



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:25 PM BST

PDB ID : 4XYK  
Title : Crystal structure of human phosphofructokinase-1 in complex with ADP, Northeast Structural Genomics Consortium Target HR9275  
Authors : Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2015-02-02  
Resolution : 3.40 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

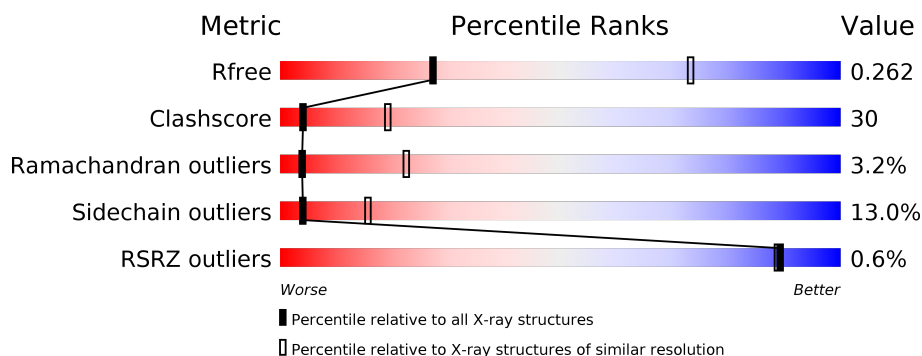
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	812	
1	B	812	
1	C	812	
1	D	812	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	803	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22897 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5640	3542	1000	1059	39			
1	B	749	Total	C	N	O	S	0	0	0
			5727	3595	1019	1074	39			
1	C	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			
1	D	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813

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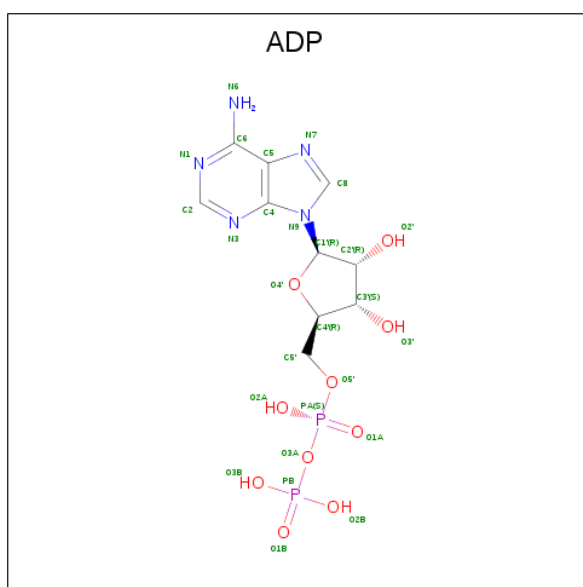
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813

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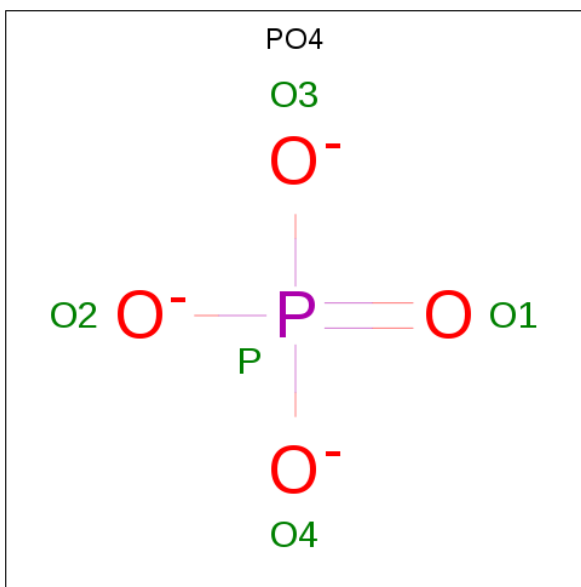
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



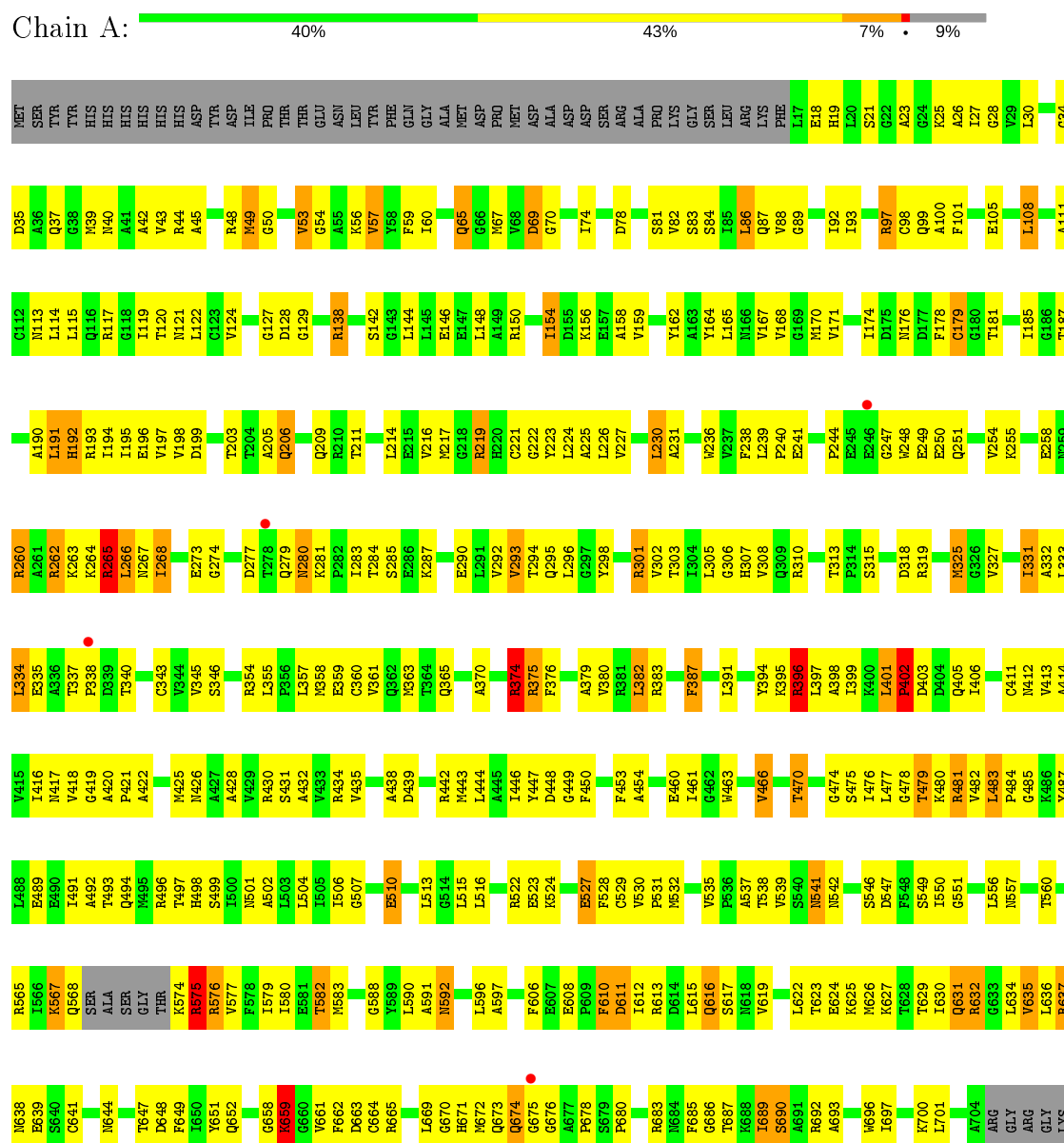
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

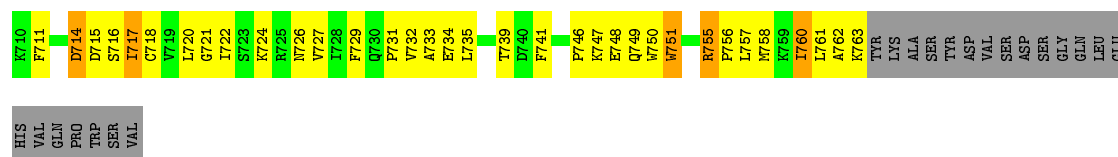


### 3 Residue-property plots

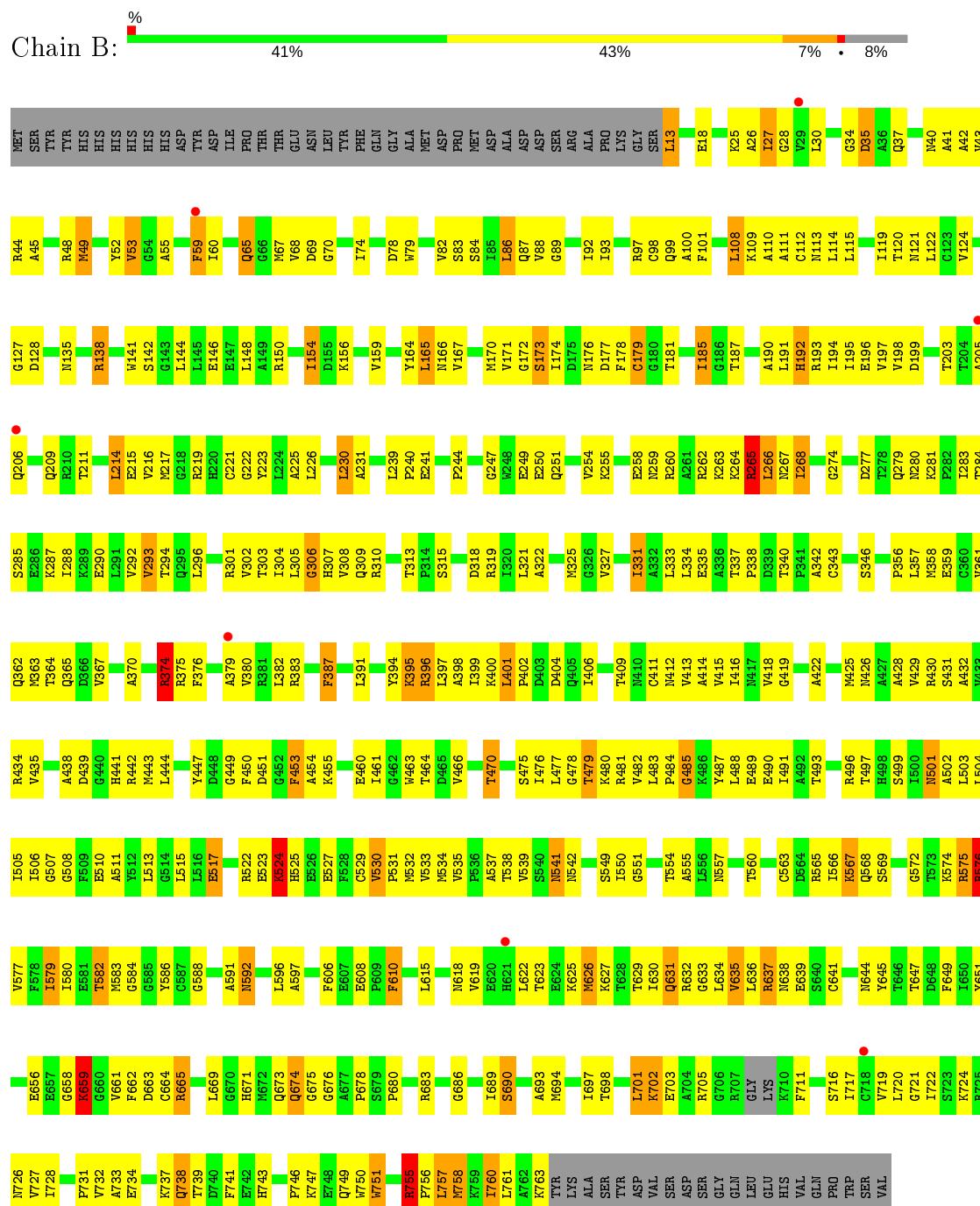
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type





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V732	R665	I580	L503	R430	L355	T278	I201	Q116
A733	I669	E581	L504	S431	M358	Q279	R202	R117
L734	T582	T582	I505	R434	E359	R280	T203	T120
L735	M583	M583	I506	V435	C360	K281	T204	A205
K736	M671	Y586	G507	D439	R363	P282	Q206	L122
Q738	Q673	C587	E510	R443	T364	T283	S207	C123
T739	Q674	G588	A511	R442	Q365	T284	R208	V124
D740	G675	Y512	Y512	M443	T386	S285	Q209	
H743	G676	A591	L515	L444	A370	K287	R210	D128
	A677	N592	L516	Y447	R374	E290	G129	S130
P746	P678	L596	E517	D443	R375	L291	L214	A138
K747	P680	A597	L518	F450	F376	V292	E215	S142
E748	R683	F606	S519	G449		T293	V216	G143
Q749	R684	A520	A521	F450	A379	T294	M217	L144
W750	N685	F610	A521	F453	V380	Q295	R219	L145
W751	G686		H525	A454	R381	L296	H220	L146
L752	L615		E526		L382	G297	C221	E147
R755	V619		E527	I458	R383	Y298	G222	E148
P756	V619		F528	K459	Q384	R301	Y223	L149
L757	E620		C529	E460	R385	V302	L224	R150
W758	H621		V530	I461	S386	T303	A225	
K759	L622		P531	G462	F387	L304	L226	
I760	T623		H532	W463	N390	L305	L230	I154
L761	E624		V533	T464	Y394	G306	L230	D155
A762	G625		M534	D465	R396	R307	A231	K156
K763	M626		V535	V466	K395	V308	W236	V159
T764	K627		A537	T470	R397	Q309	V237	Y162
L765	I630		T538		L397	R310	F238	A163
L766	Q631		V539	G474	A398	S315	L239	Y164
L767	R632		S540	I476	I399	D318	P240	L165
L768	G633		N541	L477	K400	R319	P244	M170
L769	L634		P544	G478	L401	I320	W243	V171
L770	V635		G545	T479	D403	K325	E249	T174
L771	R637		S546	K480	Q405	G326	E250	D175
L772	N638		D547	R481	I406	V327	Q251	N176
L773	E639		F548	V482	C411	I331	V254	D177
L774	S640		S549	L483	N412	A332	K255	F178
L775	C641		I550	P484	V413	L333	E258	C179
L776	N644		N557	Q485	A414	L334	T181	G180
L777	T647		T560	K486	Y487		T187	T181
L778	Q652		B565	E489	L488	T337	R260	
L779	Q652		I566	E490	I416	P338	A261	A190
L780	S655		K567	I491	V418	D339	R262	L191
L781	E656		Q568	A492	G419	T340	K263	H192
L782	E657		G572	M495	A420	C343	K264	R193
L783	G658		B575	R496	P421	V344	R265	L266
L784	K659		R576	T497	A422	V345	N267	I194
L785	G660		F577	H498	G424	S346	I268	I195
L786	V661		F578	S499	M425	H351	G274	E196
L787	F662		C664	N501	N426	R354	D277	V197
L788	D663			A502	V429			A200
L789	C664							

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.34Å 168.37Å 133.27Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	45.37 – 3.40 45.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	74.2 (45.37-3.40) 84.5 (45.37-3.40)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.256 , 0.290 0.250 , 0.262	Depositor DCC
$R_{free}$ test set	3943 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 14.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: PO4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.57	1/5730 (0.0%)	0.75	15/7735 (0.2%)
1	B	0.55	0/5819	0.85	18/7854 (0.2%)
1	C	0.54	1/5773 (0.0%)	0.81	16/7795 (0.2%)
1	D	0.53	0/5773	0.89	16/7795 (0.2%)
All	All	0.55	2/23095 (0.0%)	0.83	65/31179 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	664	CYS	CB-SG	-6.17	1.71	1.82
1	A	360	CYS	CB-SG	-5.68	1.72	1.81

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-22.12	109.24	120.30
1	D	374	ARG	NE-CZ-NH1	-21.17	109.71	120.30
1	D	374	ARG	NE-CZ-NH2	21.17	130.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	ARG	NE-CZ-NH1	-20.40	110.10	120.30
1	C	97	ARG	NE-CZ-NH1	19.91	130.25	120.30
1	D	375	ARG	NE-CZ-NH2	-17.76	111.42	120.30
1	B	575	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	B	665	ARG	NE-CZ-NH2	17.37	128.98	120.30
1	D	575	ARG	NE-CZ-NH1	16.50	128.55	120.30
1	D	375	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	B	576	ARG	NE-CZ-NH1	-16.29	112.16	120.30
1	D	150	ARG	NE-CZ-NH2	16.24	128.42	120.30
1	B	575	ARG	NE-CZ-NH2	-15.79	112.40	120.30
1	B	576	ARG	NE-CZ-NH2	15.54	128.07	120.30
1	D	575	ARG	NE-CZ-NH2	-14.22	113.19	120.30
1	C	575	ARG	NE-CZ-NH2	13.23	126.91	120.30
1	D	150	ARG	NE-CZ-NH1	-12.67	113.97	120.30
1	C	575	ARG	NE-CZ-NH1	-11.81	114.40	120.30
1	D	374	ARG	CD-NE-CZ	10.69	138.56	123.60
1	C	665	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	B	374	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	C	97	ARG	CD-NE-CZ	9.45	136.83	123.60
1	A	575	ARG	NE-CZ-NH2	8.97	124.78	120.30
1	B	665	ARG	CD-NE-CZ	8.62	135.67	123.60
1	A	665	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	D	665	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	C	375	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	D	665	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	575	ARG	CD-NE-CZ	8.00	134.79	123.60
1	C	374	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	374	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	150	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	D	150	ARG	CD-NE-CZ	7.87	134.62	123.60
1	D	375	ARG	CD-NE-CZ	7.82	134.55	123.60
1	A	576	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	D	575	ARG	CD-NE-CZ	7.67	134.34	123.60
1	C	375	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	C	665	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	375	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	C	575	ARG	CD-NE-CZ	7.25	133.75	123.60
1	A	575	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	575	ARG	CD-NE-CZ	7.18	133.66	123.60
1	C	374	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	375	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	B	375	ARG	NE-CZ-NH2	7.03	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	ARG	CD-NE-CZ	6.93	133.31	123.60
1	C	150	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	97	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	665	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	374	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	150	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	576	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	576	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	374	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	97	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	97	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	B	97	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	150	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	150	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	150	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	744	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	D	97	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	375	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	C	576	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	579	ILE	CG1-CB-CG2	-5.02	100.35	111.40

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	692	ARG	Sidechain
1	B	219	ARG	Sidechain
1	B	396	ARG	Sidechain
1	B	565	ARG	Sidechain
1	B	755	ARG	Sidechain
1	C	260	ARG	Sidechain
1	C	265	ARG	Sidechain
1	C	44	ARG	Sidechain
1	C	632	ARG	Sidechain
1	D	138	ARG	Sidechain
1	D	265	ARG	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	5640	0	5674	340	0
1	B	5727	0	5764	340	0
1	C	5681	0	5709	358	0
1	D	5681	0	5709	376	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	20	0	0	1	0
3	D	15	0	0	1	0
All	All	22897	0	22904	1376	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1376) 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:D:480:LYS:HB3	1:D:482:VAL:HG23	1.29	1.05
1:B:522:ARG:HH12	1:B:529:CYS:HA	1.25	1.00
1:D:532:MET:HB2	1:D:717:ILE:HG22	1.41	1.00
1:A:539:VAL:HG11	1:A:674:GLN:HB3	1.43	0.99
1:A:121:ASN:HB3	1:A:333:LEU:HD22	1.46	0.97
1:C:121:ASN:HB3	1:C:333:LEU:HD22	1.45	0.95
1:C:44:ARG:NH1	1:C:761:LEU:HD22	1.81	0.95
1:D:327:VAL:HG21	1:D:757:LEU:HD21	1.47	0.93
1:D:30:LEU:HD21	1:D:124:VAL:HG22	1.51	0.92
1:B:30:LEU:HD21	1:B:124:VAL:HG22	1.50	0.91
1:A:181:THR:HB	1:A:346:SER:HB2	1.53	0.91
1:B:588:GLY:HA2	1:B:638:ASN:HD22	1.36	0.90
1:A:284:THR:HG23	1:A:287:LYS:H	1.32	0.90
1:C:588:GLY:HA2	1:C:638:ASN:HD22	1.37	0.90
1:D:630:ILE:HD12	1:D:630:ILE:H	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:HB3	1:B:333:LEU:HD22	1.53	0.89
1:B:630:ILE:H	1:B:630:ILE:HD12	1.37	0.89
1:D:516:LEU:HD21	1:D:736:LYS:HE2	1.54	0.89
1:A:219:ARG:HG3	1:A:273:GLU:OE1	1.72	0.88
1:A:496:ARG:HB3	1:A:527:GLU:HG3	1.53	0.88
1:C:539:VAL:HG11	1:C:674:GLN:HB3	1.56	0.88
1:D:44:ARG:HH11	1:D:44:ARG:HG3	1.38	0.87
1:A:678:PRO:HG2	1:A:683:ARG:HD3	1.57	0.87
1:C:630:ILE:HD12	1:C:630:ILE:H	1.39	0.86
1:B:284:THR:HG23	1:B:287:LYS:H	1.37	0.86
1:D:181:THR:HB	1:D:346:SER:HB2	1.54	0.86
1:D:678:PRO:HG2	1:D:683:ARG:HD3	1.55	0.86
1:D:488:LEU:H	1:D:488:LEU:HD23	1.40	0.85
1:C:534:MET:HG2	1:C:719:VAL:HG22	1.56	0.85
1:B:522:ARG:NH1	1:B:529:CYS:HA	1.91	0.84
1:C:30:LEU:HD21	1:C:124:VAL:HG22	1.59	0.84
1:A:30:LEU:HD21	1:A:124:VAL:HG22	1.59	0.84
1:C:284:THR:HG23	1:C:287:LYS:H	1.40	0.84
1:B:262:ARG:HH22	1:B:400:LYS:HD3	1.42	0.84
1:C:181:THR:HB	1:C:346:SER:HB2	1.58	0.84
1:A:480:LYS:HB3	1:A:482:VAL:HG23	1.57	0.83
1:B:669:LEU:HB3	1:B:673:GLN:HE21	1.44	0.82
1:B:539:VAL:HG11	1:B:674:GLN:HB3	1.60	0.82
1:A:630:ILE:HD12	1:A:630:ILE:H	1.44	0.82
1:D:121:ASN:HB3	1:D:333:LEU:HD22	1.58	0.82
1:A:515:LEU:CD2	1:A:732:VAL:HG11	2.10	0.82
1:D:575:ARG:HD3	1:D:661:VAL:O	1.79	0.82
1:B:678:PRO:HG2	1:B:683:ARG:HD3	1.60	0.82
1:C:658:GLY:O	1:C:661:VAL:HG12	1.80	0.81
1:D:539:VAL:HG11	1:D:674:GLN:HB3	1.61	0.81
1:C:262:ARG:HH22	1:C:400:LYS:HD3	1.43	0.81
1:A:448:ASP:OD1	1:B:574:LYS:HG3	1.81	0.81
1:D:401:LEU:H	1:D:401:LEU:HD23	1.46	0.80
1:A:45:ALA:O	1:A:49:MET:HB2	1.82	0.80
1:B:26:ALA:HB3	1:B:119:ILE:HA	1.60	0.80
1:B:401:LEU:HD23	1:B:401:LEU:H	1.45	0.80
1:B:413:VAL:HG22	1:B:502:ALA:HB3	1.63	0.80
1:B:279:GLN:HG2	1:B:374:ARG:CZ	2.11	0.80
1:C:327:VAL:HG21	1:C:757:LEU:HD21	1.64	0.79
1:C:306:GLY:CA	1:D:303:THR:HG21	2.12	0.79
1:A:658:GLY:O	1:A:661:VAL:HG12	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ARG:NH1	1:C:529:CYS:HA	1.97	0.79
1:A:48:ARG:HH12	3:A:803:PO4:P	2.06	0.79
1:D:505:ILE:HG13	1:D:515:LEU:HD21	1.64	0.78
1:C:686:GLY:O	1:C:690:SER:HB2	1.84	0.78
1:D:284:THR:HG23	1:D:287:LYS:H	1.49	0.78
1:B:401:LEU:HD21	1:B:406:ILE:HD11	1.65	0.78
1:C:401:LEU:H	1:C:401:LEU:HD23	1.49	0.78
1:A:527:GLU:CD	1:A:527:GLU:H	1.87	0.77
1:D:503:LEU:HB3	1:D:532:MET:HG2	1.65	0.77
1:D:515:LEU:HA	1:D:518:LEU:HD12	1.65	0.77
1:B:259:ASN:HD22	1:B:267:ASN:HD21	1.33	0.77
1:A:40:ASN:OD1	1:A:92:ILE:HG23	1.85	0.76
1:B:327:VAL:HG21	1:B:757:LEU:HD21	1.68	0.76
1:B:181:THR:HB	1:B:346:SER:HB2	1.66	0.76
1:B:250:GLU:O	1:B:254:VAL:HG23	1.85	0.76
1:B:480:LYS:HB3	1:B:482:VAL:HG23	1.68	0.76
1:C:522:ARG:HE	1:C:717:ILE:HD11	1.51	0.76
1:D:630:ILE:HG22	1:D:632:ARG:HG2	1.68	0.76
1:B:70:GLY:HA3	1:B:113:ASN:ND2	2.00	0.75
1:D:266:LEU:HD22	1:D:267:ASN:N	2.02	0.75
1:D:658:GLY:O	1:D:661:VAL:HG12	1.85	0.75
1:C:412:ASN:OD1	1:C:442:ARG:HD3	1.86	0.75
1:D:262:ARG:HH22	1:D:400:LYS:HD3	1.52	0.75
1:A:515:LEU:HD22	1:A:732:VAL:HG11	1.69	0.75
1:C:413:VAL:HG22	1:C:502:ALA:HB3	1.67	0.74
1:B:606:PHE:HB2	1:B:641:CYS:HA	1.69	0.74
1:B:401:LEU:HD23	1:B:401:LEU:N	2.03	0.74
1:D:43:VAL:HG11	1:D:93:ILE:HD12	1.68	0.74
1:B:588:GLY:HA2	1:B:638:ASN:ND2	2.02	0.74
1:C:401:LEU:HD21	1:C:406:ILE:HD11	1.69	0.74
1:C:495:MET:SD	1:C:500:ILE:HD12	2.28	0.74
1:C:40:ASN:OD1	1:C:92:ILE:HG23	1.86	0.74
1:A:530:VAL:HB	1:A:531:PRO:HD2	1.70	0.73
1:C:501:ASN:O	1:C:530:VAL:HB	1.88	0.73
1:D:577:VAL:HG21	1:D:622:LEU:HD21	1.70	0.73
1:C:431:SER:HB2	1:C:687:THR:HG23	1.70	0.73
1:C:44:ARG:NH1	1:C:761:LEU:CD2	2.52	0.73
1:D:401:LEU:H	1:D:401:LEU:CD2	2.01	0.73
1:B:534:MET:HB3	1:B:719:VAL:HG12	1.71	0.73
1:D:731:PRO:HG2	1:D:734:GLU:HG2	1.68	0.73
1:B:142:SER:O	1:B:146:GLU:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:ASN:HA	1:D:549:SER:OG	1.89	0.73
1:B:401:LEU:CD2	1:B:401:LEU:H	2.02	0.73
1:C:731:PRO:HG2	1:C:734:GLU:HG2	1.68	0.73
1:D:720:LEU:HD23	1:D:721:GLY:N	2.03	0.73
1:A:83:SER:HA	3:A:803:PO4:O3	1.89	0.72
1:A:108:LEU:HG	1:A:144:LEU:HD22	1.69	0.72
1:C:588:GLY:HA2	1:C:638:ASN:ND2	2.05	0.72
1:A:577:VAL:HG21	1:A:622:LEU:HD21	1.70	0.72
1:C:171:VAL:HG11	1:C:181:THR:HG21	1.70	0.72
1:A:717:ILE:O	1:A:717:ILE:HG12	1.90	0.72
1:C:79:TRP:CZ2	1:C:763:LYS:HB2	2.25	0.72
1:C:515:LEU:HD11	1:C:534:MET:HB3	1.72	0.72
1:D:250:GLU:O	1:D:254:VAL:HG23	1.90	0.72
1:B:418:VAL:O	1:B:507:GLY:HA3	1.90	0.71
1:A:522:ARG:HH21	1:A:717:ILE:HG23	1.55	0.71
1:B:108:LEU:HG	1:B:144:LEU:HD22	1.71	0.71
1:C:250:GLU:O	1:C:254:VAL:HG23	1.90	0.71
1:D:320:ILE:HD11	1:D:597:ALA:HB2	1.70	0.71
1:D:412:ASN:OD1	1:D:442:ARG:HD3	1.90	0.71
1:D:84:SER:CB	1:D:632:ARG:HH22	2.03	0.71
1:C:301:ARG:CG	1:C:301:ARG:HH21	2.03	0.71
1:A:401:LEU:N	1:A:401:LEU:HD23	2.06	0.70
1:C:306:GLY:HA3	1:D:303:THR:HG21	1.72	0.70
1:B:503:LEU:HB3	1:B:532:MET:HG2	1.71	0.70
1:D:84:SER:HB2	1:D:632:ARG:HH22	1.55	0.70
1:B:43:VAL:HG11	1:B:93:ILE:HD12	1.71	0.70
1:C:401:LEU:N	1:C:401:LEU:HD23	2.05	0.70
1:A:191:LEU:HD22	1:A:680:PRO:HB3	1.73	0.70
1:C:401:LEU:CD2	1:C:401:LEU:H	2.04	0.70
1:B:583:MET:HG2	1:B:673:GLN:OE1	1.91	0.70
1:A:522:ARG:NH2	1:A:716:SER:HB2	2.06	0.70
1:B:731:PRO:HG2	1:B:734:GLU:HG2	1.72	0.70
1:D:40:ASN:OD1	1:D:92:ILE:HG23	1.91	0.70
1:A:700:LYS:O	1:A:711:PHE:HZ	1.75	0.70
1:B:86:LEU:HD21	1:B:597:ALA:O	1.92	0.70
1:C:505:ILE:HD12	1:C:515:LEU:HD21	1.74	0.70
1:A:401:LEU:H	1:A:401:LEU:CD2	2.06	0.69
1:B:84:SER:HB2	1:B:632:ARG:HH22	1.56	0.69
1:D:27:ILE:HG21	1:D:333:LEU:HD13	1.74	0.69
1:D:44:ARG:NH1	1:D:44:ARG:HG3	2.04	0.69
1:A:420:ALA:HB2	1:A:481:ARG:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:VAL:HG21	1:B:622:LEU:HD21	1.72	0.69
1:A:142:SER:O	1:A:146:GLU:HG2	1.93	0.69
1:D:45:ALA:O	1:D:49:MET:HB2	1.93	0.69
1:C:669:LEU:HB3	1:C:673:GLN:HE21	1.57	0.69
1:B:686:GLY:O	1:B:690:SER:HB2	1.91	0.69
1:C:108:LEU:HG	1:C:144:LEU:HD22	1.74	0.69
1:D:70:GLY:HA3	1:D:113:ASN:ND2	2.07	0.69
1:D:718:CYS:HB3	1:D:731:PRO:HA	1.75	0.69
1:C:306:GLY:HA2	1:D:303:THR:HG21	1.74	0.68
1:C:678:PRO:HG2	1:C:683:ARG:HD3	1.73	0.68
1:A:401:LEU:H	1:A:401:LEU:HD23	1.58	0.68
1:B:582:THR:HG21	1:B:591:ALA:HA	1.75	0.68
1:C:508:GLY:HA3	1:C:538:THR:HB	1.76	0.68
1:D:327:VAL:HG21	1:D:757:LEU:CD2	2.21	0.68
1:A:583:MET:HG2	1:A:673:GLN:OE1	1.93	0.68
1:B:515:LEU:HD12	1:B:732:VAL:HG11	1.75	0.68
1:B:532:MET:HB2	1:B:717:ILE:HG23	1.75	0.68
1:B:719:VAL:HG13	1:B:732:VAL:HG12	1.76	0.68
1:C:219:ARG:HH12	3:C:805:PO4:P	2.15	0.68
1:C:430:ARG:HD3	1:C:470:THR:HG23	1.73	0.68
1:C:623:THR:HG23	1:C:661:VAL:HG21	1.75	0.68
1:D:401:LEU:N	1:D:401:LEU:HD23	2.08	0.68
1:B:370:ALA:HB3	1:B:379:ALA:HB2	1.75	0.68
1:C:301:ARG:NH2	1:C:301:ARG:HG2	2.07	0.68
1:C:43:VAL:HG11	1:C:93:ILE:HD12	1.76	0.68
1:D:430:ARG:HD3	1:D:470:THR:HG23	1.76	0.67
1:B:428:ALA:HB1	1:B:506:ILE:HD13	1.77	0.67
1:A:756:PRO:O	1:A:760:ILE:HG23	1.94	0.67
1:B:756:PRO:O	1:B:760:ILE:HG23	1.94	0.67
1:C:483:LEU:CD1	1:C:484:PRO:HD2	2.24	0.67
1:A:731:PRO:HG2	1:A:734:GLU:HG2	1.75	0.67
1:B:532:MET:HB2	1:B:717:ILE:HG12	1.76	0.67
1:A:49:MET:O	1:A:53:VAL:HG22	1.95	0.67
1:D:370:ALA:HB3	1:D:379:ALA:HB2	1.77	0.66
1:A:250:GLU:O	1:A:254:VAL:HG23	1.96	0.66
1:A:430:ARG:HD3	1:A:470:THR:HG23	1.77	0.66
1:B:266:LEU:HD22	1:B:267:ASN:N	2.10	0.66
1:C:483:LEU:HD13	1:C:484:PRO:HD2	1.76	0.66
1:C:45:ALA:O	1:C:49:MET:HB2	1.95	0.66
1:A:294:THR:HG23	1:A:294:THR:O	1.96	0.66
1:A:669:LEU:HB3	1:A:673:GLN:HE21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:PHE:O	1:D:380:VAL:HG23	1.96	0.66
1:D:398:ALA:O	1:D:399:ILE:HD13	1.95	0.66
1:A:717:ILE:H	1:A:717:ILE:HD13	1.61	0.65
1:C:575:ARG:H	1:C:631:GLN:HB2	1.60	0.65
1:C:478:GLY:HA2	1:D:572:GLY:O	1.96	0.65
1:C:226:LEU:HB2	1:C:239:LEU:HD11	1.77	0.65
1:D:483:LEU:HD13	1:D:484:PRO:HD2	1.78	0.65
1:B:588:GLY:CA	1:B:638:ASN:HD22	2.09	0.65
1:D:702:LYS:HA	1:D:705:ARG:HB2	1.77	0.65
1:A:418:VAL:O	1:A:507:GLY:HA3	1.96	0.65
1:C:280:ASN:H	1:C:374:ARG:HH21	1.43	0.65
1:D:515:LEU:HD11	1:D:534:MET:HB2	1.77	0.65
1:A:515:LEU:HD21	1:A:732:VAL:HG11	1.78	0.65
1:B:401:LEU:HG	1:B:406:ILE:HG12	1.78	0.65
1:D:583:MET:HG2	1:D:673:GLN:OE1	1.96	0.65
1:A:678:PRO:HG2	1:A:683:ARG:CD	2.27	0.65
1:A:358:MET:HG3	1:A:359:GLU:H	1.63	0.64
1:B:416:ILE:HD11	1:B:449:GLY:C	2.18	0.64
1:B:483:LEU:HD22	1:B:513:LEU:HD22	1.80	0.64
1:A:70:GLY:HA3	1:A:113:ASN:ND2	2.12	0.64
1:C:693:ALA:HB2	1:C:720:LEU:HD23	1.79	0.64
1:D:16:PHE:N	1:D:16:PHE:CD2	2.64	0.64
1:D:534:MET:HB3	1:D:719:VAL:HG12	1.80	0.64
1:D:108:LEU:HG	1:D:144:LEU:HD22	1.78	0.64
1:A:419:GLY:HA2	1:A:510:GLU:HG3	1.79	0.64
1:D:512:TYR:HA	1:D:534:MET:CE	2.28	0.64
1:C:70:GLY:HA3	1:C:113:ASN:ND2	2.13	0.64
1:D:669:LEU:HB3	1:D:673:GLN:HE21	1.63	0.64
1:C:457:GLN:HA	1:C:457:GLN:NE2	2.12	0.64
1:D:412:ASN:ND2	1:D:499:SER:HB2	2.12	0.64
1:D:532:MET:O	1:D:717:ILE:HA	1.98	0.64
1:A:43:VAL:HG11	1:A:93:ILE:HD12	1.79	0.63
1:A:588:GLY:HA2	1:A:638:ASN:OD1	1.98	0.63
1:B:230:LEU:HG	1:B:394:TYR:HB2	1.79	0.63
1:B:527:GLU:H	1:B:527:GLU:CD	2.01	0.63
1:B:630:ILE:HG22	1:B:632:ARG:HG2	1.80	0.63
1:D:306:GLY:C	1:D:308:VAL:H	2.01	0.63
1:B:49:MET:HG3	1:B:327:VAL:HG13	1.80	0.63
1:D:719:VAL:HG13	1:D:732:VAL:HG12	1.79	0.63
1:B:623:THR:HG23	1:B:661:VAL:HG21	1.80	0.63
1:B:192:HIS:CE1	1:B:680:PRO:HD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:PRO:HG2	1:C:749:GLN:HG2	1.81	0.63
1:D:419:GLY:HA2	1:D:510:GLU:HG3	1.81	0.63
1:C:266:LEU:HD22	1:C:267:ASN:N	2.13	0.63
1:D:262:ARG:O	1:D:263:LYS:HB2	1.98	0.63
1:D:697:ILE:O	1:D:701:LEU:HB2	1.99	0.63
1:D:280:ASN:H	1:D:374:ARG:NH2	1.97	0.63
1:A:171:VAL:HG11	1:A:181:THR:HG21	1.80	0.63
1:B:575:ARG:H	1:B:631:GLN:HB2	1.64	0.63
1:D:320:ILE:CD1	1:D:597:ALA:HB2	2.28	0.63
1:D:507:GLY:O	1:D:537:ALA:N	2.31	0.63
1:C:416:ILE:HD11	1:C:449:GLY:C	2.19	0.62
1:A:306:GLY:C	1:A:308:VAL:H	2.02	0.62
1:A:398:ALA:O	1:A:399:ILE:HD13	1.98	0.62
1:A:280:ASN:H	1:A:374:ARG:HH21	1.45	0.62
1:D:226:LEU:HB2	1:D:239:LEU:HD11	1.81	0.62
1:C:303:THR:HG21	1:D:306:GLY:CA	2.29	0.62
1:D:280:ASN:H	1:D:374:ARG:HH21	1.47	0.62
1:A:612:ILE:HG21	1:C:616:GLN:NE2	2.15	0.62
1:B:40:ASN:OD1	1:B:92:ILE:HG23	1.99	0.62
1:C:49:MET:HG3	1:C:327:VAL:HG13	1.79	0.62
1:D:203:THR:HA	1:D:206:GLN:HG2	1.82	0.62
1:D:722:ILE:HD13	1:D:727:VAL:HG12	1.80	0.62
1:D:678:PRO:HG2	1:D:683:ARG:CD	2.28	0.62
1:B:358:MET:HG3	1:B:359:GLU:H	1.62	0.62
1:B:541:ASN:HA	1:B:549:SER:OG	2.00	0.62
1:D:454:ALA:HB1	1:D:490:GLU:HB2	1.81	0.62
1:D:512:TYR:HE1	1:D:516:LEU:HD12	1.64	0.62
1:D:27:ILE:HD13	1:D:57:VAL:HG12	1.82	0.62
1:B:18:GLU:HB2	1:B:52:TYR:OH	1.98	0.62
1:B:480:LYS:HB3	1:B:482:VAL:CG2	2.30	0.62
1:B:505:ILE:HD12	1:B:515:LEU:HD21	1.81	0.62
1:D:171:VAL:HG11	1:D:181:THR:HG21	1.80	0.62
1:A:567:LYS:HG2	1:A:632:ARG:HD3	1.82	0.61
1:A:648:ASP:O	1:A:652:GLN:HG3	2.00	0.61
1:B:84:SER:CB	1:B:632:ARG:HH22	2.12	0.61
1:C:546:SER:HA	1:C:722:ILE:O	2.00	0.61
1:D:702:LYS:HD2	1:D:705:ARG:CB	2.31	0.61
1:D:148:LEU:HB3	1:D:154:ILE:HG23	1.81	0.61
1:A:422:ALA:O	1:A:425:MET:HB2	2.00	0.61
1:C:749:GLN:OE1	1:C:751:TRP:CZ2	2.54	0.61
1:D:337:THR:OG1	1:D:340:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:MET:SD	1:D:760:ILE:HD11	2.41	0.61
1:B:79:TRP:NE1	1:B:763:LYS:HB2	2.16	0.61
1:D:120:THR:HG23	1:D:121:ASN:ND2	2.15	0.61
1:B:409:THR:HB	1:B:705:ARG:HH22	1.65	0.61
1:B:658:GLY:O	1:B:661:VAL:HG12	2.00	0.61
1:D:49:MET:HG3	1:D:327:VAL:HG13	1.80	0.61
1:A:292:VAL:O	1:A:296:LEU:HB2	2.01	0.61
1:A:416:ILE:HD11	1:A:449:GLY:C	2.21	0.61
1:D:538:THR:HG23	1:D:541:ASN:H	1.66	0.61
1:D:458:ILE:HD12	1:D:498:HIS:CD2	2.36	0.61
1:B:259:ASN:HD22	1:B:267:ASN:ND2	1.99	0.60
1:B:171:VAL:HG11	1:B:181:THR:HG21	1.82	0.60
1:C:292:VAL:O	1:C:296:LEU:HB2	2.01	0.60
1:A:454:ALA:HB2	1:A:491:ILE:HD12	1.82	0.60
1:B:428:ALA:CB	1:B:506:ILE:HD13	2.32	0.60
1:C:301:ARG:NH2	1:C:301:ARG:CG	2.62	0.60
1:C:65:GLN:HG2	1:C:98:CYS:HB2	1.84	0.60
1:B:13:LEU:N	1:B:13:LEU:HD23	2.17	0.60
1:C:514:GLY:O	1:C:518:LEU:HD23	2.01	0.60
1:C:148:LEU:HB3	1:C:154:ILE:HG23	1.83	0.60
1:C:32:SER:HB3	1:C:130:SER:OG	2.02	0.60
1:A:575:ARG:H	1:A:631:GLN:HB2	1.67	0.60
1:A:714:ASP:OD2	1:A:733:ALA:HB2	2.02	0.60
1:D:567:LYS:HG2	1:D:632:ARG:HD3	1.84	0.60
1:B:70:GLY:HA3	1:B:113:ASN:HD22	1.67	0.60
1:C:418:VAL:O	1:C:507:GLY:HA3	2.01	0.60
1:C:762:ALA:O	1:C:763:LYS:HB3	2.02	0.60
1:B:179:CYS:SG	1:B:363:MET:HB2	2.42	0.59
1:C:230:LEU:HG	1:C:394:TYR:HB2	1.84	0.59
1:D:746:PRO:HG2	1:D:749:GLN:HG2	1.84	0.59
1:A:596:LEU:HB2	1:A:758:MET:HG3	1.83	0.59
1:B:415:VAL:HG12	1:B:504:LEU:HD23	1.83	0.59
1:C:171:VAL:HG11	1:C:181:THR:CG2	2.31	0.59
1:D:720:LEU:HD12	1:D:729:PHE:CE2	2.37	0.59
1:C:541:ASN:HA	1:C:549:SER:OG	2.02	0.59
1:D:221:CYS:HA	1:D:383:ARG:NH2	2.17	0.59
1:D:503:LEU:HD21	1:D:505:ILE:HD11	1.83	0.59
1:A:535:VAL:HG13	1:A:689:ILE:HD11	1.83	0.59
1:B:493:THR:O	1:B:497:THR:HG23	2.02	0.59
1:B:79:TRP:CZ2	1:B:763:LYS:HA	2.36	0.59
1:C:361:VAL:HG12	1:C:365:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ALA:O	1:D:194:ILE:HG13	2.01	0.59
1:B:244:PRO:HD2	1:B:277:ASP:HA	1.84	0.59
1:B:398:ALA:O	1:B:399:ILE:HD13	2.02	0.59
1:C:25:LYS:CE	1:C:120:THR:HG21	2.33	0.59
1:C:398:ALA:O	1:C:399:ILE:HD13	2.02	0.59
1:D:418:VAL:O	1:D:507:GLY:HA3	2.02	0.59
1:A:226:LEU:HB2	1:A:239:LEU:HD11	1.85	0.59
1:A:582:THR:HG21	1:A:591:ALA:HA	1.84	0.59
1:B:45:ALA:O	1:B:49:MET:HB2	2.02	0.59
1:B:430:ARG:HD3	1:B:470:THR:HG23	1.84	0.59
1:C:606:PHE:HB2	1:C:641:CYS:HA	1.85	0.59
1:D:512:TYR:CE1	1:D:516:LEU:HD12	2.37	0.59
1:A:205:ALA:CB	1:A:266:LEU:HD23	2.33	0.59
1:B:266:LEU:HD11	1:B:268:ILE:HD11	1.84	0.59
1:D:290:GLU:O	1:D:294:THR:HG22	2.02	0.59
1:D:422:ALA:O	1:D:425:MET:HB2	2.01	0.59
1:A:205:ALA:HB3	1:A:266:LEU:HD23	1.85	0.59
1:C:473:GLY:CA	1:C:678:PRO:HD3	2.32	0.59
1:A:644:ASN:HD22	1:C:656:GLU:HB2	1.68	0.59
1:B:251:GLN:O	1:B:254:VAL:HB	2.03	0.58
1:C:579:ILE:N	1:C:579:ILE:HD12	2.18	0.58
1:D:358:MET:HG3	1:D:359:GLU:H	1.67	0.58
1:D:634:LEU:HD11	1:D:636:LEU:HD21	1.85	0.58
1:D:702:LYS:HD2	1:D:705:ARG:HB3	1.85	0.58
1:C:756:PRO:O	1:C:760:ILE:HG23	2.03	0.58
1:D:216:VAL:HG21	1:D:225:ALA:HA	1.85	0.58
1:D:487:TYR:N	1:D:487:TYR:HD2	2.01	0.58
1:D:579:ILE:HD12	1:D:579:ILE:N	2.18	0.58
1:A:203:THR:HA	1:A:206:GLN:HG2	1.84	0.58
1:C:221:CYS:HA	1:C:383:ARG:NH2	2.17	0.58
1:C:676:GLY:HA2	1:D:565:ARG:HG2	1.85	0.58
1:A:592:ASN:C	1:A:592:ASN:HD22	2.07	0.58
1:B:426:ASN:OD1	1:B:476:ILE:HG13	2.04	0.58
1:C:195:ILE:HD11	1:C:231:ALA:HB3	1.86	0.58
1:C:370:ALA:HB3	1:C:379:ALA:HB2	1.86	0.58
1:B:434:ARG:HG2	1:B:463:TRP:CD2	2.38	0.58
1:B:83:SER:O	1:B:84:SER:HB3	2.04	0.58
1:C:290:GLU:O	1:C:294:THR:HG22	2.04	0.58
1:A:426:ASN:OD1	1:A:476:ILE:HG13	2.04	0.58
1:B:148:LEU:HB3	1:B:154:ILE:HG23	1.84	0.58
1:D:217:MET:HG3	1:D:309:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:THR:HG23	1:D:661:VAL:HG21	1.85	0.58
1:D:658:GLY:O	1:D:659:LYS:C	2.41	0.58
1:C:542:ASN:O	1:C:746:PRO:HD3	2.04	0.58
1:A:477:LEU:HD12	1:A:477:LEU:H	1.67	0.57
1:B:634:LEU:HD11	1:B:636:LEU:HD21	1.86	0.57
1:A:401:LEU:CD2	1:A:401:LEU:N	2.66	0.57
1:B:190:ALA:O	1:B:194:ILE:HG13	2.04	0.57
1:B:195:ILE:HD11	1:B:231:ALA:HB3	1.86	0.57
1:C:176:ASN:C	1:C:178:PHE:H	2.08	0.57
1:A:649:PHE:CD1	1:C:649:PHE:CE1	2.93	0.57
1:D:762:ALA:O	1:D:763:LYS:HB2	2.04	0.57
1:A:630:ILE:HG22	1:A:632:ARG:HG2	1.87	0.57
1:B:630:ILE:H	1:B:630:ILE:CD1	2.14	0.57
1:D:401:LEU:HD21	1:D:406:ILE:HD11	1.86	0.57
1:B:30:LEU:H	1:B:30:LEU:HD23	1.70	0.57
1:B:337:THR:OG1	1:B:340:THR:HB	2.05	0.57
1:D:431:SER:HB2	1:D:687:THR:HG23	1.86	0.57
1:A:425:MET:HE1	1:A:475:SER:HB2	1.85	0.57
1:D:487:TYR:N	1:D:487:TYR:CD2	2.72	0.57
1:D:735:LEU:O	1:D:739:THR:HG22	2.05	0.57
1:B:327:VAL:HG21	1:B:757:LEU:CD2	2.35	0.57
1:C:25:LYS:HE2	1:C:120:THR:HG21	1.87	0.57
1:C:637:ARG:HE	1:C:647:THR:N	2.03	0.57
1:D:719:VAL:HG23	1:D:719:VAL:O	2.04	0.57
1:C:315:SER:O	1:C:319:ARG:HG3	2.05	0.57
1:C:583:MET:HG2	1:C:673:GLN:OE1	2.05	0.57
1:C:676:GLY:HA3	1:D:565:ARG:CD	2.34	0.57
1:C:483:LEU:HD12	1:C:517:GLU:OE1	2.05	0.56
1:B:358:MET:HG3	1:B:359:GLU:N	2.19	0.56
1:B:669:LEU:CB	1:B:673:GLN:HE21	2.15	0.56
1:D:592:ASN:HD22	1:D:592:ASN:C	2.08	0.56
1:D:756:PRO:O	1:D:760:ILE:HG23	2.04	0.56
1:A:402:PRO:HG2	1:A:405:GLN:HG3	1.88	0.56
1:A:479:THR:HG23	1:A:479:THR:O	2.05	0.56
1:A:539:VAL:HG11	1:A:674:GLN:CB	2.29	0.56
1:B:292:VAL:O	1:B:296:LEU:HB2	2.05	0.56
1:B:508:GLY:CA	1:B:538:THR:HB	2.35	0.56
1:A:612:ILE:HG21	1:C:616:GLN:HE22	1.69	0.56
1:C:608:GLU:OE1	1:C:755:ARG:HG2	2.05	0.56
1:B:484:PRO:HG2	1:B:517:GLU:HB3	1.87	0.56
1:B:525:HIS:HB3	1:B:527:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:PRO:HG2	1:B:683:ARG:CD	2.33	0.56
1:C:285:SER:HB3	1:C:302:VAL:HG21	1.87	0.56
1:D:92:ILE:HG13	1:D:93:ILE:N	2.19	0.56
1:A:181:THR:CB	1:A:346:SER:HB2	2.33	0.56
1:A:49:MET:HG3	1:A:327:VAL:HG13	1.86	0.56
1:C:419:GLY:HA2	1:C:510:GLU:HG3	1.86	0.56
1:A:606:PHE:HB2	1:A:641:CYS:HA	1.87	0.56
1:C:262:ARG:NH2	1:C:400:LYS:HD3	2.19	0.56
1:D:84:SER:HB2	1:D:632:ARG:NH2	2.21	0.56
1:A:575:ARG:HG2	1:A:661:VAL:O	2.05	0.56
1:C:156:LYS:O	1:C:159:VAL:HG12	2.06	0.56
1:D:577:VAL:HG21	1:D:622:LEU:CD2	2.36	0.56
1:A:401:LEU:HD21	1:A:406:ILE:HD11	1.88	0.56
1:A:686:GLY:O	1:A:690:SER:HB2	2.06	0.56
1:B:701:LEU:O	1:B:705:ARG:HG3	2.06	0.56
1:B:531:PRO:HA	1:B:716:SER:O	2.06	0.56
1:A:454:ALA:HB2	1:A:491:ILE:CD1	2.36	0.56
1:B:477:LEU:HD12	1:B:477:LEU:H	1.70	0.56
1:C:35:ASP:OD2	1:D:204:THR:HA	2.06	0.56
1:D:390:ASN:OD1	1:D:688:LYS:HE2	2.05	0.56
1:A:236:TRP:HZ3	1:A:399:ILE:HD11	1.71	0.55
1:C:337:THR:OG1	1:C:340:THR:HB	2.05	0.55
1:C:487:TYR:O	1:C:491:ILE:HG13	2.06	0.55
1:C:720:LEU:HD22	1:C:729:PHE:CE2	2.41	0.55
1:C:303:THR:HG21	1:D:306:GLY:HA3	1.87	0.55
1:C:579:ILE:HG13	1:C:635:VAL:CG1	2.37	0.55
1:C:534:MET:CG	1:C:719:VAL:HG22	2.33	0.55
1:A:416:ILE:HG13	1:A:446:ILE:HB	1.87	0.55
1:B:577:VAL:HG21	1:B:622:LEU:CD2	2.36	0.55
1:A:370:ALA:HB3	1:A:379:ALA:HB2	1.88	0.55
1:A:397:LEU:HD21	1:A:430:ARG:NH2	2.22	0.55
1:C:397:LEU:HD11	1:C:431:SER:HA	1.88	0.55
1:A:450:PHE:CE1	1:A:484:PRO:HD3	2.42	0.55
1:D:83:SER:O	1:D:84:SER:HB3	2.07	0.55
1:B:78:ASP:N	1:B:78:ASP:OD2	2.34	0.55
1:D:292:VAL:O	1:D:296:LEU:HB2	2.06	0.55
1:D:567:LYS:HD3	1:D:632:ARG:NH1	2.21	0.55
1:D:606:PHE:HB2	1:D:641:CYS:HA	1.89	0.55
1:A:195:ILE:HD11	1:A:231:ALA:HB3	1.89	0.55
1:C:634:LEU:HD11	1:C:636:LEU:HD21	1.87	0.55
1:A:176:ASN:C	1:A:178:PHE:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLY:HA2	1:B:572:GLY:O	2.05	0.55
1:C:579:ILE:HG13	1:C:635:VAL:HG13	1.88	0.55
1:C:680:PRO:HA	1:C:683:ARG:HG3	1.89	0.55
1:D:305:LEU:H	1:D:305:LEU:HD12	1.72	0.55
1:D:722:ILE:HD13	1:D:727:VAL:CG1	2.36	0.55
1:B:192:HIS:O	1:B:196:GLU:HG3	2.06	0.55
1:B:221:CYS:HA	1:B:383:ARG:NH2	2.22	0.55
1:A:148:LEU:HB3	1:A:154:ILE:HD12	1.89	0.55
1:A:461:ILE:HD12	1:A:461:ILE:O	2.07	0.55
1:C:25:LYS:CD	1:C:120:THR:HG21	2.37	0.55
1:C:505:ILE:HG21	1:C:511:ALA:HB1	1.88	0.55
1:C:320:ILE:HD11	1:C:597:ALA:HB2	1.88	0.55
1:C:675:GLY:O	1:D:568:GLN:HG2	2.07	0.55
1:D:637:ARG:HE	1:D:647:THR:N	2.05	0.55
1:A:658:GLY:O	1:A:659:LYS:C	2.45	0.54
1:C:301:ARG:HG2	1:C:301:ARG:HH21	1.67	0.54
1:A:358:MET:HG3	1:A:359:GLU:N	2.22	0.54
1:A:506:ILE:HD13	1:A:535:VAL:HB	1.88	0.54
1:A:649:PHE:CE1	1:C:649:PHE:CE1	2.95	0.54
1:B:401:LEU:N	1:B:401:LEU:CD2	2.68	0.54
1:B:397:LEU:HD11	1:B:431:SER:HA	1.89	0.54
1:A:634:LEU:HD11	1:A:636:LEU:HD21	1.90	0.54
1:A:669:LEU:HB3	1:A:673:GLN:NE2	2.22	0.54
1:B:205:ALA:CB	1:B:266:LEU:HD23	2.37	0.54
1:B:37:GLN:NE2	1:B:310:ARG:C	2.61	0.54
1:B:461:ILE:HD12	1:B:461:ILE:O	2.08	0.54
1:C:240:PRO:HG3	1:C:274:GLY:O	2.08	0.54
1:B:177:ASP:O	1:B:364:THR:HG23	2.06	0.54
1:C:327:VAL:HG21	1:C:757:LEU:CD2	2.37	0.54
1:C:630:ILE:HG22	1:C:632:ARG:HG2	1.90	0.54
1:D:156:LYS:O	1:D:159:VAL:HG12	2.08	0.54
1:D:582:THR:HG21	1:D:591:ALA:HA	1.90	0.54
1:B:262:ARG:O	1:B:263:LYS:HB2	2.07	0.54
1:D:588:GLY:HA2	1:D:638:ASN:HD22	1.71	0.54
1:A:541:ASN:HA	1:A:549:SER:OG	2.08	0.54
1:C:303:THR:HG21	1:D:306:GLY:HA2	1.89	0.54
1:D:434:ARG:HG2	1:D:463:TRP:CD2	2.43	0.54
1:D:661:VAL:HG13	1:D:662:PHE:CD2	2.43	0.54
1:A:315:SER:O	1:A:319:ARG:HG3	2.08	0.54
1:A:680:PRO:HA	1:A:683:ARG:HG3	1.88	0.54
1:C:114:LEU:HD22	1:C:119:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:PHE:O	1:C:380:VAL:HG23	2.07	0.54
1:D:236:TRP:CZ3	1:D:399:ILE:HD11	2.43	0.54
1:B:669:LEU:HB3	1:B:673:GLN:NE2	2.18	0.54
1:C:120:THR:HG23	1:C:121:ASN:ND2	2.23	0.54
1:C:658:GLY:O	1:C:659:LYS:C	2.45	0.54
1:D:370:ALA:CB	1:D:379:ALA:HB2	2.37	0.54
1:A:576:ARG:HA	1:A:663:ASP:O	2.08	0.53
1:A:746:PRO:HG2	1:A:749:GLN:HG2	1.90	0.53
1:B:266:LEU:CD1	1:B:268:ILE:HD11	2.38	0.53
1:B:479:THR:HG23	1:B:479:THR:O	2.08	0.53
1:C:560:THR:HG22	1:C:597:ALA:HB3	1.90	0.53
1:D:480:LYS:C	1:D:482:VAL:H	2.11	0.53
1:A:221:CYS:HA	1:A:383:ARG:NH2	2.24	0.53
1:C:567:LYS:HG2	1:C:632:ARG:HD3	1.89	0.53
1:C:737:LYS:HG3	1:C:738:GLN:N	2.22	0.53
1:A:434:ARG:HG2	1:A:463:TRP:CD2	2.43	0.53
1:A:522:ARG:HG2	1:A:528:PHE:O	2.08	0.53
1:B:240:PRO:HG3	1:B:274:GLY:O	2.08	0.53
1:D:142:SER:O	1:D:146:GLU:HG2	2.08	0.53
1:D:503:LEU:CB	1:D:532:MET:HG2	2.36	0.53
1:D:535:VAL:HG13	1:D:689:ILE:HD11	1.91	0.53
1:A:262:ARG:O	1:A:263:LYS:HB2	2.08	0.53
1:A:483:LEU:HD12	1:A:483:LEU:H	1.74	0.53
1:A:65:GLN:HG2	1:A:98:CYS:HB2	1.90	0.53
1:C:138:ARG:HA	1:C:165:LEU:HD12	1.91	0.53
1:D:503:LEU:CD2	1:D:505:ILE:HD11	2.39	0.53
1:A:577:VAL:HG21	1:A:622:LEU:CD2	2.37	0.53
1:B:409:THR:HB	1:B:705:ARG:NH2	2.23	0.53
1:C:434:ARG:HG2	1:C:463:TRP:CD2	2.43	0.53
1:D:236:TRP:HZ3	1:D:399:ILE:HD11	1.73	0.53
1:D:397:LEU:HD21	1:D:430:ARG:NH2	2.24	0.53
1:D:488:LEU:H	1:D:488:LEU:CD2	2.16	0.53
1:A:529:CYS:O	1:A:711:PHE:HB2	2.08	0.53
1:B:625:LYS:C	1:B:627:LYS:H	2.11	0.53
1:C:638:ASN:HB3	1:C:641:CYS:HB3	1.90	0.53
1:C:757:LEU:O	1:C:757:LEU:HD22	2.09	0.53
1:D:193:ARG:O	1:D:197:VAL:HG23	2.09	0.53
1:B:120:THR:HG23	1:B:121:ASN:ND2	2.24	0.53
1:B:42:ALA:HB1	1:B:170:MET:CE	2.39	0.53
1:C:25:LYS:CG	1:C:120:THR:HG21	2.39	0.53
1:C:538:THR:HG23	1:C:541:ASN:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:TYR:HA	1:D:534:MET:HE1	1.91	0.53
1:C:37:GLN:NE2	1:C:310:ARG:C	2.62	0.53
1:C:669:LEU:HB3	1:C:673:GLN:NE2	2.23	0.53
1:A:431:SER:HB2	1:A:687:THR:HG23	1.89	0.53
1:B:306:GLY:C	1:B:308:VAL:H	2.13	0.53
1:B:658:GLY:O	1:B:659:LYS:C	2.47	0.53
1:B:739:THR:HG23	1:B:741:PHE:CE1	2.44	0.53
1:D:171:VAL:HG11	1:D:181:THR:CG2	2.38	0.53
1:D:240:PRO:HG3	1:D:274:GLY:O	2.08	0.53
1:A:138:ARG:HA	1:A:165:LEU:HD12	1.90	0.53
1:A:412:ASN:HB2	1:A:499:SER:O	2.08	0.53
1:A:83:SER:O	1:A:84:SER:HB3	2.09	0.53
1:B:717:ILE:O	1:B:732:VAL:HG13	2.09	0.53
1:B:84:SER:HB2	1:B:632:ARG:NH2	2.24	0.53
1:D:27:ILE:HG23	1:D:121:ASN:HB2	1.90	0.53
1:D:480:LYS:HB3	1:D:482:VAL:CG2	2.20	0.53
1:A:515:LEU:C	1:A:515:LEU:HD23	2.29	0.52
1:B:530:VAL:HB	1:B:531:PRO:HD2	1.90	0.52
1:C:49:MET:O	1:C:53:VAL:HG22	2.09	0.52
1:A:421:PRO:HG2	1:A:674:GLN:HE22	1.74	0.52
1:B:579:ILE:HD12	1:B:579:ILE:N	2.24	0.52
1:B:680:PRO:HA	1:B:683:ARG:HG3	1.91	0.52
1:C:174:ILE:HG21	1:C:190:ALA:HB2	1.90	0.52
1:C:280:ASN:H	1:C:374:ARG:NH2	2.06	0.52
1:C:488:LEU:HD22	1:C:528:PHE:CZ	2.44	0.52
1:C:746:PRO:HD2	1:C:749:GLN:NE2	2.24	0.52
1:D:560:THR:HG22	1:D:597:ALA:HB3	1.91	0.52
1:B:315:SER:O	1:B:319:ARG:HG3	2.09	0.52
1:C:556:LEU:O	1:C:560:THR:HG23	2.09	0.52
1:C:700:LYS:HA	1:C:703:GLU:HG2	1.90	0.52
1:C:356:PRO:HG2	1:C:359:GLU:HB3	1.92	0.52
1:C:582:THR:HG21	1:C:591:ALA:HA	1.91	0.52
1:A:240:PRO:HG3	1:A:274:GLY:O	2.09	0.52
1:A:487:TYR:O	1:A:491:ILE:HD13	2.10	0.52
1:C:435:VAL:HG21	1:C:691:ALA:CB	2.40	0.52
1:D:27:ILE:HD12	1:D:27:ILE:N	2.24	0.52
1:D:397:LEU:HD11	1:D:431:SER:HA	1.91	0.52
1:A:138:ARG:HD3	1:A:165:LEU:O	2.09	0.52
1:A:395:LYS:C	1:A:397:LEU:H	2.12	0.52
1:A:483:LEU:N	1:A:483:LEU:HD12	2.23	0.52
1:A:616:GLN:HA	1:A:616:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TRP:CZ3	1:A:399:ILE:HD11	2.45	0.52
1:B:419:GLY:HA2	1:B:481:ARG:HG2	1.90	0.52
1:B:532:MET:CB	1:B:717:ILE:HG23	2.40	0.52
1:C:508:GLY:CA	1:C:538:THR:HB	2.39	0.52
1:D:176:ASN:C	1:D:178:PHE:H	2.13	0.52
1:C:516:LEU:HD22	1:C:732:VAL:HB	1.92	0.52
1:C:592:ASN:C	1:C:592:ASN:HD22	2.13	0.52
1:C:757:LEU:C	1:C:757:LEU:HD22	2.30	0.52
1:A:268:ILE:N	1:A:268:ILE:HD12	2.25	0.52
1:A:435:VAL:HG12	1:A:435:VAL:O	2.09	0.52
1:C:424:GLY:N	1:C:678:PRO:HB3	2.24	0.52
1:C:477:LEU:HD12	1:C:477:LEU:H	1.74	0.52
1:D:416:ILE:HD11	1:D:449:GLY:C	2.30	0.52
1:D:477:LEU:HD12	1:D:477:LEU:H	1.74	0.52
1:D:625:LYS:C	1:D:627:LYS:H	2.14	0.52
1:A:720:LEU:HD22	1:A:729:PHE:CE2	2.46	0.51
1:B:176:ASN:C	1:B:178:PHE:H	2.13	0.51
1:D:420:ALA:HB2	1:D:481:ARG:HH11	1.76	0.51
1:D:680:PRO:HA	1:D:683:ARG:HG3	1.91	0.51
1:A:206:GLN:O	1:A:265:ARG:NH2	2.44	0.51
1:A:396:ARG:HB3	1:A:396:ARG:HH21	1.76	0.51
1:A:50:GLY:O	1:A:53:VAL:HG23	2.11	0.51
1:B:114:LEU:HD22	1:B:119:ILE:HB	1.93	0.51
1:B:376:PHE:O	1:B:380:VAL:HG23	2.10	0.51
1:B:483:LEU:HD21	1:B:513:LEU:HD13	1.92	0.51
1:C:187:THR:HG21	1:C:223:TYR:HE2	1.75	0.51
1:C:615:LEU:O	1:C:619:VAL:HG23	2.10	0.51
1:A:42:ALA:HB1	1:A:170:MET:CE	2.40	0.51
1:B:226:LEU:HB2	1:B:239:LEU:HD11	1.91	0.51
1:B:542:ASN:O	1:B:746:PRO:HD3	2.10	0.51
1:C:181:THR:CB	1:C:346:SER:HB2	2.35	0.51
1:C:479:THR:HG23	1:C:479:THR:O	2.10	0.51
1:D:621:HIS:CE1	1:D:763:LYS:HB2	2.46	0.51
1:D:715:ASP:C	1:D:717:ILE:H	2.13	0.51
1:D:717:ILE:O	1:D:732:VAL:HG13	2.10	0.51
1:D:48:ARG:HG2	1:D:79:TRP:CE2	2.45	0.51
1:A:115:LEU:HD12	1:A:162:TYR:CD2	2.46	0.51
1:A:337:THR:OG1	1:A:340:THR:HB	2.10	0.51
1:A:527:GLU:CD	1:A:527:GLU:N	2.62	0.51
1:B:560:THR:HG22	1:B:597:ALA:HB3	1.92	0.51
1:D:65:GLN:HG2	1:D:98:CYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG21	1:A:225:ALA:HA	1.93	0.51
1:A:623:THR:HG23	1:A:661:VAL:HG21	1.93	0.51
1:B:438:ALA:HB2	1:B:463:TRP:HZ3	1.74	0.51
1:D:412:ASN:ND2	1:D:499:SER:CB	2.74	0.51
1:B:42:ALA:HB1	1:B:170:MET:HE1	1.93	0.51
1:B:216:VAL:HG21	1:B:225:ALA:HA	1.91	0.51
1:B:262:ARG:NH2	1:B:400:LYS:HD3	2.18	0.51
1:D:32:SER:HB3	1:D:130:SER:OG	2.09	0.51
1:A:28:GLY:HA3	1:A:122:LEU:HD12	1.93	0.51
1:A:579:ILE:HG13	1:A:635:VAL:HG13	1.93	0.51
1:B:592:ASN:C	1:B:592:ASN:HD22	2.14	0.51
1:C:357:LEU:O	1:C:361:VAL:HG23	2.10	0.51
1:D:66:GLY:HA2	1:D:73:ASN:HD22	1.75	0.51
1:A:99:GLN:C	1:A:101:PHE:H	2.14	0.51
1:B:443:MET:O	1:B:460:GLU:HG3	2.11	0.51
1:B:615:LEU:O	1:B:619:VAL:HG23	2.11	0.51
1:B:630:ILE:N	1:B:630:ILE:HD12	2.17	0.51
1:C:572:GLY:O	1:D:478:GLY:HA2	2.10	0.51
1:B:203:THR:HA	1:B:206:GLN:HG2	1.93	0.51
1:B:496:ARG:HB3	1:B:527:GLU:HG2	1.92	0.51
1:B:579:ILE:HG13	1:B:635:VAL:HG13	1.93	0.51
1:B:760:ILE:HG12	1:B:761:LEU:HD23	1.92	0.51
1:C:305:LEU:HD12	1:C:305:LEU:H	1.75	0.51
1:D:16:PHE:N	1:D:16:PHE:HD2	2.09	0.51
1:D:450:PHE:CD1	1:D:484:PRO:HD3	2.46	0.51
1:A:608:GLU:OE1	1:A:755:ARG:HG2	2.11	0.51
1:B:277:ASP:HB3	1:B:283:ILE:HD11	1.93	0.51
1:B:739:THR:N	1:B:747:LYS:HG3	2.26	0.51
1:C:190:ALA:O	1:C:194:ILE:HG13	2.11	0.51
1:C:262:ARG:HD3	1:C:464:THR:HG22	1.93	0.51
1:D:331:ILE:HG13	1:D:354:ARG:HH22	1.76	0.51
1:A:538:THR:HG23	1:A:541:ASN:H	1.75	0.50
1:B:737:LYS:HG3	1:B:738:GLN:HG3	1.92	0.50
1:B:750:TRP:CG	1:B:751:TRP:N	2.78	0.50
1:C:516:LEU:CD2	1:C:732:VAL:HB	2.41	0.50
1:C:522:ARG:HH12	1:C:529:CYS:HA	1.72	0.50
1:D:358:MET:HG3	1:D:359:GLU:N	2.26	0.50
1:B:92:ILE:HG13	1:B:93:ILE:N	2.26	0.50
1:C:306:GLY:C	1:C:308:VAL:H	2.14	0.50
1:C:583:MET:HA	1:C:639:GLU:HB2	1.93	0.50
1:A:171:VAL:HG11	1:A:181:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:C	2:A:801:ADP:O3B	2.49	0.50
1:B:206:GLN:O	1:B:265:ARG:NH2	2.44	0.50
1:A:174:ILE:HG21	1:A:190:ALA:HB2	1.93	0.50
1:A:483:LEU:HD23	1:A:513:LEU:HD12	1.94	0.50
1:A:625:LYS:C	1:A:627:LYS:H	2.15	0.50
1:B:26:ALA:CB	1:B:119:ILE:HA	2.35	0.50
1:B:192:HIS:HA	1:B:680:PRO:HG2	1.94	0.50
1:C:237:VAL:HG12	1:C:238:PHE:N	2.26	0.50
1:D:577:VAL:CG2	1:D:622:LEU:HD21	2.39	0.50
1:D:615:LEU:O	1:D:619:VAL:HG23	2.12	0.50
1:D:630:ILE:CD1	1:D:630:ILE:H	2.11	0.50
1:D:424:GLY:N	1:D:678:PRO:HB3	2.26	0.50
1:A:717:ILE:O	1:A:717:ILE:CG1	2.58	0.50
1:B:539:VAL:HG12	1:B:551:GLY:O	2.12	0.50
1:C:515:LEU:CD1	1:C:534:MET:HB3	2.42	0.50
1:D:211:THR:OG1	1:D:267:ASN:HB2	2.12	0.50
1:A:192:HIS:O	1:A:196:GLU:HG3	2.11	0.50
1:A:254:VAL:O	1:A:258:GLU:HG3	2.11	0.50
1:A:195:ILE:HG13	1:A:680:PRO:HG3	1.93	0.50
1:B:432:ALA:HB1	1:B:504:LEU:CD2	2.42	0.50
1:B:501:ASN:HA	1:B:530:VAL:HG11	1.92	0.50
1:B:746:PRO:HG2	1:B:749:GLN:HG2	1.94	0.50
1:C:255:LYS:HE3	1:C:399:ILE:HD13	1.93	0.50
1:C:396:ARG:HH21	1:C:396:ARG:HB3	1.75	0.50
1:C:565:ARG:HG2	1:D:676:GLY:HA2	1.92	0.50
1:A:305:LEU:HD12	1:A:305:LEU:H	1.77	0.50
1:C:522:ARG:NE	1:C:717:ILE:HD11	2.24	0.50
1:D:315:SER:O	1:D:319:ARG:HG3	2.11	0.50
1:A:611:ASP:OD1	1:A:613:ARG:HB2	2.11	0.50
1:C:84:SER:CB	1:C:632:ARG:HH22	2.25	0.50
1:D:580:ILE:N	1:D:580:ILE:HD12	2.26	0.50
1:B:290:GLU:O	1:B:294:THR:HG23	2.12	0.50
1:B:453:PHE:CG	1:B:491:ILE:HD12	2.46	0.50
1:B:538:THR:HG23	1:B:541:ASN:H	1.75	0.50
1:D:70:GLY:HA3	1:D:113:ASN:HD22	1.77	0.50
1:A:238:PHE:CD2	1:A:283:ILE:HG21	2.47	0.49
1:A:630:ILE:HD12	1:A:630:ILE:N	2.21	0.49
1:C:44:ARG:HH11	1:C:761:LEU:CD2	2.21	0.49
1:A:114:LEU:HD22	1:A:119:ILE:HB	1.94	0.49
1:A:539:VAL:O	1:A:590:LEU:HD11	2.12	0.49
1:B:49:MET:O	1:B:53:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HD11	1:D:308:VAL:HG12	1.95	0.49
1:C:429:VAL:HG11	1:C:477:LEU:HD11	1.93	0.49
1:D:306:GLY:C	1:D:308:VAL:N	2.65	0.49
1:A:266:LEU:HD22	1:A:267:ASN:N	2.26	0.49
1:A:290:GLU:O	1:A:294:THR:HG22	2.12	0.49
1:A:560:THR:HG22	1:A:597:ALA:HB3	1.94	0.49
1:B:211:THR:OG1	1:B:267:ASN:HB2	2.12	0.49
1:B:255:LYS:HE3	1:B:399:ILE:HD13	1.93	0.49
1:C:262:ARG:O	1:C:263:LYS:HB2	2.11	0.49
1:D:279:GLN:O	1:D:281:LYS:N	2.46	0.49
1:A:230:LEU:HG	1:A:394:TYR:HB2	1.94	0.49
1:B:193:ARG:O	1:B:197:VAL:HG23	2.11	0.49
1:D:395:LYS:C	1:D:397:LEU:H	2.15	0.49
1:D:447:TYR:HD2	1:D:477:LEU:HA	1.77	0.49
1:D:461:ILE:HD12	1:D:461:ILE:O	2.11	0.49
1:A:331:ILE:HG13	1:A:354:ARG:HH22	1.78	0.49
1:A:280:ASN:H	1:A:374:ARG:NH2	2.09	0.49
1:A:474:GLY:HA3	1:B:568:GLN:HE21	1.77	0.49
1:B:111:ALA:O	1:B:115:LEU:HD22	2.12	0.49
1:B:422:ALA:O	1:B:425:MET:HB2	2.12	0.49
1:C:447:TYR:HD2	1:C:477:LEU:HA	1.77	0.49
1:D:429:VAL:HG11	1:D:477:LEU:HD11	1.93	0.49
1:A:266:LEU:HD11	1:A:268:ILE:HD11	1.94	0.49
1:A:417:ASN:ND2	1:A:506:ILE:HB	2.28	0.49
1:A:542:ASN:O	1:A:746:PRO:HD3	2.13	0.49
1:A:693:ALA:HB2	1:A:720:LEU:HD23	1.93	0.49
1:B:181:THR:CB	1:B:346:SER:HB2	2.41	0.49
1:B:579:ILE:HG13	1:B:635:VAL:CG1	2.42	0.49
1:B:48:ARG:HG2	1:B:79:TRP:CE2	2.48	0.49
1:C:42:ALA:HB1	1:C:170:MET:CE	2.43	0.49
1:D:238:PHE:CD2	1:D:283:ILE:HG21	2.48	0.49
1:D:669:LEU:HB3	1:D:673:GLN:NE2	2.28	0.49
1:A:493:THR:O	1:A:497:THR:HB	2.13	0.49
1:B:539:VAL:HG11	1:B:674:GLN:CB	2.38	0.49
1:C:179:CYS:SG	1:C:363:MET:HB2	2.53	0.49
1:D:49:MET:O	1:D:53:VAL:HG22	2.12	0.49
1:A:44:ARG:HD3	1:A:86:LEU:HB2	1.95	0.49
1:B:395:LYS:C	1:B:397:LEU:H	2.15	0.49
1:D:195:ILE:HD11	1:D:231:ALA:HB3	1.95	0.49
1:D:696:TRP:CZ2	1:D:700:LYS:HD2	2.47	0.49
1:A:244:PRO:HD2	1:A:277:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:O	1:A:683:ARG:HD2	2.13	0.49
1:B:669:LEU:CB	1:B:673:GLN:NE2	2.75	0.49
1:C:264:LYS:HG2	1:C:266:LEU:O	2.12	0.49
1:C:537:ALA:HA	1:C:550:ILE:HB	1.94	0.49
1:C:539:VAL:HG12	1:C:551:GLY:O	2.13	0.49
1:C:65:GLN:HG2	1:C:98:CYS:CB	2.42	0.49
1:D:411:CYS:O	1:D:442:ARG:HG2	2.12	0.49
1:D:412:ASN:HB2	1:D:499:SER:O	2.12	0.49
1:B:737:LYS:HG3	1:B:738:GLN:N	2.27	0.49
1:C:397:LEU:HD21	1:C:430:ARG:NH2	2.28	0.49
1:C:605:ILE:HG12	1:C:755:ARG:HH21	1.76	0.49
1:C:610:PHE:N	1:C:610:PHE:CD1	2.80	0.49
1:D:99:GLN:C	1:D:101:PHE:H	2.16	0.49
1:D:27:ILE:HG21	1:D:333:LEU:CD1	2.43	0.49
1:A:268:ILE:HD12	1:A:268:ILE:H	1.77	0.48
1:D:192:HIS:O	1:D:196:GLU:HG3	2.13	0.48
1:D:501:ASN:HA	1:D:530:VAL:HG11	1.94	0.48
1:D:739:THR:N	1:D:747:LYS:HG3	2.28	0.48
1:A:266:LEU:CD1	1:A:268:ILE:HD11	2.42	0.48
1:A:532:MET:HB2	1:A:717:ILE:HG22	1.95	0.48
1:C:325:MET:HE2	1:C:345:VAL:HB	1.96	0.48
1:D:205:ALA:CB	1:D:266:LEU:HD23	2.43	0.48
1:B:174:ILE:HG21	1:B:190:ALA:HB2	1.94	0.48
1:B:645:TYR:CE1	1:D:656:GLU:HG2	2.48	0.48
1:C:501:ASN:O	1:C:531:PRO:HD2	2.13	0.48
1:D:746:PRO:HG2	1:D:749:GLN:CG	2.43	0.48
1:A:156:LYS:O	1:A:159:VAL:HG12	2.13	0.48
1:A:37:GLN:NE2	1:A:310:ARG:C	2.67	0.48
1:B:722:ILE:HD13	1:B:727:VAL:HG12	1.95	0.48
1:A:644:ASN:ND2	1:C:656:GLU:HB2	2.27	0.48
1:C:99:GLN:C	1:C:101:PHE:H	2.15	0.48
1:D:715:ASP:C	1:D:717:ILE:N	2.66	0.48
1:A:292:VAL:HG23	1:A:293:VAL:N	2.28	0.48
1:A:583:MET:HA	1:A:639:GLU:HB2	1.96	0.48
1:A:92:ILE:HG13	1:A:93:ILE:N	2.29	0.48
1:B:504:LEU:HD22	1:B:694:MET:HE1	1.95	0.48
1:B:583:MET:HA	1:B:639:GLU:HB2	1.94	0.48
1:A:522:ARG:NH1	1:A:529:CYS:HA	2.29	0.48
1:B:508:GLY:HA2	1:B:538:THR:HB	1.94	0.48
1:B:535:VAL:HG13	1:B:689:ILE:HD11	1.94	0.48
1:C:266:LEU:CD1	1:C:268:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLU:HB2	1:D:644:ASN:ND2	2.28	0.48
1:A:577:VAL:CG2	1:A:622:LEU:HD21	2.41	0.48
1:C:461:ILE:HD12	1:C:461:ILE:O	2.13	0.48
1:C:750:TRP:CG	1:C:751:TRP:N	2.81	0.48
1:D:181:THR:CB	1:D:346:SER:HB2	2.37	0.48
1:A:241:GLU:OE2	1:A:387:PHE:HE1	1.97	0.48
1:A:284:THR:HG22	1:A:287:LYS:HB2	1.96	0.48
1:A:443:MET:O	1:A:460:GLU:HG3	2.12	0.48
1:A:539:VAL:CG1	1:A:674:GLN:HB3	2.30	0.48
1:C:244:PRO:HD2	1:C:277:ASP:HA	1.93	0.48
1:C:533:VAL:HG22	1:C:696:TRP:CZ3	2.49	0.48
1:D:174:ILE:HG21	1:D:190:ALA:HB2	1.95	0.48
1:D:515:LEU:HG	1:D:534:MET:HE1	1.95	0.48
1:B:638:ASN:HB3	1:B:641:CYS:HB3	1.96	0.48
1:C:238:PHE:CD2	1:C:283:ILE:HG21	2.48	0.48
1:D:255:LYS:HE3	1:D:399:ILE:HD13	1.95	0.48
1:D:49:MET:SD	1:D:760:ILE:CD1	3.01	0.48
1:D:52:TYR:CE2	1:D:760:ILE:HB	2.49	0.48
1:A:337:THR:O	1:A:340:THR:HG22	2.13	0.47
1:A:539:VAL:HG12	1:A:551:GLY:O	2.14	0.47
1:B:156:LYS:O	1:B:159:VAL:HG12	2.13	0.47
1:C:27:ILE:CG2	1:C:121:ASN:HB2	2.44	0.47
1:C:211:THR:OG1	1:C:267:ASN:HB2	2.14	0.47
1:D:560:THR:CG2	1:D:597:ALA:HB3	2.44	0.47
1:D:596:LEU:HB2	1:D:758:MET:HG3	1.96	0.47
1:D:87:GLN:HE22	1:D:567:LYS:HE3	1.79	0.47
1:A:191:LEU:HD22	1:A:680:PRO:CB	2.44	0.47
1:B:530:VAL:CB	1:B:531:PRO:HD2	2.45	0.47
1:B:750:TRP:CD2	1:B:751:TRP:N	2.82	0.47
1:B:65:GLN:HG2	1:B:98:CYS:HB2	1.96	0.47
1:C:205:ALA:CB	1:C:266:LEU:HD23	2.44	0.47
1:C:411:CYS:O	1:C:442:ARG:HG2	2.13	0.47
1:C:539:VAL:O	1:C:590:LEU:HD11	2.14	0.47
1:C:720:LEU:HD13	1:C:729:PHE:CD2	2.49	0.47
1:C:48:ARG:HG2	1:C:79:TRP:CE2	2.49	0.47
1:A:750:TRP:CG	1:A:751:TRP:N	2.82	0.47
1:B:719:VAL:HG23	1:B:719:VAL:O	2.15	0.47
1:D:27:ILE:CG2	1:D:333:LEU:HD13	2.41	0.47
1:B:205:ALA:HB3	1:B:266:LEU:HD23	1.97	0.47
1:B:262:ARG:HD3	1:B:464:THR:HG22	1.96	0.47
1:C:192:HIS:CE1	1:C:680:PRO:HD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:HG13	1:C:57:VAL:HG12	1.96	0.47
1:D:450:PHE:CE1	1:D:484:PRO:HG3	2.49	0.47
1:B:435:VAL:O	1:B:435:VAL:HG12	2.14	0.47
1:C:451:ASP:O	1:C:455:LYS:HG3	2.14	0.47
1:D:138:ARG:HA	1:D:165:LEU:HD12	1.95	0.47
1:D:164:TYR:CD2	1:D:338:PRO:HB3	2.50	0.47
1:D:262:ARG:HD3	1:D:464:THR:HG22	1.97	0.47
1:C:197:VAL:HG13	1:D:308:VAL:HG11	1.95	0.47
1:A:494:GLN:O	1:A:497:THR:HG22	2.14	0.47
1:A:547:ASP:HB3	1:A:750:TRP:NE1	2.30	0.47
1:A:651:TYR:HE2	1:A:664:CYS:O	1.98	0.47
1:B:478:GLY:O	1:B:479:THR:HB	2.15	0.47
1:B:44:ARG:HD3	1:B:86:LEU:HB2	1.96	0.47
1:C:148:LEU:HB3	1:C:154:ILE:CG2	2.45	0.47
1:C:414:ALA:HA	1:C:444:LEU:O	2.13	0.47
1:D:27:ILE:HD12	1:D:56:LYS:O	2.14	0.47
1:C:193:ARG:O	1:C:197:VAL:HG23	2.14	0.47
1:C:661:VAL:HG13	1:C:662:PHE:CD2	2.50	0.47
1:D:191:LEU:HD22	1:D:680:PRO:HB3	1.95	0.47
1:A:306:GLY:C	1:A:308:VAL:N	2.68	0.47
1:A:23:ALA:HB1	1:A:54:GLY:O	2.14	0.47
1:A:579:ILE:HG13	1:A:635:VAL:CG1	2.44	0.47
1:A:661:VAL:HG13	1:A:662:PHE:CD2	2.49	0.47
1:C:241:GLU:OE2	1:C:387:PHE:HE1	1.97	0.47
1:A:221:CYS:SG	1:A:223:TYR:HB2	2.55	0.47
1:A:487:TYR:CD2	1:A:487:TYR:N	2.81	0.47
1:A:565:ARG:O	1:A:568:GLN:HB3	2.15	0.47
1:B:171:VAL:HG11	1:B:181:THR:CG2	2.44	0.47
1:B:254:VAL:O	1:B:258:GLU:HG3	2.15	0.47
1:B:567:LYS:HG2	1:B:632:ARG:HD3	1.97	0.47
1:B:99:GLN:C	1:B:101:PHE:H	2.18	0.47
1:C:443:MET:O	1:C:460:GLU:HG3	2.15	0.47
1:D:337:THR:O	1:D:340:THR:HG22	2.14	0.47
1:D:610:PHE:N	1:D:610:PHE:CD1	2.82	0.47
1:A:260:ARG:NH2	1:A:267:ASN:HD22	2.13	0.47
1:A:739:THR:N	1:A:747:LYS:HG3	2.30	0.47
1:B:241:GLU:O	1:B:376:PHE:HB3	2.15	0.47
1:B:508:GLY:HA3	1:B:538:THR:HB	1.96	0.47
1:B:630:ILE:CG2	1:B:632:ARG:HG2	2.45	0.47
1:B:580:ILE:HG23	1:B:669:LEU:HG	1.96	0.47
1:C:209:GLN:HA	1:C:265:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:VAL:HG12	1:C:365:GLN:HE22	1.80	0.47
1:C:651:TYR:HE2	1:C:664:CYS:O	1.97	0.47
1:C:502:ALA:HB2	1:C:701:LEU:HD11	1.95	0.47
1:A:726:ASN:OD1	1:A:726:ASN:N	2.48	0.47
1:B:726:ASN:OD1	1:B:726:ASN:N	2.47	0.47
1:C:213:VAL:O	1:C:302:VAL:HG23	2.15	0.47
1:C:596:LEU:HB2	1:C:758:MET:HG3	1.96	0.47
1:D:332:ALA:HA	1:D:354:ARG:NH1	2.30	0.47
1:D:546:SER:HA	1:D:722:ILE:O	2.15	0.47
1:A:319:ARG:HD2	1:A:597:ALA:O	2.14	0.46
1:A:750:TRP:CD2	1:A:751:TRP:N	2.83	0.46
1:B:720:LEU:HD23	1:B:721:GLY:N	2.29	0.46
1:B:722:ILE:HD13	1:B:727:VAL:CG1	2.45	0.46
1:C:121:ASN:OD1	1:C:166:ASN:HB2	2.15	0.46
1:C:199:ASP:CG	1:C:683:ARG:HH22	2.19	0.46
1:C:676:GLY:HA3	1:D:565:ARG:HD2	1.96	0.46
1:D:101:PHE:C	1:D:103:THR:H	2.17	0.46
1:D:713:THR:O	1:D:715:ASP:N	2.49	0.46
1:A:198:VAL:HG12	1:A:199:ASP:N	2.29	0.46
1:A:413:VAL:HG22	1:A:502:ALA:HB3	1.97	0.46
1:B:198:VAL:HG22	1:B:214:LEU:HD21	1.96	0.46
1:B:414:ALA:HA	1:B:444:LEU:O	2.15	0.46
1:D:414:ALA:HA	1:D:444:LEU:O	2.14	0.46
1:A:428:ALA:HB1	1:A:506:ILE:HD12	1.98	0.46
1:A:42:ALA:HB1	1:A:170:MET:HE1	1.97	0.46
1:B:661:VAL:HG13	1:B:662:PHE:CD2	2.50	0.46
1:C:420:ALA:HB2	1:C:481:ARG:NH1	2.31	0.46
1:C:750:TRP:CD2	1:C:751:TRP:N	2.83	0.46
1:D:430:ARG:HA	1:D:466:VAL:HB	1.97	0.46
1:D:481:ARG:HH12	3:D:801:PO4:P	2.39	0.46
1:D:579:ILE:HG13	1:D:635:VAL:CG1	2.45	0.46
1:A:711:PHE:HD2	1:A:716:SER:HB3	1.81	0.46
1:C:509:PHE:HE2	1:C:513:LEU:HD21	1.80	0.46
1:D:115:LEU:HD12	1:D:162:TYR:CD2	2.50	0.46
1:D:42:ALA:HB1	1:D:170:MET:HE1	1.98	0.46
1:D:262:ARG:NH2	1:D:400:LYS:HD3	2.27	0.46
1:D:426:ASN:OD1	1:D:476:ILE:HG13	2.15	0.46
1:D:752:LEU:O	1:D:755:ARG:HB2	2.14	0.46
1:D:65:GLN:HG2	1:D:98:CYS:CB	2.46	0.46
1:A:396:ARG:O	1:A:396:ARG:HD2	2.15	0.46
1:A:638:ASN:HB3	1:A:641:CYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:VAL:HG13	1:C:689:ILE:HD11	1.98	0.46
1:C:755:ARG:N	1:C:756:PRO:HD2	2.31	0.46
1:D:496:ARG:HB2	1:D:527:GLU:HG2	1.98	0.46
1:D:685:PHE:CE2	1:D:689:ILE:HG21	2.51	0.46
1:B:185:ILE:HD11	1:B:322:ALA:HA	1.98	0.46
1:B:406:ILE:HG22	1:B:406:ILE:O	2.16	0.46
1:B:493:THR:HG22	1:B:496:ARG:NH2	2.30	0.46
1:D:718:CYS:HA	1:D:732:VAL:HG13	1.97	0.46
1:B:702:LYS:HA	1:B:705:ARG:HD2	1.97	0.46
1:C:92:ILE:HG13	1:C:93:ILE:N	2.30	0.46
1:A:492:ALA:HB1	1:A:527:GLU:OE1	2.15	0.46
1:C:525:HIS:HB2	1:C:528:PHE:CE1	2.51	0.46
1:C:577:VAL:HG21	1:C:622:LEU:HD21	1.98	0.46
1:C:700:LYS:HA	1:C:703:GLU:CG	2.45	0.46
1:A:69:ASP:O	1:A:113:ASN:ND2	2.48	0.46
1:A:325:MET:HE2	1:A:345:VAL:HB	1.98	0.46
1:B:529:CYS:HB3	1:B:711:PHE:O	2.16	0.46
1:B:610:PHE:CD1	1:B:610:PHE:N	2.84	0.46
1:C:762:ALA:O	1:C:763:LYS:CB	2.64	0.46
1:A:546:SER:HB2	1:A:721:GLY:HA3	1.98	0.46
1:A:622:LEU:O	1:A:626:MET:HG2	2.16	0.46
1:A:717:ILE:N	1:A:717:ILE:HD13	2.30	0.46
1:A:735:LEU:O	1:A:739:THR:HG22	2.16	0.46
1:B:576:ARG:HD3	1:B:663:ASP:HB3	1.96	0.46
1:B:663:ASP:O	1:B:664:CYS:HB3	2.16	0.46
1:C:417:ASN:HB3	1:C:425:MET:HE3	1.98	0.46
1:C:630:ILE:HD12	1:C:630:ILE:N	2.19	0.46
1:D:214:LEU:HB3	1:D:305:LEU:HD11	1.98	0.46
1:A:148:LEU:HB3	1:A:154:ILE:HG23	1.97	0.45
1:A:174:ILE:HD11	1:A:217:MET:SD	2.56	0.45
1:A:522:ARG:C	1:A:524:LYS:H	2.18	0.45
1:A:532:MET:O	1:A:717:ILE:HA	2.16	0.45
1:B:523:GLU:O	1:B:524:LYS:C	2.54	0.45
1:C:236:TRP:CZ3	1:C:399:ILE:HD11	2.51	0.45
1:D:262:ARG:O	1:D:263:LYS:CB	2.64	0.45
1:A:138:ARG:CD	1:A:165:LEU:O	2.64	0.45
1:A:260:ARG:NH2	1:A:267:ASN:ND2	2.64	0.45
1:A:412:ASN:OD1	1:A:442:ARG:HD3	2.17	0.45
1:A:27:ILE:HD13	1:A:57:VAL:CG1	2.46	0.45
1:B:241:GLU:OE2	1:B:387:PHE:HE1	1.98	0.45
1:B:135:ASN:HB2	1:B:357:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:LEU:HB2	1:B:758:MET:HG3	1.98	0.45
1:B:88:VAL:HG12	1:B:89:GLY:N	2.31	0.45
1:D:401:LEU:HG	1:D:406:ILE:HG12	1.98	0.45
1:D:504:LEU:HD23	1:D:504:LEU:O	2.16	0.45
1:C:223:TYR:O	1:C:225:ALA:N	2.48	0.45
1:C:395:LYS:C	1:C:397:LEU:H	2.19	0.45
1:C:522:ARG:HE	1:C:717:ILE:CD1	2.23	0.45
1:D:42:ALA:HB1	1:D:170:MET:CE	2.47	0.45
1:D:507:GLY:N	1:D:537:ALA:HB3	2.32	0.45
1:C:115:LEU:HD12	1:C:162:TYR:CD2	2.52	0.45
1:C:426:ASN:OD1	1:C:476:ILE:HG13	2.16	0.45
1:C:489:GLU:OE2	1:C:525:HIS:CD2	2.69	0.45
1:D:306:GLY:O	1:D:308:VAL:N	2.50	0.45
1:D:487:TYR:O	1:D:491:ILE:HD12	2.17	0.45
1:D:750:TRP:CG	1:D:751:TRP:N	2.83	0.45
1:B:447:TYR:HD2	1:B:477:LEU:HA	1.82	0.45
1:C:277:ASP:HB3	1:C:283:ILE:HD11	1.99	0.45
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.99	0.45
1:C:577:VAL:HG22	1:C:633:GLY:HA3	1.99	0.45
1:C:746:PRO:HG2	1:C:749:GLN:CG	2.45	0.45
1:B:363:MET:O	1:B:367:VAL:HG23	2.17	0.45
1:B:483:LEU:CD2	1:B:513:LEU:HD22	2.45	0.45
1:D:536:PRO:HD3	1:D:720:LEU:O	2.16	0.45
1:D:580:ILE:HG23	1:D:669:LEU:HG	1.99	0.45
1:A:332:ALA:HA	1:A:354:ARG:NH1	2.31	0.45
1:B:537:ALA:HA	1:B:550:ILE:HB	1.98	0.45
1:C:327:VAL:O	1:C:331:ILE:HG23	2.16	0.45
1:C:450:PHE:CE1	1:C:484:PRO:HD3	2.52	0.45
1:C:67:MET:HE2	1:C:110:ALA:HB1	1.99	0.45
1:D:470:THR:O	1:D:683:ARG:HD2	2.17	0.45
1:D:701:LEU:HD23	1:D:701:LEU:HA	1.83	0.45
1:D:729:PHE:N	1:D:729:PHE:CD1	2.85	0.45
1:D:755:ARG:N	1:D:756:PRO:HD2	2.31	0.45
1:A:120:THR:HG23	1:A:121:ASN:ND2	2.31	0.45
1:A:168:VAL:HG13	1:A:168:VAL:O	2.16	0.45
1:B:356:PRO:HG2	1:B:359:GLU:HB3	1.99	0.45
1:C:409:THR:HB	1:C:705:ARG:NH2	2.32	0.45
1:C:473:GLY:HA2	1:C:678:PRO:HD3	1.98	0.45
1:D:485:GLY:O	1:D:488:LEU:HD22	2.17	0.45
1:D:481:ARG:HG3	1:D:510:GLU:CG	2.47	0.45
1:D:419:GLY:CA	1:D:510:GLU:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:PHE:HE2	1:D:689:ILE:HG21	1.81	0.45
1:A:293:VAL:HG23	1:A:298:TYR:O	2.16	0.45
1:A:354:ARG:O	1:A:355:LEU:HD23	2.16	0.45
1:A:556:LEU:O	1:A:560:THR:HG23	2.16	0.45
1:B:285:SER:HB3	1:B:302:VAL:HG21	1.98	0.45
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.98	0.45
1:C:670:GLY:C	1:C:672:MET:H	2.20	0.45
1:D:435:VAL:O	1:D:435:VAL:HG12	2.16	0.45
1:A:70:GLY:HA3	1:A:113:ASN:HD22	1.79	0.45
1:A:187:THR:HG21	1:A:223:TYR:HE2	1.82	0.45
1:A:258:GLU:O	1:A:262:ARG:HG3	2.17	0.45
1:A:39:MET:O	1:A:42:ALA:HB3	2.16	0.45
1:A:417:ASN:HD22	1:A:506:ILE:HB	1.82	0.45
1:B:450:PHE:HD1	1:B:482:VAL:O	2.00	0.45
1:B:515:LEU:HD11	1:B:534:MET:HB2	1.98	0.45
1:B:586:TYR:CG	1:B:743:HIS:HB3	2.51	0.45
1:C:519:SER:O	1:C:522:ARG:HD2	2.16	0.45
1:D:285:SER:HB3	1:D:302:VAL:HG21	1.99	0.45
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.99	0.45
1:D:59:PHE:O	1:D:74:ILE:HA	2.17	0.45
1:D:726:ASN:OD1	1:D:726:ASN:N	2.48	0.45
1:A:247:GLY:O	1:A:251:GLN:HG2	2.17	0.44
1:A:397:LEU:HD11	1:A:431:SER:HA	1.99	0.44
1:A:685:PHE:CE2	1:A:689:ILE:HG21	2.53	0.44
1:B:25:LYS:O	1:B:55:ALA:HB1	2.17	0.44
1:B:577:VAL:CG2	1:B:622:LEU:HD21	2.44	0.44
1:B:662:PHE:C	1:B:662:PHE:CD1	2.90	0.44
1:B:79:TRP:CZ2	1:B:763:LYS:CA	3.00	0.44
1:C:488:LEU:HD22	1:C:528:PHE:CE1	2.52	0.44
1:C:735:LEU:O	1:C:739:THR:HG22	2.17	0.44
1:A:174:ILE:CG2	1:A:190:ALA:HB2	2.48	0.44
1:A:284:THR:CG2	1:A:287:LYS:HB2	2.46	0.44
1:A:26:ALA:HA	1:A:56:LYS:O	2.16	0.44
1:B:533:VAL:HG21	1:B:693:ALA:HB1	1.99	0.44
1:C:50:GLY:O	1:C:53:VAL:HG23	2.18	0.44
1:C:83:SER:O	1:C:84:SER:HB3	2.18	0.44
1:D:583:MET:HA	1:D:639:GLU:HB2	1.98	0.44
1:A:696:TRP:CZ2	1:A:700:LYS:HD2	2.52	0.44
1:B:79:TRP:CE2	1:B:763:LYS:HB2	2.51	0.44
1:C:320:ILE:CD1	1:C:597:ALA:HB2	2.47	0.44
1:D:221:CYS:HA	1:D:383:ARG:HH21	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:TYR:C	1:D:512:TYR:CD1	2.91	0.44
1:D:521:ALA:O	1:D:525:HIS:HB2	2.17	0.44
1:D:530:VAL:HG12	1:D:531:PRO:HD2	1.99	0.44
1:D:579:ILE:HA	1:D:635:VAL:HG13	1.98	0.44
1:D:52:TYR:CD2	1:D:760:ILE:HB	2.52	0.44
1:B:215:GLU:OE1	1:B:304:ILE:HG12	2.18	0.44
1:C:165:LEU:HD13	1:C:167:VAL:HG13	2.00	0.44
1:D:387:PHE:HD2	1:D:387:PHE:O	2.01	0.44
1:A:496:ARG:HH21	1:A:496:ARG:HG3	1.83	0.44
1:B:138:ARG:HA	1:B:165:LEU:HD12	1.98	0.44
1:B:221:CYS:HA	1:B:383:ARG:HH21	1.82	0.44
1:B:483:LEU:CD2	1:B:513:LEU:HB3	2.48	0.44
1:C:223:TYR:C	1:C:225:ALA:N	2.69	0.44
1:D:266:LEU:HD11	1:D:268:ILE:HD11	1.99	0.44
1:D:293:VAL:HG23	1:D:298:TYR:O	2.18	0.44
1:D:416:ILE:HG22	1:D:505:ILE:HD13	1.99	0.44
1:A:285:SER:HB3	1:A:302:VAL:HG21	2.00	0.44
1:B:205:ALA:HB1	1:B:266:LEU:HD23	1.99	0.44
1:B:451:ASP:O	1:B:455:LYS:HG3	2.17	0.44
1:B:524:LYS:HD3	1:B:524:LYS:H	1.82	0.44
1:B:608:GLU:OE1	1:B:755:ARG:HG2	2.18	0.44
1:C:208:HIS:O	1:C:209:GLN:C	2.56	0.44
1:C:23:ALA:HA	1:C:54:GLY:O	2.17	0.44
1:C:326:GLY:O	1:C:330:VAL:HG23	2.18	0.44
1:C:578:PHE:C	1:C:579:ILE:HD12	2.38	0.44
1:D:27:ILE:HD12	1:D:27:ILE:H	1.83	0.44
1:D:479:THR:HG23	1:D:479:THR:O	2.16	0.44
1:D:495:MET:C	1:D:497:THR:H	2.21	0.44
1:D:413:VAL:HA	1:D:502:ALA:HB3	1.98	0.44
1:D:537:ALA:HA	1:D:550:ILE:HB	1.99	0.44
1:B:644:ASN:HD21	1:D:655:SER:HB3	1.83	0.44
1:A:306:GLY:O	1:A:308:VAL:N	2.51	0.44
1:A:720:LEU:HD13	1:A:729:PHE:CD2	2.53	0.44
1:A:78:ASP:OD2	1:A:78:ASP:N	2.43	0.44
1:B:209:GLN:HA	1:B:265:ARG:O	2.18	0.44
1:B:30:LEU:N	1:B:30:LEU:HD23	2.32	0.44
1:B:327:VAL:O	1:B:331:ILE:HG23	2.18	0.44
1:B:84:SER:C	1:B:87:GLN:HE22	2.21	0.44
1:C:221:CYS:HA	1:C:383:ARG:HH21	1.80	0.44
1:D:512:TYR:CE2	1:D:544:PRO:HG2	2.53	0.44
1:D:74:ILE:HG21	1:D:117:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HH22	1:A:267:ASN:HD22	1.66	0.44
1:B:223:TYR:C	1:B:225:ALA:N	2.70	0.44
1:B:27:ILE:HG12	1:B:333:LEU:HD13	1.99	0.44
1:B:554:THR:HG22	1:B:555:ALA:N	2.33	0.44
1:C:266:LEU:HD11	1:C:268:ILE:HD11	1.99	0.44
1:D:244:PRO:HB2	1:D:248:TRP:CG	2.53	0.44
1:D:26:ALA:HA	1:D:56:LYS:O	2.17	0.44
1:A:279:GLN:O	1:A:281:LYS:N	2.51	0.44
1:A:327:VAL:O	1:A:331:ILE:HG23	2.18	0.44
1:A:411:CYS:O	1:A:442:ARG:HG2	2.17	0.44
1:A:718:CYS:SG	1:A:731:PRO:HA	2.58	0.44
1:B:566:ILE:C	1:B:568:GLN:H	2.21	0.44
1:C:701:LEU:HD23	1:C:701:LEU:HA	1.89	0.44
1:A:370:ALA:HB2	1:A:375:ARG:NH1	2.33	0.43
1:A:414:ALA:HA	1:A:444:LEU:O	2.18	0.43
1:B:411:CYS:O	1:B:442:ARG:HG2	2.17	0.43
1:B:454:ALA:N	1:B:491:ILE:HD11	2.33	0.43
1:B:504:LEU:HD12	1:B:533:VAL:HG13	1.99	0.43
1:B:541:ASN:O	1:B:541:ASN:ND2	2.48	0.43
1:C:580:ILE:N	1:C:580:ILE:HD12	2.33	0.43
1:D:37:GLN:NE2	1:D:310:ARG:C	2.71	0.43
1:D:717:ILE:HG13	1:D:717:ILE:O	2.18	0.43
1:D:740:ASP:CG	1:D:743:HIS:HD1	2.21	0.43
1:A:193:ARG:O	1:A:197:VAL:HG23	2.18	0.43
1:A:211:THR:OG1	1:A:267:ASN:HB2	2.17	0.43
1:A:327:VAL:HG21	1:A:757:LEU:HD21	2.01	0.43
1:A:480:LYS:C	1:A:482:VAL:H	2.20	0.43
1:A:670:GLY:C	1:A:672:MET:H	2.21	0.43
1:B:370:ALA:CB	1:B:379:ALA:HB2	2.45	0.43
1:B:412:ASN:OD1	1:B:442:ARG:HD3	2.19	0.43
1:B:429:VAL:HG11	1:B:477:LEU:HD11	1.99	0.43
1:B:577:VAL:O	1:B:664:CYS:HA	2.18	0.43
1:C:70:GLY:HA3	1:C:113:ASN:HD22	1.83	0.43
1:C:414:ALA:O	1:C:503:LEU:HA	2.18	0.43
1:D:230:LEU:HG	1:D:394:TYR:HB2	2.00	0.43
1:D:244:PRO:HD2	1:D:277:ASP:HA	1.99	0.43
1:D:327:VAL:O	1:D:331:ILE:HG23	2.17	0.43
1:D:496:ARG:HD3	1:D:527:GLU:OE1	2.17	0.43
1:B:419:GLY:HA2	1:B:510:GLU:HG3	2.00	0.43
1:C:433:VAL:HG21	1:C:466:VAL:HG11	1.99	0.43
1:D:187:THR:HG21	1:D:223:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:GLY:HA3	1:D:200:ALA:O	2.18	0.43
1:A:209:GLN:HA	1:A:265:ARG:O	2.19	0.43
1:A:535:VAL:HG13	1:A:689:ILE:CD1	2.48	0.43
1:A:649:PHE:CD1	1:C:649:PHE:CD1	3.06	0.43
1:A:739:THR:HG23	1:A:741:PHE:CE1	2.53	0.43
1:D:27:ILE:HD13	1:D:57:VAL:CG1	2.47	0.43
1:D:738:GLN:O	1:D:738:GLN:HG2	2.18	0.43
1:A:244:PRO:HB2	1:A:248:TRP:CG	2.54	0.43
1:A:255:LYS:HE3	1:A:399:ILE:HD13	2.01	0.43
1:B:187:THR:HG21	1:B:223:TYR:HE2	1.82	0.43
1:B:217:MET:HG3	1:B:309:GLN:NE2	2.33	0.43
1:B:425:MET:HE2	1:B:475:SER:HB2	2.00	0.43
1:B:637:ARG:HE	1:B:647:THR:N	2.17	0.43
1:B:755:ARG:HA	1:B:755:ARG:HD2	1.70	0.43
1:C:262:ARG:HD3	1:C:464:THR:CG2	2.48	0.43
1:D:25:LYS:H	1:D:25:LYS:HG3	1.50	0.43
1:A:170:MET:HG3	1:A:345:VAL:HG23	2.01	0.43
1:B:67:MET:HE2	1:B:110:ALA:HB1	2.00	0.43
1:B:717:ILE:HG22	1:B:717:ILE:O	2.18	0.43
1:C:370:ALA:HB2	1:C:375:ARG:NH1	2.34	0.43
1:C:565:ARG:HG2	1:D:676:GLY:CA	2.49	0.43
1:C:579:ILE:HA	1:C:635:VAL:HG13	2.00	0.43
1:D:87:GLN:NE2	1:D:567:LYS:HE3	2.33	0.43
1:B:649:PHE:HD1	1:D:652:GLN:OE1	2.01	0.43
1:B:35:ASP:O	1:B:310:ARG:HD2	2.19	0.43
1:C:402:PRO:HB2	1:C:405:GLN:HG3	2.01	0.43
1:C:608:GLU:OE1	1:C:755:ARG:CG	2.66	0.43
1:C:568:GLN:HG3	1:D:474:GLY:HA3	2.01	0.43
1:A:477:LEU:N	1:A:477:LEU:HD12	2.33	0.43
1:A:59:PHE:O	1:A:74:ILE:HA	2.18	0.43
1:A:722:ILE:HD13	1:A:727:VAL:HG12	2.01	0.43
1:B:284:THR:O	1:B:288:ILE:HG13	2.18	0.43
1:B:493:THR:O	1:B:496:ARG:N	2.49	0.43
1:C:402:PRO:HG2	1:C:405:GLN:HG3	2.01	0.43
1:C:88:VAL:HG12	1:C:89:GLY:N	2.34	0.43
1:D:277:ASP:HB3	1:D:283:ILE:HD11	2.01	0.43
1:D:526:GLU:HA	1:D:529:CYS:SG	2.59	0.43
1:A:30:LEU:N	1:A:30:LEU:HD23	2.34	0.43
1:B:41:ALA:CB	1:B:86:LEU:HD12	2.48	0.43
1:C:601:ASP:O	1:C:602:ALA:HB2	2.19	0.43
1:A:438:ALA:HB2	1:A:463:TRP:HZ3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:VAL:HG23	1:B:293:VAL:N	2.34	0.43
1:B:331:ILE:O	1:B:335:GLU:HB2	2.19	0.43
1:C:308:VAL:HG12	1:D:201:ILE:HD11	2.00	0.43
1:C:30:LEU:HD23	1:C:30:LEU:N	2.33	0.43
1:C:49:MET:HG2	1:C:760:ILE:HD11	2.01	0.43
1:C:324:ARG:NE	1:C:754:LEU:HD21	2.34	0.43
1:D:148:LEU:HB3	1:D:154:ILE:CG2	2.47	0.43
1:D:481:ARG:HG3	1:D:510:GLU:HB3	2.00	0.43
1:D:519:SER:OG	1:D:717:ILE:HD11	2.18	0.43
1:A:610:PHE:CD1	1:A:610:PHE:N	2.87	0.42
1:A:685:PHE:HE2	1:A:689:ILE:HG21	1.84	0.42
1:B:121:ASN:OD1	1:B:166:ASN:HB2	2.18	0.42
1:B:247:GLY:O	1:B:251:GLN:HG2	2.19	0.42
1:B:321:LEU:O	1:B:321:LEU:HD23	2.19	0.42
1:B:567:LYS:HD3	1:B:632:ARG:NH1	2.33	0.42
1:B:68:VAL:O	1:B:109:LYS:HG3	2.19	0.42
1:B:702:LYS:HD2	1:B:705:ARG:HD2	2.01	0.42
1:C:25:LYS:HG2	1:C:120:THR:HG21	1.99	0.42
1:C:483:LEU:HD13	1:C:484:PRO:CD	2.47	0.42
1:C:739:THR:HG23	1:C:741:PHE:CE1	2.54	0.42
1:D:638:ASN:HB3	1:D:641:CYS:HB3	1.99	0.42
1:B:199:ASP:CG	1:B:683:ARG:HH22	2.23	0.42
1:B:279:GLN:O	1:B:281:LYS:N	2.52	0.42
1:B:629:THR:O	1:B:631:GLN:HG3	2.18	0.42
1:C:177:ASP:O	1:C:364:THR:HG23	2.19	0.42
1:C:42:ALA:HB1	1:C:170:MET:HE1	2.01	0.42
1:D:179:CYS:SG	1:D:363:MET:CB	3.07	0.42
1:D:443:MET:O	1:D:460:GLU:HG3	2.18	0.42
1:A:222:GLY:HA3	1:A:240:PRO:HD2	2.01	0.42
1:A:629:THR:O	1:A:631:GLN:HG3	2.19	0.42
1:B:222:GLY:HA3	1:B:240:PRO:HD2	2.01	0.42
1:B:337:THR:O	1:B:340:THR:HG22	2.19	0.42
1:C:541:ASN:ND2	1:C:541:ASN:O	2.53	0.42
1:C:86:LEU:HD21	1:C:597:ALA:O	2.19	0.42
1:D:223:TYR:O	1:D:225:ALA:N	2.52	0.42
1:D:402:PRO:HB2	1:D:405:GLN:HG3	2.00	0.42
1:D:637:ARG:CG	1:D:637:ARG:HH11	2.32	0.42
1:D:87:GLN:CD	1:D:87:GLN:H	2.23	0.42
1:A:357:LEU:O	1:A:361:VAL:HG23	2.19	0.42
1:B:164:TYR:CD2	1:B:338:PRO:HB3	2.54	0.42
1:C:223:TYR:C	1:C:225:ALA:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:MET:HG3	1:C:309:GLN:NE2	2.35	0.42
1:C:625:LYS:C	1:C:627:LYS:H	2.22	0.42
1:C:755:ARG:HA	1:C:755:ARG:HD2	1.83	0.42
1:D:540:SER:O	1:D:541:ASN:HB3	2.19	0.42
1:D:694:MET:O	1:D:697:ILE:HB	2.20	0.42
1:A:190:ALA:O	1:A:194:ILE:HG13	2.18	0.42
1:A:376:PHE:O	1:A:380:VAL:HG23	2.19	0.42
1:A:476:ILE:C	1:A:478:GLY:H	2.23	0.42
1:A:731:PRO:O	1:A:733:ALA:N	2.52	0.42
1:A:731:PRO:C	1:A:733:ALA:N	2.72	0.42
1:A:84:SER:C	1:A:87:GLN:HE22	2.23	0.42
1:B:28:GLY:HA3	1:B:122:LEU:HD12	2.01	0.42
1:B:441:HIS:NE2	1:B:698:THR:HG23	2.34	0.42
1:C:27:ILE:HG23	1:C:121:ASN:HB2	2.01	0.42
1:C:408:LYS:HG2	1:C:408:LYS:H	1.68	0.42
1:C:438:ALA:HB2	1:C:463:TRP:HZ3	1.84	0.42
1:C:662:PHE:CD1	1:C:662:PHE:C	2.93	0.42
1:D:492:ALA:HB2	1:D:528:PHE:CZ	2.55	0.42
1:D:78:ASP:OD2	1:D:78:ASP:N	2.42	0.42
1:A:171:VAL:HG23	1:A:171:VAL:O	2.19	0.42
1:A:380:VAL:C	1:A:382:LEU:H	2.22	0.42
1:A:422:ALA:HB2	1:A:538:THR:HA	2.01	0.42
1:A:411:CYS:SG	1:A:701:LEU:HD21	2.60	0.42
1:A:74:ILE:HG21	1:A:117:ARG:HG3	2.01	0.42
1:B:477:LEU:HD12	1:B:477:LEU:N	2.33	0.42
1:C:505:ILE:HD12	1:C:515:LEU:CD2	2.48	0.42
1:D:577:VAL:O	1:D:664:CYS:HA	2.20	0.42
1:A:277:ASP:HB3	1:A:283:ILE:HD11	2.00	0.42
1:A:580:ILE:HD12	1:A:580:ILE:N	2.34	0.42
1:B:112:CYS:HB2	1:B:148:LEU:CD2	2.49	0.42
1:C:21:SER:HB2	1:C:22:GLY:H	1.60	0.42
1:C:236:TRP:HZ3	1:C:399:ILE:HD11	1.85	0.42
1:C:492:ALA:O	1:C:495:MET:HB2	2.19	0.42
1:D:179:CYS:SG	1:D:363:MET:HB2	2.59	0.42
1:D:380:VAL:C	1:D:382:LEU:H	2.23	0.42
1:A:537:ALA:HA	1:A:550:ILE:HB	2.01	0.42
1:A:630:ILE:H	1:A:630:ILE:CD1	2.18	0.42
1:B:127:GLY:HA3	2:B:801:ADP:O2B	2.19	0.42
1:C:307:HIS:NE2	1:D:301:ARG:HG2	2.34	0.42
1:C:355:LEU:HB3	1:C:356:PRO:HD2	2.01	0.42
1:C:241:GLU:O	1:C:376:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:VAL:O	1:C:435:VAL:HG12	2.20	0.42
1:C:667:ASN:HD22	1:C:667:ASN:HA	1.64	0.42
1:C:84:SER:HB2	1:C:632:ARG:HH22	1.83	0.42
1:D:478:GLY:O	1:D:479:THR:HB	2.19	0.42
1:D:547:ASP:HB3	1:D:750:TRP:NE1	2.35	0.42
1:A:156:LYS:HD2	1:A:156:LYS:HA	1.84	0.42
1:A:447:TYR:HD2	1:A:477:LEU:HA	1.83	0.42
1:C:293:VAL:HG23	1:C:298:TYR:O	2.20	0.42
1:C:402:PRO:HG2	1:C:405:GLN:CD	2.40	0.42
1:C:521:ALA:O	1:C:528:PHE:HD1	2.02	0.42
1:D:413:VAL:HG22	1:D:502:ALA:HB3	2.01	0.42
1:D:416:ILE:CG2	1:D:505:ILE:HD13	2.50	0.42
1:D:534:MET:HB2	1:D:534:MET:HE2	1.87	0.42
1:D:670:GLY:C	1:D:672:MET:H	2.23	0.42
1:A:729:PHE:N	1:A:729:PHE:CD1	2.87	0.42
1:B:148:LEU:HB3	1:B:154:ILE:CG2	2.49	0.42
1:C:179:CYS:SG	1:C:363:MET:CB	3.08	0.42
1:C:244:PRO:HB2	1:C:248:TRP:CG	2.55	0.42
1:C:422:ALA:O	1:C:425:MET:HB2	2.20	0.42
1:C:48:ARG:HD3	1:C:761:LEU:O	2.20	0.42
1:C:729:PHE:N	1:C:729:PHE:CD1	2.88	0.42
1:C:717:ILE:O	1:C:732:VAL:HG22	2.20	0.42
1:D:567:LYS:HD3	1:D:632:ARG:CD	2.50	0.42
1:D:61:TYR:HA	1:D:93:ILE:O	2.20	0.42
1:A:637:ARG:HE	1:A:647:THR:N	2.18	0.41
1:B:156:LYS:HD2	1:B:156:LYS:HA	1.85	0.41
1:B:504:LEU:CD1	1:B:533:VAL:HG13	2.50	0.41
1:B:504:LEU:HD22	1:B:694:MET:CE	2.50	0.41
1:C:412:ASN:OD1	1:C:442:ARG:CD	2.63	0.41
1:C:412:ASN:ND2	1:C:498:HIS:O	2.53	0.41
1:D:205:ALA:HB3	1:D:266:LEU:HD23	2.02	0.41
1:D:717:ILE:O	1:D:732:VAL:HG22	2.21	0.41
1:B:223:TYR:C	1:B:225:ALA:H	2.24	0.41
1:B:59:PHE:O	1:B:74:ILE:HA	2.19	0.41
1:B:656:GLU:HB2	1:D:644:ASN:HD22	1.84	0.41
1:C:648:ASP:O	1:C:652:GLN:HG3	2.20	0.41
1:D:174:ILE:CG2	1:D:190:ALA:HB2	2.50	0.41
1:D:387:PHE:C	1:D:387:PHE:CD2	2.93	0.41
1:A:406:ILE:HG22	1:A:406:ILE:O	2.20	0.41
1:A:501:ASN:O	1:A:531:PRO:HD2	2.19	0.41
1:A:546:SER:HA	1:A:722:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LYS:C	1:B:266:LEU:H	2.24	0.41
1:B:214:LEU:HB3	1:B:305:LEU:HD11	2.02	0.41
1:B:530:VAL:HA	1:B:711:PHE:CD2	2.55	0.41
1:C:370:ALA:CB	1:C:379:ALA:HB2	2.49	0.41
1:C:74:ILE:HG21	1:C:117:ARG:HG3	2.02	0.41
1:D:208:HIS:C	1:D:209:GLN:HG2	2.40	0.41
1:D:294:THR:O	1:D:294:THR:HG23	2.19	0.41
1:D:48:ARG:NE	1:D:79:TRP:NE1	2.68	0.41
1:A:219:ARG:HG3	1:A:273:GLU:CD	2.38	0.41
1:A:432:ALA:HB1	1:A:504:LEU:HD23	2.02	0.41
1:A:717:ILE:O	1:A:732:VAL:HG13	2.20	0.41
1:B:357:LEU:O	1:B:361:VAL:HG23	2.20	0.41
1:B:430:ARG:HH21	1:B:470:THR:CG2	2.33	0.41
1:C:176:ASN:C	1:C:178:PHE:N	2.72	0.41
1:D:354:ARG:O	1:D:355:LEU:HD23	2.20	0.41
1:D:735:LEU:O	1:D:739:THR:CG2	2.67	0.41
1:A:264:LYS:C	1:A:266:LEU:H	2.24	0.41
1:A:478:GLY:O	1:A:479:THR:HB	2.20	0.41
1:A:88:VAL:HG12	1:A:89:GLY:N	2.35	0.41
1:B:622:LEU:O	1:B:626:MET:HG2	2.20	0.41
1:B:65:GLN:HG2	1:B:98:CYS:CB	2.50	0.41
1:B:731:PRO:C	1:B:733:ALA:N	2.74	0.41
1:D:176:ASN:C	1:D:178:PHE:N	2.73	0.41
1:D:512:TYR:HD1	1:D:512:TYR:C	2.24	0.41
1:A:494:GLN:C	1:A:497:THR:HG22	2.41	0.41
1:A:86:LEU:HD21	1:A:597:ALA:O	2.20	0.41
1:A:129:GLY:N	2:A:801:ADP:O3B	2.53	0.41
1:B:412:ASN:ND2	1:B:442:ARG:HH11	2.17	0.41
1:D:223:TYR:C	1:D:225:ALA:N	2.74	0.41
1:D:424:GLY:CA	1:D:678:PRO:HB3	2.50	0.41
1:D:481:ARG:HD3	1:D:510:GLU:OE1	2.20	0.41
1:D:731:PRO:C	1:D:733:ALA:N	2.74	0.41
1:B:138:ARG:HH11	1:B:342:ALA:HA	1.86	0.41
1:B:268:ILE:HD12	1:B:268:ILE:H	1.85	0.41
1:B:284:THR:CG2	1:B:287:LYS:HB2	2.51	0.41
1:B:397:LEU:HD21	1:B:430:ARG:NH2	2.36	0.41
1:C:52:TYR:CE2	1:C:760:ILE:HB	2.56	0.41
1:D:586:TYR:HB2	1:D:743:HIS:O	2.21	0.41
1:A:122:LEU:O	1:A:167:VAL:HA	2.21	0.41
1:A:30:LEU:HB3	1:A:60:ILE:HB	2.02	0.41
1:B:122:LEU:O	1:B:167:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLY:O	1:B:173:SER:HB2	2.19	0.41
1:B:476:ILE:C	1:B:478:GLY:H	2.22	0.41
1:B:524:LYS:CD	1:B:524:LYS:H	2.34	0.41
1:C:130:SER:HB2	2:C:801:ADP:O2A	2.20	0.41
1:C:201:ILE:HD11	1:D:308:VAL:CG1	2.50	0.41
1:C:354:ARG:O	1:C:355:LEU:HD23	2.21	0.41
1:C:512:TYR:O	1:C:516:LEU:HD23	2.21	0.41
1:C:731:PRO:C	1:C:733:ALA:N	2.74	0.41
1:D:79:TRP:CZ2	1:D:763:LYS:HA	2.55	0.41
1:A:334:LEU:HG	1:A:334:LEU:H	1.68	0.41
1:A:164:TYR:CD2	1:A:338:PRO:HB3	2.56	0.41
1:A:447:TYR:CD2	1:A:477:LEU:HA	2.56	0.41
1:A:755:ARG:N	1:A:756:PRO:HD2	2.35	0.41
1:C:214:LEU:N	1:C:214:LEU:CD1	2.84	0.41
1:C:216:VAL:HG21	1:C:225:ALA:HA	2.01	0.41
1:C:264:LYS:C	1:C:266:LEU:H	2.23	0.41
1:D:209:GLN:HA	1:D:265:ARG:O	2.20	0.41
1:D:254:VAL:O	1:D:258:GLU:HG3	2.20	0.41
1:D:284:THR:CG2	1:D:287:LYS:HB2	2.51	0.41
1:D:387:PHE:C	1:D:387:PHE:HD2	2.24	0.41
1:D:486:LYS:C	1:D:487:TYR:HD2	2.24	0.41
1:D:712:THR:O	1:D:713:THR:C	2.58	0.41
1:A:331:ILE:O	1:A:335:GLU:HB2	2.21	0.41
1:A:697:ILE:O	1:A:701:LEU:N	2.51	0.41
1:B:412:ASN:HB2	1:B:499:SER:O	2.21	0.41
1:B:485:GLY:O	1:B:488:LEU:HB2	2.21	0.41
1:B:755:ARG:N	1:B:756:PRO:HD2	2.36	0.41
1:A:67:MET:HB3	1:A:67:MET:HE2	1.92	0.41
1:B:223:TYR:O	1:B:225:ALA:N	2.54	0.41
1:C:515:LEU:HB3	1:C:717:ILE:CG2	2.51	0.41
1:C:539:VAL:HG11	1:C:674:GLN:CB	2.36	0.41
1:C:580:ILE:HG23	1:C:669:LEU:HG	2.03	0.41
1:D:222:GLY:HA3	1:D:240:PRO:HD2	2.01	0.41
1:D:266:LEU:CD1	1:D:268:ILE:HD11	2.51	0.41
1:D:579:ILE:HG13	1:D:635:VAL:HG13	2.02	0.41
1:D:67:MET:HB3	1:D:67:MET:HE2	1.89	0.41
1:D:67:MET:HE3	1:D:114:LEU:HG	2.02	0.41
1:A:251:GLN:O	1:A:254:VAL:HB	2.21	0.40
1:A:81:SER:C	1:A:83:SER:H	2.24	0.40
1:B:511:ALA:HB1	1:B:534:MET:HG3	2.03	0.40
1:C:111:ALA:O	1:C:115:LEU:HD22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLU:OE1	1:C:304:ILE:HG12	2.21	0.40
1:C:530:VAL:HB	1:C:531:PRO:HD2	2.02	0.40
1:C:78:ASP:OD2	1:C:81:SER:HB2	2.21	0.40
1:D:239:LEU:HA	1:D:240:PRO:HD3	1.86	0.40
1:D:416:ILE:HG12	1:D:417:ASN:N	2.36	0.40
1:D:750:TRP:CD2	1:D:751:TRP:N	2.89	0.40
1:A:255:LYS:HB2	1:A:255:LYS:HE2	1.91	0.40
1:A:425:MET:CE	1:A:475:SER:HB2	2.49	0.40
1:A:615:LEU:O	1:A:619:VAL:HG23	2.22	0.40
1:A:722:ILE:HD13	1:A:727:VAL:CG1	2.51	0.40
1:B:141:TRP:CG	1:B:165:LEU:HB2	2.56	0.40
1:B:577:VAL:HG22	1:B:633:GLY:HA3	2.03	0.40
1:C:139:LYS:HD3	1:C:139:LYS:HA	1.80	0.40
1:C:174:ILE:CG2	1:C:190:ALA:HB2	2.50	0.40
1:C:205:ALA:HB1	1:C:266:LEU:HD23	2.03	0.40
1:C:268:ILE:HD12	1:C:268:ILE:H	1.86	0.40
1:C:473:GLY:HA3	1:C:678:PRO:HD3	2.03	0.40
1:A:430:ARG:HA	1:A:466:VAL:HB	2.02	0.40
1:B:502:ALA:HB1	1:B:697:ILE:CG2	2.51	0.40
1:C:307:HIS:C	1:C:309:GLN:H	2.24	0.40
1:C:506:ILE:HG22	1:C:537:ALA:CB	2.52	0.40
1:D:251:GLN:OE1	1:D:251:GLN:HA	2.21	0.40
1:D:534:MET:HB3	1:D:534:MET:HE2	1.86	0.40
1:D:83:SER:O	1:D:84:SER:CB	2.69	0.40
1:A:111:ALA:O	1:A:115:LEU:HD22	2.21	0.40
1:A:224:LEU:HA	1:A:227:VAL:CG2	2.51	0.40
1:A:579:ILE:HD12	1:A:579:ILE:N	2.36	0.40
1:B:728:ILE:HA	1:B:728:ILE:HD12	1.97	0.40
1:B:756:PRO:HG2	1:B:757:LEU:H	1.86	0.40
1:C:25:LYS:HB3	1:C:120:THR:CG2	2.50	0.40
1:C:425:MET:HE1	1:C:475:SER:HB2	2.03	0.40
1:C:476:ILE:C	1:C:478:GLY:H	2.23	0.40
1:C:544:PRO:HB3	1:C:746:PRO:HB3	2.04	0.40
1:D:531:PRO:HD3	1:D:711:PHE:CD1	2.57	0.40
1:D:81:SER:C	1:D:83:SER:H	2.25	0.40
1:A:179:CYS:SG	1:A:363:MET:HB2	2.62	0.40
1:A:491:ILE:HG22	1:A:492:ALA:N	2.36	0.40
1:A:496:ARG:C	1:A:498:HIS:H	2.25	0.40
1:A:530:VAL:HB	1:A:531:PRO:CD	2.47	0.40
1:A:577:VAL:O	1:A:664:CYS:HA	2.21	0.40
1:B:239:LEU:HA	1:B:240:PRO:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:TYR:HE2	1:B:664:CYS:O	2.03	0.40
1:B:586:TYR:CE1	1:B:743:HIS:HD2	2.40	0.40
1:C:667:ASN:OD1	1:D:670:GLY:HA3	2.22	0.40
1:C:390:ASN:OD1	1:C:688:LYS:HE2	2.21	0.40
1:D:156:LYS:HD2	1:D:156:LYS:HA	1.82	0.40
1:D:23:ALA:O	1:D:25:LYS:HG3	2.21	0.40
1:D:512:TYR:HA	1:D:534:MET:HE3	2.03	0.40
1:D:506:ILE:HG23	1:D:537:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	731/812 (90%)	610 (83%)	95 (13%)	26 (4%)	3	21
1	B	745/812 (92%)	631 (85%)	87 (12%)	27 (4%)	3	21
1	C	739/812 (91%)	620 (84%)	97 (13%)	22 (3%)	4	23
1	D	739/812 (91%)	618 (84%)	101 (14%)	20 (3%)	5	26
All	All	2954/3248 (91%)	2479 (84%)	380 (13%)	95 (3%)	4	22

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	724	LYS
1	B	724	LYS
1	C	19	HIS
1	C	724	LYS
1	D	714	ASP
1	A	402	PRO

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Mol	Chain	Res	Type
1	A	523	GLU
1	A	659	LYS
1	A	675	GLY
1	B	69	ASP
1	B	374	ARG
1	B	402	PRO
1	B	485	GLY
1	B	659	LYS
1	B	675	GLY
1	B	676	GLY
1	C	69	ASP
1	C	486	LYS
1	C	659	LYS
1	C	675	GLY
1	D	69	ASP
1	D	280	ASN
1	D	307	HIS
1	D	402	PRO
1	D	659	LYS
1	D	675	GLY
1	D	724	LYS
1	D	751	TRP
1	A	19	HIS
1	A	34	GLY
1	A	158	ALA
1	A	280	ASN
1	A	307	HIS
1	A	751	TRP
1	A	762	ALA
1	B	82	VAL
1	B	280	ASN
1	B	490	GLU
1	B	524	LYS
1	B	703	GLU
1	B	751	TRP
1	C	35	ASP
1	C	82	VAL
1	C	173	SER
1	C	185	ILE
1	C	307	HIS
1	C	402	PRO
1	C	524	LYS

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Mol	Chain	Res	Type
1	D	82	VAL
1	D	100	ALA
1	D	466	VAL
1	D	676	GLY
1	D	713	THR
1	D	715	ASP
1	A	18	GLU
1	A	35	ASP
1	A	265	ARG
1	A	396	ARG
1	A	466	VAL
1	A	676	GLY
1	B	35	ASP
1	B	100	ALA
1	B	173	SER
1	B	185	ILE
1	B	265	ARG
1	B	307	HIS
1	B	466	VAL
1	B	479	THR
1	C	34	GLY
1	C	100	ALA
1	C	280	ASN
1	D	34	GLY
1	D	35	ASP
1	D	498	HIS
1	A	82	VAL
1	A	295	GLN
1	A	479	THR
1	A	485	GLY
1	A	527	GLU
1	B	626	MET
1	C	265	ARG
1	C	466	VAL
1	C	607	GLU
1	D	265	ARG
1	A	100	ALA
1	B	489	GLU
1	C	751	TRP
1	C	306	GLY
1	C	485	GLY
1	D	306	GLY

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Mol	Chain	Res	Type
1	B	34	GLY
1	B	306	GLY
1	A	185	ILE
1	B	584	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	594/658 (90%)	516 (87%)	78 (13%)	4	15
1	B	602/658 (92%)	529 (88%)	73 (12%)	5	18
1	C	598/658 (91%)	518 (87%)	80 (13%)	4	15
1	D	598/658 (91%)	517 (86%)	81 (14%)	4	14
All	All	2392/2632 (91%)	2080 (87%)	312 (13%)	4	16

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	25	LYS
1	A	49	MET
1	A	53	VAL
1	A	57	VAL
1	A	65	GLN
1	A	86	LEU
1	A	97	ARG
1	A	105	GLU
1	A	108	LEU
1	A	128	ASP
1	A	138	ARG
1	A	154	ILE
1	A	179	CYS
1	A	191	LEU
1	A	192	HIS
1	A	206	GLN

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	230	LEU
1	A	249	GLU
1	A	260	ARG
1	A	265	ARG
1	A	266	LEU
1	A	268	ILE
1	A	293	VAL
1	A	301	ARG
1	A	303	THR
1	A	313	THR
1	A	318	ASP
1	A	325	MET
1	A	331	ILE
1	A	334	LEU
1	A	343	CYS
1	A	365	GLN
1	A	374	ARG
1	A	382	LEU
1	A	387	PHE
1	A	391	LEU
1	A	396	ARG
1	A	401	LEU
1	A	402	PRO
1	A	403	ASP
1	A	439	ASP
1	A	453	PHE
1	A	470	THR
1	A	481	ARG
1	A	483	LEU
1	A	489	GLU
1	A	510	GLU
1	A	516	LEU
1	A	541	ASN
1	A	557	ASN
1	A	567	LYS
1	A	574	LYS
1	A	575	ARG
1	A	582	THR
1	A	592	ASN
1	A	610	PHE
1	A	611	ASP

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Mol	Chain	Res	Type
1	A	616	GLN
1	A	617	SER
1	A	624	GLU
1	A	631	GLN
1	A	635	VAL
1	A	637	ARG
1	A	659	LYS
1	A	671	HIS
1	A	674	GLN
1	A	689	ILE
1	A	690	SER
1	A	714	ASP
1	A	715	ASP
1	A	717	ILE
1	A	748	GLU
1	A	755	ARG
1	A	760	ILE
1	A	761	LEU
1	A	763	LYS
1	B	13	LEU
1	B	27	ILE
1	B	49	MET
1	B	53	VAL
1	B	59	PHE
1	B	65	GLN
1	B	86	LEU
1	B	108	LEU
1	B	128	ASP
1	B	138	ARG
1	B	154	ILE
1	B	165	LEU
1	B	179	CYS
1	B	191	LEU
1	B	192	HIS
1	B	214	LEU
1	B	230	LEU
1	B	249	GLU
1	B	260	ARG
1	B	265	ARG
1	B	266	LEU
1	B	268	ILE
1	B	293	VAL

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Mol	Chain	Res	Type
1	B	301	ARG
1	B	303	THR
1	B	313	THR
1	B	318	ASP
1	B	325	MET
1	B	331	ILE
1	B	334	LEU
1	B	343	CYS
1	B	362	GLN
1	B	365	GLN
1	B	382	LEU
1	B	387	PHE
1	B	391	LEU
1	B	395	LYS
1	B	396	ARG
1	B	401	LEU
1	B	404	ASP
1	B	439	ASP
1	B	453	PHE
1	B	470	THR
1	B	487	TYR
1	B	501	ASN
1	B	517	GLU
1	B	524	LYS
1	B	530	VAL
1	B	541	ASN
1	B	557	ASN
1	B	563	CYS
1	B	567	LYS
1	B	569	SER
1	B	576	ARG
1	B	582	THR
1	B	592	ASN
1	B	610	PHE
1	B	618	ASN
1	B	631	GLN
1	B	635	VAL
1	B	637	ARG
1	B	659	LYS
1	B	665	ARG
1	B	671	HIS
1	B	674	GLN

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Mol	Chain	Res	Type
1	B	690	SER
1	B	701	LEU
1	B	702	LYS
1	B	738	GLN
1	B	755	ARG
1	B	757	LEU
1	B	758	MET
1	B	760	ILE
1	C	16	PHE
1	C	18	GLU
1	C	19	HIS
1	C	21	SER
1	C	27	ILE
1	C	49	MET
1	C	57	VAL
1	C	59	PHE
1	C	65	GLN
1	C	86	LEU
1	C	87	GLN
1	C	108	LEU
1	C	128	ASP
1	C	130	SER
1	C	138	ARG
1	C	139	LYS
1	C	146	GLU
1	C	154	ILE
1	C	179	CYS
1	C	191	LEU
1	C	192	HIS
1	C	214	LEU
1	C	219	ARG
1	C	230	LEU
1	C	249	GLU
1	C	258	GLU
1	C	260	ARG
1	C	265	ARG
1	C	266	LEU
1	C	268	ILE
1	C	293	VAL
1	C	301	ARG
1	C	303	THR
1	C	308	VAL

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Mol	Chain	Res	Type
1	C	318	ASP
1	C	325	MET
1	C	331	ILE
1	C	334	LEU
1	C	343	CYS
1	C	351	HIS
1	C	358	MET
1	C	365	GLN
1	C	374	ARG
1	C	382	LEU
1	C	385	ARG
1	C	387	PHE
1	C	391	LEU
1	C	396	ARG
1	C	401	LEU
1	C	403	ASP
1	C	439	ASP
1	C	453	PHE
1	C	457	GLN
1	C	470	THR
1	C	503	LEU
1	C	524	LYS
1	C	526	GLU
1	C	530	VAL
1	C	541	ASN
1	C	557	ASN
1	C	568	GLN
1	C	575	ARG
1	C	582	THR
1	C	583	MET
1	C	592	ASN
1	C	610	PHE
1	C	624	GLU
1	C	631	GLN
1	C	635	VAL
1	C	637	ARG
1	C	659	LYS
1	C	674	GLN
1	C	689	ILE
1	C	690	SER
1	C	711	PHE
1	C	715	ASP

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Mol	Chain	Res	Type
1	C	755	ARG
1	C	757	LEU
1	C	760	ILE
1	C	761	LEU
1	D	16	PHE
1	D	20	LEU
1	D	27	ILE
1	D	29	VAL
1	D	44	ARG
1	D	49	MET
1	D	53	VAL
1	D	59	PHE
1	D	65	GLN
1	D	86	LEU
1	D	87	GLN
1	D	97	ARG
1	D	99	GLN
1	D	108	LEU
1	D	128	ASP
1	D	130	SER
1	D	138	ARG
1	D	142	SER
1	D	154	ILE
1	D	179	CYS
1	D	191	LEU
1	D	192	HIS
1	D	206	GLN
1	D	214	LEU
1	D	219	ARG
1	D	230	LEU
1	D	249	GLU
1	D	260	ARG
1	D	265	ARG
1	D	266	LEU
1	D	268	ILE
1	D	293	VAL
1	D	301	ARG
1	D	303	THR
1	D	318	ASP
1	D	325	MET
1	D	331	ILE
1	D	334	LEU

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Mol	Chain	Res	Type
1	D	351	HIS
1	D	365	GLN
1	D	374	ARG
1	D	382	LEU
1	D	385	ARG
1	D	387	PHE
1	D	396	ARG
1	D	401	LEU
1	D	403	ASP
1	D	439	ASP
1	D	453	PHE
1	D	470	THR
1	D	475	SER
1	D	487	TYR
1	D	488	LEU
1	D	489	GLU
1	D	510	GLU
1	D	512	TYR
1	D	516	LEU
1	D	519	SER
1	D	530	VAL
1	D	534	MET
1	D	540	SER
1	D	541	ASN
1	D	557	ASN
1	D	567	LYS
1	D	582	THR
1	D	592	ASN
1	D	610	PHE
1	D	624	GLU
1	D	630	ILE
1	D	637	ARG
1	D	671	HIS
1	D	674	GLN
1	D	690	SER
1	D	701	LEU
1	D	714	ASP
1	D	715	ASP
1	D	718	CYS
1	D	755	ARG
1	D	757	LEU
1	D	760	ILE

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Mol	Chain	Res	Type
1	D	763	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	73	ASN
1	A	87	GLN
1	A	116	GLN
1	A	135	ASN
1	A	206	GLN
1	A	417	ASN
1	A	616	GLN
1	A	618	ASN
1	A	667	ASN
1	A	674	GLN
1	B	65	GLN
1	B	113	ASN
1	B	116	GLN
1	B	135	ASN
1	B	153	GLN
1	B	192	HIS
1	B	208	HIS
1	B	267	ASN
1	B	417	ASN
1	B	568	GLN
1	B	644	ASN
1	B	652	GLN
1	B	673	GLN
1	C	65	GLN
1	C	73	ASN
1	C	113	ASN
1	C	116	GLN
1	C	153	GLN
1	C	192	HIS
1	C	295	GLN
1	C	365	GLN
1	C	457	GLN
1	C	498	HIS
1	C	592	ASN
1	C	616	GLN
1	C	652	GLN

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Mol	Chain	Res	Type
1	D	65	GLN
1	D	73	ASN
1	D	113	ASN
1	D	116	GLN
1	D	135	ASN
1	D	153	GLN
1	D	192	HIS
1	D	206	GLN
1	D	208	HIS
1	D	417	ASN
1	D	457	GLN
1	D	494	GLN
1	D	498	HIS
1	D	541	ASN
1	D	592	ASN
1	D	667	ASN
1	D	674	GLN
1	D	730	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	804	-	4,4,4	1.64	1 (25%)	6,6,6	0.46	0
3	PO4	D	804	-	4,4,4	1.56	0	6,6,6	0.45	0
3	PO4	C	804	-	4,4,4	1.47	0	6,6,6	0.42	0
3	PO4	A	803	-	4,4,4	1.39	0	6,6,6	0.40	0
3	PO4	D	801	-	4,4,4	1.54	0	6,6,6	0.46	0
3	PO4	C	803	-	4,4,4	1.57	0	6,6,6	0.51	0
3	PO4	C	802	-	4,4,4	1.64	1 (25%)	6,6,6	0.40	0
2	ADP	A	801	-	24,29,29	1.33	2 (8%)	29,45,45	1.26	4 (13%)
3	PO4	A	802	-	4,4,4	1.64	0	6,6,6	0.45	0
2	ADP	C	801	-	24,29,29	1.51	3 (12%)	29,45,45	1.18	3 (10%)
3	PO4	B	802	-	4,4,4	1.51	0	6,6,6	0.41	0
2	ADP	B	801	-	24,29,29	1.67	4 (16%)	29,45,45	1.25	4 (13%)
2	ADP	D	802	-	24,29,29	1.84	5 (20%)	29,45,45	1.37	4 (13%)
3	PO4	B	803	-	4,4,4	1.52	0	6,6,6	0.44	0
3	PO4	C	805	-	4,4,4	1.56	0	6,6,6	0.41	0
3	PO4	D	803	-	4,4,4	1.61	1 (25%)	6,6,6	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	801	-	-	4/12/32/32	0/3/3/3
2	ADP	C	801	-	-	3/12/32/32	0/3/3/3
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
2	ADP	D	802	-	-	1/12/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ADP	PB-O1B	6.40	1.71	1.50
2	B	801	ADP	PB-O1B	5.95	1.69	1.50
2	C	801	ADP	PB-O3B	3.85	1.69	1.54
2	A	801	ADP	PB-O3B	3.54	1.68	1.54
2	D	802	ADP	O4'-C1'	3.47	1.45	1.41
2	A	801	ADP	O4'-C1'	3.36	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ADP	C4-N3	2.98	1.39	1.35
2	B	801	ADP	C4-N3	2.67	1.39	1.35
2	C	801	ADP	O4'-C1'	2.60	1.44	1.41
2	B	801	ADP	O4'-C1'	2.37	1.44	1.41
2	D	802	ADP	C4-N3	2.26	1.38	1.35
3	D	803	PO4	P-O2	-2.20	1.48	1.54
2	D	802	ADP	C2-N3	2.18	1.35	1.32
3	A	804	PO4	P-O4	-2.04	1.48	1.54
3	C	802	PO4	P-O4	-2.04	1.48	1.54
2	D	802	ADP	PB-O2B	-2.03	1.47	1.54
2	B	801	ADP	C2-N3	2.01	1.35	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	O2B-PB-O3A	3.38	115.98	104.64
2	C	801	ADP	C5-C6-N6	3.25	125.29	120.35
2	D	802	ADP	O5'-C5'-C4'	3.18	119.92	108.99
2	D	802	ADP	C5-C6-N6	3.16	125.16	120.35
2	C	801	ADP	O2B-PB-O3A	2.80	114.03	104.64
2	B	801	ADP	O2B-PB-O3A	2.76	113.88	104.64
2	D	802	ADP	O2B-PB-O3A	2.74	113.83	104.64
2	A	801	ADP	O5'-C5'-C4'	2.74	118.42	108.99
2	B	801	ADP	C5-C6-N6	2.56	124.25	120.35
2	A	801	ADP	C5-C6-N6	2.54	124.21	120.35
2	C	801	ADP	O5'-C5'-C4'	2.47	117.50	108.99
2	B	801	ADP	O5'-C5'-C4'	2.38	117.17	108.99
2	B	801	ADP	O3B-PB-O3A	2.23	112.10	104.64
2	A	801	ADP	O4'-C1'-C2'	-2.12	103.83	106.93
2	D	802	ADP	O2B-PB-O1B	-2.09	102.49	110.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	C5'-O5'-PA-O1A
2	C	801	ADP	C3'-C4'-C5'-O5'
2	C	801	ADP	O4'-C4'-C5'-O5'
2	C	801	ADP	C4'-C5'-O5'-PA
2	A	801	ADP	C5'-O5'-PA-O3A
2	D	802	ADP	C5'-O5'-PA-O3A

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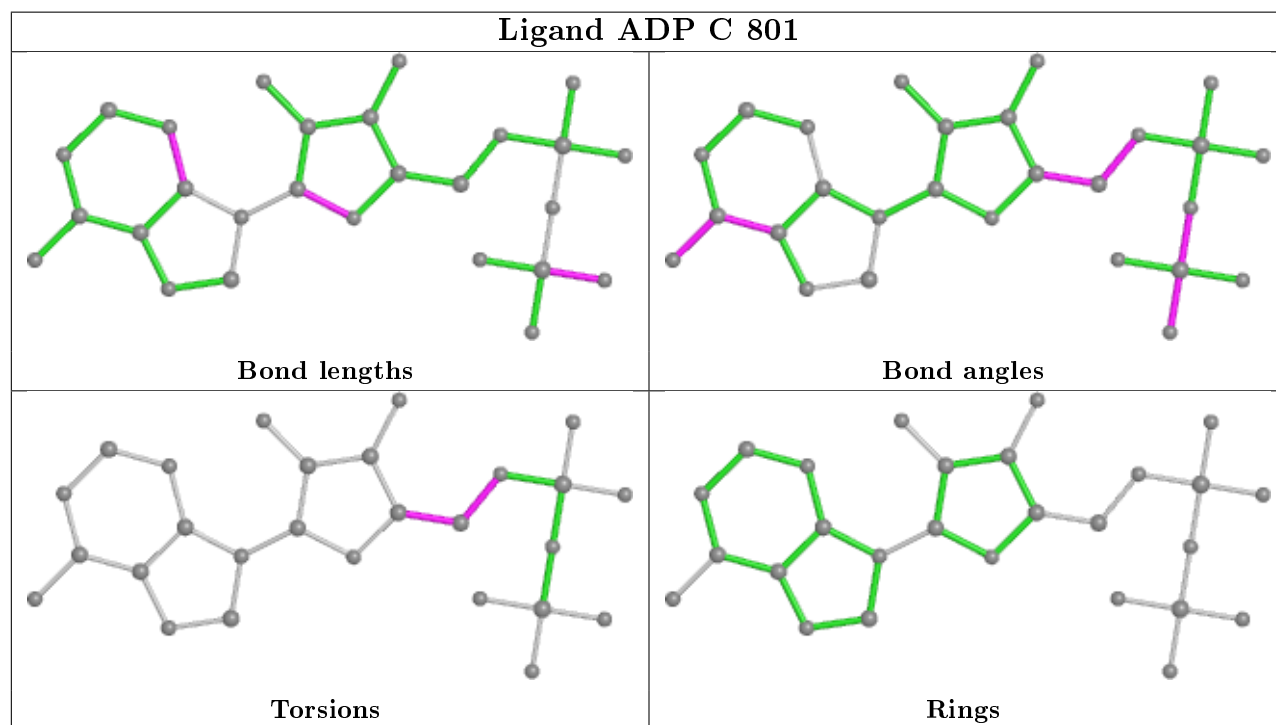
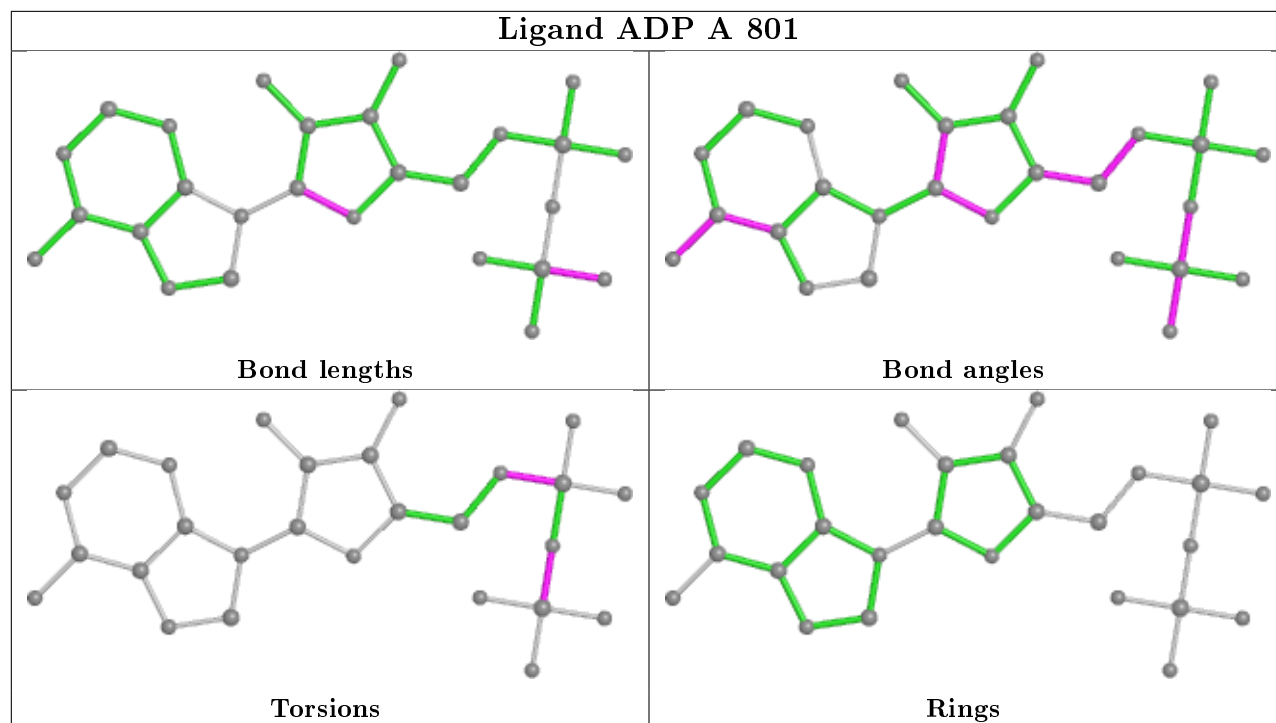
Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O3B

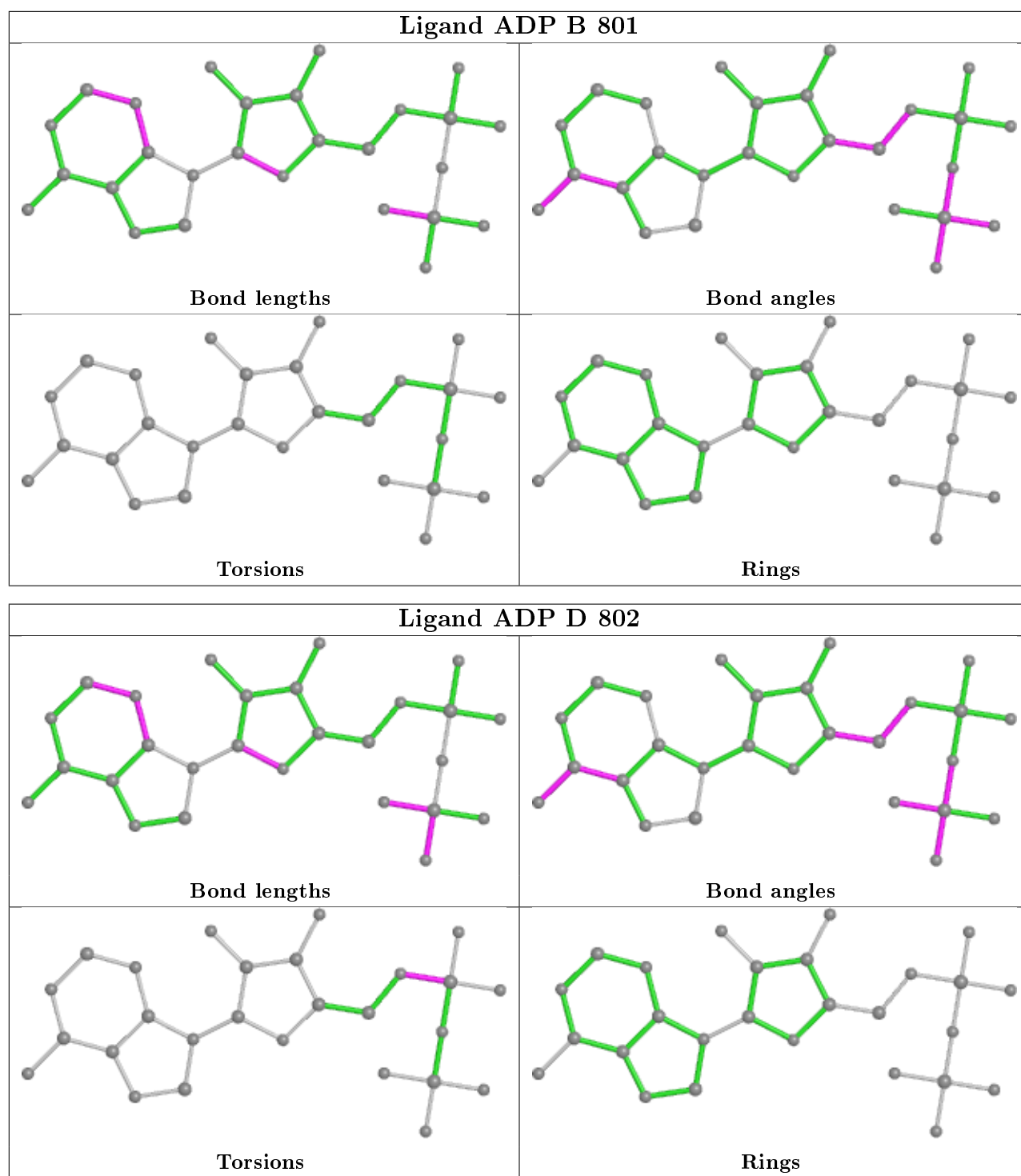
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	PO4	2	0
3	D	801	PO4	1	0
2	A	801	ADP	2	0
2	C	801	ADP	1	0
2	B	801	ADP	1	0
3	C	805	PO4	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.





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	737/812 (90%)	-0.17	4 (0%) 91 90	27, 73, 113, 162	0
1	B	749/812 (92%)	-0.11	7 (0%) 84 83	25, 75, 114, 162	0
1	C	743/812 (91%)	-0.16	2 (0%) 94 93	26, 73, 112, 161	0
1	D	743/812 (91%)	-0.14	4 (0%) 91 90	29, 74, 113, 162	0
All	All	2972/3248 (91%)	-0.14	17 (0%) 89 89	25, 74, 113, 162	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.2
1	D	343	CYS	2.9
1	B	59	PHE	2.8
1	B	205	ALA	2.8
1	B	206	GLN	2.5
1	C	347	LEU	2.5
1	B	621	HIS	2.5
1	A	246	GLU	2.4
1	D	360	CYS	2.2
1	A	675	GLY	2.2
1	B	379	ALA	2.2
1	B	29	VAL	2.2
1	D	344	VAL	2.1
1	D	122	LEU	2.1
1	A	278	THR	2.1
1	C	59	PHE	2.0
1	B	718	CYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

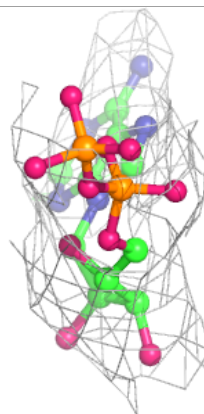
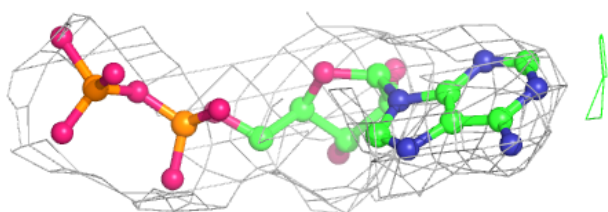
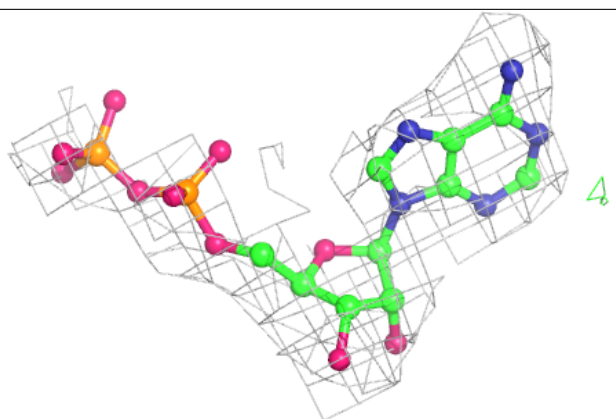
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	C	804	5/5	0.90	0.19	6,89,105,127	0
3	PO4	A	803	5/5	0.91	0.17	17,29,126,144	0
3	PO4	C	805	5/5	0.91	0.12	65,81,155,163	0
2	ADP	B	801	27/27	0.92	0.17	21,98,154,163	0
2	ADP	C	801	27/27	0.94	0.17	35,98,135,151	0
3	PO4	C	803	5/5	0.94	0.15	1,20,85,87	0
2	ADP	D	802	27/27	0.94	0.21	1,91,129,134	0
2	ADP	A	801	27/27	0.94	0.19	1,73,118,137	0
3	PO4	B	803	5/5	0.95	0.16	7,34,89,107	0
3	PO4	B	802	5/5	0.95	0.12	16,71,134,135	0
3	PO4	D	801	5/5	0.96	0.14	14,27,57,97	0
3	PO4	C	802	5/5	0.97	0.12	1,66,70,97	0
3	PO4	A	802	5/5	0.97	0.13	1,67,103,108	0
3	PO4	D	803	5/5	0.97	0.10	31,32,74,82	0
3	PO4	D	804	5/5	0.98	0.13	18,41,68,78	0
3	PO4	A	804	5/5	0.99	0.13	4,10,57,70	0

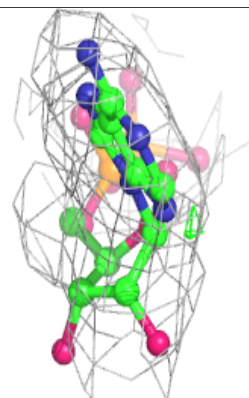
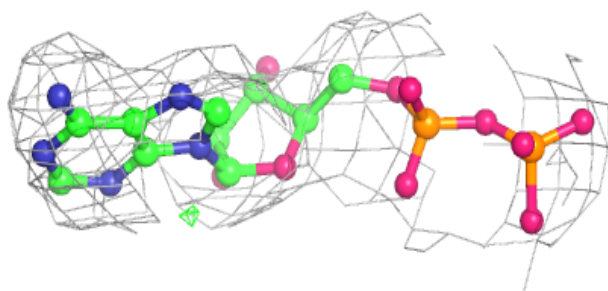
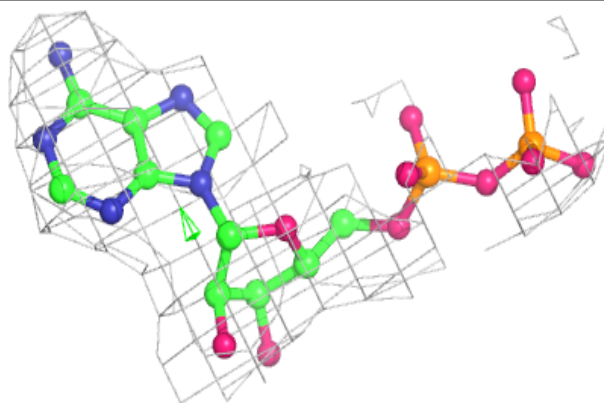
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP B 801:**

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

**Electron density around ADP C 801:**

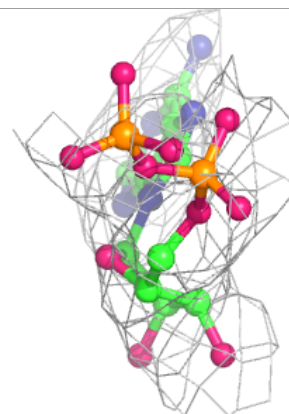
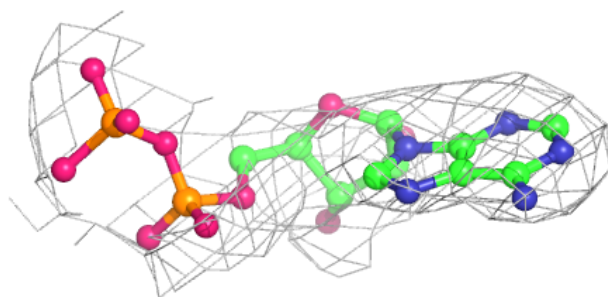
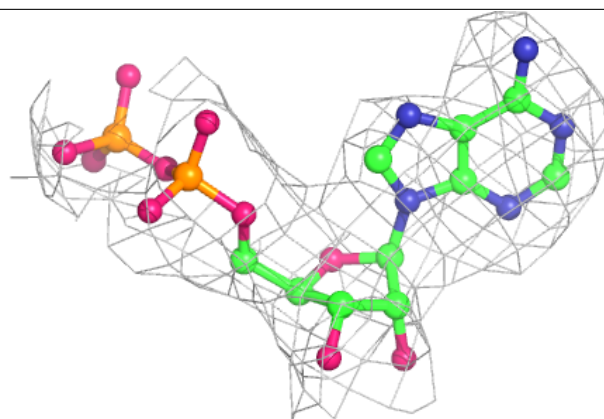
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





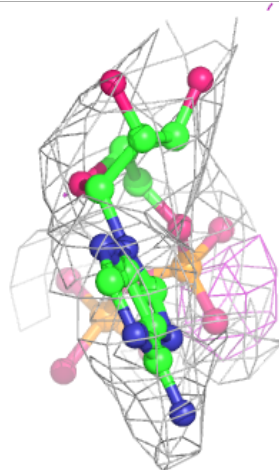
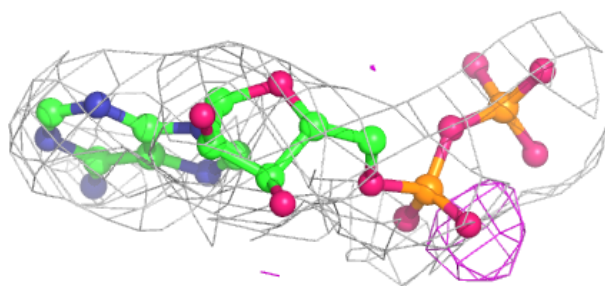
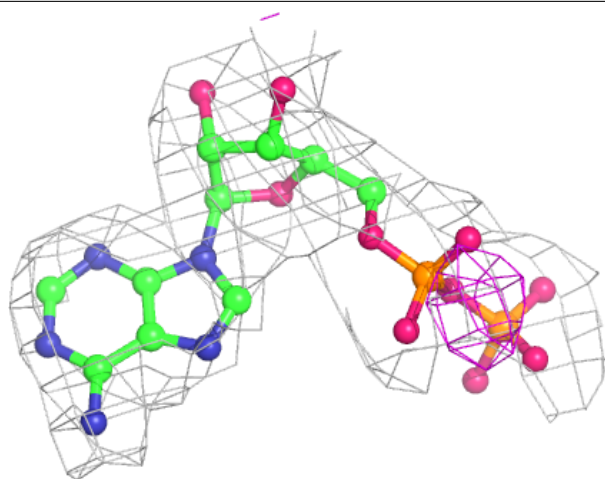
**Electron density around ADP D 802:**

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



**Electron density around ADP A 801:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.