Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 04:31 AM EDT

PDB ID	:	1GLF
Title	:	CRYSTAL STRUCTURES OF ESCHERICHIA COLI GLYCEROL KINASE AND THE MUTANT A65T IN AN INACTIVE TETRAMER: CONFORMA-TIONAL CHANGES AND IMPLICATIONS FOR ALLOSTERIC REGULA-TION
Authors	:	Feese, M.D.; Faber, H.R.; Bystrom, C.E.; Pettigrew, D.W.; Remington, S.J.
Deposited on	:	1998-08-30
Resolution	:	2.62 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:
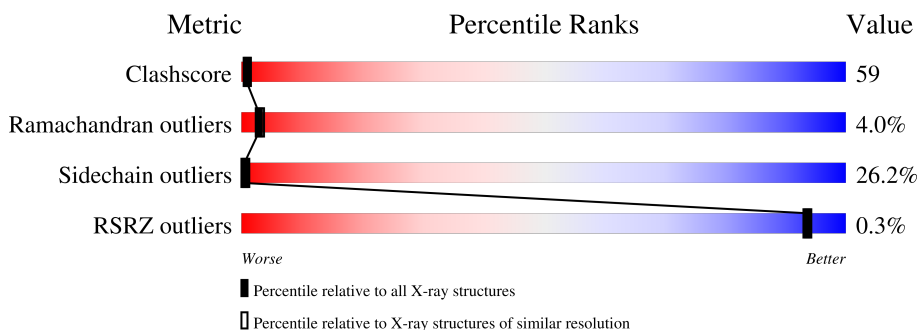
1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	Percentile Ranks	Value
Clashscore		59
Ramachandran outliers		4.0%
Sidechain outliers		26.2%
RSRZ outliers		0.3%

Worse　　　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	O	501	22% / 45% / 24% / 8%
1	X	501	21% / 49% / 24% / 5%
1	Y	501	25% / 47% / 23%
1	Z	501	23% / 50% / 19% / 7%

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:

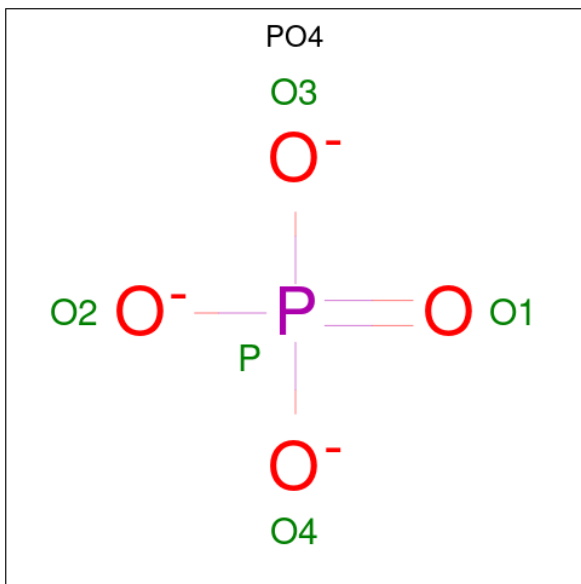| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	O	601	-	-	X	-
3	ADP	O	607	X	-	-	-
4	GOL	Z	605	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15981 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 PROTEIN (GLYCEROL KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3913	2467	684	743	19			
1	Y	499	Total	C	N	O	S	0	0	0
			3909	2465	683	742	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3907	2465	682	741	19			
1	X	498	Total	C	N	O	S	0	0	0
			3910	2467	684	740	19			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	Y	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
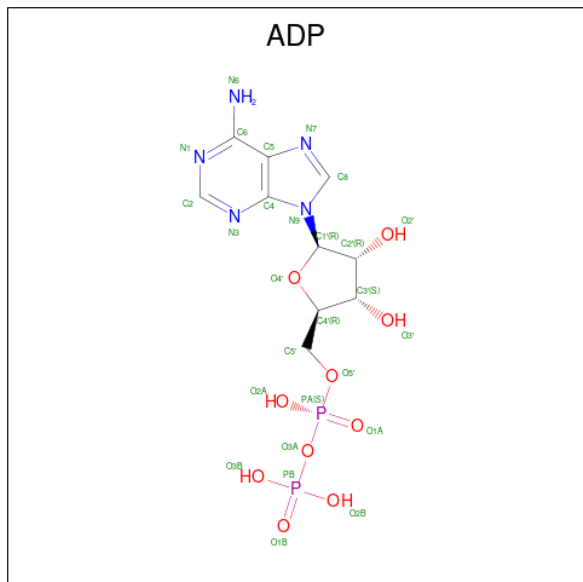
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Y	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Z	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	X	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total 6	C 3	O 3	0	0
4	Y	1	Total 6	C 3	O 3	0	0
4	Z	1	Total 6	C 3	O 3	0	0
4	X	1	Total 6	C 3	O 3	0	0
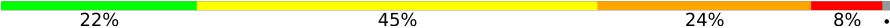
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	46	Total 46	O 46	0	0
5	Y	51	Total 51	O 51	0	0
5	Z	53	Total 53	O 53	0	0
5	X	50	Total 50	O 50	0	0

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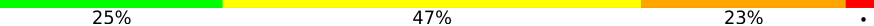
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PROTEIN (GLYCEROL KINASE)
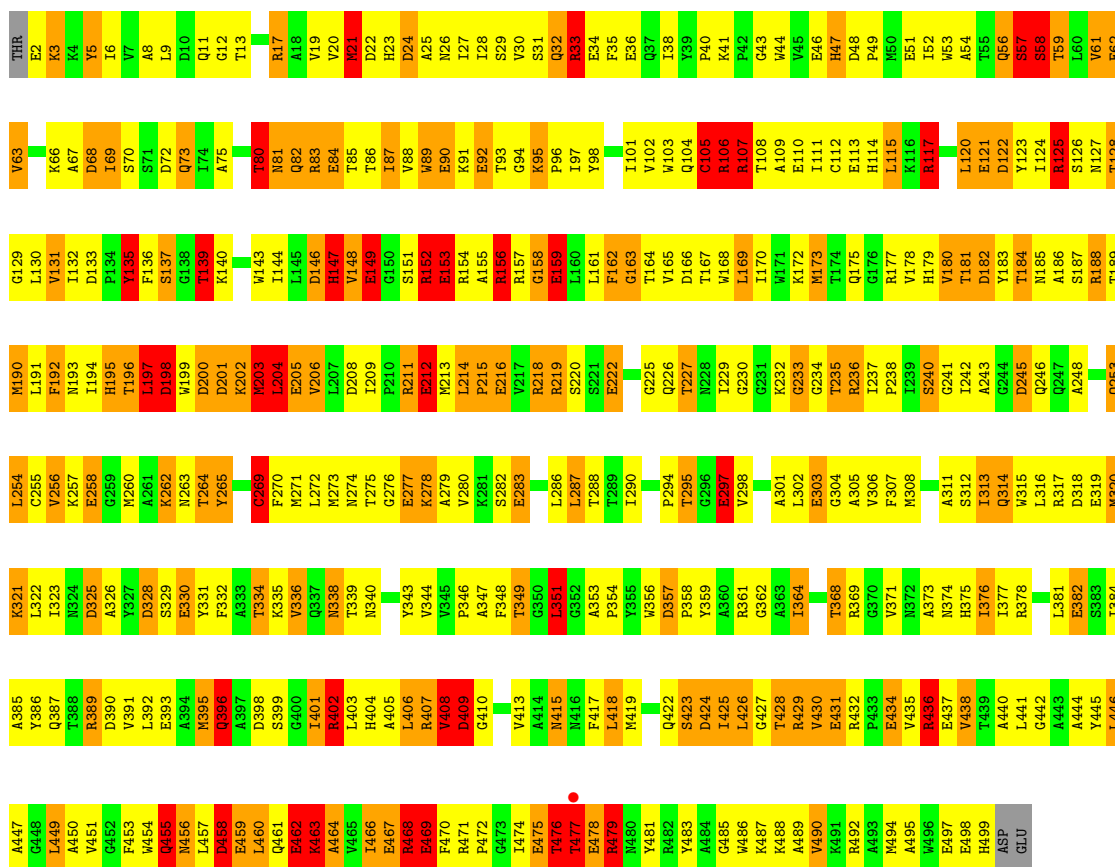
• Molecule 1: PROTEIN (GLYCEROL KINASE)

• Molecule 1: PROTEIN (GLYCEROL KINASE)

● Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain X:

21%   49%   24%   5% ●
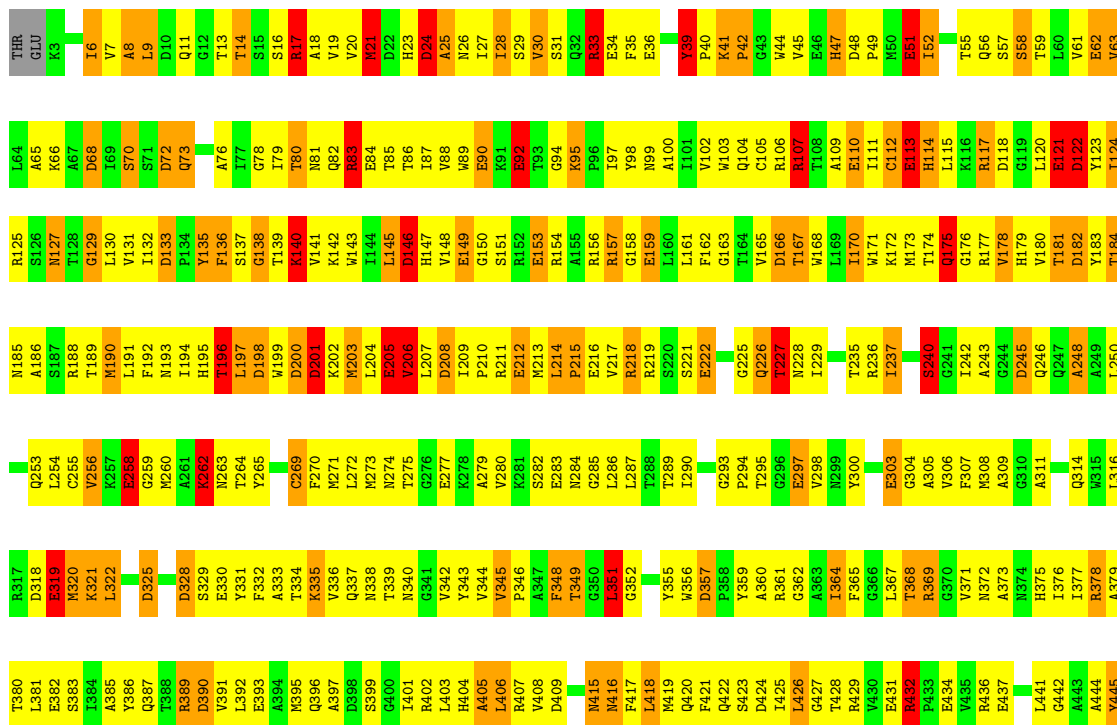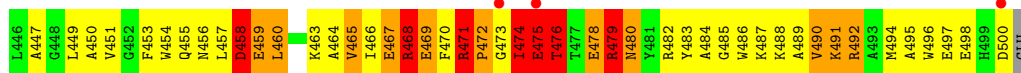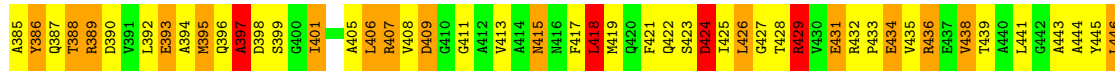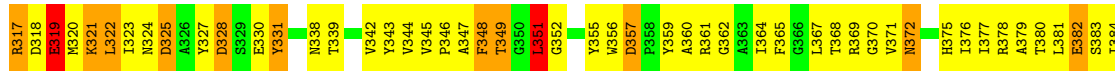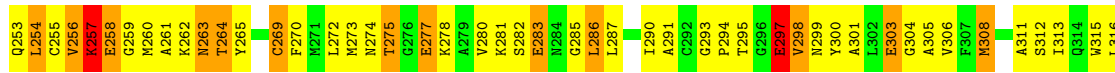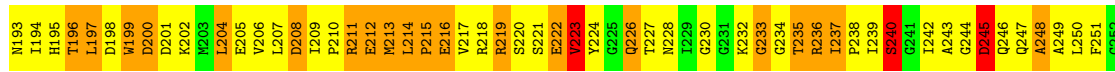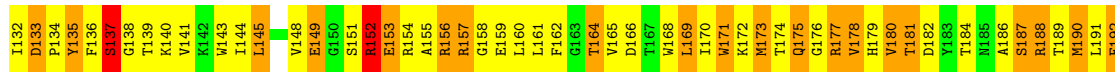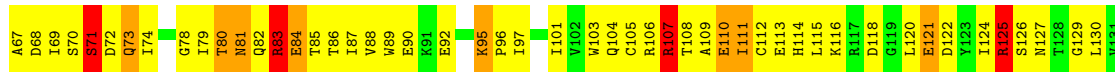
4 Data and refinement statistics ⓘ

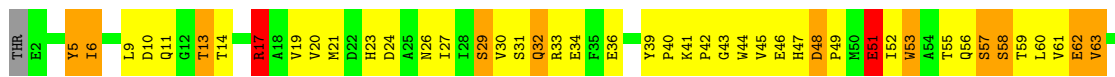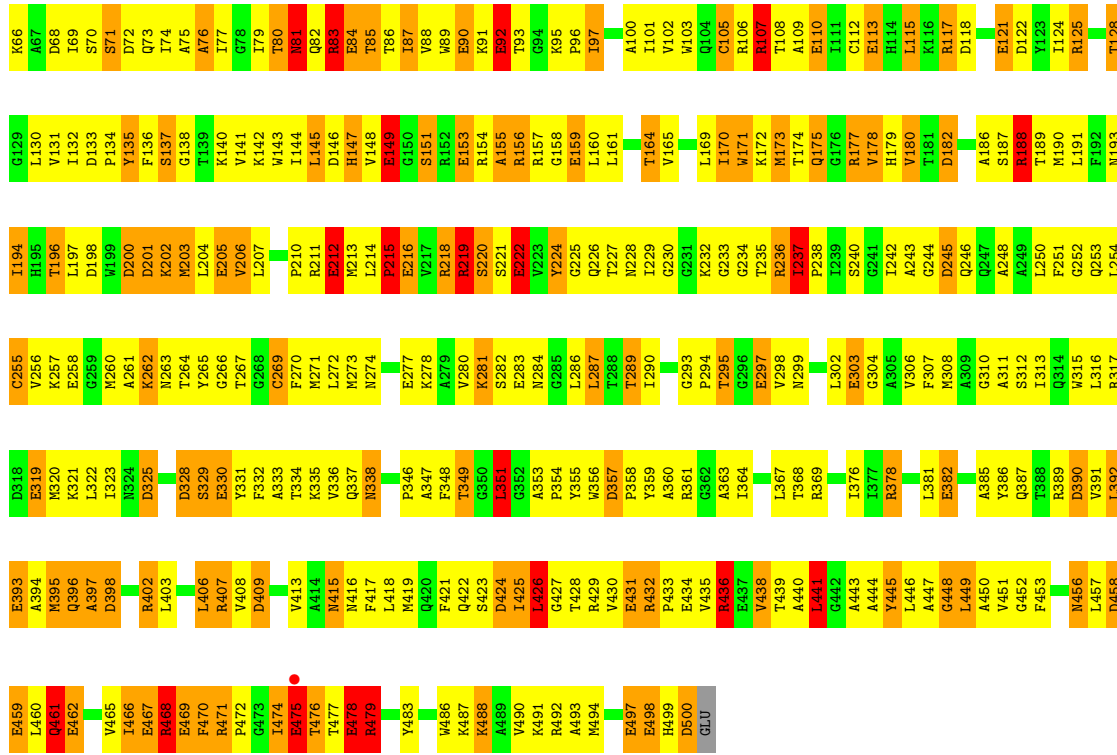| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.10Å 117.40Å 108.40Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 20.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-2.62) 84.4 (20.00-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.63Å)	Xtriage
Refinement program	TNT 5F-6	Depositor
R, R_{free}	0.146 , (Not available) 0.138 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	1.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 117.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15981	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4046e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	O	1.34	41/3993 (1.0%)	1.82	99/5416 (1.8%)
1	X	1.34	36/3990 (0.9%)	1.75	79/5411 (1.5%)
1	Y	1.32	38/3989 (1.0%)	1.77	84/5412 (1.6%)
1	Z	1.32	32/3987 (0.8%)	1.79	88/5408 (1.6%)
All	All	1.33	147/15959 (0.9%)	1.78	350/21647 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	1	1
1	Y	1	0
All	All	2	1

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	121	GLU	CD-OE1	10.08	1.36	1.25
1	O	475	GLU	CD-OE1	9.83	1.36	1.25
1	Y	277	GLU	CD-OE1	9.55	1.36	1.25
1	X	478	GLU	CD-OE1	9.33	1.35	1.25
1	Z	149	GLU	CD-OE1	9.21	1.35	1.25
1	O	149	GLU	CD-OE1	9.21	1.35	1.25
1	O	2	GLU	CD-OE1	9.19	1.35	1.25
1	Z	222	GLU	CD-OE2	8.86	1.35	1.25
1	Y	258	GLU	CD-OE2	8.82	1.35	1.25
1	X	434	GLU	CD-OE1	8.78	1.35	1.25
1	Z	216	GLU	CD-OE2	8.71	1.35	1.25
1	Y	84	GLU	CD-OE1	8.69	1.35	1.25

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	475	GLU	CD-OE2	8.60	1.35	1.25
1	Y	393	GLU	CD-OE1	8.54	1.35	1.25
1	X	36	GLU	CD-OE2	8.45	1.34	1.25
1	O	153	GLU	CD-OE1	8.40	1.34	1.25
1	Z	92	GLU	CD-OE2	8.32	1.34	1.25
1	X	149	GLU	CD-OE1	8.27	1.34	1.25
1	Y	467	GLU	CD-OE2	8.22	1.34	1.25
1	X	51	GLU	CD-OE1	8.20	1.34	1.25
1	O	462	GLU	CD-OE1	8.18	1.34	1.25
1	O	92	GLU	CD-OE2	8.18	1.34	1.25
1	Z	434	GLU	CD-OE1	8.12	1.34	1.25
1	Z	283	GLU	CD-OE1	8.08	1.34	1.25
1	X	459	GLU	CD-OE2	8.07	1.34	1.25
1	O	393	GLU	CD-OE1	8.06	1.34	1.25
1	Y	110	GLU	CD-OE1	7.97	1.34	1.25
1	X	84	GLU	CD-OE1	7.96	1.34	1.25
1	Y	62	GLU	CD-OE2	7.96	1.34	1.25
1	X	121	GLU	CD-OE1	7.93	1.34	1.25
1	Z	459	GLU	CD-OE1	7.88	1.34	1.25
1	X	277	GLU	CD-OE2	7.81	1.34	1.25
1	Z	110	GLU	CD-OE1	7.74	1.34	1.25
1	X	469	GLU	CD-OE1	7.66	1.34	1.25
1	Z	205	GLU	CD-OE2	7.61	1.34	1.25
1	Z	478	GLU	CD-OE1	7.60	1.34	1.25
1	Y	283	GLU	CD-OE1	7.56	1.33	1.25
1	Y	462	GLU	CD-OE1	7.53	1.33	1.25
1	Z	319	GLU	CD-OE2	7.49	1.33	1.25
1	Z	498	GLU	CD-OE1	7.45	1.33	1.25
1	Y	497	GLU	CD-OE2	7.42	1.33	1.25
1	X	110	GLU	CD-OE1	7.41	1.33	1.25
1	O	110	GLU	CD-OE1	7.40	1.33	1.25
1	O	498	GLU	CD-OE1	7.38	1.33	1.25
1	X	92	GLU	CD-OE1	7.32	1.33	1.25
1	O	478	GLU	CD-OE2	7.32	1.33	1.25
1	Y	153	GLU	CD-OE1	7.32	1.33	1.25
1	X	475	GLU	CD-OE2	7.27	1.33	1.25
1	Z	467	GLU	CD-OE2	7.26	1.33	1.25
1	Z	437	GLU	CD-OE2	7.25	1.33	1.25
1	Y	212	GLU	CD-OE2	7.24	1.33	1.25
1	Y	216	GLU	CD-OE1	7.23	1.33	1.25
1	X	431	GLU	CD-OE1	7.22	1.33	1.25
1	X	297	GLU	CD-OE1	7.18	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	330	GLU	CD-OE1	7.16	1.33	1.25
1	X	393	GLU	CD-OE1	7.15	1.33	1.25
1	X	462	GLU	CD-OE2	7.15	1.33	1.25
1	O	216	GLU	CD-OE2	7.09	1.33	1.25
1	Y	113	GLU	CD-OE2	7.09	1.33	1.25
1	Z	51	GLU	CD-OE1	7.08	1.33	1.25
1	X	498	GLU	CD-OE1	7.06	1.33	1.25
1	X	34	GLU	CD-OE1	7.05	1.33	1.25
1	Y	498	GLU	CD-OE1	7.05	1.33	1.25
1	O	319	GLU	CD-OE2	7.01	1.33	1.25
1	O	277	GLU	CD-OE1	6.98	1.33	1.25
1	Y	92	GLU	CD-OE1	6.89	1.33	1.25
1	Y	159	GLU	CD-OE1	6.88	1.33	1.25
1	Z	153	GLU	CD-OE1	6.87	1.33	1.25
1	X	467	GLU	CD-OE2	6.80	1.33	1.25
1	Y	51	GLU	CD-OE1	6.78	1.33	1.25
1	Y	297	GLU	CD-OE2	6.78	1.33	1.25
1	O	283	GLU	CD-OE2	6.77	1.33	1.25
1	Z	330	GLU	CD-OE1	6.77	1.33	1.25
1	X	382	GLU	CD-OE2	6.74	1.33	1.25
1	O	330	GLU	CD-OE2	6.74	1.33	1.25
1	Z	469	GLU	CD-OE2	6.69	1.33	1.25
1	O	205	GLU	CD-OE2	6.67	1.32	1.25
1	O	34	GLU	CD-OE1	6.63	1.32	1.25
1	O	62	GLU	CD-OE1	6.62	1.32	1.25
1	Y	205	GLU	CD-OE2	6.60	1.32	1.25
1	Y	434	GLU	CD-OE1	6.59	1.32	1.25
1	X	153	GLU	CD-OE1	6.59	1.32	1.25
1	Y	469	GLU	CD-OE2	6.58	1.32	1.25
1	O	51	GLU	CD-OE1	6.52	1.32	1.25
1	X	46	GLU	CD-OE2	6.51	1.32	1.25
1	O	382	GLU	CD-OE2	6.49	1.32	1.25
1	Y	46	GLU	CD-OE1	-6.44	1.18	1.25
1	X	205	GLU	CD-OE2	6.41	1.32	1.25
1	Y	475	GLU	CD-OE1	6.39	1.32	1.25
1	Z	34	GLU	CD-OE1	6.37	1.32	1.25
1	Y	149	GLU	CD-OE2	6.37	1.32	1.25
1	Z	36	GLU	CD-OE2	6.34	1.32	1.25
1	Y	121	GLU	CD-OE2	6.33	1.32	1.25
1	Z	159	GLU	CD-OE1	6.32	1.32	1.25
1	O	121	GLU	CD-OE1	6.31	1.32	1.25
1	Y	222	GLU	CD-OE2	6.31	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	62	GLU	CD-OE2	6.30	1.32	1.25
1	Z	90	GLU	CD-OE2	6.22	1.32	1.25
1	O	212	GLU	CD-OE1	6.21	1.32	1.25
1	X	258	GLU	CD-OE2	6.18	1.32	1.25
1	O	113	GLU	CD-OE1	6.16	1.32	1.25
1	Z	277	GLU	CD-OE2	6.14	1.32	1.25
1	O	222	GLU	CD-OE2	6.11	1.32	1.25
1	O	437	GLU	CD-OE1	6.09	1.32	1.25
1	O	431	GLU	CD-OE1	6.06	1.32	1.25
1	Z	497	GLU	CD-OE2	6.03	1.32	1.25
1	O	497	GLU	CD-OE2	6.01	1.32	1.25
1	Z	393	GLU	CD-OE1	6.00	1.32	1.25
1	X	283	GLU	CD-OE2	6.00	1.32	1.25
1	O	303	GLU	CD-OE2	-5.94	1.19	1.25
1	Y	90	GLU	CD-OE2	5.94	1.32	1.25
1	O	46	GLU	CD-OE2	5.94	1.32	1.25
1	Y	319	GLU	CD-OE1	5.93	1.32	1.25
1	X	497	GLU	CD-OE2	5.90	1.32	1.25
1	Y	382	GLU	CD-OE2	5.89	1.32	1.25
1	Y	459	GLU	CD-OE1	5.83	1.32	1.25
1	Z	431	GLU	CD-OE1	5.83	1.32	1.25
1	O	459	GLU	CD-OE1	5.80	1.32	1.25
1	O	469	GLU	CD-OE2	5.78	1.32	1.25
1	O	90	GLU	CD-OE2	5.77	1.31	1.25
1	O	297	GLU	CD-OE1	5.75	1.31	1.25
1	Z	129	GLY	CA-C	5.69	1.60	1.51
1	X	429	ARG	NE-CZ	5.68	1.40	1.33
1	Y	478	GLU	CD-OE2	5.59	1.31	1.25
1	Z	303	GLU	CD-OE1	5.57	1.31	1.25
1	Z	258	GLU	CD-OE2	5.50	1.31	1.25
1	X	113	GLU	CD-OE2	5.50	1.31	1.25
1	O	159	GLU	CD-OE1	5.49	1.31	1.25
1	O	258	GLU	CD-OE2	5.49	1.31	1.25
1	X	222	GLU	CD-OE2	5.44	1.31	1.25
1	O	125	ARG	NE-CZ	5.44	1.40	1.33
1	Z	113	GLU	CD-OE1	5.41	1.31	1.25
1	X	319	GLU	CD-OE2	5.39	1.31	1.25
1	Y	36	GLU	CD-OE2	5.36	1.31	1.25
1	O	36	GLU	CD-OE2	5.36	1.31	1.25
1	O	434	GLU	CD-OE1	5.33	1.31	1.25
1	X	212	GLU	CD-OE2	5.31	1.31	1.25
1	Y	34	GLU	CD-OE1	5.29	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	303	GLU	CD-OE1	5.24	1.31	1.25
1	O	330	GLU	CD-OE1	-5.21	1.20	1.25
1	Y	431	GLU	CD-OE1	5.18	1.31	1.25
1	O	163	GLY	N-CA	-5.16	1.38	1.46
1	O	467	GLU	CD-OE2	5.12	1.31	1.25
1	Y	237	ILE	C-N	-5.11	1.24	1.34
1	X	157	ARG	NE-CZ	5.10	1.39	1.33
1	X	125	ARG	NE-CZ	5.05	1.39	1.33
1	Y	330	GLU	CD-OE2	5.01	1.31	1.25

All (350) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	479	ARG	NE-CZ-NH2	-21.02	109.79	120.30
1	O	479	ARG	NE-CZ-NH1	15.27	127.93	120.30
1	Y	200	ASP	CB-CG-OD1	-14.20	105.52	118.30
1	O	245	ASP	CB-CG-OD2	-13.98	105.72	118.30
1	Y	177	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	O	152	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	X	245	ASP	CB-CG-OD2	-11.26	108.17	118.30
1	X	182	ASP	CB-CG-OD2	-11.22	108.20	118.30
1	Z	200	ASP	CB-CG-OD2	-11.01	108.39	118.30
1	Z	218	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	Z	357	ASP	CB-CG-OD2	-10.70	108.67	118.30
1	O	182	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	Z	357	ASP	CB-CG-OD1	10.57	127.81	118.30
1	Z	107	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	O	135	TYR	CB-CG-CD1	10.19	127.11	121.00
1	Z	432	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	O	200	ASP	CB-CG-OD2	-9.70	109.57	118.30
1	Y	479	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	X	357	ASP	CB-CG-OD1	9.56	126.90	118.30
1	Y	402	ARG	NE-CZ-NH2	9.55	125.08	120.30
1	X	200	ASP	CB-CG-OD1	-9.48	109.77	118.30
1	Y	492	ARG	NE-CZ-NH1	9.45	125.02	120.30
1	O	106	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	Z	83	ARG	C-N-CA	-9.28	98.51	121.70
1	X	245	ASP	CB-CG-OD1	9.26	126.63	118.30
1	X	357	ASP	CB-CG-OD2	-9.22	110.00	118.30
1	O	133	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	X	107	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	X	31	SER	N-CA-CB	9.06	124.10	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	72	ASP	CB-CG-OD1	-9.04	110.16	118.30
1	Z	245	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	Z	342	VAL	CB-CA-C	-8.91	94.47	111.40
1	Z	325	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	X	135	TYR	CB-CG-CD1	8.80	126.28	121.00
1	Y	107	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	O	429	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	O	432	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	O	133	ASP	CB-CG-OD1	8.63	126.07	118.30
1	O	182	ASP	CB-CG-OD1	8.53	125.97	118.30
1	O	83	ARG	C-N-CA	-8.42	100.65	121.70
1	Y	201	ASP	CB-CG-OD1	-8.42	110.72	118.30
1	Z	328	ASP	CB-CG-OD1	-8.40	110.73	118.30
1	O	211	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	Z	83	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	X	133	ASP	CB-CG-OD1	8.34	125.81	118.30
1	Z	468	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	X	135	TYR	CB-CG-CD2	-8.26	116.05	121.00
1	X	107	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	O	195	HIS	CA-CB-CG	-8.24	99.59	113.60
1	Z	409	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	X	152	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	Y	219	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	Y	48	ASP	CB-CG-OD1	-8.07	111.04	118.30
1	O	328	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	Y	211	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	Z	33	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	Y	155	ALA	N-CA-CB	8.02	121.33	110.10
1	X	492	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	Y	328	ASP	CB-CG-OD2	8.00	125.50	118.30
1	O	218	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	O	198	ASP	CB-CG-OD2	7.98	125.48	118.30
1	Z	309	ALA	N-CA-CB	7.94	121.21	110.10
1	Z	201	ASP	CB-CG-OD1	-7.86	111.22	118.30
1	Y	245	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	Y	436	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	Y	328	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	O	135	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	Y	424	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	Z	107	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	Z	409	ASP	CB-CG-OD1	7.81	125.33	118.30
1	O	218	ARG	NE-CZ-NH1	-7.78	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	67	ALA	CB-CA-C	7.78	121.77	110.10
1	Y	107	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	Z	17	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	O	458	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	X	10	ASP	CB-CG-OD1	-7.65	111.42	118.30
1	O	122	ASP	CB-CG-OD1	7.64	125.17	118.30
1	O	117	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	Z	351	LEU	C-N-CA	-7.64	106.26	122.30
1	Y	436	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	O	432	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	O	125	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	Z	378	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	O	146	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	X	24	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	Y	398	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	X	192	PHE	N-CA-CB	-7.46	97.17	110.60
1	Y	188	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	Z	390	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	X	378	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	Y	164	THR	N-CA-CB	7.40	124.36	110.30
1	X	390	ASP	CB-CG-OD2	7.40	124.96	118.30
1	Y	357	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	Y	432	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	Y	325	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	O	468	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	Y	125	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	Z	133	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	Y	458	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	Y	468	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	Y	409	ASP	CB-CG-OD1	7.29	124.86	118.30
1	Z	24	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	Z	118	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	O	479	ARG	CD-NE-CZ	7.27	133.78	123.60
1	Y	118	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	Z	83	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	O	68	ASP	CB-CG-OD1	-7.16	111.85	118.30
1	O	245	ASP	CB-CG-OD1	7.16	124.75	118.30
1	Z	146	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	X	451	VAL	CA-CB-CG1	7.14	121.62	110.90
1	Z	135	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	O	351	LEU	C-N-CA	-7.11	107.37	122.30
1	Y	48	ASP	CB-CG-OD2	7.08	124.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	13	THR	CA-CB-CG2	-7.05	102.54	112.40
1	X	68	ASP	CB-CG-OD1	-7.04	111.96	118.30
1	Y	72	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	X	10	ASP	CB-CG-OD2	7.03	124.62	118.30
1	Z	133	ASP	CB-CG-OD1	7.00	124.60	118.30
1	O	33	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	X	429	ARG	CD-NE-CZ	6.99	133.38	123.60
1	Y	200	ASP	CB-CG-OD2	6.98	124.58	118.30
1	Z	114	HIS	CA-CB-CG	-6.94	101.80	113.60
1	O	357	ASP	CB-CG-OD1	6.93	124.54	118.30
1	O	409	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	O	156	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	X	83	ARG	C-N-CA	-6.90	104.44	121.70
1	Z	68	ASP	CB-CG-OD1	-6.88	112.10	118.30
1	Y	146	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	X	351	LEU	C-N-CA	-6.84	107.94	122.30
1	O	122	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	X	359	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	Y	479	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	Y	177	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	Y	118	ASP	CB-CG-OD1	6.78	124.40	118.30
1	X	390	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	Z	245	ASP	CB-CG-OD1	6.71	124.34	118.30
1	Y	156	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	X	33	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	Z	196	THR	N-CA-CB	-6.65	97.67	110.30
1	O	32	GLN	N-CA-CB	6.64	122.55	110.60
1	O	328	ASP	CB-CG-OD2	6.62	124.26	118.30
1	Y	357	ASP	CB-CG-OD1	6.62	124.26	118.30
1	Y	424	ASP	CB-CG-OD1	6.60	124.24	118.30
1	Y	155	ALA	CB-CA-C	6.60	120.00	110.10
1	Z	240	SER	CB-CA-C	-6.59	97.58	110.10
1	X	318	ASP	CB-CG-OD1	6.58	124.22	118.30
1	Z	72	ASP	CB-CG-OD1	-6.56	112.40	118.30
1	O	265	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	X	182	ASP	CB-CG-OD1	6.54	124.18	118.30
1	O	198	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	Y	390	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	Z	361	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	O	72	ASP	CB-CG-OD2	6.51	124.16	118.30
1	Z	361	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	Y	255	CYS	CB-CA-C	6.50	123.40	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	83	ARG	C-N-CA	-6.49	105.47	121.70
1	X	324	ASN	CB-CA-C	6.48	123.35	110.40
1	Z	117	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	Z	471	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	O	131	VAL	N-CA-CB	-6.44	97.34	111.50
1	Z	200	ASP	CB-CG-OD1	6.43	124.08	118.30
1	O	269	CYS	CA-CB-SG	-6.42	102.44	114.00
1	Z	345	VAL	CA-CB-CG2	-6.42	101.27	110.90
1	Y	351	LEU	C-N-CA	-6.39	108.88	122.30
1	Y	81	ASN	N-CA-CB	-6.35	99.17	110.60
1	O	408	VAL	N-CA-CB	-6.32	97.60	111.50
1	O	389	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	Z	208	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	O	357	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	Y	32	GLN	N-CA-CB	6.28	121.90	110.60
1	Y	432	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	Z	287	LEU	CB-CA-C	-6.27	98.29	110.20
1	O	402	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	Y	24	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	O	407	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	Z	490	VAL	CA-CB-CG1	-6.25	101.52	110.90
1	X	223	VAL	N-CA-CB	6.25	125.24	111.50
1	X	494	MET	CG-SD-CE	-6.23	90.23	100.20
1	O	21	MET	CB-CA-C	-6.20	97.99	110.40
1	X	118	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	Z	109	ALA	CB-CA-C	6.20	119.40	110.10
1	Y	500	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	X	429	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	X	328	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	X	186	ALA	N-CA-CB	6.17	118.73	110.10
1	X	458	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	Y	219	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	X	216	GLU	N-CA-CB	6.15	121.67	110.60
1	Y	68	ASP	CB-CG-OD2	6.14	123.82	118.30
1	Y	122	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	Z	122	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	X	157	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	Z	219	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	Z	318	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	O	107	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	Z	333	ALA	N-CA-CB	-6.02	101.67	110.10
1	X	318	ASP	CB-CG-OD2	-6.01	112.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	156	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	X	424	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	Z	328	ASP	CB-CG-OD2	6.00	123.70	118.30
1	Z	389	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	O	147	HIS	CA-CB-CG	-5.98	103.43	113.60
1	X	409	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	Z	248	ALA	CB-CA-C	-5.96	101.15	110.10
1	Z	167	THR	CA-CB-CG2	-5.95	104.07	112.40
1	O	84	GLU	N-CA-CB	5.94	121.30	110.60
1	Y	83	ARG	N-CA-C	5.94	127.05	111.00
1	X	436	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	X	48	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	O	24	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	O	68	ASP	CB-CG-OD2	5.90	123.61	118.30
1	O	198	ASP	CB-CA-C	5.89	122.18	110.40
1	O	139	THR	CA-CB-CG2	-5.88	104.16	112.40
1	O	495	ALA	CB-CA-C	-5.88	101.28	110.10
1	Z	21	MET	CB-CA-C	-5.87	98.66	110.40
1	X	386	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	X	125	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	Y	68	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	Z	227	THR	CA-CB-CG2	-5.82	104.25	112.40
1	Z	369	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	Y	236	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	Y	85	THR	CA-CB-CG2	-5.82	104.26	112.40
1	O	152	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	O	334	THR	CA-CB-CG2	-5.81	104.27	112.40
1	Z	458	ASP	CB-CA-C	5.80	122.01	110.40
1	Z	157	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	Y	325	ASP	CB-CG-OD1	5.79	123.51	118.30
1	X	177	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	Y	438	VAL	CA-CB-CG1	-5.78	102.24	110.90
1	Y	245	ASP	CB-CG-OD1	5.75	123.47	118.30
1	X	500	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	O	181	THR	N-CA-CB	5.73	121.19	110.30
1	Z	445	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	O	158	GLY	C-N-CA	5.73	136.02	121.70
1	O	201	ASP	CB-CG-OD1	5.72	123.45	118.30
1	Y	182	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	Y	55	THR	CA-CB-CG2	-5.70	104.42	112.40
1	X	137	SER	N-CA-CB	5.69	119.04	110.50
1	X	386	TYR	CA-CB-CG	-5.68	102.61	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	402	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	Y	426	LEU	CB-CA-C	-5.66	99.44	110.20
1	Z	140	LYS	N-CA-CB	5.64	120.76	110.60
1	Z	195	HIS	CA-CB-CG	-5.64	104.01	113.60
1	X	357	ASP	N-CA-CB	5.64	120.75	110.60
1	O	389	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	Y	17	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	X	435	VAL	CB-CA-C	-5.62	100.72	111.40
1	X	240	SER	N-CA-CB	-5.61	102.08	110.50
1	X	257	LYS	N-CA-CB	5.60	120.67	110.60
1	O	188	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	X	171	TRP	CB-CA-C	-5.58	99.23	110.40
1	Z	325	ASP	CB-CG-OD1	5.56	123.31	118.30
1	Y	80	THR	N-CA-CB	5.56	120.87	110.30
1	Z	334	THR	CA-CB-CG2	-5.56	104.61	112.40
1	X	500	ASP	CB-CG-OD1	5.56	123.31	118.30
1	Z	472	PRO	CA-N-CD	-5.56	103.72	111.50
1	O	338	ASN	N-CA-C	-5.55	96.00	111.00
1	Y	125	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	O	468	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	Z	122	ASP	CB-CA-C	5.54	121.49	110.40
1	Y	445	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	Z	211	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	O	409	ASP	CB-CG-OD1	5.53	123.27	118.30
1	Z	262	LYS	N-CA-CB	5.52	120.53	110.60
1	O	424	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	Y	72	ASP	CB-CG-OD1	5.49	123.24	118.30
1	O	396	GLN	N-CA-CB	5.48	120.47	110.60
1	X	390	ASP	N-CA-CB	5.47	120.45	110.60
1	O	258	GLU	N-CA-CB	5.47	120.45	110.60
1	Z	390	ASP	CB-CG-OD2	5.47	123.22	118.30
1	O	83	ARG	CA-C-N	5.47	129.23	117.20
1	O	325	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	Z	39	TYR	C-N-CD	-5.45	108.62	120.60
1	O	203	MET	CG-SD-CE	-5.42	91.53	100.20
1	Y	147	HIS	CA-CB-CG	-5.42	104.39	113.60
1	Z	332	PHE	CA-CB-CG	-5.41	100.93	113.90
1	Y	329	SER	N-CA-CB	-5.40	102.39	110.50
1	X	31	SER	CB-CA-C	5.40	120.36	110.10
1	O	455	GLN	N-CA-CB	5.40	120.32	110.60
1	X	208	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	X	471	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	348	PHE	CB-CA-C	-5.39	99.63	110.40
1	X	372	ASN	CB-CA-C	-5.38	99.64	110.40
1	O	105	CYS	CA-CB-SG	-5.38	104.33	114.00
1	O	475	GLU	O-C-N	5.37	131.30	122.70
1	Y	117	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	Z	219	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	O	139	THR	CA-CB-OG1	5.36	120.26	109.00
1	O	121	GLU	N-CA-CB	5.36	120.25	110.60
1	X	33	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	X	13	THR	N-CA-CB	5.36	120.48	110.30
1	Z	8	ALA	N-CA-CB	5.35	117.59	110.10
1	X	325	ASP	CB-CG-OD1	5.34	123.11	118.30
1	Z	201	ASP	CB-CG-OD2	5.34	123.11	118.30
1	Z	47	HIS	CB-CA-C	-5.33	99.75	110.40
1	Z	135	TYR	CB-CG-CD1	5.33	124.19	121.00
1	O	197	LEU	N-CA-CB	5.31	121.03	110.40
1	O	80	THR	CA-CB-CG2	-5.31	104.97	112.40
1	O	98	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	X	418	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	X	264	THR	N-CA-CB	-5.28	100.27	110.30
1	O	83	ARG	O-C-N	-5.27	114.26	122.70
1	Y	413	VAL	CB-CA-C	5.27	121.42	111.40
1	O	429	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	O	219	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	O	5	TYR	CB-CA-C	-5.26	99.88	110.40
1	Z	479	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	Y	407	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	Y	468	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	O	455	GLN	CB-CA-C	5.24	120.87	110.40
1	O	147	HIS	N-CA-CB	5.23	120.02	110.60
1	Z	318	ASP	CB-CG-OD1	5.23	123.00	118.30
1	X	407	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	Z	117	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	X	189	THR	CA-CB-CG2	-5.22	105.09	112.40
1	X	248	ALA	CB-CA-C	-5.22	102.27	110.10
1	O	436	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Z	14	THR	N-CA-CB	-5.22	100.39	110.30
1	Z	68	ASP	CB-CG-OD2	5.20	122.98	118.30
1	Z	476	THR	N-CA-CB	-5.20	100.42	110.30
1	X	317	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	O	398	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	Y	497	GLU	CA-C-N	-5.18	105.80	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	354	PRO	CB-CA-C	-5.18	99.06	112.00
1	O	192	PHE	N-CA-CB	-5.17	101.29	110.60
1	Z	109	ALA	N-CA-CB	5.17	117.33	110.10
1	Y	386	TYR	N-CA-CB	5.16	119.89	110.60
1	O	408	VAL	CA-CB-CG1	5.16	118.64	110.90
1	X	83	ARG	N-CA-C	5.15	124.90	111.00
1	Y	106	ARG	CD-NE-CZ	-5.14	116.40	123.60
1	Y	407	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	X	122	ASP	N-CA-CB	5.14	119.85	110.60
1	X	286	LEU	CA-CB-CG	-5.14	103.48	115.30
1	O	208	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	O	490	VAL	CA-CB-CG1	-5.12	103.21	110.90
1	X	458	ASP	CB-CG-OD2	5.12	122.91	118.30
1	Z	122	ASP	CB-CG-OD1	5.12	122.91	118.30
1	O	351	LEU	N-CA-CB	5.11	120.62	110.40
1	Y	135	TYR	CB-CG-CD1	5.11	124.06	121.00
1	X	389	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	Y	39	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	Z	42	PRO	N-CA-CB	5.08	109.39	103.30
1	O	492	ARG	N-CA-CB	5.08	119.74	110.60
1	Z	127	ASN	CB-CA-C	5.07	120.54	110.40
1	Y	5	TYR	CB-CA-C	-5.06	100.28	110.40
1	Y	378	ARG	CD-NE-CZ	-5.06	116.52	123.60
1	Y	236	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	X	152	ARG	CD-NE-CZ	5.04	130.65	123.60
1	Z	218	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	X	397	ALA	CB-CA-C	5.01	117.62	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Y	155	ALA	CA
1	X	31	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	478	GLU	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3913	0	3830	495	0
1	X	3910	0	3833	478	0
1	Y	3909	0	3822	435	0
1	Z	3907	0	3826	459	0
2	O	5	0	0	2	0
2	Y	5	0	0	1	0
3	O	27	0	11	1	0
3	X	27	0	11	1	0
3	Y	27	0	12	0	0
3	Z	27	0	12	0	0
4	O	6	0	8	2	0
4	X	6	0	8	2	0
4	Y	6	0	8	3	0
4	Z	6	0	8	9	0
5	O	46	0	0	9	0
5	X	50	0	0	6	0
5	Y	51	0	0	11	0
5	Z	53	0	0	10	0
All	All	15981	0	15389	1827	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 59.

All (1827) 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:Y:200:ASP:HB3	1:Y:203:MET:HB2	1.14	1.13
1:Y:155:ALA:HB2	1:Y:160:LEU:HB2	1.10	1.08
1:Z:468:ARG:HH11	1:Z:468:ARG:HG3	1.17	1.07
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.31	1.06
1:X:422:GLN:HE21	1:X:426:LEU:HD22	1.18	1.06
1:O:211:ARG:HA	1:O:214:LEU:HD13	1.36	1.04
1:Z:33:ARG:HH21	1:Z:58:SER:HB2	1.21	1.03
1:Z:84:GLU:HB2	1:Z:103:TRP:HB3	1.37	1.03
1:Z:112:CYS:HB3	1:Z:132:ILE:HG22	1.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:84:GLU:HB2	1:X:103:TRP:HB3	1.38	1.02
1:Y:468:ARG:HG3	1:Y:468:ARG:HH11	1.21	1.01
1:O:468:ARG:HH11	1:O:468:ARG:HG3	1.21	1.01
1:O:170:ILE:HD11	1:O:242:ILE:HD11	1.38	1.00
1:O:20:VAL:HG12	1:O:28:ILE:HB	1.39	1.00
1:Z:429:ARG:NH1	1:Z:471:ARG:HH11	1.59	1.00
1:X:152:ARG:HH21	1:X:208:ASP:HB3	1.21	0.98
1:X:399:SER:HB2	1:X:401:ILE:HD12	1.44	0.98
1:X:108:THR:HA	1:X:111:ILE:HD13	1.46	0.97
1:Y:261:ALA:HB2	1:Y:273:MET:HB2	1.45	0.97
1:O:61:VAL:HG11	1:X:61:VAL:HG21	1.48	0.95
1:Z:456:ASN:HD22	1:Z:458:ASP:H	1.00	0.95
1:Y:154:ARG:HB3	1:Y:159:GLU:HG3	1.49	0.95
1:Z:456:ASN:HD22	1:Z:458:ASP:N	1.63	0.95
1:Y:142:LYS:HD2	1:Y:207:LEU:HD23	1.46	0.94
1:Y:431:GLU:HB3	1:Y:466:ILE:HG21	1.50	0.94
1:X:33:ARG:HG2	1:X:33:ARG:HH11	1.32	0.94
1:Y:81:ASN:HD22	1:Y:81:ASN:N	1.67	0.93
1:Z:196:THR:HG22	1:Z:198:ASP:H	1.34	0.93
1:X:80:THR:HG21	1:X:248:ALA:HB2	1.49	0.92
1:Y:19:VAL:HG11	1:Y:27:ILE:HD13	1.50	0.92
1:Z:6:ILE:HD11	1:Z:444:ALA:HA	1.50	0.92
1:Y:105:CYS:SG	1:Y:107:ARG:HD2	2.10	0.91
1:X:14:THR:HA	1:X:37:GLN:NE2	1.85	0.91
1:X:226:GLN:HE21	1:X:236:ARG:HB3	1.36	0.91
1:X:482:ARG:HG2	1:X:482:ARG:HH11	1.33	0.91
1:X:471:ARG:HH11	1:X:471:ARG:HG3	1.34	0.90
1:Y:61:VAL:HG21	1:Z:61:VAL:HG11	1.53	0.90
1:Z:344:VAL:HG22	1:Z:364:ILE:HG23	1.54	0.90
1:X:431:GLU:HG2	1:X:466:ILE:HG13	1.54	0.89
1:Y:406:LEU:HD13	1:Y:408:VAL:CG1	2.02	0.89
1:Z:396:GLN:NE2	1:Z:403:LEU:H	1.69	0.89
1:Z:103:TRP:HB2	1:Z:135:TYR:CD1	2.08	0.89
1:X:294:PRO:HB3	1:X:457:LEU:HD12	1.53	0.89
1:O:263:ASN:HB2	1:O:406:LEU:HD11	1.54	0.89
1:Y:468:ARG:HD2	1:Y:470:PHE:CE1	2.08	0.89
1:X:84:GLU:HB2	1:X:103:TRP:CB	2.03	0.89
1:X:193:ASN:HB3	1:X:196:THR:HG22	1.53	0.88
1:O:362:GLY:HA3	1:Y:367:LEU:HB2	1.56	0.88
1:X:111:ILE:HD12	1:X:111:ILE:H	1.39	0.87
1:Y:456:ASN:ND2	1:Y:458:ASP:H	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:17:ARG:HG3	1:X:32:GLN:HG3	1.55	0.87
1:X:458:ASP:HA	1:X:461:GLN:CG	2.04	0.87
1:Z:396:GLN:HE21	1:Z:403:LEU:H	1.17	0.87
1:X:406:LEU:HD13	1:X:408:VAL:HG12	1.56	0.87
1:O:20:VAL:CG1	1:O:28:ILE:HB	2.05	0.87
1:X:20:VAL:HG12	1:X:28:ILE:HG12	1.57	0.87
1:Y:141:VAL:HG12	1:Y:145:LEU:HD23	1.54	0.87
1:X:399:SER:HB2	1:X:401:ILE:CD1	2.05	0.87
1:O:179:HIS:NE2	1:O:215:PRO:HB3	1.90	0.86
1:Y:83:ARG:HH11	1:Y:83:ARG:HG3	1.39	0.86
1:O:12:GLY:HA3	1:O:17:ARG:HH12	1.38	0.86
1:O:180:VAL:CG2	1:O:218:ARG:HG3	2.06	0.86
1:Z:83:ARG:HH11	1:Z:83:ARG:HG3	1.41	0.85
1:O:203:MET:HA	1:O:206:VAL:HG23	1.55	0.85
1:X:45:VAL:H	1:X:105:CYS:HB2	1.41	0.85
1:O:80:THR:HG21	1:O:248:ALA:CB	2.07	0.85
1:Z:40:PRO:HG2	1:Z:44:TRP:HB3	1.59	0.85
1:Z:88:VAL:HG12	1:Z:97:ILE:HG12	1.57	0.85
1:Y:237:ILE:CG2	1:Y:238:PRO:HD2	2.06	0.84
1:Z:340:ASN:HB2	1:Z:375:HIS:CD2	2.11	0.84
1:X:179:HIS:CG	1:X:215:PRO:HB3	2.12	0.84
1:X:320:MET:HE2	1:X:322:LEU:HD21	1.60	0.84
1:O:272:LEU:HG	1:O:303:GLU:HB2	1.60	0.84
1:Y:200:ASP:HB3	1:Y:203:MET:CB	2.05	0.84
1:Y:235:THR:O	1:Y:236:ARG:HD3	1.78	0.84
1:O:353:ALA:HB2	1:O:356:TRP:CZ2	2.12	0.84
1:Y:33:ARG:HH21	1:Y:58:SER:HB2	1.41	0.84
1:O:362:GLY:CA	1:Y:367:LEU:HB2	2.07	0.83
1:Z:83:ARG:HH11	4:Z:605:GOL:H2	1.43	0.83
1:Z:193:ASN:HB3	1:Z:196:THR:CG2	2.08	0.83
1:X:105:CYS:SG	1:X:107:ARG:HD2	2.18	0.83
1:Z:320:MET:HE3	1:X:376:ILE:HD12	1.60	0.83
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.08	0.83
1:O:258:GLU:HB3	1:O:276:GLY:N	1.92	0.83
1:O:474:ILE:HG22	1:O:475:GLU:H	1.44	0.82
1:Y:468:ARG:HG3	1:Y:468:ARG:NH1	1.92	0.82
1:Y:474:ILE:HG13	1:Y:478:GLU:HG2	1.59	0.82
1:X:478:GLU:HA	1:X:481:TYR:HB3	1.61	0.82
1:Z:351:LEU:HD22	1:Z:360:ALA:HB2	1.61	0.82
1:Z:351:LEU:HD22	1:Z:360:ALA:CB	2.10	0.82
1:Z:415:ASN:HD21	1:Z:417:PHE:HB3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:179:HIS:CD2	1:X:215:PRO:HB3	2.15	0.82
1:X:81:ASN:HD22	1:X:81:ASN:N	1.76	0.82
1:X:193:ASN:HB3	1:X:196:THR:CG2	2.10	0.82
1:X:80:THR:CG2	1:X:248:ALA:HB2	2.09	0.81
1:X:308:MET:HE3	1:X:311:ALA:HB3	1.62	0.81
1:Y:179:HIS:ND1	1:Y:215:PRO:HA	1.95	0.81
1:X:70:SER:H	1:X:73:GLN:HE22	1.26	0.81
1:Z:161:LEU:HD22	1:Z:179:HIS:CE1	2.16	0.81
1:O:409:ASP:CB	1:O:438:VAL:HG21	2.10	0.81
1:Y:84:GLU:HB2	1:Y:103:TRP:HB3	1.62	0.81
1:X:145:LEU:HD12	1:X:151:SER:HB3	1.60	0.81
1:O:170:ILE:CD1	1:O:242:ILE:HD11	2.11	0.81
1:Z:6:ILE:HG12	1:Z:7:VAL:N	1.94	0.80
1:Z:173:MET:O	1:Z:227:THR:HG23	1.78	0.80
1:X:478:GLU:O	1:X:482:ARG:HG3	1.82	0.80
1:O:415:ASN:HB3	1:O:418:LEU:HB2	1.62	0.80
1:Z:382:GLU:HB3	1:Z:421:PHE:CE2	2.17	0.80
1:O:89:TRP:HH2	1:O:167:THR:HG22	1.47	0.80
1:O:192:PHE:HB2	1:O:199:TRP:CE3	2.17	0.80
1:X:407:ARG:CZ	1:X:466:ILE:HD11	2.11	0.80
1:O:91:LYS:HG3	1:O:161:LEU:HD11	1.64	0.80
1:Y:155:ALA:CB	1:Y:160:LEU:HB2	2.04	0.79
1:O:25:ALA:HB3	1:O:463:LYS:HE2	1.64	0.79
1:Z:97:ILE:HD12	1:Z:148:VAL:HG21	1.64	0.79
1:O:245:ASP:HA	1:O:248:ALA:HB3	1.62	0.79
1:Y:347:ALA:HB3	1:Y:361:ARG:O	1.82	0.79
1:Y:196:THR:HG22	1:Y:198:ASP:N	1.98	0.79
1:X:109:ALA:HA	1:X:134:PRO:HG3	1.62	0.79
1:Y:155:ALA:HB2	1:Y:160:LEU:CB	2.03	0.79
1:Z:240:SER:HB2	1:Z:447:ALA:HA	1.65	0.79
1:X:83:ARG:HG2	4:X:606:GOL:O2	1.83	0.79
1:Y:262:LYS:HZ3	1:Y:264:THR:CB	1.95	0.78
1:Z:204:LEU:HD21	1:Z:214:LEU:HD11	1.64	0.78
1:Z:137:SER:O	1:Z:141:VAL:HG23	1.82	0.78
1:Z:429:ARG:NH1	1:Z:471:ARG:NH1	2.30	0.78
1:X:81:ASN:N	1:X:81:ASN:ND2	2.29	0.78
1:O:180:VAL:HG22	1:O:218:ARG:HG3	1.65	0.78
1:O:460:LEU:O	1:O:463:LYS:HB2	1.82	0.78
1:Y:406:LEU:HD13	1:Y:408:VAL:HG12	1.64	0.77
1:Y:467:GLU:OE2	1:Y:468:ARG:HB2	1.83	0.77
1:X:120:LEU:O	1:X:124:ILE:HG13	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:399:SER:CB	1:O:401:ILE:HG23	2.13	0.77
1:X:32:GLN:O	1:X:33:ARG:HG3	1.85	0.77
1:O:11:GLN:NE2	1:O:52:ILE:HD13	1.98	0.77
1:Z:103:TRP:HB2	1:Z:135:TYR:CE1	2.20	0.77
1:Z:316:LEU:HA	1:Z:320:MET:HB2	1.66	0.77
1:X:346:PRO:HA	1:X:348:PHE:HE1	1.48	0.76
1:O:23:HIS:HA	1:O:453:PHE:CE2	2.21	0.76
1:Y:17:ARG:HG3	1:Y:32:GLN:HG2	1.66	0.76
1:Y:140:LYS:O	1:Y:144:ILE:HD12	1.85	0.76
1:X:20:VAL:HG12	1:X:28:ILE:CG1	2.14	0.76
1:Y:200:ASP:CB	1:Y:203:MET:HB2	2.07	0.76
1:X:152:ARG:NH2	1:X:208:ASP:HB3	1.99	0.76
1:O:406:LEU:HD22	1:O:407:ARG:N	2.01	0.76
1:O:431:GLU:HB3	1:O:466:ILE:HG21	1.68	0.76
1:Y:180:VAL:HG23	1:Y:216:GLU:HG3	1.66	0.76
1:Y:86:THR:OG1	1:Y:137:SER:HB3	1.85	0.76
1:Z:89:TRP:HD1	1:Z:94:GLY:HA2	1.50	0.76
1:O:203:MET:CA	1:O:206:VAL:HG23	2.16	0.76
1:X:80:THR:HG21	1:X:248:ALA:CB	2.16	0.76
1:Y:81:ASN:N	1:Y:81:ASN:ND2	2.29	0.76
1:Y:475:GLU:O	1:Y:478:GLU:HB3	1.86	0.75
1:Z:483:TYR:O	1:Z:486:TRP:HB3	1.86	0.75
1:O:31:SER:CB	1:O:59:THR:HG22	2.17	0.75
1:Y:422:GLN:HE21	1:Y:426:LEU:CD2	1.99	0.75
1:Z:35:PHE:HE2	1:Z:47:HIS:CD2	2.05	0.75
1:Z:137:SER:OG	1:Z:189:THR:HA	1.86	0.75
1:X:160:LEU:O	1:X:213:MET:HB3	1.87	0.75
1:O:216:GLU:OE2	1:O:218:ARG:HD3	1.86	0.75
1:O:399:SER:OG	1:O:401:ILE:HG23	1.87	0.75
1:Z:26:ASN:O	1:Z:28:ILE:HD13	1.85	0.75
1:X:108:THR:CA	1:X:111:ILE:HD13	2.16	0.75
1:X:320:MET:O	1:X:322:LEU:HD23	1.86	0.75
1:O:3:LYS:HA	1:O:73:GLN:O	1.86	0.75
1:O:23:HIS:HA	1:O:453:PHE:HE2	1.51	0.75
1:Y:174:THR:HG21	1:Y:178:VAL:CG1	2.16	0.75
1:Z:185:ASN:O	1:Z:188:ARG:HB2	1.87	0.75
1:X:240:SER:O	1:X:447:ALA:HA	1.87	0.74
1:X:429:ARG:NH1	1:X:471:ARG:HG2	2.01	0.74
1:O:33:ARG:NH2	1:O:58:SER:HB2	2.01	0.74
1:O:200:ASP:O	1:O:203:MET:HB2	1.87	0.74
1:X:155:ALA:HB1	1:X:210:PRO:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:344:VAL:HG23	1:X:379:ALA:CB	2.17	0.74
1:O:105:CYS:SG	1:O:107:ARG:HD2	2.27	0.74
1:X:192:PHE:HA	1:X:199:TRP:HA	1.70	0.74
1:X:269:CYS:HB2	1:X:306:VAL:HB	1.68	0.74
1:O:125:ARG:HH21	1:O:282:SER:H	1.32	0.74
1:Y:61:VAL:HG11	1:Z:61:VAL:HG21	1.70	0.74
1:O:196:THR:HG22	1:O:198:ASP:H	1.53	0.74
1:Y:351:LEU:HD22	1:Y:360:ALA:CB	2.17	0.74
1:X:202:LYS:O	1:X:206:VAL:HG23	1.87	0.74
1:X:346:PRO:HA	1:X:348:PHE:CE1	2.23	0.74
1:O:362:GLY:C	1:Y:367:LEU:HB2	2.07	0.74
1:O:196:THR:CG2	1:O:198:ASP:H	2.01	0.74
1:O:346:PRO:HA	1:O:348:PHE:CE1	2.23	0.74
1:Y:29:SER:OG	1:Y:63:VAL:HG12	1.86	0.74
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.22	0.74
1:X:145:LEU:HD12	1:X:151:SER:CB	2.18	0.74
1:X:222:GLU:O	1:X:240:SER:HA	1.88	0.74
1:Y:353:ALA:HB1	1:Y:354:PRO:HA	1.69	0.73
1:Z:389:ARG:HD2	1:Z:426:LEU:HD12	1.69	0.73
1:O:308:MET:CE	1:Y:369:ARG:HD2	2.18	0.73
1:Z:367:LEU:HB2	1:X:362:GLY:O	1.88	0.73
1:O:166:ASP:OD1	1:O:167:THR:N	2.22	0.73
1:X:20:VAL:O	1:X:28:ILE:HG12	1.88	0.73
1:X:179:HIS:CE1	1:X:215:PRO:HB3	2.23	0.73
1:X:264:THR:HA	1:X:409:ASP:O	1.89	0.73
1:O:338:ASN:HB2	5:O:653:HOH:O	1.88	0.73
1:O:456:ASN:ND2	1:O:459:GLU:HG3	2.04	0.73
1:X:482:ARG:HG2	1:X:482:ARG:NH1	1.98	0.73
1:Z:273:MET:CE	1:Z:401:ILE:HD12	2.19	0.73
1:Z:382:GLU:HB3	1:Z:421:PHE:HE2	1.51	0.73
1:Z:200:ASP:O	1:Z:204:LEU:HD13	1.88	0.73
1:X:295:THR:HG23	1:X:297:GLU:OE2	1.88	0.73
1:Z:44:TRP:HA	1:Z:105:CYS:SG	2.28	0.73
1:Y:415:ASN:HD21	1:Y:417:PHE:HB3	1.53	0.73
1:O:409:ASP:CG	1:O:438:VAL:HG21	2.09	0.72
1:Y:389:ARG:HD3	1:Y:483:TYR:CE1	2.24	0.72
1:Z:492:ARG:HD3	1:X:492:ARG:O	1.89	0.72
1:Y:80:THR:HG22	1:Y:243:ALA:O	1.89	0.72
1:Z:381:LEU:HD12	1:Z:417:PHE:CD2	2.24	0.72
1:X:86:THR:OG1	1:X:137:SER:HB3	1.89	0.72
1:O:204:LEU:HD21	1:O:214:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:237:ILE:HG23	1:O:238:PRO:HD2	1.70	0.72
1:O:409:ASP:HB2	1:O:438:VAL:HG21	1.71	0.72
1:Y:432:ARG:C	1:Y:466:ILE:HG22	2.09	0.72
1:Y:479:ARG:HG3	1:Y:479:ARG:HH11	1.54	0.72
1:Z:47:HIS:O	1:Z:49:PRO:HD3	1.89	0.72
1:Y:33:ARG:NH2	1:Y:58:SER:HB2	2.04	0.72
1:X:64:LEU:CD2	1:X:69:ILE:HB	2.20	0.72
1:O:169:LEU:O	1:O:173:MET:HG3	1.89	0.72
1:X:181:THR:O	1:X:217:VAL:HA	1.90	0.72
1:X:475:GLU:HG2	1:X:478:GLU:HG2	1.72	0.72
1:Y:264:THR:HA	1:Y:409:ASP:O	1.90	0.72
1:Y:83:ARG:HG3	1:Y:83:ARG:NH1	2.03	0.71
1:Y:387:GLN:O	1:Y:390:ASP:HB2	1.90	0.71
1:Z:325:ASP:O	1:Z:328:ASP:HB2	1.90	0.71
1:X:111:ILE:H	1:X:111:ILE:CD1	2.02	0.71
1:Z:179:HIS:CE1	1:Z:215:PRO:HB3	2.25	0.71
1:Z:345:VAL:HG22	1:Z:486:TRP:CZ3	2.25	0.71
1:Y:85:THR:HA	1:Y:101:ILE:O	1.91	0.71
1:Z:240:SER:HB2	1:Z:447:ALA:CA	2.20	0.71
1:Z:193:ASN:CG	1:Z:196:THR:HB	2.10	0.71
1:X:415:ASN:ND2	1:X:417:PHE:H	1.89	0.71
1:Z:33:ARG:NH2	1:Z:58:SER:HB2	2.02	0.71
1:Z:273:MET:SD	1:Z:401:ILE:HD12	2.31	0.71
1:X:108:THR:HB	1:X:139:THR:HB	1.72	0.71
1:O:144:ILE:O	1:O:148:VAL:HG23	1.91	0.71
1:Z:40:PRO:HG2	1:Z:44:TRP:CB	2.20	0.71
1:O:467:GLU:OE2	1:O:468:ARG:HB2	1.90	0.71
1:Y:88:VAL:CG1	1:Y:97:ILE:HD11	2.21	0.71
1:O:203:MET:O	1:O:205:GLU:N	2.24	0.71
1:X:422:GLN:NE2	1:X:426:LEU:HD22	2.02	0.71
1:O:26:ASN:O	1:O:28:ILE:HG12	1.90	0.70
1:O:240:SER:HB2	1:O:447:ALA:HA	1.73	0.70
1:O:29:SER:OG	1:O:63:VAL:HG12	1.91	0.70
1:X:308:MET:CE	1:X:311:ALA:HB3	2.21	0.70
1:X:168:TRP:O	1:X:172:LYS:HG2	1.91	0.70
1:O:399:SER:HB2	1:O:401:ILE:HG23	1.71	0.70
1:Y:170:ILE:HA	1:Y:173:MET:HG3	1.72	0.70
1:X:273:MET:CE	1:X:401:ILE:HD13	2.21	0.70
1:O:19:VAL:CG1	1:O:27:ILE:HG23	2.21	0.70
1:Y:351:LEU:HD22	1:Y:360:ALA:HB1	1.72	0.70
1:Y:406:LEU:HD22	1:Y:407:ARG:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:192:PHE:CE1	1:Z:198:ASP:HA	2.26	0.70
1:X:83:ARG:HD2	1:X:244:GLY:HA3	1.74	0.70
1:X:272:LEU:HD11	1:X:303:GLU:OE1	1.92	0.70
1:Y:171:TRP:HB2	5:Y:631:HOH:O	1.92	0.70
1:Y:325:ASP:HB3	1:Y:328:ASP:OD2	1.92	0.70
1:Z:460:LEU:O	1:Z:463:LYS:HB2	1.92	0.70
1:O:264:THR:HA	1:O:409:ASP:O	1.90	0.70
1:Y:105:CYS:HG	1:Y:107:ARG:HD2	1.55	0.70
1:X:48:ASP:HB3	1:X:51:GLU:HB3	1.73	0.70
1:X:295:THR:OG1	1:X:297:GLU:HG2	1.92	0.70
1:O:91:LYS:CG	1:O:161:LEU:HD11	2.22	0.70
1:O:147:HIS:ND1	1:O:147:HIS:N	2.35	0.70
1:X:360:ALA:HB2	1:X:494:MET:HA	1.74	0.70
1:O:204:LEU:HD23	1:O:209:ILE:O	1.90	0.70
1:O:415:ASN:O	1:O:419:MET:HG2	1.90	0.70
1:O:165:VAL:HG23	5:O:627:HOH:O	1.91	0.70
1:Z:165:VAL:HG23	5:Z:647:HOH:O	1.92	0.70
1:X:246:GLN:HA	1:X:246:GLN:OE1	1.92	0.70
1:Y:87:ILE:HD12	1:Y:87:ILE:N	2.06	0.69
1:Z:387:GLN:O	1:Z:390:ASP:HB2	1.92	0.69
1:X:200:ASP:O	1:X:204:LEU:HD13	1.92	0.69
1:Z:83:ARG:NH1	4:Z:605:GOL:H2	2.07	0.69
1:Z:322:LEU:N	1:Z:322:LEU:HD23	2.06	0.69
1:O:203:MET:O	1:O:206:VAL:HG23	1.92	0.69
1:O:431:GLU:HB3	1:O:466:ILE:CG2	2.22	0.69
1:X:344:VAL:HG23	1:X:379:ALA:HB1	1.73	0.69
1:Z:112:CYS:HB3	1:Z:132:ILE:CG2	2.20	0.69
1:O:68:ASP:HA	5:O:635:HOH:O	1.92	0.69
1:O:188:ARG:HH22	1:O:303:GLU:CD	1.96	0.69
1:O:245:ASP:HA	1:O:248:ALA:CB	2.22	0.69
1:Z:19:VAL:HG11	1:Z:27:ILE:HG23	1.74	0.69
1:X:14:THR:HA	1:X:37:GLN:HE22	1.56	0.69
1:X:381:LEU:N	1:X:381:LEU:HD23	2.06	0.69
1:O:35:PHE:HE2	1:O:47:HIS:CD2	2.10	0.69
1:X:227:THR:N	1:X:237:ILE:O	2.26	0.69
1:Z:192:PHE:HB2	1:Z:199:TRP:CZ3	2.28	0.69
1:X:406:LEU:CD1	1:X:408:VAL:HG12	2.22	0.69
1:O:203:MET:O	1:O:206:VAL:N	2.26	0.68
1:O:245:ASP:OD1	1:O:246:GLN:N	2.26	0.68
1:O:430:VAL:HG23	1:O:470:PHE:O	1.93	0.68
1:Z:154:ARG:HB3	1:Z:159:GLU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:422:GLN:HE21	1:Z:426:LEU:HD22	1.58	0.68
1:X:64:LEU:HD23	1:X:69:ILE:HB	1.75	0.68
1:O:155:ALA:HB1	1:O:213:MET:CE	2.22	0.68
1:Y:81:ASN:HD22	1:Y:81:ASN:H	1.39	0.68
1:Z:256:VAL:HG13	1:Z:294:PRO:HG3	1.76	0.68
1:X:250:LEU:HD12	1:X:255:CYS:HB2	1.75	0.68
1:Y:237:ILE:HG22	1:Y:238:PRO:HD2	1.75	0.68
1:Z:83:ARG:NH2	1:Z:303:GLU:OE2	2.27	0.68
1:X:483:TYR:O	1:X:486:TRP:HB3	1.94	0.68
1:O:295:THR:HG23	1:O:297:GLU:OE2	1.94	0.68
1:Y:262:LYS:HZ3	1:Y:264:THR:HB	1.56	0.68
1:X:66:LYS:HG3	1:X:67:ALA:N	2.07	0.68
1:Z:227:THR:HG22	1:Z:228:ASN:H	1.58	0.68
1:Z:469:GLU:OE1	1:Z:471:ARG:NH1	2.27	0.68
1:O:368:THR:HG22	1:Y:348:PHE:O	1.94	0.68
1:Y:80:THR:HG21	1:Y:248:ALA:HB2	1.76	0.68
1:X:275:THR:HG23	1:X:301:ALA:HA	1.75	0.68
1:X:422:GLN:HE21	1:X:426:LEU:CD2	2.02	0.68
1:Y:80:THR:HG21	1:Y:248:ALA:CB	2.24	0.68
1:Y:48:ASP:HB3	1:Y:51:GLU:HB2	1.76	0.67
1:Z:424:ASP:CB	1:Z:475:GLU:HG2	2.24	0.67
1:Z:480:ASN:ND2	1:Z:480:ASN:H	1.92	0.67
1:O:80:THR:HG21	1:O:245:ASP:HA	1.76	0.67
1:O:103:TRP:HB2	1:O:135:TYR:HD1	1.58	0.67
1:O:193:ASN:HB3	1:O:196:THR:HG22	1.74	0.67
1:Y:219:ARG:NH2	1:Y:295:THR:O	2.28	0.67
1:Z:486:TRP:O	1:Z:489:ALA:HB3	1.94	0.67
1:O:456:ASN:CG	1:O:459:GLU:HG3	2.14	0.67
1:Z:21:MET:HA	1:Z:26:ASN:O	1.95	0.67
1:Z:367:LEU:HB2	1:X:362:GLY:C	2.14	0.67
1:X:396:GLN:HB2	5:X:657:HOH:O	1.94	0.67
1:X:474:ILE:O	1:X:479:ARG:NH2	2.28	0.67
1:Z:424:ASP:OD1	1:Z:473:GLY:N	2.27	0.67
1:O:427:GLY:HA2	1:O:472:PRO:HB3	1.75	0.67
1:Z:381:LEU:HD12	1:Z:417:PHE:HD2	1.57	0.67
1:X:264:THR:HG23	1:X:409:ASP:OD1	1.95	0.67
1:O:84:GLU:CB	1:O:103:TRP:HB3	2.19	0.67
1:O:103:TRP:HB2	1:O:135:TYR:CD1	2.30	0.67
1:O:128:THR:HG21	1:O:190:MET:HA	1.77	0.67
1:X:415:ASN:ND2	1:X:417:PHE:N	2.42	0.67
1:O:147:HIS:N	1:O:147:HIS:HD1	1.90	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:458:ASP:HA	1:Y:461:GLN:CG	2.25	0.67
1:Z:85:THR:CG2	1:Z:100:ALA:HB1	2.24	0.67
1:Z:365:PHE:CZ	1:Z:492:ARG:HB3	2.30	0.67
1:X:273:MET:HE2	1:X:401:ILE:HD13	1.77	0.67
1:X:389:ARG:O	1:X:393:GLU:HG3	1.94	0.67
1:Y:474:ILE:O	1:Y:474:ILE:HG12	1.93	0.67
1:Z:214:LEU:HD23	1:Z:214:LEU:N	2.09	0.67
1:O:287:LEU:HD12	1:O:303:GLU:HG2	1.77	0.66
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.08	0.66
1:X:257:LYS:HG2	1:X:260:MET:SD	2.35	0.66
1:O:308:MET:HE3	1:Y:369:ARG:HD2	1.76	0.66
1:Y:83:ARG:HG3	4:Y:604:GOL:O2	1.95	0.66
1:Z:166:ASP:N	1:Z:166:ASP:OD1	2.28	0.66
1:O:226:GLN:HA	1:O:237:ILE:O	1.95	0.66
1:Z:30:VAL:HG12	1:Z:31:SER:N	2.10	0.66
1:O:192:PHE:HB2	1:O:199:TRP:CZ3	2.30	0.66
1:X:145:LEU:CD1	1:X:151:SER:HB3	2.26	0.66
1:Z:407:ARG:HG2	1:Z:407:ARG:HH11	1.60	0.66
1:X:80:THR:HG22	1:X:243:ALA:O	1.95	0.66
1:X:471:ARG:HG3	1:X:471:ARG:NH1	2.03	0.66
1:O:387:GLN:O	1:O:390:ASP:HB2	1.95	0.66
1:Z:6:ILE:HD11	1:Z:444:ALA:CA	2.22	0.66
1:O:474:ILE:O	1:O:479:ARG:NH2	2.29	0.66
1:Z:184:THR:OG1	1:Z:185:ASN:N	2.28	0.66
1:X:81:ASN:ND2	1:X:81:ASN:H	1.93	0.66
1:O:272:LEU:HD21	1:O:303:GLU:OE1	1.95	0.66
1:Y:154:ARG:NH2	5:Y:634:HOH:O	2.29	0.66
1:X:478:GLU:CA	1:X:481:TYR:HB3	2.25	0.66
1:X:84:GLU:OE2	1:X:188:ARG:NH1	2.29	0.66
1:Z:174:THR:OG1	1:Z:178:VAL:HG13	1.95	0.66
1:Z:399:SER:O	1:Z:401:ILE:HG13	1.96	0.66
1:Y:226:GLN:HA	1:Y:237:ILE:O	1.96	0.65
1:Z:115:LEU:N	1:Z:115:LEU:HD12	2.12	0.65
1:O:325:ASP:O	1:O:328:ASP:HB2	1.96	0.65
1:Y:49:PRO:HG2	1:Y:96:PRO:HG3	1.78	0.65
1:Y:251:PHE:O	1:Y:253:GLN:N	2.29	0.65
1:Z:308:MET:HE3	1:Z:348:PHE:CD2	2.31	0.65
1:X:57:SER:O	1:X:60:LEU:HB3	1.97	0.65
1:O:11:GLN:HG3	1:O:165:VAL:HG11	1.79	0.65
1:Y:10:ASP:HB3	1:Y:17:ARG:HB2	1.78	0.65
1:O:263:ASN:CB	1:O:406:LEU:HD11	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:476:THR:O	1:O:479:ARG:N	2.28	0.65
1:Y:391:VAL:HG23	1:Y:392:LEU:N	2.10	0.65
1:Y:394:ALA:O	1:Y:397:ALA:HB3	1.96	0.65
1:O:124:ILE:HG12	1:O:203:MET:HE3	1.77	0.65
1:Y:483:TYR:O	1:Y:486:TRP:HB3	1.97	0.65
1:Z:282:SER:OG	1:Z:286:LEU:HB2	1.96	0.65
1:X:317:ARG:HB2	1:X:323:ILE:HG13	1.77	0.65
1:X:388:THR:HG22	1:X:389:ARG:N	2.11	0.65
1:O:423:SER:O	1:O:427:GLY:N	2.30	0.65
1:Y:169:LEU:O	1:Y:173:MET:HG2	1.97	0.65
1:Y:173:MET:O	1:Y:227:THR:HG23	1.97	0.65
1:Y:427:GLY:HA2	1:Y:472:PRO:HG3	1.79	0.65
1:Z:70:SER:OG	1:Z:73:GLN:NE2	2.30	0.65
1:Z:174:THR:C	1:Z:175:GLN:HG2	2.16	0.65
1:O:62:GLU:OE2	1:X:33:ARG:NH2	2.30	0.65
1:Y:308:MET:CE	1:Y:349:THR:HB	2.27	0.65
1:X:237:ILE:HG22	1:X:238:PRO:HD2	1.79	0.65
1:Y:284:ASN:ND2	1:Y:397:ALA:HB1	2.12	0.65
1:O:235:THR:O	1:O:236:ARG:NE	2.29	0.65
1:Z:250:LEU:CD1	1:Z:255:CYS:HB2	2.27	0.65
1:X:17:ARG:HG3	1:X:32:GLN:CG	2.25	0.65
1:X:394:ALA:O	1:X:397:ALA:HB3	1.97	0.65
1:O:90:GLU:HB2	1:O:93:THR:OG1	1.97	0.64
1:X:135:TYR:O	1:X:140:LYS:NZ	2.30	0.64
1:O:415:ASN:HD22	1:O:418:LEU:H	1.43	0.64
1:O:17:ARG:NH2	3:O:607:ADP:O3B	2.28	0.64
1:O:104:GLN:HG2	1:O:349:THR:HG21	1.78	0.64
1:Z:23:HIS:HA	1:Z:453:PHE:CE2	2.33	0.64
1:Z:480:ASN:O	1:Z:484:ALA:N	2.29	0.64
1:O:403:LEU:H	1:O:403:LEU:HD12	1.62	0.64
1:Z:86:THR:HG23	1:Z:162:PHE:CE1	2.32	0.64
1:Z:103:TRP:HB2	1:Z:135:TYR:HD1	1.56	0.64
1:X:104:GLN:HG2	1:X:349:THR:HG21	1.79	0.64
1:Z:270:PHE:CE2	1:Z:305:ALA:HB1	2.32	0.64
1:Z:395:MET:O	1:Z:399:SER:N	2.28	0.64
1:O:203:MET:HA	1:O:206:VAL:CG2	2.26	0.64
1:Y:170:ILE:CD1	1:Y:242:ILE:HD11	2.28	0.64
1:Y:289:THR:HG23	1:Y:290:ILE:N	2.12	0.64
1:Y:490:VAL:O	1:Y:493:ALA:HB3	1.98	0.64
1:Z:156:ARG:HG3	1:Z:210:PRO:HG3	1.80	0.64
1:Z:407:ARG:HG2	1:Z:407:ARG:NH1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:247:GLN:N	1:X:247:GLN:OE1	2.30	0.64
1:Z:193:ASN:HB3	1:Z:196:THR:HG21	1.80	0.64
1:Z:86:THR:HG23	1:Z:162:PHE:HE1	1.63	0.64
1:X:152:ARG:O	1:X:155:ALA:HB3	1.98	0.64
1:X:368:THR:O	1:X:371:VAL:HG23	1.98	0.64
1:O:122:ASP:O	1:O:126:SER:N	2.27	0.63
1:Y:441:LEU:HD23	1:Y:445:TYR:CZ	2.32	0.63
1:Z:19:VAL:CG1	1:Z:27:ILE:HG23	2.28	0.63
1:Z:76:ALA:HB1	1:Z:240:SER:OG	1.98	0.63
1:X:79:ILE:HD11	1:X:173:MET:HE1	1.80	0.63
1:Z:456:ASN:ND2	1:Z:458:ASP:N	2.41	0.63
1:X:257:LYS:O	1:X:274:ASN:HB3	1.97	0.63
1:Y:41:LYS:HD3	1:Y:44:TRP:CZ2	2.33	0.63
1:Y:81:ASN:ND2	1:Y:81:ASN:H	1.94	0.63
1:Y:441:LEU:HD23	1:Y:445:TYR:CE1	2.32	0.63
1:Z:352:GLY:O	1:Z:355:TYR:N	2.31	0.63
1:O:406:LEU:HD13	1:O:408:VAL:HG23	1.80	0.63
1:Y:431:GLU:CB	1:Y:466:ILE:HG21	2.26	0.63
1:Y:432:ARG:O	1:Y:467:GLU:N	2.31	0.63
1:X:166:ASP:O	1:X:169:LEU:HB2	1.99	0.63
1:Z:89:TRP:CD1	1:Z:94:GLY:HA2	2.33	0.63
1:X:71:SER:HB2	1:X:235:THR:HG21	1.79	0.63
1:X:144:ILE:HD12	1:X:144:ILE:H	1.64	0.63
1:O:422:GLN:HE21	1:O:426:LEU:HD22	1.64	0.63
1:Y:422:GLN:HE21	1:Y:426:LEU:HD22	1.62	0.63
1:Z:218:ARG:NH1	1:Z:222:GLU:OE2	2.27	0.63
1:Z:295:THR:HB	1:Z:297:GLU:OE2	1.99	0.63
1:X:269:CYS:CB	1:X:306:VAL:HB	2.29	0.63
1:Y:102:VAL:O	1:Y:140:LYS:NZ	2.31	0.63
1:O:396:GLN:HB3	1:O:401:ILE:O	1.98	0.63
1:Z:429:ARG:HH11	1:Z:471:ARG:HH11	1.46	0.63
1:Z:295:THR:CG2	1:Z:297:GLU:HG2	2.28	0.62
1:Z:424:ASP:HB3	1:Z:475:GLU:HG2	1.79	0.62
1:O:317:ARG:O	1:O:321:LYS:HA	1.98	0.62
1:Y:294:PRO:HD2	1:Y:297:GLU:OE2	1.99	0.62
1:Z:30:VAL:HG12	1:Z:31:SER:H	1.64	0.62
1:O:154:ARG:HB3	1:O:159:GLU:HB2	1.81	0.62
1:O:408:VAL:HG13	1:O:413:VAL:HG11	1.81	0.62
1:O:245:ASP:CA	1:O:248:ALA:HB3	2.29	0.62
1:O:438:VAL:O	1:O:441:LEU:HB2	1.99	0.62
1:Z:250:LEU:HD11	1:Z:255:CYS:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:368:THR:O	1:Z:371:VAL:HB	1.99	0.62
1:Z:429:ARG:HH12	1:Z:471:ARG:NH1	1.96	0.62
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.81	0.62
1:O:415:ASN:HB3	1:O:418:LEU:CB	2.28	0.62
1:Z:193:ASN:HB3	1:Z:196:THR:HG22	1.81	0.62
1:Z:293:GLY:N	1:Z:297:GLU:O	2.33	0.62
1:X:157:ARG:HB2	1:X:159:GLU:HG3	1.82	0.62
1:O:5:TYR:CE2	1:O:69:ILE:HG12	2.34	0.62
1:Y:424:ASP:HB3	1:Y:474:ILE:HG21	1.80	0.62
1:X:460:LEU:HD12	1:X:463:LYS:CG	2.30	0.62
1:Y:448:GLY:O	1:Y:453:PHE:N	2.33	0.62
1:X:111:ILE:HD12	1:X:111:ILE:N	2.13	0.62
1:X:130:LEU:HD12	1:X:190:MET:CB	2.29	0.62
1:X:447:ALA:O	1:X:450:ALA:HB3	2.00	0.62
1:O:86:THR:C	1:O:87:ILE:HG13	2.19	0.62
1:O:476:THR:O	1:O:479:ARG:HB2	2.00	0.62
1:Z:308:MET:HE2	1:Z:348:PHE:HB2	1.80	0.62
1:Z:320:MET:CE	1:X:376:ILE:HD12	2.28	0.62
1:X:88:VAL:HG11	1:X:97:ILE:HD11	1.82	0.62
1:X:253:GLN:NE2	1:X:409:ASP:OD2	2.33	0.62
1:O:124:ILE:HD12	1:O:132:ILE:HD11	1.82	0.61
1:Y:308:MET:HE2	1:Y:349:THR:HB	1.82	0.61
1:Y:330:GLU:OE1	1:Y:416:ASN:N	2.33	0.61
1:O:24:ASP:O	1:O:463:LYS:NZ	2.26	0.61
1:O:378:ARG:O	1:O:382:GLU:HG3	2.01	0.61
1:O:436:ARG:O	1:O:438:VAL:HG22	1.99	0.61
1:Z:331:TYR:O	1:Z:335:LYS:HD3	1.99	0.61
1:X:434:GLU:N	1:X:465:VAL:O	2.28	0.61
1:O:148:VAL:HB	1:O:151:SER:OG	2.00	0.61
1:O:351:LEU:N	1:O:357:ASP:O	2.33	0.61
1:Y:360:ALA:O	1:Y:361:ARG:NH1	2.29	0.61
1:X:290:ILE:HG23	1:X:299:ASN:O	2.00	0.61
1:X:423:SER:HB2	1:X:428:THR:O	2.00	0.61
1:O:434:GLU:HA	1:O:467:GLU:HB2	1.83	0.61
1:Z:272:LEU:HD21	1:Z:303:GLU:OE1	2.00	0.61
1:O:31:SER:HB2	1:O:59:THR:HG22	1.83	0.61
1:Z:48:ASP:HB3	1:Z:51:GLU:HB2	1.82	0.61
1:Z:78:GLY:O	1:Z:79:ILE:HG13	2.00	0.61
1:Z:83:ARG:CZ	1:Z:246:GLN:HB2	2.29	0.61
1:Z:245:ASP:OD1	1:Z:246:GLN:N	2.33	0.61
1:Y:156:ARG:O	1:Y:158:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:201:ASP:OD2	1:X:211:ARG:NH2	2.34	0.61
1:O:406:LEU:HD22	1:O:407:ARG:H	1.65	0.61
1:Y:41:LYS:HG2	1:Y:44:TRP:CD2	2.36	0.61
1:Y:263:ASN:O	1:Y:408:VAL:HA	2.01	0.61
1:Y:415:ASN:HD22	1:Y:418:LEU:H	1.47	0.61
1:X:112:CYS:SG	1:X:134:PRO:HD3	2.40	0.61
1:X:294:PRO:CB	1:X:457:LEU:HD12	2.30	0.61
1:Y:180:VAL:HG23	1:Y:216:GLU:CG	2.31	0.61
1:X:106:ARG:HD2	1:X:349:THR:O	2.01	0.61
1:X:384:ILE:O	1:X:387:GLN:HB2	2.01	0.61
1:O:47:HIS:CE1	1:O:102:VAL:HG21	2.36	0.61
1:Z:80:THR:HG21	1:Z:248:ALA:CB	2.31	0.61
1:Z:255:CYS:HB3	1:Z:260:MET:HB2	1.82	0.61
1:X:348:PHE:HD1	1:X:348:PHE:H	1.48	0.61
1:O:27:ILE:HD13	1:O:27:ILE:N	2.16	0.60
1:O:183:TYR:O	1:O:186:ALA:N	2.34	0.60
1:O:336:VAL:HG23	1:O:378:ARG:HD2	1.81	0.60
1:X:316:LEU:O	1:X:321:LYS:N	2.33	0.60
1:Y:41:LYS:HD3	1:Y:44:TRP:CH2	2.36	0.60
1:Y:88:VAL:O	1:Y:97:ILE:HG13	2.01	0.60
1:Z:256:VAL:HG21	1:Z:457:LEU:HD11	1.83	0.60
1:X:474:ILE:HD13	1:X:478:GLU:CD	2.21	0.60
1:O:83:ARG:NH1	1:O:188:ARG:NH1	2.49	0.60
1:O:308:MET:HG3	1:O:348:PHE:HD1	1.65	0.60
1:Y:421:PHE:O	1:Y:424:ASP:HB2	2.00	0.60
1:Z:58:SER:O	1:Z:62:GLU:HB2	2.00	0.60
1:Z:221:SER:OG	1:Z:450:ALA:HB2	2.01	0.60
1:Y:475:GLU:OE1	1:Y:478:GLU:HB2	2.00	0.60
1:X:415:ASN:HD22	1:X:417:PHE:N	1.99	0.60
1:X:423:SER:O	1:X:427:GLY:N	2.27	0.60
1:O:457:LEU:O	1:O:459:GLU:N	2.34	0.60
1:Y:136:PHE:HZ	1:Y:287:LEU:HD11	1.67	0.60
1:Z:92:GLU:HB3	5:Z:658:HOH:O	2.00	0.60
1:Z:181:THR:HG23	1:Z:182:ASP:N	2.15	0.60
1:X:320:MET:CE	1:X:322:LEU:HD21	2.29	0.60
1:O:340:ASN:HB2	1:O:375:HIS:CD2	2.37	0.60
1:Y:58:SER:OG	1:Z:62:GLU:HG3	2.01	0.60
1:Y:174:THR:O	1:Y:177:ARG:HG3	2.01	0.60
1:Y:422:GLN:HE21	1:Y:426:LEU:HD21	1.66	0.60
1:Z:227:THR:HG22	1:Z:228:ASN:N	2.16	0.60
1:X:60:LEU:O	1:X:63:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:141:VAL:CG1	1:Y:145:LEU:HD23	2.29	0.60
1:X:84:GLU:CB	1:X:103:TRP:HB3	2.23	0.60
1:X:240:SER:HB2	1:X:450:ALA:HB3	1.83	0.60
1:X:259:GLY:N	1:X:274:ASN:O	2.28	0.60
1:X:386:TYR:O	1:X:389:ARG:HB3	2.01	0.60
1:X:455:GLN:N	1:X:459:GLU:OE1	2.29	0.60
1:O:211:ARG:HG2	1:O:211:ARG:O	2.02	0.60
1:O:335:LYS:HB2	1:O:374:ASN:ND2	2.17	0.60
1:O:405:ALA:HA	1:O:428:THR:HG23	1.83	0.60
1:X:256:VAL:HG21	1:X:294:PRO:HA	1.83	0.60
1:X:263:ASN:O	1:X:408:VAL:HA	2.01	0.60
1:O:101:ILE:HD12	1:O:144:ILE:HD11	1.83	0.60
1:Y:474:ILE:HD11	1:Y:479:ARG:HA	1.84	0.60
1:X:83:ARG:HD3	1:X:245:ASP:OD1	2.02	0.60
1:O:271:MET:HG2	1:O:395:MET:CE	2.32	0.59
1:O:474:ILE:HG22	1:O:475:GLU:N	2.16	0.59
1:Y:112:CYS:HB3	1:Y:132:ILE:HG22	1.84	0.59
1:Y:153:GLU:OE1	1:Y:153:GLU:HA	2.02	0.59
1:X:217:VAL:C	1:X:218:ARG:HG2	2.22	0.59
1:X:460:LEU:O	1:X:463:LYS:HB2	2.02	0.59
1:O:401:ILE:O	1:O:401:ILE:HG13	2.02	0.59
1:Y:457:LEU:O	1:Y:460:LEU:HB2	2.02	0.59
1:X:207:LEU:HB2	1:X:209:ILE:CD1	2.32	0.59
1:X:418:LEU:HD13	1:X:419:MET:HE3	1.84	0.59
1:X:424:ASP:O	1:X:426:LEU:N	2.35	0.59
1:Y:456:ASN:O	1:Y:459:GLU:HB2	2.00	0.59
1:Z:80:THR:CG2	1:Z:248:ALA:HB2	2.32	0.59
1:Z:84:GLU:CB	1:Z:103:TRP:HB3	2.22	0.59
1:Z:191:LEU:HD11	1:Z:209:ILE:HD12	1.84	0.59
1:Z:320:MET:O	1:Z:322:LEU:HD23	2.02	0.59
1:O:389:ARG:HH12	1:O:479:ARG:HG2	1.66	0.59
1:Y:60:LEU:O	1:Y:63:VAL:HG23	2.02	0.59
1:Y:210:PRO:HA	5:Y:657:HOH:O	2.02	0.59
1:Y:257:LYS:HG3	1:Y:260:MET:SD	2.42	0.59
1:Y:347:ALA:HA	5:Y:656:HOH:O	2.02	0.59
1:Z:456:ASN:ND2	1:Z:458:ASP:H	1.85	0.59
1:X:320:MET:HB3	1:X:322:LEU:HD21	1.84	0.59
1:X:348:PHE:N	1:X:348:PHE:CD1	2.70	0.59
1:O:410:GLY:O	1:O:413:VAL:HG22	2.02	0.59
1:Y:456:ASN:HD21	1:Y:458:ASP:H	1.47	0.59
1:Z:102:VAL:O	1:Z:140:LYS:HE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:415:ASN:ND2	1:Z:417:PHE:HB3	2.15	0.59
1:O:163:GLY:HA3	1:O:167:THR:HG21	1.83	0.59
1:O:468:ARG:HG3	1:O:468:ARG:NH1	1.96	0.59
1:Y:174:THR:HG21	1:Y:178:VAL:HG13	1.85	0.59
1:Z:182:ASP:OD1	1:Z:185:ASN:HB2	2.03	0.59
1:X:170:ILE:HA	1:X:173:MET:CE	2.32	0.59
1:Y:479:ARG:HH11	1:Y:479:ARG:CG	2.15	0.59
1:Z:427:GLY:HA3	1:Z:479:ARG:NH1	2.17	0.59
1:X:219:ARG:HH21	1:X:221:SER:HB3	1.67	0.59
1:X:254:LEU:HD13	1:X:254:LEU:N	2.17	0.59
1:X:429:ARG:NH1	1:X:469:GLU:OE2	2.35	0.59
1:Y:415:ASN:ND2	1:Y:417:PHE:HB3	2.16	0.59
1:Z:9:LEU:HG	1:Z:56:GLN:NE2	2.18	0.59
1:Y:90:GLU:HB2	1:Y:93:THR:OG1	2.02	0.59
1:Y:196:THR:HG23	1:Y:198:ASP:HB3	1.85	0.58
1:Z:90:GLU:HB3	5:Z:658:HOH:O	2.02	0.58
1:Z:121:GLU:O	1:Z:124:ILE:N	2.36	0.58
1:Z:181:THR:O	1:Z:218:ARG:N	2.34	0.58
1:X:53:TRP:O	1:X:56:GLN:N	2.36	0.58
1:O:75:ALA:O	1:O:238:PRO:HG2	2.03	0.58
1:Y:265:TYR:N	1:Y:409:ASP:O	2.32	0.58
1:Y:432:ARG:O	1:Y:466:ILE:HG22	2.02	0.58
1:Z:114:HIS:O	1:Z:117:ARG:HB2	2.02	0.58
1:Z:295:THR:HG22	1:Z:297:GLU:HG2	1.83	0.58
1:Z:336:VAL:HG11	1:Z:375:HIS:CD2	2.38	0.58
1:X:137:SER:O	1:X:140:LYS:HB2	2.02	0.58
1:X:214:LEU:N	1:X:214:LEU:HD23	2.17	0.58
1:X:237:ILE:CG2	1:X:238:PRO:HD2	2.34	0.58
1:O:153:GLU:OE1	1:O:153:GLU:HA	2.02	0.58
1:O:336:VAL:HG13	1:O:374:ASN:HB3	1.84	0.58
1:O:415:ASN:ND2	1:O:417:PHE:HB3	2.18	0.58
1:O:457:LEU:O	1:O:460:LEU:N	2.32	0.58
1:Y:338:ASN:HD22	1:Y:338:ASN:N	2.01	0.58
1:Z:188:ARG:HH22	1:Z:303:GLU:CD	2.06	0.58
1:Z:331:TYR:CE2	1:Z:335:LYS:HE2	2.38	0.58
1:X:207:LEU:CB	1:X:209:ILE:HD11	2.33	0.58
1:X:272:LEU:HG	1:X:303:GLU:HB2	1.86	0.58
1:Z:339:THR:HG21	1:Z:379:ALA:HA	1.84	0.58
1:X:347:ALA:HB2	1:X:351:LEU:HD13	1.86	0.58
1:O:84:GLU:OE2	1:O:188:ARG:HD2	2.04	0.58
1:O:120:LEU:O	1:O:124:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:362:GLY:HA3	1:Y:367:LEU:CB	2.31	0.58
1:Y:5:TYR:CE2	1:Y:69:ILE:HD13	2.38	0.58
1:Z:179:HIS:CD2	1:Z:215:PRO:HA	2.39	0.58
1:X:327:TYR:HA	5:X:616:HOH:O	2.04	0.58
1:Z:196:THR:CG2	1:Z:198:ASP:H	2.12	0.58
1:Z:240:SER:HB3	1:Z:450:ALA:HB3	1.85	0.58
1:X:148:VAL:HB	1:X:151:SER:OG	2.04	0.58
1:Y:156:ARG:C	1:Y:158:GLY:H	2.06	0.58
1:Z:6:ILE:CD1	1:Z:444:ALA:HB1	2.34	0.58
1:Z:202:LYS:O	1:Z:206:VAL:HB	2.03	0.58
1:X:344:VAL:HG23	1:X:379:ALA:HB3	1.86	0.58
1:O:154:ARG:CB	1:O:159:GLU:HB2	2.34	0.58
1:O:335:LYS:HB2	1:O:374:ASN:HD22	1.68	0.58
1:X:74:ILE:HD13	1:X:74:ILE:N	2.19	0.58
1:X:174:THR:C	1:X:175:GLN:HG2	2.23	0.58
1:O:21:MET:HG2	1:O:25:ALA:HA	1.86	0.57
1:Y:196:THR:CG2	1:Y:198:ASP:HB3	2.34	0.57
1:X:81:ASN:HD22	1:X:81:ASN:H	1.52	0.57
1:X:179:HIS:ND1	1:X:215:PRO:HB3	2.18	0.57
1:X:179:HIS:NE2	1:X:215:PRO:HB3	2.19	0.57
1:O:155:ALA:HB1	1:O:213:MET:HE1	1.84	0.57
1:O:316:LEU:HA	1:O:320:MET:HB2	1.85	0.57
1:Y:196:THR:HG22	1:Y:198:ASP:H	1.66	0.57
1:Z:196:THR:HG22	1:Z:198:ASP:N	2.13	0.57
1:X:251:PHE:HE1	1:X:293:GLY:O	1.87	0.57
1:X:265:TYR:CD2	1:X:413:VAL:HG12	2.39	0.57
1:O:152:ARG:O	1:O:155:ALA:HB3	2.04	0.57
1:O:308:MET:HE1	1:Y:369:ARG:HD2	1.86	0.57
1:Y:189:THR:OG1	1:Y:191:LEU:HB2	2.04	0.57
1:Y:262:LYS:NZ	1:Y:264:THR:HB	2.19	0.57
1:Z:200:ASP:HB3	1:Z:203:MET:HB2	1.87	0.57
1:Z:295:THR:HB	1:Z:297:GLU:CG	2.34	0.57
1:Z:319:GLU:HG3	1:X:372:ASN:HA	1.86	0.57
1:O:11:GLN:CG	1:O:165:VAL:HG11	2.34	0.57
1:O:474:ILE:CG2	1:O:475:GLU:H	2.14	0.57
1:Y:161:LEU:HD22	1:Y:179:HIS:NE2	2.19	0.57
1:O:401:ILE:HD12	1:O:402:ARG:N	2.20	0.57
1:Z:83:ARG:HG3	1:Z:83:ARG:NH1	2.09	0.57
1:Z:303:GLU:HG3	1:Z:304:GLY:N	2.18	0.57
1:Z:422:GLN:NE2	1:Z:426:LEU:HD22	2.19	0.57
1:X:261:ALA:HB2	1:X:273:MET:HA	1.86	0.57

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:256:VAL:HG21	1:O:294:PRO:HA	1.87	0.57
1:O:317:ARG:HB2	1:O:323:ILE:HG13	1.86	0.57
1:O:402:ARG:HH22	1:O:404:HIS:HA	1.69	0.57
1:Z:83:ARG:HG2	4:Z:605:GOL:O2	2.05	0.57
1:Z:316:LEU:O	1:Z:321:LYS:N	2.37	0.57
1:O:182:ASP:OD1	1:O:185:ASN:HB2	2.05	0.57
1:Y:254:LEU:N	1:Y:254:LEU:HD12	2.20	0.57
1:X:245:ASP:HA	1:X:439:THR:HG23	1.85	0.57
1:X:399:SER:CB	1:X:401:ILE:HD12	2.29	0.57
1:O:103:TRP:HA	1:O:140:LYS:NZ	2.20	0.57
1:O:270:PHE:HE2	1:O:305:ALA:HB1	1.68	0.57
1:X:125:ARG:NH1	5:X:636:HOH:O	2.34	0.57
1:X:475:GLU:HG3	1:X:477:THR:OG1	2.05	0.57
1:Y:221:SER:O	1:Y:222:GLU:HB3	2.05	0.57
1:Z:259:GLY:N	1:Z:274:ASN:O	2.27	0.57
1:X:70:SER:OG	1:X:73:GLN:NE2	2.38	0.57
1:X:221:SER:OG	1:X:446:LEU:O	2.22	0.57
1:O:20:VAL:HG12	1:O:28:ILE:CB	2.25	0.57
1:Y:17:ARG:CG	1:Y:32:GLN:HG2	2.34	0.57
1:Y:331:TYR:CE2	1:Y:335:LYS:HE2	2.40	0.57
1:Z:123:TYR:CD2	1:Z:203:MET:HE2	2.39	0.57
1:Z:166:ASP:OD1	1:Z:167:THR:N	2.29	0.57
1:Z:468:ARG:HG3	1:Z:468:ARG:NH1	1.94	0.57
1:X:21:MET:CE	1:X:444:ALA:HB2	2.34	0.57
1:X:130:LEU:HD12	1:X:190:MET:HB2	1.86	0.57
1:X:415:ASN:HD22	1:X:415:ASN:C	2.07	0.57
1:O:125:ARG:NH2	1:O:282:SER:HB3	2.19	0.56
1:O:179:HIS:CE1	1:O:215:PRO:HB3	2.39	0.56
1:Y:88:VAL:HG12	1:Y:97:ILE:HD11	1.87	0.56
1:Y:103:TRP:HA	1:Y:140:LYS:NZ	2.19	0.56
1:Y:351:LEU:HB2	1:Y:357:ASP:HB3	1.87	0.56
1:Z:415:ASN:ND2	1:Z:418:LEU:H	2.03	0.56
1:X:468:ARG:HG2	1:X:469:GLU:N	2.19	0.56
1:Z:204:LEU:HD21	1:Z:214:LEU:CD1	2.34	0.56
1:X:108:THR:CB	1:X:139:THR:HB	2.35	0.56
1:O:11:GLN:HE22	1:O:52:ILE:HD13	1.67	0.56
1:O:17:ARG:N	1:O:17:ARG:HD3	2.20	0.56
1:O:44:TRP:HA	1:O:105:CYS:SG	2.45	0.56
1:O:90:GLU:HB2	1:O:93:THR:HG1	1.70	0.56
1:O:483:TYR:O	1:O:486:TRP:HB3	2.05	0.56
1:Y:17:ARG:O	1:Y:56:GLN:NE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:429:ARG:CZ	1:Y:471:ARG:HD3	2.35	0.56
1:Z:115:LEU:HD12	1:Z:115:LEU:H	1.70	0.56
1:Z:242:ILE:HG22	1:Z:243:ALA:N	2.20	0.56
1:Z:416:ASN:ND2	1:Z:416:ASN:H	2.01	0.56
1:X:204:LEU:HB3	1:X:209:ILE:O	2.06	0.56
1:O:56:GLN:NE2	1:O:56:GLN:HA	2.20	0.56
1:Y:313:ILE:H	1:Y:313:ILE:HD12	1.70	0.56
1:Y:346:PRO:CB	1:Y:348:PHE:HE1	2.19	0.56
1:Z:135:TYR:O	1:Z:140:LYS:NZ	2.39	0.56
1:X:47:HIS:O	1:X:49:PRO:HD3	2.06	0.56
1:O:144:ILE:HG22	1:O:148:VAL:CG2	2.35	0.56
1:O:240:SER:HB2	1:O:447:ALA:CA	2.35	0.56
1:Y:497:GLU:HG3	1:Y:498:GLU:H	1.70	0.56
1:X:35:PHE:HE2	1:X:47:HIS:CD2	2.24	0.56
1:X:127:ASN:HB3	1:X:193:ASN:ND2	2.21	0.56
1:O:135:TYR:O	1:O:140:LYS:NZ	2.38	0.56
1:O:155:ALA:HB1	1:O:213:MET:HE3	1.88	0.56
1:O:227:THR:O	1:O:236:ARG:HA	2.06	0.56
1:O:265:TYR:HE1	1:O:408:VAL:HG22	1.71	0.56
1:O:269:CYS:CB	1:O:306:VAL:HB	2.36	0.56
1:O:330:GLU:O	1:O:334:THR:HG23	2.05	0.56
1:O:147:HIS:HD1	1:O:147:HIS:H	1.54	0.56
1:O:181:THR:O	1:O:218:ARG:N	2.39	0.56
1:Y:392:LEU:O	1:Y:396:GLN:HG2	2.06	0.56
1:Z:123:TYR:CE2	1:Z:203:MET:HE2	2.41	0.56
1:Z:262:LYS:HD2	1:Z:263:ASN:N	2.21	0.56
1:Z:348:PHE:O	1:X:368:THR:HG22	2.06	0.56
1:X:196:THR:O	1:X:197:LEU:HB2	2.06	0.56
1:X:320:MET:HB3	1:X:322:LEU:CD2	2.35	0.56
1:O:125:ARG:O	1:O:125:ARG:HG3	2.06	0.56
1:O:453:PHE:HD2	1:O:454:TRP:CE2	2.24	0.56
1:X:21:MET:HA	1:X:26:ASN:O	2.06	0.56
1:X:475:GLU:HG2	1:X:475:GLU:O	2.06	0.56
1:O:35:PHE:CE2	1:O:47:HIS:CD2	2.94	0.56
1:O:248:ALA:O	1:O:442:GLY:HA3	2.05	0.56
1:O:389:ARG:HB2	1:O:426:LEU:HD13	1.88	0.56
1:Y:497:GLU:HG3	1:Y:498:GLU:N	2.20	0.56
1:Z:70:SER:H	1:Z:73:GLN:HE21	1.53	0.56
1:Z:83:ARG:NH2	1:Z:188:ARG:NH2	2.54	0.56
1:X:395:MET:O	1:X:399:SER:N	2.28	0.56
1:Z:154:ARG:HB3	1:Z:159:GLU:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:389:ARG:HB2	1:Z:426:LEU:CD1	2.36	0.55
1:X:429:ARG:HG3	1:X:429:ARG:HH11	1.70	0.55
1:Y:458:ASP:HA	1:Y:461:GLN:HG2	1.88	0.55
1:Z:348:PHE:CE1	1:X:367:LEU:HB3	2.42	0.55
1:X:109:ALA:CA	1:X:134:PRO:HG3	2.33	0.55
1:X:386:TYR:CD2	1:X:486:TRP:CE3	2.94	0.55
1:O:241:GLY:HA3	1:O:447:ALA:HB2	1.89	0.55
1:O:478:GLU:O	1:O:481:TYR:N	2.40	0.55
1:Y:112:CYS:HA	1:Y:115:LEU:HD22	1.88	0.55
1:Z:423:SER:O	1:Z:472:PRO:HB3	2.07	0.55
1:X:14:THR:HA	1:X:37:GLN:HE21	1.70	0.55
1:Y:21:MET:CE	1:Y:444:ALA:HB2	2.37	0.55
1:Y:330:GLU:OE2	1:Y:416:ASN:HB2	2.06	0.55
1:Z:420:GLN:NE2	1:Z:424:ASP:OD1	2.40	0.55
1:O:430:VAL:O	1:O:469:GLU:HA	2.06	0.55
1:Y:250:LEU:HD12	1:Y:255:CYS:HB2	1.89	0.55
1:Y:332:PHE:O	1:Y:334:THR:N	2.38	0.55
1:Y:422:GLN:O	1:Y:426:LEU:HD22	2.07	0.55
1:Z:85:THR:HG21	1:Z:100:ALA:HB1	1.87	0.55
1:Z:406:LEU:HD13	1:Z:408:VAL:HG12	1.88	0.55
1:X:476:THR:HG22	1:X:477:THR:N	2.21	0.55
1:Z:227:THR:N	1:Z:237:ILE:O	2.35	0.55
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.37	0.55
1:O:275:THR:HG21	1:O:280:VAL:CG2	2.37	0.55
1:O:312:SER:O	1:O:315:TRP:HB3	2.07	0.55
1:Z:416:ASN:HA	1:Z:419:MET:HB2	1.89	0.55
1:X:89:TRP:HB2	1:X:95:LYS:O	2.07	0.55
1:X:348:PHE:HD1	1:X:348:PHE:N	2.04	0.55
1:O:11:GLN:O	1:O:82:GLN:HG2	2.06	0.55
1:O:163:GLY:HA3	1:O:167:THR:CG2	2.36	0.55
1:O:332:PHE:O	1:O:374:ASN:ND2	2.40	0.55
1:O:389:ARG:NH1	1:O:479:ARG:HG2	2.21	0.55
1:Y:306:VAL:O	1:Y:306:VAL:HG12	2.07	0.55
1:Z:351:LEU:HB2	1:Z:357:ASP:HB3	1.88	0.55
1:Z:381:LEU:CD1	1:Z:417:PHE:HD2	2.19	0.55
1:O:154:ARG:HB3	1:O:159:GLU:CB	2.37	0.55
1:Y:53:TRP:HA	1:Y:53:TRP:CE3	2.42	0.55
1:Y:83:ARG:CD	1:Y:244:GLY:HA3	2.37	0.55
1:Y:280:VAL:O	1:Y:280:VAL:HG12	2.06	0.55
1:Y:433:PRO:HA	1:Y:466:ILE:HA	1.89	0.55
1:X:115:LEU:N	1:X:115:LEU:HD23	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:363:ALA:C	1:Y:364:ILE:HG13	2.28	0.55
1:O:486:TRP:O	1:O:489:ALA:HB3	2.07	0.54
1:Y:419:MET:O	1:Y:422:GLN:HB3	2.08	0.54
1:Z:432:ARG:O	1:Z:467:GLU:N	2.35	0.54
1:X:313:ILE:H	1:X:313:ILE:HD12	1.72	0.54
1:X:474:ILE:HD13	1:X:478:GLU:OE2	2.06	0.54
1:O:275:THR:HG21	1:O:280:VAL:HG23	1.89	0.54
1:Y:142:LYS:CD	1:Y:207:LEU:HD23	2.29	0.54
1:X:112:CYS:HB3	1:X:132:ILE:HG22	1.88	0.54
1:X:315:TRP:CE3	1:X:316:LEU:HD23	2.42	0.54
1:Y:19:VAL:CG1	1:Y:27:ILE:HD13	2.31	0.54
1:Y:74:ILE:HG22	1:Y:76:ALA:H	1.72	0.54
1:Y:87:ILE:HG22	1:Y:88:VAL:N	2.23	0.54
1:Y:424:ASP:HB3	1:Y:474:ILE:CG2	2.37	0.54
1:Z:23:HIS:HA	1:Z:453:PHE:HE2	1.72	0.54
1:Z:142:LYS:O	1:Z:145:LEU:HB2	2.07	0.54
1:Z:205:GLU:O	1:Z:208:ASP:N	2.40	0.54
1:Z:344:VAL:HG23	1:Z:379:ALA:HB1	1.89	0.54
1:X:242:ILE:HG22	1:X:243:ALA:N	2.22	0.54
1:O:202:LYS:O	1:O:205:GLU:HB3	2.07	0.54
1:X:170:ILE:HA	1:X:173:MET:HE3	1.89	0.54
1:O:182:ASP:CG	1:O:242:ILE:HG22	2.27	0.54
1:O:201:ASP:HA	1:O:204:LEU:HB2	1.89	0.54
1:O:313:ILE:HD11	1:O:381:LEU:HD23	1.89	0.54
1:O:347:ALA:HA	5:O:625:HOH:O	2.08	0.54
1:O:422:GLN:NE2	1:O:426:LEU:HD22	2.22	0.54
1:Y:48:ASP:OD1	1:Y:49:PRO:HD2	2.08	0.54
1:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.89	0.54
1:Z:148:VAL:HB	1:Z:151:SER:OG	2.07	0.54
1:O:144:ILE:HG22	1:O:148:VAL:HG23	1.90	0.54
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.37	0.54
1:Y:83:ARG:NH1	4:Y:604:GOL:O2	2.40	0.54
1:Y:115:LEU:HD13	1:Y:115:LEU:N	2.22	0.54
1:Y:227:THR:HG22	1:Y:228:ASN:N	2.22	0.54
1:Z:16:SER:O	1:Z:17:ARG:HG3	2.07	0.54
1:Y:128:THR:HB	5:Y:640:HOH:O	2.07	0.54
1:Y:200:ASP:O	1:Y:204:LEU:HG	2.08	0.54
1:Z:104:GLN:O	1:Z:106:ARG:NE	2.41	0.54
1:X:144:ILE:O	1:X:148:VAL:HG23	2.08	0.54
1:X:357:ASP:OD2	1:X:494:MET:HB3	2.08	0.54
1:O:271:MET:C	1:O:272:LEU:HD12	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:331:TYR:CZ	1:Z:335:LYS:HE2	2.43	0.54
1:X:424:ASP:O	1:X:427:GLY:N	2.41	0.54
2:O:601:PO4:O2	1:X:234:GLY:N	2.36	0.54
1:Y:89:TRP:HB2	1:Y:95:LYS:C	2.28	0.54
1:Y:179:HIS:CE1	1:Y:215:PRO:N	2.76	0.54
1:Z:92:GLU:O	1:Z:92:GLU:HG2	2.08	0.54
1:Z:196:THR:HG22	1:Z:197:LEU:N	2.23	0.54
1:X:249:ALA:HA	1:X:438:VAL:HG23	1.90	0.54
1:O:58:SER:HB3	1:X:62:GLU:HB2	1.90	0.54
1:O:70:SER:H	1:O:73:GLN:NE2	2.06	0.54
1:O:349:THR:HG23	1:O:349:THR:O	2.08	0.54
1:Y:328:ASP:O	1:Y:331:TYR:HB3	2.08	0.54
1:Z:181:THR:HG23	1:Z:182:ASP:O	2.07	0.54
1:Y:225:GLY:O	1:Y:238:PRO:HA	2.07	0.53
1:Y:237:ILE:HG23	1:Y:238:PRO:HD2	1.87	0.53
1:Y:427:GLY:HA2	1:Y:472:PRO:CG	2.37	0.53
1:X:175:GLN:HA	5:X:627:HOH:O	2.08	0.53
1:Y:88:VAL:HG11	1:Y:97:ILE:HD11	1.91	0.53
1:Y:170:ILE:HD11	1:Y:242:ILE:HD11	1.90	0.53
1:Y:421:PHE:CZ	1:Y:425:ILE:HD13	2.44	0.53
1:X:45:VAL:N	1:X:105:CYS:HB2	2.17	0.53
1:X:125:ARG:O	1:X:129:GLY:HA2	2.08	0.53
1:X:274:ASN:HD21	1:X:299:ASN:HD22	1.56	0.53
1:X:290:ILE:HG22	1:X:291:ALA:O	2.08	0.53
1:O:47:HIS:HD2	1:O:52:ILE:HD11	1.72	0.53
1:O:245:ASP:O	1:O:248:ALA:HB3	2.08	0.53
1:Y:44:TRP:N	1:Y:44:TRP:CD1	2.75	0.53
1:Z:44:TRP:N	1:Z:44:TRP:CD1	2.73	0.53
1:Z:80:THR:CG2	1:Z:245:ASP:HA	2.38	0.53
1:Z:162:PHE:CD1	1:Z:163:GLY:N	2.77	0.53
1:X:22:ASP:OD1	1:X:24:ASP:N	2.40	0.53
1:X:392:LEU:HD23	1:X:392:LEU:C	2.28	0.53
1:Y:307:PHE:CD2	1:Y:349:THR:HG23	2.43	0.53
1:Z:18:ALA:CB	1:Z:63:VAL:HG21	2.38	0.53
1:Z:135:TYR:OH	4:Z:605:GOL:O1	2.26	0.53
1:X:422:GLN:O	1:X:426:LEU:HB2	2.09	0.53
1:O:179:HIS:CD2	1:O:215:PRO:HB3	2.41	0.53
1:O:216:GLU:OE2	1:O:218:ARG:NH1	2.36	0.53
1:Y:174:THR:HG21	1:Y:178:VAL:HG11	1.90	0.53
1:Z:137:SER:HA	1:Z:140:LYS:HG3	1.91	0.53
1:Z:246:GLN:HG3	1:Z:270:PHE:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:219:ARG:NH2	1:X:295:THR:O	2.41	0.53
1:X:317:ARG:HB2	1:X:323:ILE:CG1	2.38	0.53
1:Y:422:GLN:NE2	1:Y:426:LEU:HD21	2.23	0.53
1:O:271:MET:HG2	1:O:395:MET:HE1	1.90	0.53
1:O:348:PHE:O	1:Y:368:THR:HG22	2.09	0.53
1:Z:193:ASN:OD1	1:Z:196:THR:HB	2.09	0.53
1:Z:263:ASN:HB2	1:Z:406:LEU:HD11	1.90	0.53
1:Z:345:VAL:HG22	1:Z:486:TRP:CH2	2.42	0.53
1:X:64:LEU:HD22	1:X:69:ILE:HB	1.90	0.53
1:X:126:SER:O	1:X:195:HIS:HE1	1.91	0.53
1:O:152:ARG:HA	1:O:155:ALA:HB3	1.90	0.53
1:Y:348:PHE:HD1	1:Y:348:PHE:H	1.56	0.53
1:Z:246:GLN:HG3	1:Z:270:PHE:CG	2.44	0.53
1:X:169:LEU:O	1:X:173:MET:HB2	2.09	0.53
1:O:109:ALA:HA	1:O:112:CYS:HB2	1.90	0.53
1:Y:156:ARG:O	1:Y:212:GLU:OE1	2.26	0.53
1:Y:180:VAL:HG21	1:Y:218:ARG:HG3	1.91	0.53
1:Z:120:LEU:HD11	1:Z:206:VAL:CG2	2.38	0.53
1:Z:264:THR:O	1:Z:269:CYS:HA	2.09	0.53
1:Y:84:GLU:OE2	1:Y:188:ARG:NH1	2.40	0.53
1:X:207:LEU:HB3	1:X:209:ILE:HD11	1.91	0.53
1:Y:40:PRO:HG2	1:Y:44:TRP:HB3	1.90	0.52
1:X:60:LEU:C	1:X:60:LEU:HD12	2.29	0.52
1:O:128:THR:HB	1:O:130:LEU:HB2	1.92	0.52
1:O:343:TYR:OH	1:O:485:GLY:HA3	2.08	0.52
1:Y:40:PRO:HD2	1:Y:44:TRP:HB2	1.90	0.52
1:O:54:ALA:O	1:O:58:SER:OG	2.27	0.52
1:O:225:GLY:O	1:O:238:PRO:HA	2.10	0.52
1:Z:194:ILE:HD12	1:Z:300:TYR:CE1	2.43	0.52
1:Z:351:LEU:HB3	1:Z:355:TYR:HB2	1.91	0.52
1:X:41:LYS:HD3	1:X:44:TRP:CE2	2.45	0.52
1:O:102:VAL:HG12	1:O:104:GLN:HB2	1.92	0.52
1:O:353:ALA:HB2	1:O:356:TRP:HZ2	1.73	0.52
1:Z:295:THR:HB	1:Z:297:GLU:HG2	1.92	0.52
1:X:382:GLU:HB3	1:X:421:PHE:CE2	2.45	0.52
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.40	0.52
1:Y:75:ALA:O	1:Y:76:ALA:HB2	2.09	0.52
1:Y:85:THR:HG23	1:Y:102:VAL:HA	1.91	0.52
1:Y:351:LEU:HB3	1:Y:355:TYR:HB2	1.91	0.52
1:Y:440:ALA:O	1:Y:443:ALA:HB3	2.09	0.52
1:Z:18:ALA:HB1	1:Z:63:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:415:ASN:HD21	1:X:417:PHE:HB3	1.75	0.52
1:X:448:GLY:O	1:X:453:PHE:N	2.37	0.52
1:X:483:TYR:OH	1:X:487:LYS:NZ	2.40	0.52
1:O:31:SER:HB3	1:O:59:THR:HG22	1.89	0.52
1:O:348:PHE:HA	1:Y:367:LEU:O	2.10	0.52
1:Y:251:PHE:C	1:Y:253:GLN:H	2.13	0.52
1:Y:378:ARG:O	1:Y:382:GLU:HG3	2.09	0.52
1:Y:476:THR:HG22	1:Y:477:THR:N	2.25	0.52
1:Z:29:SER:OG	1:Z:66:LYS:HE2	2.10	0.52
1:Z:269:CYS:HB2	1:Z:306:VAL:HB	1.92	0.52
1:Z:279:ALA:HA	5:Z:644:HOH:O	2.09	0.52
1:X:405:ALA:CB	1:X:429:ARG:HB3	2.40	0.52
1:Y:19:VAL:HG11	1:Y:27:ILE:CD1	2.33	0.52
1:Y:109:ALA:O	1:Y:112:CYS:N	2.43	0.52
1:X:33:ARG:HG2	1:X:33:ARG:NH1	2.08	0.52
1:X:44:TRP:N	1:X:44:TRP:CD1	2.76	0.52
1:X:79:ILE:O	1:X:79:ILE:HG22	2.09	0.52
1:O:20:VAL:HG12	1:O:20:VAL:O	2.10	0.52
1:O:89:TRP:CH2	1:O:167:THR:HG22	2.37	0.52
1:O:105:CYS:SG	1:O:106:ARG:N	2.83	0.52
1:O:389:ARG:HB2	1:O:426:LEU:CD1	2.39	0.52
1:Y:148:VAL:HB	1:Y:151:SER:OG	2.09	0.52
1:Y:469:GLU:CD	1:Y:471:ARG:HH12	2.14	0.52
1:Z:352:GLY:H	1:Z:356:TRP:HA	1.75	0.52
1:X:89:TRP:HB2	1:X:95:LYS:C	2.30	0.52
1:X:218:ARG:NH2	1:X:222:GLU:OE2	2.29	0.52
1:X:263:ASN:HD22	1:X:406:LEU:CD1	2.23	0.52
1:Y:353:ALA:CB	1:Y:354:PRO:HA	2.33	0.52
1:Z:48:ASP:OD1	1:Z:49:PRO:HD2	2.09	0.52
1:Z:331:TYR:CZ	1:Z:335:LYS:NZ	2.78	0.52
1:Z:396:GLN:NE2	1:Z:403:LEU:N	2.50	0.52
1:X:457:LEU:O	1:X:460:LEU:N	2.31	0.52
1:O:204:LEU:HD21	1:O:214:LEU:CD2	2.37	0.51
1:O:258:GLU:HB3	1:O:276:GLY:H	1.73	0.51
1:Y:436:ARG:O	1:Y:438:VAL:HG22	2.09	0.51
1:Z:142:LYS:O	1:Z:146:ASP:OD1	2.28	0.51
1:X:249:ALA:O	1:X:253:GLN:HB2	2.10	0.51
1:X:256:VAL:HG12	1:X:257:LYS:NZ	2.25	0.51
1:O:314:GLN:O	1:O:318:ASP:HB2	2.11	0.51
1:O:456:ASN:ND2	1:O:459:GLU:H	2.08	0.51
1:X:45:VAL:H	1:X:105:CYS:CB	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:406:LEU:HB3	1:Y:430:VAL:HG22	1.92	0.51
1:X:85:THR:HA	1:X:101:ILE:O	2.11	0.51
1:X:90:GLU:HA	1:X:160:LEU:HD23	1.92	0.51
1:O:182:ASP:OD2	1:O:220:SER:OG	2.27	0.51
1:Z:179:HIS:NE2	1:Z:215:PRO:HB3	2.25	0.51
1:X:343:TYR:CE2	1:X:486:TRP:N	2.78	0.51
1:X:421:PHE:O	1:X:424:ASP:HB2	2.10	0.51
1:O:97:ILE:HD12	1:O:148:VAL:HG21	1.91	0.51
1:O:202:LYS:O	1:O:203:MET:O	2.28	0.51
1:Y:436:ARG:NH1	1:Y:467:GLU:OE1	2.44	0.51
1:Z:103:TRP:HA	1:Z:140:LYS:HZ1	1.76	0.51
1:Z:449:LEU:HD12	1:Z:454:TRP:O	2.11	0.51
1:X:303:GLU:HG3	1:X:304:GLY:N	2.22	0.51
1:O:28:ILE:O	1:O:29:SER:HB2	2.10	0.51
1:O:91:LYS:HG3	1:O:161:LEU:CD1	2.37	0.51
1:O:166:ASP:OD1	1:O:166:ASP:N	2.40	0.51
1:Y:79:ILE:O	1:Y:242:ILE:HA	2.11	0.51
1:Y:201:ASP:HA	1:Y:204:LEU:HD12	1.92	0.51
1:Z:263:ASN:HB2	1:Z:406:LEU:CD1	2.40	0.51
1:X:107:ARG:HG2	1:X:108:THR:HG23	1.93	0.51
1:O:102:VAL:O	1:O:140:LYS:HE2	2.10	0.51
1:Y:135:TYR:CD2	1:Y:136:PHE:CE1	2.99	0.51
1:O:124:ILE:HG12	1:O:203:MET:CE	2.41	0.51
1:O:124:ILE:HD12	1:O:132:ILE:CD1	2.40	0.51
1:O:193:ASN:HB3	1:O:196:THR:HG21	1.90	0.51
1:Y:234:GLY:H	2:Y:602:PO4:P	2.34	0.51
1:Y:263:ASN:ND2	1:Y:265:TYR:CE1	2.79	0.51
1:Y:409:ASP:CG	1:Y:438:VAL:HG21	2.30	0.51
1:Z:103:TRP:CD1	1:Z:103:TRP:N	2.79	0.51
1:Z:204:LEU:N	1:Z:204:LEU:HD12	2.25	0.51
1:Z:262:LYS:HD2	1:Z:262:LYS:C	2.32	0.51
1:Z:338:ASN:HA	1:Z:482:ARG:NH2	2.26	0.51
1:Z:368:THR:HG22	1:Z:371:VAL:HG23	1.93	0.51
1:X:153:GLU:OE1	1:X:156:ARG:NH1	2.44	0.51
1:X:232:LYS:O	1:X:233:GLY:O	2.29	0.51
1:O:29:SER:CB	1:O:63:VAL:HG12	2.41	0.51
1:O:89:TRP:HH2	1:O:167:THR:CG2	2.20	0.51
1:Y:190:MET:O	1:Y:203:MET:HG3	2.10	0.51
1:Y:266:GLY:O	1:Y:310:GLY:N	2.43	0.51
1:Z:399:SER:C	1:Z:401:ILE:H	2.14	0.51
1:X:427:GLY:C	1:X:472:PRO:HG3	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:123:TYR:HE2	1:O:203:MET:HE2	1.76	0.50
1:Y:14:THR:HB	5:Y:647:HOH:O	2.10	0.50
1:Y:154:ARG:O	1:Y:159:GLU:HG2	2.11	0.50
1:Y:316:LEU:HA	1:Y:320:MET:HB2	1.93	0.50
1:Y:456:ASN:OD1	1:Y:458:ASP:HB2	2.11	0.50
1:Z:24:ASP:O	1:Z:25:ALA:HB3	2.10	0.50
1:Z:474:ILE:C	1:Z:476:THR:H	2.05	0.50
1:X:41:LYS:HG3	1:X:42:PRO:HD2	1.93	0.50
1:X:152:ARG:NE	1:X:208:ASP:O	2.43	0.50
1:X:153:GLU:OE1	1:X:153:GLU:HA	2.11	0.50
1:O:298:VAL:O	1:O:298:VAL:HG12	2.10	0.50
1:Z:225:GLY:C	1:Z:226:GLN:HG2	2.31	0.50
1:X:396:GLN:HA	1:X:399:SER:OG	2.11	0.50
1:X:478:GLU:O	1:X:481:TYR:HB3	2.11	0.50
1:O:31:SER:HB2	1:O:63:VAL:HG22	1.94	0.50
1:X:478:GLU:C	1:X:481:TYR:HB3	2.32	0.50
1:Y:148:VAL:O	1:Y:151:SER:OG	2.28	0.50
1:Y:262:LYS:O	1:Y:271:MET:HA	2.11	0.50
1:X:3:LYS:HA	1:X:73:GLN:HA	1.93	0.50
1:X:194:ILE:O	1:X:300:TYR:OH	2.28	0.50
1:X:342:VAL:HG21	1:X:371:VAL:HG11	1.92	0.50
1:X:380:THR:O	1:X:383:SER:OG	2.30	0.50
1:O:415:ASN:CB	1:O:418:LEU:HB2	2.38	0.50
1:Y:31:SER:OG	1:Y:59:THR:HG22	2.11	0.50
1:Y:286:LEU:O	1:Y:287:LEU:HD23	2.12	0.50
1:Y:427:GLY:HA2	1:Y:472:PRO:HB3	1.92	0.50
1:Y:468:ARG:HD3	1:Y:469:GLU:O	2.12	0.50
1:Z:150:GLY:O	1:Z:154:ARG:HG3	2.12	0.50
1:Z:154:ARG:O	1:Z:159:GLU:HB2	2.12	0.50
1:Z:349:THR:HG23	1:Z:349:THR:O	2.10	0.50
1:Z:451:VAL:O	1:Z:451:VAL:HG12	2.11	0.50
1:X:140:LYS:O	1:X:143:TRP:HB3	2.11	0.50
1:X:303:GLU:OE2	1:X:305:ALA:HB2	2.12	0.50
1:O:19:VAL:HG13	1:O:27:ILE:HG23	1.92	0.50
1:Y:19:VAL:HG12	1:Y:27:ILE:HG23	1.94	0.50
1:Y:293:GLY:HA3	1:Y:297:GLU:CD	2.32	0.50
1:Z:345:VAL:O	1:Z:362:GLY:HA2	2.12	0.50
1:O:483:TYR:CE2	1:O:487:LYS:HE3	2.47	0.50
1:Y:188:ARG:NH2	1:Y:303:GLU:OE1	2.45	0.50
1:Z:133:ASP:OD2	1:Z:356:TRP:HE3	1.94	0.50
1:Z:474:ILE:O	1:Z:476:THR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:389:ARG:HG2	1:X:483:TYR:CZ	2.47	0.50
1:X:396:GLN:HG2	1:X:401:ILE:O	2.12	0.50
1:O:245:ASP:C	1:O:248:ALA:HB3	2.33	0.50
1:Y:155:ALA:HB3	1:Y:213:MET:HE1	1.93	0.50
1:Y:307:PHE:HB3	1:Y:349:THR:CG2	2.42	0.50
1:Y:382:GLU:HB3	1:Y:421:PHE:CE2	2.47	0.50
1:Y:427:GLY:HA2	1:Y:472:PRO:CB	2.41	0.50
1:O:155:ALA:CB	1:O:213:MET:HE1	2.41	0.50
1:O:457:LEU:O	1:O:460:LEU:HB2	2.12	0.50
1:Y:267:THR:HG23	1:Y:311:ALA:HB2	1.92	0.50
1:Z:322:LEU:HD23	1:Z:322:LEU:H	1.73	0.50
1:Z:432:ARG:O	1:Z:466:ILE:HG23	2.12	0.50
1:Z:432:ARG:HH11	1:Z:468:ARG:HB2	1.76	0.50
1:X:347:ALA:HB2	1:X:351:LEU:CD1	2.42	0.50
1:Y:53:TRP:HA	1:Y:53:TRP:HE3	1.76	0.49
1:Y:109:ALA:HA	1:Y:134:PRO:HG3	1.94	0.49
1:Y:235:THR:C	1:Y:236:ARG:HD3	2.32	0.49
1:X:499:HIS:CD2	1:X:499:HIS:N	2.79	0.49
1:O:47:HIS:CD2	1:O:52:ILE:HD11	2.47	0.49
1:O:80:THR:CG2	1:O:245:ASP:HA	2.41	0.49
1:O:241:GLY:N	1:O:447:ALA:HB2	2.27	0.49
1:O:362:GLY:N	1:Y:367:LEU:O	2.29	0.49
1:Y:245:ASP:HA	1:Y:248:ALA:HB3	1.94	0.49
1:Y:245:ASP:O	1:Y:248:ALA:HB3	2.11	0.49
1:X:226:GLN:NE2	1:X:236:ARG:HB3	2.17	0.49
1:X:235:THR:C	1:X:236:ARG:HD3	2.32	0.49
1:X:285:GLY:O	1:X:286:LEU:HD23	2.12	0.49
1:O:83:ARG:HB2	4:O:603:GOL:H12	1.93	0.49
1:O:193:ASN:OD1	1:O:195:HIS:N	2.40	0.49
1:O:328:ASP:O	1:O:331:TYR:HB3	2.13	0.49
1:Z:322:LEU:N	1:Z:322:LEU:CD2	2.75	0.49
1:X:352:GLY:O	1:X:356:TRP:N	2.40	0.49
1:Y:270:PHE:CD1	1:Y:270:PHE:N	2.79	0.49
1:X:156:ARG:C	1:X:158:GLY:H	2.16	0.49
1:X:349:THR:O	1:X:349:THR:HG23	2.12	0.49
1:O:62:GLU:HG3	1:X:54:ALA:HB1	1.93	0.49
1:O:154:ARG:HA	1:O:159:GLU:HG3	1.94	0.49
1:O:184:THR:O	1:O:187:SER:OG	2.26	0.49
1:O:232:LYS:O	1:O:233:GLY:O	2.30	0.49
1:Y:40:PRO:HG2	1:Y:44:TRP:CB	2.41	0.49
1:Y:45:VAL:H	1:Y:105:CYS:HB2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:427:GLY:CA	1:Y:472:PRO:HG3	2.42	0.49
1:Z:113:GLU:O	1:Z:117:ARG:HG3	2.11	0.49
1:Z:293:GLY:C	1:Z:295:THR:H	2.15	0.49
1:X:110:GLU:O	1:X:114:HIS:HD2	1.96	0.49
1:X:160:LEU:C	1:X:161:LEU:HD23	2.33	0.49
1:X:212:GLU:H	1:X:212:GLU:CD	2.16	0.49
1:O:84:GLU:HB2	1:O:103:TRP:CB	2.22	0.49
1:Y:130:LEU:HD11	1:Y:188:ARG:HA	1.94	0.49
1:Z:143:TRP:O	1:Z:147:HIS:ND1	2.35	0.49
1:Z:289:THR:OG1	1:Z:290:ILE:N	2.45	0.49
1:Z:476:THR:HG23	1:Z:479:ARG:HH11	1.78	0.49
1:X:461:GLN:C	1:X:463:LYS:H	2.16	0.49
1:O:43:GLY:C	1:O:44:TRP:HD1	2.16	0.49
1:O:44:TRP:N	1:O:44:TRP:CD1	2.78	0.49
1:O:270:PHE:CE2	1:O:305:ALA:HB1	2.46	0.49
1:Y:108:THR:OG1	1:Y:134:PRO:HB3	2.13	0.49
1:Y:468:ARG:HD2	1:Y:470:PHE:CD1	2.47	0.49
1:X:196:THR:CG2	1:X:197:LEU:N	2.75	0.49
1:O:8:ALA:HB3	1:O:440:ALA:HB1	1.93	0.49
1:O:115:LEU:CD1	1:O:115:LEU:N	2.75	0.49
1:O:340:ASN:N	5:O:653:HOH:O	2.45	0.49
1:Y:83:ARG:HD3	1:Y:244:GLY:HA3	1.93	0.49
1:Z:161:LEU:HD22	1:Z:179:HIS:NE2	2.27	0.49
1:Z:166:ASP:CG	1:Z:167:THR:H	2.16	0.49
1:Z:174:THR:O	1:Z:177:ARG:N	2.45	0.49
1:Z:189:THR:HB	1:Z:191:LEU:HB2	1.94	0.49
1:Z:485:GLY:O	1:Z:488:LYS:HB3	2.12	0.49
1:X:44:TRP:HA	1:X:105:CYS:SG	2.53	0.49
1:Y:83:ARG:NH1	1:Y:246:GLN:HG2	2.27	0.49
1:Z:98:TYR:CD2	1:Z:99:ASN:N	2.81	0.49
1:Z:445:TYR:O	1:Z:449:LEU:HB2	2.13	0.49
1:X:135:TYR:CD2	1:X:136:PHE:CE1	3.01	0.49
1:X:177:ARG:HB3	1:X:177:ARG:HH11	1.78	0.49
1:X:180:VAL:HA	1:X:216:GLU:O	2.12	0.49
1:X:406:LEU:O	1:X:431:GLU:N	2.38	0.49
1:O:17:ARG:HA	1:O:31:SER:O	2.12	0.49
1:Y:84:GLU:HB2	1:Y:103:TRP:CB	2.36	0.49
1:Y:145:LEU:HD12	1:Y:151:SER:HB2	1.94	0.49
1:X:226:GLN:HA	1:X:237:ILE:O	2.13	0.49
1:O:85:THR:OG1	1:O:103:TRP:HD1	1.96	0.48
1:O:425:ILE:HD12	1:O:425:ILE:HA	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:80:THR:CG2	1:Y:248:ALA:HB2	2.43	0.48
1:Y:261:ALA:CB	1:Y:273:MET:HB2	2.32	0.48
1:Y:307:PHE:CB	1:Y:349:THR:HG22	2.43	0.48
1:Z:115:LEU:H	1:Z:115:LEU:CD1	2.25	0.48
1:Z:246:GLN:HG3	1:Z:270:PHE:HB2	1.95	0.48
1:Z:331:TYR:CD2	1:Z:335:LYS:HE2	2.48	0.48
1:Y:179:HIS:CE1	1:Y:215:PRO:CA	2.97	0.48
1:Y:415:ASN:ND2	1:Y:418:LEU:H	2.08	0.48
1:Z:41:LYS:HB2	1:Z:42:PRO:HD2	1.95	0.48
1:Z:171:TRP:CE2	1:Z:176:GLY:HA2	2.48	0.48
1:Z:415:ASN:HD22	1:Z:418:LEU:H	1.60	0.48
1:O:255:CYS:HB3	1:O:260:MET:HB2	1.95	0.48
1:O:270:PHE:HE2	1:O:305:ALA:CB	2.26	0.48
1:Y:117:ARG:O	1:Y:117:ARG:HG3	2.13	0.48
1:Y:178:VAL:HG23	1:Y:179:HIS:N	2.28	0.48
1:Z:246:GLN:HB3	1:Z:272:LEU:HD11	1.94	0.48
1:X:171:TRP:CD1	1:X:176:GLY:HA2	2.48	0.48
1:X:381:LEU:O	1:X:384:ILE:HB	2.12	0.48
1:X:427:GLY:HA2	1:X:472:PRO:HG3	1.94	0.48
1:O:178:VAL:HG12	1:O:179:HIS:N	2.27	0.48
1:Y:47:HIS:CD2	1:Y:82:GLN:HE22	2.31	0.48
1:Y:60:LEU:O	1:Y:60:LEU:HD12	2.13	0.48
1:Y:154:ARG:CB	1:Y:159:GLU:HG3	2.34	0.48
1:Y:261:ALA:HA	1:Y:272:LEU:O	2.12	0.48
1:X:130:LEU:HD13	1:X:136:PHE:CG	2.49	0.48
1:O:253:GLN:HE22	1:O:409:ASP:HB3	1.79	0.48
1:O:303:GLU:HG3	1:O:304:GLY:N	2.27	0.48
1:Y:328:ASP:O	1:Y:331:TYR:N	2.47	0.48
1:Y:468:ARG:HD3	1:Y:469:GLU:N	2.28	0.48
1:Z:55:THR:O	1:Z:59:THR:OG1	2.30	0.48
1:Z:95:LYS:O	1:Z:95:LYS:HG2	2.14	0.48
1:Z:115:LEU:N	1:Z:115:LEU:CD1	2.77	0.48
1:X:71:SER:HB2	1:X:235:THR:CG2	2.42	0.48
1:X:207:LEU:HB2	1:X:209:ILE:HD11	1.94	0.48
1:O:127:ASN:HB3	1:O:193:ASN:ND2	2.28	0.48
1:O:137:SER:OG	1:O:189:THR:HA	2.13	0.48
1:Y:160:LEU:O	1:Y:213:MET:HB3	2.13	0.48
1:Z:19:VAL:HG12	1:Z:20:VAL:N	2.28	0.48
1:X:401:ILE:HD12	1:X:401:ILE:H	1.77	0.48
1:O:80:THR:HG21	1:O:248:ALA:HB1	1.90	0.48
1:O:182:ASP:OD2	1:O:184:THR:OG1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:257:LYS:O	1:O:260:MET:HG3	2.13	0.48
1:O:272:LEU:HA	1:O:302:LEU:O	2.13	0.48
1:Y:23:HIS:HA	1:Y:453:PHE:HE2	1.78	0.48
1:Y:110:GLU:O	1:Y:113:GLU:HB2	2.13	0.48
1:Z:352:GLY:O	1:Z:356:TRP:N	2.35	0.48
1:O:140:LYS:O	1:O:143:TRP:HB3	2.14	0.48
1:Y:21:MET:HA	1:Y:26:ASN:O	2.14	0.48
1:Y:143:TRP:O	1:Y:147:HIS:ND1	2.29	0.48
1:Z:7:VAL:O	1:Z:7:VAL:HG12	2.13	0.48
1:Z:18:ALA:HB3	1:Z:63:VAL:CG2	2.44	0.48
1:Z:242:ILE:CG2	1:Z:243:ALA:N	2.77	0.48
1:X:83:ARG:NH1	4:X:606:GOL:O1	2.46	0.48
1:O:282:SER:O	1:O:283:GLU:HG2	2.14	0.48
1:O:409:ASP:HB2	1:O:438:VAL:CG2	2.42	0.48
1:Y:19:VAL:HG12	1:Y:20:VAL:N	2.29	0.48
1:Y:202:LYS:O	1:Y:206:VAL:HB	2.14	0.48
1:Y:331:TYR:CZ	1:Y:335:LYS:HE2	2.48	0.48
1:Z:80:THR:HG22	1:Z:245:ASP:HA	1.94	0.48
1:Z:429:ARG:HG2	1:Z:471:ARG:HA	1.95	0.48
1:O:270:PHE:CD2	1:O:305:ALA:HA	2.48	0.48
1:Y:103:TRP:HA	1:Y:140:LYS:HZ2	1.79	0.48
1:Y:196:THR:HG22	1:Y:197:LEU:N	2.29	0.48
1:Y:381:LEU:HA	1:Y:381:LEU:HD23	1.60	0.48
1:O:125:ARG:O	1:O:129:GLY:N	2.47	0.47
1:O:477:THR:HG22	1:O:478:GLU:N	2.28	0.47
1:Y:159:GLU:HG2	1:Y:159:GLU:H	1.30	0.47
1:Z:84:GLU:OE2	1:Z:188:ARG:HD2	2.14	0.47
1:Z:156:ARG:C	1:Z:158:GLY:H	2.16	0.47
1:Z:476:THR:HG23	1:Z:479:ARG:NH1	2.28	0.47
1:X:154:ARG:HB2	1:X:160:LEU:CD1	2.44	0.47
1:O:173:MET:O	1:O:227:THR:HG23	2.14	0.47
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.78	0.47
1:Y:359:TYR:CZ	1:Y:499:HIS:CD2	3.02	0.47
1:Y:448:GLY:CA	1:Y:453:PHE:HB3	2.44	0.47
1:Z:83:ARG:HH11	4:Z:605:GOL:C2	2.19	0.47
1:X:190:MET:HE3	1:X:190:MET:HB3	1.76	0.47
1:X:381:LEU:HA	1:X:384:ILE:HD12	1.96	0.47
1:O:21:MET:N	1:O:21:MET:CE	2.77	0.47
1:Y:142:LYS:HD2	1:Y:207:LEU:CD2	2.32	0.47
1:Y:250:LEU:HA	1:Y:262:LYS:HG2	1.95	0.47
1:Z:286:LEU:HD11	1:Z:395:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:460:LEU:HD13	1:X:460:LEU:HA	1.70	0.47
1:X:467:GLU:O	1:X:467:GLU:HG2	2.14	0.47
1:O:477:THR:CG2	1:O:478:GLU:N	2.77	0.47
1:Y:272:LEU:HA	1:Y:302:LEU:O	2.15	0.47
1:Y:281:LYS:O	1:Y:281:LYS:HG3	2.04	0.47
1:Z:161:LEU:HA	1:Z:161:LEU:HD23	1.71	0.47
1:Z:206:VAL:CG1	1:Z:207:LEU:N	2.78	0.47
1:X:360:ALA:O	1:X:361:ARG:NH1	2.42	0.47
1:X:396:GLN:HA	1:X:399:SER:HG	1.80	0.47
1:O:165:VAL:HG12	1:O:169:LEU:HD22	1.95	0.47
1:O:318:ASP:HA	1:O:321:LYS:HE3	1.95	0.47
1:Y:49:PRO:HG2	1:Y:96:PRO:CG	2.42	0.47
1:Y:450:ALA:C	1:Y:452:GLY:H	2.18	0.47
1:Z:85:THR:HG22	1:Z:100:ALA:HB1	1.93	0.47
1:X:250:LEU:CD1	1:X:255:CYS:HB2	2.43	0.47
1:X:265:TYR:HD2	1:X:413:VAL:HG12	1.78	0.47
1:X:344:VAL:CG2	1:X:379:ALA:HB3	2.44	0.47
1:O:123:TYR:CE2	1:O:203:MET:HE2	2.50	0.47
1:O:199:TRP:HB3	1:O:204:LEU:HD11	1.97	0.47
1:O:270:PHE:CE2	1:O:305:ALA:CB	2.98	0.47
1:O:278:LYS:HG3	1:O:279:ALA:N	2.27	0.47
1:Y:57:SER:O	1:Y:61:VAL:HG23	2.15	0.47
1:Z:154:ARG:C	1:Z:159:GLU:HB2	2.35	0.47
1:Z:183:TYR:CD1	1:Z:217:VAL:CG1	2.98	0.47
1:X:372:ASN:OD1	1:X:375:HIS:ND1	2.47	0.47
1:O:254:LEU:HD12	1:O:254:LEU:HA	1.60	0.47
1:O:476:THR:O	1:O:478:GLU:N	2.47	0.47
1:Y:41:LYS:CG	1:Y:44:TRP:CD2	2.97	0.47
1:Y:170:ILE:HD13	1:Y:242:ILE:HD11	1.95	0.47
1:Y:269:CYS:HB3	1:Y:306:VAL:HB	1.97	0.47
1:Y:312:SER:O	1:Y:315:TRP:HB3	2.14	0.47
1:Y:359:TYR:CE2	1:Y:499:HIS:CD2	3.03	0.47
1:Y:500:ASP:OD1	1:Y:500:ASP:N	2.48	0.47
1:Z:83:ARG:HG2	4:Z:605:GOL:HO2	1.79	0.47
1:Z:140:LYS:O	1:Z:143:TRP:HB3	2.15	0.47
1:Z:174:THR:CB	1:Z:178:VAL:HG13	2.44	0.47
1:Z:307:PHE:HB3	1:Z:349:THR:CG2	2.44	0.47
1:Z:308:MET:HE2	1:Z:348:PHE:CB	2.44	0.47
1:Z:376:ILE:HD12	1:X:320:MET:SD	2.55	0.47
1:Z:445:TYR:N	1:Z:445:TYR:CD1	2.83	0.47
1:X:73:GLN:HE21	1:X:73:GLN:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:86:THR:HG21	1:X:141:VAL:HG22	1.95	0.47
1:X:347:ALA:HB3	1:X:361:ARG:O	2.14	0.47
1:Y:194:ILE:HB	1:Y:290:ILE:HD11	1.97	0.47
1:Z:21:MET:HE2	1:Z:21:MET:N	2.28	0.47
1:Z:83:ARG:NH1	4:Z:605:GOL:O1	2.48	0.47
1:Z:319:GLU:HG3	1:X:372:ASN:CA	2.45	0.47
1:O:81:ASN:HD22	1:O:81:ASN:N	2.13	0.47
1:O:230:GLY:N	1:X:230:GLY:CA	2.77	0.47
1:O:242:ILE:CG2	1:O:243:ALA:N	2.78	0.47
1:Z:14:THR:HB	5:Z:659:HOH:O	2.15	0.47
1:Z:47:HIS:O	1:Z:99:ASN:HB3	2.13	0.47
1:Z:404:HIS:O	1:Z:405:ALA:HB2	2.15	0.47
1:X:21:MET:HE3	1:X:444:ALA:HB2	1.96	0.47
1:X:298:VAL:HG13	1:X:299:ASN:N	2.30	0.47
1:X:392:LEU:HD23	1:X:392:LEU:O	2.15	0.47
1:Y:271:MET:HE1	1:Y:391:VAL:HG23	1.96	0.47
1:Y:428:THR:CG2	1:Y:429:ARG:N	2.77	0.47
1:X:263:ASN:HD22	1:X:406:LEU:HD11	1.79	0.47
1:X:286:LEU:HD22	1:X:304:GLY:HA2	1.96	0.47
1:Y:156:ARG:HG3	1:Y:210:PRO:HB3	1.97	0.46
1:Y:438:VAL:H	1:Y:438:VAL:HG13	1.40	0.46
1:Z:80:THR:HG23	1:Z:248:ALA:HB2	1.97	0.46
1:X:84:GLU:HB2	1:X:103:TRP:HB2	1.94	0.46
1:X:449:LEU:HA	1:X:449:LEU:HD12	1.60	0.46
1:Z:13:THR:O	1:Z:13:THR:HG22	2.15	0.46
1:Z:80:THR:HG21	1:Z:248:ALA:HB3	1.98	0.46
1:Z:328:ASP:O	1:Z:331:TYR:N	2.48	0.46
1:Z:343:TYR:OH	1:Z:482:ARG:O	2.29	0.46
1:X:30:VAL:HG12	1:X:31:SER:N	2.30	0.46
1:X:258:GLU:HA	1:X:274:ASN:O	2.15	0.46
1:X:269:CYS:HB2	1:X:306:VAL:CB	2.39	0.46
1:Y:169:LEU:HD23	1:Y:169:LEU:HA	1.77	0.46
1:O:331:TYR:O	1:O:334:THR:OG1	2.31	0.46
1:O:430:VAL:HG23	1:O:470:PHE:HB2	1.97	0.46
1:Y:363:ALA:O	1:Y:364:ILE:HG13	2.16	0.46
1:X:385:ALA:HA	1:X:422:GLN:OE1	2.16	0.46
1:O:57:SER:O	1:O:61:VAL:HG23	2.16	0.46
1:O:122:ASP:O	1:O:126:SER:OG	2.34	0.46
1:Z:456:ASN:ND2	1:Z:458:ASP:CA	2.79	0.46
1:X:342:VAL:HG12	1:X:343:TYR:N	2.30	0.46
1:Y:271:MET:O	1:Y:304:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:271:MET:SD	1:Y:395:MET:HE2	2.56	0.46
1:Y:448:GLY:HA3	1:Y:453:PHE:HB3	1.98	0.46
1:Y:450:ALA:O	1:Y:452:GLY:N	2.49	0.46
1:Z:65:ALA:O	1:Z:68:ASP:N	2.45	0.46
1:Z:137:SER:HG	1:Z:189:THR:HA	1.78	0.46
1:Z:201:ASP:O	1:Z:205:GLU:N	2.48	0.46
1:Z:253:GLN:HB3	1:Z:255:CYS:SG	2.55	0.46
1:Z:418:LEU:HD23	1:Z:418:LEU:HA	1.54	0.46
1:X:103:TRP:CD1	1:X:103:TRP:N	2.77	0.46
1:X:445:TYR:N	1:X:445:TYR:CD1	2.84	0.46
1:X:449:LEU:C	1:X:451:VAL:H	2.19	0.46
1:Y:115:LEU:HD12	1:Y:115:LEU:HA	1.50	0.46
1:Y:145:LEU:CD1	1:Y:151:SER:HB2	2.46	0.46
1:Y:274:ASN:HD21	1:Y:299:ASN:HD22	1.63	0.46
1:Y:376:ILE:HG23	1:Y:376:ILE:HD12	1.63	0.46
1:Y:456:ASN:HD21	1:Y:458:ASP:HB2	1.81	0.46
1:Z:139:THR:O	1:Z:142:LYS:HB3	2.16	0.46
1:Z:197:LEU:HD12	1:Z:197:LEU:HA	1.69	0.46
1:Z:248:ALA:O	1:Z:442:GLY:HA3	2.15	0.46
1:Z:331:TYR:CZ	1:Z:335:LYS:CE	2.99	0.46
1:X:180:VAL:CG2	1:X:218:ARG:HG3	2.46	0.46
1:X:295:THR:H	1:X:297:GLU:CG	2.27	0.46
1:O:88:VAL:O	1:O:88:VAL:HG12	2.15	0.46
1:O:212:GLU:OE1	1:O:212:GLU:N	2.49	0.46
1:O:271:MET:HG2	1:O:395:MET:HE2	1.98	0.46
1:Y:84:GLU:OE2	1:Y:188:ARG:HD3	2.16	0.46
1:Y:391:VAL:CG2	1:Y:392:LEU:N	2.78	0.46
1:Z:21:MET:HB2	1:Z:21:MET:HE3	1.38	0.46
1:Z:49:PRO:HA	1:Z:52:ILE:HG13	1.97	0.46
1:Z:348:PHE:HD1	1:X:368:THR:CA	2.29	0.46
1:Z:389:ARG:HB2	1:Z:426:LEU:HD11	1.98	0.46
1:Z:422:GLN:O	1:Z:425:ILE:HG22	2.15	0.46
1:X:13:THR:O	1:X:13:THR:HG22	2.15	0.46
1:X:204:LEU:N	1:X:204:LEU:CD1	2.78	0.46
1:X:328:ASP:O	1:X:331:TYR:HB3	2.16	0.46
1:O:108:THR:HB	1:O:139:THR:HB	1.97	0.46
1:O:227:THR:O	1:O:237:ILE:N	2.46	0.46
1:O:307:PHE:HB3	1:O:349:THR:CG2	2.45	0.46
1:O:357:ASP:HA	1:O:358:PRO:HD2	1.60	0.46
1:Y:145:LEU:HA	1:Y:145:LEU:HD13	1.47	0.46
1:Y:262:LYS:HE3	1:Y:272:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:284:ASN:ND2	1:Y:397:ALA:CB	2.79	0.46
1:Y:457:LEU:HD23	1:Y:460:LEU:HD12	1.97	0.46
1:Z:250:LEU:HD12	1:Z:255:CYS:HB2	1.97	0.46
1:Z:316:LEU:HA	1:Z:320:MET:CB	2.41	0.46
1:X:372:ASN:OD1	1:X:372:ASN:N	2.29	0.46
1:O:30:VAL:HG12	1:O:31:SER:N	2.31	0.46
1:O:83:ARG:HB2	4:O:603:GOL:O2	2.16	0.46
1:O:376:ILE:HG22	1:O:377:ILE:N	2.30	0.46
1:O:389:ARG:HA	1:O:426:LEU:HD11	1.98	0.46
5:O:638:HOH:O	1:Y:369:ARG:HG3	2.15	0.46
1:Y:161:LEU:CD2	1:Y:179:HIS:CE1	2.98	0.46
1:Y:287:LEU:HB2	1:Y:303:GLU:HB3	1.97	0.46
1:Y:307:PHE:CD2	1:Y:349:THR:CG2	2.99	0.46
1:Z:132:ILE:O	1:Z:133:ASP:HB2	2.15	0.46
1:Z:157:ARG:HG2	1:Z:157:ARG:O	2.16	0.46
1:Z:240:SER:HB2	1:Z:447:ALA:CB	2.46	0.46
1:X:124:ILE:HD12	1:X:132:ILE:HG12	1.97	0.46
1:X:386:TYR:HB3	1:X:486:TRP:CE2	2.50	0.46
1:O:361:ARG:HD2	1:Y:368:THR:CG2	2.46	0.45
1:O:455:GLN:HG3	1:O:459:GLU:OE2	2.16	0.45
1:Y:179:HIS:CE1	1:Y:215:PRO:HA	2.50	0.45
1:Z:135:TYR:HH	4:Z:605:GOL:HO1	1.61	0.45
1:Z:295:THR:HB	1:Z:297:GLU:CD	2.36	0.45
1:X:152:ARG:HH11	1:X:152:ARG:CG	2.28	0.45
1:X:174:THR:OG1	1:X:178:VAL:HG13	2.15	0.45
1:Y:193:ASN:OD1	1:Y:196:THR:HB	2.16	0.45
1:Y:353:ALA:HB2	1:Y:356:TRP:CZ2	2.51	0.45
1:Y:447:ALA:O	1:Y:450:ALA:N	2.48	0.45
1:Y:447:ALA:O	1:Y:449:LEU:N	2.49	0.45
1:Z:346:PRO:C	1:Z:348:PHE:H	2.19	0.45
1:X:287:LEU:HD12	1:X:303:GLU:HG2	1.98	0.45
1:X:431:GLU:CG	1:X:466:ILE:HG13	2.38	0.45
1:X:499:HIS:CD2	1:X:499:HIS:H	2.34	0.45
1:O:58:SER:HA	1:O:61:VAL:CG2	2.47	0.45
1:O:399:SER:HB2	1:O:401:ILE:CG2	2.43	0.45
1:Y:348:PHE:CD1	1:Y:348:PHE:N	2.81	0.45
1:Z:39:TYR:HE2	1:X:369:ARG:HD3	1.81	0.45
1:Z:90:GLU:O	1:Z:94:GLY:N	2.49	0.45
1:Z:316:LEU:CA	1:Z:320:MET:HB2	2.41	0.45
1:X:133:ASP:OD1	1:X:134:PRO:HD2	2.17	0.45
1:X:177:ARG:CB	1:X:177:ARG:NH1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:17:ARG:N	1:O:17:ARG:CD	2.79	0.45
1:O:225:GLY:C	1:O:226:GLN:HG2	2.37	0.45
1:O:340:ASN:HD22	1:O:371:VAL:CG2	2.30	0.45
1:O:359:TYR:CE2	1:O:499:HIS:CD2	3.05	0.45
1:O:406:LEU:CD2	1:O:407:ARG:H	2.29	0.45
1:Z:8:ALA:O	1:Z:9:LEU:HD12	2.17	0.45
1:X:438:VAL:HA	1:X:441:LEU:HD12	1.98	0.45
1:O:83:ARG:NH1	1:O:188:ARG:CZ	2.79	0.45
1:O:175:GLN:HG2	1:O:177:ARG:NH2	2.31	0.45
1:O:230:GLY:HA2	1:X:228:ASN:CG	2.37	0.45
1:O:463:LYS:HB3	1:O:464:ALA:H	1.33	0.45
1:Y:83:ARG:HD2	1:Y:244:GLY:HA3	1.97	0.45
1:Y:206:VAL:CG1	1:Y:207:LEU:N	2.80	0.45
1:Y:357:ASP:OD2	1:Y:494:MET:HB3	2.17	0.45
1:Y:385:ALA:HA	1:Y:422:GLN:OE1	2.17	0.45
1:Z:39:TYR:HA	1:Z:40:PRO:HD2	1.56	0.45
1:X:41:LYS:O	1:X:44:TRP:HB2	2.16	0.45
1:X:352:GLY:O	1:X:355:TYR:N	2.49	0.45
1:X:427:GLY:CA	1:X:472:PRO:HG3	2.47	0.45
1:X:456:ASN:ND2	1:X:459:GLU:H	2.13	0.45
1:O:130:LEU:HD22	1:O:136:PHE:CZ	2.52	0.45
1:O:175:GLN:HG3	1:O:177:ARG:HH21	1.80	0.45
1:Y:13:THR:O	1:Y:13:THR:HG22	2.16	0.45
1:Y:44:TRP:N	1:Y:44:TRP:HD1	2.15	0.45
1:Y:130:LEU:HD13	1:Y:136:PHE:CG	2.50	0.45
1:Y:284:ASN:HD21	1:Y:397:ALA:HB1	1.81	0.45
1:X:429:ARG:HH12	1:X:471:ARG:HG2	1.79	0.45
1:O:114:HIS:HA	1:O:117:ARG:HB2	1.99	0.45
1:O:203:MET:C	1:O:206:VAL:HG23	2.37	0.45
1:O:359:TYR:CZ	1:O:499:HIS:CD2	3.05	0.45
1:Z:194:ILE:HD12	1:Z:300:TYR:HE1	1.82	0.45
1:Z:200:ASP:HA	5:Z:656:HOH:O	2.16	0.45
1:Z:295:THR:CB	1:Z:297:GLU:HG2	2.47	0.45
1:X:160:LEU:O	1:X:161:LEU:HD23	2.17	0.45
1:X:389:ARG:HG2	1:X:483:TYR:CE1	2.51	0.45
1:X:482:ARG:HH11	1:X:482:ARG:CG	2.18	0.45
1:O:56:GLN:NE2	1:O:56:GLN:CA	2.78	0.45
1:O:103:TRP:HA	1:O:140:LYS:HZ3	1.80	0.45
1:Y:60:LEU:HD12	1:Y:60:LEU:C	2.36	0.45
1:Y:389:ARG:HD3	1:Y:483:TYR:CZ	2.51	0.45
1:O:234:GLY:H	2:O:601:PO4:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:272:LEU:CG	1:O:303:GLU:HB2	2.41	0.45
1:O:316:LEU:O	1:O:321:LYS:N	2.49	0.45
1:O:391:VAL:CG2	1:O:392:LEU:N	2.79	0.45
1:O:435:VAL:CG2	1:O:436:ARG:N	2.79	0.45
1:Y:349:THR:HG23	1:Y:349:THR:O	2.17	0.45
1:Y:357:ASP:HA	1:Y:358:PRO:HD2	1.84	0.45
1:Y:488:LYS:HE3	1:Y:488:LYS:HB3	1.81	0.45
1:Z:270:PHE:CD2	1:Z:305:ALA:CB	3.00	0.45
1:Z:392:LEU:O	1:Z:392:LEU:HG	2.16	0.45
1:O:114:HIS:CD2	1:O:114:HIS:H	2.34	0.45
1:O:162:PHE:CG	1:O:163:GLY:N	2.85	0.45
1:O:218:ARG:NH2	1:O:222:GLU:OE2	2.49	0.45
1:O:477:THR:HG22	1:O:478:GLU:H	1.81	0.45
1:Y:475:GLU:H	1:Y:475:GLU:HG3	1.44	0.45
1:Y:479:ARG:HG3	1:Y:479:ARG:NH1	2.29	0.45
1:Z:6:ILE:HD13	1:Z:444:ALA:HB1	1.98	0.45
1:Z:80:THR:O	1:Z:81:ASN:HB3	2.17	0.45
1:Z:338:ASN:HA	1:Z:482:ARG:HH22	1.82	0.45
1:X:418:LEU:HD13	1:X:419:MET:CE	2.45	0.45
1:X:494:MET:HE2	1:X:494:MET:HB2	1.62	0.45
1:O:407:ARG:HG3	1:O:408:VAL:N	2.31	0.44
1:Y:13:THR:HG1	1:Y:103:TRP:HE1	1.63	0.44
1:Z:88:VAL:CG1	1:Z:97:ILE:HG12	2.37	0.44
1:Z:271:MET:CE	1:Z:391:VAL:HG23	2.47	0.44
1:O:81:ASN:N	1:O:81:ASN:ND2	2.65	0.44
1:O:175:GLN:CG	1:O:177:ARG:NH2	2.80	0.44
1:Y:5:TYR:O	1:Y:74:ILE:HA	2.17	0.44
1:Y:245:ASP:OD1	1:Y:246:GLN:N	2.50	0.44
1:Y:445:TYR:O	1:Y:449:LEU:HB2	2.17	0.44
1:Y:474:ILE:HD11	1:Y:479:ARG:CA	2.47	0.44
1:Z:204:LEU:N	1:Z:204:LEU:CD1	2.80	0.44
1:Z:212:GLU:OE1	1:Z:212:GLU:N	2.50	0.44
1:X:164:THR:HB	1:X:165:VAL:H	1.61	0.44
1:O:88:VAL:CG1	1:O:97:ILE:HD11	2.47	0.44
1:O:214:LEU:N	1:O:214:LEU:HD12	2.32	0.44
1:O:307:PHE:HB3	1:O:349:THR:HG22	1.99	0.44
1:O:396:GLN:CD	1:O:402:ARG:HA	2.37	0.44
1:Y:202:LYS:O	1:Y:205:GLU:HB3	2.17	0.44
1:Z:282:SER:CB	1:Z:286:LEU:HB2	2.47	0.44
1:X:180:VAL:HG21	1:X:218:ARG:HG3	1.99	0.44
1:O:73:GLN:HE21	1:O:73:GLN:HB2	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:95:LYS:HA	1:O:96:PRO:HD3	1.71	0.44
1:Y:418:LEU:CD1	1:Y:419:MET:CE	2.95	0.44
1:X:220:SER:HB3	1:X:242:ILE:O	2.18	0.44
1:X:286:LEU:HD13	1:X:395:MET:CE	2.47	0.44
1:O:391:VAL:HG23	1:O:392:LEU:N	2.31	0.44
1:O:456:ASN:O	1:O:459:GLU:HB2	2.18	0.44
1:Z:83:ARG:HG3	4:Z:605:GOL:C2	2.47	0.44
1:X:15:SER:HA	1:X:33:ARG:O	2.18	0.44
1:X:83:ARG:HH11	1:X:83:ARG:CG	2.30	0.44
1:X:130:LEU:HD12	1:X:190:MET:CA	2.48	0.44
1:Y:325:ASP:O	1:Y:328:ASP:HB2	2.18	0.44
1:Y:389:ARG:O	1:Y:393:GLU:HG3	2.18	0.44
1:Z:111:ILE:O	1:Z:115:LEU:HD13	2.18	0.44
1:Z:136:PHE:O	1:Z:140:LYS:HG3	2.17	0.44
1:X:428:THR:HG22	1:X:429:ARG:N	2.33	0.44
1:X:446:LEU:HD12	1:X:446:LEU:HA	1.82	0.44
1:O:320:MET:HB3	1:O:322:LEU:HG	1.99	0.44
1:O:340:ASN:HD22	1:O:371:VAL:HG22	1.81	0.44
1:Y:90:GLU:HB3	5:Y:634:HOH:O	2.17	0.44
1:Y:110:GLU:HA	5:Y:653:HOH:O	2.18	0.44
1:Z:83:ARG:HH21	1:Z:188:ARG:NH2	2.14	0.44
1:Z:331:TYR:CE1	1:Z:335:LYS:HE2	2.53	0.44
1:X:342:VAL:CG1	1:X:343:TYR:N	2.80	0.44
1:X:342:VAL:HA	1:X:365:PHE:O	2.18	0.44
1:O:200:ASP:OD1	1:O:202:LYS:HB3	2.17	0.44
1:O:241:GLY:CA	1:O:447:ALA:HB2	2.47	0.44
1:O:346:PRO:HG2	1:O:387:GLN:HE22	1.82	0.44
1:Y:186:ALA:N	5:Y:618:HOH:O	2.50	0.44
1:Y:428:THR:HG22	1:Y:429:ARG:O	2.17	0.44
1:Z:377:ILE:H	1:Z:377:ILE:HG13	1.56	0.44
1:Z:385:ALA:HB1	1:Z:425:ILE:HG21	2.00	0.44
1:X:88:VAL:CG1	1:X:97:ILE:HD11	2.46	0.44
1:X:396:GLN:O	1:X:397:ALA:O	2.36	0.44
1:X:415:ASN:ND2	1:X:415:ASN:C	2.71	0.44
1:X:468:ARG:CG	1:X:469:GLU:N	2.81	0.44
1:O:395:MET:O	1:O:399:SER:N	2.35	0.44
1:Z:35:PHE:CE2	1:Z:47:HIS:CD2	2.95	0.44
1:Z:194:ILE:HB	1:Z:290:ILE:HD11	2.00	0.44
1:Z:458:ASP:N	1:Z:458:ASP:OD1	2.51	0.44
1:X:154:ARG:HB2	1:X:160:LEU:HD11	2.00	0.44
1:X:184:THR:O	1:X:187:SER:OG	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:238:PRO:C	1:X:239:ILE:HG13	2.34	0.44
1:X:423:SER:O	1:X:424:ASP:O	2.35	0.44
1:O:9:LEU:O	1:O:80:THR:N	2.42	0.43
1:O:38:ILE:HG22	1:O:40:PRO:HD3	1.99	0.43
1:Y:156:ARG:C	1:Y:158:GLY:N	2.72	0.43
1:Y:263:ASN:HA	1:Y:270:PHE:O	2.17	0.43
1:Y:441:LEU:CD2	1:Y:445:TYR:CZ	3.00	0.43
1:X:228:ASN:HA	5:X:638:HOH:O	2.18	0.43
1:X:315:TRP:CZ3	1:X:316:LEU:HD23	2.53	0.43
1:O:211:ARG:CA	1:O:214:LEU:HD13	2.27	0.43
1:O:288:THR:HA	1:O:301:ALA:O	2.18	0.43
1:X:85:THR:OG1	1:X:103:TRP:HD1	2.02	0.43
1:X:154:ARG:HB3	1:X:159:GLU:HB2	1.99	0.43
1:X:263:ASN:HA	1:X:270:PHE:O	2.18	0.43
1:O:82:GLN:HE21	1:O:82:GLN:HB2	1.45	0.43
1:O:200:ASP:O	1:O:204:LEU:HD12	2.18	0.43
1:O:474:ILE:CG2	1:O:475:GLU:N	2.79	0.43
1:Y:151:SER:O	1:Y:155:ALA:N	2.40	0.43
1:Y:490:VAL:HG12	1:Y:491:LYS:N	2.33	0.43
1:Z:40:PRO:CG	1:Z:44:TRP:HB3	2.40	0.43
1:Z:89:TRP:N	1:Z:89:TRP:CE3	2.86	0.43
1:Z:123:TYR:HD2	1:Z:203:MET:CE	2.31	0.43
1:Z:476:THR:HA	1:Z:479:ARG:HD3	1.99	0.43
1:X:434:GLU:HA	1:X:467:GLU:HB2	2.01	0.43
1:O:6:ILE:CG2	1:O:444:ALA:HB1	2.49	0.43
1:O:70:SER:H	1:O:73:GLN:HE22	1.64	0.43
1:O:262:LYS:NZ	1:O:264:THR:HB	2.34	0.43
1:O:369:ARG:HD2	1:Y:308:MET:CE	2.48	0.43
1:O:430:VAL:N	1:O:470:PHE:O	2.51	0.43
1:O:490:VAL:O	1:O:494:MET:HG3	2.18	0.43
1:Z:83:ARG:NE	1:Z:246:GLN:HB2	2.34	0.43
1:Z:449:LEU:HD12	1:Z:449:LEU:HA	1.63	0.43
1:X:478:GLU:HA	1:X:481:TYR:CB	2.40	0.43
1:O:114:HIS:O	1:O:117:ARG:N	2.52	0.43
1:O:336:VAL:CG2	1:O:378:ARG:HD2	2.48	0.43
1:Y:218:ARG:HD2	1:Y:222:GLU:OE2	2.19	0.43
1:Y:317:ARG:HB2	1:Y:323:ILE:HG13	1.99	0.43
1:Z:87:ILE:HD12	1:Z:168:TRP:CB	2.48	0.43
1:Z:138:GLY:N	1:Z:189:THR:O	2.52	0.43
1:Z:271:MET:HE1	1:Z:391:VAL:HG23	2.00	0.43
1:Z:378:ARG:O	1:Z:382:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:282:SER:OG	1:X:398:ASP:OD2	2.28	0.43
1:X:405:ALA:HB2	1:X:429:ARG:HB3	2.00	0.43
1:O:83:ARG:CZ	1:O:188:ARG:NH1	2.82	0.43
1:O:156:ARG:C	1:O:158:GLY:H	2.22	0.43
1:O:193:ASN:CG	1:O:196:THR:HB	2.39	0.43
1:O:196:THR:CG2	1:O:197:LEU:N	2.82	0.43
1:Y:186:ALA:O	1:Y:189:THR:HG23	2.19	0.43
1:Y:457:LEU:HD23	1:Y:457:LEU:HA	1.72	0.43
1:Z:59:THR:O	1:Z:62:GLU:N	2.51	0.43
1:Z:125:ARG:O	1:Z:129:GLY:N	2.49	0.43
1:X:33:ARG:NH1	1:X:33:ARG:CG	2.79	0.43
1:X:89:TRP:HB3	1:X:96:PRO:HA	2.01	0.43
1:X:320:MET:HA	1:X:320:MET:HE3	2.00	0.43
1:X:494:MET:HB3	1:X:494:MET:HE3	1.59	0.43
1:O:115:LEU:HD13	1:O:115:LEU:H	1.83	0.43
1:O:143:TRP:O	1:O:147:HIS:ND1	2.40	0.43
1:O:154:ARG:O	1:O:159:GLU:HB2	2.19	0.43
1:O:399:SER:C	1:O:401:ILE:H	2.22	0.43
1:O:438:VAL:HA	1:O:441:LEU:HD12	1.99	0.43
1:Y:190:MET:HA	5:Y:640:HOH:O	2.19	0.43
1:Z:369:ARG:O	1:X:319:GLU:HG2	2.19	0.43
1:X:86:THR:HG23	1:X:162:PHE:HE1	1.84	0.43
1:X:432:ARG:HA	1:X:433:PRO:HD3	1.79	0.43
1:O:461:GLN:C	1:O:463:LYS:H	2.21	0.43
1:Z:258:GLU:HA	1:Z:274:ASN:O	2.19	0.43
1:Z:357:ASP:O	1:Z:359:TYR:N	2.51	0.43
1:Z:367:LEU:HB2	1:X:362:GLY:CA	2.49	0.43
1:X:179:HIS:CE1	1:X:215:PRO:CB	2.99	0.43
1:X:209:ILE:HA	1:X:210:PRO:HD3	1.72	0.43
1:O:125:ARG:HA	1:O:130:LEU:O	2.19	0.43
1:O:273:MET:HG2	1:O:274:ASN:N	2.33	0.43
1:O:462:GLU:H	1:O:462:GLU:HG2	1.30	0.43
1:Y:41:LYS:HD3	1:Y:44:TRP:CE2	2.53	0.43
1:Y:80:THR:C	1:Y:81:ASN:HD22	2.20	0.43
1:Z:188:ARG:HD3	1:Z:188:ARG:HA	1.79	0.43
1:Z:419:MET:HB3	1:Z:470:PHE:CE1	2.54	0.43
1:X:95:LYS:HA	1:X:96:PRO:HD3	1.87	0.43
1:O:31:SER:HB3	1:O:59:THR:CG2	2.48	0.43
1:O:386:TYR:CD2	1:O:486:TRP:CE3	3.07	0.43
1:O:456:ASN:ND2	1:O:459:GLU:CG	2.80	0.43
1:Y:155:ALA:CB	1:Y:213:MET:HE1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:178:VAL:CG2	1:Y:179:HIS:N	2.79	0.43
1:Y:262:LYS:HE3	1:Y:272:LEU:CD1	2.49	0.43
1:Y:468:ARG:NH1	1:Y:468:ARG:CG	2.73	0.43
1:Y:477:THR:HG22	1:Y:478:GLU:N	2.33	0.43
1:Z:123:TYR:O	1:Z:127:ASN:N	2.29	0.43
1:Z:308:MET:CE	1:X:369:ARG:HG2	2.49	0.43
1:Z:320:MET:C	1:Z:322:LEU:HD23	2.39	0.43
1:Z:372:ASN:O	1:Z:375:HIS:HB2	2.18	0.43
1:X:177:ARG:HH11	1:X:177:ARG:CB	2.32	0.43
1:X:258:GLU:HB2	1:X:275:THR:C	2.39	0.43
1:O:220:SER:HB3	1:O:446:LEU:HD21	2.01	0.42
1:O:346:PRO:CA	1:O:348:PHE:CE1	2.99	0.42
1:Z:104:GLN:HG2	1:Z:349:THR:HG21	2.00	0.42
1:Z:202:LYS:O	1:Z:206:VAL:N	2.49	0.42
1:Z:285:GLY:O	1:Z:356:TRP:NE1	2.44	0.42
1:X:157:ARG:CB	1:X:159:GLU:HG3	2.48	0.42
1:X:192:PHE:HB2	1:X:199:TRP:CE3	2.54	0.42
1:Y:87:ILE:HG13	1:Y:100:ALA:HB2	2.01	0.42
1:Z:197:LEU:N	1:Z:197:LEU:HD13	2.34	0.42
1:Z:308:MET:CE	1:Z:348:PHE:HB2	2.48	0.42
1:Z:488:LYS:HD3	1:X:496:TRP:CZ3	2.54	0.42
1:X:144:ILE:HD12	1:X:144:ILE:N	2.31	0.42
1:O:21:MET:N	1:O:21:MET:HE3	2.32	0.42
1:O:88:VAL:HG11	1:O:97:ILE:HD11	2.01	0.42
1:O:308:MET:SD	1:O:311:ALA:CB	3.08	0.42
1:Y:155:ALA:HB1	1:Y:213:MET:CE	2.48	0.42
1:Y:203:MET:O	1:Y:206:VAL:HG12	2.19	0.42
1:Z:27:ILE:H	1:Z:27:ILE:HG12	1.44	0.42
1:Z:391:VAL:CG2	1:Z:392:LEU:N	2.82	0.42
1:X:88:VAL:HA	1:X:161:LEU:O	2.19	0.42
1:X:263:ASN:HB3	1:X:406:LEU:HD11	2.00	0.42
1:O:196:THR:CG2	1:O:198:ASP:N	2.76	0.42
1:O:344:VAL:HG22	1:O:364:ILE:HG23	2.00	0.42
1:O:399:SER:O	1:O:401:ILE:HG22	2.18	0.42
1:Y:23:HIS:HA	1:Y:453:PHE:CE2	2.54	0.42
1:Y:191:LEU:HD23	1:Y:203:MET:HB3	2.00	0.42
1:X:21:MET:SD	1:X:444:ALA:CB	3.07	0.42
1:X:52:ILE:HG23	1:X:52:ILE:HD13	1.62	0.42
1:X:286:LEU:HD13	1:X:395:MET:HE2	2.00	0.42
1:X:462:GLU:HG3	1:X:462:GLU:O	2.19	0.42
1:O:227:THR:O	1:O:236:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:237:ILE:CG2	1:O:238:PRO:CD	2.98	0.42
1:Y:19:VAL:CG1	1:Y:27:ILE:CG2	2.98	0.42
1:Z:308:MET:HB2	5:Z:642:HOH:O	2.19	0.42
1:Z:351:LEU:HD12	1:Z:351:LEU:HA	1.60	0.42
1:Z:373:ALA:O	1:Z:376:ILE:HB	2.19	0.42
1:Z:407:ARG:HD3	1:Z:408:VAL:N	2.35	0.42
1:X:78:GLY:HA3	1:X:443:ALA:O	2.20	0.42
1:X:108:THR:HA	1:X:111:ILE:CD1	2.32	0.42
1:X:214:LEU:HA	1:X:215:PRO:HD3	1.82	0.42
1:X:253:GLN:C	1:X:254:LEU:HD22	2.40	0.42
1:O:163:GLY:CA	1:O:167:THR:HG21	2.48	0.42
1:O:453:PHE:CD2	1:O:454:TRP:CE2	3.05	0.42
1:X:83:ARG:CZ	1:X:188:ARG:NH1	2.82	0.42
1:X:191:LEU:HD23	1:X:191:LEU:HA	1.77	0.42
1:X:291:ALA:HB2	1:X:301:ALA:HB2	2.01	0.42
1:X:445:TYR:N	1:X:445:TYR:HD1	2.16	0.42
1:O:97:ILE:H	1:O:97:ILE:HG13	1.72	0.42
1:O:144:ILE:O	1:O:148:VAL:N	2.29	0.42
1:O:237:ILE:HG23	1:O:238:PRO:CD	2.44	0.42
1:O:381:LEU:O	1:O:384:ILE:HB	2.20	0.42
1:O:403:LEU:HD12	1:O:403:LEU:N	2.31	0.42
1:Y:189:THR:O	1:Y:190:MET:HB3	2.19	0.42
1:Z:181:THR:HG21	1:Z:186:ALA:HB2	2.01	0.42
1:Z:425:ILE:HA	1:Z:425:ILE:HD12	1.40	0.42
1:X:251:PHE:C	1:X:253:GLN:H	2.22	0.42
1:O:56:GLN:CA	1:O:56:GLN:HE21	2.32	0.42
1:O:120:LEU:HD13	1:O:206:VAL:HG11	2.01	0.42
1:O:196:THR:HG22	1:O:197:LEU:N	2.35	0.42
1:O:415:ASN:ND2	1:O:418:LEU:H	2.14	0.42
1:O:436:ARG:H	1:O:436:ARG:HG2	1.58	0.42
1:Y:180:VAL:CG2	1:Y:218:ARG:HG3	2.49	0.42
1:Y:361:ARG:HD3	1:Y:361:ARG:HA	1.83	0.42
1:Y:392:LEU:O	1:Y:392:LEU:HG	2.20	0.42
1:Z:88:VAL:HG12	1:Z:97:ILE:CG1	2.38	0.42
1:Z:386:TYR:HB3	1:Z:486:TRP:CE2	2.55	0.42
1:Z:392:LEU:O	1:Z:395:MET:HB3	2.19	0.42
1:Y:21:MET:HE3	1:Y:444:ALA:HB2	2.02	0.42
1:Y:71:SER:HA	1:Y:74:ILE:HD12	2.00	0.42
1:Y:164:THR:HB	1:Y:165:VAL:H	1.54	0.42
1:Y:394:ALA:O	1:Y:398:ASP:HB2	2.20	0.42
1:Z:18:ALA:CB	1:Z:63:VAL:CG2	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:87:ILE:HG22	1:Z:88:VAL:N	2.35	0.42
1:O:153:GLU:O	1:O:157:ARG:N	2.47	0.42
1:Z:197:LEU:N	1:Z:197:LEU:CD1	2.83	0.42
1:Z:210:PRO:O	1:Z:213:MET:HG2	2.20	0.42
1:X:256:VAL:HG12	1:X:257:LYS:HZ2	1.84	0.42
1:X:367:LEU:HA	1:X:367:LEU:HD23	1.63	0.42
1:X:370:GLY:HA3	5:X:654:HOH:O	2.19	0.42
1:X:389:ARG:HD2	1:X:426:LEU:CD1	2.50	0.42
1:O:12:GLY:CA	1:O:17:ARG:HH12	2.22	0.41
1:O:53:TRP:O	1:O:57:SER:OG	2.38	0.41
1:O:93:THR:OG1	1:O:94:GLY:N	2.51	0.41
1:O:153:GLU:C	1:O:155:ALA:N	2.73	0.41
1:O:269:CYS:HB2	1:O:306:VAL:HB	2.01	0.41
1:O:339:THR:N	5:O:643:HOH:O	2.45	0.41
1:Y:41:LYS:HG2	1:Y:44:TRP:CG	2.55	0.41
1:Z:200:ASP:OD1	1:Z:202:LYS:HB3	2.19	0.41
1:Z:250:LEU:HD22	1:Z:272:LEU:CB	2.50	0.41
1:X:86:THR:CG2	1:X:141:VAL:HG22	2.50	0.41
1:X:411:GLY:HA3	3:X:610:ADP:H5'2	2.01	0.41
1:O:111:ILE:HA	1:O:114:HIS:HD2	1.85	0.41
1:O:351:LEU:HD12	1:O:351:LEU:HA	1.90	0.41
1:Y:257:LYS:N	1:Y:260:MET:SD	2.87	0.41
1:Y:307:PHE:CB	1:Y:349:THR:CG2	2.99	0.41
1:Y:336:VAL:HG23	1:Y:338:ASN:O	2.20	0.41
1:Y:435:VAL:O	1:Y:435:VAL:HG12	2.18	0.41
1:Z:6:ILE:CD1	1:Z:444:ALA:CA	2.97	0.41
1:Z:40:PRO:HG2	1:Z:44:TRP:HE3	1.85	0.41
1:Z:120:LEU:O	1:Z:124:ILE:HG13	2.20	0.41
1:Z:170:ILE:HD13	1:Z:242:ILE:HD11	2.01	0.41
1:Z:340:ASN:HD22	1:Z:371:VAL:HA	1.83	0.41
1:X:345:VAL:O	1:X:362:GLY:HA2	2.20	0.41
1:O:106:ARG:HD2	1:O:349:THR:O	2.20	0.41
1:O:442:GLY:O	1:O:445:TYR:HB2	2.19	0.41
1:Y:84:GLU:OE1	4:Y:604:GOL:O1	2.27	0.41
1:Y:227:THR:HG22	1:Y:228:ASN:H	1.84	0.41
1:Z:284:ASN:OD1	1:Z:397:ALA:HB3	2.21	0.41
1:X:290:ILE:HG21	1:X:298:VAL:HG22	2.02	0.41
1:X:429:ARG:NH1	1:X:471:ARG:CG	2.78	0.41
1:X:457:LEU:HD23	1:X:457:LEU:HA	1.93	0.41
1:X:475:GLU:HG2	1:X:478:GLU:H	1.85	0.41
1:O:381:LEU:HD23	1:O:381:LEU:HA	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:286:LEU:C	1:Y:287:LEU:HD23	2.39	0.41
1:Y:322:LEU:HD23	1:Y:322:LEU:HA	1.95	0.41
1:Z:190:MET:N	5:Z:657:HOH:O	2.29	0.41
1:Z:196:THR:CG2	1:Z:197:LEU:N	2.81	0.41
1:Z:339:THR:CG2	1:Z:379:ALA:HA	2.48	0.41
1:Z:345:VAL:CG2	1:Z:486:TRP:CZ3	3.00	0.41
1:X:312:SER:O	1:X:315:TRP:HB3	2.20	0.41
1:O:189:THR:OG1	1:O:191:LEU:HB2	2.21	0.41
1:O:197:LEU:N	1:O:197:LEU:HD13	2.34	0.41
1:O:241:GLY:O	1:O:242:ILE:HD12	2.20	0.41
1:O:385:ALA:HA	1:O:422:GLN:OE1	2.21	0.41
1:O:418:LEU:HD13	1:O:419:MET:CE	2.50	0.41
1:O:424:ASP:N	1:O:424:ASP:OD1	2.50	0.41
1:Y:23:HIS:CE1	1:Y:453:PHE:O	2.73	0.41
1:Y:187:SER:CB	1:Y:290:ILE:HD12	2.50	0.41
1:X:343:TYR:CD2	1:X:486:TRP:HA	2.55	0.41
1:O:152:ARG:HA	1:O:155:ALA:CB	2.51	0.41
1:O:385:ALA:HB1	1:O:422:GLN:HA	2.02	0.41
1:O:449:LEU:HA	1:O:449:LEU:HD12	1.51	0.41
1:Y:219:ARG:HH21	1:Y:221:SER:HB3	1.85	0.41
1:Y:423:SER:OG	1:Y:472:PRO:N	2.54	0.41
1:Z:6:ILE:CD1	1:Z:444:ALA:CB	2.98	0.41
1:Z:9:LEU:HD12	1:Z:9:LEU:HA	1.79	0.41
1:Z:271:MET:CE	1:Z:391:VAL:CG2	2.99	0.41
1:X:5:TYR:CE2	1:X:69:ILE:HD13	2.56	0.41
1:X:386:TYR:HD2	1:X:486:TRP:CE3	2.35	0.41
1:X:424:ASP:HA	1:X:472:PRO:HB3	2.02	0.41
1:O:48:ASP:HA	1:O:49:PRO:HD3	1.68	0.41
1:O:230:GLY:HA2	1:X:228:ASN:OD1	2.20	0.41
1:O:240:SER:CB	1:O:450:ALA:HB3	2.50	0.41
1:O:240:SER:HB3	1:O:450:ALA:HB3	2.02	0.41
1:Y:14:THR:N	5:Y:647:HOH:O	2.37	0.41
1:Y:30:VAL:HG12	1:Y:31:SER:N	2.36	0.41
1:Y:70:SER:H	1:Y:73:GLN:NE2	2.19	0.41
1:Z:269:CYS:CB	1:Z:306:VAL:HB	2.50	0.41
1:Z:271:MET:HE3	1:Z:391:VAL:CG2	2.51	0.41
1:Z:340:ASN:HD22	1:Z:371:VAL:CG2	2.34	0.41
1:X:9:LEU:HD12	1:X:9:LEU:HA	1.47	0.41
1:X:83:ARG:NH1	1:X:83:ARG:CG	2.84	0.41
1:X:156:ARG:O	1:X:212:GLU:HG2	2.20	0.41
1:X:222:GLU:CG	1:X:223:VAL:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:257:LYS:O	1:X:260:MET:HB2	2.20	0.41
1:X:316:LEU:HA	1:X:320:MET:HB2	2.02	0.41
1:X:467:GLU:O	1:X:468:ARG:HB2	2.20	0.41
1:O:173:MET:O	1:O:227:THR:CG2	2.69	0.41
1:Y:89:TRP:HB2	1:Y:95:LYS:O	2.21	0.41
1:Z:44:TRP:HA	1:Z:105:CYS:HG	1.85	0.41
1:Z:121:GLU:CG	1:Z:125:ARG:CD	2.99	0.41
1:Z:349:THR:HG22	5:Z:645:HOH:O	2.20	0.41
1:Z:380:THR:O	1:Z:383:SER:OG	2.29	0.41
1:Z:491:LYS:HA	1:Z:494:MET:HG3	2.03	0.41
1:X:80:THR:HA	1:X:243:ALA:O	2.20	0.41
1:X:377:ILE:O	1:X:380:THR:HB	2.20	0.41
1:X:441:LEU:HD23	1:X:441:LEU:HA	1.92	0.41
1:O:114:HIS:O	1:O:117:ARG:HB3	2.21	0.41
1:O:173:MET:HB3	1:O:227:THR:HG21	2.03	0.41
1:O:237:ILE:CG2	1:O:238:PRO:N	2.84	0.41
1:O:278:LYS:HG2	1:O:280:VAL:HG22	2.03	0.41
1:O:316:LEU:HA	1:O:316:LEU:HD23	1.82	0.41
1:Y:6:ILE:HD13	1:Y:448:GLY:CA	2.51	0.41
1:Y:80:THR:CA	1:Y:81:ASN:HD22	2.34	0.41
1:Y:230:GLY:HA2	1:Z:228:ASN:ND2	2.36	0.41
1:Y:424:ASP:CB	1:Y:474:ILE:CG2	2.98	0.41
1:Z:81:ASN:N	1:Z:81:ASN:ND2	2.69	0.41
1:Z:172:LYS:HA	1:Z:172:LYS:HD2	1.92	0.41
1:Z:191:LEU:HD23	1:Z:191:LEU:HA	1.60	0.41
1:Z:473:GLY:O	1:Z:475:GLU:N	2.54	0.41
1:X:60:LEU:O	1:X:60:LEU:HD12	2.19	0.41
1:X:103:TRP:HA	1:X:140:LYS:NZ	2.35	0.41
1:X:174:THR:HB	1:X:177:ARG:NH1	2.35	0.41
1:X:320:MET:HE3	1:X:320:MET:CA	2.50	0.41
1:X:474:ILE:HG23	1:X:475:GLU:N	2.36	0.41
1:O:428:THR:HG22	1:O:429:ARG:O	2.21	0.41
1:Y:133:ASP:CG	1:Y:134:PRO:HD2	2.42	0.41
1:Z:392:LEU:C	1:Z:392:LEU:HD23	2.41	0.41
1:Z:403:LEU:N	1:Z:403:LEU:HD12	2.36	0.41
1:Z:406:LEU:CD1	1:Z:408:VAL:CG1	2.99	0.41
1:X:17:ARG:HH11	1:X:17:ARG:HD3	1.77	0.41
1:X:224:TYR:CE2	1:X:242:ILE:HG13	2.56	0.41
1:X:429:ARG:HA	1:X:470:PHE:O	2.21	0.41
1:O:130:LEU:HD13	1:O:136:PHE:CD2	2.56	0.40
1:O:178:VAL:CG1	1:O:179:HIS:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:308:MET:SD	1:O:311:ALA:HB3	2.61	0.40
1:O:326:ALA:O	1:O:329:SER:OG	2.27	0.40
1:O:435:VAL:HG22	1:O:436:ARG:N	2.33	0.40
1:O:451:VAL:HG12	1:O:451:VAL:O	2.20	0.40
1:X:41:LYS:CB	1:X:42:PRO:HD2	2.50	0.40
1:X:193:ASN:OD1	1:X:194:ILE:N	2.55	0.40
1:O:108:THR:CB	1:O:139:THR:HB	2.51	0.40
1:O:123:TYR:CD2	1:O:203:MET:HE1	2.56	0.40
1:O:194:ILE:HG13	1:O:195:HIS:CE1	2.55	0.40
1:O:237:ILE:HA	1:O:238:PRO:HD2	1.76	0.40
1:O:434:GLU:HA	1:O:467:GLU:CB	2.51	0.40
1:Y:175:GLN:HE21	1:Y:175:GLN:HB3	1.44	0.40
1:Y:220:SER:O	1:Y:224:TYR:OH	2.39	0.40
1:Y:260:MET:O	1:Y:274:ASN:N	2.46	0.40
1:Z:110:GLU:O	1:Z:113:GLU:N	2.54	0.40
1:Z:120:LEU:HD11	1:Z:206:VAL:HG21	2.03	0.40
1:Z:183:TYR:CD1	1:Z:217:VAL:HG11	2.56	0.40
1:Z:275:THR:HG21	1:Z:280:VAL:HG23	2.02	0.40
1:X:265:TYR:HD2	1:X:413:VAL:CG1	2.35	0.40
1:O:22:ASP:HB2	5:O:640:HOH:O	2.21	0.40
1:O:83:ARG:HH12	1:O:188:ARG:NH1	2.19	0.40
1:O:165:VAL:O	1:O:168:TRP:N	2.54	0.40
1:O:202:LYS:HD3	1:O:202:LYS:HA	1.67	0.40
1:O:279:ALA:HA	5:O:611:HOH:O	2.19	0.40
1:O:282:SER:HB3	1:O:286:LEU:O	2.21	0.40
1:O:373:ALA:O	1:O:376:ILE:HB	2.21	0.40
1:Y:43:GLY:C	1:Y:44:TRP:HD1	2.24	0.40
1:Y:424:ASP:O	1:Y:479:ARG:NH1	2.55	0.40
1:Y:438:VAL:HA	1:Y:441:LEU:HB2	2.04	0.40
1:Z:30:VAL:CG1	1:Z:31:SER:N	2.81	0.40
1:Z:41:LYS:HB2	1:Z:42:PRO:CD	2.52	0.40
1:Z:44:TRP:CZ2	1:Z:107:ARG:HB2	2.56	0.40
1:Z:311:ALA:O	1:Z:314:GLN:HB3	2.21	0.40
1:Z:474:ILE:C	1:Z:476:THR:N	2.71	0.40
1:X:177:ARG:NH1	1:X:177:ARG:HB2	2.36	0.40
1:Y:295:THR:N	1:Y:297:GLU:OE1	2.47	0.40
1:Y:409:ASP:CB	1:Y:438:VAL:HG21	2.51	0.40
1:Z:20:VAL:HG23	1:Z:63:VAL:HG11	2.03	0.40
1:Z:45:VAL:H	1:Z:105:CYS:HB2	1.87	0.40
1:Z:130:LEU:HD21	5:Z:627:HOH:O	2.21	0.40
1:Z:406:LEU:HD13	1:Z:408:VAL:CG1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:487:LYS:HA	1:Z:487:LYS:HD2	1.93	0.40
1:X:28:ILE:O	1:X:29:SER:HB2	2.22	0.40
1:X:236:ARG:HD2	1:X:236:ARG:HA	1.82	0.40
1:X:237:ILE:HA	1:X:238:PRO:HD3	1.75	0.40
1:X:250:LEU:O	1:X:253:GLN:HB3	2.21	0.40
1:O:91:LYS:CB	1:O:161:LEU:CD1	2.99	0.40
1:O:218:ARG:NE	1:O:222:GLU:OE2	2.53	0.40
1:O:441:LEU:HA	1:O:441:LEU:HD23	1.81	0.40
1:Y:6:ILE:HD11	1:Y:448:GLY:N	2.37	0.40
1:Y:271:MET:SD	1:Y:395:MET:CE	3.10	0.40
1:Z:83:ARG:NH2	1:Z:303:GLU:OE1	2.55	0.40
1:Z:256:VAL:CG1	1:Z:294:PRO:HG3	2.45	0.40
1:Z:426:LEU:HD12	1:Z:426:LEU:HA	1.97	0.40
1:X:466:ILE:HD12	1:X:466:ILE:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	496/501 (99%)	409 (82%)	65 (13%)	22 (4%)	2	3
1	X	496/501 (99%)	411 (83%)	69 (14%)	16 (3%)	4	5
1	Y	497/501 (99%)	414 (83%)	60 (12%)	23 (5%)	2	2
1	Z	496/501 (99%)	425 (86%)	52 (10%)	19 (4%)	3	4
All	All	1985/2004 (99%)	1659 (84%)	246 (12%)	80 (4%)	3	3

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	149	GLU

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Mol	Chain	Res	Type
1	O	159	GLU
1	O	203	MET
1	O	204	LEU
1	O	233	GLY
1	O	458	ASP
1	O	476	THR
1	O	477	THR
1	Y	149	GLU
1	Y	212	GLU
1	Y	232	LYS
1	Y	233	GLY
1	Y	333	ALA
1	Z	121	GLU
1	Z	149	GLU
1	Z	329	SER
1	X	149	GLU
1	X	233	GLY
1	X	424	ASP
1	X	425	ILE
1	X	461	GLN
1	O	92	GLU
1	O	105	CYS
1	O	120	LEU
1	O	215	PRO
1	O	463	LYS
1	O	479	ARG
1	Y	92	GLU
1	Y	138	GLY
1	Y	157	ARG
1	Y	252	GLY
1	Y	329	SER
1	Y	397	ALA
1	Y	448	GLY
1	Y	461	GLN
1	Z	138	GLY
1	Z	475	GLU
1	Z	495	ALA
1	Z	496	TRP
1	X	197	LEU
1	X	215	PRO
1	X	450	ALA
1	X	458	ASP

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Mol	Chain	Res	Type
1	O	3	LYS
1	O	57	SER
1	O	58	SER
1	O	464	ALA
1	Y	76	ALA
1	Y	107	ARG
1	Y	222	GLU
1	Y	441	LEU
1	Z	122	ASP
1	Z	405	ALA
1	X	71	SER
1	X	397	ALA
1	O	121	GLU
1	O	184	THR
1	Y	53	TRP
1	Y	105	CYS
1	Z	474	ILE
1	X	199	TRP
1	X	457	LEU
1	X	473	GLY
1	Y	42	PRO
1	Y	57	SER
1	Y	451	VAL
1	Z	175	GLN
1	Z	190	MET
1	Z	215	PRO
1	Z	298	VAL
1	Z	464	ALA
1	Z	465	VAL
1	X	138	GLY
1	X	331	TYR
1	O	336	VAL
1	O	446	LEU
1	Z	25	ALA
1	Z	184	THR
1	Z	206	VAL
1	Y	215	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	406/412 (98%)	294 (72%)	112 (28%)	0	1
1	X	405/412 (98%)	295 (73%)	110 (27%)	0	1
1	Y	405/412 (98%)	305 (75%)	100 (25%)	0	1
1	Z	405/412 (98%)	303 (75%)	102 (25%)	0	1
All	All	1621/1648 (98%)	1197 (74%)	424 (26%)	0	1

All (424) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	13	THR
1	O	17	ARG
1	O	21	MET
1	O	32	GLN
1	O	33	ARG
1	O	41	LYS
1	O	47	HIS
1	O	56	GLN
1	O	57	SER
1	O	58	SER
1	O	59	THR
1	O	61	VAL
1	O	63	VAL
1	O	66	LYS
1	O	69	ILE
1	O	73	GLN
1	O	80	THR
1	O	81	ASN
1	O	82	GLN
1	O	87	ILE
1	O	89	TRP
1	O	95	LYS
1	O	106	ARG
1	O	107	ARG
1	O	115	LEU
1	O	117	ARG
1	O	125	ARG
1	O	128	THR

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Mol	Chain	Res	Type
1	O	131	VAL
1	O	135	TYR
1	O	137	SER
1	O	139	THR
1	O	146	ASP
1	O	147	HIS
1	O	148	VAL
1	O	149	GLU
1	O	152	ARG
1	O	153	GLU
1	O	156	ARG
1	O	162	PHE
1	O	164	THR
1	O	169	LEU
1	O	172	LYS
1	O	173	MET
1	O	180	VAL
1	O	190	MET
1	O	196	THR
1	O	197	LEU
1	O	198	ASP
1	O	202	LYS
1	O	204	LEU
1	O	206	VAL
1	O	212	GLU
1	O	214	LEU
1	O	219	ARG
1	O	227	THR
1	O	229	ILE
1	O	235	THR
1	O	236	ARG
1	O	240	SER
1	O	253	GLN
1	O	254	LEU
1	O	256	VAL
1	O	262	LYS
1	O	264	THR
1	O	269	CYS
1	O	277	GLU
1	O	278	LYS
1	O	287	LEU
1	O	290	ILE

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Mol	Chain	Res	Type
1	O	295	THR
1	O	297	GLU
1	O	313	ILE
1	O	314	GLN
1	O	320	MET
1	O	321	LYS
1	O	349	THR
1	O	351	LEU
1	O	364	ILE
1	O	368	THR
1	O	376	ILE
1	O	395	MET
1	O	396	GLN
1	O	401	ILE
1	O	402	ARG
1	O	406	LEU
1	O	408	VAL
1	O	409	ASP
1	O	415	ASN
1	O	418	LEU
1	O	423	SER
1	O	425	ILE
1	O	426	LEU
1	O	428	THR
1	O	430	VAL
1	O	436	ARG
1	O	438	VAL
1	O	449	LEU
1	O	455	GLN
1	O	456	ASN
1	O	458	ASP
1	O	460	LEU
1	O	462	GLU
1	O	463	LYS
1	O	466	ILE
1	O	468	ARG
1	O	469	GLU
1	O	471	ARG
1	O	476	THR
1	O	477	THR
1	O	479	ARG
1	O	488	LYS

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Mol	Chain	Res	Type
1	Y	6	ILE
1	Y	9	LEU
1	Y	11	GLN
1	Y	17	ARG
1	Y	29	SER
1	Y	51	GLU
1	Y	52	ILE
1	Y	58	SER
1	Y	62	GLU
1	Y	63	VAL
1	Y	66	LYS
1	Y	71	SER
1	Y	77	ILE
1	Y	81	ASN
1	Y	83	ARG
1	Y	87	ILE
1	Y	91	LYS
1	Y	92	GLU
1	Y	97	ILE
1	Y	107	ARG
1	Y	115	LEU
1	Y	121	GLU
1	Y	124	ILE
1	Y	125	ARG
1	Y	128	THR
1	Y	131	VAL
1	Y	137	SER
1	Y	145	LEU
1	Y	149	GLU
1	Y	151	SER
1	Y	170	ILE
1	Y	171	TRP
1	Y	172	LYS
1	Y	173	MET
1	Y	175	GLN
1	Y	178	VAL
1	Y	180	VAL
1	Y	182	ASP
1	Y	188	ARG
1	Y	194	ILE
1	Y	196	THR
1	Y	202	LYS

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Mol	Chain	Res	Type
1	Y	203	MET
1	Y	206	VAL
1	Y	212	GLU
1	Y	214	LEU
1	Y	215	PRO
1	Y	218	ARG
1	Y	219	ARG
1	Y	220	SER
1	Y	222	GLU
1	Y	224	TYR
1	Y	229	ILE
1	Y	237	ILE
1	Y	240	SER
1	Y	256	VAL
1	Y	262	LYS
1	Y	269	CYS
1	Y	278	LYS
1	Y	281	LYS
1	Y	282	SER
1	Y	287	LEU
1	Y	289	THR
1	Y	295	THR
1	Y	298	VAL
1	Y	319	GLU
1	Y	321	LYS
1	Y	337	GLN
1	Y	338	ASN
1	Y	349	THR
1	Y	351	LEU
1	Y	392	LEU
1	Y	395	MET
1	Y	396	GLN
1	Y	402	ARG
1	Y	403	LEU
1	Y	406	LEU
1	Y	415	ASN
1	Y	425	ILE
1	Y	426	LEU
1	Y	436	ARG
1	Y	439	THR
1	Y	441	LEU
1	Y	446	LEU

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Mol	Chain	Res	Type
1	Y	449	LEU
1	Y	456	ASN
1	Y	461	GLN
1	Y	462	GLU
1	Y	465	VAL
1	Y	466	ILE
1	Y	468	ARG
1	Y	470	PHE
1	Y	471	ARG
1	Y	474	ILE
1	Y	475	GLU
1	Y	476	THR
1	Y	478	GLU
1	Y	479	ARG
1	Y	487	LYS
1	Y	488	LYS
1	Z	6	ILE
1	Z	9	LEU
1	Z	11	GLN
1	Z	17	ARG
1	Z	21	MET
1	Z	24	ASP
1	Z	28	ILE
1	Z	30	VAL
1	Z	33	ARG
1	Z	39	TYR
1	Z	41	LYS
1	Z	51	GLU
1	Z	52	ILE
1	Z	57	SER
1	Z	58	SER
1	Z	62	GLU
1	Z	63	VAL
1	Z	70	SER
1	Z	72	ASP
1	Z	73	GLN
1	Z	80	THR
1	Z	82	GLN
1	Z	83	ARG
1	Z	92	GLU
1	Z	95	LYS
1	Z	107	ARG

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Mol	Chain	Res	Type
1	Z	112	CYS
1	Z	113	GLU
1	Z	122	ASP
1	Z	124	ILE
1	Z	131	VAL
1	Z	136	PHE
1	Z	140	LYS
1	Z	145	LEU
1	Z	146	ASP
1	Z	153	GLU
1	Z	166	ASP
1	Z	170	ILE
1	Z	175	GLN
1	Z	178	VAL
1	Z	180	VAL
1	Z	181	THR
1	Z	182	ASP
1	Z	196	THR
1	Z	197	LEU
1	Z	198	ASP
1	Z	201	ASP
1	Z	203	MET
1	Z	205	GLU
1	Z	206	VAL
1	Z	212	GLU
1	Z	214	LEU
1	Z	226	GLN
1	Z	227	THR
1	Z	229	ILE
1	Z	235	THR
1	Z	236	ARG
1	Z	237	ILE
1	Z	240	SER
1	Z	254	LEU
1	Z	256	VAL
1	Z	258	GLU
1	Z	262	LYS
1	Z	265	TYR
1	Z	269	CYS
1	Z	297	GLU
1	Z	319	GLU
1	Z	320	MET

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Mol	Chain	Res	Type
1	Z	321	LYS
1	Z	322	LEU
1	Z	335	LYS
1	Z	337	GLN
1	Z	349	THR
1	Z	351	LEU
1	Z	364	ILE
1	Z	368	THR
1	Z	402	ARG
1	Z	406	LEU
1	Z	415	ASN
1	Z	416	ASN
1	Z	418	LEU
1	Z	426	LEU
1	Z	428	THR
1	Z	432	ARG
1	Z	436	ARG
1	Z	441	LEU
1	Z	455	GLN
1	Z	458	ASP
1	Z	459	GLU
1	Z	460	LEU
1	Z	465	VAL
1	Z	468	ARG
1	Z	471	ARG
1	Z	474	ILE
1	Z	476	THR
1	Z	478	GLU
1	Z	479	ARG
1	Z	480	ASN
1	Z	490	VAL
1	Z	491	LYS
1	Z	492	ARG
1	Z	500	ASP
1	X	3	LYS
1	X	4	LYS
1	X	9	LEU
1	X	14	THR
1	X	17	ARG
1	X	28	ILE
1	X	33	ARG
1	X	41	LYS

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Mol	Chain	Res	Type
1	X	45	VAL
1	X	47	HIS
1	X	50	MET
1	X	52	ILE
1	X	57	SER
1	X	58	SER
1	X	60	LEU
1	X	66	LYS
1	X	71	SER
1	X	72	ASP
1	X	73	GLN
1	X	80	THR
1	X	81	ASN
1	X	82	GLN
1	X	83	ARG
1	X	87	ILE
1	X	95	LYS
1	X	107	ARG
1	X	111	ILE
1	X	116	LYS
1	X	121	GLU
1	X	125	ARG
1	X	137	SER
1	X	145	LEU
1	X	152	ARG
1	X	164	THR
1	X	169	LEU
1	X	173	MET
1	X	175	GLN
1	X	178	VAL
1	X	180	VAL
1	X	181	THR
1	X	187	SER
1	X	188	ARG
1	X	190	MET
1	X	196	THR
1	X	198	ASP
1	X	204	LEU
1	X	211	ARG
1	X	213	MET
1	X	214	LEU
1	X	219	ARG

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Mol	Chain	Res	Type
1	X	223	VAL
1	X	226	GLN
1	X	235	THR
1	X	236	ARG
1	X	237	ILE
1	X	240	SER
1	X	245	ASP
1	X	254	LEU
1	X	256	VAL
1	X	257	LYS
1	X	262	LYS
1	X	263	ASN
1	X	269	CYS
1	X	275	THR
1	X	277	GLU
1	X	278	LYS
1	X	280	VAL
1	X	281	LYS
1	X	283	GLU
1	X	297	GLU
1	X	298	VAL
1	X	303	GLU
1	X	308	MET
1	X	319	GLU
1	X	321	LYS
1	X	322	LEU
1	X	325	ASP
1	X	338	ASN
1	X	339	THR
1	X	348	PHE
1	X	349	THR
1	X	351	LEU
1	X	364	ILE
1	X	388	THR
1	X	395	MET
1	X	401	ILE
1	X	406	LEU
1	X	415	ASN
1	X	418	LEU
1	X	426	LEU
1	X	429	ARG
1	X	436	ARG

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Mol	Chain	Res	Type
1	X	438	VAL
1	X	446	LEU
1	X	451	VAL
1	X	456	ASN
1	X	460	LEU
1	X	462	GLU
1	X	466	ILE
1	X	469	GLU
1	X	471	ARG
1	X	474	ILE
1	X	475	GLU
1	X	476	THR
1	X	477	THR
1	X	479	ARG
1	X	482	ARG
1	X	492	ARG
1	X	494	MET
1	X	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	11	GLN
1	O	23	HIS
1	O	56	GLN
1	O	73	GLN
1	O	81	ASN
1	O	82	GLN
1	O	185	ASN
1	O	253	GLN
1	O	340	ASN
1	O	374	ASN
1	O	387	GLN
1	O	415	ASN
1	O	456	ASN
1	O	461	GLN
1	Y	23	HIS
1	Y	47	HIS
1	Y	73	GLN
1	Y	81	ASN
1	Y	175	GLN
1	Y	179	HIS

Continued from previous page...

Mol	Chain	Res	Type
1	Y	195	HIS
1	Y	226	GLN
1	Y	253	GLN
1	Y	299	ASN
1	Y	314	GLN
1	Y	337	GLN
1	Y	338	ASN
1	Y	387	GLN
1	Y	415	ASN
1	Y	422	GLN
1	Y	456	ASN
1	Y	461	GLN
1	Y	499	HIS
1	Z	73	GLN
1	Z	175	GLN
1	Z	226	GLN
1	Z	337	GLN
1	Z	340	ASN
1	Z	396	GLN
1	Z	415	ASN
1	Z	422	GLN
1	Z	455	GLN
1	Z	456	ASN
1	Z	480	ASN
1	X	23	HIS
1	X	73	GLN
1	X	81	ASN
1	X	127	ASN
1	X	175	GLN
1	X	185	ASN
1	X	195	HIS
1	X	226	GLN
1	X	263	ASN
1	X	299	ASN
1	X	337	GLN
1	X	415	ASN
1	X	420	GLN
1	X	422	GLN
1	X	456	ASN
1	X	499	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	PO4	Y	602	-	4,4,4	2.76	3 (75%)	6,6,6	0.86	0
3	ADP	Y	608	-	24,29,29	1.17	2 (8%)	29,45,45	2.58	9 (31%)
2	PO4	O	601	-	4,4,4	2.07	1 (25%)	6,6,6	1.07	0
4	GOL	Y	604	-	5,5,5	0.69	0	5,5,5	0.49	0
3	ADP	X	610	-	24,29,29	1.35	3 (12%)	29,45,45	2.82	6 (20%)
4	GOL	X	606	-	5,5,5	0.62	0	5,5,5	0.74	0
4	GOL	O	603	-	5,5,5	0.61	0	5,5,5	0.25	0
3	ADP	Z	609	-	24,29,29	0.86	0	29,45,45	2.27	7 (24%)
3	ADP	O	607	-	24,29,29	1.43	2 (8%)	29,45,45	3.20	8 (27%)
4	GOL	Z	605	-	5,5,5	0.52	0	5,5,5	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	Y	608	-	-	8/12/32/32	0/3/3/3
4	GOL	Y	604	-	-	0/4/4/4	-
3	ADP	X	610	-	-	8/12/32/32	0/3/3/3
4	GOL	X	606	-	-	2/4/4/4	-
4	GOL	O	603	-	-	2/4/4/4	-
3	ADP	Z	609	-	-	2/12/32/32	0/3/3/3
3	ADP	O	607	-	1/1/6/6	0/12/32/32	0/3/3/3
4	GOL	Z	605	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	607	ADP	O2'-C2'	4.17	1.52	1.43
3	O	607	ADP	C2'-C1'	-4.02	1.47	1.53
3	X	610	ADP	C2-N3	3.65	1.38	1.32
2	O	601	PO4	P-O4	-3.48	1.44	1.54
2	Y	602	PO4	P-O2	3.34	1.64	1.54
3	Y	608	ADP	O4'-C1'	3.18	1.45	1.41
2	Y	602	PO4	P-O3	3.04	1.63	1.54
2	Y	602	PO4	P-O4	-3.04	1.45	1.54
3	X	610	ADP	C2-N1	2.93	1.39	1.33
3	X	610	ADP	PB-O2B	-2.31	1.45	1.54
3	Y	608	ADP	C2-N3	2.29	1.35	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	607	ADP	C1'-N9-C4	-12.88	104.00	126.64
3	X	610	ADP	C1'-N9-C4	-9.87	109.31	126.64
3	Y	608	ADP	C1'-N9-C4	-9.79	109.44	126.64
3	X	610	ADP	O2'-C2'-C3'	8.09	138.00	111.82
3	Z	609	ADP	C1'-N9-C4	7.85	140.43	126.64
3	O	607	ADP	O2'-C2'-C1'	7.36	138.02	110.85
3	X	610	ADP	PA-O3A-PB	-5.65	113.44	132.83
3	Y	608	ADP	PA-O3A-PB	-4.75	116.54	132.83
3	Z	609	ADP	O2'-C2'-C3'	4.66	126.89	111.82
3	Z	609	ADP	O2'-C2'-C1'	-4.32	94.90	110.85
3	O	607	ADP	PA-O3A-PB	-3.97	119.22	132.83
3	Y	608	ADP	O2'-C2'-C3'	-3.94	99.06	111.82
3	Z	609	ADP	PA-O3A-PB	-3.78	119.85	132.83
3	O	607	ADP	C5-C6-N6	3.36	125.46	120.35
3	O	607	ADP	O4'-C1'-C2'	3.29	111.73	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	608	ADP	C3'-C2'-C1'	3.09	105.62	100.98
3	O	607	ADP	C3'-C2'-C1'	3.05	105.56	100.98
3	X	610	ADP	O2'-C2'-C1'	-2.77	100.61	110.85
3	Z	609	ADP	O2B-PB-O3A	2.75	113.87	104.64
3	Y	608	ADP	C5-C6-N6	2.58	124.28	120.35
3	O	607	ADP	O2B-PB-O3A	2.45	112.86	104.64
3	O	607	ADP	O4'-C4'-C3'	2.36	109.78	105.11
3	Z	609	ADP	O5'-PA-O1A	-2.31	100.06	109.07
3	X	610	ADP	C3'-C2'-C1'	2.30	104.44	100.98
3	Y	608	ADP	C4-C5-N7	2.26	111.75	109.40
3	Y	608	ADP	O2B-PB-O3A	2.25	112.18	104.64
3	X	610	ADP	C2-N1-C6	-2.19	115.02	118.75
3	Y	608	ADP	C2'-C3'-C4'	2.17	106.85	102.64
3	Z	609	ADP	O3B-PB-O3A	2.04	111.49	104.64
3	Y	608	ADP	O2'-C2'-C1'	2.04	118.39	110.85

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	O	607	ADP	C2'

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	608	ADP	PA-O3A-PB-O2B
3	Y	608	ADP	C5'-O5'-PA-O1A
3	Y	608	ADP	C5'-O5'-PA-O2A
3	Y	608	ADP	C3'-C4'-C5'-O5'
3	X	610	ADP	PA-O3A-PB-O2B
3	X	610	ADP	C5'-O5'-PA-O3A
3	X	610	ADP	O4'-C4'-C5'-O5'
4	O	603	GOL	O1-C1-C2-C3
4	Z	605	GOL	O1-C1-C2-C3
4	X	606	GOL	O1-C1-C2-C3
3	X	610	ADP	C3'-C4'-C5'-O5'
4	O	603	GOL	O1-C1-C2-O2
4	Z	605	GOL	O1-C1-C2-O2
3	Y	608	ADP	O4'-C4'-C5'-O5'
3	X	610	ADP	PB-O3A-PA-O1A
4	X	606	GOL	O1-C1-C2-O2
3	Y	608	ADP	PB-O3A-PA-O2A
3	X	610	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	Y	608	ADP	PB-O3A-PA-O1A
3	Y	608	ADP	PA-O3A-PB-O3B
3	X	610	ADP	PA-O3A-PB-O3B
3	Z	609	ADP	PB-O3A-PA-O1A
3	X	610	ADP	PB-O3A-PA-O2A
3	Z	609	ADP	C5'-O5'-PA-O1A
4	Z	605	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	602	PO4	1	0
2	O	601	PO4	2	0
4	Y	604	GOL	3	0
3	X	610	ADP	1	0
4	X	606	GOL	2	0
4	O	603	GOL	2	0
3	O	607	ADP	1	0
4	Z	605	GOL	9	0

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

Ligand ADP Y 608

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP X 610

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP Z 609

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP O 607

Bond lengths

Bond angles

Torsions

Rings
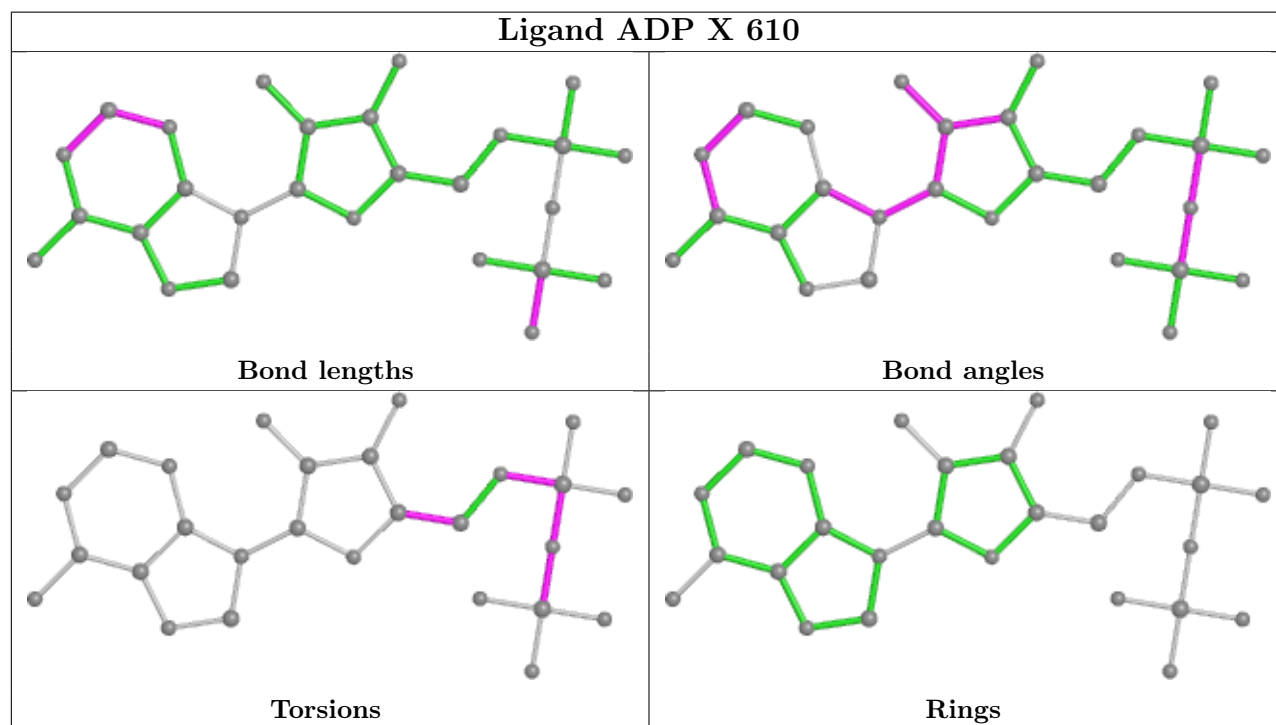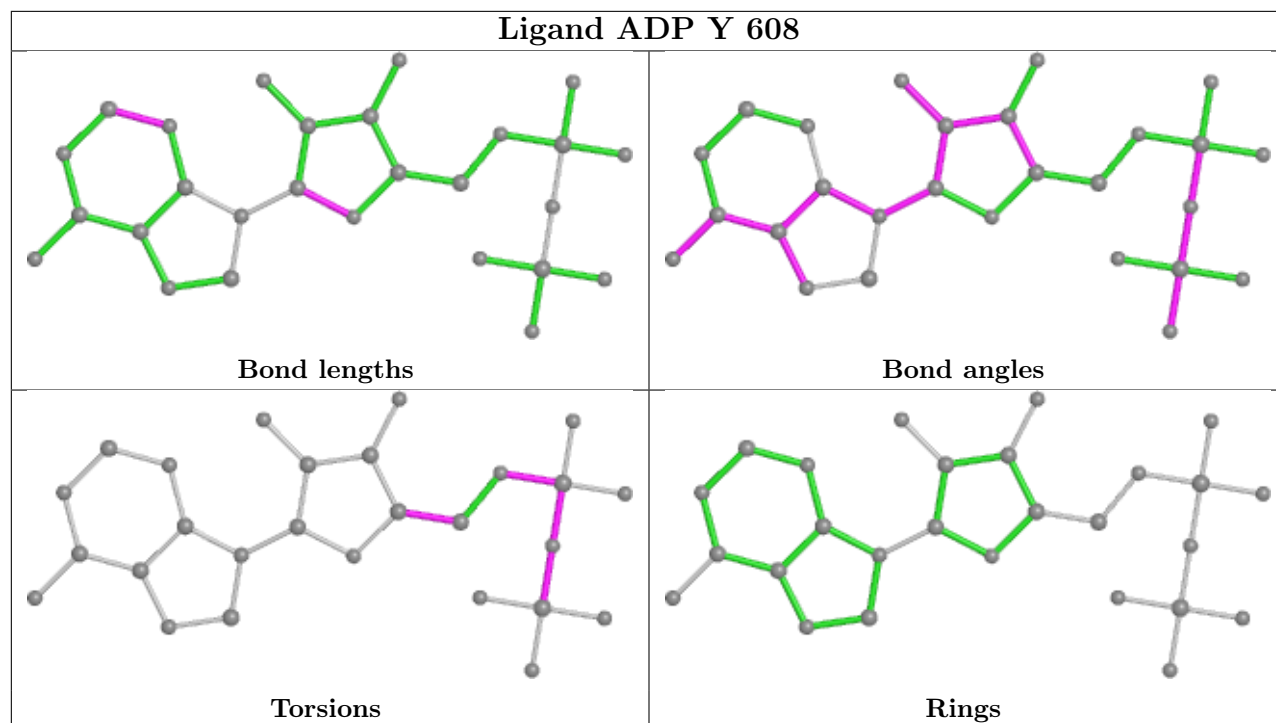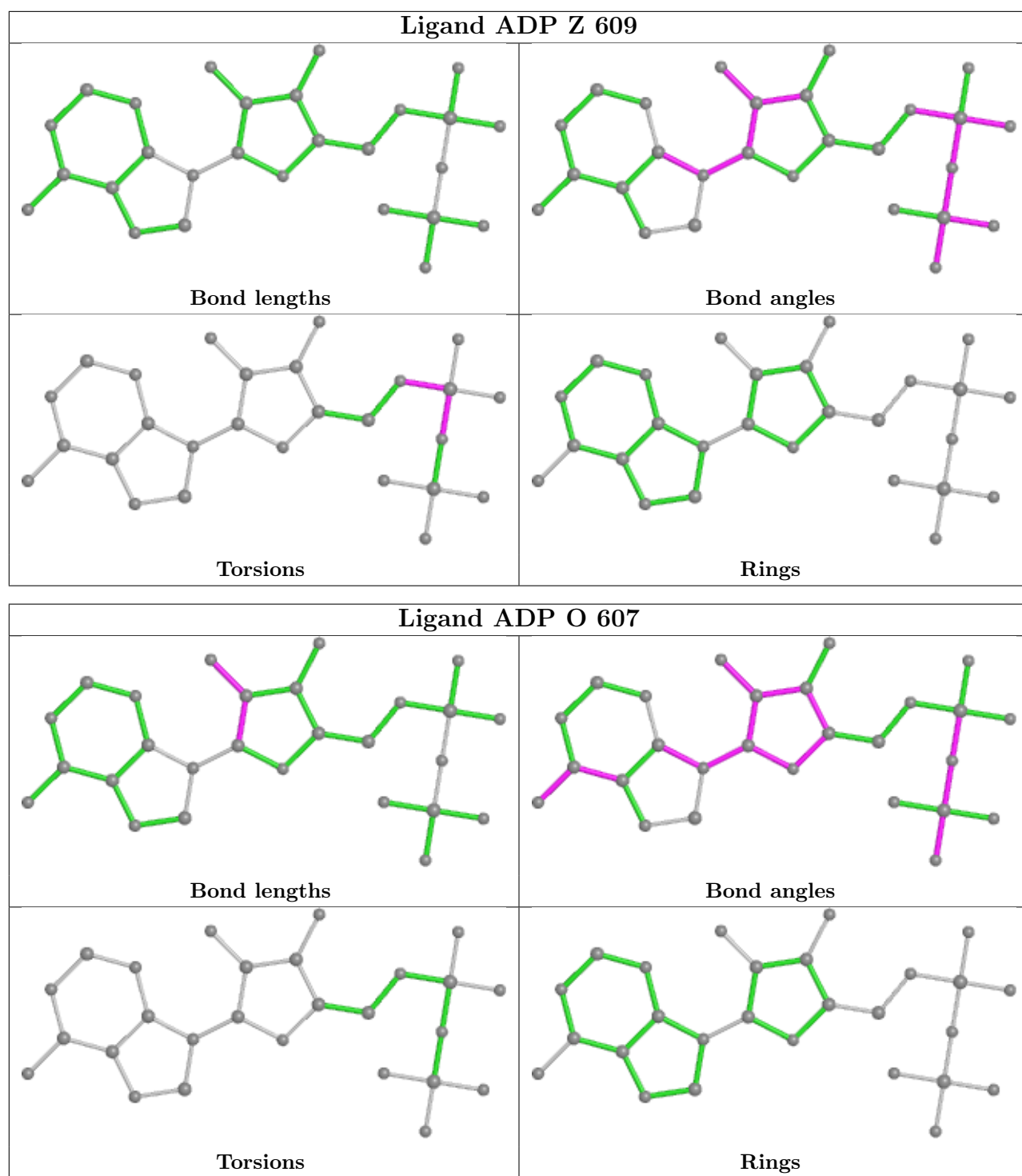
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	O	498/501 (99%)	-0.90	1 (0%)	95	95	7, 28, 61, 75	0
1	X	498/501 (99%)	-0.92	1 (0%)	95	95	7, 27, 60, 75	0
1	Y	499/501 (99%)	-0.91	1 (0%)	95	95	6, 27, 59, 73	0
1	Z	498/501 (99%)	-1.01	3 (0%)	89	88	6, 24, 58, 75	0
All	All	1993/2004 (99%)	-0.94	6 (0%)	94	93	6, 26, 60, 75	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	500	ASP	3.1
1	O	477	THR	2.9
1	Y	475	GLU	2.7
1	Z	473	GLY	2.6
1	X	500	ASP	2.2
1	Z	475	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	PO4	Y	602	5/5	0.97	0.12	29,31,53,75	0
4	GOL	O	603	6/6	0.97	0.12	5,7,49,55	0
3	ADP	Y	608	27/27	0.98	0.08	5,27,75,75	0
3	ADP	Z	609	27/27	0.98	0.09	5,26,57,75	0
3	ADP	X	610	27/27	0.98	0.10	5,49,75,75	0
3	ADP	O	607	27/27	0.98	0.09	5,39,75,75	0
4	GOL	X	606	6/6	0.98	0.10	5,18,38,43	0
4	GOL	Y	604	6/6	0.99	0.13	5,19,42,48	0
4	GOL	Z	605	6/6	0.99	0.08	5,10,25,51	0
2	PO4	O	601	5/5	0.99	0.09	5,31,56,59	0

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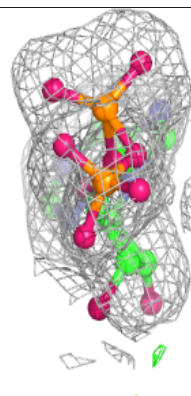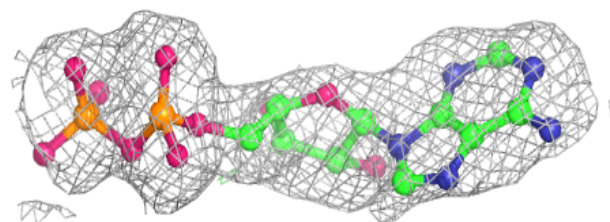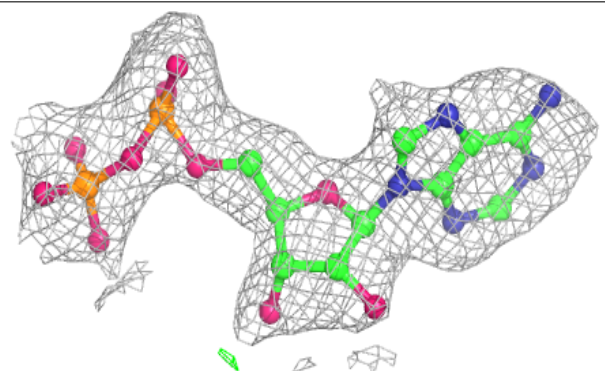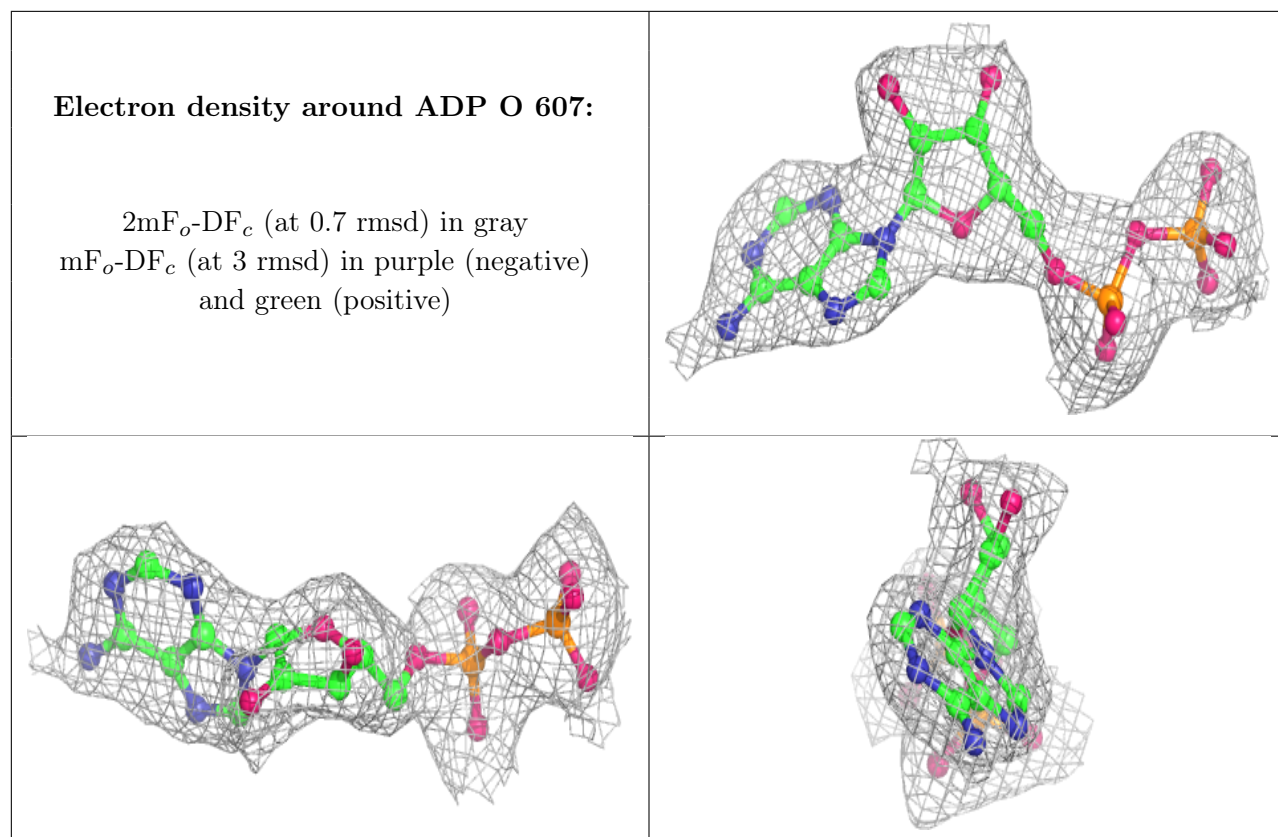

Electron density around ADP Y 608:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
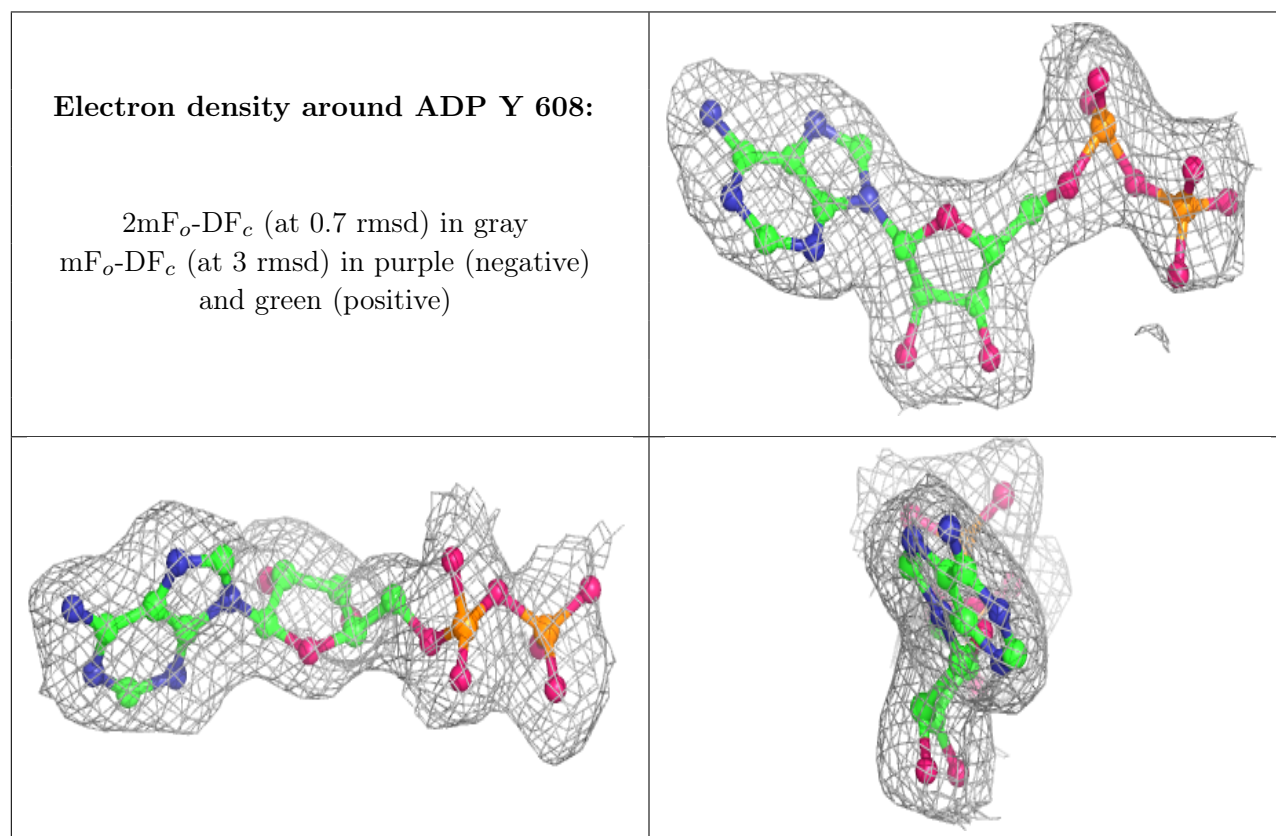
Electron density around ADP Z 609:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
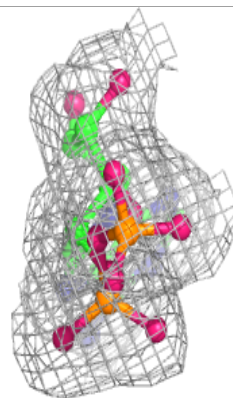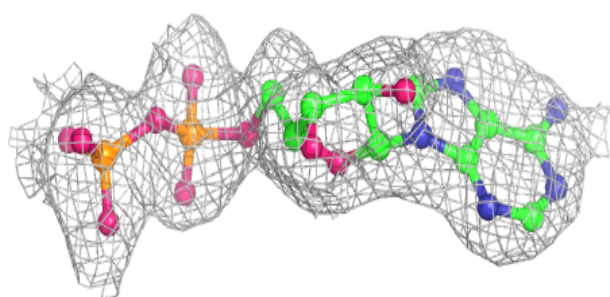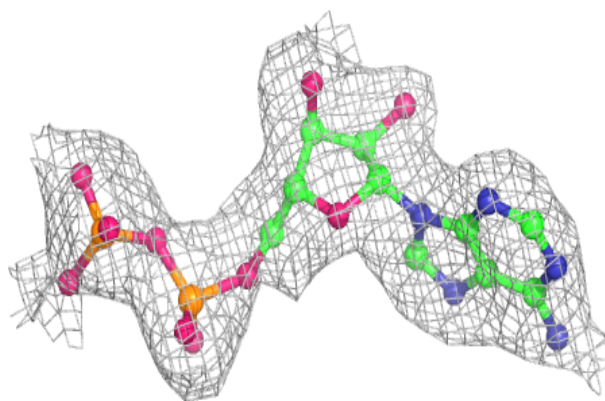
Electron density around ADP X 610:

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

Electron density around ADP O 607:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.