Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:54 AM GMT

PDB ID	:	3GG5
Title	:	Replacement of Val3 in Human Thymidylate Synthase Affects Its Kinetic Properties and Intracellular Stability
Authors	:	Huang, X.; Gibson, L.M.; Bell, B.J.; Lovelace, L.L.; Lebioda, L.
Deposited on	:	2009-02-27
Resolution	:	2.77 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

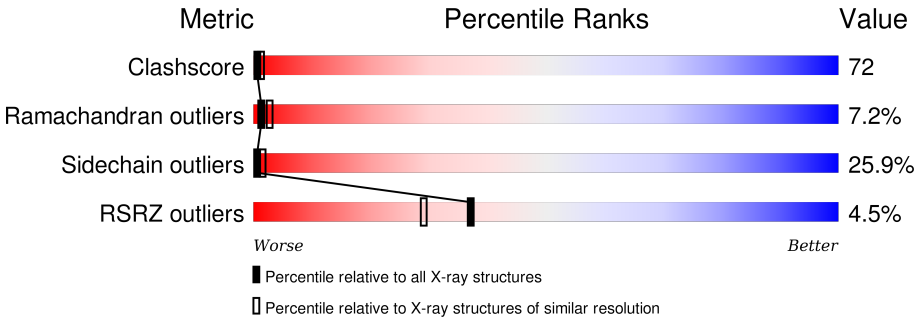
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	313	2% 15% 35% 28% 13% 10%
1	B	313	6% 15% 31% 34% 9% 10%
1	C	313	3% 15% 37% 25% 13% 10%
1	D	313	6% 11% 35% 33% 12% 10%

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	SO4	A	616	-	X	-	-
3	PO4	B	616	-	-	X	-
3	PO4	D	616	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9174 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.

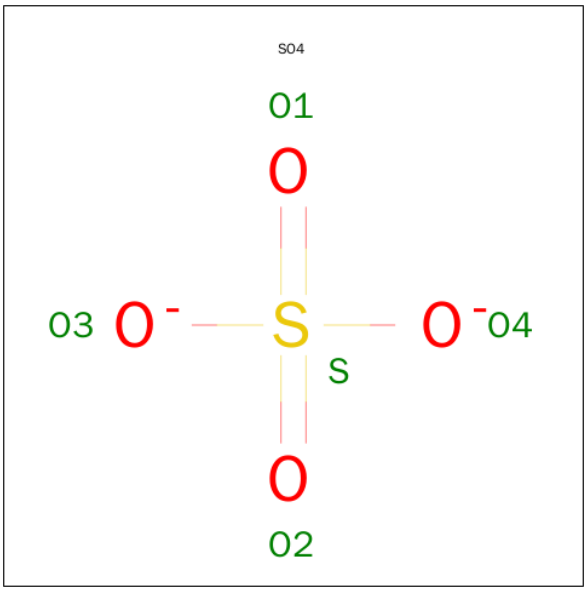
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	B	281	Total	C	N	O	S	0	0	0
			2270	1451	397	411	11			
1	C	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			
1	D	283	Total	C	N	O	S	0	0	0
			2287	1463	400	413	11			

There are 4 discrepancies between the modelled and reference sequences:

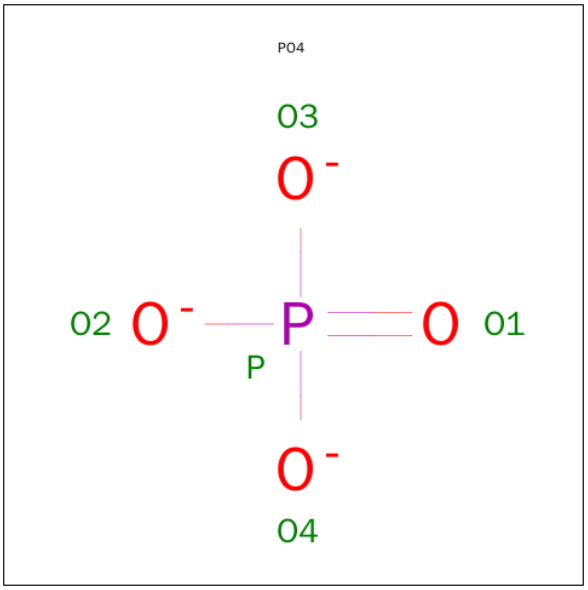
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	TYR	VAL	ENGINEERED	UNP P04818
B	3	TYR	VAL	ENGINEERED	UNP P04818
C	3	TYR	VAL	ENGINEERED	UNP P04818
D	3	TYR	VAL	ENGINEERED	UNP P04818

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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



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

- Molecule 4 is water.

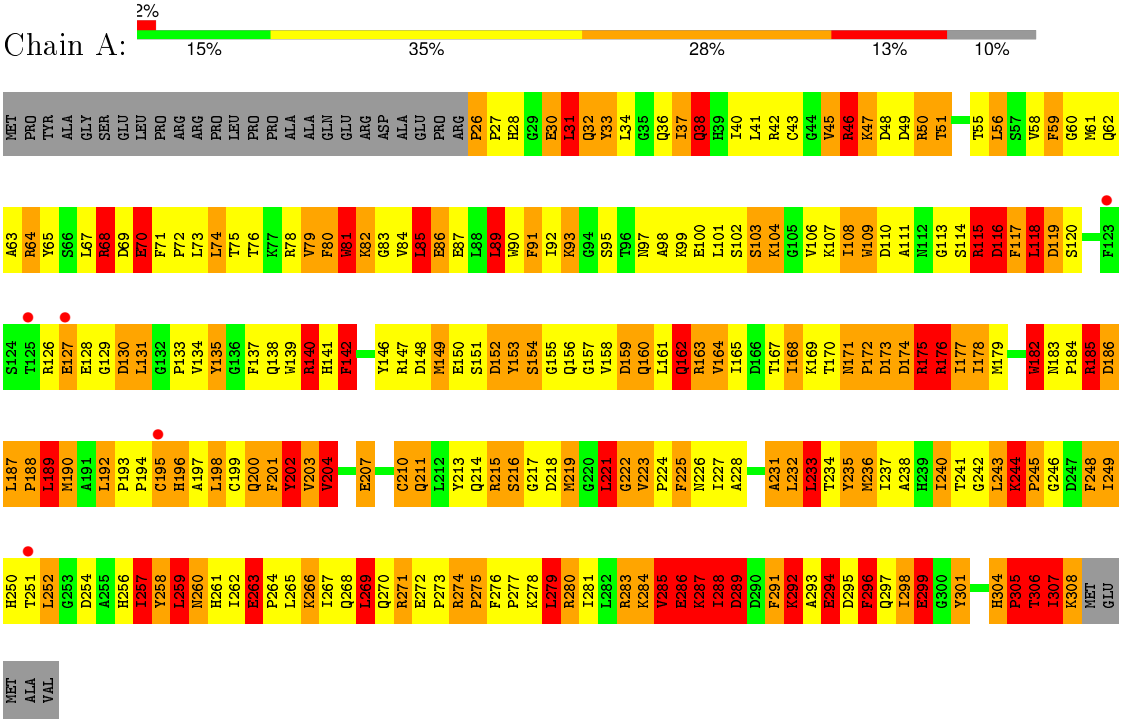
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	7	Total O 7 7	0	0
4	C	5	Total O 5 5	0	0
4	D	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

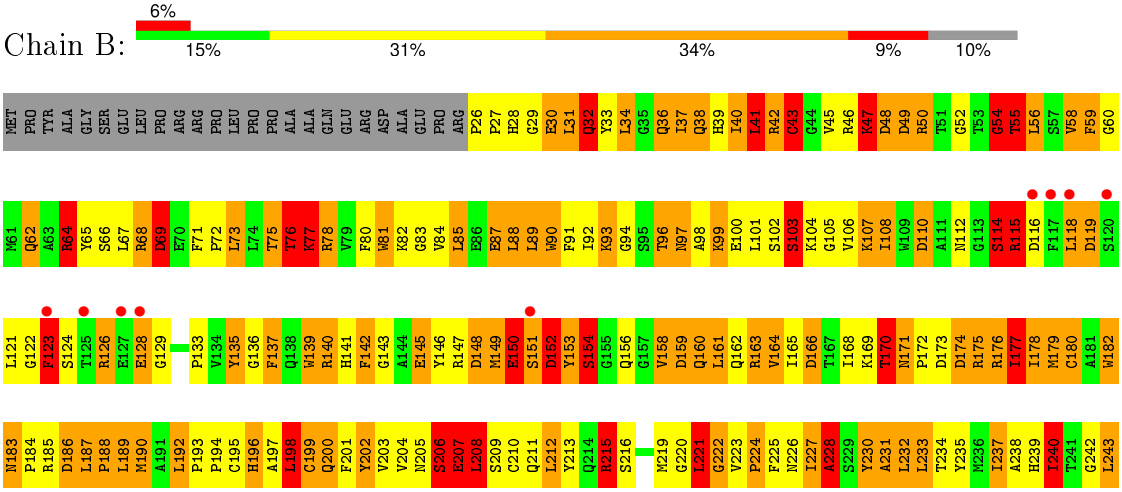
- Molecule 1: Thymidylate synthase

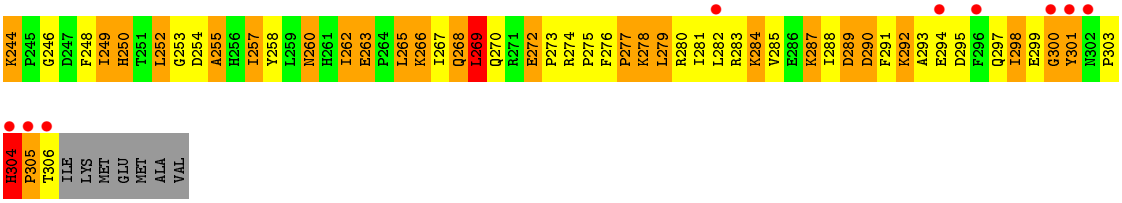
Chain A:



- Molecule 1: Thymidylate synthase

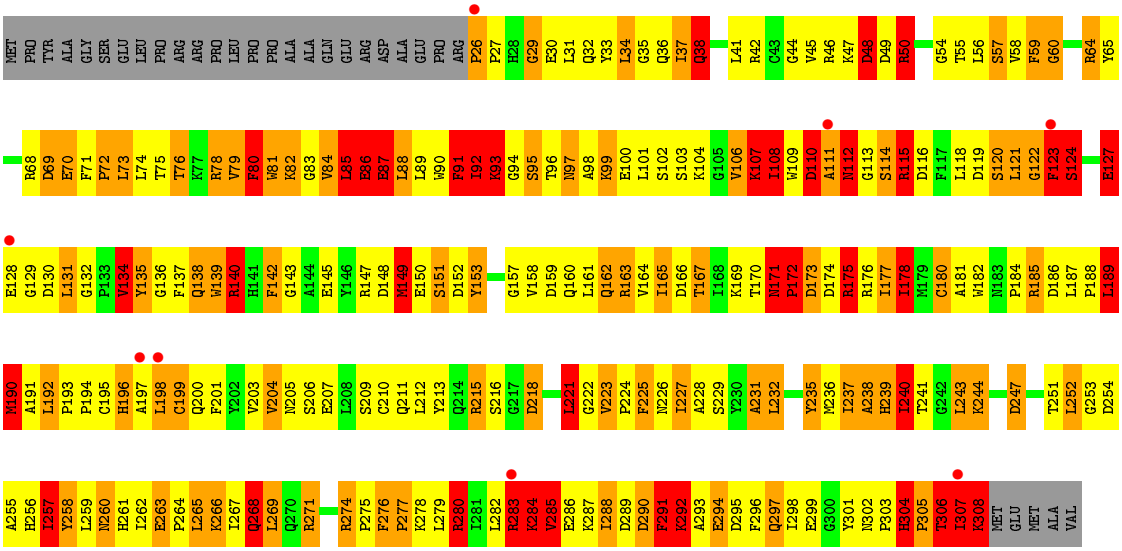
Chain B:





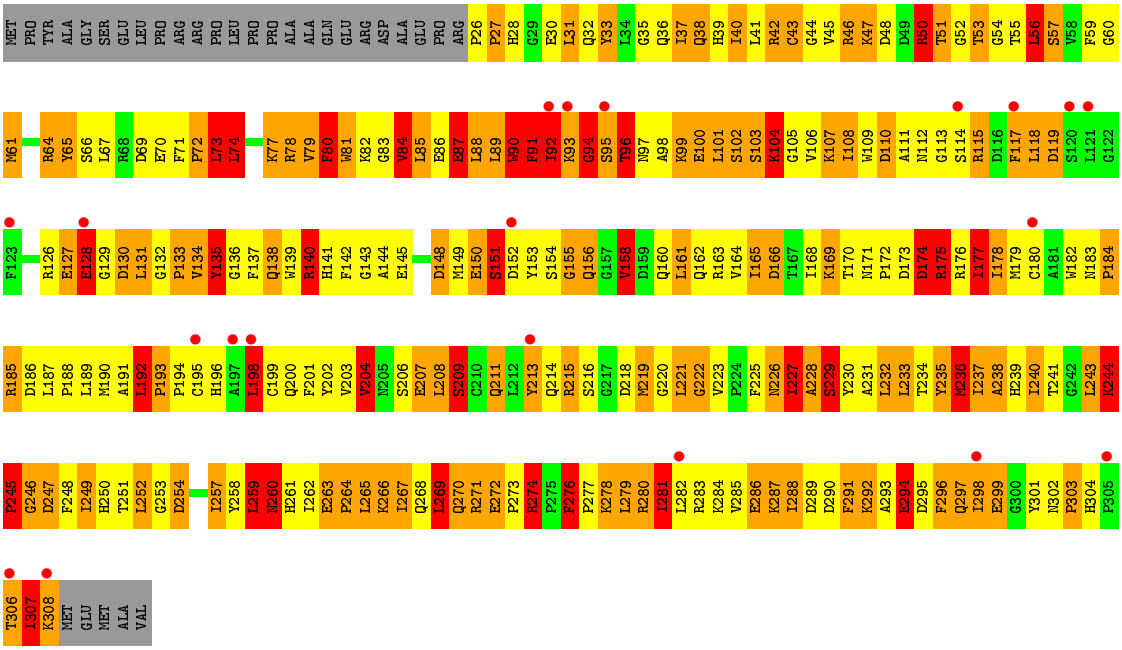
- Molecule 1: Thymidylate synthase

Chain C:



- Molecule 1: Thymidylate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.56Å 94.86Å 130.86Å 90.00° 122.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.77 40.16 – 2.77	Depositor EDS
% Data completeness (in resolution range)	89.3 (50.00-2.77) 80.4 (40.16-2.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.254 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 36191 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9174	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	2.66	136/2347 (5.8%)	2.72	132/3175 (4.2%)
1	B	2.32	104/2330 (4.5%)	2.14	91/3153 (2.9%)
1	C	2.38	102/2347 (4.3%)	2.29	113/3175 (3.6%)
1	D	2.24	81/2347 (3.5%)	2.18	98/3175 (3.1%)
All	All	2.41	423/9371 (4.5%)	2.34	434/12678 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	10
1	D	0	4
All	All	0	26

All (423) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	PHE	CE2-CZ	19.68	1.74	1.37
1	A	200	GLN	C-O	19.56	1.60	1.23
1	A	185	ARG	CZ-NH2	16.97	1.55	1.33
1	A	203	VAL	CB-CG2	-14.60	1.22	1.52
1	A	185	ARG	NE-CZ	-13.65	1.15	1.33
1	C	65	TYR	CD1-CE1	13.56	1.59	1.39
1	C	292	LYS	CD-CE	12.70	1.82	1.51
1	A	38	GLN	CG-CD	12.60	1.80	1.51
1	A	185	ARG	CG-CD	12.56	1.83	1.51
1	C	38	GLN	CG-CD	12.39	1.79	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	GLU	CD-OE2	11.80	1.38	1.25
1	D	43	CYS	CB-SG	11.41	2.01	1.82
1	C	114	SER	CA-C	-11.37	1.23	1.52
1	C	292	LYS	CE-NZ	11.26	1.77	1.49
1	A	175	ARG	CZ-NH2	11.18	1.47	1.33
1	C	299	GLU	CG-CD	11.01	1.68	1.51
1	A	286	GLU	CG-CD	10.93	1.68	1.51
1	A	294	GLU	CD-OE1	10.92	1.37	1.25
1	A	225	PHE	CE2-CZ	10.90	1.58	1.37
1	C	280	ARG	CG-CD	10.84	1.79	1.51
1	B	202	TYR	CD1-CE1	10.70	1.55	1.39
1	D	47	LYS	CD-CE	10.51	1.77	1.51
1	D	207	GLU	CD-OE2	10.51	1.37	1.25
1	A	79	VAL	CB-CG1	-10.49	1.30	1.52
1	A	175	ARG	NE-CZ	10.48	1.46	1.33
1	D	65	TYR	CD1-CE1	-10.15	1.24	1.39
1	D	204	VAL	CB-CG2	-10.13	1.31	1.52
1	D	90	TRP	CB-CG	-10.11	1.32	1.50
1	C	135	TYR	CD1-CE1	10.06	1.54	1.39
1	A	286	GLU	CB-CG	10.03	1.71	1.52
1	A	200	GLN	N-CA	-9.96	1.26	1.46
1	B	58	VAL	C-O	9.95	1.42	1.23
1	B	145	GLU	CD-OE1	9.70	1.36	1.25
1	A	201	PHE	CG-CD1	9.67	1.53	1.38
1	A	79	VAL	CA-CB	-9.62	1.34	1.54
1	B	107	LYS	CD-CE	9.42	1.74	1.51
1	A	263	GLU	CG-CD	9.34	1.66	1.51
1	B	263	GLU	CG-CD	9.25	1.65	1.51
1	A	203	VAL	CA-CB	-9.01	1.35	1.54
1	A	203	VAL	C-O	-8.96	1.06	1.23
1	A	185	ARG	CZ-NH1	-8.95	1.21	1.33
1	C	69	ASP	CB-CG	-8.93	1.33	1.51
1	C	153	TYR	CB-CG	8.84	1.65	1.51
1	A	175	ARG	CG-CD	8.80	1.74	1.51
1	C	238	ALA	CA-CB	-8.69	1.34	1.52
1	A	284	LYS	CD-CE	8.67	1.73	1.51
1	B	197	ALA	CA-CB	-8.67	1.34	1.52
1	B	145	GLU	CD-OE2	8.65	1.35	1.25
1	A	43	CYS	CB-SG	-8.60	1.67	1.82
1	A	235	TYR	CD2-CE2	8.51	1.52	1.39
1	D	266	LYS	CB-CG	8.39	1.75	1.52
1	B	65	TYR	CD1-CE1	8.33	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	201	PHE	CE1-CZ	-8.33	1.21	1.37
1	C	65	TYR	CB-CG	-8.27	1.39	1.51
1	C	180	CYS	CB-SG	-8.27	1.68	1.82
1	D	235	TYR	CZ-OH	8.26	1.51	1.37
1	B	58	VAL	CB-CG2	-8.17	1.35	1.52
1	D	235	TYR	CD2-CE2	8.14	1.51	1.39
1	C	280	ARG	CZ-NH2	8.14	1.43	1.33
1	B	139	TRP	CB-CG	-8.12	1.35	1.50
1	B	230	TYR	CZ-OH	8.10	1.51	1.37
1	B	27	PRO	N-CA	8.09	1.61	1.47
1	B	153	TYR	CD1-CE1	8.09	1.51	1.39
1	B	114	SER	CA-CB	-8.09	1.40	1.52
1	D	195	CYS	CB-SG	-8.02	1.68	1.82
1	A	284	LYS	CG-CD	8.01	1.79	1.52
1	D	100	GLU	CG-CD	8.01	1.64	1.51
1	D	294	GLU	CG-CD	8.00	1.64	1.51
1	B	42	ARG	CB-CG	7.97	1.74	1.52
1	A	203	VAL	N-CA	7.97	1.62	1.46
1	A	235	TYR	C-O	7.92	1.38	1.23
1	A	45	VAL	CB-CG2	-7.91	1.36	1.52
1	C	235	TYR	CB-CG	7.89	1.63	1.51
1	C	235	TYR	CE1-CZ	-7.83	1.28	1.38
1	A	284	LYS	CB-CG	7.81	1.73	1.52
1	C	285	VAL	CB-CG1	7.80	1.69	1.52
1	C	291	PHE	CD2-CE2	7.78	1.54	1.39
1	B	202	TYR	CD2-CE2	7.77	1.51	1.39
1	C	244	LYS	CE-NZ	7.77	1.68	1.49
1	A	223	VAL	CB-CG1	-7.76	1.36	1.52
1	C	42	ARG	CG-CD	7.74	1.71	1.51
1	B	59	PHE	CD2-CE2	7.68	1.54	1.39
1	A	201	PHE	CB-CG	-7.66	1.38	1.51
1	B	114	SER	N-CA	7.62	1.61	1.46
1	A	63	ALA	CA-CB	-7.57	1.36	1.52
1	C	307	ILE	N-CA	7.56	1.61	1.46
1	D	201	PHE	CG-CD2	-7.56	1.27	1.38
1	C	38	GLN	CB-CG	7.51	1.72	1.52
1	B	207	GLU	N-CA	-7.46	1.31	1.46
1	C	87	GLU	CB-CG	-7.43	1.38	1.52
1	B	244	LYS	CG-CD	7.41	1.77	1.52
1	D	87	GLU	CD-OE1	7.41	1.33	1.25
1	A	106	VAL	CB-CG1	-7.39	1.37	1.52
1	A	137	PHE	CD2-CE2	7.38	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	ILE	CA-CB	-7.37	1.37	1.54
1	A	306	THR	C-O	7.37	1.37	1.23
1	D	299	GLU	CG-CD	7.35	1.62	1.51
1	A	285	VAL	CB-CG2	-7.30	1.37	1.52
1	C	239	HIS	N-CA	-7.24	1.31	1.46
1	B	207	GLU	CD-OE2	7.21	1.33	1.25
1	A	202	TYR	C-N	7.17	1.50	1.34
1	D	216	SER	CB-OG	7.17	1.51	1.42
1	B	266	LYS	CD-CE	7.16	1.69	1.51
1	D	229	SER	C-O	7.12	1.36	1.23
1	A	244	LYS	CE-NZ	7.12	1.66	1.49
1	A	223	VAL	CB-CG2	-7.11	1.38	1.52
1	A	254	ASP	CB-CG	7.11	1.66	1.51
1	C	111	ALA	N-CA	7.08	1.60	1.46
1	A	301	TYR	CD1-CE1	7.05	1.50	1.39
1	A	85	LEU	C-O	7.02	1.36	1.23
1	C	225	PHE	CE2-CZ	7.02	1.50	1.37
1	C	216	SER	CB-OG	7.01	1.51	1.42
1	D	215	ARG	N-CA	7.01	1.60	1.46
1	B	81	TRP	CB-CG	-7.00	1.37	1.50
1	B	42	ARG	CG-CD	6.98	1.69	1.51
1	B	230	TYR	CE2-CZ	6.96	1.47	1.38
1	D	151	SER	CA-CB	6.96	1.63	1.52
1	B	301	TYR	CB-CG	6.94	1.62	1.51
1	B	54	GLY	C-O	-6.93	1.12	1.23
1	B	249	ILE	CA-CB	-6.92	1.39	1.54
1	B	123	PHE	CB-CG	-6.87	1.39	1.51
1	C	33	TYR	CB-CG	-6.86	1.41	1.51
1	A	45	VAL	CA-CB	-6.86	1.40	1.54
1	A	248	PHE	CB-CG	-6.84	1.39	1.51
1	B	30	GLU	CG-CD	6.83	1.62	1.51
1	B	237	ILE	CA-CB	-6.83	1.39	1.54
1	B	253	GLY	N-CA	6.81	1.56	1.46
1	B	174	ASP	C-O	6.80	1.36	1.23
1	B	244	LYS	CD-CE	6.80	1.68	1.51
1	B	108	ILE	CA-CB	6.80	1.70	1.54
1	A	248	PHE	CG-CD2	-6.76	1.28	1.38
1	A	116	ASP	CB-CG	6.72	1.65	1.51
1	A	172	PRO	N-CA	-6.70	1.35	1.47
1	B	263	GLU	CB-CG	6.68	1.64	1.52
1	B	50	ARG	NE-CZ	6.68	1.41	1.33
1	A	175	ARG	CB-CG	6.67	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	GLN	CD-NE2	-6.67	1.16	1.32
1	B	242	GLY	C-O	-6.65	1.13	1.23
1	C	308	LYS	CD-CE	6.64	1.67	1.51
1	A	153	TYR	CE1-CZ	6.64	1.47	1.38
1	C	81	TRP	CZ3-CH2	6.63	1.50	1.40
1	B	287	LYS	CB-CG	6.62	1.70	1.52
1	D	100	GLU	CB-CG	6.62	1.64	1.52
1	A	200	GLN	CB-CG	6.61	1.70	1.52
1	A	135	TYR	CE2-CZ	-6.60	1.29	1.38
1	A	162	GLN	CB-CG	6.58	1.70	1.52
1	C	44	GLY	C-O	-6.58	1.13	1.23
1	A	65	TYR	CD1-CE1	6.56	1.49	1.39
1	A	231	ALA	CA-CB	-6.56	1.38	1.52
1	A	216	SER	C-O	-6.55	1.10	1.23
1	A	245	PRO	N-CA	6.54	1.58	1.47
1	C	292	LYS	CG-CD	6.53	1.74	1.52
1	A	307	ILE	CA-C	6.52	1.70	1.52
1	D	65	TYR	CD2-CE2	-6.52	1.29	1.39
1	A	178	ILE	CA-CB	-6.52	1.39	1.54
1	D	258	TYR	CE1-CZ	-6.51	1.30	1.38
1	B	235	TYR	N-CA	6.50	1.59	1.46
1	C	247	ASP	CB-CG	-6.48	1.38	1.51
1	B	59	PHE	CB-CG	-6.48	1.40	1.51
1	A	292	LYS	CB-CG	6.47	1.70	1.52
1	C	269	LEU	N-CA	-6.45	1.33	1.46
1	A	225	PHE	CB-CG	-6.44	1.40	1.51
1	A	266	LYS	CD-CE	6.44	1.67	1.51
1	B	235	TYR	CG-CD2	-6.44	1.30	1.39
1	A	175	ARG	CZ-NH1	6.43	1.41	1.33
1	C	210	CYS	CB-SG	6.42	1.93	1.82
1	C	26	PRO	CA-C	6.41	1.65	1.52
1	A	287	LYS	CD-CE	6.41	1.67	1.51
1	C	26	PRO	CB-CG	6.41	1.81	1.50
1	C	199	CYS	CB-SG	-6.38	1.71	1.82
1	C	251	THR	N-CA	-6.37	1.33	1.46
1	A	305	PRO	CA-C	6.37	1.65	1.52
1	B	182	TRP	CE3-CZ3	6.32	1.49	1.38
1	A	60	GLY	CA-C	-6.31	1.41	1.51
1	A	217	GLY	N-CA	-6.31	1.36	1.46
1	B	164	VAL	CB-CG1	-6.31	1.39	1.52
1	B	142	PHE	CD1-CE1	6.31	1.51	1.39
1	B	266	LYS	CE-NZ	6.31	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	GLU	CD-OE2	6.30	1.32	1.25
1	D	299	GLU	CD-OE1	6.29	1.32	1.25
1	B	178	ILE	CB-CG2	-6.28	1.33	1.52
1	C	162	GLN	CA-C	-6.28	1.36	1.52
1	C	60	GLY	N-CA	6.27	1.55	1.46
1	A	219	MET	CB-CG	-6.27	1.31	1.51
1	C	240	ILE	C-O	-6.27	1.11	1.23
1	C	232	LEU	C-O	6.25	1.35	1.23
1	A	221	LEU	CG-CD2	6.25	1.75	1.51
1	A	80	PHE	CE1-CZ	6.24	1.49	1.37
1	B	177	ILE	CB-CG2	6.22	1.72	1.52
1	A	215	ARG	CG-CD	-6.22	1.36	1.51
1	D	134	VAL	CB-CG2	-6.21	1.39	1.52
1	C	58	VAL	CB-CG2	-6.21	1.39	1.52
1	C	221	LEU	CG-CD1	6.20	1.74	1.51
1	A	61	MET	C-O	6.19	1.35	1.23
1	C	251	THR	CA-CB	-6.18	1.37	1.53
1	C	299	GLU	CB-CG	6.18	1.63	1.52
1	A	177	ILE	C-O	6.18	1.35	1.23
1	B	208	LEU	CG-CD2	-6.17	1.29	1.51
1	A	78	ARG	CZ-NH1	6.17	1.41	1.33
1	D	104	LYS	CE-NZ	6.17	1.64	1.49
1	B	244	LYS	CB-CG	6.16	1.69	1.52
1	A	301	TYR	CZ-OH	6.16	1.48	1.37
1	A	197	ALA	CA-CB	-6.15	1.39	1.52
1	C	107	LYS	CG-CD	6.15	1.73	1.52
1	C	254	ASP	CB-CG	6.14	1.64	1.51
1	B	135	TYR	C-O	6.13	1.35	1.23
1	B	175	ARG	CZ-NH1	6.12	1.41	1.33
1	B	154	SER	CB-OG	-6.12	1.34	1.42
1	C	167	THR	CA-CB	-6.11	1.37	1.53
1	D	245	PRO	CB-CG	6.09	1.80	1.50
1	B	36	GLN	CD-OE1	6.08	1.37	1.24
1	C	38	GLN	CD-NE2	6.07	1.48	1.32
1	A	26	PRO	CB-CG	6.07	1.80	1.50
1	C	266	LYS	CD-CE	6.06	1.66	1.51
1	A	84	VAL	CB-CG1	-6.05	1.40	1.52
1	A	296	PHE	CB-CG	-6.05	1.41	1.51
1	A	93	LYS	CE-NZ	6.04	1.64	1.49
1	B	196	HIS	N-CA	-6.04	1.34	1.46
1	D	192	LEU	CG-CD2	6.03	1.74	1.51
1	B	228	ALA	C-O	6.03	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	GLN	CD-NE2	6.03	1.48	1.32
1	A	33	TYR	CG-CD2	6.00	1.47	1.39
1	D	211	GLN	CG-CD	6.00	1.64	1.51
1	B	260	ASN	CB-CG	5.99	1.64	1.51
1	A	117	PHE	CE1-CZ	5.97	1.48	1.37
1	A	299	GLU	CD-OE1	5.97	1.32	1.25
1	D	93	LYS	C-N	-5.97	1.22	1.33
1	B	178	ILE	CA-CB	-5.96	1.41	1.54
1	A	86	GLU	CD-OE2	5.96	1.32	1.25
1	C	165	ILE	CB-CG2	-5.96	1.34	1.52
1	C	308	LYS	CE-NZ	5.94	1.63	1.49
1	C	82	LYS	CD-CE	5.92	1.66	1.51
1	C	275	PRO	CA-C	-5.92	1.41	1.52
1	C	177	ILE	CB-CG2	-5.92	1.34	1.52
1	D	296	PHE	CA-C	-5.92	1.37	1.52
1	A	87	GLU	CD-OE2	5.91	1.32	1.25
1	C	266	LYS	CE-NZ	5.91	1.63	1.49
1	C	258	TYR	CB-CG	-5.91	1.42	1.51
1	A	70	GLU	C-N	-5.90	1.20	1.34
1	D	263	GLU	CB-CG	5.89	1.63	1.52
1	B	301	TYR	CD2-CE2	5.88	1.48	1.39
1	B	192	LEU	CG-CD2	5.88	1.73	1.51
1	D	135	TYR	CB-CG	-5.87	1.42	1.51
1	C	91	PHE	CD2-CE2	5.86	1.50	1.39
1	A	213	TYR	CZ-OH	5.86	1.47	1.37
1	B	159	ASP	C-O	5.85	1.34	1.23
1	D	209	SER	CB-OG	5.82	1.49	1.42
1	A	201	PHE	CA-CB	-5.82	1.41	1.53
1	B	169	LYS	CE-NZ	5.81	1.63	1.49
1	B	206	SER	C-O	5.81	1.34	1.23
1	D	96	THR	C-N	-5.81	1.20	1.34
1	C	35	GLY	N-CA	-5.80	1.37	1.46
1	A	185	ARG	CB-CG	5.80	1.68	1.52
1	C	142	PHE	CD1-CE1	5.80	1.50	1.39
1	B	304	HIS	CA-CB	5.78	1.66	1.53
1	C	209	SER	C-O	5.78	1.34	1.23
1	A	59	PHE	CB-CG	-5.78	1.41	1.51
1	A	296	PHE	CE1-CZ	5.76	1.48	1.37
1	D	166	ASP	CA-CB	-5.76	1.41	1.53
1	D	77	LYS	CB-CG	5.75	1.68	1.52
1	D	247	ASP	CG-OD2	5.74	1.38	1.25
1	D	279	LEU	C-O	5.74	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	175	ARG	N-CA	-5.74	1.34	1.46
1	A	81	TRP	CZ3-CH2	5.73	1.49	1.40
1	C	34	LEU	CG-CD1	5.73	1.73	1.51
1	D	89	LEU	N-CA	5.72	1.57	1.46
1	D	59	PHE	CB-CG	-5.70	1.41	1.51
1	D	107	LYS	CD-CE	5.67	1.65	1.51
1	C	139	TRP	CD1-NE1	5.67	1.47	1.38
1	D	87	GLU	CG-CD	5.67	1.60	1.51
1	D	245	PRO	CG-CD	-5.67	1.31	1.50
1	C	107	LYS	CD-CE	5.67	1.65	1.51
1	B	90	TRP	CE3-CZ3	5.66	1.48	1.38
1	B	294	GLU	CD-OE2	5.66	1.31	1.25
1	D	39	HIS	N-CA	-5.64	1.35	1.46
1	B	59	PHE	N-CA	-5.63	1.35	1.46
1	D	296	PHE	CB-CG	-5.63	1.41	1.51
1	C	91	PHE	CB-CG	-5.62	1.41	1.51
1	D	244	LYS	CD-CE	5.62	1.65	1.51
1	D	91	PHE	CE2-CZ	5.62	1.48	1.37
1	D	278	LYS	CD-CE	5.62	1.65	1.51
1	A	203	VAL	CA-C	5.62	1.67	1.52
1	C	268	GLN	CB-CG	-5.62	1.37	1.52
1	A	26	PRO	CA-C	5.61	1.64	1.52
1	A	37	ILE	CA-CB	-5.61	1.42	1.54
1	D	145	GLU	CD-OE1	5.61	1.31	1.25
1	C	110	ASP	C-N	5.61	1.47	1.34
1	C	26	PRO	N-CA	5.60	1.56	1.47
1	A	174	ASP	C-O	5.60	1.33	1.23
1	A	201	PHE	CD1-CE1	5.58	1.50	1.39
1	D	180	CYS	CB-SG	5.58	1.91	1.82
1	B	183	ASN	CG-OD1	5.58	1.36	1.24
1	B	30	GLU	CD-OE2	5.58	1.31	1.25
1	D	134	VAL	CA-C	5.57	1.67	1.52
1	B	188	PRO	CG-CD	5.57	1.69	1.50
1	A	252	LEU	N-CA	-5.56	1.35	1.46
1	A	278	LYS	CE-NZ	5.56	1.62	1.49
1	C	123	PHE	C-N	-5.56	1.21	1.34
1	B	255	ALA	CA-CB	-5.55	1.40	1.52
1	B	276	PHE	CB-CG	5.55	1.60	1.51
1	A	137	PHE	CE1-CZ	5.54	1.47	1.37
1	B	58	VAL	CB-CG1	-5.53	1.41	1.52
1	B	304	HIS	N-CA	5.53	1.57	1.46
1	D	77	LYS	CD-CE	5.52	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	ALA	CA-CB	-5.51	1.40	1.52
1	B	301	TYR	CD1-CE1	5.51	1.47	1.39
1	A	42	ARG	CZ-NH1	5.50	1.40	1.33
1	C	59	PHE	CD2-CE2	-5.50	1.28	1.39
1	A	140	ARG	CG-CD	5.50	1.65	1.51
1	D	33	TYR	CD1-CE1	5.50	1.47	1.39
1	A	174	ASP	N-CA	-5.49	1.35	1.46
1	D	259	LEU	CA-CB	-5.48	1.41	1.53
1	B	37	ILE	CA-CB	-5.48	1.42	1.54
1	D	61	MET	C-O	5.47	1.33	1.23
1	A	202	TYR	C-O	-5.47	1.12	1.23
1	C	114	SER	CA-CB	-5.47	1.44	1.52
1	B	142	PHE	CD2-CE2	5.46	1.50	1.39
1	B	65	TYR	CG-CD1	5.46	1.46	1.39
1	B	137	PHE	CE1-CZ	5.46	1.47	1.37
1	A	210	CYS	C-O	-5.46	1.12	1.23
1	D	44	GLY	C-O	-5.45	1.15	1.23
1	B	77	LYS	CD-CE	5.45	1.64	1.51
1	A	75	THR	C-O	5.43	1.33	1.23
1	A	274	ARG	C-O	-5.43	1.13	1.23
1	A	178	ILE	N-CA	-5.43	1.35	1.46
1	A	185	ARG	CD-NE	-5.42	1.37	1.46
1	D	135	TYR	CG-CD2	-5.41	1.32	1.39
1	C	244	LYS	CD-CE	5.41	1.64	1.51
1	B	43	CYS	CB-SG	-5.39	1.73	1.81
1	B	87	GLU	CG-CD	5.39	1.60	1.51
1	B	243	LEU	CG-CD2	5.39	1.71	1.51
1	C	165	ILE	C-O	5.39	1.33	1.23
1	C	162	GLN	C-N	-5.38	1.21	1.34
1	D	297	GLN	CG-CD	5.38	1.63	1.51
1	D	259	LEU	CG-CD1	5.38	1.71	1.51
1	D	38	GLN	CD-OE1	5.37	1.35	1.24
1	B	110	ASP	CB-CG	5.35	1.62	1.51
1	A	249	ILE	CA-CB	-5.35	1.42	1.54
1	A	279	LEU	CG-CD2	5.35	1.71	1.51
1	C	163	ARG	CB-CG	5.35	1.67	1.52
1	C	86	GLU	CB-CG	5.33	1.62	1.52
1	A	292	LYS	CD-CE	5.32	1.64	1.51
1	B	177	ILE	CA-CB	-5.32	1.42	1.54
1	B	219	MET	C-O	-5.31	1.13	1.23
1	C	71	PHE	CE2-CZ	-5.31	1.27	1.37
1	D	70	GLU	N-CA	5.31	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	223	VAL	CB-CG1	-5.31	1.41	1.52
1	A	50	ARG	CB-CG	5.30	1.66	1.52
1	A	258	TYR	CG-CD2	-5.30	1.32	1.39
1	A	142	PHE	CE2-CZ	5.29	1.47	1.37
1	B	146	TYR	CA-CB	-5.28	1.42	1.53
1	A	223	VAL	CA-CB	-5.28	1.43	1.54
1	B	150	GLU	CG-CD	5.26	1.59	1.51
1	A	163	ARG	CZ-NH2	5.25	1.39	1.33
1	C	27	PRO	CG-CD	5.25	1.68	1.50
1	A	131	LEU	CG-CD2	-5.25	1.32	1.51
1	C	280	ARG	CD-NE	5.25	1.55	1.46
1	C	112	ASN	CA-C	5.25	1.66	1.52
1	A	43	CYS	CA-C	-5.25	1.39	1.52
1	D	166	ASP	CA-C	-5.23	1.39	1.52
1	B	59	PHE	CD1-CE1	5.23	1.49	1.39
1	B	107	LYS	CB-CG	5.23	1.66	1.52
1	C	237	ILE	CA-CB	-5.22	1.42	1.54
1	B	207	GLU	CB-CG	-5.22	1.42	1.52
1	D	228	ALA	C-O	5.22	1.33	1.23
1	C	36	GLN	CB-CG	5.22	1.66	1.52
1	A	46	ARG	CZ-NH1	5.21	1.39	1.33
1	A	207	GLU	CA-CB	-5.21	1.42	1.53
1	B	213	TYR	CD1-CE1	5.20	1.47	1.39
1	D	170	THR	C-O	-5.20	1.13	1.23
1	A	210	CYS	CB-SG	-5.19	1.73	1.81
1	D	193	PRO	N-CA	5.19	1.56	1.47
1	B	221	LEU	CG-CD1	5.19	1.71	1.51
1	B	252	LEU	C-O	5.19	1.33	1.23
1	A	48	ASP	CG-OD1	5.19	1.37	1.25
1	D	100	GLU	CD-OE2	5.18	1.31	1.25
1	C	297	GLN	CG-CD	5.18	1.62	1.51
1	B	142	PHE	CE2-CZ	5.18	1.47	1.37
1	C	65	TYR	CZ-OH	5.18	1.46	1.37
1	C	142	PHE	CD2-CE2	5.17	1.49	1.39
1	C	280	ARG	NE-CZ	5.17	1.39	1.33
1	C	204	VAL	CA-CB	-5.16	1.44	1.54
1	A	177	ILE	N-CA	-5.16	1.36	1.46
1	B	200	GLN	C-O	5.15	1.33	1.23
1	D	135	TYR	CE1-CZ	-5.15	1.31	1.38
1	B	135	TYR	CE2-CZ	-5.14	1.31	1.38
1	D	192	LEU	CG-CD1	5.14	1.70	1.51
1	D	128	GLU	CG-CD	5.14	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	213	TYR	CG-CD2	5.14	1.45	1.39
1	A	30	GLU	CA-CB	-5.13	1.42	1.53
1	C	172	PRO	N-CA	-5.13	1.38	1.47
1	D	98	ALA	CA-CB	-5.13	1.41	1.52
1	B	192	LEU	CG-CD1	5.12	1.70	1.51
1	B	235	TYR	CE2-CZ	-5.12	1.31	1.38
1	D	213	TYR	CG-CD1	-5.12	1.32	1.39
1	B	73	LEU	CG-CD2	5.12	1.70	1.51
1	C	70	GLU	CA-C	-5.11	1.39	1.52
1	C	54	GLY	C-O	-5.10	1.15	1.23
1	A	215	ARG	CB-CG	-5.09	1.38	1.52
1	A	33	TYR	CG-CD1	5.09	1.45	1.39
1	A	109	TRP	CE3-CZ3	5.09	1.47	1.38
1	C	223	VAL	CA-CB	-5.09	1.44	1.54
1	D	298	ILE	CB-CG2	5.08	1.68	1.52
1	C	284	LYS	CE-NZ	5.07	1.61	1.49
1	D	174	ASP	CB-CG	5.07	1.62	1.51
1	A	78	ARG	CD-NE	5.06	1.55	1.46
1	C	221	LEU	CG-CD2	5.06	1.70	1.51
1	D	104	LYS	CD-CE	5.06	1.64	1.51
1	C	41	LEU	CG-CD2	-5.05	1.33	1.51
1	D	201	PHE	C-O	5.05	1.32	1.23
1	A	162	GLN	CG-CD	5.04	1.62	1.51
1	C	33	TYR	CA-CB	-5.04	1.42	1.53
1	B	76	THR	CA-CB	5.04	1.66	1.53
1	D	33	TYR	C-O	5.03	1.32	1.23
1	C	225	PHE	CD1-CE1	5.03	1.49	1.39
1	A	159	ASP	C-O	5.03	1.32	1.23
1	B	257	ILE	CA-CB	-5.02	1.43	1.54
1	C	45	VAL	CB-CG1	-5.02	1.42	1.52
1	D	232	LEU	C-O	5.02	1.32	1.23
1	A	306	THR	CA-C	5.01	1.66	1.52
1	D	51	THR	CA-CB	5.01	1.66	1.53
1	A	117	PHE	CE2-CZ	5.01	1.46	1.37
1	D	307	ILE	CG1-CD1	5.00	1.84	1.50

All (434) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ARG	NE-CZ-NH1	60.36	150.48	120.30
1	A	185	ARG	NE-CZ-NH2	-53.62	93.49	120.30
1	A	185	ARG	CD-NE-CZ	23.59	156.63	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	123	PHE	O-C-N	19.79	154.36	122.70
1	D	175	ARG	NE-CZ-NH2	18.91	129.75	120.30
1	B	50	ARG	NE-CZ-NH1	18.14	129.37	120.30
1	A	70	GLU	O-C-N	-17.29	95.03	122.70
1	C	123	PHE	CA-C-N	-16.73	80.39	117.20
1	C	64	ARG	NE-CZ-NH2	16.11	128.35	120.30
1	C	180	CYS	CA-CB-SG	-16.03	85.14	114.00
1	A	42	ARG	NE-CZ-NH2	-15.17	112.72	120.30
1	C	69	ASP	CB-CG-OD2	-13.64	106.03	118.30
1	A	42	ARG	NE-CZ-NH1	13.33	126.97	120.30
1	A	68	ARG	O-C-N	13.15	143.73	122.70
1	A	50	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	C	178	ILE	CG1-CB-CG2	-12.95	82.91	111.40
1	B	48	ASP	CB-CG-OD2	-12.82	106.76	118.30
1	D	192	LEU	CA-CB-CG	12.77	144.66	115.30
1	D	281	ILE	N-CA-C	-12.60	76.98	111.00
1	A	221	LEU	CB-CG-CD2	12.60	132.41	111.00
1	B	254	ASP	CB-CG-OD2	12.59	129.63	118.30
1	C	64	ARG	NE-CZ-NH1	-12.48	114.06	120.30
1	C	283	ARG	O-C-N	-12.44	102.79	122.70
1	D	92	ILE	O-C-N	-12.23	103.13	122.70
1	C	122	GLY	O-C-N	12.11	142.08	122.70
1	D	175	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	D	74	LEU	CB-CG-CD1	-11.77	90.99	111.00
1	C	123	PHE	C-N-CA	11.74	151.05	121.70
1	C	198	LEU	CB-CG-CD1	-11.66	91.17	111.00
1	D	254	ASP	CB-CG-OD2	11.63	128.77	118.30
1	A	306	THR	N-CA-C	11.52	142.10	111.00
1	A	70	GLU	CA-C-N	11.39	142.26	117.20
1	D	215	ARG	NE-CZ-NH1	11.37	125.99	120.30
1	D	243	LEU	CA-CB-CG	-11.28	89.35	115.30
1	A	176	ARG	NE-CZ-NH1	-11.09	114.75	120.30
1	A	221	LEU	CB-CG-CD1	-10.98	92.33	111.00
1	D	198	LEU	CB-CG-CD1	-10.87	92.53	111.00
1	C	121	LEU	C-N-CA	-10.86	99.49	122.30
1	C	58	VAL	CG1-CB-CG2	-10.84	93.56	110.90
1	A	174	ASP	CB-CG-OD2	-10.72	108.65	118.30
1	D	192	LEU	CB-CG-CD2	10.70	129.19	111.00
1	B	198	LEU	CB-CG-CD2	-10.54	93.09	111.00
1	D	46	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	B	114	SER	O-C-N	10.41	139.35	122.70
1	A	46	ARG	NE-CZ-NH2	-10.26	115.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	59	PHE	CB-CG-CD1	10.23	127.96	120.80
1	D	283	ARG	NE-CZ-NH1	-10.17	115.22	120.30
1	A	203	VAL	CB-CA-C	-10.16	92.09	111.40
1	B	89	LEU	CB-CG-CD1	-9.97	94.05	111.00
1	B	49	ASP	CB-CG-OD1	-9.95	109.35	118.30
1	A	175	ARG	NE-CZ-NH2	9.93	125.27	120.30
1	B	243	LEU	CB-CG-CD1	-9.92	94.14	111.00
1	A	175	ARG	CA-CB-CG	9.90	135.18	113.40
1	D	274	ARG	NE-CZ-NH1	-9.89	115.36	120.30
1	B	41	LEU	CB-CG-CD1	-9.86	94.23	111.00
1	A	203	VAL	CG1-CB-CG2	-9.62	95.51	110.90
1	C	199	CYS	CA-CB-SG	-9.54	96.83	114.00
1	D	104	LYS	CD-CE-NZ	9.41	133.34	111.70
1	A	298	ILE	CB-CA-C	-9.28	93.03	111.60
1	A	182	TRP	O-C-N	9.24	137.48	122.70
1	A	68	ARG	CA-C-N	-9.23	96.90	117.20
1	B	34	LEU	CA-CB-CG	-9.23	94.08	115.30
1	A	201	PHE	CZ-CE2-CD2	-9.18	109.08	120.10
1	D	189	LEU	CA-CB-CG	-9.02	94.56	115.30
1	C	215	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	C	48	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	B	68	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	203	VAL	CA-CB-CG2	-8.94	97.50	110.90
1	C	123	PHE	CB-CG-CD1	-8.90	114.57	120.80
1	D	215	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	186	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	D	254	ASP	CB-CG-OD1	-8.81	110.37	118.30
1	C	290	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	B	118	LEU	CA-CB-CG	8.77	135.46	115.30
1	C	274	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	C	306	THR	N-CA-C	8.74	134.59	111.00
1	C	252	LEU	CA-CB-CG	-8.72	95.24	115.30
1	C	171	ASN	C-N-CD	-8.66	101.55	120.60
1	D	131	LEU	CA-CB-CG	8.64	135.19	115.30
1	B	78	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	233	LEU	CA-CB-CG	-8.59	95.55	115.30
1	A	159	ASP	CB-CG-OD1	8.57	126.02	118.30
1	A	175	ARG	CB-CA-C	8.53	127.46	110.40
1	A	131	LEU	CB-CG-CD1	-8.50	96.55	111.00
1	C	299	GLU	OE1-CD-OE2	-8.31	113.33	123.30
1	D	274	ARG	C-N-CD	8.30	145.84	128.40
1	A	289	ASP	CB-CG-OD2	-8.29	110.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	42	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	152	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	A	219	MET	CB-CA-C	-8.26	93.88	110.40
1	D	243	LEU	CB-CG-CD2	-8.23	97.00	111.00
1	D	222	GLY	N-CA-C	-8.21	92.56	113.10
1	C	70	GLU	N-CA-C	-8.19	88.88	111.00
1	A	201	PHE	CG-CD2-CE2	8.18	129.80	120.80
1	A	163	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	A	175	ARG	NH1-CZ-NH2	-8.16	110.42	119.40
1	D	269	LEU	CA-CB-CG	8.16	134.07	115.30
1	A	42	ARG	CD-NE-CZ	8.16	135.02	123.60
1	B	180	CYS	CA-CB-SG	-8.15	99.32	114.00
1	D	94	GLY	O-C-N	8.13	135.72	122.70
1	B	177	ILE	CG1-CB-CG2	8.09	129.19	111.40
1	A	47	LYS	CD-CE-NZ	8.05	130.21	111.70
1	D	92	ILE	CA-C-N	8.04	134.88	117.20
1	C	173	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	D	252	LEU	CA-CB-CG	-7.99	96.92	115.30
1	A	68	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	C	190	MET	CG-SD-CE	7.98	112.96	100.20
1	A	203	VAL	CA-CB-CG1	7.97	122.86	110.90
1	D	207	GLU	CG-CD-OE1	-7.95	102.41	118.30
1	A	91	PHE	CB-CA-C	-7.94	94.51	110.40
1	B	175	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	C	271	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	C	176	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	185	ARG	CG-CD-NE	-7.89	95.24	111.80
1	D	296	PHE	N-CA-C	-7.88	89.73	111.00
1	B	47	LYS	CD-CE-NZ	7.87	129.79	111.70
1	D	61	MET	CA-CB-CG	-7.84	99.97	113.30
1	A	175	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	C	287	LYS	N-CA-C	-7.79	89.95	111.00
1	B	64	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	257	ILE	CB-CA-C	-7.73	96.14	111.60
1	B	77	LYS	CD-CE-NZ	7.67	129.35	111.70
1	C	49	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	C	114	SER	O-C-N	7.59	134.84	122.70
1	B	48	ASP	CB-CG-OD1	7.57	125.11	118.30
1	D	247	ASP	CB-CG-OD2	7.57	125.11	118.30
1	C	106	VAL	CB-CA-C	7.54	125.72	111.40
1	D	161	LEU	CA-CB-CG	-7.53	97.99	115.30
1	A	171	ASN	N-CA-CB	7.50	124.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	269	LEU	CB-CG-CD1	-7.49	98.27	111.00
1	C	103	SER	N-CA-CB	-7.48	99.28	110.50
1	A	201	PHE	CB-CG-CD2	-7.42	115.61	120.80
1	B	176	ARG	CG-CD-NE	7.40	127.33	111.80
1	B	163	ARG	CB-CG-CD	-7.37	92.43	111.60
1	A	243	LEU	CB-CG-CD2	-7.36	98.49	111.00
1	C	252	LEU	CB-CG-CD2	-7.32	98.56	111.00
1	A	65	TYR	CB-CG-CD1	7.31	125.39	121.00
1	C	108	ILE	C-N-CA	-7.30	103.44	121.70
1	B	107	LYS	CD-CE-NZ	7.25	128.38	111.70
1	A	50	ARG	CD-NE-CZ	7.24	133.73	123.60
1	D	50	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	71	PHE	C-N-CD	7.19	143.50	128.40
1	C	265	LEU	CA-CB-CG	-7.17	98.81	115.30
1	A	89	LEU	CA-CB-CG	-7.16	98.84	115.30
1	A	294	GLU	OE1-CD-OE2	7.15	131.88	123.30
1	D	40	ILE	CG1-CB-CG2	-7.14	95.68	111.40
1	B	166	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	140	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	140	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	C	247	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	A	46	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	124	SER	N-CA-CB	-7.04	99.94	110.50
1	A	305	PRO	CB-CA-C	7.00	129.51	112.00
1	B	145	GLU	OE1-CD-OE2	7.00	131.70	123.30
1	B	170	THR	CB-CA-C	-6.99	92.72	111.60
1	D	88	LEU	CB-CG-CD2	6.99	122.88	111.00
1	A	307	ILE	N-CA-C	6.99	129.87	111.00
1	A	187	LEU	CB-CG-CD1	-6.98	99.13	111.00
1	C	73	LEU	CB-CG-CD1	-6.96	99.17	111.00
1	A	79	VAL	N-CA-CB	-6.96	96.20	111.50
1	A	305	PRO	CA-C-N	-6.95	101.92	117.20
1	C	284	LYS	CB-CA-C	6.94	124.28	110.40
1	D	266	LYS	CA-CB-CG	6.94	128.67	113.40
1	C	306	THR	CB-CA-C	-6.93	92.89	111.60
1	B	59	PHE	CG-CD1-CE1	6.93	128.42	120.80
1	B	221	LEU	CB-CG-CD2	-6.89	99.29	111.00
1	A	41	LEU	CB-CG-CD2	6.88	122.70	111.00
1	D	166	ASP	CB-CG-OD2	-6.87	112.11	118.30
1	A	32	GLN	CA-CB-CG	6.83	128.43	113.40
1	B	40	ILE	CG1-CB-CG2	6.83	126.43	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	91	PHE	CB-CA-C	-6.83	96.74	110.40
1	C	283	ARG	C-N-CA	-6.82	104.65	121.70
1	B	189	LEU	CA-CB-CG	6.77	130.87	115.30
1	D	213	TYR	CD1-CE1-CZ	6.77	125.89	119.80
1	D	103	SER	N-CA-CB	-6.74	100.38	110.50
1	D	254	ASP	CB-CA-C	6.72	123.84	110.40
1	C	113	GLY	O-C-N	6.72	133.45	122.70
1	A	171	ASN	C-N-CD	-6.71	105.84	120.60
1	C	110	ASP	O-C-N	-6.71	111.97	122.70
1	A	163	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	B	88	LEU	CB-CG-CD2	6.68	122.36	111.00
1	B	192	LEU	CA-CB-CG	-6.65	100.00	115.30
1	A	200	GLN	N-CA-C	-6.64	93.08	111.00
1	D	46	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	A	198	LEU	CA-CB-CG	6.61	130.51	115.30
1	D	47	LYS	CD-CE-NZ	6.59	126.86	111.70
1	A	50	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	249	ILE	CG1-CB-CG2	6.57	125.86	111.40
1	A	43	CYS	CA-CB-SG	-6.57	102.17	114.00
1	A	189	LEU	CA-CB-CG	6.56	130.39	115.30
1	C	97	ASN	CB-CA-C	-6.56	97.28	110.40
1	C	135	TYR	CA-CB-CG	6.53	125.81	113.40
1	A	218	ASP	CB-CA-C	-6.52	97.36	110.40
1	B	266	LYS	CD-CE-NZ	6.52	126.69	111.70
1	B	40	ILE	CB-CA-C	-6.50	98.59	111.60
1	B	47	LYS	CA-CB-CG	6.50	127.70	113.40
1	C	290	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	53	THR	N-CA-CB	6.45	122.56	110.30
1	C	236	MET	CA-CB-CG	-6.44	102.36	113.30
1	C	58	VAL	CA-CB-CG2	-6.43	101.25	110.90
1	A	64	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	288	ILE	CB-CA-C	-6.42	98.76	111.60
1	C	189	LEU	CA-CB-CG	6.41	130.05	115.30
1	B	114	SER	CA-C-N	-6.41	103.11	117.20
1	C	243	LEU	CA-CB-CG	-6.41	100.56	115.30
1	C	215	ARG	NH1-CZ-NH2	6.40	126.44	119.40
1	B	135	TYR	CB-CG-CD1	6.40	124.84	121.00
1	D	209	SER	CB-CA-C	-6.38	97.97	110.10
1	A	173	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	252	LEU	CB-CA-C	-6.38	98.07	110.20
1	B	301	TYR	N-CA-CB	-6.38	99.12	110.60
1	A	296	PHE	CB-CA-C	-6.35	97.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	247	ASP	CB-CA-C	-6.33	97.74	110.40
1	A	202	TYR	C-N-CA	-6.33	105.88	121.70
1	B	269	LEU	CA-CB-CG	6.32	129.84	115.30
1	B	190	MET	CB-CG-SD	-6.32	93.44	112.40
1	D	140	ARG	CA-CB-CG	6.30	127.27	113.40
1	A	89	LEU	CB-CG-CD2	6.30	121.70	111.00
1	D	48	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	276	PHE	CB-CA-C	-6.29	97.81	110.40
1	C	122	GLY	CA-C-N	-6.29	103.36	117.20
1	C	251	THR	OG1-CB-CG2	-6.26	95.61	110.00
1	C	271	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	115	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	31	LEU	CB-CG-CD2	6.24	121.61	111.00
1	D	31	LEU	CB-CG-CD2	-6.24	100.39	111.00
1	C	301	TYR	CB-CA-C	-6.22	97.96	110.40
1	B	68	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	D	90	TRP	CA-CB-CG	-6.21	101.91	113.70
1	A	175	ARG	N-CA-C	-6.20	94.25	111.00
1	B	115	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	C	69	ASP	N-CA-C	6.19	127.70	111.00
1	B	78	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	202	TYR	CG-CD2-CE2	-6.17	116.36	121.30
1	B	206	SER	CA-CB-OG	-6.17	94.54	111.20
1	A	199	CYS	C-N-CA	-6.16	106.31	121.70
1	B	88	LEU	CA-CB-CG	6.15	129.45	115.30
1	C	50	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	D	56	LEU	N-CA-CB	-6.13	98.14	110.40
1	A	176	ARG	N-CA-C	6.12	127.52	111.00
1	D	279	LEU	CB-CG-CD2	-6.12	100.60	111.00
1	A	289	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	306	THR	N-CA-C	6.11	127.51	111.00
1	A	73	LEU	CA-CB-CG	-6.08	101.31	115.30
1	A	182	TRP	CA-C-N	-6.08	103.82	117.20
1	A	223	VAL	CA-CB-CG1	-6.08	101.78	110.90
1	C	37	ILE	CG1-CB-CG2	-6.08	98.02	111.40
1	B	254	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	D	57	SER	N-CA-CB	-6.05	101.43	110.50
1	B	73	LEU	CB-CG-CD1	-6.04	100.74	111.00
1	B	235	TYR	N-CA-CB	6.04	121.47	110.60
1	A	203	VAL	O-C-N	-6.03	113.06	122.70
1	C	175	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	48	ASP	CB-CG-OD2	-6.02	112.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	42	ARG	CB-CA-C	-6.01	98.39	110.40
1	B	50	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	244	LYS	CA-CB-CG	5.99	126.58	113.40
1	A	168	ILE	CG1-CB-CG2	5.98	124.55	111.40
1	B	37	ILE	CB-CA-C	-5.97	99.67	111.60
1	B	55	THR	N-CA-C	-5.95	94.93	111.00
1	B	265	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	259	LEU	CB-CG-CD2	5.94	121.10	111.00
1	D	232	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	176	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	B	258	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	244	LYS	CD-CE-NZ	5.93	125.34	111.70
1	D	299	GLU	CA-CB-CG	5.92	126.42	113.40
1	C	171	ASN	C-N-CA	5.92	146.85	122.00
1	D	202	TYR	CZ-CE2-CD2	5.90	125.11	119.80
1	A	305	PRO	CA-C-O	5.88	134.32	120.20
1	A	80	PHE	N-CA-CB	-5.88	100.02	110.60
1	D	41	LEU	CB-CG-CD2	5.88	120.99	111.00
1	C	84	VAL	CB-CA-C	-5.87	100.25	111.40
1	A	140	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	145	GLU	C-N-CA	-5.82	107.14	121.70
1	A	106	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	A	115	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	169	LYS	CB-CG-CD	-5.81	96.49	111.60
1	A	202	TYR	CZ-CE2-CD2	5.81	125.03	119.80
1	B	265	LEU	CB-CG-CD2	5.80	120.86	111.00
1	C	123	PHE	CB-CG-CD2	5.80	124.86	120.80
1	D	155	GLY	N-CA-C	5.80	127.59	113.10
1	D	215	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	258	TYR	CG-CD1-CE1	5.79	125.93	121.30
1	A	79	VAL	CB-CA-C	-5.78	100.42	111.40
1	B	212	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	C	231	ALA	N-CA-CB	5.76	118.17	110.10
1	C	69	ASP	OD1-CG-OD2	5.75	134.23	123.30
1	A	182	TRP	CB-CA-C	-5.74	98.92	110.40
1	D	56	LEU	O-C-N	-5.74	113.52	122.70
1	A	304	HIS	C-N-CD	5.73	140.43	128.40
1	A	259	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	C	171	ASN	N-CA-C	5.71	126.40	111.00
1	A	202	TYR	CD1-CE1-CZ	-5.70	114.67	119.80
1	A	118	LEU	CB-CG-CD1	5.70	120.69	111.00
1	D	47	LYS	N-CA-CB	5.70	120.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	283	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	A	70	GLU	C-N-CA	5.69	135.93	121.70
1	C	283	ARG	CA-C-N	5.69	129.71	117.20
1	B	199	CYS	CA-CB-SG	-5.69	103.77	114.00
1	B	114	SER	N-CA-CB	-5.68	101.98	110.50
1	D	99	LYS	CD-CE-NZ	5.68	124.76	111.70
1	A	294	GLU	CB-CA-C	-5.67	99.07	110.40
1	B	161	LEU	CB-CA-C	-5.66	99.45	110.20
1	B	301	TYR	N-CA-C	5.66	126.27	111.00
1	A	187	LEU	C-N-CD	5.65	140.26	128.40
1	D	89	LEU	CA-CB-CG	-5.64	102.32	115.30
1	D	227	ILE	CG1-CB-CG2	-5.64	98.99	111.40
1	D	207	GLU	OE1-CD-OE2	5.63	130.05	123.30
1	A	173	ASP	CB-CA-C	-5.60	99.21	110.40
1	A	202	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	C	149	MET	CG-SD-CE	-5.59	91.25	100.20
1	D	175	ARG	CA-CB-CG	5.59	125.71	113.40
1	A	169	LYS	CD-CE-NZ	-5.57	98.89	111.70
1	B	279	LEU	CA-CB-CG	-5.57	102.49	115.30
1	C	304	HIS	C-N-CD	5.57	140.09	128.40
1	A	74	LEU	CB-CG-CD2	5.56	120.45	111.00
1	C	227	ILE	CG1-CB-CG2	5.56	123.63	111.40
1	C	79	VAL	CB-CA-C	-5.55	100.85	111.40
1	C	85	LEU	CB-CA-C	5.55	120.75	110.20
1	C	165	ILE	CG1-CB-CG2	-5.55	99.19	111.40
1	C	85	LEU	CB-CG-CD2	-5.55	101.57	111.00
1	B	59	PHE	CD1-CG-CD2	-5.54	111.10	118.30
1	B	175	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	232	LEU	CA-CB-CG	-5.54	102.57	115.30
1	C	80	PHE	CB-CA-C	5.54	121.47	110.40
1	A	63	ALA	C-N-CA	5.53	135.53	121.70
1	C	307	ILE	N-CA-C	5.53	125.93	111.00
1	B	50	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	B	232	LEU	CB-CG-CD1	-5.50	101.64	111.00
1	C	204	VAL	CA-C-N	-5.50	105.10	117.20
1	D	73	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	46	ARG	N-CA-C	-5.49	96.19	111.00
1	A	93	LYS	CD-CE-NZ	5.48	124.30	111.70
1	D	294	GLU	OE1-CD-OE2	-5.47	116.73	123.30
1	C	64	ARG	CG-CD-NE	-5.46	100.32	111.80
1	D	297	GLN	CB-CA-C	5.46	121.32	110.40
1	A	197	ALA	N-CA-CB	-5.46	102.46	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	145	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	B	42	ARG	CB-CA-C	5.45	121.30	110.40
1	A	269	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	43	CYS	CB-CA-C	-5.44	99.53	110.40
1	D	138	GLN	CA-CB-CG	-5.43	101.45	113.40
1	D	92	ILE	CB-CA-C	-5.43	100.75	111.60
1	D	219	MET	CA-C-O	5.42	131.48	120.10
1	A	210	CYS	CB-CA-C	-5.41	99.59	110.40
1	D	235	TYR	N-CA-C	-5.40	96.41	111.00
1	A	283	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	29	GLY	O-C-N	-5.40	114.06	122.70
1	C	215	ARG	CG-CD-NE	-5.40	100.46	111.80
1	D	89	LEU	CB-CG-CD2	5.39	120.17	111.00
1	B	62	GLN	CB-CA-C	-5.39	99.62	110.40
1	A	279	LEU	CB-CG-CD2	5.38	120.15	111.00
1	C	110	ASP	CA-C-N	5.38	129.03	117.20
1	A	37	ILE	CA-CB-CG1	-5.37	100.80	111.00
1	A	87	GLU	C-N-CA	-5.36	108.30	121.70
1	D	204	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	A	68	ARG	C-N-CA	5.36	135.09	121.70
1	D	253	GLY	N-CA-C	-5.33	99.78	113.10
1	A	292	LYS	CA-CB-CG	5.32	125.11	113.40
1	A	56	LEU	N-CA-CB	-5.32	99.76	110.40
1	A	115	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	250	HIS	CB-CA-C	-5.32	99.76	110.40
1	D	266	LYS	N-CA-CB	5.31	120.16	110.60
1	B	152	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	37	ILE	CB-CA-C	-5.29	101.02	111.60
1	A	196	HIS	N-CA-CB	-5.29	101.08	110.60
1	C	34	LEU	CB-CG-CD1	5.28	119.97	111.00
1	C	134	VAL	CB-CA-C	5.25	121.38	111.40
1	C	289	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	B	215	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	237	ILE	CB-CA-C	5.25	122.09	111.60
1	D	179	MET	CA-CB-CG	-5.25	104.38	113.30
1	C	299	GLU	CA-CB-CG	5.24	124.94	113.40
1	C	153	TYR	CA-CB-CG	5.24	123.35	113.40
1	D	130	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	263	GLU	CA-CB-CG	-5.24	101.88	113.40
1	A	259	LEU	CB-CG-CD2	5.23	119.89	111.00
1	A	233	LEU	CB-CA-C	-5.23	100.27	110.20
1	D	148	ASP	CB-CA-C	-5.22	99.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	ILE	CA-CB-CG1	-5.21	101.10	111.00
1	C	294	GLU	CA-CB-CG	-5.21	101.94	113.40
1	D	56	LEU	C-N-CA	-5.21	108.69	121.70
1	D	177	ILE	CB-CA-C	-5.21	101.19	111.60
1	D	269	LEU	CB-CG-CD1	5.21	119.85	111.00
1	C	108	ILE	N-CA-C	-5.20	96.95	111.00
1	A	269	LEU	CB-CA-C	5.20	120.08	110.20
1	C	124	SER	N-CA-C	5.19	125.02	111.00
1	C	240	ILE	O-C-N	-5.19	114.39	122.70
1	B	206	SER	C-N-CA	-5.19	108.73	121.70
1	C	308	LYS	CD-CE-NZ	5.19	123.63	111.70
1	C	163	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	D	193	PRO	C-N-CD	5.17	139.26	128.40
1	C	185	ARG	C-N-CA	-5.17	108.79	121.70
1	C	269	LEU	CB-CG-CD2	5.16	119.77	111.00
1	B	240	ILE	CB-CA-C	-5.16	101.29	111.60
1	C	196	HIS	CB-CA-C	5.16	120.71	110.40
1	C	178	ILE	N-CA-C	5.14	124.89	111.00
1	D	283	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	292	LYS	CD-CE-NZ	5.13	123.51	111.70
1	B	285	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	B	69	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	135	TYR	CG-CD2-CE2	5.12	125.40	121.30
1	A	284	LYS	CG-CD-CE	5.12	127.27	111.90
1	D	232	LEU	CB-CG-CD1	5.12	119.70	111.00
1	C	215	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	257	ILE	CA-CB-CG2	5.12	121.13	110.90
1	A	51	THR	CA-C-N	5.12	126.43	116.20
1	D	185	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	75	THR	CB-CA-C	-5.10	97.82	111.60
1	B	183	ASN	CB-CA-C	-5.10	100.20	110.40
1	D	94	GLY	CA-C-N	-5.10	105.98	117.20
1	C	34	LEU	CB-CG-CD2	5.10	119.67	111.00
1	C	97	ASN	N-CA-C	5.10	124.76	111.00
1	D	208	LEU	CB-CG-CD2	5.08	119.64	111.00
1	B	114	SER	CB-CA-C	5.08	119.75	110.10
1	D	231	ALA	N-CA-CB	5.08	117.21	110.10
1	B	75	THR	N-CA-CB	5.07	119.94	110.30
1	C	42	ARG	CD-NE-CZ	5.07	130.70	123.60
1	B	135	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	D	134	VAL	N-CA-C	5.06	124.66	111.00
1	C	169	LYS	CD-CE-NZ	-5.05	100.08	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	TYR	CZ-CE2-CD2	5.05	124.34	119.80
1	A	175	ARG	CB-CG-CD	5.03	124.68	111.60
1	B	41	LEU	C-N-CA	-5.03	109.12	121.70
1	C	259	LEU	CA-CB-CG	5.02	126.85	115.30
1	B	33	TYR	N-CA-CB	-5.02	101.57	110.60
1	D	291	PHE	C-N-CA	-5.02	109.15	121.70
1	D	73	LEU	N-CA-C	-5.01	97.47	111.00
1	D	247	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	B	182	TRP	N-CA-C	-5.01	97.47	111.00
1	A	175	ARG	N-CA-CB	-5.00	101.60	110.60
1	C	92	ILE	CG1-CB-CG2	-5.00	100.40	111.40

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	PRO	Peptide
1	A	200	GLN	Mainchain
1	A	202	TYR	Mainchain
1	A	286	GLU	Peptide
1	A	70	GLU	Mainchain,Peptide
1	B	114	SER	Peptide
1	B	123	PHE	Peptide
1	B	222	GLY	Peptide
1	B	304	HIS	Peptide
1	B	54	GLY	Peptide
1	B	69	ASP	Peptide
1	C	120	SER	Peptide
1	C	121	LEU	Peptide
1	C	127	GLU	Mainchain
1	C	138	GLN	Peptide
1	C	282	LEU	Peptide
1	C	283	ARG	Peptide
1	C	284	LYS	Peptide
1	C	285	VAL	Peptide
1	C	304	HIS	Peptide
1	C	92	ILE	Peptide
1	D	110	ASP	Peptide
1	D	174	ASP	Peptide
1	D	245	PRO	Peptide
1	D	92	ILE	Mainchain

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	A	2287	0	2257	306	0
1	B	2270	0	2232	351	0
1	C	2287	0	2258	316	0
1	D	2287	0	2259	392	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	B	5	0	0	7	0
3	D	5	0	0	4	0
4	A	6	0	0	0	0
4	B	7	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
All	All	9174	0	9006	1310	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 72.

All (1310) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CZ	1:A:201:PHE:CE2	1.74	1.64
1:B:107:LYS:CD	1:B:107:LYS:CE	1.74	1.64
1:B:244:LYS:CD	1:B:244:LYS:CG	1.77	1.62
1:D:266:LYS:CB	1:D:266:LYS:CG	1.75	1.62
1:A:221:LEU:CD2	1:A:221:LEU:CG	1.75	1.62
1:C:292:LYS:CD	1:C:292:LYS:CG	1.74	1.61
1:C:221:LEU:CD1	1:C:221:LEU:CG	1.74	1.60
1:D:47:LYS:CD	1:D:47:LYS:CE	1.77	1.59
1:C:280:ARG:CD	1:C:280:ARG:CG	1.79	1.56
1:A:284:LYS:CG	1:A:284:LYS:CD	1.79	1.56
1:C:292:LYS:CD	1:C:292:LYS:CE	1.83	1.55
1:C:244:LYS:CE	1:C:244:LYS:NZ	1.68	1.53
1:D:307:ILE:CG1	1:D:307:ILE:CD1	1.85	1.53
1:A:185:ARG:CG	1:A:185:ARG:CD	1.83	1.53
1:C:38:GLN:CD	1:C:38:GLN:CG	1.79	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD23	1:B:301:TYR:CE1	1.43	1.50
1:A:38:GLN:CD	1:A:38:GLN:CG	1.80	1.48
1:D:43:CYS:SG	1:D:43:CYS:CB	2.01	1.47
1:C:292:LYS:CE	1:C:292:LYS:NZ	1.77	1.46
1:C:26:PRO:CG	1:C:26:PRO:CB	1.82	1.46
1:A:26:PRO:CB	1:A:26:PRO:CG	1.80	1.43
1:D:97:ASN:ND2	1:D:99:LYS:HB2	1.23	1.43
1:A:263:GLU:HB3	1:A:264:PRO:CD	1.43	1.41
1:C:115:ARG:NH2	1:C:128:GLU:HB3	1.26	1.40
1:D:188:PRO:CB	1:D:188:PRO:CG	1.74	1.39
1:B:73:LEU:HD23	1:B:301:TYR:CZ	1.61	1.34
1:D:245:PRO:CG	1:D:245:PRO:CB	1.80	1.28
1:C:160:GLN:O	1:C:164:VAL:HG23	1.10	1.28
1:C:115:ARG:HH21	1:C:128:GLU:CB	1.56	1.19
1:B:73:LEU:CD2	1:B:301:TYR:CZ	2.25	1.17
1:C:115:ARG:NH2	1:C:128:GLU:CB	2.07	1.17
1:A:260:ASN:ND2	1:A:260:ASN:H	1.33	1.17
1:D:308:LYS:C	1:D:308:LYS:HD2	1.63	1.16
1:B:32:GLN:HE21	1:B:32:GLN:HA	1.11	1.15
1:B:177:ILE:CG2	1:B:201:PHE:H	1.59	1.15
1:B:305:PRO:CB	1:B:306:THR:HA	1.63	1.15
1:A:260:ASN:HD22	1:A:260:ASN:N	1.38	1.15
1:C:240:ILE:HG22	1:C:241:THR:HG22	1.27	1.14
1:D:97:ASN:ND2	1:D:99:LYS:CB	2.09	1.14
1:C:115:ARG:CZ	1:C:128:GLU:HB3	1.76	1.14
1:B:177:ILE:HG22	1:B:201:PHE:H	1.03	1.14
1:B:160:GLN:HE22	1:B:180:CYS:N	1.45	1.13
1:B:287:LYS:HD3	1:B:288:ILE:H	0.97	1.13
1:A:263:GLU:CB	1:A:264:PRO:HD3	1.76	1.13
1:C:240:ILE:HG22	1:C:241:THR:CG2	1.80	1.11
1:B:287:LYS:HD3	1:B:288:ILE:N	1.65	1.11
1:C:119:ASP:HA	1:C:122:GLY:HA3	1.30	1.11
1:C:107:LYS:HA	1:C:110:ASP:OD1	1.51	1.10
1:A:176:ARG:HH12	1:B:193:PRO:HG2	1.04	1.09
1:A:50:ARG:HH11	1:B:176:ARG:NH2	1.48	1.09
1:B:287:LYS:CD	1:B:288:ILE:HG22	1.81	1.08
1:D:53:THR:HG22	1:D:54:GLY:O	1.53	1.08
1:C:160:GLN:O	1:C:164:VAL:CG2	2.00	1.08
1:C:148:ASP:OD2	1:C:151:SER:HB2	1.54	1.07
1:B:215:ARG:HG2	1:B:215:ARG:HH11	1.17	1.07
1:D:112:ASN:ND2	1:D:191:ALA:HB1	1.70	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:SER:OG	1:D:100:GLU:OE2	1.68	1.07
1:A:176:ARG:HH12	1:B:193:PRO:CG	1.66	1.07
1:D:183:ASN:HB3	1:D:186:ASP:HB2	1.34	1.06
1:C:50:ARG:HA	1:C:50:ARG:HE	0.98	1.06
1:D:204:VAL:O	1:D:207:GLU:HB2	1.54	1.06
1:D:115:ARG:HH21	1:D:127:GLU:HA	1.15	1.06
1:B:97:ASN:HB2	1:B:149:MET:SD	1.95	1.06
1:B:73:LEU:HD21	1:B:301:TYR:OH	1.55	1.05
1:D:176:ARG:HH12	3:D:616:PO4:P	1.80	1.05
1:A:74:LEU:CD1	1:A:224:PRO:HB3	1.85	1.05
1:D:138:GLN:HA	1:D:138:GLN:OE1	1.57	1.05
1:A:74:LEU:HD12	1:A:224:PRO:CB	1.87	1.05
1:B:160:GLN:NE2	1:B:180:CYS:H	1.55	1.04
1:A:257:ILE:HD11	1:A:262:ILE:HG13	1.34	1.04
1:A:67:LEU:O	1:A:69:ASP:N	1.89	1.04
1:B:85:LEU:HD12	1:B:85:LEU:O	1.56	1.04
1:C:292:LYS:O	1:C:295:ASP:N	1.91	1.03
1:B:73:LEU:CD2	1:B:301:TYR:CE1	2.39	1.03
1:B:32:GLN:NE2	1:B:32:GLN:HA	1.73	1.03
1:A:288:ILE:O	1:A:288:ILE:HG13	1.54	1.03
1:D:198:LEU:HD12	1:D:198:LEU:C	1.76	1.03
1:D:280:ARG:HD2	1:D:299:GLU:OE2	1.58	1.02
1:A:292:LYS:HE3	1:A:292:LYS:HA	1.32	1.02
1:C:263:GLU:OE1	1:C:263:GLU:HA	1.23	1.02
1:B:32:GLN:CA	1:B:32:GLN:HE21	1.72	1.01
1:A:195:CYS:O	1:A:214:GLN:HA	1.60	1.01
1:B:287:LYS:CD	1:B:288:ILE:H	1.73	1.01
1:B:100:GLU:O	1:B:103:SER:HB2	1.61	1.01
1:C:72:PRO:HA	1:C:276:PHE:CE1	1.96	1.01
1:B:119:ASP:OD1	1:B:122:GLY:HA2	1.60	1.01
1:C:203:VAL:O	1:C:204:VAL:HG23	1.58	1.00
1:B:305:PRO:HB2	1:B:306:THR:HA	1.42	1.00
1:C:263:GLU:OE1	1:C:266:LYS:HD3	1.61	1.00
1:C:260:ASN:H	1:C:260:ASN:ND2	1.48	1.00
1:B:76:THR:O	1:B:305:PRO:HD3	1.63	0.98
1:C:50:ARG:HA	1:C:50:ARG:NE	1.77	0.98
1:A:240:ILE:HD11	1:A:288:ILE:HA	1.43	0.98
1:A:221:LEU:CD2	1:A:221:LEU:HG	1.92	0.97
1:D:235:TYR:O	1:D:238:ALA:HB3	1.63	0.97
1:B:287:LYS:HD3	1:B:288:ILE:HG22	1.45	0.97
1:C:76:THR:HB	1:C:268:GLN:HE21	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:NH1	1:B:193:PRO:CG	2.26	0.97
1:C:257:ILE:HD11	1:C:262:ILE:HG13	1.47	0.97
1:C:119:ASP:HA	1:C:122:GLY:CA	1.96	0.96
1:C:263:GLU:CA	1:C:263:GLU:OE1	2.13	0.95
1:C:50:ARG:CA	1:C:50:ARG:HE	1.78	0.95
1:D:209:SER:HB3	1:D:247:ASP:O	1.65	0.95
1:D:286:GLU:HA	1:D:286:GLU:OE1	1.65	0.95
1:D:40:ILE:HG21	1:D:257:ILE:HG13	1.44	0.95
1:B:73:LEU:CD2	1:B:301:TYR:OH	2.13	0.95
1:B:148:ASP:OD1	1:B:150:GLU:N	2.00	0.95
1:D:112:ASN:HD22	1:D:191:ALA:HB1	1.28	0.94
1:C:92:ILE:O	1:C:140:ARG:NH1	2.00	0.94
1:A:257:ILE:CD1	1:A:262:ILE:HG13	1.98	0.94
1:B:29:GLY:O	1:B:32:GLN:HB2	1.67	0.94
1:B:287:LYS:HG3	1:B:289:ASP:OD1	1.67	0.94
1:B:287:LYS:HD2	1:B:288:ILE:HG22	1.50	0.93
1:C:260:ASN:H	1:C:260:ASN:HD22	0.97	0.93
1:D:149:MET:HG3	1:D:150:GLU:H	1.33	0.93
1:D:97:ASN:HD22	1:D:99:LYS:HB2	1.18	0.93
1:D:144:ALA:HB2	1:D:156:GLN:O	1.67	0.93
1:C:143:GLY:HA2	1:D:185:ARG:NH2	1.84	0.93
1:D:135:TYR:C	1:D:137:PHE:H	1.73	0.92
1:D:26:PRO:N	1:D:27:PRO:HD2	1.81	0.92
1:B:301:TYR:O	1:B:303:PRO:HD3	1.70	0.92
1:B:161:LEU:O	1:B:164:VAL:HB	1.69	0.91
1:B:299:GLU:O	1:B:301:TYR:N	2.03	0.91
1:C:119:ASP:CA	1:C:122:GLY:HA3	2.00	0.91
1:A:176:ARG:NH1	1:B:193:PRO:HG2	1.82	0.91
1:A:263:GLU:CB	1:A:264:PRO:CD	2.26	0.90
1:A:187:LEU:HA	1:A:190:MET:HE3	1.51	0.90
1:D:78:ARG:NH1	1:D:303:PRO:HG2	1.86	0.90
1:C:97:ASN:HB2	1:C:149:MET:SD	2.10	0.90
1:A:72:PRO:HA	1:A:276:PHE:CE1	2.06	0.90
1:B:39:HIS:O	1:B:43:CYS:HB2	1.70	0.89
1:B:283:ARG:HG2	1:B:284:LYS:H	1.38	0.89
1:B:177:ILE:HG22	1:B:201:PHE:N	1.86	0.89
1:B:143:GLY:HA2	1:B:185:ARG:HH22	1.33	0.89
1:D:176:ARG:NH1	3:D:616:PO4:P	2.44	0.89
1:C:143:GLY:CA	1:D:185:ARG:NH2	2.36	0.89
1:D:101:LEU:HD23	1:D:102:SER:N	1.87	0.89
1:C:204:VAL:HG11	1:D:45:VAL:HG21	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HH21	1:A:246:GLY:HA2	1.36	0.89
1:B:299:GLU:O	1:B:300:GLY:C	2.10	0.89
1:D:160:GLN:O	1:D:164:VAL:HG23	1.74	0.88
1:D:292:LYS:O	1:D:295:ASP:OD2	1.90	0.88
1:D:112:ASN:HD22	1:D:191:ALA:CB	1.85	0.88
1:D:223:VAL:O	1:D:227:ILE:HG12	1.72	0.88
1:D:133:PRO:O	1:D:190:MET:CE	2.22	0.88
1:C:186:ASP:O	1:C:190:MET:HG2	1.74	0.87
1:B:110:ASP:O	1:B:112:ASN:N	2.06	0.87
1:D:198:LEU:CD1	1:D:198:LEU:C	2.42	0.87
1:B:177:ILE:O	1:B:177:ILE:CG2	2.21	0.87
1:D:203:VAL:CG2	1:D:208:LEU:HD13	2.04	0.87
1:A:279:LEU:HD12	1:A:280:ARG:N	1.89	0.87
1:C:130:ASP:HB2	1:C:149:MET:HG2	1.56	0.87
1:D:108:ILE:O	1:D:108:ILE:HG13	1.72	0.87
1:B:115:ARG:HD3	1:B:128:GLU:OE2	1.74	0.87
1:C:221:LEU:CD1	1:C:221:LEU:HG	2.06	0.86
1:A:185:ARG:CG	1:A:185:ARG:NE	2.38	0.86
1:A:187:LEU:HA	1:A:190:MET:CE	2.04	0.86
1:C:101:LEU:O	1:C:104:LYS:HB2	1.75	0.86
1:B:176:ARG:NH1	3:B:616:PO4:O3	2.09	0.86
1:A:102:SER:HB2	1:A:110:ASP:OD2	1.75	0.85
1:D:37:ILE:CG2	1:D:269:LEU:HD21	2.07	0.85
1:B:177:ILE:O	1:B:177:ILE:HG22	1.72	0.85
1:B:176:ARG:NH1	3:B:616:PO4:P	2.49	0.85
1:B:289:ASP:N	1:B:289:ASP:OD1	2.09	0.85
1:D:176:ARG:NH1	3:D:616:PO4:O4	2.09	0.85
1:B:211:GLN:HG3	1:B:249:ILE:HB	1.55	0.85
1:B:304:HIS:HB2	1:B:305:PRO:HA	1.59	0.85
1:A:187:LEU:HD23	1:A:190:MET:HE3	1.57	0.84
1:D:67:LEU:HB2	1:D:245:PRO:HB2	1.57	0.84
1:A:70:GLU:OE1	1:A:276:PHE:HD2	1.60	0.84
1:B:273:PRO:HA	1:B:304:HIS:CE1	2.13	0.84
1:B:172:PRO:CB	1:B:203:VAL:HG11	2.08	0.83
1:D:150:GLU:OE1	1:D:150:GLU:N	2.12	0.83
1:B:305:PRO:CB	1:B:306:THR:CA	2.55	0.83
1:C:239:HIS:HE1	1:C:284:LYS:HG3	1.42	0.83
1:D:196:HIS:CE1	1:D:226:ASN:ND2	2.47	0.83
1:C:239:HIS:CE1	1:C:284:LYS:HG3	2.14	0.83
1:D:301:TYR:CZ	1:D:303:PRO:HG3	2.13	0.82
1:C:198:LEU:C	1:C:198:LEU:HD12	2.00	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:SER:O	1:B:105:GLY:N	2.12	0.82
1:A:68:ARG:HH21	1:A:246:GLY:CA	1.90	0.82
1:D:37:ILE:HG21	1:D:269:LEU:HD21	1.61	0.82
1:C:69:ASP:OD1	1:C:69:ASP:C	2.17	0.82
1:B:152:ASP:OD2	1:B:154:SER:HB3	1.80	0.82
1:C:260:ASN:HD22	1:C:260:ASN:N	1.76	0.82
1:D:133:PRO:C	1:D:190:MET:HE2	1.99	0.82
1:D:115:ARG:NH2	1:D:127:GLU:HA	1.93	0.82
1:A:183:ASN:HB3	1:A:186:ASP:HB2	1.61	0.82
1:D:133:PRO:O	1:D:190:MET:HE1	1.78	0.82
1:D:73:LEU:HD12	1:D:228:ALA:HB2	1.59	0.81
1:D:80:PHE:O	1:D:83:GLY:N	2.12	0.81
1:B:177:ILE:CG2	1:B:201:PHE:N	2.42	0.81
1:C:184:PRO:HA	1:C:187:LEU:CD1	2.11	0.81
1:C:119:ASP:C	1:C:122:GLY:HA3	2.01	0.81
1:B:283:ARG:CG	1:B:284:LYS:H	1.94	0.81
1:A:85:LEU:O	1:A:85:LEU:HD12	1.79	0.81
1:A:85:LEU:HD11	1:A:89:LEU:HD11	1.63	0.81
1:B:184:PRO:HA	1:B:187:LEU:HD12	1.63	0.81
1:D:232:LEU:O	1:D:235:TYR:N	2.14	0.81
1:B:292:LYS:N	1:B:295:ASP:OD1	2.14	0.81
1:B:165:ILE:HG21	1:B:287:LYS:NZ	1.96	0.80
1:B:215:ARG:HG2	1:B:215:ARG:NH1	1.90	0.80
1:A:292:LYS:HE3	1:A:292:LYS:CA	2.10	0.80
1:D:37:ILE:HG21	1:D:269:LEU:CD2	2.11	0.80
1:C:240:ILE:CG2	1:C:241:THR:HG22	2.08	0.80
1:A:30:GLU:HG3	1:A:74:LEU:HD22	1.63	0.80
1:C:32:GLN:HE22	1:C:64:ARG:H	1.26	0.80
1:A:263:GLU:HB3	1:A:264:PRO:HD3	0.80	0.80
1:B:100:GLU:O	1:B:103:SER:CB	2.28	0.80
1:A:50:ARG:HH11	1:B:176:ARG:HH21	1.27	0.80
1:D:196:HIS:NE2	1:D:226:ASN:ND2	2.29	0.80
1:B:37:ILE:HG22	1:B:38:GLN:N	1.94	0.80
1:C:140:ARG:O	1:C:159:ASP:HA	1.82	0.80
1:B:73:LEU:HD21	1:B:301:TYR:CZ	2.14	0.80
1:C:76:THR:HB	1:C:268:GLN:NE2	1.96	0.80
1:A:56:LEU:HD13	1:A:259:LEU:HD23	1.63	0.79
1:A:279:LEU:O	1:A:280:ARG:NH1	2.15	0.79
1:D:86:GLU:OE2	1:D:104:LYS:NZ	2.15	0.79
1:A:176:ARG:NH1	1:B:193:PRO:HG3	1.96	0.79
1:A:99:LYS:HG3	1:A:129:GLY:HA3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:OE1	1:C:76:THR:OG1	2.00	0.79
1:C:143:GLY:HA2	1:D:185:ARG:HH21	1.47	0.79
1:C:184:PRO:O	1:C:185:ARG:C	2.17	0.79
1:B:239:HIS:HD1	1:B:281:ILE:HD13	1.47	0.79
1:C:130:ASP:CB	1:C:149:MET:HG2	2.13	0.78
1:B:305:PRO:HB3	1:B:306:THR:HA	1.63	0.78
1:D:135:TYR:O	1:D:137:PHE:N	2.15	0.78
1:B:176:ARG:HH12	3:B:616:PO4:P	2.05	0.78
1:B:305:PRO:HB2	1:B:306:THR:CA	2.11	0.78
1:C:260:ASN:ND2	1:C:260:ASN:N	2.28	0.78
1:C:140:ARG:HD2	1:C:140:ARG:N	1.98	0.78
1:B:73:LEU:HD23	1:B:301:TYR:HE1	1.45	0.78
1:C:88:LEU:O	1:C:91:PHE:HB2	1.83	0.78
1:A:269:LEU:HD12	1:A:269:LEU:O	1.84	0.78
1:A:307:ILE:O	1:A:308:LYS:NZ	2.14	0.77
1:C:204:VAL:CG2	1:D:47:LYS:HD2	2.14	0.77
1:B:151:SER:O	1:B:153:TYR:CD1	2.36	0.77
1:C:91:PHE:CE1	1:C:135:TYR:HB2	2.19	0.77
1:C:147:ARG:N	1:C:153:TYR:OH	2.17	0.77
1:A:97:ASN:HB2	1:A:149:MET:HE3	1.65	0.77
1:C:145:GLU:OE1	1:C:185:ARG:NH2	2.17	0.77
1:B:135:TYR:HE1	1:B:196:HIS:HB2	1.50	0.77
1:C:48:ASP:N	1:C:48:ASP:OD2	2.13	0.77
1:A:307:ILE:HD12	1:A:308:LYS:H	1.47	0.77
1:A:184:PRO:O	1:A:188:PRO:HD3	1.85	0.77
1:A:176:ARG:CZ	1:B:193:PRO:HG3	2.15	0.77
1:C:239:HIS:NE2	1:C:284:LYS:HB2	1.99	0.77
1:D:164:VAL:HG13	1:D:177:ILE:HG22	1.67	0.77
1:D:73:LEU:HD12	1:D:228:ALA:CB	2.14	0.76
1:D:183:ASN:CB	1:D:186:ASP:HB2	2.13	0.76
1:A:67:LEU:O	1:A:69:ASP:CA	2.33	0.76
1:C:178:ILE:HG22	1:C:199:CYS:O	1.84	0.76
1:C:76:THR:CB	1:C:268:GLN:HE21	1.98	0.76
1:C:139:TRP:C	1:C:140:ARG:HD2	2.05	0.76
1:C:274:ARG:HD2	1:C:304:HIS:CD2	2.21	0.76
1:C:187:LEU:HB2	1:C:188:PRO:HD3	1.67	0.76
1:D:135:TYR:C	1:D:137:PHE:N	2.37	0.76
1:A:85:LEU:C	1:A:85:LEU:HD12	2.06	0.76
1:A:85:LEU:HD12	1:A:89:LEU:HD12	1.68	0.75
1:D:94:GLY:HA3	1:D:136:GLY:O	1.85	0.75
1:A:67:LEU:O	1:A:69:ASP:HA	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:CE1	1:A:194:PRO:HB3	2.21	0.75
1:A:187:LEU:O	1:A:189:LEU:N	2.19	0.75
1:D:296:PHE:O	1:D:297:GLN:HG3	1.86	0.75
1:D:79:VAL:HG11	1:D:225:PHE:HA	1.67	0.75
1:C:283:ARG:HG2	1:C:285:VAL:CG2	2.16	0.75
1:C:32:GLN:HE22	1:C:64:ARG:N	1.85	0.74
1:B:172:PRO:HB3	1:B:203:VAL:HG11	1.67	0.74
1:C:213:TYR:HD2	1:D:213:TYR:HD1	1.35	0.74
1:B:28:HIS:ND1	1:B:29:GLY:N	2.34	0.74
1:B:288:ILE:O	1:B:291:PHE:HD2	1.70	0.74
1:B:163:ARG:HA	1:B:166:ASP:OD1	1.87	0.74
1:A:74:LEU:HD12	1:A:224:PRO:HB3	0.91	0.74
1:D:97:ASN:HD21	1:D:99:LYS:CG	2.00	0.74
1:C:257:ILE:O	1:C:257:ILE:HG13	1.82	0.74
1:C:199:CYS:HA	1:C:211:GLN:O	1.88	0.74
1:C:185:ARG:O	1:C:188:PRO:HD2	1.87	0.73
1:D:213:TYR:C	1:D:213:TYR:CD2	2.60	0.73
1:D:112:ASN:ND2	1:D:191:ALA:CB	2.46	0.73
1:B:143:GLY:HA2	1:B:185:ARG:NH2	2.02	0.73
1:B:47:LYS:O	1:B:55:THR:HB	1.88	0.73
1:D:97:ASN:HD21	1:D:99:LYS:HG3	1.53	0.73
1:D:115:ARG:HG2	1:D:128:GLU:OE1	1.88	0.73
1:B:287:LYS:HD3	1:B:288:ILE:CG2	2.17	0.73
1:D:203:VAL:HG22	1:D:208:LEU:HD13	1.70	0.73
1:C:192:LEU:HD13	1:C:192:LEU:O	1.88	0.73
1:D:80:PHE:CE1	1:D:82:LYS:HB2	2.24	0.72
1:B:231:ALA:O	1:B:234:THR:N	2.22	0.72
1:D:203:VAL:HA	1:D:207:GLU:O	1.89	0.72
1:A:192:LEU:N	1:A:192:LEU:HD12	2.04	0.72
1:D:270:GLN:OE1	1:D:270:GLN:HA	1.88	0.72
1:B:32:GLN:CA	1:B:32:GLN:NE2	2.41	0.72
1:C:178:ILE:HG23	1:C:200:GLN:HB2	1.70	0.72
1:C:148:ASP:OD2	1:C:151:SER:CB	2.35	0.72
1:D:308:LYS:C	1:D:308:LYS:CD	2.46	0.72
1:A:185:ARG:HB3	1:A:185:ARG:NH2	2.04	0.72
1:D:239:HIS:ND1	1:D:281:ILE:HD13	2.04	0.72
1:C:292:LYS:N	1:C:295:ASP:OD1	2.23	0.72
1:A:50:ARG:NH1	1:B:176:ARG:NH2	2.33	0.72
1:B:172:PRO:HB2	1:B:203:VAL:CG1	2.20	0.72
1:B:75:THR:O	1:B:77:LYS:N	2.23	0.72
1:A:149:MET:O	1:A:150:GLU:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ARG:HH22	1:C:307:ILE:HG22	1.54	0.72
1:C:308:LYS:HA	1:C:308:LYS:HE2	1.72	0.71
1:D:26:PRO:N	1:D:27:PRO:CD	2.52	0.71
1:D:213:TYR:HD2	1:D:213:TYR:O	1.72	0.71
1:B:239:HIS:CE1	1:B:281:ILE:HG21	2.25	0.71
1:C:285:VAL:CG1	1:C:286:GLU:H	2.04	0.71
1:D:101:LEU:HA	1:D:104:LYS:HE3	1.73	0.71
1:C:240:ILE:HG22	1:C:241:THR:HG23	1.68	0.71
1:D:54:GLY:HA3	1:D:259:LEU:HD11	1.71	0.71
1:D:138:GLN:OE1	1:D:138:GLN:CA	2.38	0.71
1:B:263:GLU:HG2	1:B:266:LYS:NZ	2.06	0.71
1:D:80:PHE:CE1	1:D:82:LYS:CB	2.74	0.70
1:A:91:PHE:CD1	1:A:135:TYR:HB2	2.25	0.70
1:B:283:ARG:HG2	1:B:284:LYS:N	2.06	0.70
1:C:258:TYR:HB3	1:C:260:ASN:HD21	1.57	0.70
1:B:143:GLY:CA	1:B:185:ARG:HH22	2.05	0.70
1:A:85:LEU:CD1	1:A:89:LEU:CD1	2.70	0.70
1:B:176:ARG:NH1	3:B:616:PO4:O1	2.25	0.70
1:A:130:ASP:CG	1:A:149:MET:HG2	2.10	0.70
1:B:160:GLN:HE22	1:B:180:CYS:H	0.77	0.70
1:D:80:PHE:O	1:D:84:VAL:HG23	1.91	0.70
1:A:68:ARG:NH2	1:A:246:GLY:HA2	2.07	0.70
1:A:85:LEU:CD1	1:A:89:LEU:HD11	2.22	0.69
1:A:148:ASP:OD1	1:A:150:GLU:N	2.24	0.69
1:D:265:LEU:HA	1:D:268:GLN:HB3	1.74	0.69
1:A:67:LEU:C	1:A:69:ASP:N	2.41	0.69
1:B:119:ASP:HA	1:B:122:GLY:N	2.07	0.69
1:B:274:ARG:CZ	1:B:304:HIS:HD2	2.06	0.69
1:C:93:LYS:NZ	1:C:100:GLU:HG3	2.07	0.69
1:D:47:LYS:O	1:D:55:THR:HG22	1.92	0.69
1:C:115:ARG:NH2	1:C:128:GLU:CA	2.54	0.69
1:B:133:PRO:HG2	1:B:190:MET:HG3	1.75	0.69
1:C:112:ASN:HD22	1:C:112:ASN:H	1.41	0.69
1:A:259:LEU:O	1:A:260:ASN:C	2.29	0.69
1:B:282:LEU:HD11	1:B:297:GLN:HG2	1.74	0.69
1:B:277:PRO:HB3	1:B:301:TYR:CD1	2.27	0.69
1:D:164:VAL:HG13	1:D:177:ILE:CG2	2.23	0.69
1:D:280:ARG:HD2	1:D:299:GLU:CD	2.12	0.69
1:A:240:ILE:CD1	1:A:288:ILE:HA	2.20	0.69
1:A:288:ILE:HG23	1:A:289:ASP:N	2.07	0.69
1:D:220:GLY:C	1:D:221:LEU:HG	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ASP:OD2	1:D:166:ASP:N	2.16	0.69
1:A:76:THR:OG1	1:A:268:GLN:NE2	2.22	0.69
1:D:91:PHE:O	1:D:136:GLY:HA2	1.93	0.69
1:D:133:PRO:O	1:D:190:MET:HE2	1.90	0.69
1:A:32:GLN:NE2	1:A:64:ARG:H	1.91	0.69
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.74	0.69
1:C:215:ARG:HD2	1:D:175:ARG:O	1.91	0.69
1:C:47:LYS:O	1:C:55:THR:N	2.23	0.68
1:A:97:ASN:HB3	1:A:100:GLU:H	1.59	0.68
1:D:47:LYS:O	1:D:55:THR:CG2	2.41	0.68
1:A:115:ARG:HH22	1:A:127:GLU:HA	1.58	0.68
1:D:279:LEU:HG	1:D:280:ARG:N	2.08	0.68
1:C:118:LEU:O	1:C:122:GLY:O	2.12	0.68
1:A:59:PHE:O	1:B:64:ARG:NH1	2.25	0.68
1:D:223:VAL:O	1:D:227:ILE:CG1	2.41	0.68
1:B:267:ILE:O	1:B:270:GLN:N	2.24	0.68
1:D:97:ASN:HB3	1:D:100:GLU:HG3	1.74	0.68
1:D:97:ASN:CG	1:D:99:LYS:HB2	2.07	0.67
1:B:262:ILE:HG22	1:B:263:GLU:N	2.09	0.67
1:A:81:TRP:CD2	1:A:298:ILE:HD11	2.29	0.67
1:D:115:ARG:NH2	1:D:126:ARG:O	2.27	0.67
1:B:187:LEU:H	1:B:188:PRO:HD2	1.58	0.67
1:D:101:LEU:C	1:D:103:SER:N	2.45	0.67
1:C:285:VAL:CG1	1:C:286:GLU:N	2.57	0.67
1:B:177:ILE:HG21	1:B:201:PHE:HB2	1.77	0.67
1:B:205:ASN:O	1:B:206:SER:HB2	1.93	0.67
1:A:134:VAL:O	1:A:135:TYR:C	2.32	0.67
1:B:283:ARG:CG	1:B:284:LYS:N	2.57	0.67
1:A:171:ASN:O	1:A:174:ASP:HB2	1.95	0.67
1:D:54:GLY:C	1:D:259:LEU:HD11	2.14	0.67
1:D:96:THR:CG2	1:D:134:VAL:CG2	2.73	0.67
1:D:225:PHE:O	1:D:226:ASN:C	2.32	0.67
1:D:165:ILE:HG22	1:D:166:ASP:N	2.10	0.67
1:A:204:VAL:HG21	1:B:45:VAL:CG2	2.24	0.67
1:A:91:PHE:CE1	1:A:135:TYR:HB2	2.30	0.66
1:A:31:LEU:HD22	1:A:273:PRO:HG2	1.77	0.66
1:D:54:GLY:CA	1:D:259:LEU:HD11	2.24	0.66
1:D:281:ILE:HA	1:D:295:ASP:O	1.96	0.66
1:B:97:ASN:ND2	1:B:100:GLU:H	1.92	0.66
1:B:188:PRO:O	1:B:190:MET:N	2.28	0.66
1:D:135:TYR:HD2	1:D:135:TYR:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ASN:ND2	1:D:99:LYS:CG	2.58	0.66
1:A:85:LEU:HD12	1:A:89:LEU:CD1	2.25	0.66
1:C:98:ALA:HB2	1:C:131:LEU:HD21	1.78	0.66
1:C:88:LEU:HD22	1:C:232:LEU:HD23	1.76	0.66
1:C:72:PRO:HA	1:C:276:PHE:CZ	2.30	0.66
1:D:274:ARG:HH11	1:D:274:ARG:CG	2.09	0.66
1:D:213:TYR:O	1:D:213:TYR:CD2	2.49	0.65
1:A:28:HIS:HB3	1:A:31:LEU:HD23	1.78	0.65
1:C:257:ILE:HD11	1:C:262:ILE:CG1	2.24	0.65
1:A:187:LEU:HD23	1:A:190:MET:CE	2.26	0.65
1:D:130:ASP:OD1	1:D:149:MET:HG2	1.97	0.65
1:C:283:ARG:HG2	1:C:285:VAL:HG22	1.76	0.65
1:D:274:ARG:HH11	1:D:274:ARG:HB2	1.61	0.65
1:C:69:ASP:O	1:C:69:ASP:OD1	2.13	0.65
1:A:140:ARG:O	1:A:141:HIS:CG	2.49	0.65
1:A:192:LEU:H	1:A:192:LEU:HD12	1.61	0.65
1:D:163:ARG:O	1:D:164:VAL:C	2.29	0.65
1:D:88:LEU:O	1:D:91:PHE:N	2.30	0.65
1:A:176:ARG:NH2	1:B:193:PRO:HG3	2.12	0.65
1:A:149:MET:O	1:A:149:MET:HE2	1.97	0.65
1:A:184:PRO:HA	1:A:187:LEU:HG	1.78	0.65
1:C:186:ASP:O	1:C:189:LEU:HB2	1.97	0.65
1:A:260:ASN:ND2	1:A:260:ASN:N	2.09	0.65
1:C:288:ILE:HD13	1:C:291:PHE:HD2	1.60	0.65
1:A:298:ILE:HG22	1:A:299:GLU:N	2.11	0.65
1:D:30:GLU:HG2	1:D:30:GLU:O	1.94	0.65
1:C:204:VAL:HG23	1:D:47:LYS:HD2	1.79	0.65
1:D:169:LYS:HD2	1:D:241:THR:HG22	1.78	0.65
1:B:223:VAL:O	1:B:227:ILE:HG13	1.96	0.65
1:B:172:PRO:CB	1:B:203:VAL:CG1	2.75	0.65
1:A:55:THR:HG22	1:A:258:TYR:HA	1.78	0.65
1:C:90:TRP:CE3	1:C:101:LEU:HD22	2.32	0.65
1:B:278:LYS:HB3	1:B:299:GLU:HB3	1.78	0.64
1:C:88:LEU:O	1:C:92:ILE:HG12	1.96	0.64
1:B:97:ASN:HA	1:B:129:GLY:O	1.95	0.64
1:B:76:THR:C	1:B:305:PRO:HD3	2.16	0.64
1:D:261:HIS:C	1:D:264:PRO:HD2	2.18	0.64
1:A:279:LEU:HD12	1:A:279:LEU:C	2.15	0.64
1:D:30:GLU:OE1	1:D:74:LEU:HB3	1.97	0.64
1:B:88:LEU:HD21	1:B:233:LEU:HD13	1.78	0.64
1:B:272:GLU:O	1:B:304:HIS:CE1	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:LYS:O	1:D:285:VAL:HG22	1.98	0.64
1:B:177:ILE:O	1:B:200:GLN:HA	1.98	0.64
1:D:259:LEU:O	1:D:260:ASN:C	2.35	0.64
1:A:195:CYS:O	1:A:214:GLN:CA	2.43	0.64
1:B:178:ILE:HG22	1:B:179:MET:N	2.13	0.64
1:A:114:SER:HB2	1:A:116:ASP:OD2	1.97	0.64
1:D:126:ARG:HD2	1:D:130:ASP:CG	2.18	0.64
1:D:89:LEU:HD22	1:D:291:PHE:O	1.98	0.64
1:C:115:ARG:HH21	1:C:128:GLU:CA	2.07	0.64
1:A:288:ILE:O	1:A:288:ILE:CG1	2.37	0.64
1:C:292:LYS:HG3	1:C:294:GLU:OE1	1.97	0.64
1:B:177:ILE:C	1:B:178:ILE:HG13	2.16	0.64
1:D:261:HIS:O	1:D:264:PRO:HD2	1.97	0.64
1:B:105:GLY:C	1:B:106:VAL:CG2	2.66	0.64
1:B:40:ILE:HG21	1:B:257:ILE:HD12	1.79	0.64
1:D:307:ILE:HG23	1:D:308:LYS:H	1.62	0.64
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.28	0.64
1:D:160:GLN:O	1:D:161:LEU:C	2.35	0.64
1:B:198:LEU:C	1:B:198:LEU:HD12	2.18	0.64
1:C:204:VAL:CG1	1:D:45:VAL:HG21	2.27	0.63
1:B:165:ILE:HG21	1:B:287:LYS:HZ1	1.63	0.63
1:B:287:LYS:CD	1:B:288:ILE:N	2.45	0.63
1:B:91:PHE:HB3	1:B:139:TRP:CZ3	2.34	0.63
1:B:304:HIS:CB	1:B:305:PRO:HA	2.27	0.63
1:B:97:ASN:HD21	1:B:100:GLU:H	1.44	0.63
1:C:76:THR:O	1:C:271:ARG:NH1	2.28	0.63
1:C:285:VAL:HG12	1:C:286:GLU:N	2.13	0.63
1:C:68:ARG:O	1:C:69:ASP:OD2	2.16	0.63
1:B:145:GLU:HB2	1:B:147:ARG:NH2	2.14	0.63
1:B:220:GLY:O	1:B:221:LEU:HD12	1.98	0.63
1:B:222:GLY:O	1:B:225:PHE:HB3	1.98	0.63
1:B:174:ASP:OD1	1:B:176:ARG:HG3	1.98	0.63
1:D:282:LEU:HD11	1:D:297:GLN:HB2	1.81	0.63
1:A:207:GLU:HA	1:A:244:LYS:O	1.99	0.63
1:D:218:ASP:C	1:D:220:GLY:H	2.02	0.63
1:D:112:ASN:HB3	1:D:131:LEU:HD22	1.80	0.63
1:C:85:LEU:HD11	1:C:89:LEU:HD11	1.81	0.63
1:B:287:LYS:CG	1:B:289:ASP:OD1	2.45	0.63
1:B:135:TYR:CE1	1:B:196:HIS:HB2	2.33	0.63
1:B:105:GLY:O	1:B:106:VAL:HG22	1.98	0.63
1:A:32:GLN:HE21	1:A:64:ARG:H	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:PRO:HD2	1:D:142:PHE:CE2	2.34	0.62
1:C:88:LEU:CD2	1:C:232:LEU:HD23	2.29	0.62
1:C:307:ILE:HD13	1:C:307:ILE:O	1.99	0.62
1:A:262:ILE:HG22	1:A:266:LYS:HD3	1.80	0.62
1:D:101:LEU:HG	1:D:106:VAL:HB	1.81	0.62
1:D:263:GLU:HB2	1:D:264:PRO:HD3	1.80	0.62
1:D:78:ARG:HD2	1:D:301:TYR:OH	1.99	0.62
1:A:279:LEU:HG	1:A:279:LEU:O	1.99	0.62
1:A:85:LEU:O	1:A:89:LEU:HD12	2.00	0.62
1:D:133:PRO:HG2	1:D:190:MET:CE	2.30	0.62
1:C:204:VAL:HG21	1:D:47:LYS:HD2	1.80	0.62
1:C:97:ASN:OD1	1:C:98:ALA:N	2.32	0.62
1:B:160:GLN:NE2	1:B:180:CYS:N	2.29	0.62
1:C:308:LYS:HA	1:C:308:LYS:CE	2.29	0.62
1:A:130:ASP:C	1:A:130:ASP:OD2	2.37	0.62
1:B:29:GLY:O	1:B:32:GLN:CB	2.45	0.62
1:D:32:GLN:NE2	1:D:32:GLN:HA	2.15	0.62
1:D:85:LEU:O	1:D:89:LEU:HD12	2.00	0.62
1:D:97:ASN:C	1:D:99:LYS:N	2.52	0.62
1:D:149:MET:HG3	1:D:150:GLU:N	2.10	0.61
1:D:80:PHE:C	1:D:84:VAL:HG23	2.19	0.61
1:D:60:GLY:HA2	1:D:252:LEU:O	1.99	0.61
1:D:96:THR:HG21	1:D:134:VAL:CG2	2.30	0.61
1:D:47:LYS:CG	1:D:47:LYS:CE	2.73	0.61
1:A:115:ARG:NH2	1:A:127:GLU:HA	2.13	0.61
1:A:283:ARG:CZ	1:A:285:VAL:CG2	2.77	0.61
1:B:301:TYR:O	1:B:303:PRO:CD	2.46	0.61
1:C:57:SER:HB2	1:C:256:HIS:HB3	1.82	0.61
1:B:41:LEU:N	1:B:41:LEU:HD23	2.14	0.61
1:D:101:LEU:O	1:D:102:SER:C	2.39	0.61
1:D:101:LEU:O	1:D:103:SER:N	2.33	0.61
1:D:85:LEU:O	1:D:89:LEU:CD1	2.48	0.61
1:C:284:LYS:HA	1:C:285:VAL:HG23	1.83	0.61
1:A:115:ARG:O	1:A:116:ASP:C	2.38	0.61
1:D:280:ARG:CD	1:D:299:GLU:OE2	2.44	0.60
1:A:113:GLY:O	1:A:118:LEU:HD12	1.99	0.60
1:A:34:LEU:HD11	1:A:76:THR:HG21	1.82	0.60
1:B:177:ILE:HG21	1:B:201:PHE:H	1.62	0.60
1:B:263:GLU:HG2	1:B:266:LYS:HZ2	1.65	0.60
1:D:274:ARG:NH1	1:D:274:ARG:CG	2.61	0.60
1:C:115:ARG:O	1:C:118:LEU:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:N	1:B:290:ASP:OD2	2.34	0.60
1:D:259:LEU:O	1:D:262:ILE:N	2.34	0.60
1:D:274:ARG:HG2	1:D:274:ARG:NH1	2.15	0.60
1:C:206:SER:O	1:C:244:LYS:HG2	2.02	0.60
1:C:184:PRO:HA	1:C:187:LEU:HD12	1.84	0.60
1:B:119:ASP:C	1:B:122:GLY:H	2.04	0.60
1:A:85:LEU:HD11	1:A:89:LEU:CD1	2.30	0.60
1:B:279:LEU:HD12	1:B:297:GLN:O	2.01	0.60
1:C:186:ASP:HB3	1:C:189:LEU:HD13	1.84	0.60
1:D:192:LEU:HD23	1:D:193:PRO:O	2.02	0.60
1:B:85:LEU:HD12	1:B:85:LEU:C	2.22	0.60
1:C:143:GLY:CA	1:D:185:ARG:HH21	2.10	0.60
1:B:288:ILE:O	1:B:291:PHE:CD2	2.54	0.60
1:B:41:LEU:HD12	1:B:262:ILE:HD12	1.84	0.60
1:D:218:ASP:C	1:D:218:ASP:OD2	2.39	0.60
1:C:95:SER:OG	1:C:96:THR:N	2.34	0.59
1:A:292:LYS:HA	1:A:292:LYS:CE	2.20	0.59
1:C:170:THR:O	1:C:171:ASN:HB3	2.02	0.59
1:B:100:GLU:C	1:B:103:SER:HB2	2.22	0.59
1:C:293:ALA:O	1:C:296:PHE:HB2	2.02	0.59
1:C:207:GLU:HA	1:C:244:LYS:O	2.03	0.59
1:D:67:LEU:CB	1:D:245:PRO:HB2	2.31	0.59
1:B:178:ILE:HA	1:B:199:CYS:O	2.02	0.59
1:A:178:ILE:HD11	1:B:215:ARG:HG3	1.83	0.59
1:D:109:TRP:HB3	1:D:131:LEU:HD21	1.83	0.59
1:B:119:ASP:OD1	1:B:122:GLY:CA	2.45	0.59
1:D:101:LEU:C	1:D:103:SER:H	2.06	0.59
1:D:220:GLY:O	1:D:221:LEU:HD23	2.03	0.59
1:C:83:GLY:O	1:C:87:GLU:HB2	2.02	0.59
1:D:96:THR:HG21	1:D:134:VAL:HG22	1.83	0.59
1:D:67:LEU:HB3	1:D:235:TYR:CE2	2.37	0.59
1:B:234:THR:O	1:B:237:ILE:N	2.34	0.59
1:A:70:GLU:OE1	1:A:276:PHE:CD2	2.51	0.59
1:D:248:PHE:C	1:D:249:ILE:HG12	2.22	0.59
1:A:184:PRO:O	1:A:185:ARG:C	2.38	0.59
1:D:101:LEU:CD2	1:D:106:VAL:O	2.51	0.59
1:C:119:ASP:C	1:C:122:GLY:CA	2.70	0.59
1:B:77:LYS:HB2	1:B:268:GLN:NE2	2.18	0.59
1:C:70:GLU:HB3	1:C:276:PHE:HB3	1.84	0.59
1:C:72:PRO:HG2	1:C:72:PRO:O	2.00	0.59
1:D:74:LEU:HD23	1:D:74:LEU:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ILE:O	1:D:178:ILE:HG22	2.01	0.59
1:A:267:ILE:O	1:A:270:GLN:HB2	2.03	0.58
1:D:92:ILE:HG23	1:D:161:LEU:CD2	2.33	0.58
1:C:178:ILE:HG23	1:C:200:GLN:HA	1.85	0.58
1:C:114:SER:OG	1:C:114:SER:O	2.18	0.58
1:B:175:ARG:HG2	3:B:616:PO4:O4	2.02	0.58
1:D:86:GLU:O	1:D:88:LEU:N	2.35	0.58
1:B:304:HIS:HB2	1:B:305:PRO:CA	2.31	0.58
1:A:126:ARG:HD3	1:A:130:ASP:CG	2.24	0.58
1:A:98:ALA:HB2	1:A:131:LEU:HD21	1.85	0.58
1:A:187:LEU:C	1:A:189:LEU:N	2.56	0.58
1:A:219:MET:HA	1:A:223:VAL:HB	1.84	0.58
1:B:299:GLU:HG3	1:B:300:GLY:H	1.67	0.58
1:D:102:SER:HB3	1:D:110:ASP:OD2	2.02	0.58
1:A:292:LYS:CE	1:A:292:LYS:CA	2.80	0.58
1:D:265:LEU:O	1:D:269:LEU:N	2.35	0.58
1:C:123:PHE:HA	1:C:124:SER:OG	2.02	0.58
1:A:50:ARG:HD2	1:B:176:ARG:NH1	2.17	0.58
1:D:177:ILE:CD1	1:D:177:ILE:N	2.67	0.58
1:B:139:TRP:CD2	1:B:179:MET:HE3	2.39	0.58
1:B:208:LEU:HD12	1:B:209:SER:N	2.18	0.58
1:B:88:LEU:HD21	1:B:233:LEU:HA	1.85	0.58
1:C:213:TYR:CD2	1:D:213:TYR:HD1	2.18	0.58
1:A:114:SER:OG	1:A:117:PHE:HB2	2.02	0.58
1:C:115:ARG:CZ	1:C:118:LEU:HD22	2.34	0.58
1:C:307:ILE:O	1:C:307:ILE:CG1	2.52	0.58
1:D:43:CYS:SG	1:D:43:CYS:CA	2.90	0.58
1:C:151:SER:HB3	1:C:153:TYR:CE1	2.38	0.58
1:A:114:SER:OG	1:A:114:SER:O	2.20	0.58
1:A:69:ASP:HA	1:A:235:TYR:OH	2.04	0.58
1:A:149:MET:HE2	1:A:150:GLU:HG3	1.86	0.58
1:D:148:ASP:C	1:D:148:ASP:OD2	2.43	0.58
1:A:187:LEU:CA	1:A:190:MET:HE3	2.28	0.57
1:D:90:TRP:NE1	1:D:101:LEU:HB3	2.18	0.57
1:C:237:ILE:O	1:C:241:THR:HG23	2.03	0.57
1:A:81:TRP:O	1:A:82:LYS:C	2.42	0.57
1:D:80:PHE:CE1	1:D:82:LYS:HB3	2.37	0.57
1:A:204:VAL:CG2	1:B:45:VAL:HG21	2.34	0.57
1:D:274:ARG:CB	1:D:274:ARG:HH11	2.17	0.57
1:B:227:ILE:HG23	1:B:248:PHE:CE2	2.38	0.57
1:C:175:ARG:HG3	1:D:254:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LYS:CD	1:B:244:LYS:CB	2.80	0.57
1:B:160:GLN:NE2	1:B:179:MET:HA	2.18	0.57
1:C:277:PRO:C	1:C:278:LYS:HG2	2.23	0.57
1:A:271:ARG:NH2	1:A:307:ILE:HB	2.19	0.57
1:B:68:ARG:O	1:B:69:ASP:HB2	2.03	0.57
1:D:50:ARG:C	1:D:52:GLY:H	2.05	0.57
1:A:62:GLN:HG3	1:A:251:THR:OG1	2.02	0.57
1:D:101:LEU:HD21	1:D:106:VAL:O	2.05	0.57
1:B:123:PHE:HB3	1:B:126:ARG:HD2	1.87	0.57
1:B:240:ILE:O	1:B:240:ILE:CG2	2.52	0.57
1:A:50:ARG:NH1	1:B:176:ARG:HH21	2.00	0.57
1:C:288:ILE:HD13	1:C:291:PHE:CD2	2.39	0.57
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.86	0.57
1:C:178:ILE:HG23	1:C:200:GLN:CB	2.33	0.57
1:D:204:VAL:O	1:D:207:GLU:CB	2.42	0.57
1:C:277:PRO:O	1:C:278:LYS:HG2	2.05	0.57
1:A:33:TYR:HA	1:A:36:GLN:HG3	1.87	0.57
1:D:263:GLU:N	1:D:264:PRO:CD	2.67	0.57
1:A:202:TYR:O	1:A:202:TYR:CD2	2.58	0.57
1:C:218:ASP:OD1	1:C:218:ASP:C	2.41	0.56
1:D:203:VAL:CG2	1:D:208:LEU:CD1	2.82	0.56
1:A:72:PRO:HA	1:A:276:PHE:CD1	2.40	0.56
1:A:140:ARG:C	1:A:141:HIS:CG	2.79	0.56
1:B:299:GLU:C	1:B:301:TYR:N	2.58	0.56
1:A:56:LEU:HD13	1:A:259:LEU:CD2	2.35	0.56
1:B:290:ASP:O	1:B:292:LYS:HE3	2.05	0.56
1:A:177:ILE:C	1:A:178:ILE:HG13	2.25	0.56
1:A:68:ARG:NH2	1:A:246:GLY:CA	2.66	0.56
1:A:183:ASN:O	1:A:187:LEU:HG	2.05	0.56
1:A:185:ARG:HB3	1:A:185:ARG:HH21	1.67	0.56
1:D:183:ASN:ND2	1:D:186:ASP:OD1	2.38	0.56
1:B:40:ILE:HD13	1:B:58:VAL:HB	1.87	0.56
1:D:222:GLY:O	1:D:226:ASN:OD1	2.24	0.56
1:B:94:GLY:HA2	1:B:136:GLY:O	2.05	0.56
1:C:239:HIS:CE1	1:C:284:LYS:HB2	2.41	0.56
1:A:268:GLN:C	1:A:270:GLN:N	2.55	0.56
1:D:178:ILE:HG13	1:D:200:GLN:HG3	1.86	0.56
1:D:148:ASP:OD2	1:D:151:SER:OG	2.23	0.56
1:A:79:VAL:HG12	1:A:80:PHE:N	2.11	0.56
1:D:92:ILE:O	1:D:92:ILE:HG22	2.06	0.56
1:A:49:ASP:OD2	1:A:49:ASP:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ALA:HB1	1:B:243:LEU:O	2.06	0.56
1:D:135:TYR:CD2	1:D:135:TYR:N	2.73	0.56
1:D:135:TYR:O	1:D:136:GLY:C	2.44	0.56
1:B:205:ASN:O	1:B:206:SER:CB	2.48	0.56
1:D:86:GLU:C	1:D:88:LEU:N	2.54	0.56
1:D:263:GLU:N	1:D:264:PRO:HD2	2.21	0.56
1:B:105:GLY:C	1:B:106:VAL:HG23	2.25	0.56
1:D:176:ARG:NH1	3:D:616:PO4:O1	2.39	0.56
1:B:118:LEU:O	1:B:123:PHE:HB2	2.05	0.56
1:C:93:LYS:HZ1	1:C:100:GLU:HG3	1.70	0.56
1:A:130:ASP:CB	1:A:149:MET:HG2	2.35	0.56
1:B:58:VAL:O	1:B:255:ALA:N	2.38	0.56
1:C:280:ARG:HA	1:C:280:ARG:HD3	1.86	0.55
1:A:187:LEU:N	1:A:188:PRO:HD3	2.21	0.55
1:A:202:TYR:CE1	1:B:47:LYS:HE3	2.41	0.55
1:C:79:VAL:HG12	1:C:80:PHE:N	2.21	0.55
1:A:85:LEU:C	1:A:85:LEU:CD1	2.73	0.55
1:B:265:LEU:O	1:B:269:LEU:HB2	2.07	0.55
1:C:112:ASN:ND2	1:C:112:ASN:H	2.03	0.55
1:C:184:PRO:HA	1:C:187:LEU:CG	2.37	0.55
1:D:86:GLU:HB2	1:D:106:VAL:HG21	1.89	0.55
1:C:97:ASN:CB	1:C:149:MET:SD	2.91	0.55
1:B:287:LYS:CD	1:B:288:ILE:CG2	2.72	0.55
1:C:107:LYS:C	1:C:109:TRP:N	2.54	0.55
1:A:116:ASP:N	1:A:116:ASP:OD1	2.38	0.55
1:A:263:GLU:O	1:A:266:LYS:HB2	2.07	0.55
1:B:82:LYS:HD3	1:B:106:VAL:HG22	1.89	0.55
1:D:218:ASP:C	1:D:220:GLY:N	2.58	0.55
1:A:81:TRP:O	1:A:83:GLY:N	2.40	0.55
1:D:266:LYS:CB	1:D:266:LYS:CD	2.80	0.55
1:C:186:ASP:O	1:C:190:MET:CG	2.52	0.55
1:D:115:ARG:HH21	1:D:127:GLU:CA	2.05	0.55
1:D:140:ARG:O	1:D:141:HIS:CG	2.60	0.55
1:B:145:GLU:HB2	1:B:147:ARG:HH21	1.72	0.55
1:C:115:ARG:NE	1:C:128:GLU:HB3	2.21	0.55
1:D:87:GLU:O	1:D:87:GLU:HG2	2.06	0.55
1:C:130:ASP:HB2	1:C:149:MET:CG	2.33	0.55
1:C:107:LYS:CA	1:C:110:ASP:OD1	2.42	0.55
1:B:118:LEU:O	1:B:123:PHE:N	2.38	0.55
1:C:213:TYR:CD1	1:C:213:TYR:C	2.80	0.55
1:A:183:ASN:HD21	1:A:185:ARG:NH2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:HG23	1:D:208:LEU:HD13	1.86	0.55
1:A:103:SER:OG	1:A:104:LYS:NZ	2.40	0.55
1:A:152:ASP:OD1	1:A:152:ASP:C	2.46	0.55
1:B:75:THR:O	1:B:304:HIS:O	2.26	0.54
1:A:175:ARG:NH2	1:B:55:THR:HG21	2.21	0.54
1:B:34:LEU:HD11	1:B:76:THR:HG21	1.88	0.54
1:D:198:LEU:HD13	1:D:199:CYS:N	2.22	0.54
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.43	0.54
1:D:97:ASN:O	1:D:100:GLU:N	2.30	0.54
1:A:307:ILE:CD1	1:A:308:LYS:H	2.17	0.54
1:C:170:THR:O	1:C:171:ASN:CB	2.51	0.54
1:A:296:PHE:CD1	1:A:296:PHE:N	2.74	0.54
1:A:221:LEU:CD2	1:A:221:LEU:CD1	2.80	0.54
1:A:187:LEU:N	1:A:188:PRO:CD	2.70	0.54
1:D:187:LEU:O	1:D:188:PRO:C	2.42	0.54
1:B:76:THR:OG1	1:B:268:GLN:NE2	2.35	0.54
1:D:264:PRO:O	1:D:267:ILE:HB	2.07	0.54
1:C:130:ASP:CG	1:C:149:MET:HG2	2.28	0.54
1:A:268:GLN:C	1:A:270:GLN:H	2.08	0.54
1:D:133:PRO:HG2	1:D:190:MET:HE3	1.90	0.54
1:D:218:ASP:O	1:D:220:GLY:N	2.40	0.54
1:A:288:ILE:CG2	1:A:289:ASP:N	2.71	0.54
1:D:153:TYR:O	1:D:156:GLN:HG3	2.08	0.54
1:D:92:ILE:O	1:D:140:ARG:HD3	2.08	0.54
1:C:100:GLU:OE1	1:C:100:GLU:HA	2.08	0.54
1:A:164:VAL:O	1:A:168:ILE:HG12	2.07	0.54
1:D:214:GLN:OE1	1:D:250:HIS:NE2	2.39	0.54
1:B:171:ASN:ND2	1:B:171:ASN:O	2.41	0.54
1:B:177:ILE:HG21	1:B:201:PHE:CB	2.37	0.54
1:D:274:ARG:N	1:D:274:ARG:HD3	2.23	0.54
1:C:91:PHE:O	1:C:136:GLY:HA2	2.08	0.54
1:C:283:ARG:NH1	1:C:290:ASP:OD2	2.41	0.54
1:A:101:LEU:HD12	1:A:101:LEU:O	2.08	0.54
1:A:135:TYR:CZ	1:A:194:PRO:HB3	2.43	0.53
1:A:195:CYS:HA	1:A:215:ARG:HG2	1.89	0.53
1:A:50:ARG:HD2	1:B:176:ARG:CZ	2.37	0.53
1:C:223:VAL:O	1:C:227:ILE:HG13	2.09	0.53
1:D:30:GLU:HG3	1:D:74:LEU:HD13	1.88	0.53
1:A:187:LEU:HA	1:A:190:MET:HE2	1.88	0.53
1:D:113:GLY:HA3	1:D:129:GLY:HA2	1.89	0.53
1:B:274:ARG:CZ	1:B:304:HIS:CD2	2.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LEU:O	1:C:122:GLY:HA2	2.09	0.53
1:C:131:LEU:HD12	1:C:134:VAL:HG21	1.91	0.53
1:B:273:PRO:HA	1:B:304:HIS:HE1	1.71	0.53
1:D:148:ASP:O	1:D:148:ASP:OD2	2.26	0.53
1:C:85:LEU:CD1	1:C:89:LEU:HD11	2.38	0.53
1:B:135:TYR:OH	1:B:195:CYS:N	2.31	0.53
1:C:307:ILE:O	1:C:307:ILE:CD1	2.56	0.53
1:C:94:GLY:HA2	1:C:136:GLY:HA3	1.91	0.53
1:D:301:TYR:CZ	1:D:303:PRO:CG	2.89	0.53
1:C:178:ILE:CG2	1:C:200:GLN:HB2	2.38	0.53
1:A:210:CYS:HB3	1:A:248:PHE:HD1	1.73	0.53
1:D:73:LEU:CD1	1:D:228:ALA:CB	2.86	0.53
1:D:88:LEU:HD23	1:D:232:LEU:HD23	1.89	0.53
1:C:97:ASN:OD1	1:C:97:ASN:C	2.44	0.53
1:B:139:TRP:CE2	1:B:179:MET:HE2	2.42	0.53
1:B:88:LEU:O	1:B:89:LEU:C	2.46	0.53
1:B:102:SER:O	1:B:103:SER:C	2.46	0.53
1:B:124:SER:C	1:B:126:ARG:H	2.11	0.53
1:D:271:ARG:HB3	1:D:304:HIS:CE1	2.44	0.53
1:A:74:LEU:O	1:A:301:TYR:OH	2.11	0.53
1:C:283:ARG:CG	1:C:285:VAL:CG2	2.86	0.53
1:C:88:LEU:CD2	1:C:232:LEU:CD2	2.87	0.53
1:D:60:GLY:O	1:D:61:MET:HG3	2.08	0.53
1:A:299:GLU:HG2	1:A:299:GLU:O	2.09	0.52
1:A:154:SER:O	1:A:156:GLN:N	2.42	0.52
1:B:211:GLN:HA	1:B:249:ILE:O	2.09	0.52
1:B:305:PRO:HB2	1:B:306:THR:HG22	1.91	0.52
1:D:37:ILE:HG22	1:D:269:LEU:HD21	1.86	0.52
1:C:88:LEU:HD23	1:C:232:LEU:CD2	2.39	0.52
1:A:196:HIS:N	1:A:196:HIS:CD2	2.75	0.52
1:D:142:PHE:CD2	1:D:143:GLY:N	2.78	0.52
1:A:257:ILE:HD11	1:A:262:ILE:CG1	2.23	0.52
1:B:92:ILE:O	1:B:140:ARG:HD3	2.09	0.52
1:D:177:ILE:HD12	1:D:177:ILE:N	2.24	0.52
1:A:102:SER:CB	1:A:110:ASP:OD2	2.53	0.52
1:A:184:PRO:CA	1:A:187:LEU:HG	2.39	0.52
1:C:81:TRP:O	1:C:84:VAL:N	2.43	0.52
1:B:301:TYR:O	1:B:301:TYR:CG	2.61	0.52
1:D:233:LEU:HD11	1:D:237:ILE:HD11	1.91	0.52
1:C:68:ARG:O	1:C:69:ASP:CG	2.48	0.52
1:A:283:ARG:NH1	1:A:285:VAL:CG2	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:MET:HG3	1:D:150:GLU:OE1	2.10	0.52
1:B:239:HIS:CD2	1:B:239:HIS:C	2.83	0.52
1:B:288:ILE:HD12	1:B:291:PHE:CE2	2.45	0.52
1:B:30:GLU:OE1	1:B:76:THR:HG23	2.10	0.52
1:B:182:TRP:CZ3	1:B:194:PRO:HD2	2.44	0.52
1:C:261:HIS:O	1:C:265:LEU:HB2	2.10	0.52
1:C:285:VAL:HG12	1:C:286:GLU:H	1.70	0.52
1:A:204:VAL:CG2	1:B:45:VAL:CG2	2.88	0.52
1:D:65:TYR:N	1:D:248:PHE:O	2.40	0.52
1:B:277:PRO:HB3	1:B:301:TYR:HD1	1.71	0.52
1:D:87:GLU:OE1	1:D:91:PHE:HE2	1.93	0.52
1:B:76:THR:HA	1:B:304:HIS:ND1	2.25	0.52
1:D:272:GLU:OE2	1:D:273:PRO:HD2	2.10	0.52
1:A:283:ARG:CZ	1:A:285:VAL:HG22	2.40	0.52
1:C:221:LEU:CD1	1:C:221:LEU:CB	2.79	0.52
1:C:132:GLY:O	1:C:134:VAL:N	2.43	0.52
1:B:88:LEU:HD11	1:B:233:LEU:HD13	1.92	0.52
1:A:154:SER:C	1:A:156:GLN:H	2.13	0.52
1:A:215:ARG:NH1	1:B:175:ARG:O	2.43	0.51
1:D:87:GLU:O	1:D:90:TRP:HB3	2.10	0.51
1:B:178:ILE:CG2	1:B:179:MET:N	2.73	0.51
1:D:261:HIS:HA	1:D:264:PRO:HG2	1.92	0.51
1:A:294:GLU:CD	1:A:294:GLU:H	2.12	0.51
1:C:172:PRO:O	1:C:203:VAL:HB	2.10	0.51
1:C:190:MET:O	1:C:191:ALA:C	2.49	0.51
1:D:177:ILE:CD1	1:D:177:ILE:H	2.22	0.51
1:C:96:THR:CG2	1:C:137:PHE:HB2	2.41	0.51
1:B:97:ASN:HD21	1:B:100:GLU:N	2.09	0.51
1:C:178:ILE:H	1:C:178:ILE:HD12	1.75	0.51
1:B:47:LYS:O	1:B:55:THR:CG2	2.58	0.51
1:C:134:VAL:O	1:C:138:GLN:CG	2.58	0.51
1:B:94:GLY:HA3	1:B:140:ARG:HG3	1.93	0.51
1:B:97:ASN:ND2	1:B:97:ASN:O	2.43	0.51
1:C:93:LYS:HZ3	1:C:100:GLU:HG3	1.73	0.51
1:B:110:ASP:C	1:B:112:ASN:N	2.64	0.51
1:C:292:LYS:CG	1:C:294:GLU:OE1	2.58	0.51
1:C:115:ARG:HH22	1:C:127:GLU:C	2.12	0.51
1:B:274:ARG:NE	1:B:304:HIS:CD2	2.79	0.51
1:C:76:THR:CB	1:C:268:GLN:NE2	2.66	0.51
1:D:35:GLY:O	1:D:38:GLN:HB3	2.10	0.51
1:C:184:PRO:HA	1:C:187:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD21	1:B:233:LEU:CD1	2.39	0.51
1:B:88:LEU:HD12	1:B:92:ILE:HG12	1.92	0.51
1:D:162:GLN:O	1:D:166:ASP:OD2	2.28	0.51
1:A:232:LEU:HD12	1:A:232:LEU:C	2.23	0.51
1:C:307:ILE:HG12	1:C:307:ILE:O	2.10	0.51
1:C:307:ILE:O	1:C:308:LYS:HE2	2.11	0.51
1:B:145:GLU:CB	1:B:147:ARG:NH2	2.73	0.51
1:A:97:ASN:ND2	1:A:99:LYS:HB2	2.25	0.51
1:C:205:ASN:O	1:C:206:SER:OG	2.21	0.51
1:A:195:CYS:O	1:A:214:GLN:HG3	2.10	0.51
1:C:190:MET:SD	1:C:194:PRO:HD2	2.50	0.51
1:A:190:MET:HB2	1:A:192:LEU:O	2.11	0.51
1:C:165:ILE:HG21	1:C:240:ILE:HG21	1.91	0.51
1:A:130:ASP:OD1	1:A:149:MET:HG2	2.11	0.51
1:D:284:LYS:O	1:D:285:VAL:CG2	2.58	0.51
1:C:59:PHE:HA	1:C:253:GLY:O	2.11	0.51
1:D:67:LEU:HB3	1:D:235:TYR:HE2	1.76	0.50
1:B:90:TRP:HA	1:B:93:LYS:HE3	1.93	0.50
1:C:152:ASP:OD1	1:C:153:TYR:N	2.44	0.50
1:D:101:LEU:HD23	1:D:102:SER:H	1.72	0.50
1:D:80:PHE:CZ	1:D:82:LYS:HD3	2.45	0.50
1:D:97:ASN:OD1	1:D:129:GLY:C	2.50	0.50
1:A:99:LYS:O	1:A:101:LEU:N	2.45	0.50
1:D:192:LEU:HD23	1:D:194:PRO:HA	1.93	0.50
1:C:142:PHE:CD2	1:D:184:PRO:HG2	2.47	0.50
1:C:294:GLU:C	1:C:296:PHE:H	2.13	0.50
1:C:97:ASN:OD1	1:C:129:GLY:HA3	2.11	0.50
1:D:165:ILE:O	1:D:168:ILE:N	2.44	0.50
1:A:108:ILE:HG13	1:A:109:TRP:N	2.25	0.50
1:A:38:GLN:HG2	1:A:269:LEU:HD21	1.92	0.50
1:D:135:TYR:N	1:D:135:TYR:HD2	2.09	0.50
1:C:276:PHE:HD1	1:C:277:PRO:HD2	1.76	0.50
1:A:118:LEU:HD22	1:A:126:ARG:O	2.11	0.50
1:B:84:VAL:HG22	1:B:225:PHE:CE1	2.47	0.50
1:D:240:ILE:HD11	1:D:291:PHE:CE2	2.46	0.50
1:C:130:ASP:N	1:C:149:MET:SD	2.85	0.50
1:B:287:LYS:HD3	1:B:288:ILE:CA	2.41	0.50
1:B:77:LYS:HB2	1:B:268:GLN:HE22	1.76	0.50
1:D:232:LEU:O	1:D:236:MET:N	2.34	0.50
1:D:92:ILE:C	1:D:94:GLY:N	2.60	0.50
1:A:46:ARG:HA	1:A:55:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:HG23	1:D:208:LEU:CD1	2.42	0.50
1:D:251:THR:HG22	1:D:252:LEU:N	2.25	0.50
1:C:142:PHE:CZ	1:D:184:PRO:HD2	2.47	0.50
1:A:139:TRP:O	1:A:140:ARG:CB	2.58	0.50
1:D:81:TRP:N	1:D:84:VAL:HG23	2.26	0.50
1:B:230:TYR:O	1:B:233:LEU:HB3	2.12	0.50
1:C:192:LEU:N	1:C:192:LEU:CD1	2.74	0.50
1:B:266:LYS:O	1:B:269:LEU:HB3	2.12	0.50
1:D:47:LYS:O	1:D:55:THR:HG23	2.10	0.49
1:A:50:ARG:CD	3:B:616:PO4:O3	2.60	0.49
1:D:79:VAL:HG11	1:D:225:PHE:CA	2.41	0.49
1:B:30:GLU:OE2	1:B:273:PRO:HB2	2.12	0.49
1:B:170:THR:HB	1:B:171:ASN:HB3	1.94	0.49
1:B:76:THR:OG1	1:B:268:GLN:HG3	2.12	0.49
1:B:160:GLN:O	1:B:164:VAL:HG23	2.12	0.49
1:D:298:ILE:CG2	1:D:301:TYR:HB2	2.42	0.49
1:D:135:TYR:O	1:D:139:TRP:HB2	2.12	0.49
1:B:119:ASP:HA	1:B:122:GLY:H	1.76	0.49
1:D:268:GLN:C	1:D:270:GLN:N	2.66	0.49
1:A:186:ASP:O	1:A:189:LEU:HB3	2.12	0.49
1:C:237:ILE:HD13	1:C:237:ILE:N	2.28	0.49
1:B:36:GLN:O	1:B:39:HIS:HB3	2.13	0.49
1:B:176:ARG:NH1	3:B:616:PO4:O4	2.44	0.49
1:D:101:LEU:HD23	1:D:101:LEU:C	2.32	0.49
1:D:111:ALA:O	1:D:112:ASN:C	2.51	0.49
1:D:84:VAL:HG22	1:D:225:PHE:CE1	2.47	0.49
1:D:204:VAL:CG1	1:D:204:VAL:O	2.59	0.49
1:C:92:ILE:C	1:C:94:GLY:N	2.66	0.49
1:C:143:GLY:O	1:D:185:ARG:NH2	2.46	0.49
1:A:142:PHE:O	1:A:142:PHE:CD2	2.66	0.49
1:D:155:GLY:C	1:D:156:GLN:HG2	2.33	0.49
1:C:99:LYS:C	1:C:101:LEU:N	2.66	0.49
1:C:211:GLN:HG3	1:C:212:LEU:N	2.28	0.49
1:D:32:GLN:HE21	1:D:32:GLN:HA	1.77	0.49
1:B:292:LYS:O	1:B:295:ASP:OD1	2.30	0.49
1:D:259:LEU:O	1:D:261:HIS:N	2.46	0.49
1:D:211:GLN:HG3	1:D:249:ILE:O	2.12	0.49
1:D:232:LEU:O	1:D:233:LEU:C	2.51	0.48
1:A:261:HIS:O	1:A:262:ILE:C	2.50	0.48
1:D:77:LYS:CG	1:D:78:ARG:H	2.26	0.48
1:D:86:GLU:O	1:D:90:TRP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PRO:HA	1:C:276:PHE:CD1	2.44	0.48
1:C:34:LEU:O	1:C:38:GLN:N	2.42	0.48
1:C:184:PRO:CA	1:C:187:LEU:HD12	2.42	0.48
1:D:115:ARG:NH1	1:D:119:ASP:OD2	2.46	0.48
1:D:92:ILE:HG23	1:D:161:LEU:HD22	1.95	0.48
1:C:98:ALA:CB	1:C:131:LEU:HD21	2.42	0.48
1:C:96:THR:O	1:C:131:LEU:HG	2.13	0.48
1:D:251:THR:CG2	1:D:252:LEU:N	2.76	0.48
1:C:201:PHE:N	1:C:201:PHE:CD2	2.81	0.48
1:A:147:ARG:HB2	1:A:151:SER:OG	2.13	0.48
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.31	0.48
1:D:268:GLN:O	1:D:270:GLN:N	2.47	0.48
1:C:212:LEU:HD12	1:C:213:TYR:H	1.79	0.48
1:D:126:ARG:HB3	1:D:130:ASP:HB3	1.95	0.48
1:C:116:ASP:O	1:C:119:ASP:N	2.46	0.48
1:B:135:TYR:CZ	1:B:194:PRO:HA	2.49	0.48
1:C:257:ILE:CD1	1:C:258:TYR:O	2.62	0.48
1:B:263:GLU:CG	1:B:266:LYS:HZ1	2.27	0.48
1:D:74:LEU:HD23	1:D:74:LEU:H	1.78	0.48
1:A:135:TYR:O	1:A:139:TRP:N	2.46	0.48
1:D:137:PHE:C	1:D:137:PHE:CD2	2.87	0.48
1:C:257:ILE:HD12	1:C:258:TYR:O	2.13	0.48
1:C:83:GLY:HA2	1:C:106:VAL:HG21	1.94	0.48
1:D:172:PRO:O	1:D:174:ASP:N	2.46	0.48
1:D:187:LEU:N	1:D:187:LEU:HD23	2.28	0.48
1:C:162:GLN:HG3	1:C:166:ASP:OD1	2.13	0.48
1:D:265:LEU:HA	1:D:268:GLN:CB	2.43	0.48
1:C:228:ALA:O	1:C:229:SER:C	2.49	0.48
1:B:172:PRO:O	1:B:203:VAL:HG12	2.14	0.48
1:A:91:PHE:O	1:A:92:ILE:C	2.51	0.48
1:C:92:ILE:O	1:C:93:LYS:C	2.52	0.48
1:D:285:VAL:HG13	1:D:290:ASP:HB2	1.96	0.48
1:A:62:GLN:HA	1:A:250:HIS:O	2.14	0.48
1:B:299:GLU:CG	1:B:300:GLY:H	2.26	0.48
1:D:105:GLY:HA2	1:D:107:LYS:NZ	2.29	0.48
1:C:161:LEU:O	1:C:164:VAL:HB	2.14	0.48
1:B:40:ILE:CG2	1:B:257:ILE:HD12	2.42	0.48
1:D:45:VAL:HG23	1:D:46:ARG:O	2.13	0.48
1:A:183:ASN:O	1:A:187:LEU:N	2.47	0.48
1:B:164:VAL:O	1:B:168:ILE:HG12	2.13	0.48
1:B:200:GLN:O	1:B:210:CYS:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:LEU:HA	1:D:262:ILE:HD12	1.95	0.48
1:D:54:GLY:HA3	1:D:259:LEU:CD1	2.42	0.48
1:A:236:MET:HG2	1:A:291:PHE:CE2	2.48	0.48
1:C:138:GLN:O	1:C:160:GLN:NE2	2.47	0.47
1:C:90:TRP:NE1	1:C:95:SER:HB3	2.30	0.47
1:C:178:ILE:HD13	1:D:182:TRP:CZ2	2.48	0.47
1:C:292:LYS:O	1:C:293:ALA:C	2.51	0.47
1:B:41:LEU:H	1:B:41:LEU:HD23	1.79	0.47
1:C:145:GLU:HA	1:C:145:GLU:OE1	2.14	0.47
1:D:142:PHE:N	1:D:158:VAL:O	2.34	0.47
1:B:119:ASP:OD2	1:B:124:SER:HB3	2.14	0.47
1:B:298:ILE:HG23	1:B:299:GLU:N	2.29	0.47
1:B:75:THR:C	1:B:77:LYS:H	2.16	0.47
1:A:240:ILE:HG22	1:A:241:THR:N	2.24	0.47
1:A:268:GLN:O	1:A:270:GLN:N	2.47	0.47
1:B:159:ASP:O	1:B:160:GLN:C	2.52	0.47
1:B:228:ALA:O	1:B:231:ALA:HB3	2.13	0.47
1:D:198:LEU:CD1	1:D:199:CYS:N	2.78	0.47
1:A:222:GLY:O	1:A:223:VAL:C	2.51	0.47
1:A:147:ARG:N	1:A:153:TYR:OH	2.43	0.47
1:D:64:ARG:CG	1:D:64:ARG:O	2.60	0.47
1:D:177:ILE:H	1:D:177:ILE:HD13	1.79	0.47
1:C:97:ASN:OD1	1:C:129:GLY:CA	2.62	0.47
1:B:273:PRO:HA	1:B:304:HIS:NE2	2.29	0.47
1:B:105:GLY:O	1:B:106:VAL:CG2	2.62	0.47
1:B:223:VAL:HG12	1:B:227:ILE:HD11	1.95	0.47
1:C:177:ILE:O	1:C:201:PHE:N	2.39	0.47
1:C:184:PRO:O	1:C:186:ASP:N	2.48	0.47
1:D:115:ARG:HG2	1:D:128:GLU:CD	2.35	0.47
1:D:114:SER:O	1:D:118:LEU:HB2	2.15	0.47
1:C:162:GLN:C	1:C:164:VAL:N	2.61	0.47
1:B:41:LEU:CD2	1:B:41:LEU:N	2.77	0.47
1:D:265:LEU:O	1:D:268:GLN:N	2.48	0.47
1:A:72:PRO:HA	1:A:276:PHE:CZ	2.47	0.47
1:C:32:GLN:NE2	1:C:64:ARG:O	2.48	0.47
1:D:96:THR:HG23	1:D:134:VAL:HG23	1.97	0.47
1:C:115:ARG:NH2	1:C:118:LEU:HD22	2.30	0.47
1:C:78:ARG:CZ	1:C:303:PRO:HG3	2.45	0.47
1:A:183:ASN:ND2	1:A:185:ARG:HH22	2.13	0.46
1:B:299:GLU:CG	1:B:300:GLY:N	2.77	0.46
1:D:111:ALA:O	1:D:113:GLY:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ASP:C	1:C:159:ASP:OD1	2.54	0.46
1:D:225:PHE:O	1:D:228:ALA:N	2.48	0.46
1:B:165:ILE:HG21	1:B:287:LYS:HZ2	1.79	0.46
1:B:177:ILE:CG2	1:B:201:PHE:HD2	2.28	0.46
1:C:269:LEU:HA	1:C:269:LEU:HD12	1.27	0.46
1:D:66:SER:O	1:D:67:LEU:HD23	2.15	0.46
1:A:271:ARG:HB3	1:A:304:HIS:CE1	2.50	0.46
1:D:50:ARG:C	1:D:52:GLY:N	2.68	0.46
1:B:60:GLY:HA2	1:B:252:LEU:O	2.16	0.46
1:A:183:ASN:HD21	1:A:185:ARG:HH22	1.63	0.46
1:D:81:TRP:CA	1:D:84:VAL:HG23	2.46	0.46
1:C:198:LEU:HD12	1:C:199:CYS:N	2.30	0.46
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.59	0.46
1:A:152:ASP:OD1	1:A:154:SER:OG	2.31	0.46
1:D:134:VAL:O	1:D:137:PHE:HB3	2.16	0.46
1:C:134:VAL:O	1:C:138:GLN:HG2	2.16	0.46
1:B:34:LEU:HD23	1:B:34:LEU:N	2.19	0.46
1:C:225:PHE:O	1:C:226:ASN:C	2.52	0.46
1:A:201:PHE:CD2	1:A:201:PHE:N	2.82	0.46
1:B:64:ARG:HG3	1:B:249:ILE:CD1	2.46	0.46
1:C:148:ASP:OD1	1:C:150:GLU:HB3	2.15	0.46
1:B:96:THR:CG2	1:B:137:PHE:HB2	2.45	0.46
1:D:280:ARG:O	1:D:296:PHE:HA	2.16	0.46
1:D:86:GLU:CD	1:D:104:LYS:NZ	2.69	0.46
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.80	0.46
1:C:285:VAL:HG13	1:C:286:GLU:H	1.79	0.46
1:A:81:TRP:CE3	1:A:298:ILE:HD11	2.51	0.46
1:D:33:TYR:OH	1:D:219:MET:O	2.32	0.46
1:C:85:LEU:O	1:C:85:LEU:HD12	2.15	0.46
1:A:292:LYS:O	1:A:293:ALA:C	2.52	0.46
1:D:149:MET:HE2	1:D:150:GLU:HB3	1.98	0.46
1:D:86:GLU:C	1:D:88:LEU:H	2.17	0.46
1:C:50:ARG:CA	1:C:50:ARG:NE	2.53	0.46
1:A:93:LYS:HZ1	1:A:100:GLU:HG3	1.81	0.46
1:A:202:TYR:CD1	1:B:59:PHE:CD2	3.04	0.46
1:D:171:ASN:O	1:D:172:PRO:C	2.52	0.46
1:A:37:ILE:O	1:A:38:GLN:C	2.51	0.46
1:C:193:PRO:HA	1:C:194:PRO:HD2	1.55	0.46
1:A:260:ASN:H	1:A:260:ASN:HD22	0.58	0.46
1:D:207:GLU:HA	1:D:207:GLU:OE1	2.15	0.46
1:C:29:GLY:O	1:C:30:GLU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:CG2	1:A:299:GLU:N	2.76	0.46
1:A:211:GLN:HB2	1:A:249:ILE:HB	1.98	0.45
1:A:187:LEU:CD2	1:A:190:MET:HE3	2.38	0.45
1:D:92:ILE:CG2	1:D:161:LEU:CD2	2.94	0.45
1:B:140:ARG:HE	1:B:140:ARG:HB3	1.42	0.45
1:B:288:ILE:HD12	1:B:291:PHE:HE2	1.81	0.45
1:A:175:ARG:HB2	1:A:175:ARG:HH11	1.81	0.45
1:D:61:MET:HB2	1:D:252:LEU:HB2	1.98	0.45
1:C:223:VAL:N	1:C:224:PRO:CD	2.79	0.45
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.71	0.45
1:A:214:GLN:HB3	1:A:252:LEU:HD23	1.98	0.45
1:D:140:ARG:C	1:D:141:HIS:CG	2.89	0.45
1:D:97:ASN:HD22	1:D:99:LYS:CB	2.02	0.45
1:B:233:LEU:HD12	1:B:233:LEU:O	2.15	0.45
1:B:182:TRP:CZ3	1:B:215:ARG:CD	3.00	0.45
1:B:97:ASN:C	1:B:97:ASN:ND2	2.70	0.45
1:C:72:PRO:CA	1:C:276:PHE:CE1	2.86	0.45
1:A:119:ASP:O	1:A:120:SER:C	2.55	0.45
1:A:138:GLN:O	1:A:160:GLN:NE2	2.44	0.45
1:A:133:PRO:HD3	1:A:146:TYR:CD2	2.51	0.45
1:D:112:ASN:HD22	1:D:191:ALA:HB3	1.75	0.45
1:B:274:ARG:NE	1:B:304:HIS:HD2	2.13	0.45
1:B:49:ASP:HB2	1:B:50:ARG:H	1.60	0.45
1:C:88:LEU:O	1:C:92:ILE:CG1	2.64	0.45
1:D:28:HIS:C	1:D:28:HIS:ND1	2.69	0.45
1:C:139:TRP:N	1:C:139:TRP:CD1	2.84	0.45
1:D:79:VAL:HG12	1:D:225:PHE:HD1	1.82	0.45
1:D:87:GLU:OE1	1:D:91:PHE:CE2	2.70	0.45
1:B:293:ALA:C	1:B:295:ASP:H	2.19	0.45
1:B:274:ARG:HD2	1:B:304:HIS:CD2	2.51	0.45
1:D:169:LYS:CD	1:D:241:THR:HG22	2.45	0.45
1:A:45:VAL:HG21	1:B:204:VAL:HG21	1.98	0.45
1:D:36:GLN:O	1:D:37:ILE:C	2.54	0.45
1:C:222:GLY:O	1:C:226:ASN:N	2.30	0.45
1:A:182:TRP:CZ3	1:A:194:PRO:HD2	2.51	0.45
1:D:85:LEU:O	1:D:89:LEU:HD11	2.16	0.45
1:C:99:LYS:C	1:C:101:LEU:H	2.19	0.45
1:B:101:LEU:O	1:B:102:SER:C	2.56	0.45
1:B:81:TRP:C	1:B:83:GLY:N	2.67	0.45
1:A:102:SER:C	1:A:104:LYS:N	2.68	0.45
1:C:264:PRO:O	1:C:267:ILE:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ASP:C	1:A:190:MET:HE2	2.37	0.45
1:B:102:SER:O	1:B:104:LYS:N	2.49	0.45
1:A:113:GLY:O	1:A:118:LEU:CD1	2.65	0.45
1:C:305:PRO:O	1:C:306:THR:HG22	2.16	0.45
1:C:280:ARG:HA	1:C:280:ARG:CD	2.47	0.45
1:D:234:THR:O	1:D:235:TYR:C	2.56	0.45
1:C:95:SER:OG	1:C:97:ASN:N	2.43	0.45
1:C:257:ILE:HD13	1:C:265:LEU:HD12	1.99	0.45
1:C:239:HIS:CE1	1:C:284:LYS:CG	2.93	0.45
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.64	0.45
1:C:57:SER:HA	1:C:255:ALA:O	2.17	0.45
1:D:229:SER:HB3	1:D:230:TYR:HD2	1.82	0.45
1:D:135:TYR:HA	1:D:138:GLN:HB2	2.00	0.44
1:B:231:ALA:O	1:B:232:LEU:C	2.56	0.44
1:B:80:PHE:CE1	1:B:82:LYS:HB3	2.52	0.44
1:D:78:ARG:CZ	1:D:303:PRO:HG2	2.44	0.44
1:B:55:THR:HA	1:B:257:ILE:O	2.17	0.44
1:B:171:ASN:HA	1:B:172:PRO:HD3	1.43	0.44
1:D:96:THR:HG22	1:D:96:THR:O	2.17	0.44
1:D:97:ASN:HB2	1:D:149:MET:CE	2.48	0.44
1:D:301:TYR:OH	1:D:303:PRO:HG3	2.15	0.44
1:A:68:ARG:NE	1:A:207:GLU:OE2	2.50	0.44
1:C:178:ILE:HG23	1:C:200:GLN:CA	2.46	0.44
1:C:173:ASP:O	1:C:174:ASP:C	2.52	0.44
1:C:238:ALA:O	1:C:243:LEU:N	2.50	0.44
1:D:244:LYS:HE2	1:D:244:LYS:HB2	1.68	0.44
1:C:37:ILE:HG23	1:C:37:ILE:HD12	1.57	0.44
1:A:140:ARG:C	1:A:141:HIS:CD2	2.90	0.44
1:D:115:ARG:CG	1:D:128:GLU:OE1	2.60	0.44
1:D:141:HIS:HB3	1:D:144:ALA:HB3	1.99	0.44
1:D:238:ALA:O	1:D:240:ILE:N	2.50	0.44
1:B:304:HIS:C	1:B:305:PRO:O	2.56	0.44
1:B:98:ALA:N	1:B:129:GLY:O	2.42	0.44
1:C:288:ILE:C	1:C:290:ASP:H	2.20	0.44
1:C:69:ASP:HA	1:C:235:TYR:OH	2.18	0.44
1:A:175:ARG:HB2	1:A:175:ARG:NH1	2.33	0.44
1:A:227:ILE:O	1:A:228:ALA:C	2.56	0.44
1:B:142:PHE:HB3	1:B:158:VAL:HB	2.00	0.44
1:B:192:LEU:HG	1:B:193:PRO:HD2	1.99	0.44
1:B:223:VAL:N	1:B:224:PRO:HD2	2.32	0.44
1:A:182:TRP:HD1	1:A:184:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:CG1	1:A:257:ILE:O	2.46	0.44
1:B:139:TRP:CE2	1:B:179:MET:CE	3.00	0.44
1:A:232:LEU:HD12	1:A:232:LEU:O	2.18	0.44
1:A:225:PHE:O	1:A:228:ALA:HB3	2.17	0.44
1:D:206:SER:HA	1:D:243:LEU:HD21	1.99	0.44
1:C:186:ASP:HA	1:C:189:LEU:HD12	2.00	0.44
1:D:261:HIS:O	1:D:262:ILE:C	2.54	0.44
1:B:82:LYS:O	1:B:82:LYS:HG2	2.16	0.44
1:C:143:GLY:C	1:D:185:ARG:NH2	2.71	0.44
1:C:212:LEU:HD12	1:C:213:TYR:N	2.32	0.44
1:B:297:GLN:HA	1:B:297:GLN:OE1	2.18	0.44
1:A:287:LYS:HE3	1:A:287:LYS:HB2	1.21	0.44
1:D:276:PHE:O	1:D:277:PRO:C	2.56	0.44
1:D:164:VAL:CG1	1:D:177:ILE:CG2	2.94	0.44
1:D:298:ILE:O	1:D:298:ILE:HG22	2.17	0.44
1:A:93:LYS:NZ	1:A:100:GLU:HG3	2.33	0.44
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.60	0.44
1:B:66:SER:O	1:B:67:LEU:HD23	2.18	0.44
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.27	0.44
1:D:126:ARG:NH1	1:D:132:GLY:N	2.65	0.44
1:D:79:VAL:HG12	1:D:225:PHE:CD1	2.52	0.44
1:B:272:GLU:OE2	1:B:273:PRO:HD2	2.18	0.44
1:B:304:HIS:CB	1:B:305:PRO:CA	2.95	0.44
1:B:215:ARG:NH1	1:B:215:ARG:CG	2.64	0.44
1:A:202:TYR:O	1:A:202:TYR:HD2	2.00	0.44
1:C:279:LEU:HD13	1:C:298:ILE:HD13	2.00	0.44
1:A:216:SER:OG	1:A:256:HIS:HE1	2.01	0.44
1:C:184:PRO:CA	1:C:187:LEU:CD1	2.91	0.43
1:D:86:GLU:O	1:D:87:GLU:C	2.56	0.43
1:A:207:GLU:HG3	1:A:244:LYS:HG3	2.00	0.43
1:A:102:SER:HB2	1:A:110:ASP:CG	2.37	0.43
1:A:173:ASP:O	1:A:174:ASP:C	2.53	0.43
1:A:196:HIS:NE2	1:A:226:ASN:ND2	2.66	0.43
1:A:45:VAL:CG2	1:B:204:VAL:HG21	2.48	0.43
1:A:203:VAL:HG13	1:A:243:LEU:HD13	1.99	0.43
1:B:87:GLU:O	1:B:90:TRP:HB3	2.16	0.43
1:A:47:LYS:HD2	1:B:204:VAL:HG23	2.01	0.43
1:B:177:ILE:HG21	1:B:201:PHE:N	2.25	0.43
1:C:31:LEU:O	1:C:32:GLN:C	2.55	0.43
1:A:194:PRO:O	1:A:215:ARG:NE	2.43	0.43
1:D:101:LEU:HA	1:D:104:LYS:CE	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ILE:O	1:B:178:ILE:HG13	2.18	0.43
1:C:165:ILE:HG23	1:C:241:THR:CG2	2.49	0.43
1:B:186:ASP:O	1:B:190:MET:HE3	2.17	0.43
1:A:97:ASN:O	1:A:100:GLU:N	2.52	0.43
1:C:305:PRO:O	1:C:306:THR:CG2	2.66	0.43
1:C:86:GLU:O	1:C:87:GLU:C	2.56	0.43
1:D:71:PHE:HA	1:D:72:PRO:HD2	1.68	0.43
1:D:126:ARG:HH12	1:D:132:GLY:N	2.17	0.43
1:D:142:PHE:C	1:D:144:ALA:N	2.72	0.43
1:D:236:MET:HG2	1:D:291:PHE:CE2	2.54	0.43
1:D:240:ILE:CG2	1:D:240:ILE:O	2.66	0.43
1:B:177:ILE:HG23	1:B:201:PHE:HD2	1.84	0.43
1:B:199:CYS:HB2	1:B:211:GLN:O	2.18	0.43
1:A:142:PHE:C	1:A:142:PHE:CD2	2.92	0.43
1:A:79:VAL:CG1	1:A:80:PHE:N	2.73	0.43
1:B:62:GLN:HA	1:B:250:HIS:O	2.18	0.43
1:B:203:VAL:HA	1:B:207:GLU:O	2.18	0.43
1:B:174:ASP:OD1	1:B:176:ARG:CG	2.67	0.43
1:D:118:LEU:O	1:D:119:ASP:C	2.57	0.43
1:C:84:VAL:O	1:C:84:VAL:HG12	2.19	0.43
1:B:140:ARG:NH2	1:B:159:ASP:OD2	2.25	0.43
1:C:148:ASP:OD1	1:C:150:GLU:CB	2.66	0.43
1:C:231:ALA:O	1:C:232:LEU:C	2.57	0.43
1:A:142:PHE:CD2	1:B:184:PRO:HG2	2.54	0.43
1:C:73:LEU:HD21	1:C:81:TRP:HB2	2.00	0.43
1:B:207:GLU:HB3	1:B:244:LYS:O	2.18	0.43
1:D:142:PHE:C	1:D:144:ALA:H	2.22	0.43
1:D:85:LEU:O	1:D:85:LEU:HD12	2.19	0.43
1:C:99:LYS:O	1:C:101:LEU:N	2.52	0.43
1:C:135:TYR:O	1:C:136:GLY:C	2.55	0.43
1:C:112:ASN:N	1:C:112:ASN:ND2	2.66	0.43
1:D:284:LYS:C	1:D:285:VAL:CG2	2.87	0.43
1:B:159:ASP:C	1:B:161:LEU:N	2.72	0.43
1:D:287:LYS:O	1:D:289:ASP:N	2.52	0.43
1:D:233:LEU:CD1	1:D:237:ILE:HD11	2.49	0.42
1:A:148:ASP:C	1:A:148:ASP:OD1	2.58	0.42
1:A:304:HIS:HB3	1:A:305:PRO:CD	2.49	0.42
1:B:298:ILE:HG23	1:B:301:TYR:HB2	2.00	0.42
1:D:67:LEU:HG	1:D:246:GLY:O	2.19	0.42
1:C:96:THR:HG22	1:C:137:PHE:HB2	2.00	0.42
1:B:201:PHE:HA	1:B:209:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TRP:CE2	1:A:298:ILE:HD11	2.54	0.42
1:B:172:PRO:HB2	1:B:203:VAL:HG11	1.81	0.42
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.56	0.42
1:D:227:ILE:HG23	1:D:227:ILE:HD13	1.75	0.42
1:B:91:PHE:O	1:B:92:ILE:C	2.56	0.42
1:A:283:ARG:NH1	1:A:285:VAL:HG21	2.35	0.42
1:C:175:ARG:CG	1:D:254:ASP:OD1	2.66	0.42
1:B:140:ARG:HH21	1:B:159:ASP:CG	2.16	0.42
1:C:139:TRP:O	1:C:140:ARG:HD2	2.19	0.42
1:C:92:ILE:HG23	1:C:92:ILE:HD13	1.73	0.42
1:A:91:PHE:CD1	1:A:135:TYR:CB	3.00	0.42
1:D:86:GLU:OE2	1:D:86:GLU:CA	2.67	0.42
1:C:115:ARG:HH21	1:C:128:GLU:HB2	1.69	0.42
1:B:88:LEU:O	1:B:92:ILE:N	2.49	0.42
1:C:192:LEU:HD13	1:C:192:LEU:N	2.34	0.42
1:A:291:PHE:HA	1:A:295:ASP:OD1	2.19	0.42
1:D:86:GLU:OE2	1:D:86:GLU:HA	2.19	0.42
1:A:257:ILE:HG13	1:A:258:TYR:O	2.20	0.42
1:C:161:LEU:O	1:C:164:VAL:N	2.52	0.42
1:C:89:LEU:O	1:C:90:TRP:C	2.55	0.42
1:A:274:ARG:O	1:A:275:PRO:C	2.55	0.42
1:A:140:ARG:HA	1:A:159:ASP:HA	2.02	0.42
1:D:225:PHE:O	1:D:227:ILE:N	2.53	0.42
1:D:89:LEU:O	1:D:90:TRP:C	2.57	0.42
1:C:55:THR:HB	1:C:257:ILE:O	2.20	0.42
1:A:102:SER:O	1:A:103:SER:C	2.54	0.42
1:A:90:TRP:CD2	1:A:101:LEU:HD22	2.54	0.42
1:D:32:GLN:CA	1:D:32:GLN:NE2	2.80	0.42
1:D:71:PHE:O	1:D:277:PRO:HG2	2.19	0.42
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.83	0.42
1:D:107:LYS:O	1:D:110:ASP:HB2	2.20	0.42
1:D:268:GLN:C	1:D:270:GLN:H	2.22	0.42
1:A:162:GLN:O	1:A:163:ARG:C	2.57	0.42
1:C:204:VAL:HG21	1:D:47:LYS:CD	2.49	0.42
1:B:298:ILE:HG22	1:B:298:ILE:O	2.20	0.42
1:D:117:PHE:O	1:D:118:LEU:C	2.58	0.42
1:B:162:GLN:O	1:B:165:ILE:N	2.53	0.42
1:C:258:TYR:HB2	1:C:261:HIS:CD2	2.55	0.42
1:A:202:TYR:CZ	1:B:59:PHE:HB2	2.54	0.42
1:A:164:VAL:HG12	1:A:165:ILE:N	2.34	0.42
1:B:140:ARG:O	1:B:141:HIS:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LYS:HA	1:B:305:PRO:HD2	2.01	0.42
1:B:119:ASP:CA	1:B:122:GLY:H	2.33	0.42
1:A:102:SER:OG	1:A:107:LYS:HD3	2.20	0.42
1:A:127:GLU:O	1:A:128:GLU:C	2.58	0.42
1:D:32:GLN:O	1:D:33:TYR:C	2.58	0.42
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.74	0.42
1:A:71:PHE:CZ	1:A:231:ALA:HB3	2.55	0.42
1:A:284:LYS:CD	1:A:284:LYS:CB	2.90	0.41
1:C:240:ILE:CG2	1:C:240:ILE:O	2.67	0.41
1:A:176:ARG:HD2	1:A:176:ARG:HH11	1.56	0.41
1:A:176:ARG:HH22	1:B:193:PRO:HG3	1.83	0.41
1:C:135:TYR:OH	1:C:195:CYS:N	2.51	0.41
1:B:48:ASP:OD2	1:B:54:GLY:HA2	2.20	0.41
1:B:99:LYS:HB2	1:B:99:LYS:HZ3	1.84	0.41
1:A:299:GLU:CG	1:A:299:GLU:O	2.67	0.41
1:A:203:VAL:O	1:A:204:VAL:HB	2.19	0.41
1:A:306:THR:O	1:A:306:THR:CG2	2.67	0.41
1:B:160:GLN:NE2	1:B:179:MET:CA	2.83	0.41
1:B:118:LEU:HB3	1:B:123:PHE:O	2.20	0.41
1:C:143:GLY:CA	1:D:185:ARG:CZ	2.98	0.41
1:A:32:GLN:O	1:A:36:GLN:HG3	2.21	0.41
1:D:30:GLU:OE2	1:D:273:PRO:HB3	2.20	0.41
1:B:84:VAL:HG22	1:B:225:PHE:CZ	2.55	0.41
1:C:182:TRP:CE2	1:D:178:ILE:HG21	2.55	0.41
1:C:203:VAL:C	1:C:204:VAL:HG23	2.35	0.41
1:D:142:PHE:CG	1:D:143:GLY:N	2.89	0.41
1:D:161:LEU:HD12	1:D:161:LEU:HA	1.65	0.41
1:D:237:ILE:H	1:D:237:ILE:HG13	1.53	0.41
1:D:257:ILE:HD13	1:D:265:LEU:CD1	2.50	0.41
1:C:178:ILE:N	1:C:178:ILE:HD12	2.34	0.41
1:B:41:LEU:H	1:B:41:LEU:CD2	2.33	0.41
1:A:167:THR:O	1:A:168:ILE:C	2.57	0.41
1:A:238:ALA:O	1:A:242:GLY:N	2.53	0.41
1:B:164:VAL:O	1:B:165:ILE:C	2.56	0.41
1:A:142:PHE:O	1:A:142:PHE:HD2	2.02	0.41
1:D:238:ALA:C	1:D:240:ILE:N	2.74	0.41
1:B:178:ILE:HG23	1:B:199:CYS:O	2.21	0.41
1:C:108:ILE:HG13	1:C:109:TRP:N	2.27	0.41
1:A:171:ASN:HA	1:A:172:PRO:HD3	1.17	0.41
1:B:173:ASP:O	1:B:174:ASP:C	2.59	0.41
1:D:118:LEU:O	1:D:119:ASP:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:THR:C	1:D:236:MET:N	2.70	0.41
1:B:141:HIS:CD2	1:B:153:TYR:HB3	2.55	0.41
1:B:119:ASP:C	1:B:121:LEU:N	2.74	0.41
1:C:68:ARG:HH22	1:C:247:ASP:CG	2.24	0.41
1:C:304:HIS:O	1:C:305:PRO:C	2.59	0.41
1:B:223:VAL:O	1:B:224:PRO:C	2.58	0.41
1:C:174:ASP:CG	1:C:175:ARG:H	2.24	0.41
1:B:240:ILE:O	1:B:240:ILE:HG22	2.19	0.41
1:C:134:VAL:O	1:C:138:GLN:HG3	2.21	0.41
1:B:231:ALA:HB3	1:B:232:LEU:H	1.60	0.41
1:B:88:LEU:O	1:B:91:PHE:HB2	2.20	0.41
1:B:123:PHE:HA	1:B:123:PHE:HD1	1.60	0.41
1:C:177:ILE:HG21	1:C:177:ILE:HD13	1.77	0.41
1:C:60:GLY:O	1:D:64:ARG:NH1	2.54	0.41
1:A:234:THR:O	1:A:237:ILE:N	2.54	0.41
1:D:55:THR:OG1	1:D:56:LEU:N	2.54	0.41
1:D:85:LEU:HD11	1:D:296:PHE:CD1	2.56	0.41
1:A:176:ARG:NH2	1:B:50:ARG:NH1	2.68	0.41
1:B:97:ASN:O	1:B:100:GLU:HB2	2.21	0.41
1:C:265:LEU:HA	1:C:265:LEU:HD23	1.61	0.41
1:C:88:LEU:HD23	1:C:232:LEU:HG	2.03	0.41
1:A:90:TRP:CD1	1:A:95:SER:HB3	2.55	0.41
1:A:175:ARG:HH21	1:B:55:THR:HG21	1.83	0.41
1:B:263:GLU:CG	1:B:266:LYS:NZ	2.78	0.41
1:A:114:SER:CB	1:A:116:ASP:OD2	2.66	0.41
1:A:167:THR:HG21	1:A:174:ASP:OD1	2.21	0.41
1:A:71:PHE:O	1:A:277:PRO:HD2	2.20	0.41
1:C:294:GLU:C	1:C:296:PHE:N	2.74	0.41
1:A:158:VAL:HG12	1:A:159:ASP:N	2.36	0.41
1:A:202:TYR:C	1:A:202:TYR:CD2	2.94	0.41
1:A:182:TRP:CD1	1:A:184:PRO:HD3	2.56	0.40
1:D:79:VAL:O	1:D:81:TRP:N	2.46	0.40
1:A:58:VAL:CG1	1:A:59:PHE:N	2.80	0.40
1:B:30:GLU:CD	1:B:76:THR:HG23	2.42	0.40
1:A:177:ILE:HD13	1:A:177:ILE:HG21	1.62	0.40
1:A:109:TRP:O	1:A:111:ALA:N	2.54	0.40
1:D:101:LEU:HD23	1:D:106:VAL:O	2.21	0.40
1:D:113:GLY:CA	1:D:129:GLY:HA2	2.50	0.40
1:D:240:ILE:HD11	1:D:291:PHE:CZ	2.57	0.40
1:B:208:LEU:O	1:B:246:GLY:N	2.51	0.40
1:B:232:LEU:O	1:B:233:LEU:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HA	1:D:208:LEU:HD12	1.61	0.40
1:B:31:LEU:N	1:B:31:LEU:CD2	2.84	0.40
1:D:307:ILE:CG2	1:D:308:LYS:H	2.32	0.40
1:D:236:MET:O	1:D:238:ALA:N	2.54	0.40
1:B:135:TYR:OH	1:B:194:PRO:HA	2.21	0.40
1:B:81:TRP:O	1:B:85:LEU:N	2.46	0.40
1:D:26:PRO:O	1:D:27:PRO:C	2.60	0.40
1:C:298:ILE:HA	1:C:298:ILE:HD13	1.76	0.40
1:C:181:ALA:HB3	1:C:196:HIS:O	2.21	0.40
1:B:56:LEU:HD12	1:B:56:LEU:HA	1.88	0.40
1:D:307:ILE:CD1	1:D:307:ILE:CB	2.88	0.40
1:D:99:LYS:O	1:D:103:SER:OG	2.39	0.40
1:D:73:LEU:CD1	1:D:228:ALA:HB1	2.51	0.40
1:D:261:HIS:O	1:D:264:PRO:CD	2.67	0.40
1:D:301:TYR:CE2	1:D:303:PRO:CG	3.04	0.40
1:C:32:GLN:NE2	1:C:64:ARG:N	2.62	0.40
1:B:225:PHE:C	1:B:225:PHE:CD2	2.95	0.40
1:D:235:TYR:O	1:D:238:ALA:CB	2.51	0.40
1:B:274:ARG:HB3	1:B:275:PRO:HD2	2.04	0.40
1:D:260:ASN:OD1	1:D:260:ASN:N	2.54	0.40
1:B:183:ASN:HB3	1:B:186:ASP:HB2	2.04	0.40
1:A:130:ASP:HB2	1:A:149:MET:HG2	2.02	0.40
1:D:274:ARG:NH1	1:D:302:ASN:O	2.53	0.40
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	281/313 (90%)	225 (80%)	37 (13%)	19 (7%)	1 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	279/313 (89%)	205 (74%)	57 (20%)	17 (6%)	2 4
1	C	281/313 (90%)	228 (81%)	41 (15%)	12 (4%)	3 9
1	D	281/313 (90%)	193 (69%)	55 (20%)	33 (12%)	0 1
All	All	1122/1252 (90%)	851 (76%)	190 (17%)	81 (7%)	1 3

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	116	ASP
1	A	305	PRO
1	B	38	GLN
1	B	76	THR
1	B	186	ASP
1	D	27	PRO
1	D	81	TRP
1	D	238	ALA
1	D	264	PRO
1	D	265	LEU
1	D	271	ARG
1	D	307	ILE
1	A	68	ARG
1	A	119	ASP
1	A	142	PHE
1	A	291	PHE
1	B	32	GLN
1	B	52	GLY
1	B	103	SER
1	B	115	ARG
1	B	189	LEU
1	B	228	ALA
1	B	231	ALA
1	B	300	GLY
1	C	127	GLU
1	C	157	GLY
1	C	172	PRO
1	C	277	PRO
1	D	85	LEU
1	D	87	GLU
1	D	102	SER
1	D	173	ASP

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Mol	Chain	Res	Type
1	D	227	ILE
1	D	236	MET
1	D	260	ASN
1	D	294	GLU
1	A	27	PRO
1	A	81	TRP
1	A	115	ARG
1	A	118	LEU
1	A	155	GLY
1	A	189	LEU
1	B	72	PRO
1	B	160	GLN
1	B	305	PRO
1	C	111	ALA
1	C	306	THR
1	D	80	PHE
1	D	119	ASP
1	D	226	ASN
1	D	237	ILE
1	D	269	LEU
1	D	288	ILE
1	A	140	ARG
1	A	204	VAL
1	B	187	LEU
1	C	93	LYS
1	C	134	VAL
1	D	84	VAL
1	D	135	TYR
1	D	151	SER
1	D	293	ALA
1	A	233	LEU
1	C	123	PHE
1	C	305	PRO
1	D	72	PRO
1	D	90	TRP
1	D	158	VAL
1	A	222	GLY
1	B	158	VAL
1	C	124	SER
1	C	149	MET
1	D	175	ARG
1	A	157	GLY

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Mol	Chain	Res	Type
1	D	184	PRO
1	D	303	PRO
1	D	246	GLY
1	D	94	GLY
1	A	263	GLU
1	B	277	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/271 (91%)	183 (74%)	64 (26%)	0	1
1	B	245/271 (90%)	184 (75%)	61 (25%)	1	2
1	C	247/271 (91%)	187 (76%)	60 (24%)	1	2
1	D	247/271 (91%)	177 (72%)	70 (28%)	0	1
All	All	986/1084 (91%)	731 (74%)	255 (26%)	0	1

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	38	GLN
1	A	40	ILE
1	A	46	ARG
1	A	51	THR
1	A	68	ARG
1	A	85	LEU
1	A	86	GLU
1	A	89	LEU
1	A	103	SER
1	A	104	LYS
1	A	108	ILE
1	A	116	ASP
1	A	118	LEU
1	A	127	GLU

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Mol	Chain	Res	Type
1	A	140	ARG
1	A	149	MET
1	A	152	ASP
1	A	154	SER
1	A	160	GLN
1	A	162	GLN
1	A	164	VAL
1	A	170	THR
1	A	175	ARG
1	A	176	ARG
1	A	179	MET
1	A	182	TRP
1	A	185	ARG
1	A	189	LEU
1	A	190	MET
1	A	192	LEU
1	A	195	CYS
1	A	198	LEU
1	A	202	TYR
1	A	204	VAL
1	A	211	GLN
1	A	221	LEU
1	A	233	LEU
1	A	236	MET
1	A	240	ILE
1	A	244	LYS
1	A	257	ILE
1	A	259	LEU
1	A	260	ASN
1	A	269	LEU
1	A	271	ARG
1	A	272	GLU
1	A	275	PRO
1	A	279	LEU
1	A	280	ARG
1	A	281	ILE
1	A	285	VAL
1	A	286	GLU
1	A	287	LYS
1	A	288	ILE
1	A	289	ASP
1	A	292	LYS

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Mol	Chain	Res	Type
1	A	294	GLU
1	A	296	PHE
1	A	297	GLN
1	A	299	GLU
1	A	306	THR
1	A	307	ILE
1	A	308	LYS
1	B	26	PRO
1	B	31	LEU
1	B	32	GLN
1	B	41	LEU
1	B	42	ARG
1	B	43	CYS
1	B	47	LYS
1	B	55	THR
1	B	56	LEU
1	B	64	ARG
1	B	76	THR
1	B	77	LYS
1	B	78	ARG
1	B	85	LEU
1	B	93	LYS
1	B	96	THR
1	B	97	ASN
1	B	99	LYS
1	B	103	SER
1	B	108	ILE
1	B	114	SER
1	B	116	ASP
1	B	119	ASP
1	B	126	ARG
1	B	128	GLU
1	B	140	ARG
1	B	148	ASP
1	B	149	MET
1	B	150	GLU
1	B	151	SER
1	B	152	ASP
1	B	154	SER
1	B	156	GLN
1	B	170	THR
1	B	171	ASN

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Mol	Chain	Res	Type
1	B	177	ILE
1	B	179	MET
1	B	198	LEU
1	B	202	TYR
1	B	206	SER
1	B	207	GLU
1	B	208	LEU
1	B	212	LEU
1	B	215	ARG
1	B	216	SER
1	B	221	LEU
1	B	224	PRO
1	B	226	ASN
1	B	240	ILE
1	B	260	ASN
1	B	262	ILE
1	B	268	GLN
1	B	269	LEU
1	B	272	GLU
1	B	278	LYS
1	B	280	ARG
1	B	284	LYS
1	B	289	ASP
1	B	290	ASP
1	B	292	LYS
1	B	298	ILE
1	C	38	GLN
1	C	46	ARG
1	C	48	ASP
1	C	50	ARG
1	C	56	LEU
1	C	57	SER
1	C	72	PRO
1	C	74	LEU
1	C	76	THR
1	C	78	ARG
1	C	80	PHE
1	C	82	LYS
1	C	85	LEU
1	C	86	GLU
1	C	87	GLU
1	C	88	LEU

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Mol	Chain	Res	Type
1	C	91	PHE
1	C	93	LYS
1	C	95	SER
1	C	99	LYS
1	C	102	SER
1	C	107	LYS
1	C	108	ILE
1	C	110	ASP
1	C	112	ASN
1	C	115	ARG
1	C	120	SER
1	C	123	PHE
1	C	127	GLU
1	C	131	LEU
1	C	140	ARG
1	C	151	SER
1	C	158	VAL
1	C	163	ARG
1	C	167	THR
1	C	171	ASN
1	C	175	ARG
1	C	178	ILE
1	C	180	CYS
1	C	189	LEU
1	C	190	MET
1	C	192	LEU
1	C	218	ASP
1	C	221	LEU
1	C	240	ILE
1	C	257	ILE
1	C	260	ASN
1	C	263	GLU
1	C	268	GLN
1	C	276	PHE
1	C	280	ARG
1	C	283	ARG
1	C	284	LYS
1	C	288	ILE
1	C	291	PHE
1	C	292	LYS
1	C	297	GLN
1	C	302	ASN

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Mol	Chain	Res	Type
1	C	307	ILE
1	C	308	LYS
1	D	31	LEU
1	D	42	ARG
1	D	50	ARG
1	D	51	THR
1	D	56	LEU
1	D	57	SER
1	D	64	ARG
1	D	69	ASP
1	D	73	LEU
1	D	74	LEU
1	D	78	ARG
1	D	79	VAL
1	D	80	PHE
1	D	84	VAL
1	D	90	TRP
1	D	91	PHE
1	D	92	ILE
1	D	93	LYS
1	D	95	SER
1	D	96	THR
1	D	101	LEU
1	D	104	LYS
1	D	108	ILE
1	D	115	ARG
1	D	117	PHE
1	D	118	LEU
1	D	127	GLU
1	D	128	GLU
1	D	133	PRO
1	D	135	TYR
1	D	140	ARG
1	D	150	GLU
1	D	151	SER
1	D	152	ASP
1	D	154	SER
1	D	156	GLN
1	D	158	VAL
1	D	165	ILE
1	D	169	LYS
1	D	174	ASP

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Mol	Chain	Res	Type
1	D	177	ILE
1	D	178	ILE
1	D	192	LEU
1	D	198	LEU
1	D	204	VAL
1	D	209	SER
1	D	215	ARG
1	D	221	LEU
1	D	229	SER
1	D	233	LEU
1	D	236	MET
1	D	240	ILE
1	D	244	LYS
1	D	259	LEU
1	D	260	ASN
1	D	267	ILE
1	D	270	GLN
1	D	272	GLU
1	D	274	ARG
1	D	276	PHE
1	D	278	LYS
1	D	280	ARG
1	D	281	ILE
1	D	286	GLU
1	D	287	LYS
1	D	288	ILE
1	D	292	LYS
1	D	294	GLU
1	D	306	THR
1	D	308	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	226	ASN
1	A	256	HIS
1	A	260	ASN
1	A	268	GLN
1	A	270	GLN
1	B	32	GLN
1	B	39	HIS

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	112	ASN
1	B	138	GLN
1	B	160	GLN
1	B	171	ASN
1	B	205	ASN
1	B	304	HIS
1	C	32	GLN
1	C	112	ASN
1	C	226	ASN
1	C	239	HIS
1	C	260	ASN
1	C	268	GLN
1	D	32	GLN
1	D	97	ASN
1	D	112	ASN
1	D	160	GLN
1	D	200	GLN
1	D	211	GLN
1	D	226	ASN
1	D	256	HIS
1	D	297	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	616	-	4,4,4	1.95	2 (50%)	6,6,6	2.72	4 (66%)
3	PO4	B	616	-	4,4,4	1.51	1 (25%)	6,6,6	0.59	0
2	SO4	C	616	-	4,4,4	1.27	0	6,6,6	1.60	2 (33%)
3	PO4	D	616	-	4,4,4	0.68	0	6,6,6	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	616	-	-	0/0/0/0	0/0/0/0
3	PO4	B	616	-	-	0/0/0/0	0/0/0/0
2	SO4	C	616	-	-	0/0/0/0	0/0/0/0
3	PO4	D	616	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	616	PO4	P-O2	2.04	1.60	1.53
2	A	616	SO4	O2-S	2.62	1.56	1.47
2	A	616	SO4	O1-S	2.70	1.56	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	616	SO4	O2-S-O1	-3.25	99.20	109.50
2	A	616	SO4	O4-S-O1	-2.87	83.52	110.19
2	A	616	SO4	O3-S-O2	-2.03	91.33	110.19
2	C	616	SO4	O4-S-O3	2.16	117.76	108.98
2	A	616	SO4	O3-S-O1	2.53	133.71	110.19
2	A	616	SO4	O2-S-O1	4.91	125.06	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	616	PO4	7	0
3	D	616	PO4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	283/313 (90%)	-0.05	5 (1%)	71	65	26, 53, 94, 116	0
1	B	281/313 (89%)	0.21	18 (6%)	23	16	30, 67, 111, 149	0
1	C	283/313 (90%)	-0.05	8 (2%)	56	49	25, 58, 109, 144	0
1	D	283/313 (90%)	0.17	20 (7%)	19	12	29, 71, 115, 130	0
All	All	1130/1252 (90%)	0.07	51 (4%)	37	29	25, 63, 109, 149	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	8.9
1	D	123	PHE	7.0
1	B	305	PRO	6.2
1	D	121	LEU	5.9
1	B	306	THR	5.6
1	B	128	GLU	5.4
1	B	120	SER	4.7
1	C	123	PHE	4.6
1	C	111	ALA	4.6
1	B	302	ASN	4.4
1	D	117	PHE	4.1
1	D	95	SER	3.9
1	B	304	HIS	3.9
1	B	301	TYR	3.8
1	B	300	GLY	3.6
1	C	128	GLU	3.5
1	B	116	ASP	3.5
1	A	127	GLU	3.3
1	C	26	PRO	3.0
1	B	151	SER	2.9
1	B	123	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	282	LEU	2.8
1	B	117	PHE	2.7
1	D	282	LEU	2.7
1	A	125	THR	2.6
1	D	213	TYR	2.5
1	C	283	ARG	2.5
1	B	125	THR	2.5
1	D	305	PRO	2.5
1	B	127	GLU	2.5
1	D	92	ILE	2.5
1	B	118	LEU	2.5
1	D	120	SER	2.4
1	D	198	LEU	2.4
1	D	195	CYS	2.3
1	D	308	LYS	2.3
1	A	251	THR	2.3
1	D	93	LYS	2.3
1	D	128	GLU	2.3
1	C	198	LEU	2.3
1	C	307	ILE	2.2
1	A	195	CYS	2.2
1	B	294	GLU	2.2
1	D	152	ASP	2.2
1	C	197	ALA	2.2
1	D	298	ILE	2.2
1	D	114	SER	2.1
1	D	180	CYS	2.1
1	D	306	THR	2.1
1	B	296	PHE	2.0
1	D	197	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	C	616	5/5	0.96	0.22	0.19	68,69,70,71	0
3	PO4	B	616	5/5	0.95	0.17	-0.97	54,58,58,61	0
2	SO4	A	616	5/5	0.97	0.16	-1.01	61,62,66,67	0
3	PO4	D	616	5/5	0.98	0.14	-1.35	58,58,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.