



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 01:08 AM EDT

PDB ID : 1EFR  
Title : BOVINE MITOCHONDRIAL F1-ATPASE COMPLEXED WITH THE PEP-  
TIDE ANTIBIOTIC EFRAPEPTIN  
Authors : Abrahams, J.P.; Buchanan, S.K.; Van Raaij, M.J.; Fearnley, I.M.; Leslie,  
A.G.W.; Walker, J.E.  
Deposited on : unknown  
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

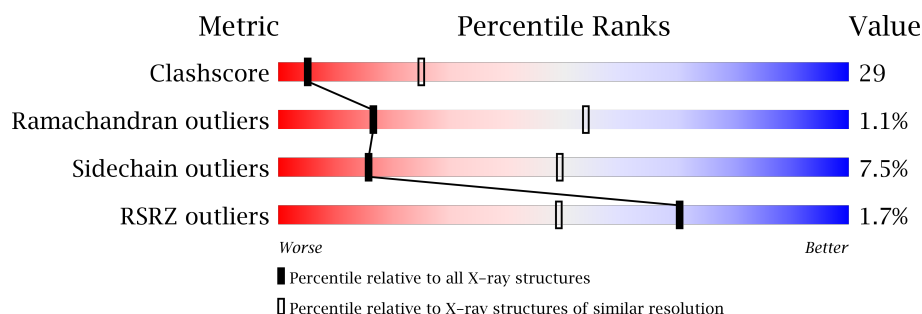
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



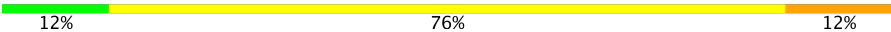
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

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Mol	Chain	Length	Quality of chain
4	Q	17	 <div>12% 76% 12%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AIB	Q	12	-	-	X	-
4	AIB	Q	2	-	-	X	-
5	MG	D	601	-	-	-	X
5	MG	F	601	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23527 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 BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	10	0	0
			3715	2341	656	706	12			
1	B	487	Total	C	N	O	S	59	0	0
			3715	2341	656	706	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CONFLICT	UNP P19483
B	481	GLY	SER	CONFLICT	UNP P19483
C	481	GLY	SER	CONFLICT	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	122	Total	C	N	O	S	0	0	0
			945	591	171	176	7			

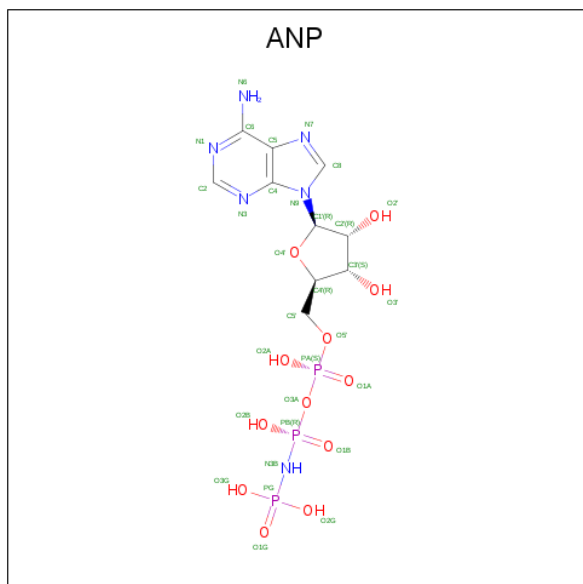
- Molecule 4 is a protein called EFRAPEPTIN C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Q	17	Total	C	N	O	0	0	0
			114	80	18	16			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

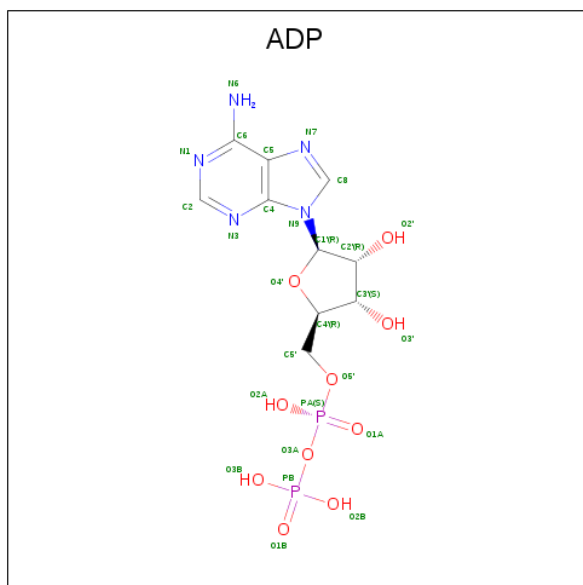
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

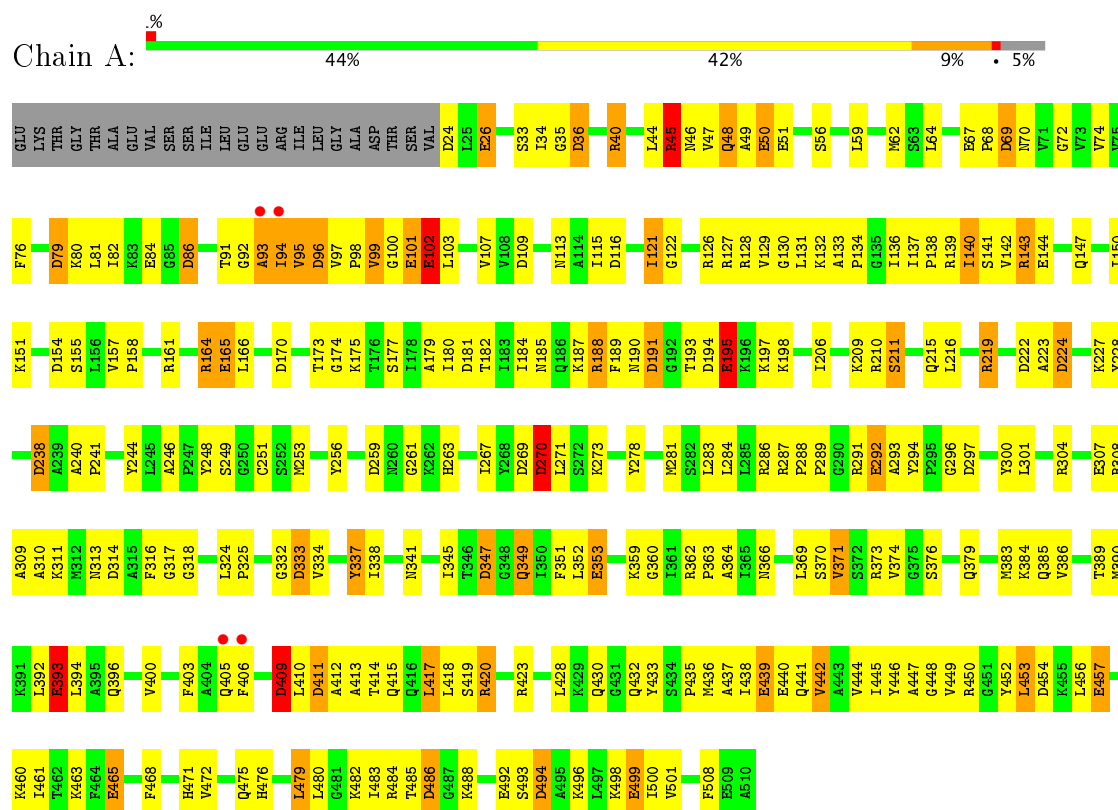
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	89	Total O 89 89	0	0
8	B	86	Total O 86 86	0	0
8	C	120	Total O 120 120	0	0
8	D	92	Total O 92 92	0	0
8	E	44	Total O 44 44	0	0
8	F	97	Total O 97 97	0	0
8	G	7	Total O 7 7	0	0

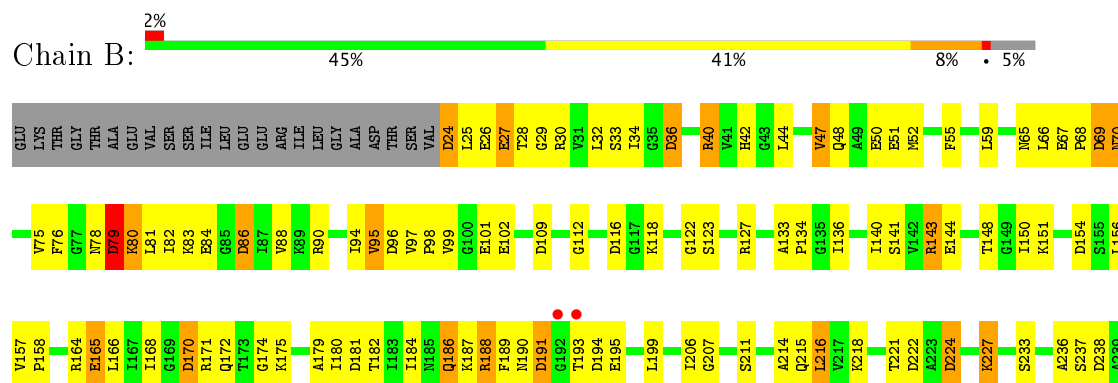
### 3 Residue-property plots

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

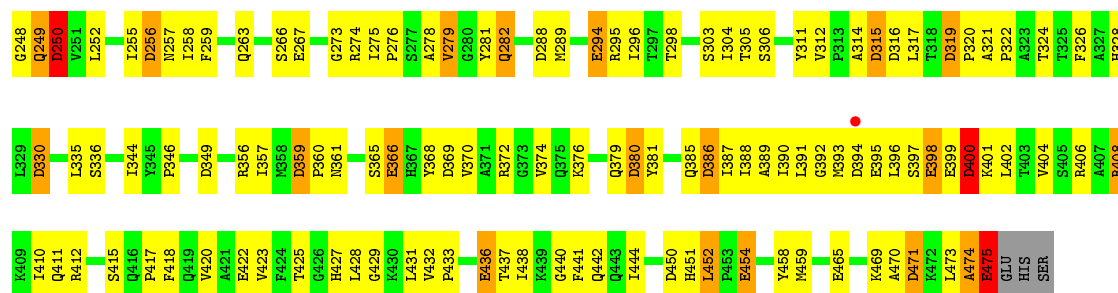
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT ALPHA



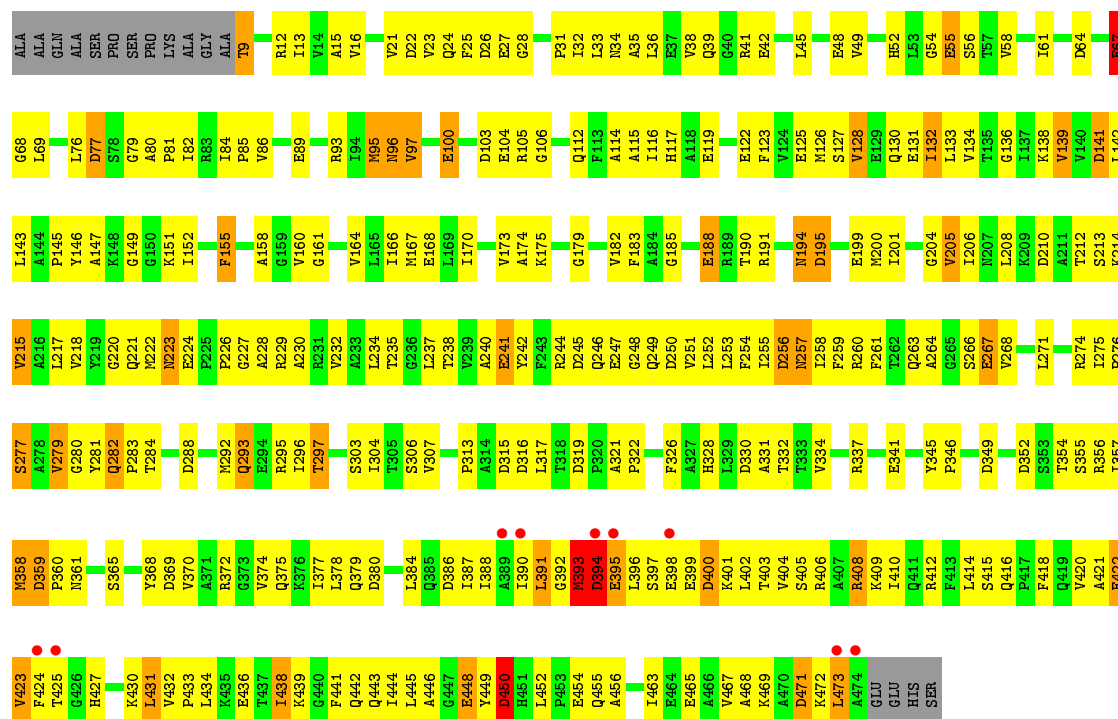
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT ALPHA



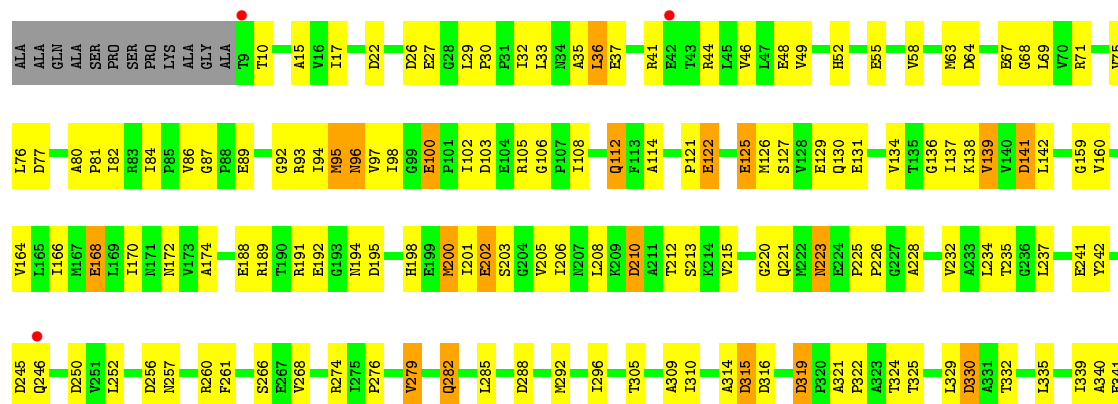


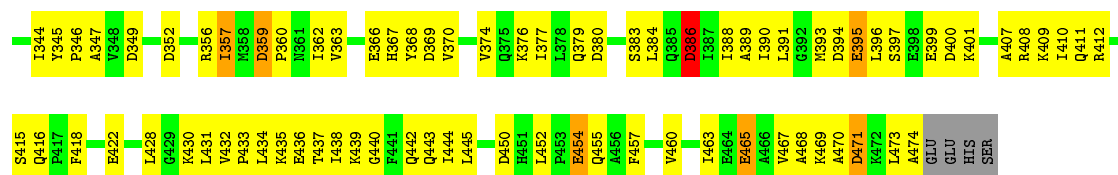


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT BETA

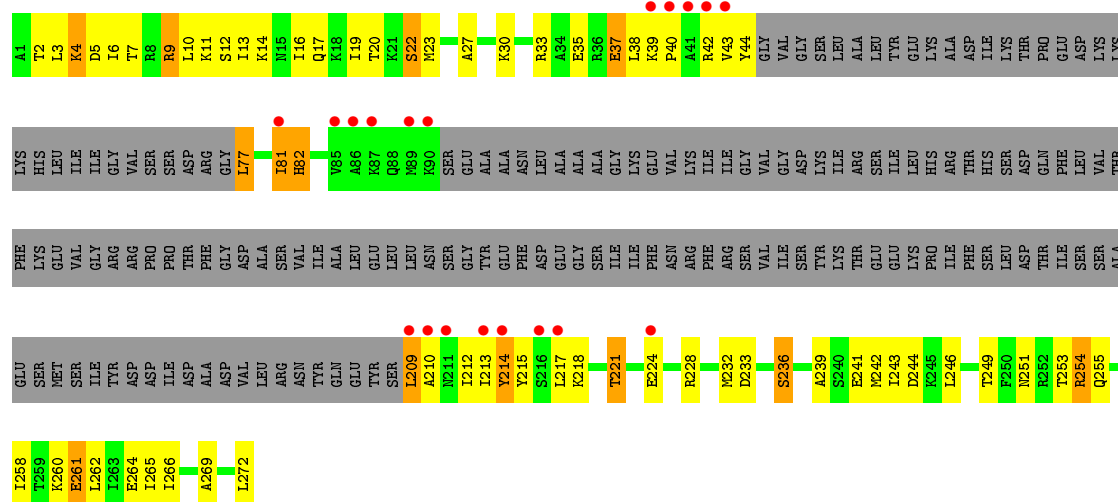
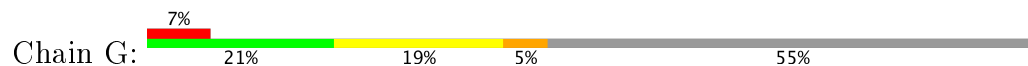


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT BETA





• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE SUBUNIT GAMMA



• Molecule 4: EFRAPEPTIN C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	285.70 Å   107.40 Å   139.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	5.50 – 3.10 19.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.50-3.10) 88.0 (19.99-3.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.56 (at 3.09 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.177 , 0.220 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 90.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: MG, TLX, ACE, ADP, YCP, ANP, BAL, AIB

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	0.76	15/3766 (0.4%)	1.17	51/5080 (1.0%)
1	B	0.75	15/3766 (0.4%)	1.16	50/5080 (1.0%)
1	C	0.77	18/3799 (0.5%)	1.16	54/5126 (1.1%)
2	D	0.81	17/3596 (0.5%)	1.15	52/4879 (1.1%)
2	E	0.81	21/3587 (0.6%)	1.15	50/4867 (1.0%)
2	F	0.81	21/3587 (0.6%)	1.12	44/4867 (0.9%)
3	G	0.71	5/949 (0.5%)	1.03	6/1266 (0.5%)
4	Q	0.47	0/23	0.99	0/29
All	All	0.78	112/23073 (0.5%)	1.15	307/31194 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	Q	0	3

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	355	GLU	CD-OE2	6.33	1.32	1.25
2	F	55	GLU	CD-OE2	5.74	1.31	1.25
2	E	100	GLU	CD-OE2	5.73	1.31	1.25
1	C	457	GLU	CD-OE1	5.68	1.31	1.25
2	F	37	GLU	CD-OE2	5.63	1.31	1.25
1	A	465	GLU	CD-OE2	5.59	1.31	1.25
1	B	292	GLU	CD-OE2	5.53	1.31	1.25
1	B	491	GLU	CD-OE1	5.52	1.31	1.25
2	F	192	GLU	CD-OE2	5.50	1.31	1.25
1	B	84	GLU	CD-OE2	5.50	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	440	GLU	CD-OE2	5.49	1.31	1.25
2	D	168	GLU	CD-OE2	5.46	1.31	1.25
1	A	84	GLU	CD-OE2	5.46	1.31	1.25
2	E	341	GLU	CD-OE1	5.42	1.31	1.25
2	E	454	GLU	CD-OE2	5.42	1.31	1.25
1	C	51	GLU	CD-OE2	5.42	1.31	1.25
2	E	241	GLU	CD-OE2	5.41	1.31	1.25
1	B	26	GLU	CD-OE2	5.40	1.31	1.25
2	F	422	GLU	CD-OE2	5.40	1.31	1.25
3	G	241	GLU	CD-OE2	5.40	1.31	1.25
2	F	129	GLU	CD-OE2	5.39	1.31	1.25
2	D	395	GLU	CD-OE2	5.38	1.31	1.25
1	A	440	GLU	CD-OE1	5.37	1.31	1.25
2	F	27	GLU	CD-OE2	5.36	1.31	1.25
2	E	119	GLU	CD-OE2	5.35	1.31	1.25
2	E	247	GLU	CD-OE2	5.35	1.31	1.25
1	C	393	GLU	CD-OE1	5.34	1.31	1.25
2	F	122	GLU	CD-OE2	5.34	1.31	1.25
1	B	492	GLU	CD-OE2	5.34	1.31	1.25
2	F	399	GLU	CD-OE1	5.33	1.31	1.25
3	G	35	GLU	CD-OE2	5.33	1.31	1.25
2	D	366	GLU	CD-OE2	5.32	1.31	1.25
1	A	101	GLU	CD-OE2	5.31	1.31	1.25
2	F	395	GLU	CD-OE2	5.30	1.31	1.25
1	C	255	GLU	CD-OE2	5.30	1.31	1.25
2	D	398	GLU	CD-OE2	5.30	1.31	1.25
2	E	267	GLU	CD-OE2	5.29	1.31	1.25
2	E	27	GLU	CD-OE2	5.27	1.31	1.25
2	E	67	GLU	CD-OE2	5.27	1.31	1.25
1	B	355	GLU	CD-OE2	5.26	1.31	1.25
1	C	50	GLU	CD-OE2	5.26	1.31	1.25
1	A	102	GLU	CD-OE2	5.26	1.31	1.25
2	E	131	GLU	CD-OE1	5.26	1.31	1.25
2	E	48	GLU	CD-OE2	5.26	1.31	1.25
2	E	395	GLU	CD-OE1	5.25	1.31	1.25
1	A	51	GLU	CD-OE2	5.25	1.31	1.25
3	G	261	GLU	CD-OE2	5.24	1.31	1.25
2	E	188	GLU	CD-OE2	5.24	1.31	1.25
1	A	393	GLU	CD-OE2	5.23	1.31	1.25
2	E	399	GLU	CD-OE2	5.22	1.31	1.25
1	C	491	GLU	CD-OE2	5.22	1.31	1.25
2	F	188	GLU	CD-OE2	5.22	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	465	GLU	CD-OE2	5.21	1.31	1.25
1	A	499	GLU	CD-OE1	5.20	1.31	1.25
2	E	55	GLU	CD-OE2	5.20	1.31	1.25
1	C	492	GLU	CD-OE1	5.20	1.31	1.25
1	B	255	GLU	CD-OE2	5.20	1.31	1.25
2	E	398	GLU	CD-OE2	5.18	1.31	1.25
2	D	436	GLU	CD-OE2	5.18	1.31	1.25
2	F	202	GLU	CD-OE2	5.18	1.31	1.25
2	D	241	GLU	CD-OE2	5.17	1.31	1.25
1	B	440	GLU	CD-OE2	5.17	1.31	1.25
2	D	42	GLU	CD-OE2	5.17	1.31	1.25
2	D	465	GLU	CD-OE2	5.17	1.31	1.25
2	F	131	GLU	CD-OE1	5.17	1.31	1.25
2	F	341	GLU	CD-OE2	5.16	1.31	1.25
2	F	454	GLU	CD-OE1	5.15	1.31	1.25
1	C	328	GLU	CD-OE2	5.15	1.31	1.25
1	C	292	GLU	CD-OE2	5.15	1.31	1.25
2	D	27	GLU	CD-OE2	5.14	1.31	1.25
2	D	399	GLU	CD-OE2	5.14	1.31	1.25
2	D	475	GLU	CD-OE2	5.14	1.31	1.25
2	F	125	GLU	CD-OE2	5.14	1.31	1.25
2	F	241	GLU	CD-OE2	5.13	1.31	1.25
2	F	168	GLU	CD-OE2	5.13	1.31	1.25
2	D	294	GLU	CD-OE2	5.13	1.31	1.25
2	D	454	GLU	CD-OE2	5.13	1.31	1.25
2	D	100	GLU	CD-OE2	5.12	1.31	1.25
2	E	104	GLU	CD-OE2	5.12	1.31	1.25
1	C	509	GLU	CD-OE2	5.11	1.31	1.25
2	E	465	GLU	CD-OE2	5.11	1.31	1.25
2	E	422	GLU	CD-OE2	5.09	1.31	1.25
1	B	499	GLU	CD-OE2	5.09	1.31	1.25
1	A	195	GLU	CD-OE1	5.08	1.31	1.25
1	B	27	GLU	CD-OE2	5.08	1.31	1.25
1	A	165	GLU	CD-OE2	5.08	1.31	1.25
1	B	165	GLU	CD-OE2	5.08	1.31	1.25
2	D	119	GLU	CD-OE2	5.08	1.31	1.25
1	C	27	GLU	CD-OE2	5.07	1.31	1.25
1	C	84	GLU	CD-OE2	5.06	1.31	1.25
2	D	188	GLU	CD-OE2	5.06	1.31	1.25
2	D	125	GLU	CD-OE2	5.06	1.31	1.25
1	C	195	GLU	CD-OE1	5.06	1.31	1.25
2	F	465	GLU	CD-OE2	5.06	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	48	GLU	CD-OE2	5.05	1.31	1.25
1	B	439	GLU	CD-OE2	5.05	1.31	1.25
2	F	366	GLU	CD-OE2	5.05	1.31	1.25
1	A	292	GLU	CD-OE2	5.05	1.31	1.25
2	F	100	GLU	CD-OE2	5.05	1.31	1.25
1	A	353	GLU	CD-OE2	5.04	1.31	1.25
1	A	26	GLU	CD-OE1	5.04	1.31	1.25
1	A	492	GLU	CD-OE2	5.04	1.31	1.25
1	B	50	GLU	CD-OE2	5.04	1.31	1.25
3	G	37	GLU	CD-OE2	5.04	1.31	1.25
2	E	448	GLU	CD-OE2	5.03	1.31	1.25
2	E	42	GLU	CD-OE2	5.02	1.31	1.25
1	C	165	GLU	CD-OE1	5.02	1.31	1.25
1	B	144	GLU	CD-OE2	5.01	1.31	1.25
1	C	307	GLU	CD-OE1	5.01	1.31	1.25
1	A	457	GLU	CD-OE2	5.01	1.31	1.25
1	B	426	GLU	CD-OE2	5.00	1.31	1.25
3	G	224	GLU	CD-OE2	5.00	1.31	1.25

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ASP	CB-CG-OD1	8.55	126.00	118.30
1	A	270	ASP	CB-CG-OD2	-7.57	111.48	118.30
2	E	64	ASP	CB-CG-OD2	-7.56	111.49	118.30
2	E	77	ASP	CB-CG-OD2	-7.13	111.88	118.30
2	D	408	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	109	ASP	CB-CG-OD1	7.01	124.61	118.30
2	D	316	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	194	ASP	CB-CG-OD2	-6.87	112.12	118.30
2	F	103	ASP	CB-CG-OD2	-6.85	112.13	118.30
2	E	77	ASP	CB-CG-OD1	6.84	124.45	118.30
2	E	64	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	116	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	C	224	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	154	ASP	CB-CG-OD2	-6.75	112.22	118.30
2	D	316	ASP	CB-CG-OD2	-6.74	112.23	118.30
2	F	359	ASP	CB-CG-OD2	-6.73	112.24	118.30
2	D	210	ASP	CB-CG-OD1	6.71	124.34	118.30
2	D	315	ASP	CB-CG-OD2	-6.70	112.27	118.30
2	E	96	ASN	N-CA-CB	-6.70	98.54	110.60
2	E	316	ASP	CB-CG-OD2	-6.70	112.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	96	ASP	CB-CG-OD2	-6.67	112.29	118.30
2	D	77	ASP	CB-CG-OD2	-6.67	112.30	118.30
2	E	359	ASP	CB-CG-OD2	-6.66	112.30	118.30
2	D	256	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	24	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	270	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	45	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	79	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	D	103	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	109	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	154	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	238	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	F	288	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	270	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	A	494	ASP	CB-CG-OD2	-6.54	112.41	118.30
2	D	349	ASP	CB-CG-OD2	-6.54	112.41	118.30
2	F	319	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	D	210	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	E	349	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	E	195	ASP	CB-CG-OD2	-6.50	112.45	118.30
2	E	26	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	222	ASP	CB-CG-OD2	-6.44	112.51	118.30
2	F	22	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	36	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	96	ASP	CB-CG-OD1	6.42	124.07	118.30
1	B	486	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	486	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	E	330	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	D	349	ASP	CB-CG-OD1	6.39	124.05	118.30
2	D	250	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	154	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	36	ASP	CB-CG-OD1	-6.35	112.58	118.30
3	G	233	ASP	CB-CG-OD1	6.35	124.02	118.30
2	F	256	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	B	314	ASP	CB-CG-OD1	-6.33	112.60	118.30
2	E	450	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	D	330	ASP	CB-CG-OD2	-6.33	112.61	118.30
2	F	386	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	C	86	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	116	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	D	369	ASP	CB-CG-OD2	-6.30	112.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	B	454	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	194	ASP	CB-CG-OD2	-6.26	112.67	118.30
2	E	359	ASP	CB-CG-OD1	6.24	123.92	118.30
2	E	471	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	333	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	C	238	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	40	ARG	NE-CZ-NH1	6.23	123.42	120.30
2	E	319	ASP	CB-CG-OD1	-6.23	112.70	118.30
2	F	77	ASP	CB-CG-OD2	-6.22	112.70	118.30
2	F	141	ASP	CB-CG-OD2	-6.21	112.71	118.30
2	D	288	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	154	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	269	ASP	CB-CG-OD1	-6.18	112.74	118.30
2	D	450	ASP	CB-CG-OD2	-6.17	112.74	118.30
3	G	233	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	C	409	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	194	ASP	CB-CG-OD1	6.16	123.85	118.30
2	E	386	ASP	CB-CG-OD2	-6.16	112.76	118.30
2	D	359	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	224	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	269	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	222	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	181	ASP	CB-CG-OD2	-6.13	112.79	118.30
2	D	195	ASP	CB-CG-OD2	-6.13	112.79	118.30
2	E	22	ASP	CB-CG-OD1	6.13	123.81	118.30
1	C	69	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	B	222	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	E	195	ASP	CB-CG-OD1	6.09	123.78	118.30
2	D	77	ASP	CB-CG-OD1	6.09	123.78	118.30
2	E	22	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	C	79	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	194	ASP	CB-CG-OD2	-6.07	112.84	118.30
2	E	103	ASP	CB-CG-OD2	-6.06	112.84	118.30
2	E	380	ASP	CB-CG-OD2	-6.06	112.85	118.30
2	E	369	ASP	CB-CG-OD2	-6.05	112.85	118.30
2	F	77	ASP	CB-CG-OD1	6.05	123.75	118.30
2	F	195	ASP	CB-CG-OD2	-6.05	112.85	118.30
2	D	394	ASP	CB-CG-OD2	-6.05	112.86	118.30
2	E	394	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	A	154	ASP	CB-CG-OD1	6.04	123.73	118.30
2	D	369	ASP	CB-CG-OD1	6.04	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	316	ASP	CB-CG-OD1	6.03	123.72	118.30
1	C	191	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	F	380	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	C	269	ASP	CB-CG-OD2	-6.01	112.89	118.30
2	E	26	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	170	ASP	CB-CG-OD1	6.00	123.70	118.30
2	D	319	ASP	CB-CG-OD2	-6.00	112.90	118.30
2	F	103	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	86	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	E	408	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	E	141	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	238	ASP	CB-CG-OD1	5.99	123.69	118.30
2	F	26	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	C	314	ASP	CB-CG-OD2	-5.97	112.92	118.30
2	F	330	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	314	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	191	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	D	26	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	B	494	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	E	141	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	116	ASP	CB-CG-OD2	-5.95	112.95	118.30
2	D	22	ASP	CB-CG-OD2	-5.92	112.97	118.30
2	E	245	ASP	CB-CG-OD2	-5.92	112.97	118.30
2	F	64	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	170	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	B	36	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	181	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	170	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	409	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	270	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	36	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	454	ASP	CB-CG-OD1	5.90	123.61	118.30
2	D	103	ASP	CB-CG-OD1	5.90	123.61	118.30
2	F	450	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	F	359	ASP	CB-CG-OD1	5.89	123.61	118.30
2	F	256	ASP	CB-CG-OD1	5.89	123.60	118.30
2	F	369	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	224	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	E	349	ASP	CB-CG-OD1	5.88	123.59	118.30
2	E	319	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	297	ASP	CB-CG-OD2	-5.87	113.02	118.30
2	D	386	ASP	CB-CG-OD2	-5.87	113.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	B	96	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	238	ASP	CB-CG-OD1	5.85	123.57	118.30
1	C	411	ASP	CB-CG-OD2	-5.84	113.04	118.30
2	F	386	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	79	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	454	ASP	CB-CG-OD2	-5.82	113.07	118.30
2	E	256	ASP	CB-CG-OD2	-5.81	113.07	118.30
3	G	5	ASP	CB-CG-OD1	-5.81	113.07	118.30
2	F	141	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	79	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	24	ASP	CB-CG-OD2	-5.80	113.08	118.30
3	G	9	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	F	250	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	116	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	333	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	D	64	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	F	400	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	F	288	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	69	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	411	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	B	314	ASP	CB-CG-OD2	5.74	123.47	118.30
2	F	352	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	494	ASP	CB-CG-OD1	-5.72	113.15	118.30
2	E	250	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	F	394	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	258	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	191	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	347	ASP	CB-CG-OD2	-5.70	113.17	118.30
2	E	400	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	181	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	411	ASP	CB-CG-OD2	-5.69	113.18	118.30
2	D	22	ASP	CB-CG-OD1	5.68	123.41	118.30
2	E	450	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	194	ASP	CB-CG-OD1	5.67	123.40	118.30
2	E	288	ASP	CB-CG-OD2	-5.66	113.20	118.30
2	E	471	ASP	CB-CG-OD1	5.66	123.40	118.30
2	F	369	ASP	CB-CG-OD1	5.66	123.39	118.30
2	E	380	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	20	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	191	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	C	270	ASP	CB-CG-OD1	5.63	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	ASP	CB-CG-OD1	5.63	123.36	118.30
2	D	195	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	224	ASP	CB-CG-OD1	5.62	123.36	118.30
2	F	210	ASP	CB-CG-OD2	-5.62	113.24	118.30
2	F	195	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	259	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	116	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	69	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	A	409	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	C	69	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	347	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	486	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	191	ASP	CB-CG-OD1	5.57	123.32	118.30
2	F	315	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	86	ASP	CB-CG-OD1	5.55	123.30	118.30
2	E	315	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	B	96	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	411	ASP	CB-CG-OD1	5.55	123.29	118.30
2	E	408	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	297	ASP	CB-CG-OD2	-5.54	113.31	118.30
2	D	386	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	494	ASP	CB-CG-OD1	5.54	123.28	118.30
1	C	86	ASP	CB-CG-OD1	5.54	123.28	118.30
2	F	380	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	314	ASP	CB-CG-OD1	5.53	123.28	118.30
2	D	256	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	405	GLN	C-N-CA	5.53	135.51	121.70
2	F	471	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	A	314	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	79	ASP	CB-CG-OD1	5.52	123.27	118.30
2	D	26	ASP	CB-CG-OD2	5.51	123.26	118.30
2	E	394	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	79	ASP	N-CA-CB	5.51	120.51	110.60
1	C	222	ASP	CB-CG-OD1	5.48	123.23	118.30
1	C	494	ASP	CB-CG-OD2	5.47	123.22	118.30
2	F	349	ASP	CB-CG-OD2	-5.47	113.38	118.30
2	D	319	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	270	ASP	CB-CA-C	-5.47	99.47	110.40
1	B	222	ASP	CB-CG-OD1	5.46	123.21	118.30
2	D	141	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	E	330	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	224	ASP	CB-CG-OD1	5.45	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	380	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	C	454	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	86	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	24	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	C	304	ARG	N-CA-CB	-5.43	100.82	110.60
2	E	386	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	454	ASP	CB-CG-OD1	5.41	123.17	118.30
2	E	369	ASP	CB-CG-OD1	5.41	123.17	118.30
2	F	64	ASP	CB-CG-OD1	5.40	123.16	118.30
2	D	394	ASP	CB-CG-OD1	5.39	123.16	118.30
2	F	319	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	297	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	F	96	ASN	CB-CA-C	-5.39	99.63	110.40
2	F	352	ASP	CB-CG-OD1	5.39	123.15	118.30
2	D	288	ASP	CB-CG-OD1	5.38	123.15	118.30
1	B	238	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	297	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	222	ASP	CB-CG-OD1	5.36	123.12	118.30
2	D	380	ASP	CB-CG-OD1	5.36	123.12	118.30
2	D	400	ASP	CB-CG-OD2	5.35	123.12	118.30
1	C	154	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	194	ASP	CB-CG-OD1	5.35	123.11	118.30
1	C	269	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	269	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	486	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	409	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	494	ASP	CB-CG-OD1	5.33	123.09	118.30
2	D	245	ASP	CB-CG-OD1	5.32	123.09	118.30
2	D	408	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	D	315	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	347	ASP	CB-CG-OD1	5.31	123.08	118.30
2	D	245	ASP	CB-CG-OD2	-5.31	113.52	118.30
2	F	316	ASP	CB-CG-OD2	-5.29	113.53	118.30
2	F	22	ASP	CB-CG-OD1	5.29	123.06	118.30
2	E	352	ASP	CB-CG-OD1	-5.28	113.55	118.30
3	G	5	ASP	CB-CG-OD2	5.27	123.05	118.30
2	E	256	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	411	ASP	CB-CG-OD2	5.26	123.04	118.30
2	F	26	ASP	CB-CG-OD2	5.25	123.03	118.30
2	E	103	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	347	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	269	ASP	CB-CG-OD1	5.24	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	245	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	36	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	347	ASP	CB-CG-OD1	5.22	123.00	118.30
2	D	471	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	D	64	ASP	CB-CG-OD1	5.21	122.99	118.30
2	D	330	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	333	ASP	CB-CG-OD1	5.21	122.98	118.30
1	B	24	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	170	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	69	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	181	ASP	CB-CG-OD1	5.17	122.96	118.30
1	C	24	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	45	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	337	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	371	VAL	CB-CA-C	-5.15	101.61	111.40
1	A	96	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	36	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	259	ASP	CB-CG-OD1	5.13	122.92	118.30
2	E	245	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	333	ASP	CB-CG-OD1	-5.09	113.72	118.30
2	E	277	SER	N-CA-CB	5.09	118.14	110.50
1	B	69	ASP	CB-CG-OD1	5.09	122.88	118.30
2	F	210	ASP	CB-CG-OD1	5.09	122.88	118.30
2	D	222	MET	CB-CA-C	-5.08	100.24	110.40
2	D	450	ASP	CB-CG-OD1	5.08	122.87	118.30
2	D	471	ASP	CB-CG-OD1	5.08	122.87	118.30
3	G	244	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	C	259	ASP	CB-CG-OD1	5.07	122.86	118.30
2	D	359	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	411	ASP	CB-CG-OD1	5.04	122.83	118.30
2	D	141	ASP	CB-CG-OD1	5.03	122.83	118.30
2	F	400	ASP	CB-CG-OD1	5.03	122.82	118.30
2	E	250	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	164	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	291	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Q	6	LEU	Mainchain,Peptide
4	Q	7	BAL	Mainchain

## 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	3715	0	3815	252	0
1	B	3715	0	3815	230	0
1	C	3748	0	3844	216	0
2	D	3539	0	3593	227	0
2	E	3530	0	3587	278	0
2	F	3530	0	3587	179	0
3	G	945	0	1019	79	0
4	Q	114	0	137	37	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	31	0	13	2	0
6	B	31	0	13	8	0
6	C	31	0	13	8	0
6	F	31	0	13	3	0
7	D	27	0	12	1	0
8	A	89	0	0	7	0
8	B	86	0	0	12	0
8	C	120	0	0	18	0
8	D	92	0	0	6	0
8	E	44	0	0	7	0
8	F	97	0	0	5	0
8	G	7	0	0	1	0
All	All	23527	0	23461	1365	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 29.

All (1365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:NE2	2:E:356:ARG:HH12	1.45	1.14
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.29	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:HH12	1:C:255:GLU:HB2	1.01	1.08
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.32	1.06
2:E:275:ILE:HG23	3:G:266:ILE:HD13	1.36	1.05
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.37	1.05
1:B:456:LEU:HD12	1:B:457:GLU:H	1.22	1.03
1:A:68:PRO:HD3	2:E:15:ALA:HB2	1.37	1.02
2:E:276:PRO:HD2	3:G:266:ILE:HD11	1.38	1.01
2:D:223:ASN:N	2:D:223:ASN:HD22	1.57	0.98
2:E:223:ASN:H	2:E:223:ASN:ND2	1.62	0.97
2:F:220:GLY:HA3	2:F:232:VAL:HG21	1.48	0.95
2:D:282:GLN:H	2:D:282:GLN:HE21	1.14	0.94
2:D:31:PRO:HD2	2:D:34:ASN:ND2	1.83	0.94
2:D:178:GLY:H	2:D:214:LYS:HZ3	0.96	0.94
2:D:178:GLY:N	2:D:214:LYS:HZ3	1.65	0.93
1:B:172:GLN:HA	6:B:600:ANP:HNB1	1.32	0.93
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.84	0.92
2:F:223:ASN:HD22	2:F:223:ASN:H	1.00	0.92
2:D:223:ASN:ND2	2:D:223:ASN:H	1.63	0.92
3:G:17:GLN:HB2	3:G:239:ALA:HB1	1.52	0.91
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.51	0.91
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.52	0.91
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.52	0.91
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.06	0.90
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.06	0.90
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.85	0.90
1:B:172:GLN:HE22	2:E:356:ARG:HH12	1.17	0.90
1:A:333:ASP:HA	4:Q:2:AIB:HB21	1.51	0.90
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.52	0.89
2:E:223:ASN:HD22	2:E:223:ASN:N	1.66	0.88
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.55	0.87
2:D:84:ILE:HB	2:D:95:MET:HE3	1.55	0.87
2:D:136:GLY:HA3	2:D:431:LEU:HD11	1.54	0.87
1:B:354:THR:HG22	1:B:358:TYR:HE2	1.39	0.87
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.54	0.86
2:F:223:ASN:ND2	2:F:223:ASN:H	1.74	0.86
2:F:95:MET:HE3	2:F:108:ILE:HD13	1.54	0.86
2:F:205:VAL:HG12	2:F:215:VAL:HG23	1.57	0.85
1:C:215:GLN:HG3	2:F:356:ARG:HH22	1.42	0.85
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.12	0.85
1:B:334:VAL:HG11	1:B:351:PHE:HE2	1.41	0.85
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.41	0.84
1:B:353:GLU:HB2	1:B:356:LEU:HD12	1.56	0.84
1:A:121:ILE:H	1:A:121:ILE:HD13	1.42	0.84
2:E:223:ASN:H	2:E:223:ASN:HD22	0.84	0.84
2:D:136:GLY:HA3	2:D:431:LEU:CD1	2.08	0.83
2:D:390:ILE:HD13	3:G:16:ILE:HD11	1.59	0.83
2:D:178:GLY:H	2:D:214:LYS:NZ	1.77	0.83
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.93	0.83
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.59	0.82
2:F:252:LEU:HD23	2:F:305:THR:HB	1.58	0.82
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.59	0.82
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.14	0.82
2:F:159:GLY:HA2	6:F:600:ANP:HNB1	1.44	0.81
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.61	0.81
2:D:391:LEU:HD13	3:G:19:ILE:HG21	1.61	0.81
1:B:389:THR:HA	1:B:392:LEU:HD12	1.63	0.81
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.14	0.81
1:B:389:THR:HA	1:B:392:LEU:CD1	2.09	0.81
2:D:218:VAL:HG11	2:D:235:THR:HG22	1.63	0.81
2:D:402:LEU:HD21	2:D:406:ARG:NH2	1.96	0.80
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.46	0.80
2:E:313:PRO:HD2	2:E:322:PRO:CG	2.11	0.80
3:G:17:GLN:HB2	3:G:239:ALA:CB	2.11	0.80
1:C:488:LYS:HG2	1:C:489:ILE:H	1.47	0.79
1:C:78:ASN:ND2	1:C:80:LYS:HD3	1.96	0.79
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.48	0.79
2:E:155:PHE:HE2	4:Q:12:AIB:HB11	1.45	0.79
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.66	0.78
2:D:178:GLY:N	2:D:214:LYS:NZ	2.31	0.78
2:D:404:VAL:O	2:D:408:ARG:HG3	1.83	0.78
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.82	0.78
1:C:211:SER:O	1:C:215:GLN:HG2	1.83	0.78
2:D:225:PRO:HB2	8:D:2006:HOH:O	1.83	0.78
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.14	0.78
2:F:223:ASN:N	2:F:223:ASN:HD22	1.68	0.78
1:A:142:VAL:HG22	1:A:161:ARG:O	1.84	0.77
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.67	0.77
2:E:96:ASN:HB3	2:E:100:GLU:H	1.49	0.77
1:A:44:LEU:O	1:A:47:VAL:HG22	1.85	0.76
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.67	0.76
1:B:354:THR:HG22	1:B:358:TYR:CE2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.15	0.76
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.68	0.76
2:D:196:LEU:O	2:D:200:MET:HG2	1.85	0.76
1:B:456:LEU:HD12	1:B:457:GLU:N	1.99	0.75
1:B:479:LEU:HD22	1:B:482:LYS:HD2	1.69	0.75
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.21	0.75
1:A:360:GLY:HA2	1:A:362:ARG:HH12	1.51	0.75
2:D:63:MET:HE3	2:D:228:ALA:HA	1.68	0.75
1:A:403:PHE:CE1	3:G:22:SER:HB2	2.21	0.75
2:D:223:ASN:H	2:D:223:ASN:HD22	0.81	0.75
2:E:97:VAL:HG13	2:E:232:VAL:HG22	1.68	0.75
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.22	0.74
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.68	0.74
1:C:336:ALA:HB3	1:C:339:PRO:HG2	1.69	0.74
1:A:472:VAL:HG12	1:A:480:LEU:HD11	1.68	0.74
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.70	0.74
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.69	0.74
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.17	0.74
1:B:187:LYS:HE3	1:B:191:ASP:OD2	1.88	0.74
2:D:282:GLN:H	2:D:282:GLN:NE2	1.85	0.74
2:D:391:LEU:CD1	3:G:19:ILE:HG21	2.17	0.74
1:B:172:GLN:NE2	2:E:356:ARG:NH1	2.30	0.73
4:Q:2:AIB:HB13	4:Q:3:YCP:HEA	1.70	0.73
4:Q:5:AIB:O	4:Q:6:LEU:HD23	1.88	0.73
1:C:44:LEU:O	1:C:47:VAL:HG22	1.88	0.73
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.17	0.73
2:E:275:ILE:HG23	3:G:266:ILE:CD1	2.18	0.73
3:G:20:THR:HG21	3:G:236:SER:N	2.03	0.73
2:E:397:SER:O	2:E:401:LYS:HG3	1.88	0.73
2:E:408:ARG:O	2:E:412:ARG:HG3	1.89	0.73
2:D:136:GLY:HA2	2:D:432:VAL:O	1.89	0.73
1:C:173:THR:CG2	1:C:354:THR:HG22	2.18	0.73
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.70	0.73
2:E:434:LEU:O	2:E:438:ILE:HG12	1.88	0.73
2:F:95:MET:CE	2:F:108:ILE:HD13	2.19	0.73
2:E:228:ALA:O	2:E:232:VAL:HG23	1.89	0.73
1:C:398:ARG:HG2	8:C:2100:HOH:O	1.87	0.72
2:D:263:GLN:O	2:D:267:GLU:HG3	1.88	0.72
2:F:200:MET:HG2	2:F:206:ILE:HG12	1.71	0.72
1:B:172:GLN:CA	6:B:600:ANP:HNB1	2.00	0.72
2:D:160:VAL:CG1	2:D:335:LEU:HB3	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:ALA:O	2:F:232:VAL:HG23	1.90	0.72
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.72	0.72
2:E:149:GLY:HA2	2:E:304:ILE:O	1.88	0.72
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.72	0.72
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.70	0.72
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.72	0.72
2:E:155:PHE:CE2	4:Q:12:AIB:HB11	2.24	0.72
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.88	0.72
2:E:388:ILE:HG23	2:E:393:MET:CG	2.20	0.72
1:C:52:MET:O	1:C:91:THR:HB	1.90	0.72
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.71	0.72
1:B:400:VAL:HG11	1:B:418:LEU:HD11	1.70	0.71
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.71	0.71
2:D:218:VAL:HG11	2:D:235:THR:CG2	2.19	0.71
2:F:10:THR:HG22	2:F:76:LEU:HD12	1.72	0.71
1:A:187:LYS:HE2	1:A:191:ASP:OD2	1.90	0.71
2:D:346:PRO:HG3	2:D:418:PHE:CZ	2.25	0.71
2:D:172:ASN:ND2	2:D:431:LEU:HD13	2.04	0.71
1:B:102:GLU:HG3	1:B:122:GLY:O	1.90	0.71
1:B:270:ASP:OD1	1:B:273:LYS:HG3	1.91	0.71
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.90	0.71
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.73	0.71
2:E:182:VAL:HG21	2:E:240:ALA:HB2	1.71	0.70
1:A:68:PRO:HD3	2:E:15:ALA:CB	2.19	0.70
1:C:139:ARG:HD3	8:C:2072:HOH:O	1.91	0.70
2:D:203:SER:OG	2:D:205:VAL:HG23	1.91	0.70
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.26	0.70
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.92	0.70
1:A:334:VAL:HG22	4:Q:3:YCP:HA	1.74	0.70
2:D:160:VAL:HG12	2:D:335:LEU:HB3	1.74	0.70
2:F:92:GLY:HA2	2:F:206:ILE:HD13	1.74	0.70
3:G:3:LEU:HD21	3:G:253:THR:HG22	1.74	0.70
1:C:175:LYS:HE3	6:C:600:ANP:O1B	1.91	0.69
2:D:475:GLU:OE1	2:D:475:GLU:HA	1.92	0.69
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.74	0.69
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.28	0.69
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.74	0.69
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.28	0.69
4:Q:14:LEU:O	4:Q:16:TLX:H9	1.93	0.69
2:F:434:LEU:O	2:F:438:ILE:HG12	1.93	0.68
2:E:346:PRO:HG3	2:E:418:PHE:HZ	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.74	0.68
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.27	0.68
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.58	0.68
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.58	0.68
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.05	0.68
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.75	0.68
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.74	0.68
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.76	0.68
2:E:360:PRO:HD3	2:E:368:TYR:CE1	2.29	0.68
1:C:173:THR:HG22	1:C:354:THR:HG22	1.75	0.67
1:B:261:GLY:HA2	1:B:317:GLY:O	1.94	0.67
2:D:244:ARG:O	2:D:248:GLY:HA2	1.93	0.67
2:E:421:ALA:O	2:E:425:THR:HB	1.95	0.67
1:B:141:SER:O	1:B:143:ARG:HD2	1.94	0.67
2:E:155:PHE:CD2	4:Q:12:AIB:HB21	2.30	0.67
2:E:359:ASP:OD1	2:E:360:PRO:HD2	1.95	0.67
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.77	0.67
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.77	0.67
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.57	0.67
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.76	0.67
1:B:297:ASP:HA	8:B:2070:HOH:O	1.95	0.67
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.10	0.67
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.30	0.67
3:G:2:THR:HG22	3:G:4:LYS:H	1.59	0.67
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.58	0.66
1:C:127:ARG:HH12	1:C:255:GLU:CB	1.94	0.66
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.76	0.66
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.58	0.66
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.78	0.66
3:G:38:LEU:HD21	3:G:42:ARG:CZ	2.26	0.66
1:A:300:TYR:O	1:A:304:ARG:HG2	1.96	0.66
1:B:334:VAL:HG11	1:B:351:PHE:CE2	2.29	0.66
1:B:439:GLU:OE1	1:B:484:ARG:HB2	1.93	0.66
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.59	0.66
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.30	0.66
1:B:171:ARG:HG2	1:B:328:GLU:OE2	1.96	0.66
1:C:381:ARG:O	1:C:385:GLN:HG3	1.96	0.66
1:C:404:ALA:C	1:C:406:PHE:H	1.95	0.66
2:F:63:MET:CE	2:F:97:VAL:HG11	2.26	0.66
1:B:179:ALA:CB	1:B:267:ILE:HD13	2.17	0.66
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LYS:HE2	1:A:430:GLN:HG3	1.76	0.66
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.78	0.66
3:G:77:LEU:HD13	3:G:232:MET:SD	2.35	0.66
1:B:354:THR:CG2	1:B:358:TYR:HE2	2.08	0.66
1:A:134:PRO:O	1:A:139:ARG:NH2	2.29	0.65
2:D:282:GLN:HE21	2:D:282:GLN:N	1.91	0.65
2:E:388:ILE:HD12	2:E:393:MET:HG2	1.78	0.65
2:F:89:GLU:N	2:F:89:GLU:OE1	2.28	0.65
1:A:175:LYS:NZ	8:A:2031:HOH:O	2.29	0.65
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.77	0.65
4:Q:10:AIB:N	4:Q:11:YCP:HEA	2.12	0.65
1:B:83:LYS:HG2	8:B:2006:HOH:O	1.96	0.65
1:A:26:GLU:HG2	1:A:46:ASN:ND2	2.11	0.65
1:C:488:LYS:HG2	1:C:489:ILE:N	2.12	0.65
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.79	0.65
2:E:85:PRO:HD2	2:E:95:MET:CE	2.26	0.65
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.79	0.65
2:D:97:VAL:HG22	2:D:232:VAL:HG13	1.77	0.65
1:B:215:GLN:HE22	2:E:130:GLN:NE2	1.95	0.65
1:A:99:VAL:HG23	1:A:253:MET:HA	1.79	0.64
1:A:390:MET:CE	1:A:428:LEU:HD21	2.25	0.64
1:A:195:GLU:HG3	1:A:198:LYS:CE	2.28	0.64
1:C:45:ARG:NH2	1:C:68:PRO:O	2.29	0.64
2:E:375:GLN:O	2:E:379:GLN:HG3	1.97	0.64
1:B:349:GLN:NE2	8:B:2083:HOH:O	2.30	0.64
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.79	0.64
2:F:408:ARG:NE	2:F:454:GLU:OE2	2.30	0.64
2:D:63:MET:CE	2:D:228:ALA:HA	2.28	0.64
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.62	0.64
1:C:399:GLU:OE2	2:D:408:ARG:NH2	2.30	0.64
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.12	0.64
1:A:383:MET:HE2	1:A:438:ILE:HD11	1.79	0.64
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.31	0.64
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.60	0.64
1:A:457:GLU:HB3	1:A:460:LYS:CD	2.28	0.64
1:C:362:ARG:NH1	8:C:2090:HOH:O	2.29	0.64
2:E:185:GLY:HA3	2:E:188:GLU:HG3	1.80	0.64
1:B:288:PRO:HB3	2:F:276:PRO:HG3	1.80	0.64
1:C:419:SER:O	1:C:423:ARG:HG2	1.96	0.64
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.80	0.64
2:E:12:ARG:NH2	2:E:24:GLN:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:263:GLN:O	2:E:267:GLU:HG3	1.97	0.63
2:E:293:GLN:HA	2:E:293:GLN:NE2	2.13	0.63
8:C:2018:HOH:O	2:F:52:HIS:HB3	1.96	0.63
1:A:392:LEU:O	1:A:396:GLN:HG3	1.97	0.63
2:D:408:ARG:NH1	2:D:454:GLU:OE2	2.29	0.63
1:B:215:GLN:NE2	2:E:130:GLN:NE2	2.46	0.63
1:A:175:LYS:HG3	1:A:352:LEU:HD12	1.80	0.63
1:B:237:SER:HB3	8:E:2036:HOH:O	1.97	0.63
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.27	0.63
1:C:211:SER:HB3	2:F:126:MET:HE3	1.80	0.63
1:B:379:GLN:HB3	1:B:384:LYS:CE	2.22	0.63
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.80	0.63
1:B:422:VAL:O	1:B:426:GLU:HG2	1.97	0.63
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.12	0.63
2:F:170:ILE:O	2:F:174:ALA:HB3	1.98	0.63
3:G:7:THR:HG23	4:Q:1:YCP:HG	1.80	0.63
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.79	0.63
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.80	0.63
1:C:102:GLU:HG2	1:C:122:GLY:O	1.99	0.63
1:C:171:ARG:NH2	8:C:2042:HOH:O	2.25	0.63
1:C:99:VAL:HG22	1:C:253:MET:HA	1.81	0.63
1:B:40:ARG:NH1	8:B:2005:HOH:O	2.30	0.63
2:E:267:GLU:O	2:E:271:LEU:HG	1.98	0.63
1:B:218:LYS:HB2	2:E:128:VAL:CG1	2.29	0.62
1:B:413:ALA:O	1:B:417:LEU:HG	1.99	0.62
2:E:126:MET:HE2	2:E:297:THR:HG21	1.81	0.62
2:E:282:GLN:NE2	2:E:282:GLN:H	1.97	0.62
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.81	0.62
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.80	0.62
2:F:469:LYS:O	2:F:473:LEU:HG	1.97	0.62
1:B:479:LEU:CD2	1:B:482:LYS:HD2	2.29	0.62
1:C:406:PHE:O	1:C:408:SER:N	2.32	0.62
1:C:215:GLN:CG	2:F:356:ARG:HH22	2.12	0.62
1:A:383:MET:CE	1:A:438:ILE:HD11	2.29	0.62
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.62
2:E:155:PHE:HE2	4:Q:12:AIB:CB1	2.12	0.62
1:A:270:ASP:OD1	1:A:273:LYS:HG3	1.99	0.62
2:E:16:VAL:HG22	2:E:21:VAL:HG13	1.79	0.62
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.35	0.62
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.82	0.62
2:E:200:MET:HB2	2:E:206:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:PRO:HD2	2:E:34:ASN:ND2	2.15	0.62
1:C:432:GLN:HG3	6:C:600:ANP:C5	2.29	0.62
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.65	0.61
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.35	0.61
1:B:118:LYS:NZ	8:B:2014:HOH:O	2.32	0.61
2:E:377:ILE:HG21	2:E:410:ILE:HD13	1.82	0.61
1:B:390:MET:HE3	1:B:424:LEU:HD22	1.82	0.61
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.66	0.61
2:F:252:LEU:CD2	2:F:305:THR:HB	2.28	0.61
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.00	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
2:E:122:GLU:N	2:E:125:GLU:OE2	2.30	0.61
3:G:3:LEU:HD21	3:G:253:THR:CG2	2.31	0.61
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.29	0.61
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.00	0.61
1:C:248:TYR:OH	1:C:301:LEU:HD12	2.01	0.61
1:C:267:ILE:N	1:C:267:ILE:HD12	2.15	0.61
2:F:205:VAL:CG1	2:F:215:VAL:HG23	2.30	0.61
1:A:34:ILE:HD12	1:A:35:GLY:N	2.15	0.61
1:A:446:TYR:HA	1:A:449:VAL:HG12	1.82	0.61
1:B:432:GLN:OE1	6:B:600:ANP:H2'	2.00	0.61
1:B:55:PHE:CD1	1:B:88:VAL:HG22	2.36	0.61
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.83	0.61
2:E:400:ASP:O	2:E:404:VAL:HG23	2.01	0.61
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.18	0.61
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.82	0.61
1:B:363:PRO:O	1:B:365:ILE:N	2.30	0.60
1:B:390:MET:CE	1:B:428:LEU:HD21	2.31	0.60
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.83	0.60
1:A:359:LYS:HG3	2:D:379:GLN:CG	2.32	0.60
2:E:97:VAL:HG13	2:E:232:VAL:CG2	2.31	0.60
1:A:94:ILE:HG21	1:A:128:ARG:NH2	2.17	0.60
2:E:443:GLN:HG2	2:E:448:GLU:CD	2.21	0.60
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.66	0.60
1:B:48:GLN:HB3	2:F:68:GLY:HA2	1.81	0.60
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.16	0.60
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.82	0.60
2:D:398:GLU:HA	2:D:401:LYS:CG	2.32	0.60
2:E:112:GLN:NE2	2:E:242:TYR:HE2	1.98	0.60
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.83	0.60
3:G:13:ILE:HD13	3:G:242:MET:SD	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.32	0.60
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.84	0.60
2:F:200:MET:HG2	2:F:206:ILE:CG1	2.32	0.60
3:G:23:MET:HB2	3:G:232:MET:HE2	1.84	0.60
2:F:395:GLU:OE2	3:G:77:LEU:HA	2.00	0.60
1:A:195:GLU:HG3	1:A:198:LYS:HE3	1.83	0.60
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.83	0.60
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.32	0.60
1:A:438:ILE:O	1:A:442:VAL:HG13	2.02	0.60
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.16	0.60
2:E:200:MET:CB	2:E:206:ILE:HD12	2.32	0.60
1:A:417:LEU:HD23	1:A:417:LEU:H	1.67	0.59
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.84	0.59
2:E:443:GLN:O	2:E:446:ALA:HB3	2.03	0.59
2:E:251:VAL:HG12	2:E:252:LEU:N	2.17	0.59
2:D:167:MET:CB	2:D:420:VAL:HG11	2.31	0.59
3:G:82:HIS:CD2	3:G:82:HIS:H	2.19	0.59
1:A:369:LEU:HD22	4:Q:6:LEU:HB2	1.84	0.59
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.83	0.59
1:B:362:ARG:HA	1:B:363:PRO:C	2.22	0.59
2:E:84:ILE:HB	2:E:95:MET:HE2	1.83	0.59
1:B:195:GLU:HB3	8:B:2039:HOH:O	2.00	0.59
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.03	0.59
2:D:278:ALA:HB1	3:G:261:GLU:OE2	2.02	0.59
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.38	0.59
1:A:141:SER:HB2	1:A:143:ARG:HD3	1.85	0.59
2:F:234:LEU:O	2:F:237:LEU:HB3	2.02	0.59
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.33	0.59
1:A:341:ASN:O	1:A:345:ILE:HG13	2.02	0.59
1:C:143:ARG:HD2	8:C:2029:HOH:O	2.02	0.59
1:A:349:GLN:NE2	1:A:370:SER:HA	2.18	0.59
1:C:172:GLN:HA	6:C:600:ANP:HNB1	1.67	0.59
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.85	0.59
3:G:239:ALA:O	3:G:243:ILE:HG13	2.03	0.59
2:E:332:THR:HG23	4:Q:16:TLX:CM'	2.31	0.59
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.18	0.59
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.84	0.59
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.68	0.59
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.84	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.84	0.58
4:Q:15:AIB:O	4:Q:16:TLX:H5'2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:NZ	1:A:318:GLY:O	2.30	0.58
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.38	0.58
3:G:9:ARG:HH22	3:G:242:MET:HE1	1.68	0.58
1:C:278:TYR:CD2	1:C:295:PRO:HG2	2.37	0.58
2:F:266:SER:HB3	2:F:282:GLN:NE2	2.18	0.58
2:F:97:VAL:HG22	2:F:232:VAL:HG22	1.85	0.58
1:A:136:ILE:HG22	8:A:2020:HOH:O	2.04	0.58
1:A:177:SER:OG	6:A:600:ANP:H8	2.02	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.38	0.58
2:D:108:ILE:HG22	2:D:110:THR:HG23	1.85	0.58
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.68	0.58
1:C:48:GLN:HB3	2:D:68:GLY:C	2.23	0.58
2:E:391:LEU:HD23	2:E:391:LEU:N	2.18	0.58
3:G:30:LYS:HA	3:G:33:ARG:HE	1.69	0.58
1:C:83:LYS:HB3	2:F:52:HIS:HE1	1.68	0.58
1:A:211:SER:N	2:D:126:MET:HE2	2.18	0.58
1:A:403:PHE:CD1	3:G:22:SER:HB2	2.39	0.58
1:C:400:VAL:HG13	8:C:2099:HOH:O	2.03	0.58
1:B:27:GLU:O	1:B:90:ARG:HG3	2.04	0.58
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.84	0.58
2:D:87:GLY:HA2	2:D:242:TYR:CE1	2.38	0.58
2:E:313:PRO:CD	2:E:322:PRO:HG3	2.22	0.58
2:F:384:LEU:O	2:F:388:ILE:HG12	2.04	0.58
1:B:434:SER:N	1:B:435:PRO:HD3	2.19	0.58
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.86	0.58
2:D:422:GLU:HG2	2:D:427:HIS:O	2.02	0.58
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.85	0.58
3:G:37:GLU:OE1	3:G:218:LYS:HE3	2.03	0.58
1:C:52:MET:CE	1:C:95:VAL:HG22	2.32	0.57
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.34	0.57
2:E:152:ILE:HA	2:E:331:ALA:O	2.04	0.57
2:E:89:GLU:N	2:E:89:GLU:OE1	2.29	0.57
2:F:63:MET:HE3	2:F:97:VAL:HG11	1.84	0.57
4:Q:2:AIB:HB13	4:Q:3:YCP:CE	2.34	0.57
1:B:218:LYS:O	1:B:218:LYS:HD3	2.04	0.57
1:B:385:GLN:OE1	1:B:488:LYS:HG3	2.03	0.57
1:B:400:VAL:HG12	1:B:418:LEU:HD11	1.85	0.57
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.03	0.57
1:C:354:THR:HG23	8:C:2085:HOH:O	2.03	0.57
2:D:402:LEU:O	2:D:406:ARG:HG3	2.04	0.57
2:E:224:GLU:HG2	8:E:2017:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:TYR:HB3	2:E:282:GLN:HE21	1.69	0.57
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.35	0.57
1:B:391:LYS:O	1:B:395:ALA:N	2.38	0.57
1:C:102:GLU:OE1	1:C:123:SER:HA	2.04	0.57
1:C:33:SER:HB2	2:F:52:HIS:O	2.04	0.57
1:C:432:GLN:HB3	1:C:433:TYR:CD2	2.39	0.57
1:B:171:ARG:HG3	8:B:2031:HOH:O	2.04	0.57
2:E:397:SER:H	2:E:400:ASP:HB2	1.69	0.57
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.34	0.57
2:F:433:PRO:O	2:F:436:GLU:HB2	2.05	0.57
8:E:2041:HOH:O	4:Q:16:TLX:H4'	2.03	0.57
2:D:440:GLY:O	2:D:444:ILE:HG13	2.04	0.57
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.04	0.57
2:E:244:ARG:HG3	2:E:303:SER:N	2.19	0.57
1:A:291:ARG:HA	3:G:262:LEU:HD13	1.86	0.57
1:A:472:VAL:HG13	1:A:476:HIS:HB2	1.85	0.57
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.87	0.57
2:E:444:ILE:HD13	2:E:449:TYR:HD2	1.70	0.57
1:B:441:GLN:O	1:B:445:ILE:HG12	2.05	0.57
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.87	0.57
2:F:200:MET:HG3	2:F:205:VAL:HB	1.86	0.57
2:F:84:ILE:HD13	2:F:235:THR:HG23	1.87	0.57
3:G:210:ALA:HA	3:G:213:ILE:HB	1.87	0.57
3:G:38:LEU:HD11	3:G:42:ARG:NE	2.20	0.57
1:A:446:TYR:HA	1:A:449:VAL:CG1	2.35	0.57
2:E:221:GLN:N	2:E:224:GLU:OE2	2.38	0.57
2:E:431:LEU:C	2:E:431:LEU:HD12	2.25	0.57
2:F:112:GLN:N	2:F:112:GLN:OE1	2.37	0.57
1:B:24:ASP:O	1:B:28:THR:HB	2.05	0.56
2:D:139:VAL:HG23	8:D:2083:HOH:O	2.05	0.56
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.86	0.56
1:A:143:ARG:CZ	1:A:143:ARG:HB2	2.35	0.56
1:A:170:ASP:O	1:A:173:THR:HG23	2.06	0.56
1:B:172:GLN:N	6:B:600:ANP:HNB1	2.03	0.56
1:B:240:ALA:HB3	1:B:241:PRO:HD3	1.87	0.56
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.36	0.56
2:F:225:PRO:HB2	8:F:2038:HOH:O	2.03	0.56
1:B:214:ALA:HA	2:E:123:PHE:CZ	2.41	0.56
1:B:423:ARG:HG3	1:B:423:ARG:HH11	1.71	0.56
2:E:282:GLN:HE21	2:E:282:GLN:H	1.53	0.56
2:F:390:ILE:C	2:F:391:LEU:HD23	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.87	0.56
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.41	0.56
2:E:77:ASP:OD1	2:E:79:GLY:N	2.30	0.56
2:F:138:LYS:HD3	2:F:432:VAL:HG21	1.87	0.56
2:F:463:ILE:HG22	8:F:2094:HOH:O	2.04	0.56
3:G:10:LEU:O	3:G:14:LYS:HG3	2.04	0.56
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.41	0.56
2:F:396:LEU:O	2:F:401:LYS:HE3	2.06	0.56
1:A:94:ILE:HG21	1:A:128:ARG:CZ	2.36	0.56
1:A:34:ILE:HD12	1:A:35:GLY:H	1.69	0.56
2:D:398:GLU:HA	2:D:401:LYS:HG2	1.86	0.56
1:B:33:SER:HB2	2:E:52:HIS:O	2.06	0.56
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.87	0.56
2:D:298:THR:HG23	2:D:303:SER:HA	1.87	0.56
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.38	0.56
2:E:263:GLN:HB3	8:E:2025:HOH:O	2.04	0.56
2:E:388:ILE:CG2	2:E:393:MET:HG3	2.32	0.56
1:C:174:GLY:HA2	6:C:600:ANP:PA	2.45	0.56
2:E:472:LYS:C	2:E:473:LEU:HD23	2.27	0.56
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.25	0.56
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.87	0.56
2:E:32:ILE:HA	2:E:49:VAL:HG12	1.88	0.56
2:F:390:ILE:HD11	3:G:242:MET:SD	2.45	0.56
2:F:440:GLY:O	2:F:444:ILE:HG13	2.06	0.56
3:G:6:ILE:HG23	3:G:246:LEU:HD22	1.87	0.56
1:B:423:ARG:HH11	1:B:423:ARG:CG	2.18	0.56
1:C:362:ARG:HA	1:C:363:PRO:C	2.25	0.56
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.70	0.55
1:C:467:ALA:O	1:C:470:SER:HB2	2.05	0.55
2:D:391:LEU:HD12	3:G:19:ILE:HD13	1.89	0.55
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.86	0.55
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.87	0.55
1:B:151:LYS:NZ	1:B:427:LEU:O	2.31	0.55
2:D:84:ILE:CD1	2:D:95:MET:HE1	2.35	0.55
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.87	0.55
1:C:436:MET:CE	1:C:469:LEU:HD21	2.36	0.55
1:C:436:MET:HE1	1:C:469:LEU:HD21	1.88	0.55
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.36	0.55
2:E:220:GLY:CA	2:E:232:VAL:HG21	2.35	0.55
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.87	0.55
1:B:265:LEU:HD12	1:B:322:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.21	0.55
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.87	0.55
2:E:182:VAL:CG2	2:E:240:ALA:HB2	2.35	0.55
2:E:345:TYR:HA	2:E:346:PRO:C	2.27	0.55
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.22	0.55
2:F:467:VAL:O	2:F:470:ALA:HB3	2.06	0.55
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.88	0.55
1:A:62:MET:CE	1:A:76:PHE:HZ	2.20	0.55
1:B:351:PHE:CD1	1:B:369:LEU:HB3	2.42	0.55
1:B:442:VAL:HG11	1:B:489:ILE:HD11	1.89	0.55
2:E:468:ALA:O	2:E:471:ASP:HB2	2.07	0.55
1:B:65:ASN:HD22	2:F:17:ILE:CG1	2.20	0.55
3:G:81:ILE:HG22	3:G:82:HIS:HD2	1.71	0.55
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.71	0.55
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.07	0.55
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.88	0.55
2:D:359:ASP:OD1	2:D:360:PRO:HD2	2.06	0.55
2:E:116:ILE:HA	2:E:238:THR:OG1	2.06	0.55
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.42	0.55
1:B:390:MET:HE1	1:B:428:LEU:HD21	1.89	0.54
2:E:12:ARG:O	2:E:23:VAL:HG13	2.07	0.54
1:A:334:VAL:HG11	4:Q:6:LEU:HD11	1.88	0.54
1:A:351:PHE:HE1	1:A:353:GLU:CG	2.20	0.54
1:C:48:GLN:HB3	2:D:68:GLY:O	2.07	0.54
2:E:82:ILE:O	2:E:116:ILE:HG23	2.07	0.54
2:E:160:VAL:CG1	2:E:337:ARG:HA	2.37	0.54
1:B:69:ASP:O	1:B:70:ASN:HB3	2.07	0.54
1:C:399:GLU:HB3	8:C:2099:HOH:O	2.08	0.54
2:E:167:MET:SD	2:E:200:MET:HA	2.47	0.54
1:A:185:ASN:O	1:A:188:ARG:HG3	2.08	0.54
1:A:36:ASP:O	1:A:284:LEU:HD13	2.07	0.54
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.42	0.54
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.43	0.54
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.89	0.54
2:E:293:GLN:HE21	2:E:293:GLN:CA	2.19	0.54
2:D:387:ILE:HG23	3:G:19:ILE:HD13	1.89	0.54
1:C:52:MET:HE1	1:C:76:PHE:CE2	2.43	0.54
1:C:339:PRO:O	1:C:343:ILE:HG13	2.07	0.54
2:D:107:PRO:HG2	2:D:109:LYS:HE3	1.90	0.54
2:E:174:ALA:HB3	2:E:214:LYS:HD3	1.89	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:HG3	1:A:198:LYS:NZ	2.22	0.54
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.90	0.54
1:A:392:LEU:HG	1:A:396:GLN:NE2	2.20	0.54
1:B:280:GLN:CD	2:E:284:THR:HG22	2.28	0.54
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.90	0.54
2:F:357:ILE:O	2:F:359:ASP:N	2.41	0.54
1:A:248:TYR:O	1:A:251:CYS:N	2.41	0.53
1:A:206:ILE:O	1:A:273:LYS:HD2	2.08	0.53
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.08	0.53
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.73	0.53
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.43	0.53
1:C:432:GLN:HG3	6:C:600:ANP:C6	2.38	0.53
2:E:105:ARG:NH1	8:E:2009:HOH:O	2.31	0.53
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.42	0.53
3:G:20:THR:HG22	3:G:236:SER:CB	2.38	0.53
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.73	0.53
2:D:65:GLY:HA3	2:D:67:GLU:OE2	2.08	0.53
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.89	0.53
2:F:408:ARG:HB3	2:F:454:GLU:OE2	2.09	0.53
4:Q:4:AIB:O	4:Q:7:BAL:HB3	2.08	0.53
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.89	0.53
2:D:83:ARG:HA	2:D:114:ALA:O	2.08	0.53
2:E:93:ARG:NH2	2:E:106:GLY:O	2.34	0.53
2:E:402:LEU:O	2:E:406:ARG:HG3	2.08	0.53
3:G:39:LYS:HB2	3:G:40:PRO:CD	2.33	0.53
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.89	0.53
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.24	0.53
1:C:441:GLN:O	1:C:445:ILE:HG12	2.09	0.53
2:E:251:VAL:HG12	2:E:252:LEU:H	1.72	0.53
2:F:44:ARG:NH2	8:F:2002:HOH:O	2.31	0.53
1:C:167:ILE:HD13	1:C:178:ILE:HB	1.90	0.53
2:D:112:GLN:N	2:D:112:GLN:OE1	2.36	0.53
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.91	0.53
2:E:61:ILE:O	2:E:61:ILE:HG13	2.09	0.53
2:F:159:GLY:HA2	6:F:600:ANP:N3B	2.18	0.53
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.89	0.53
2:E:246:GLN:NE2	2:E:246:GLN:HA	2.24	0.53
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.90	0.53
2:F:10:THR:CG2	2:F:76:LEU:HD12	2.37	0.53
1:B:101:GLU:OE2	1:B:262:LYS:NZ	2.30	0.53
2:D:408:ARG:HD3	2:D:454:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:LEU:HD23	2:E:414:LEU:HD21	1.89	0.53
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.39	0.53
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.74	0.53
1:C:460:LYS:NZ	1:C:463:LYS:NZ	2.57	0.53
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.91	0.53
2:F:329:LEU:HD13	2:F:332:THR:HG22	1.89	0.53
1:A:121:ILE:CD1	1:A:121:ILE:H	2.16	0.53
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.38	0.53
1:B:171:ARG:NH1	1:B:171:ARG:HB2	2.24	0.52
2:D:438:ILE:O	2:D:442:GLN:HB2	2.09	0.52
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.24	0.52
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.44	0.52
2:E:414:LEU:HG	2:E:441:PHE:CE2	2.44	0.52
2:E:438:ILE:O	2:E:442:GLN:HB2	2.09	0.52
1:B:65:ASN:HD22	2:F:17:ILE:HG13	1.73	0.52
1:C:129:VAL:HG21	1:C:245:LEU:HD11	1.92	0.52
2:D:390:ILE:HD12	2:D:390:ILE:N	2.25	0.52
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.74	0.52
1:B:211:SER:HB3	2:E:126:MET:HE2	1.91	0.52
2:D:387:ILE:HG23	2:D:391:LEU:HD12	1.91	0.52
2:D:67:GLU:CD	2:D:67:GLU:H	2.12	0.52
2:D:391:LEU:CD1	3:G:19:ILE:HD13	2.39	0.52
1:A:95:VAL:O	1:A:129:VAL:HG22	2.10	0.52
1:B:496:LYS:O	1:B:500:ILE:HG13	2.09	0.52
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.92	0.52
3:G:43:VAL:HG12	3:G:43:VAL:O	2.10	0.52
1:C:359:LYS:HG3	2:F:379:GLN:HG2	1.92	0.52
2:D:289:MET:SD	2:D:324:THR:HG22	2.49	0.52
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.54	0.52
2:E:151:LYS:HD3	2:E:328:HIS:O	2.10	0.52
2:F:32:ILE:HA	2:F:49:VAL:HG12	1.91	0.52
1:B:218:LYS:CG	2:E:128:VAL:HG11	2.40	0.52
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.19	0.52
2:D:273:GLY:HA2	3:G:272:LEU:HD22	1.92	0.52
1:B:28:THR:HG22	1:B:29:GLY:N	2.25	0.52
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.39	0.52
1:C:52:MET:CE	1:C:76:PHE:HE2	2.23	0.52
2:D:366:GLU:O	2:D:370:VAL:HG23	2.09	0.52
1:A:136:ILE:HG13	2:E:194:ASN:HB2	1.91	0.52
2:F:93:ARG:NH2	2:F:106:GLY:O	2.39	0.52
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:MET:HE2	1:A:438:ILE:CD1	2.40	0.52
2:D:469:LYS:O	2:D:473:LEU:HG	2.10	0.52
1:A:359:LYS:HG3	2:D:379:GLN:HG2	1.90	0.52
2:D:205:VAL:HG12	2:D:215:VAL:HG23	1.92	0.52
2:F:41:ARG:HH11	2:F:69:LEU:HD23	1.74	0.52
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.74	0.52
1:A:74:VAL:HG12	1:A:74:VAL:O	2.10	0.52
1:C:213:VAL:O	1:C:217:VAL:HG13	2.10	0.52
1:C:420:ARG:HH11	1:C:420:ARG:HG3	1.75	0.52
2:D:63:MET:HE1	2:D:231:ARG:HB2	1.91	0.52
2:E:173:VAL:HG12	2:E:179:GLY:O	2.09	0.52
2:E:223:ASN:N	2:E:223:ASN:ND2	2.35	0.52
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.39	0.52
3:G:7:THR:HG23	4:Q:1:YCP:CG	2.40	0.52
1:A:45:ARG:CG	1:A:45:ARG:HH11	2.16	0.51
1:C:405:GLN:C	1:C:406:PHE:HD1	2.14	0.51
1:A:209:LYS:NZ	2:D:330:ASP:OD1	2.38	0.51
2:E:155:PHE:HB2	2:E:334:VAL:HA	1.92	0.51
2:F:223:ASN:N	2:F:223:ASN:ND2	2.40	0.51
2:E:332:THR:HG23	4:Q:16:TLX:HM'3	1.91	0.51
1:A:485:THR:HG22	1:A:486:ASP:N	2.26	0.51
2:D:223:ASN:N	2:D:223:ASN:ND2	2.32	0.51
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.39	0.51
1:A:94:ILE:HD13	1:A:128:ARG:HD3	1.93	0.51
1:C:99:VAL:CG1	1:C:256:TYR:HB2	2.39	0.51
1:C:469:LEU:O	1:C:473:ILE:HG13	2.11	0.51
1:A:210:ARG:HG3	2:D:294:GLU:OE2	2.10	0.51
2:D:400:ASP:O	2:D:404:VAL:HG23	2.11	0.51
1:C:211:SER:HB3	2:F:126:MET:CE	2.40	0.51
1:A:165:GLU:O	1:A:325:PRO:HD2	2.10	0.51
1:A:99:VAL:CG2	1:A:253:MET:HA	2.40	0.51
1:C:143:ARG:HB2	8:C:2029:HOH:O	2.10	0.51
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.93	0.51
1:B:283:LEU:CD1	2:E:277:SER:HB3	2.40	0.51
1:A:414:THR:HA	1:A:417:LEU:HD21	1.92	0.51
2:E:296:ILE:HD13	2:E:306:SER:HB2	1.92	0.51
1:A:130:GLY:H	1:A:308:ARG:HH12	1.57	0.51
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.92	0.51
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.93	0.51
1:C:170:ASP:O	1:C:175:LYS:HE2	2.11	0.51
2:D:417:PRO:O	2:D:429:GLY:HA2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HD13	1:C:367:VAL:CG2	2.41	0.51
1:C:359:LYS:HG3	2:F:379:GLN:CG	2.40	0.51
2:D:357:ILE:O	2:D:359:ASP:N	2.44	0.51
2:D:63:MET:HE2	2:D:97:VAL:HG11	1.92	0.51
2:F:200:MET:CG	2:F:206:ILE:HG12	2.39	0.51
3:G:82:HIS:CD2	3:G:82:HIS:N	2.79	0.51
1:B:440:GLU:O	1:B:444:VAL:HG13	2.11	0.51
1:C:142:VAL:C	1:C:143:ARG:HG3	2.31	0.51
2:E:374:VAL:O	2:E:377:ILE:HG22	2.10	0.51
2:E:463:ILE:O	2:E:467:VAL:HG23	2.11	0.51
1:A:423:ARG:NH2	1:A:456:LEU:O	2.41	0.50
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.93	0.50
2:F:393:MET:O	2:F:396:LEU:HB2	2.11	0.50
3:G:13:ILE:HD13	3:G:242:MET:HG2	1.92	0.50
1:B:353:GLU:HB2	1:B:356:LEU:CD1	2.36	0.50
1:C:23:VAL:O	1:C:23:VAL:HG12	2.10	0.50
1:C:304:ARG:NH1	8:C:2068:HOH:O	2.44	0.50
2:E:258:ILE:O	2:E:261:PHE:HB3	2.11	0.50
1:A:33:SER:HB2	2:D:52:HIS:O	2.11	0.50
1:B:175:LYS:HE3	6:B:600:ANP:O1B	2.11	0.50
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.92	0.50
1:C:433:TYR:C	1:C:435:PRO:HD3	2.31	0.50
2:E:210:ASP:CG	2:E:212:THR:HG23	2.31	0.50
2:E:431:LEU:O	2:E:431:LEU:HD12	2.11	0.50
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.41	0.50
2:E:136:GLY:HA2	2:E:432:VAL:O	2.11	0.50
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.76	0.50
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.42	0.50
2:E:143:LEU:HD22	2:E:375:GLN:HG3	1.94	0.50
1:A:444:VAL:CG1	1:A:465:GLU:HG3	2.41	0.50
1:A:151:LYS:NZ	1:A:465:GLU:OE1	2.45	0.50
2:D:389:ALA:HB3	2:D:390:ILE:HD12	1.94	0.50
1:A:360:GLY:HA2	1:A:362:ARG:NH1	2.23	0.50
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.46	0.50
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.42	0.50
2:F:92:GLY:HA2	2:F:206:ILE:CD1	2.40	0.50
1:A:224:ASP:OD1	1:A:227:LYS:HE3	2.12	0.50
1:A:155:SER:O	1:A:379:GLN:NE2	2.45	0.50
1:B:334:VAL:HG12	1:B:334:VAL:O	2.12	0.50
1:B:52:MET:HG2	1:B:95:VAL:HG22	1.94	0.50
2:D:122:GLU:HA	2:D:122:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.93	0.50
2:D:94:ILE:HG22	2:D:102:ILE:HD11	1.94	0.50
1:A:49:ALA:O	1:A:50:GLU:HB2	2.12	0.49
1:B:170:ASP:O	1:B:175:LYS:HE2	2.12	0.49
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.95	0.49
2:F:41:ARG:NH1	2:F:69:LEU:HD23	2.26	0.49
3:G:7:THR:HG23	4:Q:1:YCP:CB	2.42	0.49
1:B:442:VAL:CG1	1:B:489:ILE:HD11	2.42	0.49
2:E:237:LEU:HD21	2:E:295:ARG:HB2	1.93	0.49
2:F:44:ARG:NH1	2:F:98:ILE:HD12	2.27	0.49
2:D:220:GLY:HA3	2:D:232:VAL:HG21	1.93	0.49
2:E:112:GLN:N	2:E:112:GLN:OE1	2.45	0.49
2:F:407:ALA:O	2:F:411:GLN:HB2	2.12	0.49
2:F:471:ASP:O	2:F:474:ALA:N	2.46	0.49
1:A:359:LYS:HG3	2:D:379:GLN:HG3	1.93	0.49
1:B:302:HIS:ND1	8:B:2072:HOH:O	2.34	0.49
1:B:44:LEU:O	1:B:47:VAL:HG22	2.13	0.49
2:D:319:ASP:O	2:D:322:PRO:HD2	2.12	0.49
3:G:217:LEU:O	3:G:221:THR:HG23	2.12	0.49
1:C:465:GLU:O	1:C:469:LEU:HB2	2.13	0.49
1:A:34:ILE:CG2	2:D:52:HIS:HB2	2.42	0.49
1:A:109:ASP:CG	1:A:113:ASN:HB2	2.33	0.49
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.94	0.49
2:D:279:VAL:HG12	2:D:279:VAL:O	2.11	0.49
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.94	0.49
1:B:172:GLN:HE22	2:E:356:ARG:NH1	1.99	0.49
1:B:479:LEU:HA	1:B:482:LYS:HG3	1.94	0.49
1:C:102:GLU:HG2	1:C:122:GLY:C	2.32	0.49
1:C:188:ARG:HH11	1:C:188:ARG:HG3	1.78	0.49
1:B:389:THR:HA	1:B:392:LEU:CG	2.42	0.49
1:C:420:ARG:HH21	1:C:451:GLY:HA3	1.78	0.49
2:E:54:GLY:O	2:E:55:GLU:HB2	2.12	0.49
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.93	0.49
2:F:324:THR:O	2:F:324:THR:HG22	2.13	0.49
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.12	0.49
3:G:81:ILE:HG22	3:G:82:HIS:N	2.28	0.49
2:E:332:THR:HG23	4:Q:16:TLX:HM'2	1.94	0.49
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.94	0.49
1:A:261:GLY:HA2	1:A:317:GLY:O	2.12	0.49
1:B:443:ALA:O	1:B:446:TYR:HB3	2.12	0.49
2:E:244:ARG:HG3	2:E:303:SER:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLN:CD	2:E:356:ARG:HH12	2.11	0.49
1:A:479:LEU:HD22	1:A:483:ILE:HD12	1.94	0.49
1:B:211:SER:O	1:B:215:GLN:HG3	2.12	0.49
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.95	0.49
1:B:36:ASP:OD1	2:E:274:ARG:NH2	2.46	0.49
2:E:86:VAL:HG11	2:E:114:ALA:HB3	1.94	0.49
4:Q:11:YCP:O	4:Q:14:LEU:HB2	2.13	0.49
2:D:96:ASN:HB2	2:D:100:GLU:H	1.78	0.48
3:G:9:ARG:HH22	3:G:242:MET:CE	2.25	0.48
1:A:175:LYS:CG	1:A:352:LEU:HD12	2.41	0.48
1:B:148:THR:HG22	1:B:182:THR:OG1	2.12	0.48
1:B:48:GLN:HB3	2:F:68:GLY:CA	2.42	0.48
1:C:357:PHE:CE2	1:C:362:ARG:HD3	2.48	0.48
1:C:406:PHE:N	1:C:406:PHE:CD1	2.81	0.48
3:G:214:TYR:CZ	3:G:218:LYS:HG3	2.47	0.48
1:B:502:THR:HG22	1:B:503:ASN:N	2.27	0.48
2:D:167:MET:HB2	2:D:420:VAL:HG11	1.94	0.48
2:E:167:MET:HE3	2:E:420:VAL:HG11	1.95	0.48
1:A:441:GLN:O	1:A:445:ILE:HG12	2.12	0.48
2:D:393:MET:CE	2:D:404:VAL:HG11	2.44	0.48
2:E:414:LEU:HG	2:E:441:PHE:CZ	2.49	0.48
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.95	0.48
1:B:358:TYR:CE2	4:Q:16:TLX:H61	2.48	0.48
1:A:96:ASP:HA	1:A:128:ARG:HA	1.94	0.48
1:B:423:ARG:HE	1:B:458:PRO:CD	2.26	0.48
1:C:129:VAL:O	1:C:308:ARG:NH2	2.46	0.48
2:D:105:ARG:HH11	2:D:208:LEU:HD22	1.78	0.48
3:G:20:THR:HG22	3:G:236:SER:OG	2.13	0.48
3:G:251:ASN:O	3:G:255:GLN:HG3	2.14	0.48
4:Q:16:TLX:HN'1	4:Q:16:TLX:H9	1.78	0.48
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.14	0.48
1:A:444:VAL:HG11	1:A:465:GLU:HG3	1.95	0.48
1:B:283:LEU:HD21	1:B:289:PRO:HB3	1.95	0.48
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.48
2:D:425:THR:HG21	2:D:459:MET:HE1	1.94	0.48
2:E:32:ILE:O	2:E:33:LEU:HB2	2.14	0.48
1:C:209:LYS:NZ	2:F:330:ASP:OD1	2.43	0.48
1:C:48:GLN:CB	2:D:68:GLY:HA2	2.43	0.48
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.96	0.48
1:C:172:GLN:NE2	6:C:600:ANP:O3G	2.37	0.48
2:D:118:ALA:O	2:D:295:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HG13	1:A:324:LEU:HB2	1.96	0.48
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.96	0.48
8:C:2028:HOH:O	2:D:198:HIS:HE1	1.97	0.48
2:E:254:PHE:CE1	2:E:307:VAL:HB	2.48	0.48
2:E:279:VAL:HG12	2:E:279:VAL:O	2.14	0.48
1:B:51:GLU:HA	1:B:94:ILE:HA	1.95	0.48
2:D:207:ASN:ND2	2:D:210:ASP:OD1	2.47	0.48
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.76	0.47
1:A:332:GLY:C	4:Q:2:AIB:HB11	2.33	0.47
1:B:311:LYS:HD2	1:B:312:MET:O	2.14	0.47
1:B:383:MET:O	1:B:387:ALA:N	2.43	0.47
2:F:205:VAL:CG1	2:F:215:VAL:CG2	2.92	0.47
2:F:433:PRO:HG2	2:F:436:GLU:HG3	1.96	0.47
1:A:144:GLU:O	1:A:161:ARG:HG3	2.14	0.47
1:B:420:ARG:O	1:B:423:ARG:N	2.46	0.47
1:C:292:GLU:O	1:C:293:ALA:HB3	2.14	0.47
1:C:481:GLY:O	1:C:485:THR:HB	2.15	0.47
2:D:314:ALA:O	2:D:315:ASP:HB2	2.12	0.47
2:E:23:VAL:O	2:E:58:VAL:HG22	2.14	0.47
1:A:479:LEU:O	1:A:479:LEU:HD23	2.15	0.47
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.96	0.47
1:A:82:ILE:HA	1:A:86:ASP:OD2	2.14	0.47
1:B:499:GLU:O	1:B:502:THR:HB	2.13	0.47
1:A:289:PRO:HG3	2:D:275:ILE:HG21	1.96	0.47
2:E:155:PHE:CD1	2:E:155:PHE:N	2.83	0.47
2:E:158:ALA:C	2:E:160:VAL:H	2.18	0.47
2:F:442:GLN:O	2:F:445:LEU:HB2	2.14	0.47
1:A:139:ARG:HD3	8:A:2062:HOH:O	2.13	0.47
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.50	0.47
2:E:222:MET:HE3	2:E:260:ARG:NH1	2.29	0.47
2:E:253:LEU:O	2:E:306:SER:HA	2.13	0.47
2:E:346:PRO:HG3	2:E:418:PHE:CE1	2.47	0.47
2:F:374:VAL:O	2:F:377:ILE:HG22	2.14	0.47
1:A:102:GLU:HG3	1:A:122:GLY:O	2.14	0.47
1:A:351:PHE:CE1	1:A:353:GLU:CG	2.97	0.47
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.62	0.47
1:C:434:SER:N	1:C:435:PRO:HD3	2.30	0.47
1:C:63:SER:OG	1:C:71:VAL:HG11	2.14	0.47
2:D:163:THR:O	2:D:166:ILE:HG22	2.15	0.47
2:E:95:MET:HA	2:E:100:GLU:O	2.15	0.47
3:G:254:ARG:O	3:G:258:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.28	0.47
2:E:234:LEU:O	2:E:237:LEU:HB3	2.15	0.47
2:F:160:VAL:HG12	2:F:335:LEU:HB3	1.97	0.47
2:F:203:SER:OG	2:F:205:VAL:HG23	2.15	0.47
2:F:266:SER:N	2:F:282:GLN:HE22	2.13	0.47
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.97	0.47
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.14	0.47
1:C:352:LEU:HA	1:C:364:ALA:O	2.15	0.47
1:C:32:LEU:HB2	1:C:40:ARG:O	2.15	0.47
2:F:221:GLN:CA	2:F:221:GLN:HE21	2.23	0.47
3:G:7:THR:O	3:G:11:LYS:HG3	2.15	0.47
1:A:107:VAL:O	1:A:115:ILE:HG12	2.15	0.47
1:A:36:ASP:HB3	1:A:284:LEU:HD13	1.97	0.47
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.30	0.47
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.96	0.47
2:D:170:ILE:O	2:D:174:ALA:HB3	2.15	0.47
2:D:471:ASP:O	2:D:474:ALA:HB3	2.15	0.47
1:A:446:TYR:CA	1:A:449:VAL:HG12	2.44	0.47
1:B:381:ARG:O	1:B:384:LYS:HB2	2.15	0.47
1:B:481:GLY:O	1:B:485:THR:HB	2.14	0.47
2:E:422:GLU:HG2	2:E:427:HIS:O	2.14	0.47
1:A:48:GLN:HB3	2:E:68:GLY:O	2.14	0.47
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.96	0.47
2:F:138:LYS:HE2	2:F:416:GLN:HB2	1.97	0.47
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.47
1:A:184:ILE:HD12	1:A:223:ALA:HB3	1.97	0.47
1:B:171:ARG:NH2	4:Q:15:AIB:HB11	2.30	0.47
1:B:439:GLU:CD	1:B:484:ARG:HB2	2.34	0.47
1:C:251:CYS:O	1:C:255:GLU:HG3	2.14	0.47
1:B:136:ILE:HG23	2:F:194:ASN:HA	1.97	0.47
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.50	0.47
1:A:190:ASN:ND2	1:A:228:TYR:CG	2.83	0.47
1:A:373:ARG:NH1	1:A:373:ARG:HG3	2.30	0.47
1:A:411:ASP:OD1	1:A:413:ALA:HB3	2.15	0.47
2:D:209:LYS:HA	2:D:209:LYS:HD3	1.62	0.47
2:E:222:MET:CE	2:E:260:ARG:HH11	2.27	0.47
2:E:405:SER:OG	2:E:406:ARG:N	2.48	0.47
2:F:172:ASN:ND2	2:F:431:LEU:HD13	2.30	0.47
1:C:164:ARG:HD2	1:C:306:LEU:O	2.15	0.46
2:E:151:LYS:NZ	8:E:2013:HOH:O	2.40	0.46
2:E:152:ILE:HD12	2:E:152:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:439:LYS:HG2	2:F:443:GLN:HE21	1.79	0.46
3:G:209:LEU:HB3	3:G:210:ALA:H	1.57	0.46
3:G:6:ILE:HD13	3:G:249:THR:HG22	1.97	0.46
1:A:94:ILE:CG2	1:A:128:ARG:NH2	2.77	0.46
1:B:224:ASP:OD2	1:B:227:LYS:NZ	2.42	0.46
1:B:351:PHE:HE1	1:B:369:LEU:O	1.99	0.46
2:E:256:ASP:HA	2:E:257:ASN:HA	1.58	0.46
2:E:354:THR:CG2	2:E:355:SER:N	2.78	0.46
2:E:425:THR:HG22	2:E:427:HIS:HB2	1.97	0.46
2:E:441:PHE:O	2:E:445:LEU:HG	2.15	0.46
1:A:307:GLU:OE1	2:E:190:THR:HB	2.15	0.46
2:D:103:ASP:O	2:D:104:GLU:HB2	2.15	0.46
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.97	0.46
1:A:389:THR:O	1:A:393:GLU:HG2	2.15	0.46
1:B:389:THR:HA	1:B:392:LEU:HG	1.98	0.46
1:C:423:ARG:NH2	1:C:454:ASP:O	2.48	0.46
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.77	0.46
1:C:36:ASP:CG	2:F:274:ARG:HH21	2.18	0.46
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.97	0.46
2:D:397:SER:OG	2:D:400:ASP:HB2	2.15	0.46
2:E:377:ILE:HD11	2:E:403:THR:HB	1.98	0.46
2:E:67:GLU:H	2:E:67:GLU:HG3	1.17	0.46
2:F:226:PRO:HB2	2:F:268:VAL:CG1	2.45	0.46
2:F:314:ALA:O	2:F:315:ASP:HB2	2.16	0.46
2:D:387:ILE:CG2	3:G:19:ILE:HD13	2.45	0.46
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.51	0.46
1:A:161:ARG:HH11	1:A:263:HIS:CB	2.29	0.46
1:A:369:LEU:CD2	4:Q:7:BAL:N	2.78	0.46
1:B:133:ALA:HB1	1:B:134:PRO:HD2	1.96	0.46
1:C:47:VAL:O	2:D:70:VAL:HG13	2.15	0.46
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.97	0.46
1:A:157:VAL:N	1:A:158:PRO:CD	2.78	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.99	0.46
1:A:390:MET:HE1	1:A:428:LEU:HD21	1.97	0.46
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.98	0.46
2:D:130:GLN:OE1	2:D:357:ILE:HG22	2.16	0.46
2:D:54:GLY:O	2:D:55:GLU:HB2	2.16	0.46
2:E:292:MET:SD	2:E:293:GLN:NE2	2.89	0.46
2:F:266:SER:CA	2:F:282:GLN:NE2	2.79	0.46
1:A:238:ASP:HA	8:A:2043:HOH:O	2.15	0.46
1:A:34:ILE:HG22	2:D:52:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ILE:HG23	2:D:415:SER:HB3	1.98	0.46
2:D:95:MET:CE	2:D:99:GLY:HA2	2.45	0.46
2:E:155:PHE:CD2	4:Q:12:AIB:CB2	2.97	0.46
1:A:195:GLU:CG	1:A:198:LYS:NZ	2.79	0.46
1:C:19:ALA:O	1:C:21:THR:HG23	2.16	0.46
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.31	0.46
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.30	0.46
4:Q:10:AIB:N	4:Q:11:YCP:CE	2.79	0.46
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.80	0.46
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.51	0.46
2:D:220:GLY:CA	2:D:232:VAL:HG11	2.46	0.46
1:A:406:PHE:CE1	2:D:387:ILE:HG21	2.51	0.46
2:F:35:ALA:HB1	2:F:46:VAL:CG1	2.45	0.46
2:F:386:ASP:O	2:F:389:ALA:HB3	2.16	0.46
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.99	0.45
6:B:600:ANP:O2B	6:B:600:ANP:O2G	2.34	0.45
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.46	0.45
8:B:2021:HOH:O	2:F:198:HIS:CE1	2.68	0.45
2:F:438:ILE:O	2:F:442:GLN:HG3	2.16	0.45
1:A:136:ILE:O	2:E:194:ASN:HB2	2.16	0.45
1:A:287:ARG:HB3	1:A:288:PRO:HD2	1.97	0.45
1:A:62:MET:HE2	1:A:76:PHE:HZ	1.81	0.45
1:B:65:ASN:ND2	2:F:17:ILE:HG23	2.32	0.45
1:C:442:VAL:HG11	1:C:489:ILE:HD11	1.98	0.45
2:D:156:GLY:HA2	8:D:2019:HOH:O	2.16	0.45
2:D:335:LEU:N	2:D:335:LEU:CD1	2.79	0.45
2:E:85:PRO:HD2	2:E:95:MET:HE2	1.98	0.45
2:F:285:LEU:C	2:F:285:LEU:HD23	2.37	0.45
3:G:27:ALA:HB2	3:G:228:ARG:HG2	1.98	0.45
1:A:151:LYS:HG2	1:A:441:GLN:HG2	1.97	0.45
1:A:69:ASP:O	1:A:70:ASN:HB3	2.15	0.45
1:B:75:VAL:HG21	1:B:82:ILE:HD12	1.97	0.45
2:E:175:LYS:HD3	2:E:431:LEU:HD23	1.97	0.45
2:E:39:GLN:CD	2:E:76:LEU:HD12	2.37	0.45
2:F:391:LEU:N	2:F:391:LEU:HD23	2.31	0.45
1:B:356:LEU:HB2	1:B:364:ALA:HB1	1.98	0.45
1:B:496:LYS:HG2	1:B:500:ILE:HD11	1.98	0.45
1:B:97:VAL:HB	1:B:98:PRO:HD2	1.98	0.45
1:C:172:GLN:HA	6:C:600:ANP:N3B	2.30	0.45
1:C:37:GLY:O	1:C:38:ILE:HD13	2.17	0.45
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:ASN:CB	2:D:100:GLU:H	2.29	0.45
2:E:222:MET:CE	2:E:260:ARG:NH1	2.79	0.45
2:F:266:SER:CB	2:F:282:GLN:NE2	2.80	0.45
1:A:40:ARG:HD3	1:A:72:GLY:HA2	1.98	0.45
1:B:140:ILE:HG13	1:B:141:SER:N	2.31	0.45
1:B:34:ILE:HG21	1:B:82:ILE:O	2.17	0.45
1:C:151:LYS:HE3	1:C:430:GLN:CG	2.46	0.45
1:C:49:ALA:O	1:C:50:GLU:HB2	2.16	0.45
2:F:172:ASN:ND2	2:F:431:LEU:CD1	2.80	0.45
2:F:468:ALA:O	2:F:471:ASP:N	2.48	0.45
1:A:140:ILE:HG13	1:A:141:SER:N	2.29	0.45
1:A:92:GLY:O	1:A:93:ALA:HB2	2.16	0.45
1:B:187:LYS:NZ	1:B:224:ASP:HB3	2.32	0.45
1:C:420:ARG:NH1	1:C:420:ARG:HG3	2.32	0.45
1:C:177:SER:OG	6:C:600:ANP:H8	2.17	0.45
2:D:105:ARG:NH1	2:D:208:LEU:CD2	2.80	0.45
2:D:151:LYS:HD3	2:D:328:HIS:O	2.17	0.45
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.98	0.45
2:E:456:ALA:O	2:E:469:LYS:HD2	2.17	0.45
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.84	0.45
1:C:74:VAL:HG13	1:C:241:PRO:HG3	1.97	0.45
1:A:211:SER:N	2:D:126:MET:CE	2.80	0.45
2:F:142:LEU:HB2	2:F:437:THR:CG2	2.47	0.45
3:G:13:ILE:HD13	3:G:242:MET:CG	2.46	0.45
1:A:334:VAL:CG2	4:Q:3:YCP:HA	2.46	0.45
1:A:210:ARG:HB2	2:D:126:MET:HE2	1.98	0.45
1:A:448:GLY:HA2	1:A:453:LEU:HG	1.98	0.45
1:B:165:GLU:O	1:B:325:PRO:HD2	2.16	0.45
1:B:249:SER:O	1:B:253:MET:HG3	2.16	0.45
1:B:353:GLU:OE2	1:B:366:ASN:ND2	2.49	0.45
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.17	0.45
1:C:105:GLY:HA2	1:C:226:MET:O	2.17	0.45
1:C:469:LEU:HD12	1:C:469:LEU:HA	1.76	0.45
1:C:48:GLN:HB3	2:D:68:GLY:CA	2.47	0.45
2:D:98:ILE:HG13	2:D:100:GLU:HG3	1.98	0.45
2:D:386:ASP:HB3	3:G:12:SER:HB2	1.99	0.45
8:B:2029:HOH:O	2:F:189:ARG:HG2	2.16	0.45
2:F:221:GLN:CA	2:F:221:GLN:NE2	2.80	0.45
4:Q:9:AIB:O	4:Q:12:AIB:HB22	2.17	0.45
1:A:62:MET:CE	1:A:76:PHE:CZ	3.00	0.45
1:B:186:GLN:HB3	1:B:190:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:PHE:CD1	1:C:241:PRO:HB2	2.52	0.45
2:D:312:VAL:O	2:D:312:VAL:HG12	2.16	0.45
2:D:471:ASP:O	2:D:474:ALA:N	2.50	0.45
2:D:35:ALA:HB2	2:D:82:ILE:HG13	1.99	0.45
2:E:253:LEU:O	2:E:307:VAL:N	2.40	0.45
3:G:9:ARG:NH2	3:G:242:MET:CE	2.80	0.45
1:A:209:LYS:HZ1	2:D:330:ASP:CG	2.18	0.45
1:A:267:ILE:N	1:A:267:ILE:HD12	2.32	0.45
1:A:310:ALA:HB1	8:A:2062:HOH:O	2.17	0.45
1:B:211:SER:HB3	2:E:126:MET:CE	2.47	0.45
1:B:206:ILE:CD1	1:B:247:PRO:HG3	2.47	0.45
1:B:174:GLY:HA2	6:B:600:ANP:PA	2.57	0.45
2:D:259:PHE:CG	2:D:311:TYR:HB3	2.52	0.45
2:D:64:ASP:CG	2:D:65:GLY:H	2.20	0.45
2:D:84:ILE:HD12	2:D:95:MET:CE	2.39	0.45
2:E:105:ARG:HD2	2:E:208:LEU:CD2	2.46	0.45
2:E:218:VAL:HG12	2:E:232:VAL:HG13	1.99	0.45
2:E:275:ILE:O	2:E:283:PRO:HG3	2.17	0.45
2:E:317:LEU:HD11	4:Q:12:AIB:HB12	1.99	0.45
3:G:254:ARG:NH2	8:G:2003:HOH:O	2.50	0.45
1:B:150:ILE:HA	1:B:430:GLN:OE1	2.16	0.44
1:B:434:SER:N	1:B:435:PRO:CD	2.80	0.44
1:C:424:LEU:HD23	1:C:424:LEU:HA	1.90	0.44
1:C:91:THR:HG22	1:C:93:ALA:H	1.82	0.44
2:E:204:GLY:O	2:E:206:ILE:N	2.51	0.44
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.95	0.44
1:B:28:THR:CG2	1:B:29:GLY:N	2.79	0.44
1:B:292:GLU:O	1:B:293:ALA:HB3	2.17	0.44
1:B:67:GLU:O	2:F:71:ARG:NH1	2.42	0.44
1:C:353:GLU:O	1:C:364:ALA:HB1	2.17	0.44
1:C:498:LYS:O	1:C:502:THR:OG1	2.29	0.44
2:D:275:ILE:CG2	2:D:276:PRO:HD2	2.47	0.44
2:D:346:PRO:HG3	2:D:418:PHE:HZ	1.81	0.44
2:E:168:GLU:OE1	2:E:420:VAL:HG23	2.18	0.44
8:B:2021:HOH:O	2:F:198:HIS:HE1	2.00	0.44
1:A:137:ILE:N	1:A:138:PRO:CD	2.81	0.44
1:A:351:PHE:HE1	1:A:353:GLU:OE2	2.00	0.44
1:B:452:TYR:HH	1:B:498:LYS:HG3	1.80	0.44
1:C:52:MET:CE	1:C:76:PHE:CE2	3.01	0.44
2:D:393:MET:HE3	2:D:404:VAL:HG11	2.00	0.44
1:C:145:PRO:HB3	1:C:378:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:ILE:HG23	2:D:276:PRO:HD2	2.00	0.44
2:E:416:GLN:NE2	2:E:430:LYS:O	2.50	0.44
1:A:157:VAL:N	1:A:158:PRO:HD3	2.32	0.44
1:B:171:ARG:HH11	1:B:171:ARG:CB	2.30	0.44
1:B:271:LEU:HA	1:B:271:LEU:HD23	1.77	0.44
1:B:294:TYR:CE2	1:B:338:ILE:CD1	3.00	0.44
1:B:156:LEU:CD2	1:B:391:LYS:HD2	2.45	0.44
1:C:210:ARG:NH1	2:F:121:PRO:O	2.51	0.44
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.46	0.44
2:E:41:ARG:NH2	2:E:67:GLU:O	2.46	0.44
2:F:160:VAL:CG1	2:F:335:LEU:HB3	2.48	0.44
4:Q:12:AIB:C	4:Q:14:LEU:H	2.21	0.44
1:A:351:PHE:HE1	1:A:353:GLU:HG2	1.83	0.44
1:A:390:MET:HE2	1:A:428:LEU:HD21	1.99	0.44
2:D:178:GLY:CA	2:D:214:LYS:NZ	2.80	0.44
2:D:432:VAL:CG1	2:D:433:PRO:HD2	2.47	0.44
2:D:84:ILE:O	2:D:86:VAL:HG13	2.18	0.44
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.98	0.44
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.82	0.44
1:A:296:GLY:HA3	2:E:271:LEU:CD2	2.48	0.44
1:B:450:ARG:CB	1:B:452:TYR:CE2	3.00	0.44
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.98	0.44
2:D:433:PRO:HD2	2:D:436:GLU:HB2	2.00	0.44
2:E:293:GLN:NE2	2:E:293:GLN:CA	2.79	0.44
1:A:286:ARG:HH22	3:G:272:LEU:HD13	1.82	0.44
2:E:439:LYS:O	2:E:442:GLN:HB3	2.17	0.44
1:B:34:ILE:HD11	1:B:79:ASP:CB	2.48	0.44
2:D:96:ASN:ND2	2:D:100:GLU:HB2	2.33	0.44
2:E:358:MET:CE	2:E:372:ARG:NE	2.80	0.44
2:E:96:ASN:OD1	2:E:97:VAL:N	2.51	0.44
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.99	0.43
1:A:349:GLN:HE22	1:A:370:SER:HA	1.83	0.43
1:B:157:VAL:N	1:B:158:PRO:HD3	2.33	0.43
1:B:285:LEU:O	1:B:286:ARG:HB2	2.18	0.43
1:C:267:ILE:N	1:C:267:ILE:CD1	2.81	0.43
1:C:273:LYS:HB3	8:C:2061:HOH:O	2.18	0.43
1:C:151:LYS:HA	1:C:441:GLN:OE1	2.18	0.43
2:D:356:ARG:HG2	2:D:356:ARG:O	2.18	0.43
1:C:373:ARG:HA	7:D:600:ADP:O3'	2.18	0.43
1:A:132:LYS:HA	8:A:2019:HOH:O	2.17	0.43
1:B:172:GLN:H	6:B:600:ANP:HNB1	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:ILE:O	2:F:33:LEU:HB2	2.18	0.43
2:F:408:ARG:O	2:F:412:ARG:HD2	2.18	0.43
3:G:212:ILE:O	3:G:215:TYR:HB3	2.17	0.43
1:A:244:TYR:CG	1:A:281:MET:HE1	2.53	0.43
1:A:138:PRO:HB3	1:A:316:PHE:CE2	2.52	0.43
1:B:218:LYS:HG2	2:E:128:VAL:HG11	2.00	0.43
1:B:367:VAL:CG1	1:B:391:LYS:HE3	2.48	0.43
2:D:387:ILE:HG23	3:G:19:ILE:CD1	2.47	0.43
2:E:167:MET:C	2:E:420:VAL:HG21	2.39	0.43
1:A:130:GLY:HA2	1:A:308:ARG:NH1	2.33	0.43
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.79	0.43
1:B:32:LEU:HD21	1:B:42:HIS:HB2	2.01	0.43
1:C:345:ILE:HA	2:D:222:MET:CE	2.49	0.43
1:C:457:GLU:HG2	8:C:2111:HOH:O	2.17	0.43
2:D:105:ARG:NH1	2:D:208:LEU:HD22	2.33	0.43
2:D:149:GLY:HA2	2:D:304:ILE:O	2.19	0.43
2:E:210:ASP:OD1	2:E:212:THR:N	2.42	0.43
2:E:36:LEU:N	2:E:36:LEU:HD23	2.33	0.43
2:E:415:SER:O	2:E:416:GLN:HB2	2.18	0.43
2:E:167:MET:HE3	2:E:420:VAL:CG1	2.48	0.43
2:F:134:VAL:HG13	2:F:141:ASP:OD2	2.18	0.43
1:B:66:LEU:O	2:F:15:ALA:HA	2.19	0.43
1:A:121:ILE:N	1:A:121:ILE:HD13	2.21	0.43
1:A:102:GLU:HG3	1:A:122:GLY:C	2.39	0.43
1:A:460:LYS:HD2	1:A:460:LYS:N	2.33	0.43
1:B:157:VAL:N	1:B:158:PRO:CD	2.82	0.43
1:C:485:THR:HG22	1:C:486:ASP:N	2.33	0.43
2:D:89:GLU:HG3	2:D:109:LYS:O	2.19	0.43
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.18	0.43
1:C:344:SER:O	2:D:222:MET:HE2	2.18	0.43
2:D:63:MET:CE	2:D:97:VAL:HG11	2.48	0.43
2:E:224:GLU:HB3	2:E:228:ALA:HB3	2.00	0.43
2:E:358:MET:HE3	2:E:372:ARG:NE	2.33	0.43
2:E:394:ASP:C	2:E:396:LEU:H	2.20	0.43
2:E:423:VAL:HG12	2:E:424:PHE:CD2	2.54	0.43
1:A:139:ARG:C	1:A:140:ILE:HG22	2.38	0.43
1:A:240:ALA:N	1:A:241:PRO:HD2	2.34	0.43
1:B:479:LEU:C	1:B:479:LEU:HD13	2.38	0.43
1:C:444:VAL:HG11	1:C:469:LEU:HD22	1.99	0.43
2:D:259:PHE:CB	2:D:311:TYR:HB3	2.48	0.43
2:E:126:MET:CE	2:E:297:THR:HG21	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:ILE:HA	2:F:49:VAL:CG1	2.49	0.43
2:F:36:LEU:HD23	2:F:36:LEU:N	2.33	0.43
1:B:484:ARG:HB3	1:B:484:ARG:HH11	1.84	0.43
1:C:173:THR:HG23	1:C:354:THR:HG22	1.99	0.43
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.19	0.43
1:A:211:SER:HA	2:D:126:MET:HE3	2.01	0.43
2:D:24:GLN:HG3	2:D:57:THR:OG1	2.19	0.43
2:E:244:ARG:O	2:E:248:GLY:HA2	2.18	0.43
2:F:139:VAL:HG23	8:F:2089:HOH:O	2.19	0.43
2:F:257:ASN:HB3	2:F:260:ARG:HG2	2.01	0.43
1:A:403:PHE:CZ	3:G:22:SER:HB2	2.54	0.43
1:A:142:VAL:CG1	1:A:374:VAL:HG11	2.49	0.43
1:A:161:ARG:NH1	1:A:263:HIS:CB	2.81	0.43
1:B:445:ILE:O	1:B:449:VAL:HG23	2.18	0.43
1:C:455:LYS:HB2	1:C:455:LYS:HE3	1.89	0.43
1:C:47:VAL:HG13	1:C:90:ARG:HG2	2.00	0.43
2:D:82:ILE:HD12	8:D:2005:HOH:O	2.18	0.43
2:E:377:ILE:HD12	2:E:377:ILE:HA	1.77	0.43
1:A:94:ILE:HD13	1:A:128:ARG:CD	2.49	0.43
1:B:207:GLY:HA3	1:B:273:LYS:HD3	2.00	0.43
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.33	0.43
1:B:388:GLY:O	1:B:392:LEU:HG	2.19	0.43
1:C:347:ASP:C	1:C:373:ARG:HG3	2.39	0.43
8:A:2010:HOH:O	2:D:29:LEU:HD21	2.19	0.43
2:D:381:TYR:O	2:D:385:GLN:HG3	2.19	0.43
1:B:140:ILE:CG2	1:B:311:LYS:HG3	2.47	0.43
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.84	0.43
1:C:362:ARG:HH11	1:C:362:ARG:CG	2.31	0.43
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.34	0.43
2:E:33:LEU:HD13	2:E:117:HIS:CD2	2.54	0.43
2:F:430:LYS:NZ	2:F:465:GLU:OE1	2.52	0.43
1:A:436:MET:HG3	1:A:441:GLN:HG2	2.01	0.42
1:A:453:LEU:HD13	1:A:461:ILE:HG23	2.01	0.42
1:C:151:LYS:HE2	1:C:436:MET:SD	2.59	0.42
1:C:474:SER:OG	1:C:475:GLN:N	2.51	0.42
1:C:30:ARG:HA	1:C:86:ASP:O	2.19	0.42
2:D:252:LEU:HD23	2:D:305:THR:HB	2.01	0.42
2:F:29:LEU:HD11	2:F:58:VAL:HG13	2.00	0.42
3:G:261:GLU:O	3:G:264:GLU:HB2	2.19	0.42
4:Q:16:TLX:H2'	4:Q:16:TLX:H22	1.64	0.42
1:C:101:GLU:HG3	8:C:2057:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:VAL:HB	2:E:45:LEU:HB3	2.00	0.42
3:G:212:ILE:HD13	3:G:212:ILE:HA	1.84	0.42
3:G:81:ILE:CG2	3:G:82:HIS:HD2	2.31	0.42
1:A:296:GLY:HA3	2:E:271:LEU:HD21	2.02	0.42
1:A:360:GLY:CA	1:A:362:ARG:HH12	2.28	0.42
1:A:436:MET:CE	1:A:441:GLN:HA	2.49	0.42
1:B:336:ALA:HB3	1:B:339:PRO:HD2	2.00	0.42
1:A:436:MET:HG3	1:A:441:GLN:CG	2.49	0.42
1:A:64:LEU:HD12	1:A:74:VAL:HG21	2.02	0.42
1:B:358:TYR:C	1:B:360:GLY:H	2.23	0.42
1:C:261:GLY:HA2	1:C:317:GLY:O	2.19	0.42
1:C:266:ILE:C	1:C:267:ILE:HD12	2.39	0.42
1:C:34:ILE:HD12	1:C:35:GLY:H	1.83	0.42
2:E:254:PHE:HA	2:E:307:VAL:O	2.19	0.42
2:F:376:LYS:HG2	2:F:376:LYS:O	2.20	0.42
1:A:219:ARG:HH11	1:A:219:ARG:CB	2.22	0.42
1:A:383:MET:HE3	1:A:438:ILE:HD11	2.02	0.42
1:B:362:ARG:HA	1:B:364:ALA:N	2.34	0.42
1:B:416:GLN:NE2	1:B:417:LEU:HD23	2.34	0.42
1:B:488:LYS:HG2	1:B:489:ILE:N	2.34	0.42
1:B:76:PHE:O	1:B:242:LEU:HD21	2.18	0.42
1:C:158:PRO:HB3	1:C:379:GLN:HG3	2.02	0.42
1:C:52:MET:HG3	1:C:61:GLY:O	2.20	0.42
2:E:138:LYS:O	2:E:142:LEU:HB3	2.19	0.42
2:E:264:ALA:O	2:E:268:VAL:HG23	2.20	0.42
2:F:266:SER:N	2:F:282:GLN:NE2	2.67	0.42
1:A:244:TYR:CE1	1:A:301:LEU:HD11	2.54	0.42
1:A:219:ARG:HG2	1:A:433:TYR:CE1	2.54	0.42
1:B:291:ARG:HD3	8:B:2065:HOH:O	2.20	0.42
1:B:427:LEU:HD11	1:B:448:GLY:HA3	2.00	0.42
2:D:160:VAL:HG12	2:D:335:LEU:CB	2.46	0.42
2:D:30:PRO:HA	2:D:31:PRO:HD3	1.95	0.42
2:D:53:LEU:HD21	2:D:59:ARG:HB2	2.01	0.42
2:E:146:TYR:N	8:E:2011:HOH:O	2.30	0.42
2:E:378:LEU:HD23	2:E:378:LEU:HA	1.85	0.42
2:E:392:GLY:O	2:E:394:ASP:N	2.47	0.42
3:G:20:THR:HA	3:G:232:MET:HE3	2.01	0.42
1:A:447:ALA:HB1	1:A:453:LEU:HD21	2.01	0.42
1:B:206:ILE:HD13	1:B:247:PRO:HG3	2.02	0.42
1:B:166:LEU:HD11	1:B:327:ILE:HB	2.01	0.42
1:B:381:ARG:O	1:B:385:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ARG:HB2	1:B:452:TYR:CE2	2.54	0.42
1:C:107:VAL:HG12	1:C:115:ILE:HD11	2.01	0.42
1:C:269:ASP:HA	1:C:270:ASP:HA	1.82	0.42
1:C:300:TYR:O	1:C:304:ARG:HB2	2.19	0.42
1:C:99:VAL:HG13	1:C:256:TYR:CB	2.47	0.42
2:E:35:ALA:N	2:E:80:ALA:O	2.40	0.42
1:A:174:GLY:HA2	6:A:600:ANP:O5'	2.20	0.42
1:C:392:LEU:HB3	2:D:458:TYR:OH	2.20	0.42
1:C:303:SER:HB2	2:D:222:MET:HB3	2.02	0.42
2:D:281:TYR:CD2	2:D:320:PRO:HG2	2.55	0.42
2:D:406:ARG:O	2:D:410:ILE:HG13	2.20	0.42
2:F:370:VAL:HG22	2:F:442:GLN:HG2	2.01	0.42
1:A:142:VAL:HG12	1:A:374:VAL:HG11	2.01	0.42
1:A:414:THR:HA	1:A:417:LEU:CD2	2.50	0.42
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.55	0.42
1:B:479:LEU:HD23	1:B:496:LYS:HD3	2.02	0.42
1:C:163:GLN:O	1:C:322:THR:HG23	2.20	0.42
2:D:136:GLY:HA3	2:D:431:LEU:HD12	1.93	0.42
2:D:200:MET:HB3	2:D:206:ILE:HG13	2.00	0.42
2:E:292:MET:CE	2:E:293:GLN:NE2	2.83	0.42
3:G:17:GLN:HB2	3:G:239:ALA:HB3	1.97	0.42
1:A:456:LEU:HD23	1:A:461:ILE:HD13	2.00	0.42
1:B:247:PRO:HB3	1:B:268:TYR:CD1	2.55	0.42
1:B:353:GLU:CB	1:B:356:LEU:HD12	2.40	0.42
1:C:137:ILE:HB	8:D:2012:HOH:O	2.20	0.42
1:C:192:GLY:O	1:C:198:LYS:NZ	2.51	0.42
1:C:390:MET:HE2	1:C:428:LEU:HD11	2.01	0.42
2:D:170:ILE:HG23	2:D:174:ALA:HB3	2.01	0.42
2:D:410:ILE:HG23	2:D:441:PHE:HE1	1.83	0.42
2:E:387:ILE:HG22	2:E:388:ILE:N	2.34	0.42
1:B:358:TYR:CZ	4:Q:16:TLX:H61	2.54	0.42
1:A:140:ILE:HG22	1:A:313:ASN:HB3	2.02	0.41
1:A:185:ASN:OD1	1:A:435:PRO:HB2	2.20	0.41
1:A:496:LYS:O	1:A:500:ILE:HG13	2.20	0.41
1:B:400:VAL:CB	1:B:418:LEU:HD21	2.48	0.41
1:B:469:LEU:HA	1:B:469:LEU:HD12	1.90	0.41
1:B:468:PHE:CE1	1:B:501:VAL:HG12	2.55	0.41
1:B:59:LEU:HA	1:B:59:LEU:HD12	1.86	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.20	0.41
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.55	0.41
1:C:460:LYS:NZ	1:C:463:LYS:HZ3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:MET:HE2	1:C:76:PHE:HE2	1.83	0.41
2:D:172:ASN:ND2	2:D:431:LEU:CD1	2.79	0.41
2:D:83:ARG:HA	2:D:115:ALA:HA	2.01	0.41
2:E:360:PRO:HA	2:E:368:TYR:HB2	2.02	0.41
2:F:205:VAL:HG12	2:F:215:VAL:CG2	2.38	0.41
2:F:164:VAL:HG23	6:F:600:ANP:O1A	2.19	0.41
1:A:278:TYR:HA	1:A:281:MET:CE	2.50	0.41
1:A:351:PHE:CE1	1:A:353:GLU:HG2	2.55	0.41
1:B:416:GLN:NE2	1:B:417:LEU:CD2	2.83	0.41
2:E:142:LEU:HD21	2:E:374:VAL:HG21	2.02	0.41
2:E:25:PHE:O	2:E:56:SER:HB3	2.20	0.41
2:E:432:VAL:HA	2:E:433:PRO:HD3	1.82	0.41
2:E:473:LEU:N	2:E:473:LEU:HD23	2.35	0.41
2:F:205:VAL:O	2:F:213:SER:HA	2.19	0.41
2:F:242:TYR:O	2:F:246:GLN:HB2	2.19	0.41
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.56	0.41
1:B:475:GLN:NE2	1:B:475:GLN:HA	2.34	0.41
1:C:460:LYS:NZ	1:C:463:LYS:HZ1	2.18	0.41
2:E:358:MET:HE3	2:E:372:ARG:NH2	2.35	0.41
2:F:340:ALA:HB2	2:F:347:ALA:HB2	2.02	0.41
2:F:433:PRO:HG2	2:F:436:GLU:CG	2.51	0.41
1:A:309:ALA:O	1:A:310:ALA:HB2	2.20	0.41
1:B:460:LYS:HA	1:B:460:LYS:HD3	1.83	0.41
1:C:132:LYS:HE3	2:D:224:GLU:OE1	2.20	0.41
2:D:11:GLY:N	2:D:25:PHE:CE1	2.88	0.41
1:B:32:LEU:HB2	1:B:40:ARG:O	2.21	0.41
1:B:400:VAL:HG11	1:B:418:LEU:CD1	2.44	0.41
1:B:433:TYR:C	1:B:435:PRO:HD3	2.41	0.41
1:C:83:LYS:HE3	1:C:83:LYS:HB2	1.80	0.41
2:E:155:PHE:HD1	2:E:155:PHE:N	2.17	0.41
1:A:296:GLY:O	2:E:267:GLU:HB3	2.20	0.41
2:E:9:THR:HG21	2:E:28:GLY:O	2.21	0.41
2:E:472:LYS:O	2:E:473:LEU:HD23	2.20	0.41
2:F:138:LYS:NZ	2:F:460:VAL:O	2.45	0.41
3:G:20:THR:HG22	3:G:236:SER:HB3	2.01	0.41
1:A:379:GLN:O	1:A:384:LYS:HE3	2.20	0.41
1:A:468:PHE:CZ	1:A:501:VAL:HG12	2.56	0.41
1:C:351:PHE:CE2	1:C:369:LEU:HD12	2.56	0.41
1:C:476:HIS:N	1:C:476:HIS:ND1	2.69	0.41
2:D:237:LEU:HD13	2:D:296:ILE:HG12	2.02	0.41
2:E:200:MET:HB3	2:E:206:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:HA	2:E:69:LEU:O	2.21	0.41
2:F:52:HIS:CD2	2:F:58:VAL:HG12	2.55	0.41
2:D:387:ILE:HG12	3:G:19:ILE:HD11	2.02	0.41
1:A:292:GLU:O	1:A:293:ALA:HB3	2.21	0.41
1:B:450:ARG:HA	1:B:450:ARG:HD3	1.88	0.41
1:B:34:ILE:CG1	1:B:79:ASP:HB2	2.51	0.41
1:C:187:LYS:HE2	1:C:227:LYS:NZ	2.35	0.41
1:C:96:ASP:O	1:C:97:VAL:HG13	2.21	0.41
2:D:30:PRO:HB3	2:D:77:ASP:CG	2.41	0.41
2:E:179:GLY:HA2	2:E:249:GLN:OE1	2.21	0.41
2:F:10:THR:HA	2:F:75:VAL:O	2.20	0.41
2:F:201:ILE:HG22	2:F:202:GLU:N	2.34	0.41
1:A:294:TYR:CE2	1:A:338:ILE:HD13	2.56	0.41
1:B:473:ILE:O	1:B:477:GLN:HG2	2.21	0.41
1:C:106:ARG:NH2	1:C:118:LYS:HB2	2.35	0.41
1:C:398:ARG:NH1	8:C:2100:HOH:O	2.52	0.41
2:D:256:ASP:HA	2:D:257:ASN:HA	1.79	0.41
2:E:168:GLU:HA	2:E:420:VAL:CG2	2.51	0.41
2:E:253:LEU:CD2	2:E:255:ILE:HD11	2.51	0.41
2:F:252:LEU:HA	2:F:252:LEU:HD23	1.87	0.41
1:A:40:ARG:HD2	1:A:70:ASN:OD1	2.20	0.41
1:B:99:VAL:HG21	1:B:127:ARG:HB3	2.03	0.41
1:B:423:ARG:CG	1:B:423:ARG:NH1	2.78	0.41
1:C:137:ILE:HA	1:C:137:ILE:HD13	1.96	0.41
1:C:286:ARG:NH1	8:F:2052:HOH:O	2.54	0.41
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.77	0.41
2:D:321:ALA:HB3	2:D:322:PRO:HD3	2.03	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.03	0.41
2:F:86:VAL:HG11	2:F:114:ALA:HB3	2.02	0.41
2:F:122:GLU:O	2:F:125:GLU:HB2	2.20	0.41
2:F:319:ASP:O	2:F:322:PRO:HD2	2.21	0.41
2:F:357:ILE:HA	2:F:357:ILE:HD13	1.71	0.41
1:B:75:VAL:HG21	1:B:82:ILE:CD1	2.51	0.41
1:B:99:VAL:CG1	1:B:256:TYR:HB2	2.50	0.41
1:C:353:GLU:CD	1:C:366:ASN:HD22	2.24	0.41
2:D:376:LYS:NZ	2:D:380:ASP:OD2	2.54	0.41
2:E:404:VAL:O	2:E:408:ARG:HG3	2.20	0.41
2:E:425:THR:O	2:E:427:HIS:ND1	2.29	0.41
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.21	0.41
2:F:309:ALA:C	2:F:310:ILE:HG13	2.40	0.41
1:A:215:GLN:NE2	2:D:130:GLN:HE21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HA	1:A:418:LEU:HD23	1.93	0.41
1:C:165:GLU:O	1:C:325:PRO:HD2	2.21	0.41
1:C:345:ILE:HA	2:D:222:MET:HE1	2.03	0.41
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.56	0.41
2:D:387:ILE:CG2	3:G:19:ILE:CD1	2.99	0.41
2:E:195:ASP:O	2:E:199:GLU:HG3	2.21	0.41
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.41
2:F:345:TYR:HA	2:F:346:PRO:C	2.41	0.41
4:Q:8:GLY:O	4:Q:9:AIB:HB23	2.20	0.41
1:A:439:GLU:HG2	1:A:484:ARG:CB	2.41	0.40
1:A:423:ARG:HG3	1:A:461:ILE:HD11	2.03	0.40
1:B:295:PRO:HG2	1:B:298:VAL:HG13	2.03	0.40
2:D:229:ARG:NH1	8:D:2034:HOH:O	2.48	0.40
2:D:130:GLN:HE22	2:D:356:ARG:CD	2.33	0.40
2:D:451:HIS:NE2	2:D:452:LEU:HD23	2.36	0.40
2:E:227:GLY:O	2:E:230:ALA:HB3	2.22	0.40
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.55	0.40
1:A:69:ASP:N	1:A:69:ASP:OD1	2.53	0.40
1:B:168:ILE:O	1:B:351:PHE:HA	2.21	0.40
1:B:218:LYS:CG	2:E:128:VAL:CG1	3.00	0.40
1:C:137:ILE:HG13	2:D:103:ASP:HA	2.04	0.40
2:D:96:ASN:HD22	2:D:100:GLU:HB2	1.87	0.40
2:E:166:ILE:O	2:E:170:ILE:HG13	2.22	0.40
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.22	0.40
1:A:179:ALA:O	1:A:182:THR:HB	2.22	0.40
1:A:161:ARG:NH2	1:A:197:LYS:O	2.50	0.40
1:A:362:ARG:HA	1:A:363:PRO:C	2.40	0.40
1:B:269:ASP:HA	1:B:270:ASP:HA	1.90	0.40
1:C:287:ARG:HD3	8:C:2064:HOH:O	2.20	0.40
1:C:344:SER:HA	8:C:2093:HOH:O	2.20	0.40
1:C:390:MET:CE	1:C:424:LEU:HD22	2.51	0.40
1:C:46:ASN:HB2	1:C:90:ARG:HH11	1.86	0.40
2:D:142:LEU:HB2	2:D:437:THR:CG2	2.52	0.40
2:D:84:ILE:HB	2:D:85:PRO:HD2	2.01	0.40
2:E:354:THR:HG22	2:E:355:SER:N	2.36	0.40
1:B:412:ALA:O	1:B:415:GLN:HB2	2.20	0.40
1:C:206:ILE:HD13	1:C:247:PRO:HG3	2.03	0.40
2:D:388:ILE:HG23	2:D:392:GLY:O	2.22	0.40
2:D:470:ALA:O	2:D:474:ALA:N	2.55	0.40
2:E:438:ILE:H	2:E:438:ILE:HG12	1.66	0.40
2:E:456:ALA:HA	2:E:469:LYS:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:435:LYS:HG3	2:F:436:GLU:N	2.35	0.40
3:G:23:MET:SD	3:G:232:MET:HE1	2.61	0.40
3:G:260:LYS:HE3	3:G:260:LYS:HB2	1.82	0.40
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.25	0.40
1:B:207:GLY:HA3	1:B:273:LYS:CD	2.51	0.40
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.37	0.40
1:B:98:PRO:HG2	1:B:112:GLY:HA3	2.02	0.40
2:E:13:ILE:HD13	2:E:21:VAL:HG11	2.04	0.40
2:E:317:LEU:HD22	2:E:326:PHE:CE2	2.57	0.40
2:E:384:LEU:O	2:E:388:ILE:HG12	2.22	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	485/510 (95%)	436 (90%)	43 (9%)	6 (1%)	15	51
1	B	485/510 (95%)	434 (90%)	44 (9%)	7 (1%)	13	47
1	C	490/510 (96%)	450 (92%)	34 (7%)	6 (1%)	15	51
2	D	465/482 (96%)	419 (90%)	39 (8%)	7 (2%)	12	45
2	E	464/482 (96%)	411 (89%)	47 (10%)	6 (1%)	14	48
2	F	464/482 (96%)	428 (92%)	35 (8%)	1 (0%)	51	84
3	G	116/272 (43%)	102 (88%)	13 (11%)	1 (1%)	20	60
4	Q	4/17 (24%)	2 (50%)	2 (50%)	0	100	100
All	All	2973/3265 (91%)	2682 (90%)	257 (9%)	34 (1%)	17	54

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ALA
1	A	95	VAL
1	C	407	GLY
1	C	411	ASP
2	E	393	MET
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	476	HIS
2	D	28	GLY
2	D	177	HIS
2	E	161	GLY
2	E	205	VAL
2	E	455	GLN
3	G	81	ILE
1	B	411	ASP
1	A	364	ALA
1	B	506	ALA
1	C	57	SER
2	D	249	GLN
2	D	474	ALA
1	B	70	ASN
1	B	236	ALA
1	C	475	GLN
2	D	250	ASP
2	D	33	LEU
2	F	279	VAL
1	C	332	GLY
2	E	279	VAL
1	B	95	VAL
1	A	246	ALA
1	B	458	PRO
2	D	279	VAL
2	E	423	VAL

### 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	393/412 (95%)	354 (90%)	39 (10%)	9	34
1	B	393/412 (95%)	358 (91%)	35 (9%)	11	41
1	C	397/412 (96%)	373 (94%)	24 (6%)	22	58
2	D	377/386 (98%)	356 (94%)	21 (6%)	25	61
2	E	376/386 (97%)	345 (92%)	31 (8%)	13	45
2	F	376/386 (97%)	355 (94%)	21 (6%)	25	61
3	G	102/230 (44%)	92 (90%)	10 (10%)	9	35
4	Q	2/2 (100%)	2 (100%)	0	100	100
All	All	2416/2626 (92%)	2235 (92%)	181 (8%)	16	49

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	45	ARG
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	79	ASP
1	A	80	LYS
1	A	91	THR
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	102	GLU
1	A	103	LEU
1	A	121	ILE
1	A	140	ILE
1	A	143	ARG
1	A	147	GLN
1	A	164	ARG
1	A	188	ARG
1	A	189	PHE
1	A	193	THR
1	A	195	GLU
1	A	211	SER
1	A	219	ARG
1	A	270	ASP
1	A	349	GLN
1	A	371	VAL

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Mol	Chain	Res	Type
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP
1	A	410	LEU
1	A	417	LEU
1	A	419	SER
1	A	420	ARG
1	A	439	GLU
1	A	442	VAL
1	A	453	LEU
1	A	479	LEU
1	A	499	GLU
1	B	47	VAL
1	B	79	ASP
1	B	80	LYS
1	B	123	SER
1	B	143	ARG
1	B	164	ARG
1	B	186	GLN
1	B	188	ARG
1	B	189	PHE
1	B	193	THR
1	B	216	LEU
1	B	221	THR
1	B	227	LYS
1	B	233	SER
1	B	256	TYR
1	B	270	ASP
1	B	298	VAL
1	B	349	GLN
1	B	351	PHE
1	B	361	ILE
1	B	371	VAL
1	B	380	THR
1	B	381	ARG
1	B	399	GLU
1	B	414	THR
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	444	VAL
1	B	456	LEU

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Mol	Chain	Res	Type
1	B	474	SER
1	B	484	ARG
1	B	485	THR
1	B	490	SER
1	B	505	LEU
1	C	34	ILE
1	C	45	ARG
1	C	47	VAL
1	C	56	SER
1	C	57	SER
1	C	63	SER
1	C	64	LEU
1	C	83	LYS
1	C	87	ILE
1	C	99	VAL
1	C	189	PHE
1	C	195	GLU
1	C	208	GLN
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	349	GLN
1	C	399	GLU
1	C	406	PHE
1	C	414	THR
1	C	444	VAL
1	C	474	SER
1	C	479	LEU
1	C	505	LEU
2	D	27	GLU
2	D	67	GLU
2	D	88	PRO
2	D	89	GLU
2	D	95	MET
2	D	112	GLN
2	D	137	ILE
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	250	ASP
2	D	282	GLN
2	D	306	SER

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Mol	Chain	Res	Type
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	400	ASP
2	D	423	VAL
2	D	428	LEU
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	67	GLU
2	E	95	MET
2	E	97	VAL
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	155	PHE
2	E	164	VAL
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	266	SER
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	358	MET
2	E	365	SER
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	431	LEU
2	E	438	ILE
2	E	450	ASP
2	E	452	LEU
2	E	473	LEU
2	F	36	LEU
2	F	67	GLU
2	F	95	MET

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Mol	Chain	Res	Type
2	F	112	GLN
2	F	127	SER
2	F	137	ILE
2	F	139	VAL
2	F	166	ILE
2	F	191	ARG
2	F	200	MET
2	F	223	ASN
2	F	261	PHE
2	F	279	VAL
2	F	282	GLN
2	F	292	MET
2	F	357	ILE
2	F	383	SER
2	F	386	ASP
2	F	397	SER
2	F	428	LEU
2	F	455	GLN
3	G	4	LYS
3	G	22	SER
3	G	44	TYR
3	G	77	LEU
3	G	82	HIS
3	G	209	LEU
3	G	214	TYR
3	G	221	THR
3	G	236	SER
3	G	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	215	GLN
1	A	396	GLN
1	A	476	HIS
1	B	48	GLN
1	B	65	ASN
1	B	172	GLN
1	B	349	GLN
1	B	475	GLN
1	B	503	ASN

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Mol	Chain	Res	Type
1	C	208	GLN
1	C	260	ASN
1	C	349	GLN
2	D	34	ASN
2	D	194	ASN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	361	ASN
2	D	442	GLN
2	E	130	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	282	GLN
2	E	293	GLN
2	E	308	GLN
2	E	367	HIS
2	F	51	GLN
2	F	96	ASN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	443	GLN
3	G	82	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	YCP	Q	1	4	8,8,9	0.80	0	7,9,11	2.03	3 (42%)
4	AIB	Q	10	4	2,5,6	0.77	0	0,7,9	0.00	-
4	YCP	Q	11	4	8,8,9	0.59	0	7,9,11	1.13	1 (14%)
4	AIB	Q	12	4	2,5,6	0.81	0	0,7,9	0.00	-
4	AIB	Q	15	4	2,5,6	0.51	0	0,7,9	0.00	-
4	AIB	Q	2	4	2,5,6	0.61	0	0,7,9	0.00	-
4	YCP	Q	3	4	8,8,9	1.26	1 (12%)	7,9,11	1.13	1 (14%)
4	AIB	Q	4	4	2,5,6	0.60	0	0,7,9	0.00	-
4	AIB	Q	5	4	2,5,6	0.81	0	0,7,9	0.00	-
4	BAL	Q	7	4	4,4,5	0.46	0	2,3,5	0.94	0
4	AIB	Q	9	4	2,5,6	0.70	0	0,7,9	0.00	-

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
4	YCP	Q	1	4	-	0/1/10/12	0/1/1/1
4	AIB	Q	10	4	-	0/2/3/6	0/0/0/0
4	YCP	Q	11	4	-	0/1/10/12	0/1/1/1
4	AIB	Q	12	4	-	0/2/3/6	0/0/0/0
4	AIB	Q	15	4	-	0/2/3/6	0/0/0/0
4	AIB	Q	2	4	-	0/2/3/6	0/0/0/0
4	YCP	Q	3	4	-	0/1/10/12	0/1/1/1
4	AIB	Q	4	4	-	0/2/3/6	0/0/0/0
4	AIB	Q	5	4	-	0/2/3/6	0/0/0/0
4	BAL	Q	7	4	-	0/1/2/3	0/0/0/0
4	AIB	Q	9	4	-	0/2/3/6	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	3	YCP	CA-C	3.11	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	1	YCP	O-C-CA	-3.32	117.41	125.15
4	Q	3	YCP	CE-N-CA	2.16	116.70	111.92
4	Q	1	YCP	CG-CB-CA	2.21	114.50	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	11	YCP	CE-N-CA	2.59	117.66	111.92
4	Q	1	YCP	CE-N-CA	3.17	118.94	111.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	YCP	3	0
4	Q	10	AIB	2	0
4	Q	11	YCP	3	0
4	Q	12	AIB	8	0
4	Q	15	AIB	2	0
4	Q	2	AIB	4	0
4	Q	3	YCP	4	0
4	Q	4	AIB	1	0
4	Q	5	AIB	1	0
4	Q	7	BAL	2	0
4	Q	9	AIB	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	ANP	A	600	5	29,33,33	1.50	7 (24%)	28,52,52	1.63	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ANP	B	600	5	29,33,33	1.61	7 (24%)	28,52,52	1.65	4 (14%)
6	ANP	C	600	5	29,33,33	1.62	7 (24%)	28,52,52	1.90	6 (21%)
7	ADP	D	600	5	25,29,29	1.02	2 (8%)	24,45,45	1.30	2 (8%)
6	ANP	F	600	5	29,33,33	1.45	7 (24%)	28,52,52	1.81	5 (17%)

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
6	ANP	A	600	5	-	0/13/38/38	0/3/3/3
6	ANP	B	600	5	-	0/13/38/38	0/3/3/3
6	ANP	C	600	5	-	0/13/38/38	0/3/3/3
7	ADP	D	600	5	-	0/12/32/32	0/3/3/3
6	ANP	F	600	5	-	1/13/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PG-O3G	-2.88	1.48	1.56
6	B	600	ANP	PB-O2B	-2.79	1.49	1.56
6	A	600	ANP	PG-O3G	-2.75	1.49	1.56
6	A	600	ANP	PG-O2G	-2.71	1.49	1.56
6	C	600	ANP	PB-O2B	-2.70	1.49	1.56
6	F	600	ANP	PG-O2G	-2.66	1.49	1.56
7	D	600	ADP	PA-O5'	-2.59	1.48	1.59
6	B	600	ANP	PG-O3G	-2.59	1.49	1.56
6	A	600	ANP	PB-O2B	-2.58	1.49	1.56
6	B	600	ANP	PG-O2G	-2.55	1.49	1.56
6	C	600	ANP	PG-O2G	-2.55	1.49	1.56
6	F	600	ANP	PB-O2B	-2.51	1.49	1.56
6	F	600	ANP	PG-O3G	-2.51	1.49	1.56
6	C	600	ANP	PA-O5'	-2.42	1.48	1.59
6	F	600	ANP	PA-O5'	-2.32	1.49	1.59
6	B	600	ANP	PA-O5'	-2.25	1.49	1.59
6	A	600	ANP	PA-O5'	-2.04	1.50	1.59
6	A	600	ANP	PG-O1G	2.51	1.49	1.46
6	A	600	ANP	PB-O1B	2.55	1.49	1.46
7	D	600	ADP	PB-O3A	2.65	1.64	1.60
6	F	600	ANP	PB-O1B	2.77	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	600	ANP	PB-O1B	2.86	1.49	1.46
6	F	600	ANP	PG-O1G	3.05	1.49	1.46
6	C	600	ANP	PG-O1G	3.05	1.49	1.46
6	B	600	ANP	PG-O1G	3.19	1.49	1.46
6	F	600	ANP	PB-O3A	3.36	1.63	1.59
6	B	600	ANP	PB-O1B	3.63	1.50	1.46
6	B	600	ANP	PB-O3A	3.99	1.64	1.59
6	A	600	ANP	PB-O3A	4.16	1.64	1.59
6	C	600	ANP	PB-O3A	4.65	1.64	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	600	ANP	O1G-PG-N3B	-5.82	103.09	111.79
6	F	600	ANP	O1G-PG-N3B	-5.32	103.84	111.79
6	A	600	ANP	O1G-PG-N3B	-4.83	104.57	111.79
6	B	600	ANP	O1G-PG-N3B	-4.77	104.65	111.79
6	A	600	ANP	O1B-PB-N3B	-4.25	105.44	111.79
6	F	600	ANP	O1B-PB-N3B	-3.96	105.86	111.79
6	F	600	ANP	PA-O3A-PB	-3.43	120.29	132.38
6	B	600	ANP	O1B-PB-N3B	-2.66	107.81	111.79
6	C	600	ANP	C1'-N9-C4	-2.48	122.35	126.64
6	C	600	ANP	O1B-PB-N3B	-2.34	108.29	111.79
6	C	600	ANP	PA-O3A-PB	-2.01	125.27	132.38
6	F	600	ANP	O3G-PG-O2G	2.17	113.78	107.69
7	D	600	ADP	C4-C5-N7	2.19	111.53	109.41
6	B	600	ANP	O3G-PG-O2G	2.23	113.95	107.69
6	C	600	ANP	O2G-PG-O1G	2.34	119.36	113.41
6	A	600	ANP	O3G-PG-O2G	2.47	114.61	107.69
6	A	600	ANP	O2B-PB-O1B	4.22	118.64	109.87
7	D	600	ADP	C1'-N9-C4	4.58	134.55	126.64
6	F	600	ANP	O2B-PB-O1B	4.61	119.45	109.87
6	B	600	ANP	O2B-PB-O1B	5.66	121.63	109.87
6	C	600	ANP	O2B-PB-O1B	5.72	121.76	109.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ANP	O1G-PG-N3B-PB

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ANP	2	0
6	B	600	ANP	8	0
6	C	600	ANP	8	0
7	D	600	ADP	1	0
6	F	600	ANP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	485/510 (95%)	-0.59	4 (0%) 86 71	17, 39, 72, 98	0
1	B	479/510 (93%)	-0.54	9 (1%) 67 46	13, 38, 82, 100	0
1	C	492/510 (96%)	-0.67	6 (1%) 79 61	11, 33, 66, 101	0
2	D	467/482 (96%)	-0.68	1 (0%) 94 89	11, 34, 69, 95	0
2	E	466/482 (96%)	-0.39	9 (1%) 67 46	18, 46, 85, 103	0
2	F	466/482 (96%)	-0.64	3 (0%) 89 77	14, 34, 69, 92	0
3	G	122/272 (44%)	0.30	19 (15%) 2 1	13, 64, 101, 107	0
4	Q	4/17 (23%)	-0.65	0 100 100	22, 26, 26, 27	0
All	All	2981/3265 (91%)	-0.55	51 (1%) 70 49	11, 38, 78, 107	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	89	MET	5.0
2	E	473	LEU	5.0
1	C	407	GLY	4.7
3	G	86	ALA	4.3
3	G	210	ALA	3.8
3	G	213	ILE	3.7
1	C	405	GLN	3.7
2	D	394	ASP	3.7
1	C	409	ASP	3.6
1	C	408	SER	3.3
2	E	389	ALA	3.1
3	G	41	ALA	3.0
2	F	9	THR	3.0
3	G	90	LYS	3.0
1	A	94	ILE	2.9
3	G	217	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	401	ALA	2.9
1	A	406	PHE	2.8
3	G	211	ASN	2.8
1	B	193	THR	2.8
3	G	85	VAL	2.8
3	G	42	ARG	2.8
3	G	43	VAL	2.8
2	E	474	ALA	2.7
2	F	42	GLU	2.7
2	E	398	GLU	2.6
2	E	424	PHE	2.6
1	B	506	ALA	2.6
2	E	390	ILE	2.5
3	G	40	PRO	2.5
1	A	405	GLN	2.5
3	G	39	LYS	2.5
3	G	216	SER	2.4
3	G	87	LYS	2.4
2	F	246	GLN	2.4
2	E	395	GLU	2.3
1	B	413	ALA	2.3
2	E	394	ASP	2.3
1	B	192	GLY	2.2
3	G	209	LEU	2.2
1	C	406	PHE	2.2
1	B	458	PRO	2.2
1	B	392	LEU	2.2
1	A	93	ALA	2.2
1	C	193	THR	2.2
3	G	214	TYR	2.2
1	B	411	ASP	2.2
3	G	224	GLU	2.1
3	G	81	ILE	2.1
1	B	412	ALA	2.1
2	E	425	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	AIB	Q	12	6/7	0.98	0.11	-	14,22,27,28	0
4	AIB	Q	5	6/7	0.97	0.13	-	19,24,28,29	0
4	YCP	Q	3	8/9	0.97	0.10	-	12,21,23,26	0
4	BAL	Q	7	5/6	0.97	0.23	-	18,23,36,45	0
4	YCP	Q	11	8/9	0.98	0.12	-	12,23,25,32	0
4	AIB	Q	9	6/7	0.98	0.15	-	15,22,22,25	0
4	AIB	Q	10	6/7	0.98	0.14	-	17,18,30,32	0
4	AIB	Q	2	6/7	0.95	0.18	-	21,26,31,39	0
4	AIB	Q	15	6/7	0.97	0.19	-	19,28,40,40	0
4	YCP	Q	1	8/9	0.98	0.12	-	17,23,30,38	0
4	AIB	Q	4	6/7	0.97	0.17	-	14,24,26,29	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	F	601	1/1	0.97	0.39	24.72	25,25,25,25	0
5	MG	D	601	1/1	0.98	0.47	14.63	26,26,26,26	0
7	ADP	D	600	27/27	0.97	0.13	-0.11	12,25,33,55	0
6	ANP	A	600	31/31	0.97	0.11	-0.31	12,31,51,56	0
6	ANP	B	600	31/31	0.96	0.14	-0.32	8,32,52,59	0
6	ANP	F	600	31/31	0.98	0.13	-0.39	20,28,37,42	0
6	ANP	C	600	31/31	0.98	0.11	-0.77	16,25,31,38	0
5	MG	A	601	1/1	0.96	0.18	-	29,29,29,29	0
5	MG	C	601	1/1	0.95	0.33	-	23,23,23,23	0
5	MG	B	601	1/1	0.94	0.29	-	34,34,34,34	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.