:CD2	1:E:218:ARG:HD2	2.44	0.47
1:G:162:ILE:CD1	1:G:171:VAL:HG21	2.44	0.47
1:C:162:ILE:HD11	1:C:171:VAL:HG21	1.96	0.47
1:D:71:LEU:HD11	1:G:53:LYS:HE2	1.94	0.47
1:E:105:ASN:ND2	1:E:107:ARG:N	2.60	0.47
1:G:170:GLU:O	1:G:173:ASP:HB2	2.14	0.47
1:H:171:VAL:HG12	1:H:175:LEU:CD1	2.44	0.47
1:A:47:THR:HG22	1:A:52:TRP:CD1	2.49	0.47
1:F:164:SER:OG	1:F:167:GLU:CG	2.58	0.47
1:A:143:VAL:O	1:A:143:VAL:HG22	2.15	0.47
1:A:57:LEU:HA	1:A:61:GLU:OE2	2.14	0.47
1:E:72:ASN:O	1:E:73:HIS:HB2	2.15	0.47
1:G:85:THR:HG22	1:G:86:ARG:N	2.29	0.47
1:C:116:MET:SD	1:C:156:LEU:HD23	2.55	0.47
1:D:26:PHE:O	1:D:30:VAL:HG13	2.14	0.47
1:G:88:LYS:HG3	1:G:135:VAL:HG21	1.96	0.47
1:C:179:GLY:N	1:C:180:PRO:HD2	2.29	0.47
1:E:166:GLU:C	1:E:168:ALA:N	2.68	0.47
1:E:264:HIS:CE1	1:E:268:GLN:HG3	2.50	0.47
1:E:87:ASP:OD2	1:E:89:SER:HB2	2.14	0.47
1:F:190:LEU:O	1:F:192:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:LEU:HA	1:F:61:GLU:OE2	2.14	0.47
1:G:234:GLY:O	1:G:237:PHE:HB3	2.15	0.47
1:H:162:ILE:HD11	1:H:171:VAL:HG21	1.96	0.47
1:H:72:ASN:O	1:H:73:HIS:HB2	2.14	0.47
1:B:179:GLY:N	1:B:180:PRO:HD2	2.30	0.47
1:D:88:LYS:HA	1:D:132:LEU:HD23	1.97	0.47
1:E:219:ILE:HD11	1:E:256:CYS:SG	2.55	0.47
1:F:273:CYS:O	1:F:276:ALA:HB3	2.15	0.47
1:H:11:GLN:O	1:H:39:ASN:HA	2.14	0.47
1:H:166:GLU:O	1:H:167:GLU:C	2.53	0.47
1:C:18:TYR:OH	1:H:34:GLU:OE1	2.26	0.47
1:H:85:THR:HG22	1:H:86:ARG:N	2.29	0.47
1:C:85:THR:HG21	1:C:90:PHE:HB3	1.97	0.47
1:F:186:THR:O	1:F:187:SER:HB3	2.15	0.47
1:B:130:ASP:CG	1:C:164:SER:HB2	2.35	0.47
1:B:12:SER:HA	1:B:41:VAL:HG22	1.96	0.47
1:B:72:ASN:OD1	1:F:49:TYR:HB3	2.15	0.47
1:D:6:ARG:HD2	1:D:76:GLN:O	2.15	0.47
1:E:11:GLN:O	1:E:39:ASN:HA	2.14	0.47
1:A:247:LYS:HG3	1:A:248:HIS:CE1	2.50	0.46
1:B:172:MET:HE1	1:B:202:LEU:HB3	1.96	0.46
1:B:247:LYS:HG3	1:B:248:HIS:CE1	2.50	0.46
1:E:234:GLY:O	1:E:237:PHE:HB3	2.15	0.46
1:F:176:HIS:HE1	1:F:181:ASP:O	1.98	0.46
1:F:43:PHE:HA	1:F:54:GLY:HA3	1.96	0.46
1:G:108:LEU:HD23	1:G:109:VAL:N	2.29	0.46
1:H:87:ASP:OD2	1:H:89:SER:HB2	2.15	0.46
1:D:8:LEU:HB2	1:D:77:TYR:CD2	2.50	0.46
1:F:119:GLN:HE21	1:F:150:ASN:HD21	1.63	0.46
1:F:63:GLN:OE1	1:F:93:MET:HE1	2.16	0.46
1:H:143:VAL:O	1:H:143:VAL:HG22	2.16	0.46
1:H:176:HIS:CE1	1:H:181:ASP:O	2.68	0.46
1:B:72:ASN:O	1:B:73:HIS:HB2	2.14	0.46
1:D:166:GLU:O	1:D:167:GLU:C	2.53	0.46
1:E:170:GLU:O	1:E:173:ASP:HB2	2.15	0.46
1:F:171:VAL:HG12	1:F:175:LEU:HD11	1.98	0.46
1:F:193:PRO:HG2	1:F:220:ARG:HH12	1.81	0.46
1:H:247:LYS:HG3	1:H:248:HIS:CE1	2.50	0.46
1:A:107:ARG:CG	1:A:107:ARG:NH1	2.75	0.46
1:A:240:MET:HE3	1:A:263:MET:SD	2.55	0.46
1:A:87:ASP:HB3	1:A:90:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLN:NE2	1:B:103:GLN:N	2.56	0.46
1:B:265:HIS:O	1:B:266:VAL:C	2.53	0.46
1:B:63:GLN:OE1	1:B:93:MET:CE	2.63	0.46
1:C:85:THR:HG22	1:C:87:ASP:N	2.21	0.46
1:E:273:CYS:O	1:E:276:ALA:HB3	2.15	0.46
1:A:39:ASN:N	1:E:42:GLN:HE22	1.90	0.46
1:G:149:PRO:HG2	1:G:185:ILE:HD13	1.96	0.46
1:B:161:LYS:NZ	5:B:1423:HOH:O	2.47	0.46
1:B:236:LEU:HG	1:B:240:MET:HE2	1.98	0.46
1:B:41:VAL:HB	1:B:43:PHE:CE1	2.51	0.46
1:C:234:GLY:O	1:C:237:PHE:HB3	2.15	0.46
1:D:280:GLU:H	1:D:280:GLU:HG3	1.34	0.46
1:E:149:PRO:HG2	1:E:185:ILE:HD13	1.96	0.46
1:E:56:VAL:HG12	1:E:57:LEU:N	2.31	0.46
1:G:208:ARG:NH1	5:G:6406:HOH:O	2.47	0.46
1:H:226:VAL:O	1:H:228:ALA:N	2.45	0.46
1:C:42:GLN:NE2	1:H:39:ASN:H	2.13	0.46
1:C:88:LYS:HA	1:C:132:LEU:HD23	1.98	0.46
1:D:88:LYS:HA	1:D:132:LEU:CD2	2.46	0.46
1:D:138:GLU:O	1:D:142:PRO:HG2	2.16	0.46
1:D:46:HIS:CE1	1:D:48:GLY:HA3	2.51	0.46
1:F:235:ASP:OD2	3:F:5401:PLP:O3P	2.33	0.46
1:H:43:PHE:HA	1:H:54:GLY:HA3	1.96	0.46
1:A:44:SER:OG	1:A:45:ASN:ND2	2.49	0.46
1:B:220:ARG:HB2	1:B:312:LEU:HD11	1.97	0.46
1:C:55:GLN:HE21	1:H:57:LEU:HD21	1.80	0.46
1:F:171:VAL:O	1:F:175:LEU:HG	2.16	0.46
1:G:117:GLY:HA3	1:G:126:MET:HA	1.98	0.46
1:G:85:THR:HG21	1:G:90:PHE:HB3	1.98	0.46
1:C:172:MET:HA	1:C:175:LEU:HD12	1.97	0.46
1:E:14:VAL:HG23	1:E:14:VAL:O	2.16	0.46
1:E:133:LEU:HD13	1:E:156:LEU:HD23	1.97	0.46
1:F:59:SER:OG	1:F:89:SER:HB3	2.15	0.46
1:G:59:SER:OG	1:G:89:SER:HB3	2.16	0.46
1:H:169:LEU:HD22	1:H:218:ARG:HD2	1.98	0.46
1:A:85:THR:HG21	1:A:90:PHE:HB3	1.97	0.46
1:A:93:MET:O	1:A:97:ILE:HG13	2.16	0.46
1:C:108:LEU:HD23	1:C:109:VAL:N	2.30	0.46
1:C:47:THR:HG22	1:C:52:TRP:CD1	2.51	0.46
1:E:176:HIS:HE1	1:E:181:ASP:O	1.99	0.46
1:E:208:ARG:HG2	1:E:214:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ASP:HB3	1:E:90:PHE:HB2	1.98	0.46
1:F:28:LEU:HD21	1:F:239:ALA:O	2.16	0.46
1:G:105:ASN:C	1:G:105:ASN:HD22	2.18	0.46
1:A:149:PRO:HG2	1:A:185:ILE:CD1	2.46	0.46
1:A:43:PHE:HA	1:A:54:GLY:HA3	1.97	0.46
1:B:105:ASN:C	1:B:105:ASN:HD22	2.19	0.46
1:B:166:GLU:O	1:B:168:ALA:N	2.49	0.46
1:E:59:SER:OG	1:E:89:SER:HB3	2.16	0.46
1:F:103:GLN:N	1:F:103:GLN:NE2	2.55	0.46
1:F:158:THR:HG21	1:F:171:VAL:CG1	2.40	0.46
1:F:164:SER:HG	1:F:167:GLU:HG2	1.81	0.46
1:F:191:LEU:HD23	1:F:191:LEU:N	2.32	0.46
1:F:200:MET:HA	1:F:221:MET:O	2.15	0.46
1:F:169:LEU:HD22	1:F:218:ARG:HD2	1.98	0.46
1:G:235:ASP:OD2	3:G:6401:PLP:H5A1	2.16	0.46
1:A:190:LEU:O	1:A:192:SER:N	2.50	0.45
1:A:264:HIS:CE1	1:A:268:GLN:HG3	2.50	0.45
1:A:8:LEU:HB2	1:A:77:TYR:CD2	2.51	0.45
1:E:242:LEU:C	1:E:242:LEU:CD2	2.83	0.45
1:F:1:MET:CE	1:F:5:CYS:HB2	2.46	0.45
1:F:208:ARG:CG	1:F:208:ARG:NH1	2.74	0.45
1:B:88:LYS:HA	1:B:132:LEU:HD23	1.98	0.45
1:B:129:PRO:HG3	1:C:191:LEU:O	2.17	0.45
1:C:248:HIS:HB3	1:C:251:ASN:CB	2.46	0.45
1:D:242:LEU:CD2	1:D:242:LEU:C	2.84	0.45
1:D:280:GLU:O	1:D:282:VAL:HG23	2.16	0.45
1:E:91:LEU:O	1:E:94:VAL:HB	2.16	0.45
1:G:193:PRO:HG2	1:G:220:ARG:NH1	2.30	0.45
1:H:88:LYS:HG3	1:H:135:VAL:HG21	1.98	0.45
1:A:248:HIS:HB3	1:A:251:ASN:CB	2.46	0.45
1:C:305:ILE:HD12	1:C:305:ILE:H	1.79	0.45
1:D:105:ASN:HD22	1:D:105:ASN:C	2.20	0.45
1:F:140:VAL:O	1:F:143:VAL:HG12	2.15	0.45
1:G:105:ASN:C	1:G:105:ASN:ND2	2.67	0.45
1:A:200:MET:HA	1:A:221:MET:O	2.16	0.45
1:B:118:ASP:O	1:B:124:GLY:HA3	2.16	0.45
1:A:164:SER:OG	1:A:167:GLU:HG3	2.17	0.45
1:B:200:MET:HA	1:B:221:MET:O	2.17	0.45
1:B:273:CYS:SG	1:B:277:LYS:HE3	2.56	0.45
1:B:88:LYS:HG3	1:B:135:VAL:HG21	1.99	0.45
1:D:114:PRO:HG3	1:D:149:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PRO:HG2	1:D:185:ILE:CD1	2.45	0.45
1:E:283:LYS:NZ	5:E:4422:HOH:O	2.49	0.45
1:E:43:PHE:HA	1:E:54:GLY:HA3	1.99	0.45
1:G:46:HIS:HE1	1:G:48:GLY:HA3	1.80	0.45
1:H:88:LYS:HA	1:H:132:LEU:CD2	2.47	0.45
1:H:141:VAL:N	1:H:142:PRO:CD	2.79	0.45
1:A:80:VAL:HG23	1:A:108:LEU:HD11	1.99	0.45
1:C:79:TYR:HA	1:C:109:VAL:O	2.16	0.45
1:D:16:ARG:HG2	1:D:17:GLY:N	2.32	0.45
1:D:1:MET:HE3	1:D:32:GLY:O	2.17	0.45
1:D:19:VAL:O	1:D:22:ARG:HB2	2.17	0.45
1:E:208:ARG:CG	1:E:208:ARG:NH1	2.78	0.45
1:E:211:ASP:OD1	1:E:213:SER:OG	2.26	0.45
1:G:88:LYS:HA	1:G:132:LEU:CD2	2.47	0.45
1:G:47:THR:HG22	1:G:52:TRP:CD1	2.52	0.45
1:H:265:HIS:O	1:H:266:VAL:C	2.54	0.45
1:A:218:ARG:NH1	5:A:438:HOH:O	2.50	0.45
1:B:191:LEU:N	1:B:191:LEU:HD23	2.32	0.45
1:E:226:VAL:HG11	1:E:230:PHE:HZ	1.82	0.45
1:F:11:GLN:O	1:F:39:ASN:HA	2.17	0.45
1:F:19:VAL:O	1:F:22:ARG:HB2	2.17	0.45
1:G:114:PRO:HG3	1:G:149:PRO:HB3	1.99	0.45
1:D:37:ALA:O	1:G:15:VAL:HA	2.17	0.45
1:B:236:LEU:HD23	1:B:263:MET:HE3	1.98	0.45
1:B:5:CYS:SG	1:B:246:HIS:CE1	3.10	0.45
1:C:12:SER:HB3	1:C:84:TYR:CD2	2.51	0.45
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.82	0.45
1:F:179:GLY:N	1:F:180:PRO:HD2	2.32	0.45
1:H:147:ILE:HD11	1:H:183:VAL:HG22	1.99	0.45
1:D:80:VAL:HG23	1:D:108:LEU:HD11	1.98	0.45
1:E:248:HIS:HB3	1:E:251:ASN:CB	2.47	0.45
1:H:115:VAL:HA	1:H:153:GLU:OE2	2.16	0.45
1:B:11:GLN:O	1:B:39:ASN:HA	2.17	0.45
1:D:79:TYR:CD2	1:D:109:VAL:HB	2.52	0.45
1:A:191:LEU:HD12	1:D:129:PRO:N	2.31	0.45
1:D:174:MET:O	1:D:178:MET:HG3	2.17	0.45
1:F:233:THR:HB	4:F:5402:ADP:H5'1	1.98	0.45
1:F:87:ASP:HB3	1:F:90:PHE:HB2	1.98	0.45
1:G:116:MET:O	1:G:128:VAL:HG22	2.17	0.45
1:G:88:LYS:HA	1:G:132:LEU:HD23	1.99	0.45
1:C:34:GLU:OE1	1:H:18:TYR:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:TYR:OH	1:H:287:ALA:HA	2.16	0.45
1:A:85:THR:HG22	1:A:86:ARG:N	2.32	0.44
1:B:166:GLU:O	1:B:169:LEU:N	2.50	0.44
1:C:273:CYS:O	1:C:276:ALA:HB3	2.17	0.44
1:C:46:HIS:CE1	1:C:48:GLY:HA3	2.53	0.44
1:D:11:GLN:O	1:D:39:ASN:HA	2.17	0.44
1:G:166:GLU:O	1:G:168:ALA:N	2.50	0.44
1:H:105:ASN:ND2	1:H:105:ASN:C	2.70	0.44
1:A:227:ASP:HB2	5:A:409:HOH:O	2.17	0.44
1:A:236:LEU:HG	1:A:240:MET:CE	2.48	0.44
1:C:172:MET:HG2	1:C:183:VAL:CG1	2.48	0.44
1:D:39:ASN:H	1:G:42:GLN:NE2	2.12	0.44
1:H:292:ARG:NH2	1:H:295:GLN:HE21	2.15	0.44
1:A:129:PRO:CA	1:B:191:LEU:HD12	2.47	0.44
1:C:236:LEU:HG	1:C:240:MET:CE	2.48	0.44
1:E:149:PRO:HG2	1:E:185:ILE:CD1	2.47	0.44
1:F:88:LYS:HA	1:F:132:LEU:CD2	2.48	0.44
1:G:208:ARG:NH1	1:G:208:ARG:CG	2.79	0.44
1:G:46:HIS:ND1	1:G:48:GLY:N	2.63	0.44
1:A:194:ARG:HG2	1:A:222:GLU:OE1	2.18	0.44
1:A:47:THR:HG22	1:A:52:TRP:NE1	2.33	0.44
1:C:16:ARG:HG3	1:C:16:ARG:HH11	1.83	0.44
1:H:114:PRO:HG3	1:H:149:PRO:HB3	2.00	0.44
1:A:164:SER:OG	1:A:167:GLU:HG2	2.16	0.44
1:A:8:LEU:HB2	1:A:77:TYR:CE2	2.52	0.44
1:B:133:LEU:HD22	1:B:156:LEU:HG	1.99	0.44
1:C:264:HIS:CE1	1:C:268:GLN:HG3	2.53	0.44
1:D:70:LYS:NZ	1:D:75:ASN:HD21	2.16	0.44
1:E:284:PRO:HB2	1:E:289:LEU:HD21	2.00	0.44
1:F:244:TRP:O	1:F:247:LYS:HB3	2.17	0.44
1:F:26:PHE:N	1:F:27:PRO:CD	2.81	0.44
1:H:136:TYR:O	1:H:141:VAL:HG23	2.18	0.44
1:H:1:MET:HE1	1:H:5:CYS:HB2	1.99	0.44
1:A:110:TYR:CD2	1:A:110:TYR:C	2.91	0.44
1:A:24:ALA:C	1:A:27:PRO:HD2	2.38	0.44
1:B:116:MET:SD	1:B:156:LEU:HD23	2.57	0.44
1:B:170:GLU:O	1:B:173:ASP:HB2	2.17	0.44
1:B:63:GLN:OE1	1:B:93:MET:HE2	2.17	0.44
1:C:1:MET:HE1	1:C:5:CYS:H	1.82	0.44
1:G:164:SER:OG	1:G:167:GLU:CG	2.64	0.44
1:H:117:GLY:HA3	1:H:126:MET:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PHE:O	1:A:30:VAL:HG13	2.18	0.44
1:A:1:MET:HE2	1:A:5:CYS:HB2	1.98	0.44
1:B:205:GLN:HB2	1:B:252:LEU:HD22	1.99	0.44
1:B:242:LEU:CD2	1:B:242:LEU:C	2.84	0.44
1:B:236:LEU:CB	1:B:263:MET:HE1	2.39	0.44
1:B:29:GLN:C	1:B:31:LEU:N	2.69	0.44
1:B:59:SER:OG	1:B:89:SER:HB3	2.17	0.44
1:G:79:TYR:HA	1:G:109:VAL:O	2.18	0.44
1:H:162:ILE:CD1	1:H:171:VAL:HG21	2.48	0.44
1:H:63:GLN:OE1	1:H:93:MET:HE1	2.17	0.44
1:D:63:GLN:OE1	1:D:93:MET:HE1	2.17	0.44
1:F:79:TYR:HA	1:F:109:VAL:O	2.18	0.44
1:G:270:THR:HA	1:G:292:ARG:HG3	2.00	0.44
1:B:46:HIS:ND1	1:B:48:GLY:N	2.64	0.44
1:D:295:GLN:CD	1:D:295:GLN:H	2.18	0.44
1:D:5:CYS:SG	1:D:246:HIS:CE1	3.11	0.44
1:E:46:HIS:HE1	1:E:48:GLY:HA3	1.81	0.44
1:G:172:MET:HA	1:G:175:LEU:HD12	1.99	0.44
1:G:6:ARG:HD2	1:G:76:GLN:O	2.17	0.44
1:G:63:GLN:OE1	1:G:93:MET:CE	2.65	0.44
1:H:56:VAL:HG12	1:H:57:LEU:N	2.33	0.44
1:A:163:HIS:NE2	1:A:167:GLU:OE1	2.51	0.43
1:B:85:THR:HG22	1:B:87:ASP:N	2.19	0.43
1:C:244:TRP:CE3	1:C:244:TRP:HA	2.53	0.43
1:D:44:SER:OG	1:D:45:ASN:ND2	2.51	0.43
1:E:57:LEU:HA	1:E:61:GLU:OE2	2.17	0.43
1:F:170:GLU:O	1:F:173:ASP:N	2.51	0.43
1:F:235:ASP:OD2	3:F:5401:PLP:H5A1	2.18	0.43
1:H:175:LEU:O	1:H:176:HIS:C	2.56	0.43
1:A:85:THR:HG23	5:A:412:HOH:O	2.19	0.43
1:B:105:ASN:ND2	1:B:107:ARG:N	2.63	0.43
1:C:172:MET:HG2	1:C:183:VAL:HG12	2.00	0.43
1:D:172:MET:HA	1:D:175:LEU:HD12	2.00	0.43
1:E:41:VAL:HG12	1:E:56:VAL:HG13	1.99	0.43
1:F:166:GLU:O	1:F:168:ALA:N	2.50	0.43
1:F:248:HIS:HB3	1:F:251:ASN:CB	2.48	0.43
1:H:87:ASP:HB3	1:H:90:PHE:CB	2.49	0.43
1:A:63:GLN:OE1	1:A:93:MET:HE2	2.18	0.43
1:B:147:ILE:HB	1:B:149:PRO:HD3	2.00	0.43
1:C:166:GLU:O	1:C:168:ALA:N	2.51	0.43
1:D:28:LEU:HD21	1:D:239:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:THR:HG22	1:D:86:ARG:N	2.32	0.43
1:F:103:GLN:CA	1:F:103:GLN:NE2	2.78	0.43
1:B:53:LYS:HE2	1:F:71:LEU:HD11	2.00	0.43
1:C:305:ILE:CD1	1:C:305:ILE:H	2.32	0.43
1:C:56:VAL:HG12	1:C:57:LEU:N	2.34	0.43
1:D:107:ARG:HH11	1:D:107:ARG:CG	2.31	0.43
1:D:273:CYS:O	1:D:276:ALA:HB3	2.18	0.43
1:D:270:THR:HA	1:D:292:ARG:HG3	2.00	0.43
1:E:1:MET:CE	1:E:5:CYS:HB2	2.45	0.43
1:G:186:THR:O	1:G:187:SER:HB3	2.19	0.43
1:G:27:PRO:HG2	1:G:236:LEU:CD1	2.49	0.43
1:G:11:GLN:O	1:G:39:ASN:HA	2.18	0.43
1:A:11:GLN:O	1:A:39:ASN:HA	2.19	0.43
1:B:190:LEU:O	1:B:192:SER:N	2.51	0.43
1:B:29:GLN:O	1:F:294:VAL:HG13	2.18	0.43
1:D:110:TYR:CD2	1:D:110:TYR:C	2.90	0.43
1:D:193:PRO:HD3	1:D:200:MET:HE3	2.01	0.43
1:F:158:THR:OG1	1:F:171:VAL:HG13	2.18	0.43
1:H:221:MET:HG2	1:H:309:ALA:HA	1.99	0.43
1:H:47:THR:CG2	1:H:52:TRP:CE2	2.96	0.43
1:A:88:LYS:HA	1:A:132:LEU:CD2	2.48	0.43
1:C:149:PRO:HG2	1:C:185:ILE:HD13	1.99	0.43
1:C:235:ASP:OD2	3:C:2401:PLP:H5A1	2.18	0.43
1:C:269:ARG:HD3	1:C:295:GLN:HB3	2.00	0.43
1:C:85:THR:HG22	1:C:86:ARG:N	2.33	0.43
1:H:105:ASN:C	1:H:105:ASN:HD22	2.22	0.43
1:A:169:LEU:HA	1:A:172:MET:HE3	2.01	0.43
1:C:143:VAL:HG22	1:C:143:VAL:O	2.17	0.43
1:D:105:ASN:ND2	1:D:107:ARG:N	2.61	0.43
1:D:29:GLN:C	1:D:31:LEU:N	2.71	0.43
1:G:57:LEU:HA	1:G:61:GLU:OE2	2.17	0.43
1:G:233:THR:HB	4:G:6402:ADP:H5'1	2.00	0.43
1:A:236:LEU:HD23	1:A:263:MET:HE3	2.01	0.43
1:B:193:PRO:HD3	1:B:200:MET:HE3	2.00	0.43
1:B:36:ASP:OD2	1:F:16:ARG:HB2	2.18	0.43
1:B:9:SER:HA	1:B:81:LEU:O	2.19	0.43
1:C:12:SER:HB3	1:C:84:TYR:HB3	2.01	0.43
1:C:269:ARG:HG3	5:C:2423:HOH:O	2.19	0.43
1:C:59:SER:OG	1:C:89:SER:HB3	2.19	0.43
1:D:79:TYR:HA	1:D:109:VAL:O	2.19	0.43
1:D:26:PHE:N	1:D:27:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:GLN:HB2	1:F:187:SER:O	2.19	0.43
1:G:149:PRO:HD2	1:G:184:VAL:O	2.19	0.43
1:G:26:PHE:CE2	1:G:30:VAL:HG11	2.53	0.43
1:H:79:TYR:HA	1:H:109:VAL:O	2.18	0.43
1:B:110:TYR:CD2	1:B:110:TYR:C	2.92	0.43
1:B:90:PHE:O	1:B:94:VAL:HG23	2.19	0.43
1:C:134:PRO:HB3	1:D:281:GLY:HA3	2.00	0.43
1:D:158:THR:OG1	1:D:171:VAL:HG13	2.19	0.43
1:D:179:GLY:N	1:D:180:PRO:HD2	2.32	0.43
1:D:12:SER:HB3	1:D:84:TYR:HB3	2.01	0.43
1:F:56:VAL:HG12	1:F:57:LEU:N	2.34	0.43
1:C:15:VAL:HG11	1:H:69:LEU:HD11	1.99	0.43
1:A:140:VAL:O	1:A:143:VAL:HG12	2.17	0.43
1:B:193:PRO:HG2	1:B:220:ARG:HH12	1.82	0.43
1:B:305:ILE:H	1:B:305:ILE:CD1	2.32	0.43
1:C:140:VAL:C	1:C:142:PRO:HD2	2.39	0.43
1:C:19:VAL:O	1:C:22:ARG:HB2	2.19	0.43
1:D:296:SER:O	1:D:297:LYS:C	2.57	0.43
1:H:199:LEU:HB3	1:H:223:MET:CE	2.49	0.43
1:H:233:THR:HB	4:H:7402:ADP:H5'1	2.01	0.43
1:A:172:MET:O	1:A:176:HIS:CD2	2.72	0.42
1:A:26:PHE:N	1:A:27:PRO:CD	2.82	0.42
1:D:72:ASN:O	1:D:73:HIS:HB2	2.18	0.42
1:E:158:THR:HG21	1:E:171:VAL:CG1	2.38	0.42
1:F:162:ILE:HD11	1:F:171:VAL:HG21	2.01	0.42
1:G:140:VAL:O	1:G:143:VAL:HG12	2.19	0.42
1:H:248:HIS:HB3	1:H:251:ASN:CB	2.49	0.42
1:A:9:SER:HA	1:A:81:LEU:O	2.19	0.42
1:C:140:VAL:O	1:C:143:VAL:HG12	2.19	0.42
1:C:1:MET:HE3	1:C:32:GLY:O	2.19	0.42
1:D:186:THR:O	1:D:187:SER:HB3	2.19	0.42
1:H:26:PHE:N	1:H:27:PRO:CD	2.82	0.42
1:C:292:ARG:NH2	1:H:4:GLU:OE2	2.52	0.42
1:D:53:LYS:HE2	1:G:71:LEU:CD1	2.49	0.42
1:E:46:HIS:ND1	1:E:48:GLY:N	2.63	0.42
1:G:115:VAL:HA	1:G:153:GLU:OE2	2.19	0.42
1:G:133:LEU:CD2	1:G:156:LEU:HG	2.48	0.42
1:B:39:ASN:O	1:B:57:LEU:HD13	2.19	0.42
1:C:307:VAL:HG23	1:C:307:VAL:O	2.19	0.42
1:C:87:ASP:OD2	1:C:89:SER:N	2.51	0.42
1:D:140:VAL:C	1:D:142:PRO:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:LEU:HA	1:E:199:LEU:HD23	1.91	0.42
1:A:105:ASN:C	1:A:105:ASN:ND2	2.72	0.42
1:B:133:LEU:CD2	1:B:156:LEU:HG	2.50	0.42
1:C:71:LEU:HD13	1:H:51:HIS:CB	2.44	0.42
1:E:19:VAL:O	1:E:22:ARG:HB2	2.20	0.42
1:F:251:ASN:O	1:F:252:LEU:C	2.57	0.42
1:D:194:ARG:HG2	1:D:222:GLU:OE1	2.20	0.42
1:E:211:ASP:CG	1:E:213:SER:HG	2.21	0.42
1:F:227:ASP:HB2	5:F:5414:HOH:O	2.18	0.42
1:H:103:GLN:NE2	1:H:103:GLN:CA	2.79	0.42
1:H:107:ARG:HH11	1:H:107:ARG:CG	2.33	0.42
1:H:280:GLU:O	1:H:282:VAL:HG23	2.19	0.42
1:A:103:GLN:HE21	1:A:103:GLN:HA	1.83	0.42
1:B:162:ILE:HD11	1:B:171:VAL:HG21	2.01	0.42
1:B:261:SER:HB3	1:B:304:GLU:O	2.20	0.42
1:B:280:GLU:HG3	1:B:280:GLU:H	1.43	0.42
1:C:285:SER:HB2	1:C:286:PRO:HD2	2.01	0.42
1:C:11:GLN:O	1:C:39:ASN:HA	2.20	0.42
1:D:29:GLN:O	1:G:294:VAL:CG1	2.68	0.42
1:E:120:ARG:NH1	5:E:4444:HOH:O	2.52	0.42
1:F:283:LYS:HD3	1:F:284:PRO:CD	2.50	0.42
1:G:110:TYR:CD2	1:G:110:TYR:C	2.93	0.42
1:G:179:GLY:N	1:G:180:PRO:HD2	2.34	0.42
1:G:264:HIS:CE1	1:G:268:GLN:HG3	2.54	0.42
1:A:128:VAL:C	1:B:191:LEU:CD1	2.82	0.42
1:A:12:SER:HA	1:A:41:VAL:HG22	2.01	0.42
1:C:19:VAL:CG2	1:C:231:VAL:HG12	2.50	0.42
1:D:244:TRP:CE3	1:D:244:TRP:HA	2.54	0.42
1:D:257:GLU:OE2	1:D:308:GLN:HA	2.20	0.42
1:E:162:ILE:CD1	1:E:171:VAL:HG21	2.50	0.42
1:E:193:PRO:HD3	1:E:200:MET:HE3	2.02	0.42
1:E:79:TYR:HA	1:E:109:VAL:O	2.20	0.42
1:F:162:ILE:CD1	1:F:171:VAL:HG21	2.50	0.42
1:F:199:LEU:HB3	1:F:223:MET:CE	2.50	0.42
1:B:39:ASN:N	1:F:42:GLN:HE22	1.92	0.42
1:G:265:HIS:O	1:G:266:VAL:C	2.57	0.42
1:G:280:GLU:H	1:G:280:GLU:HG3	1.49	0.42
1:A:151:GLN:OE1	1:A:188:SER:HB2	2.18	0.42
1:B:38:VAL:HG23	1:F:15:VAL:HG13	2.02	0.42
1:D:155:GLU:HG2	1:D:162:ILE:HG12	2.01	0.42
1:D:171:VAL:O	1:D:175:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:SER:OG	1:E:167:GLU:CG	2.66	0.42
1:E:251:ASN:O	1:E:252:LEU:C	2.57	0.42
1:E:270:THR:HA	1:E:292:ARG:HG3	2.01	0.42
1:A:53:LYS:HE2	1:E:71:LEU:HD11	2.01	0.42
1:F:114:PRO:HG3	1:F:149:PRO:HB3	2.02	0.42
1:F:70:LYS:HD2	1:F:70:LYS:HA	1.84	0.42
1:G:103:GLN:CA	1:G:103:GLN:NE2	2.70	0.42
1:G:162:ILE:HD11	1:G:171:VAL:HG21	2.01	0.42
1:G:166:GLU:O	1:G:169:LEU:N	2.53	0.42
1:H:133:LEU:HD22	1:H:156:LEU:HG	2.02	0.42
1:H:174:MET:O	1:H:178:MET:HG3	2.19	0.42
1:A:88:LYS:HA	1:A:132:LEU:HD23	2.02	0.42
1:C:12:SER:HA	1:C:41:VAL:HG22	2.01	0.42
1:C:63:GLN:OE1	1:C:93:MET:HE2	2.20	0.42
1:D:103:GLN:NE2	1:D:103:GLN:CA	2.79	0.42
1:D:118:ASP:O	1:D:124:GLY:HA3	2.20	0.42
1:E:39:ASN:O	1:E:57:LEU:HD13	2.20	0.42
1:F:87:ASP:OD2	1:F:89:SER:HB2	2.20	0.42
1:H:112:CYS:O	1:H:147:ILE:HA	2.20	0.42
1:H:273:CYS:O	1:H:276:ALA:HB3	2.20	0.42
1:A:12:SER:HB3	1:A:84:TYR:HB3	2.01	0.41
1:C:176:HIS:CE1	1:C:181:ASP:O	2.71	0.41
1:D:19:VAL:HG21	1:D:231:VAL:HG12	2.02	0.41
1:D:8:LEU:HB2	1:D:77:TYR:CE2	2.55	0.41
1:E:35:VAL:HG12	1:E:36:ASP:N	2.35	0.41
1:E:70:LYS:HD2	1:E:70:LYS:HA	1.76	0.41
1:G:163:HIS:NE2	1:G:167:GLU:OE1	2.53	0.41
1:H:46:HIS:ND1	1:H:48:GLY:N	2.67	0.41
1:A:130:ASP:OD1	1:B:164:SER:HA	2.21	0.41
1:A:147:ILE:HB	1:A:149:PRO:HD3	2.02	0.41
1:C:186:THR:O	1:C:187:SER:HB3	2.21	0.41
1:C:19:VAL:HG21	1:C:231:VAL:HG12	2.01	0.41
1:C:53:LYS:HE2	1:H:71:LEU:HD11	2.01	0.41
1:E:151:GLN:HB2	1:E:187:SER:O	2.21	0.41
1:H:283:LYS:HA	1:H:284:PRO:HD3	1.95	0.41
1:A:169:LEU:HD22	1:A:218:ARG:HD2	2.02	0.41
1:B:233:THR:HB	4:B:1402:ADP:H5'1	2.03	0.41
1:B:43:PHE:HA	1:B:54:GLY:HA3	2.02	0.41
1:B:91:LEU:O	1:B:94:VAL:HB	2.21	0.41
1:D:87:ASP:OD2	1:D:89:SER:N	2.54	0.41
1:E:179:GLY:N	1:E:180:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:THR:HG22	1:F:52:TRP:CD2	2.55	0.41
1:D:133:LEU:HD13	1:D:156:LEU:HD23	2.01	0.41
1:D:24:ALA:C	1:D:27:PRO:HD2	2.41	0.41
1:F:208:ARG:NH1	5:F:5405:HOH:O	2.54	0.41
1:G:151:GLN:HB2	1:G:187:SER:O	2.20	0.41
1:H:170:GLU:O	1:H:173:ASP:N	2.53	0.41
1:C:55:GLN:NE2	1:H:57:LEU:HD21	2.35	0.41
1:D:261:SER:HB3	1:D:304:GLU:O	2.20	0.41
1:C:88:LYS:CE	1:D:280:GLU:CD	2.89	0.41
1:D:305:ILE:CD1	1:D:305:ILE:H	2.33	0.41
1:F:307:VAL:O	1:F:307:VAL:CG2	2.69	0.41
1:H:155:GLU:HB3	1:H:160:ARG:O	2.20	0.41
1:H:6:ARG:HD2	1:H:76:GLN:O	2.21	0.41
1:C:105:ASN:C	1:C:105:ASN:ND2	2.74	0.41
1:C:133:LEU:O	1:C:137:ARG:HB2	2.21	0.41
1:C:233:THR:HB	4:C:2402:ADP:H5'1	2.01	0.41
1:C:6:ARG:HD2	1:C:76:GLN:O	2.20	0.41
1:D:47:THR:HG22	1:D:52:TRP:CD2	2.55	0.41
1:E:140:VAL:O	1:E:143:VAL:HG12	2.19	0.41
1:E:296:SER:O	1:E:297:LYS:C	2.58	0.41
1:G:296:SER:O	1:G:297:LYS:C	2.59	0.41
1:H:9:SER:HA	1:H:81:LEU:O	2.20	0.41
1:A:133:LEU:HD22	1:A:156:LEU:HG	2.03	0.41
1:B:72:ASN:O	1:B:73:HIS:CB	2.69	0.41
1:G:19:VAL:O	1:G:22:ARG:HB2	2.20	0.41
1:G:56:VAL:HG12	1:G:57:LEU:N	2.35	0.41
1:H:296:SER:O	1:H:297:LYS:C	2.57	0.41
1:B:79:TYR:HA	1:B:109:VAL:O	2.21	0.41
1:C:193:PRO:HD3	1:C:200:MET:HE3	2.03	0.41
1:E:219:ILE:O	1:E:219:ILE:HG13	2.21	0.41
1:F:295:GLN:H	1:F:295:GLN:CD	2.21	0.41
1:A:265:HIS:O	1:A:266:VAL:C	2.59	0.41
1:B:87:ASP:OD2	1:B:89:SER:HB2	2.20	0.41
1:C:236:LEU:HG	1:C:240:MET:HE2	2.03	0.41
1:C:34:GLU:OE1	1:H:18:TYR:CZ	2.73	0.41
1:F:31:LEU:HD23	1:F:31:LEU:HA	1.87	0.41
1:G:280:GLU:O	1:G:282:VAL:HG23	2.21	0.41
1:H:149:PRO:HD2	1:H:184:VAL:O	2.21	0.41
1:A:233:THR:HB	4:A:402:ADP:H5'1	2.03	0.41
1:B:235:ASP:OD2	3:B:1401:PLP:H5A1	2.21	0.41
1:B:208:ARG:NH1	1:B:208:ARG:CG	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASP:O	1:C:124:GLY:HA3	2.21	0.41
1:C:151:GLN:HB2	1:C:187:SER:O	2.21	0.41
1:D:169:LEU:HD22	1:D:218:ARG:HD2	2.03	0.41
1:D:19:VAL:CG2	1:D:231:VAL:HG12	2.51	0.41
1:E:118:ASP:O	1:E:124:GLY:HA3	2.21	0.41
1:E:175:LEU:O	1:E:176:HIS:C	2.59	0.41
1:E:176:HIS:CE1	1:E:181:ASP:O	2.74	0.41
1:E:307:VAL:CG2	1:E:307:VAL:O	2.68	0.41
1:E:47:THR:HG22	1:E:52:TRP:CD2	2.55	0.41
1:F:107:ARG:HH11	1:F:107:ARG:CG	2.34	0.41
1:F:120:ARG:NH2	5:F:5421:HOH:O	2.53	0.41
1:F:166:GLU:C	1:F:168:ALA:N	2.72	0.41
1:F:46:HIS:ND1	1:F:48:GLY:N	2.64	0.41
1:G:166:GLU:C	1:G:168:ALA:N	2.73	0.41
1:G:291:LEU:HG	5:G:6411:HOH:O	2.21	0.41
1:G:261:SER:HB3	1:G:304:GLU:O	2.21	0.41
1:H:110:TYR:CD2	1:H:110:TYR:C	2.92	0.41
1:A:155:GLU:HG2	1:A:162:ILE:HG12	2.02	0.41
1:B:273:CYS:O	1:B:276:ALA:HB3	2.21	0.41
1:D:265:HIS:O	1:D:266:VAL:C	2.59	0.41
1:E:191:LEU:N	1:E:191:LEU:HD23	2.36	0.41
1:E:63:GLN:OE1	1:E:93:MET:CE	2.69	0.41
1:F:147:ILE:HD11	1:F:183:VAL:HG22	2.02	0.41
1:F:220:ARG:HB2	1:F:312:LEU:HD11	2.03	0.41
1:G:16:ARG:HG3	1:G:16:ARG:HH11	1.86	0.41
1:C:38:VAL:CG2	1:H:15:VAL:HG13	2.51	0.41
1:B:269:ARG:HD3	1:B:295:GLN:HB3	2.02	0.40
1:D:155:GLU:HB3	1:D:160:ARG:O	2.21	0.40
1:E:105:ASN:HD22	1:E:107:ARG:H	1.68	0.40
1:G:29:GLN:C	1:G:31:LEU:N	2.73	0.40
1:H:292:ARG:O	1:H:296:SER:OG	2.32	0.40
1:H:58:ASN:OD1	1:H:60:ASP:HB2	2.20	0.40
1:A:63:GLN:OE1	1:A:93:MET:HE1	2.21	0.40
1:B:85:THR:HG22	1:B:86:ARG:N	2.36	0.40
1:C:280:GLU:H	1:C:280:GLU:HG3	1.48	0.40
1:E:297:LYS:O	1:E:301:GLU:HG3	2.20	0.40
1:G:6:ARG:HG2	1:G:77:TYR:HD2	1.85	0.40
1:H:280:GLU:H	1:H:280:GLU:HG3	1.46	0.40
1:C:4:GLU:CD	1:H:292:ARG:NH2	2.62	0.40
1:H:70:LYS:HA	1:H:70:LYS:HD2	1.86	0.40
1:H:187:SER:OG	4:H:7402:ADP:O2A	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:HA	1:A:284:PRO:HD3	1.95	0.40
1:B:166:GLU:C	1:B:168:ALA:N	2.73	0.40
1:B:173:ASP:OD2	1:B:218:ARG:NH2	2.47	0.40
1:B:200:MET:HE2	1:B:220:ARG:HD3	2.02	0.40
1:B:244:TRP:HA	1:B:244:TRP:CE3	2.57	0.40
1:B:8:LEU:HB2	1:B:77:TYR:CD2	2.56	0.40
1:C:112:CYS:O	1:C:147:ILE:HA	2.22	0.40
1:C:147:ILE:HD11	1:C:183:VAL:HG22	2.02	0.40
1:C:200:MET:HE1	1:C:220:ARG:NE	2.36	0.40
1:C:6:ARG:HG2	1:C:77:TYR:HD2	1.87	0.40
1:C:93:MET:O	1:C:97:ILE:HG13	2.21	0.40
1:D:193:PRO:HG2	1:D:220:ARG:HH12	1.85	0.40
1:E:163:HIS:CE1	1:E:167:GLU:CD	2.95	0.40
1:F:108:LEU:CD2	1:F:108:LEU:C	2.81	0.40
1:B:71:LEU:HD11	1:F:53:LYS:HE2	2.02	0.40
1:F:88:LYS:HA	1:F:132:LEU:HD23	2.04	0.40
1:A:193:PRO:HD3	1:A:200:MET:HE3	2.03	0.40
1:B:26:PHE:N	1:B:27:PRO:CD	2.84	0.40
1:A:15:VAL:HA	1:E:37:ALA:O	2.20	0.40
1:H:166:GLU:C	1:H:168:ALA:N	2.75	0.40
1:H:16:ARG:HG3	1:H:16:ARG:NH1	2.37	0.40
1:H:236:LEU:HG	1:H:240:MET:CE	2.52	0.40
1:H:244:TRP:CE3	1:H:244:TRP:HA	2.57	0.40
1:H:29:GLN:C	1:H:31:LEU:N	2.75	0.40
1:H:307:VAL:O	1:H:307:VAL:CG2	2.70	0.40
1:A:207:THR:O	1:A:214:VAL:HA	2.21	0.40
1:B:12:SER:HB3	1:B:84:TYR:HB3	2.03	0.40
1:C:163:HIS:NE2	1:C:167:GLU:OE1	2.55	0.40
1:G:199:LEU:HB3	1:G:223:MET:CE	2.51	0.40
1:G:26:PHE:O	1:G:30:VAL:HG13	2.21	0.40
1:G:5:CYS:SG	1:G:246:HIS:CE1	3.15	0.40

There are no symmetry-related clashes.

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	310/312 (99%)	279 (90%)	29 (9%)	2 (1%)	25	56
1	B	310/312 (99%)	276 (89%)	30 (10%)	4 (1%)	12	36
1	C	310/312 (99%)	272 (88%)	34 (11%)	4 (1%)	12	36
1	D	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	25	56
1	E	310/312 (99%)	274 (88%)	31 (10%)	5 (2%)	9	31
1	F	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	25	56
1	G	310/312 (99%)	275 (89%)	32 (10%)	3 (1%)	15	44
1	H	310/312 (99%)	271 (87%)	36 (12%)	3 (1%)	15	44
All	All	2480/2496 (99%)	2195 (88%)	260 (10%)	25 (1%)	15	44

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	D	191	LEU
1	H	191	LEU
1	B	191	LEU
1	C	191	LEU
1	E	191	LEU
1	F	191	LEU
1	G	191	LEU
1	B	47	THR
1	C	47	THR
1	B	190	LEU
1	E	167	GLU
1	F	293	MET
1	B	293	MET
1	C	293	MET
1	D	190	LEU
1	E	47	THR
1	E	293	MET
1	G	47	THR
1	G	167	GLU
1	H	227	ASP
1	H	293	MET
1	A	47	THR
1	C	190	LEU
1	E	166	GLU

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	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	B	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	C	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	D	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	E	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	F	273/273 (100%)	251 (92%)	22 (8%)	11	33
1	G	273/273 (100%)	250 (92%)	23 (8%)	11	31
1	H	273/273 (100%)	248 (91%)	25 (9%)	9	27
All	All	2184/2184 (100%)	1994 (91%)	190 (9%)	10	30

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	19	VAL
1	A	21	ASN
1	A	55	GLN
1	A	59	SER
1	A	103	GLN
1	A	105	ASN
1	A	107	ARG
1	A	118	ASP
1	A	127	TYR
1	A	131	ASP
1	A	150	ASN
1	A	163	HIS
1	A	177	SER
1	A	189	ASN
1	A	194	ARG
1	A	197	ASP
1	A	208	ARG

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Mol	Chain	Res	Type
1	A	227	ASP
1	A	251	ASN
1	A	263	MET
1	A	280	GLU
1	A	308	GLN
1	B	1	MET
1	B	2	GLU
1	B	3	GLU
1	B	19	VAL
1	B	59	SER
1	B	74	VAL
1	B	103	GLN
1	B	105	ASN
1	B	107	ARG
1	B	110	TYR
1	B	118	ASP
1	B	130	ASP
1	B	131	ASP
1	B	150	ASN
1	B	177	SER
1	B	189	ASN
1	B	194	ARG
1	B	197	ASP
1	B	206	ARG
1	B	208	ARG
1	B	251	ASN
1	B	263	MET
1	B	280	GLU
1	B	308	GLN
1	C	1	MET
1	C	3	GLU
1	C	19	VAL
1	C	45	ASN
1	C	55	GLN
1	C	59	SER
1	C	74	VAL
1	C	103	GLN
1	C	107	ARG
1	C	110	TYR
1	C	118	ASP
1	C	127	TYR
1	C	130	ASP

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Mol	Chain	Res	Type
1	C	131	ASP
1	C	150	ASN
1	C	177	SER
1	C	189	ASN
1	C	194	ARG
1	C	197	ASP
1	C	208	ARG
1	C	251	ASN
1	C	263	MET
1	C	280	GLU
1	C	308	GLN
1	D	1	MET
1	D	2	GLU
1	D	3	GLU
1	D	5	CYS
1	D	19	VAL
1	D	21	ASN
1	D	59	SER
1	D	103	GLN
1	D	105	ASN
1	D	107	ARG
1	D	110	TYR
1	D	118	ASP
1	D	127	TYR
1	D	130	ASP
1	D	131	ASP
1	D	150	ASN
1	D	189	ASN
1	D	194	ARG
1	D	197	ASP
1	D	208	ARG
1	D	251	ASN
1	D	263	MET
1	D	280	GLU
1	D	308	GLN
1	E	1	MET
1	E	3	GLU
1	E	19	VAL
1	E	59	SER
1	E	74	VAL
1	E	103	GLN
1	E	105	ASN

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Mol	Chain	Res	Type
1	E	107	ARG
1	E	112	CYS
1	E	118	ASP
1	E	127	TYR
1	E	130	ASP
1	E	131	ASP
1	E	150	ASN
1	E	177	SER
1	E	189	ASN
1	E	190	LEU
1	E	191	LEU
1	E	194	ARG
1	E	197	ASP
1	E	208	ARG
1	E	263	MET
1	E	280	GLU
1	E	308	GLN
1	F	1	MET
1	F	3	GLU
1	F	19	VAL
1	F	59	SER
1	F	74	VAL
1	F	103	GLN
1	F	105	ASN
1	F	107	ARG
1	F	118	ASP
1	F	119	GLN
1	F	127	TYR
1	F	130	ASP
1	F	150	ASN
1	F	163	HIS
1	F	177	SER
1	F	189	ASN
1	F	191	LEU
1	F	194	ARG
1	F	197	ASP
1	F	208	ARG
1	F	280	GLU
1	F	308	GLN
1	G	1	MET
1	G	3	GLU
1	G	19	VAL

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Mol	Chain	Res	Type
1	G	59	SER
1	G	74	VAL
1	G	103	GLN
1	G	105	ASN
1	G	107	ARG
1	G	112	CYS
1	G	118	ASP
1	G	127	TYR
1	G	130	ASP
1	G	131	ASP
1	G	150	ASN
1	G	177	SER
1	G	189	ASN
1	G	190	LEU
1	G	194	ARG
1	G	197	ASP
1	G	208	ARG
1	G	263	MET
1	G	280	GLU
1	G	308	GLN
1	H	1	MET
1	H	3	GLU
1	H	19	VAL
1	H	21	ASN
1	H	59	SER
1	H	103	GLN
1	H	105	ASN
1	H	107	ARG
1	H	110	TYR
1	H	118	ASP
1	H	127	TYR
1	H	130	ASP
1	H	131	ASP
1	H	150	ASN
1	H	163	HIS
1	H	177	SER
1	H	189	ASN
1	H	191	LEU
1	H	194	ARG
1	H	197	ASP
1	H	208	ARG
1	H	251	ASN

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Mol	Chain	Res	Type
1	H	263	MET
1	H	280	GLU
1	H	308	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	21	ASN
1	A	42	GLN
1	A	45	ASN
1	A	103	GLN
1	A	104	GLN
1	A	105	ASN
1	A	119	GLN
1	A	150	ASN
1	A	308	GLN
1	B	13	HIS
1	B	21	ASN
1	B	42	GLN
1	B	45	ASN
1	B	103	GLN
1	B	104	GLN
1	B	105	ASN
1	B	150	ASN
1	B	251	ASN
1	B	308	GLN
1	C	21	ASN
1	C	42	GLN
1	C	45	ASN
1	C	103	GLN
1	C	104	GLN
1	C	105	ASN
1	C	119	GLN
1	C	150	ASN
1	D	13	HIS
1	D	21	ASN
1	D	42	GLN
1	D	45	ASN
1	D	75	ASN
1	D	103	GLN
1	D	104	GLN

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Mol	Chain	Res	Type
1	D	105	ASN
1	D	119	GLN
1	D	150	ASN
1	D	308	GLN
1	E	13	HIS
1	E	21	ASN
1	E	42	GLN
1	E	45	ASN
1	E	103	GLN
1	E	104	GLN
1	E	105	ASN
1	E	150	ASN
1	E	308	GLN
1	F	21	ASN
1	F	42	GLN
1	F	45	ASN
1	F	51	HIS
1	F	103	GLN
1	F	104	GLN
1	F	105	ASN
1	F	150	ASN
1	F	268	GLN
1	F	308	GLN
1	G	13	HIS
1	G	21	ASN
1	G	42	GLN
1	G	45	ASN
1	G	51	HIS
1	G	103	GLN
1	G	104	GLN
1	G	105	ASN
1	G	150	ASN
1	G	308	GLN
1	H	21	ASN
1	H	42	GLN
1	H	45	ASN
1	H	55	GLN
1	H	103	GLN
1	H	104	GLN
1	H	105	ASN
1	H	150	ASN
1	H	268	GLN

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Mol	Chain	Res	Type
1	H	308	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	PLP	D	3401	2	15,15,16	1.62	2 (13%)	20,22,23	2.16	4 (20%)
4	ADP	A	402	2	24,29,29	1.19	2 (8%)	29,45,45	1.60	4 (13%)
4	ADP	B	1402	2	24,29,29	1.72	7 (29%)	29,45,45	1.55	3 (10%)
3	PLP	G	6401	2	15,15,16	1.73	3 (20%)	20,22,23	2.05	5 (25%)
3	PLP	C	2401	2	15,15,16	1.69	3 (20%)	20,22,23	2.01	5 (25%)
4	ADP	H	7402	2	24,29,29	1.68	6 (25%)	29,45,45	1.55	3 (10%)
4	ADP	E	4402	2	24,29,29	1.64	6 (25%)	29,45,45	1.53	3 (10%)
3	PLP	H	7401	2	15,15,16	1.55	3 (20%)	20,22,23	2.01	4 (20%)
3	PLP	A	401	2	15,15,16	2.02	3 (20%)	20,22,23	2.32	6 (30%)
4	ADP	F	5402	2	24,29,29	1.71	7 (29%)	29,45,45	1.57	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLP	B	1401	2	15,15,16	1.59	3 (20%)	20,22,23	2.09	6 (30%)
4	ADP	C	2402	2	24,29,29	1.72	6 (25%)	29,45,45	1.55	2 (6%)
3	PLP	E	4401	2	15,15,16	1.54	2 (13%)	20,22,23	2.09	5 (25%)
4	ADP	G	6402	2	24,29,29	1.67	6 (25%)	29,45,45	1.53	3 (10%)
3	PLP	F	5401	2	15,15,16	1.65	2 (13%)	20,22,23	2.07	4 (20%)
4	ADP	D	3402	2	24,29,29	1.68	6 (25%)	29,45,45	1.57	3 (10%)

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	PLP	D	3401	2	-	2/6/6/8	0/1/1/1
4	ADP	A	402	2	-	7/12/32/32	0/3/3/3
4	ADP	B	1402	2	-	2/12/32/32	0/3/3/3
3	PLP	G	6401	2	-	2/6/6/8	0/1/1/1
3	PLP	C	2401	2	-	2/6/6/8	0/1/1/1
4	ADP	H	7402	2	-	2/12/32/32	0/3/3/3
4	ADP	E	4402	2	-	3/12/32/32	0/3/3/3
3	PLP	H	7401	2	-	2/6/6/8	0/1/1/1
3	PLP	A	401	2	-	4/6/6/8	0/1/1/1
4	ADP	F	5402	2	-	2/12/32/32	0/3/3/3
3	PLP	B	1401	2	-	1/6/6/8	0/1/1/1
4	ADP	C	2402	2	-	2/12/32/32	0/3/3/3
3	PLP	E	4401	2	-	1/6/6/8	0/1/1/1
4	ADP	G	6402	2	-	2/12/32/32	0/3/3/3
3	PLP	F	5401	2	-	2/6/6/8	0/1/1/1
4	ADP	D	3402	2	-	2/12/32/32	0/3/3/3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PLP	C5-C4	5.56	1.46	1.40
3	C	2401	PLP	C5-C4	4.35	1.45	1.40
3	D	3401	PLP	C5-C4	4.26	1.45	1.40
3	G	6401	PLP	C5-C4	4.12	1.45	1.40
3	B	1401	PLP	C5-C4	4.01	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5401	PLP	C5-C4	4.00	1.44	1.40
3	H	7401	PLP	C5-C4	3.49	1.44	1.40
4	G	6402	ADP	PB-O3B	-3.29	1.42	1.54
4	C	2402	ADP	C5'-C4'	3.28	1.61	1.51
4	B	1402	ADP	PB-O3B	-3.26	1.42	1.54
4	E	4402	ADP	PB-O2B	3.25	1.67	1.54
4	H	7402	ADP	PB-O3B	-3.22	1.42	1.54
4	G	6402	ADP	PB-O2B	3.17	1.67	1.54
4	F	5402	ADP	C2'-C3'	-3.17	1.44	1.53
4	E	4402	ADP	PB-O3B	-3.16	1.42	1.54
3	E	4401	PLP	C3-C2	-3.15	1.37	1.40
4	C	2402	ADP	PB-O3B	-3.14	1.42	1.54
3	A	401	PLP	C4A-C4	3.12	1.58	1.51
4	F	5402	ADP	PB-O2B	3.11	1.66	1.54
4	D	3402	ADP	PB-O3B	-3.11	1.42	1.54
4	F	5402	ADP	PB-O3B	-3.08	1.43	1.54
4	B	1402	ADP	PB-O2B	3.07	1.66	1.54
4	D	3402	ADP	C2'-C3'	-3.06	1.45	1.53
4	G	6402	ADP	C5'-C4'	3.05	1.61	1.51
4	H	7402	ADP	PB-O2B	3.05	1.66	1.54
4	H	7402	ADP	C3'-C4'	-3.02	1.45	1.53
4	B	1402	ADP	C5'-C4'	3.02	1.61	1.51
3	E	4401	PLP	C5-C4	3.01	1.43	1.40
4	H	7402	ADP	C2'-C3'	-3.00	1.45	1.53
4	B	1402	ADP	C2'-C3'	-3.00	1.45	1.53
4	C	2402	ADP	PB-O2B	2.99	1.66	1.54
4	D	3402	ADP	C3'-C4'	-2.97	1.45	1.53
4	C	2402	ADP	C3'-C4'	-2.97	1.45	1.53
4	G	6402	ADP	C2'-C3'	-2.96	1.45	1.53
4	A	402	ADP	PB-O3B	-2.95	1.43	1.54
4	E	4402	ADP	C2'-C3'	-2.89	1.45	1.53
4	F	5402	ADP	C3'-C4'	-2.87	1.45	1.53
4	C	2402	ADP	C2'-C3'	-2.85	1.45	1.53
4	E	4402	ADP	C5'-C4'	2.82	1.60	1.51
4	G	6402	ADP	C3'-C4'	-2.78	1.45	1.53
4	B	1402	ADP	C3'-C4'	-2.78	1.45	1.53
4	E	4402	ADP	C3'-C4'	-2.76	1.45	1.53
4	D	3402	ADP	PB-O2B	2.75	1.65	1.54
4	F	5402	ADP	C5'-C4'	2.68	1.60	1.51
3	G	6401	PLP	C3-C2	-2.68	1.38	1.40
4	D	3402	ADP	C5'-C4'	2.67	1.59	1.51
4	H	7402	ADP	C5'-C4'	2.64	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2401	PLP	C2-N1	2.52	1.38	1.33
4	D	3402	ADP	C5-N7	-2.52	1.30	1.39
3	H	7401	PLP	C2A-C2	2.41	1.54	1.50
3	D	3401	PLP	C2-N1	2.41	1.38	1.33
4	C	2402	ADP	C5-N7	-2.38	1.31	1.39
3	B	1401	PLP	C3-C2	-2.30	1.38	1.40
4	F	5402	ADP	C5-N7	-2.30	1.31	1.39
4	H	7402	ADP	C5-N7	-2.29	1.31	1.39
4	B	1402	ADP	C5-N7	-2.25	1.31	1.39
3	H	7401	PLP	C4A-C4	2.25	1.56	1.51
3	A	401	PLP	C3-C2	-2.24	1.38	1.40
4	G	6402	ADP	C5-N7	-2.23	1.31	1.39
3	B	1401	PLP	C2-N1	2.22	1.38	1.33
3	F	5401	PLP	C3-C2	-2.20	1.38	1.40
4	E	4402	ADP	C5-N7	-2.17	1.31	1.39
4	A	402	ADP	C5-N7	-2.14	1.31	1.39
3	G	6401	PLP	C2-N1	2.14	1.37	1.33
4	B	1402	ADP	PA-O1A	-2.07	1.43	1.50
4	F	5402	ADP	PA-O1A	-2.01	1.43	1.50
3	C	2401	PLP	C3-C2	-2.00	1.38	1.40

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3401	PLP	O4P-C5A-C5	6.99	122.67	109.35
4	D	3402	ADP	N3-C2-N1	-6.31	118.81	128.68
3	A	401	PLP	O4P-C5A-C5	6.29	121.33	109.35
3	G	6401	PLP	O4P-C5A-C5	6.25	121.27	109.35
4	A	402	ADP	N3-C2-N1	-6.25	118.91	128.68
3	B	1401	PLP	O4P-C5A-C5	6.19	121.15	109.35
4	C	2402	ADP	N3-C2-N1	-6.18	119.02	128.68
4	H	7402	ADP	N3-C2-N1	-6.16	119.05	128.68
4	B	1402	ADP	N3-C2-N1	-6.16	119.06	128.68
4	F	5402	ADP	N3-C2-N1	-6.11	119.13	128.68
3	H	7401	PLP	O4P-C5A-C5	6.09	120.95	109.35
3	C	2401	PLP	O4P-C5A-C5	6.02	120.83	109.35
3	F	5401	PLP	O4P-C5A-C5	5.97	120.72	109.35
4	G	6402	ADP	N3-C2-N1	-5.93	119.40	128.68
4	E	4402	ADP	N3-C2-N1	-5.85	119.54	128.68
3	E	4401	PLP	O4P-C5A-C5	5.79	120.38	109.35
3	A	401	PLP	C4A-C4-C5	4.37	125.44	120.94
3	E	4401	PLP	C5A-C5-C6	-4.19	112.48	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5401	PLP	C5A-C5-C6	-3.91	112.94	119.37
3	A	401	PLP	C5A-C5-C6	-3.82	113.09	119.37
3	B	1401	PLP	C5A-C5-C6	-3.47	113.66	119.37
3	G	6401	PLP	C5A-C5-C6	-3.35	113.86	119.37
3	H	7401	PLP	C5A-C5-C6	-3.34	113.88	119.37
3	D	3401	PLP	C5A-C5-C6	-3.32	113.91	119.37
3	C	2401	PLP	C5A-C5-C6	-3.23	114.05	119.37
4	A	402	ADP	C3'-C2'-C1'	3.13	105.70	100.98
3	E	4401	PLP	C4A-C4-C5	3.11	124.14	120.94
3	F	5401	PLP	C4A-C4-C5	3.00	124.03	120.94
3	B	1401	PLP	C4A-C4-C5	2.90	123.92	120.94
4	A	402	ADP	C4-C5-N7	-2.80	106.48	109.40
3	H	7401	PLP	O2P-P-O4P	-2.62	99.76	106.73
3	A	401	PLP	C4A-C4-C3	-2.58	116.12	120.50
3	C	2401	PLP	C4A-C4-C5	2.57	123.59	120.94
3	A	401	PLP	C5-C6-N1	-2.57	119.53	123.82
3	D	3401	PLP	C4A-C4-C5	2.56	123.57	120.94
4	G	6402	ADP	C4-C5-N7	-2.49	106.80	109.40
4	F	5402	ADP	O5'-C5'-C4'	-2.49	100.42	108.99
3	G	6401	PLP	C4A-C4-C5	2.49	123.50	120.94
3	G	6401	PLP	O2P-P-O4P	-2.47	100.16	106.73
3	E	4401	PLP	O2P-P-O4P	-2.47	100.17	106.73
4	E	4402	ADP	C4-C5-N7	-2.40	106.89	109.40
4	B	1402	ADP	C4-C5-N7	-2.37	106.93	109.40
4	E	4402	ADP	O5'-C5'-C4'	-2.36	100.86	108.99
4	D	3402	ADP	C4-C5-N7	-2.34	106.96	109.40
4	H	7402	ADP	C4-C5-N7	-2.34	106.96	109.40
3	C	2401	PLP	O2P-P-O4P	-2.32	100.56	106.73
3	B	1401	PLP	O2P-P-O4P	-2.29	100.65	106.73
4	F	5402	ADP	C4-C5-N7	-2.29	107.02	109.40
4	D	3402	ADP	O5'-C5'-C4'	-2.28	101.14	108.99
3	F	5401	PLP	O2P-P-O4P	-2.25	100.75	106.73
3	A	401	PLP	C6-N1-C2	2.25	123.33	119.17
4	C	2402	ADP	C4-C5-N7	-2.23	107.08	109.40
3	C	2401	PLP	C5-C6-N1	-2.20	120.15	123.82
4	A	402	ADP	C2'-C3'-C4'	2.20	106.92	102.64
3	B	1401	PLP	C5-C6-N1	-2.20	120.16	123.82
3	D	3401	PLP	O2P-P-O4P	-2.19	100.92	106.73
4	B	1402	ADP	O5'-C5'-C4'	-2.19	101.47	108.99
4	G	6402	ADP	O5'-C5'-C4'	-2.16	101.55	108.99
3	B	1401	PLP	C4A-C4-C3	-2.13	116.88	120.50
3	H	7401	PLP	C4A-C4-C5	2.13	123.13	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7402	ADP	O5'-C5'-C4'	-2.12	101.68	108.99
3	G	6401	PLP	C5-C6-N1	-2.09	120.34	123.82
3	E	4401	PLP	C4A-C4-C3	-2.07	116.99	120.50

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	6402	ADP	O4'-C4'-C5'-O5'
3	D	3401	PLP	C4-C5-C5A-O4P
4	A	402	ADP	C5'-O5'-PA-O3A
4	D	3402	ADP	O4'-C4'-C5'-O5'
3	G	6401	PLP	C4-C5-C5A-O4P
3	C	2401	PLP	C4-C5-C5A-O4P
3	H	7401	PLP	C4-C5-C5A-O4P
4	H	7402	ADP	O4'-C4'-C5'-O5'
4	B	1402	ADP	O4'-C4'-C5'-O5'
3	A	401	PLP	C4-C5-C5A-O4P
3	A	401	PLP	C6-C5-C5A-O4P
3	A	401	PLP	C5A-O4P-P-O1P
3	F	5401	PLP	C4-C5-C5A-O4P
4	E	4402	ADP	C3'-C4'-C5'-O5'
4	G	6402	ADP	C3'-C4'-C5'-O5'
4	E	4402	ADP	O4'-C4'-C5'-O5'
4	C	2402	ADP	O4'-C4'-C5'-O5'
4	C	2402	ADP	C3'-C4'-C5'-O5'
4	A	402	ADP	O4'-C4'-C5'-O5'
4	A	402	ADP	C3'-C4'-C5'-O5'
4	D	3402	ADP	C3'-C4'-C5'-O5'
4	F	5402	ADP	O4'-C4'-C5'-O5'
4	F	5402	ADP	C3'-C4'-C5'-O5'
4	H	7402	ADP	C3'-C4'-C5'-O5'
4	B	1402	ADP	C3'-C4'-C5'-O5'
3	D	3401	PLP	C6-C5-C5A-O4P
3	C	2401	PLP	C6-C5-C5A-O4P
3	H	7401	PLP	C6-C5-C5A-O4P
3	F	5401	PLP	C6-C5-C5A-O4P
3	A	401	PLP	C5A-O4P-P-O2P
4	A	402	ADP	PA-O3A-PB-O2B
4	A	402	ADP	PA-O3A-PB-O3B
3	B	1401	PLP	C4-C5-C5A-O4P
3	E	4401	PLP	C4-C5-C5A-O4P

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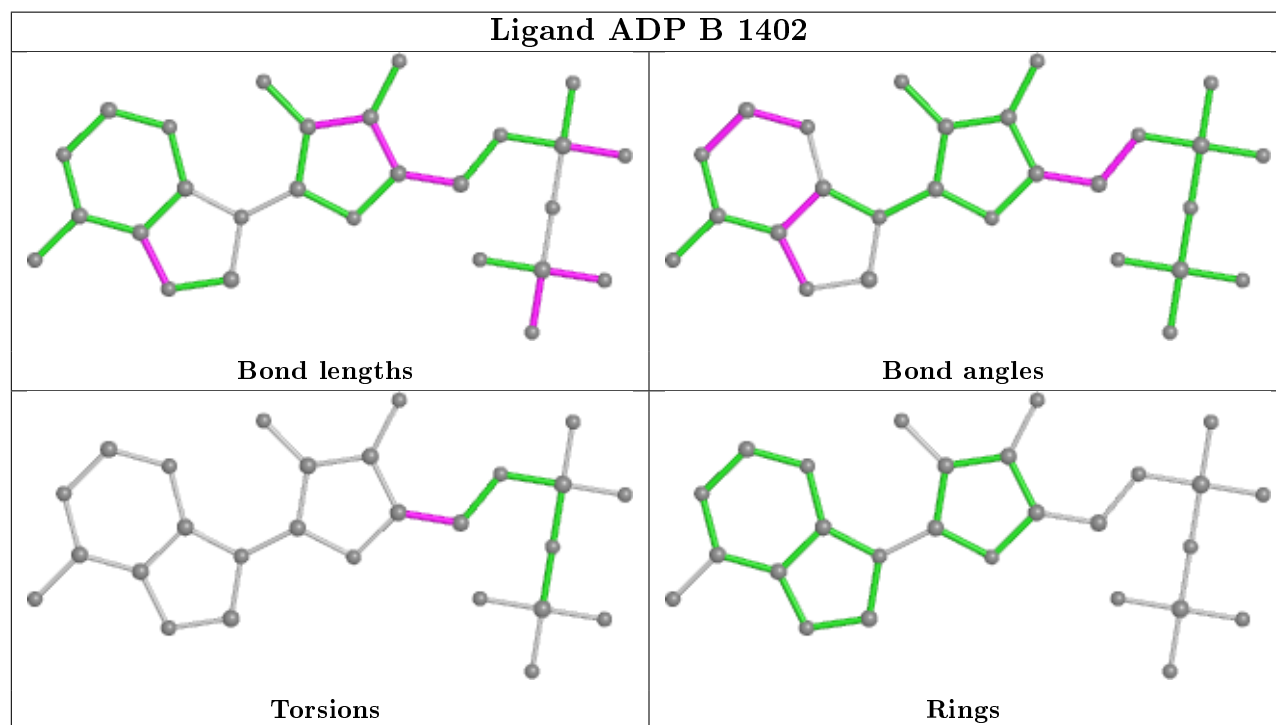
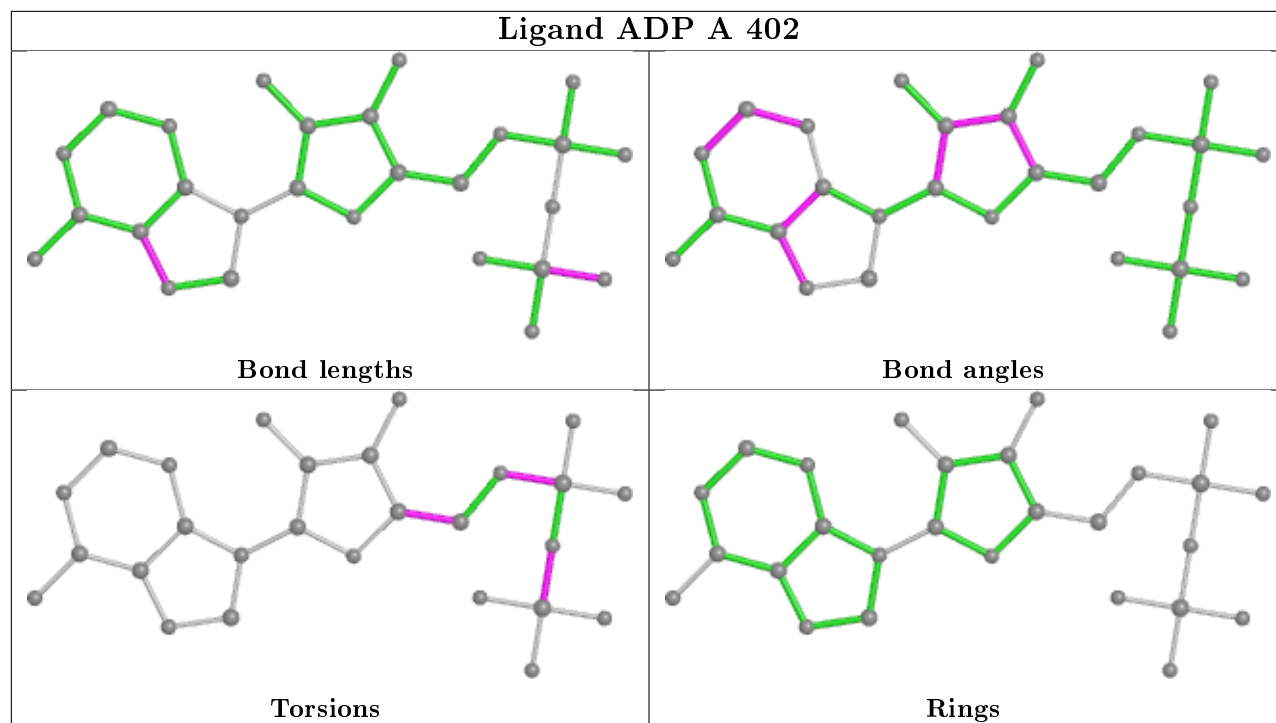
Mol	Chain	Res	Type	Atoms
4	A	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	C5'-O5'-PA-O2A
3	G	6401	PLP	C6-C5-C5A-O4P
4	E	4402	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

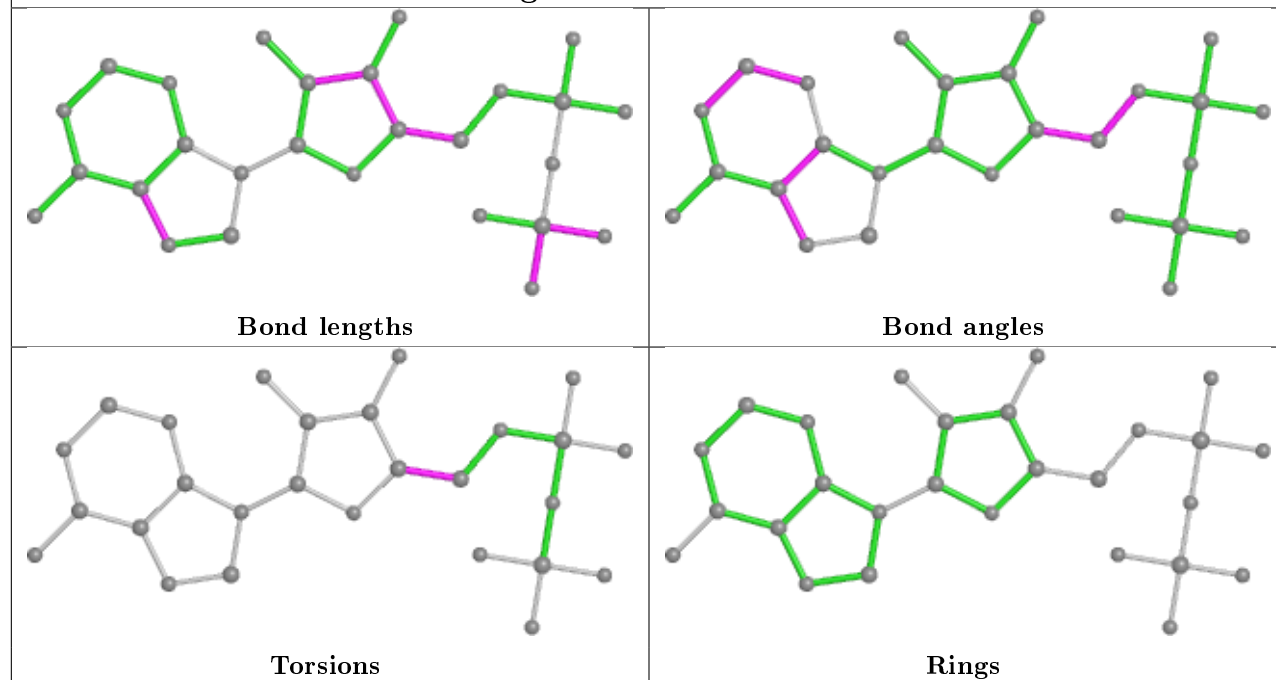
16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3401	PLP	1	0
4	A	402	ADP	3	0
4	B	1402	ADP	2	0
3	G	6401	PLP	1	0
3	C	2401	PLP	1	0
4	H	7402	ADP	2	0
4	E	4402	ADP	1	0
3	H	7401	PLP	1	0
3	A	401	PLP	2	0
4	F	5402	ADP	2	0
3	B	1401	PLP	1	0
4	C	2402	ADP	1	0
3	E	4401	PLP	1	0
4	G	6402	ADP	1	0
3	F	5401	PLP	2	0
4	D	3402	ADP	1	0

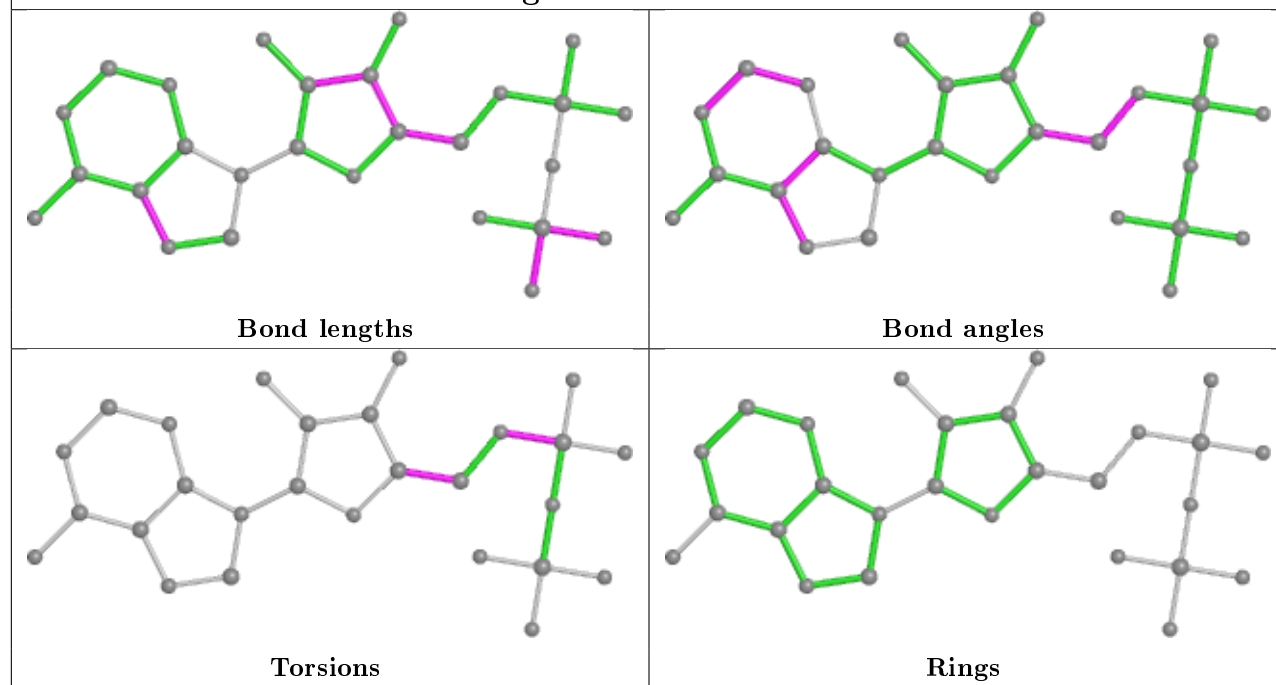
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



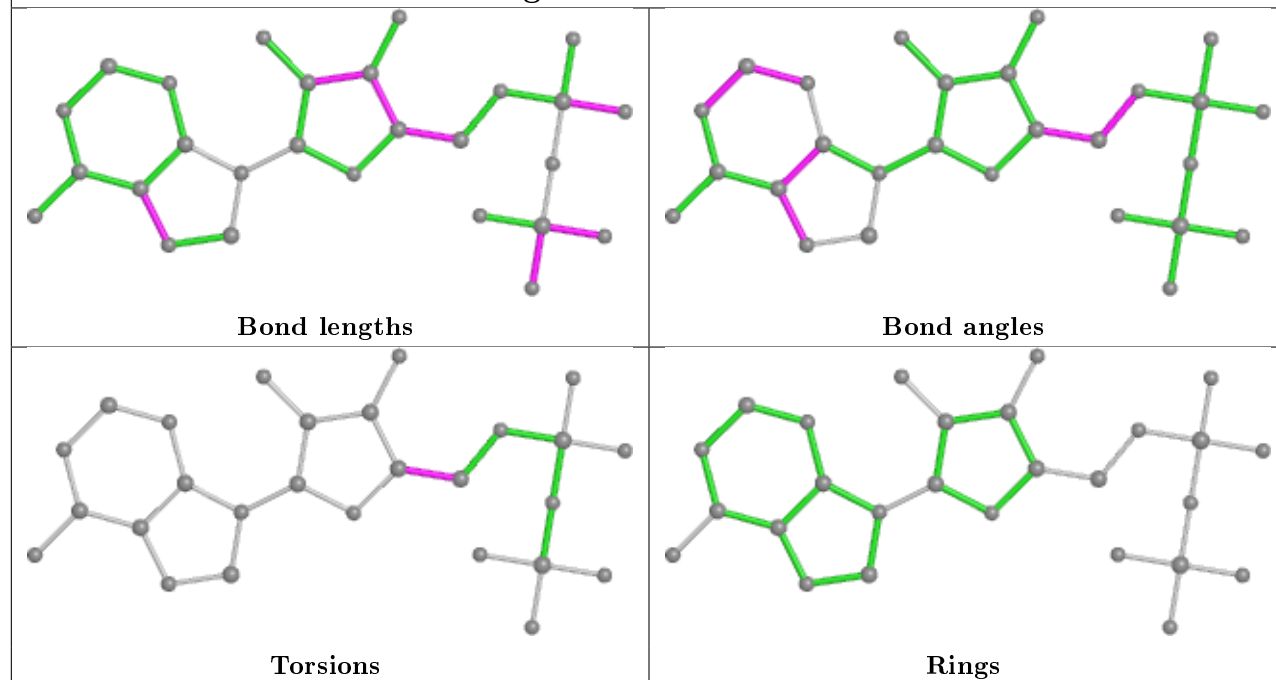
Ligand ADP H 7402



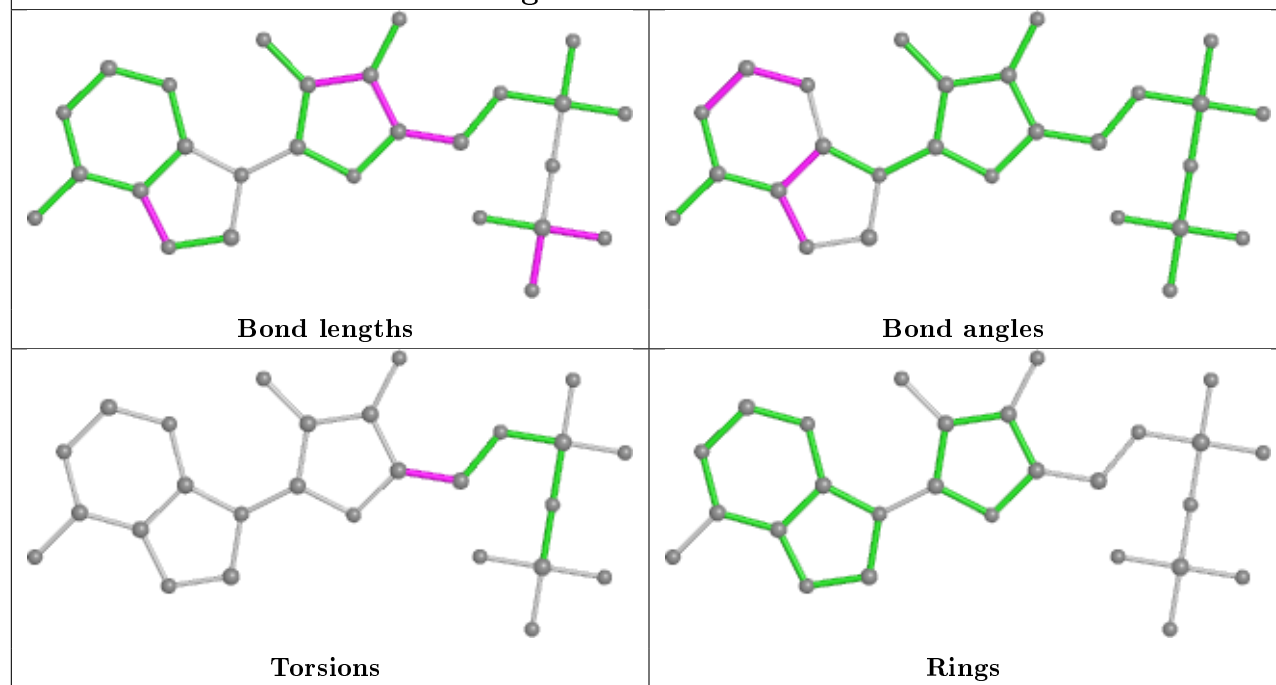
Ligand ADP E 4402

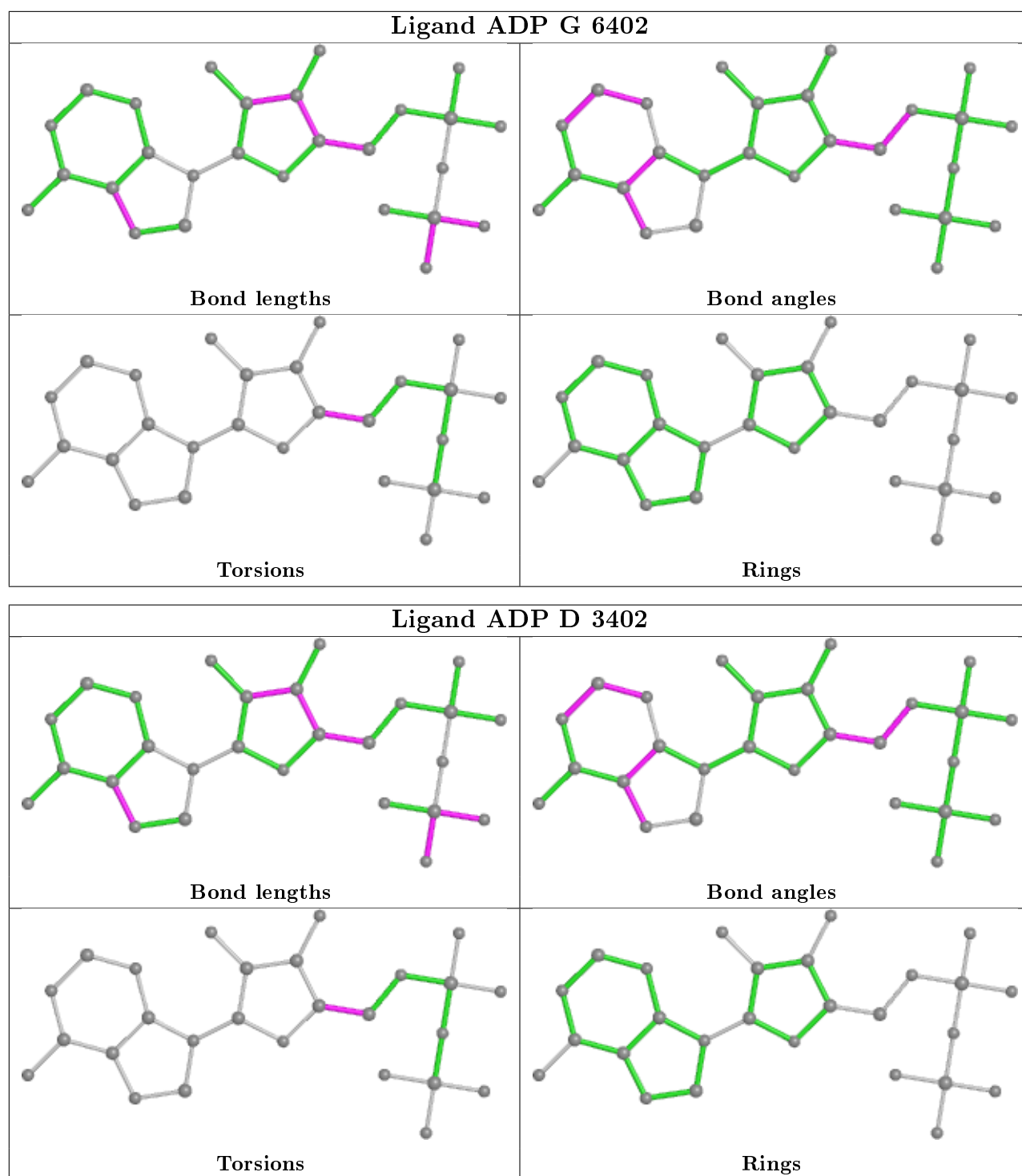


Ligand ADP F 5402



Ligand ADP C 2402





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	312/312 (100%)	-0.16	0 100 100	13, 35, 55, 69	0
1	B	312/312 (100%)	-0.22	1 (0%) 94 93	15, 32, 49, 66	0
1	C	312/312 (100%)	-0.19	3 (0%) 82 77	19, 36, 50, 65	0
1	D	312/312 (100%)	-0.13	7 (2%) 62 52	23, 40, 54, 65	0
1	E	312/312 (100%)	-0.26	0 100 100	9, 31, 47, 61	0
1	F	312/312 (100%)	-0.20	1 (0%) 94 93	7, 32, 49, 65	0
1	G	312/312 (100%)	-0.24	1 (0%) 94 93	20, 37, 53, 63	0
1	H	312/312 (100%)	-0.16	3 (0%) 82 77	24, 39, 52, 61	0
All	All	2496/2496 (100%)	-0.19	16 (0%) 89 86	7, 35, 52, 69	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	SER	4.5
1	C	209	ALA	4.3
1	H	310	THR	3.5
1	D	1	MET	3.1
1	D	309	ALA	2.9
1	G	122	GLY	2.6
1	B	122	GLY	2.5
1	C	122	GLY	2.5
1	F	119	GLN	2.5
1	H	279	GLY	2.3
1	D	197	ASP	2.2
1	D	278	SER	2.2
1	H	122	GLY	2.2
1	D	2	GLU	2.1
1	C	143	VAL	2.1
1	D	193	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

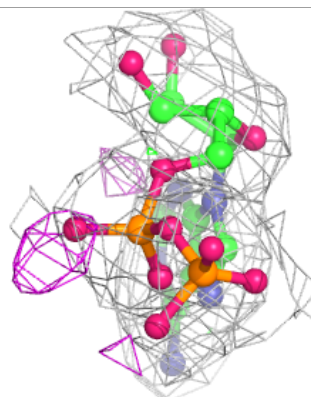
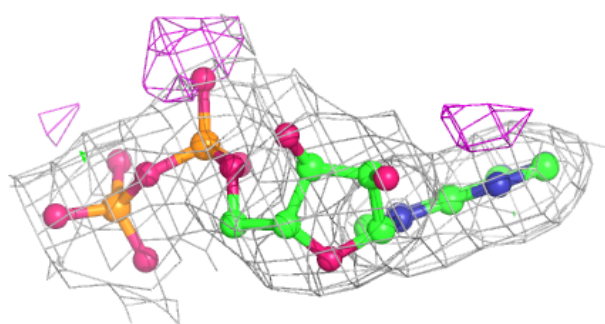
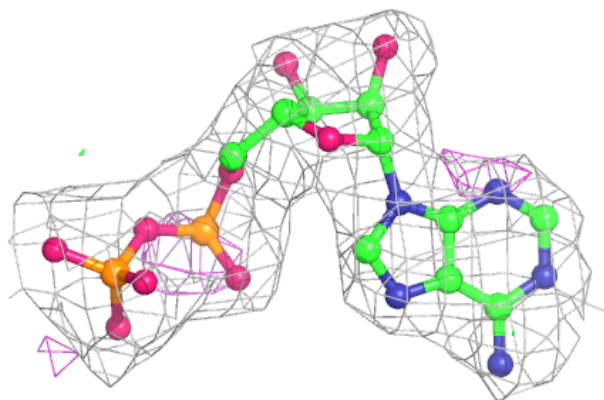
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	E	4403	1/1	0.94	0.14	59,59,59,59	0
3	PLP	D	3401	15/16	0.95	0.16	40,42,55,56	0
3	PLP	A	401	15/16	0.95	0.16	17,21,44,44	0
4	ADP	E	4402	27/27	0.96	0.18	17,27,32,35	0
4	ADP	D	3402	27/27	0.96	0.17	32,42,50,51	0
2	ZN	B	1403	1/1	0.96	0.17	54,54,54,54	0
3	PLP	C	2401	15/16	0.96	0.20	44,45,55,55	0
4	ADP	H	7402	27/27	0.96	0.15	41,43,53,54	0
2	ZN	G	6403	1/1	0.96	0.12	85,85,85,85	0
4	ADP	A	402	27/27	0.96	0.17	19,26,32,33	0
2	ZN	C	2403	1/1	0.97	0.10	49,49,49,49	0
2	ZN	H	7403	1/1	0.97	0.12	59,59,59,59	0
4	ADP	C	2402	27/27	0.97	0.16	30,33,37,39	0
3	PLP	H	7401	15/16	0.97	0.16	25,26,32,33	0
4	ADP	F	5402	27/27	0.97	0.16	26,31,36,37	0
2	ZN	D	3403	1/1	0.97	0.09	45,45,45,45	0
2	ZN	F	5403	1/1	0.97	0.15	52,52,52,52	0
3	PLP	B	1401	15/16	0.97	0.17	19,24,39,40	0
3	PLP	G	6401	15/16	0.97	0.17	29,32,41,42	0
2	ZN	A	403	1/1	0.97	0.14	48,48,48,48	0
3	PLP	F	5401	15/16	0.97	0.17	14,17,29,31	0
4	ADP	B	1402	27/27	0.98	0.17	17,25,32,32	0
3	PLP	E	4401	15/16	0.98	0.17	11,13,25,26	0
4	ADP	G	6402	27/27	0.98	0.15	30,34,38,39	0

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

orientation to approximate a three-dimensional view.

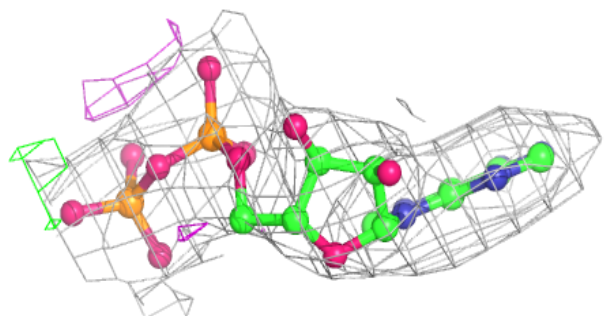
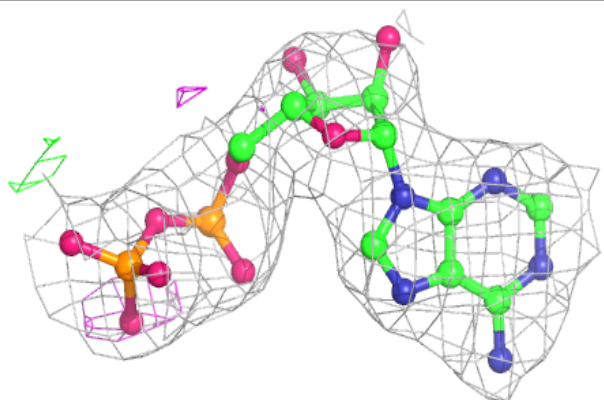
Electron density around ADP E 4402:

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



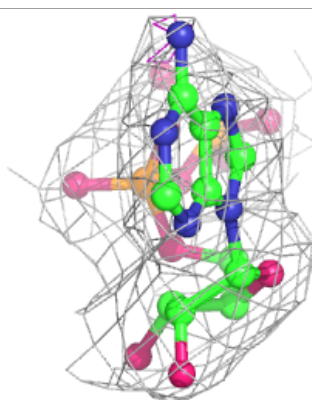
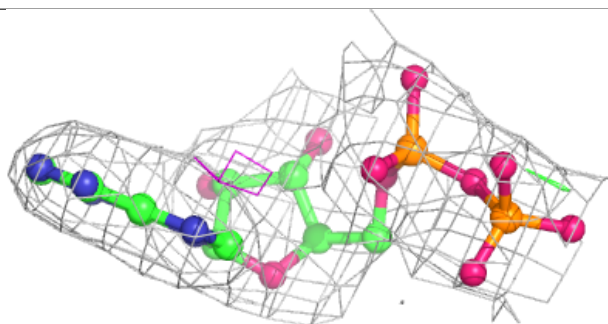
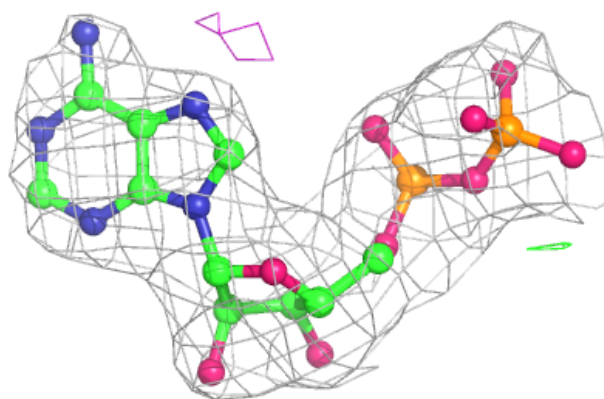
Electron density around ADP D 3402:

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

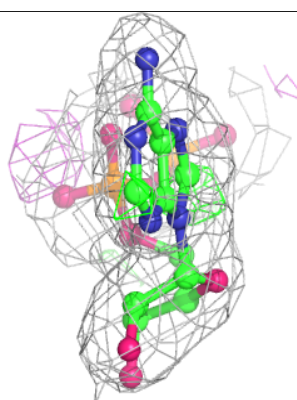
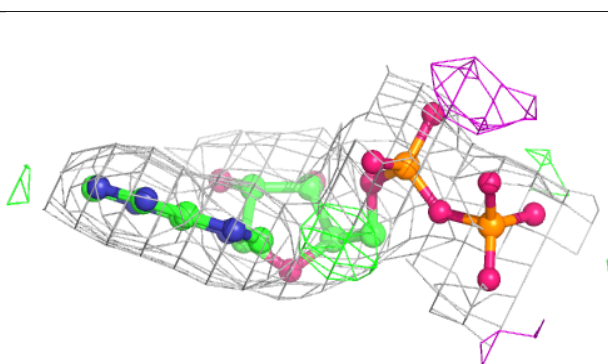
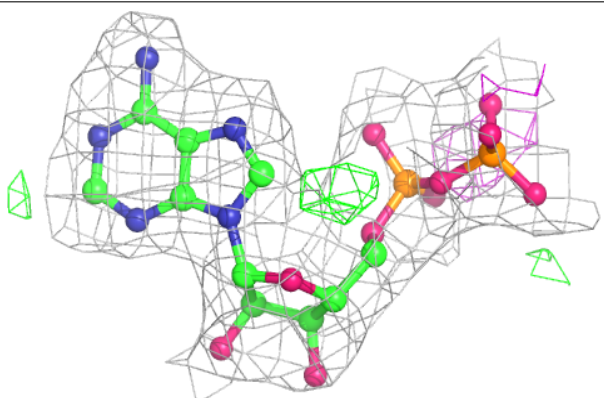


Electron density around ADP H 7402:

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

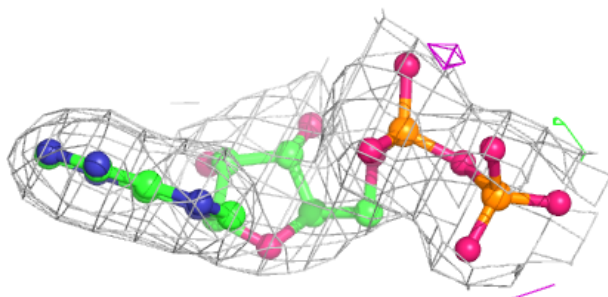
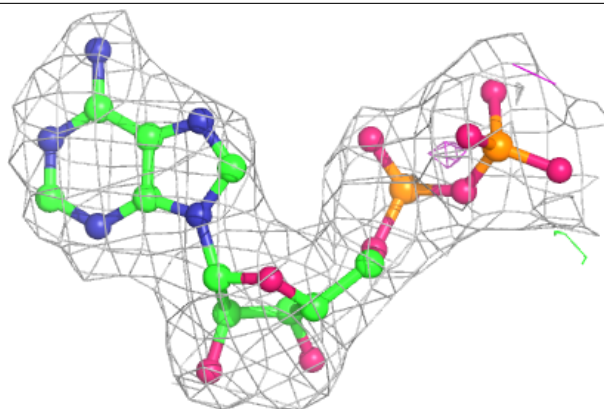
**Electron density around ADP A 402:**

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

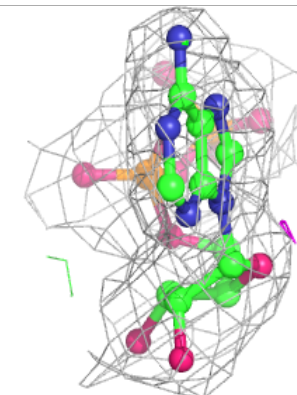
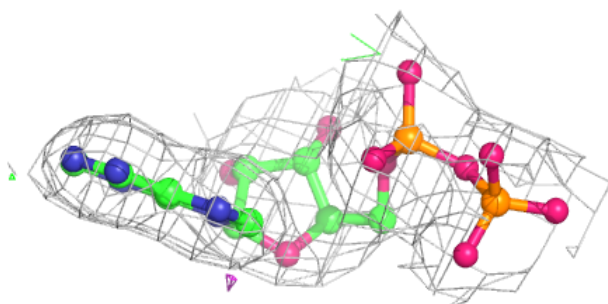
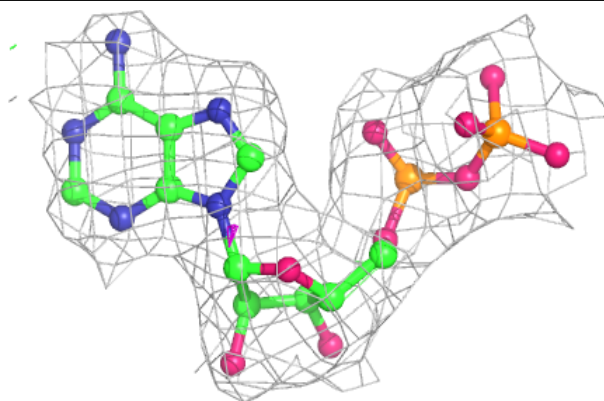


Electron density around ADP C 2402:

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

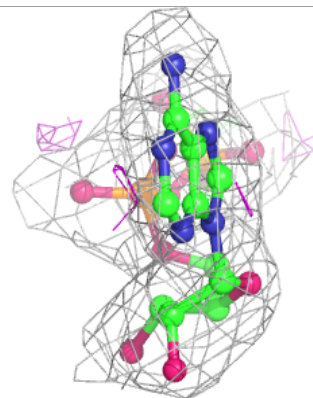
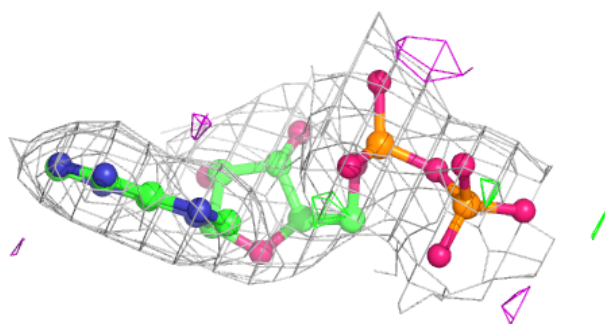
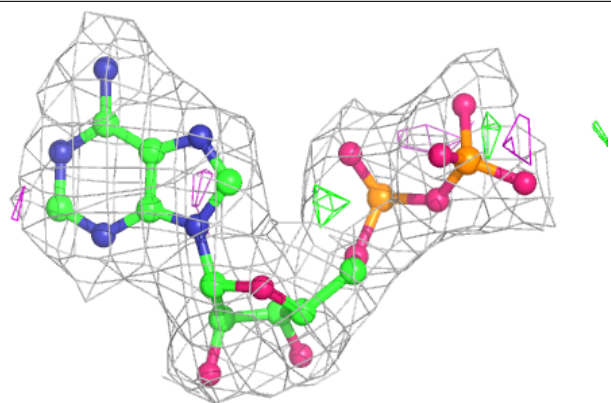
**Electron density around ADP F 5402:**

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

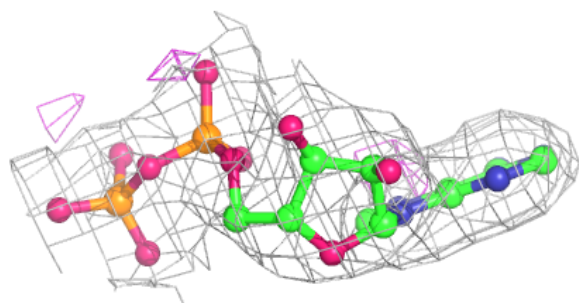
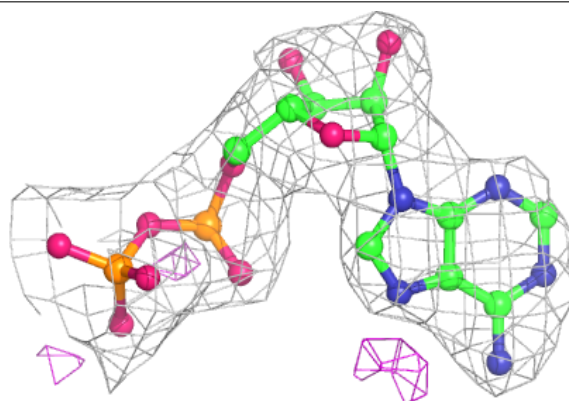


Electron density around ADP B 1402:

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

**Electron density around ADP G 6402:**

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



6.5 Other polymers

There are no such residues in this entry.