Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 02:28 PM EST

PDB ID	:	1C30
Title	:	CRYSTAL STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT MUTATION C269S
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Deposited on	:	1999-07-24
Resolution	:	2.00 Å(reported)

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

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

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

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

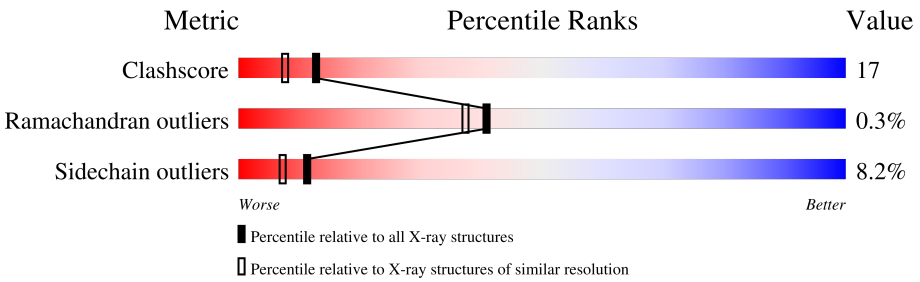
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	61% 30% 7% ••
1	C	1073	59% 31% 7% ••
1	E	1073	64% 28% 7% •
1	G	1073	52% 38% 8% ••
2	B	382	58% 35% 6% •
2	D	382	57% 35% 6% ••
2	F	382	53% 38% 8% •
2	H	382	45% 45% 8% •

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
6	PO4	C	4025	-	X	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 48668 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 CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1058	8189	5141	1429	1574	45	0	6	0
1	C	1058	8165	5126	1422	1572	45	0	1	0
1	E	1058	8188	5141	1426	1575	46	0	6	0
1	G	1058	8178	5137	1424	1572	45	0	4	0

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	379	2895	1825	508	553	9	0	0	0
2	D	379	2895	1825	508	553	9	0	0	0
2	F	379	2895	1825	508	553	9	0	0	0
2	H	379	2900	1828	508	555	9	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	SER	CYS	engineered mutation	UNP P00907
D	269	SER	CYS	engineered mutation	UNP P00907
F	269	SER	CYS	engineered mutation	UNP P00907
H	269	SER	CYS	engineered mutation	UNP P00907

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	3	3	3	0	0
3	C	3	3	3	0	0
3	E	3	3	3	0	0
3	G	3	3	3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	7	7	7	0	0
4	B	1	1	1	0	0
4	C	7	7	7	0	0
4	D	1	1	1	0	0
4	E	7	7	7	0	0
4	F	1	1	1	0	0
4	G	7	7	7	0	0
4	H	1	1	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	3	3	3	0	0
5	B	1	1	1	0	0
5	C	3	3	3	0	0
5	D	1	1	1	0	0
5	E	3	3	3	0	0
5	F	1	1	1	0	0

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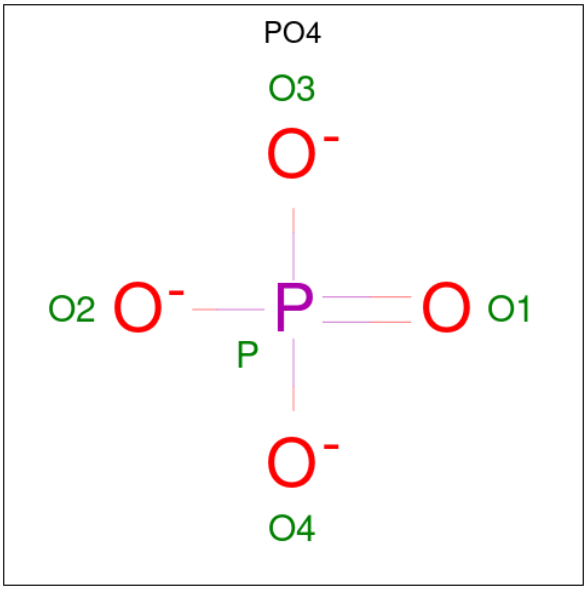
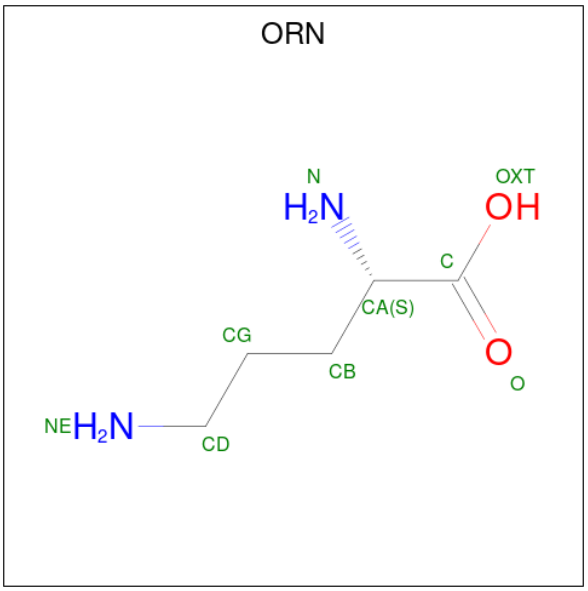
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	G	3	3	3	0	0
			Total	Cl		
5	H	1	1	1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



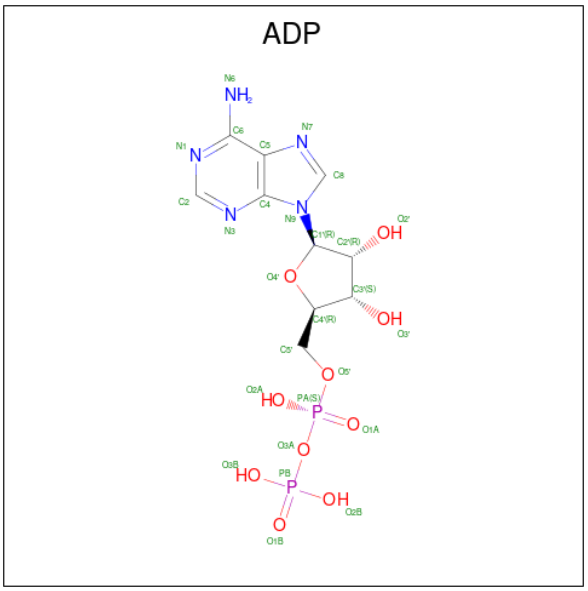
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
6	A	1	5	4	1	0	0
			Total	O	P		
6	C	1	5	4	1	0	0
			Total	O	P		
6	C	1	5	4	1	0	0
			Total	O	P		
6	E	1	5	4	1	0	0
			Total	O	P		
6	E	1	5	4	1	0	0
			Total	O	P		
6	G	1	5	4	1	0	0

- Molecule 7 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



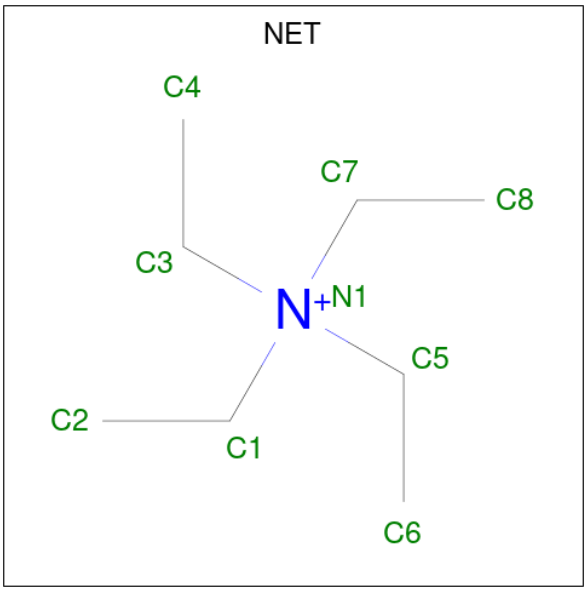
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	9	5	2	2	0	0
			Total	C	N	O		
7	A	1	8	5	2	1	0	0
			Total	C	N	O		
7	A	1	8	5	2	1	0	0
			Total	C	N	O		
7	A	1	9	5	2	2	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	E	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	E	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	G	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
8	G	1	27	10	5	10	2	0	0

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
9	A	1	9	8	1	0	0
			Total	C	N		
9	C	1	9	8	1	0	0
			Total	C	N		
9	E	1	9	8	1	0	0
			Total	C	N		
9	G	1	9	8	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	830	830	830	0	0
			Total	O		
10	B	230	230	230	0	0
			Total	O		
10	C	683	683	683	0	0
			Total	O		
10	D	238	238	238	0	0
			Total	O		
10	E	884	884	884	0	0
			Total	O		
10	F	272	272	272	0	0
			Total	O		
10	G	666	666	666	0	0
			Total	O		
10	H	184	184	184	0	0

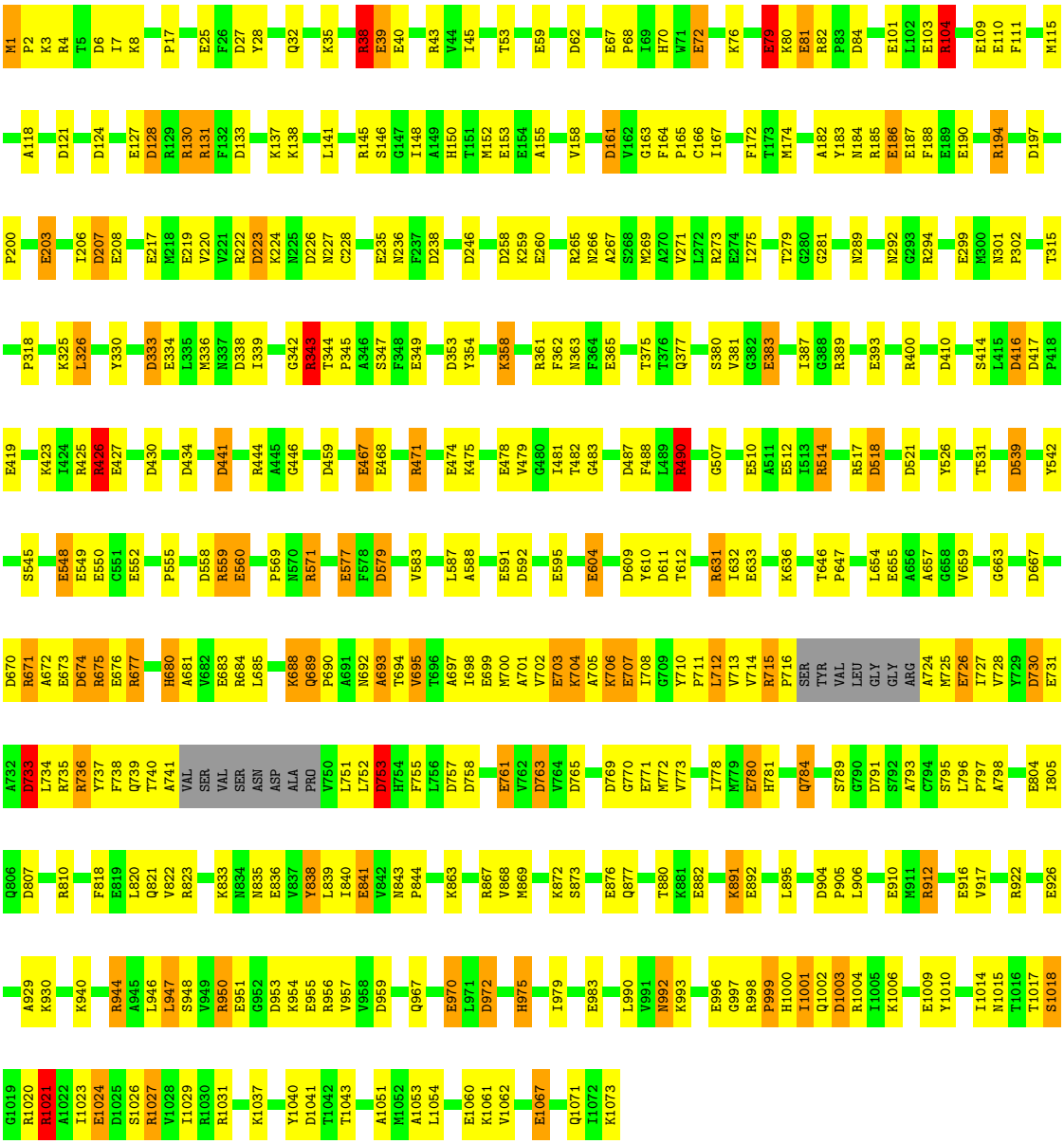
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain A: 61% 30% 7% ••



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C: 59% 31% 7% ••

M1 P2 K3 D6 I7 K8 S9 I10 L11 I12 P17 C24 E25 F26 D27 Y28 Q32 L37 R38 E39 E40 G41 Y42 R43 V44 I45 N48 P51 M55 T56 D57 P58 E59 M60 A61 D62 A63 T64 Y65 I66 E67 P68 I69 E72 V73 V74 R75 K76 I77 I78 E79

K80 E81 R82 P83 D84 L102 E103 R104 V107 L108 E109 E110 F111 D121 D124 K125 A126 E127 D128 R129 R130 R131 F132 D133 E142 R145 S146 H150 E153 E154 A159 A160 D161 P165 C166 I167 I168 R169 F172 T173 M174 A182 Y183 N184 R185 E186 E187 F188

E189 E190 R194 G195 L196 D197 K202 E203 L204 L205 I206 D207 E208 W213 E217 M218 E219 R222 D223 D226 S233 N236 F237 D238 I248 T249 V250 L256 T257 D258 K259 E260 R265 N266 A267 V271 E278 N289 N292 G293 R294 I298 E299

P302 K313 A320 K321 K325 Y330 T331 L332 D333 E334 L335 M336 N337 D338 I339 T340 G341 G342 R343 T344 P345 A346 S347 F348 E349 V356 T357 K358 N363 F364 E365 A368 D372 T375 T376 Q377 E383 R400 E403 K412 V413 S414 L415 D416 E419

R426 E427 D430 D434 R435 D441 I458 D459 R460 W461 E467 E468 L469 V470 R471 L472 E473 E474 E478 T482 D487 R490 Q491 L492 K493 R494 K495 D499 A503 R509 E510 A511 E512 I513 R514 D518 D521 L522 K527 R528 V529 D530 A534 E535

D539 Y542 M543 Y544 E548 E549 E550 N554 P555 S556 T557 D558 R559 E560 K561 I562 M563 R571 I576 E577 E578 D579 Y580 R590 E591 D592 E595 D609 Y610 D611 D614 L623 E624 D625 R631 I632 E633 K634 P635 I639 G644 Q645 T646 P647 L648

R652 A653 L654 E655 S665 P666 D667 A668 I669 D670 R671 A672 E673 D674 R675 E676 R677 F678 Q679 H680 E683 R684 L685 K686 L687 P690 A691 N692 A693 T694 V695 T696 A697 I698 E699 M700 A701 V702 E703 K704 A705 K706 E707 I708 P711 L712 V713 V714 R715 P716 SER TYR VAL LEU GLY GLY

ARG A724 M725 E726 I727 V728 Y729 D730 E731 A732 D733 L734 R735 R736 Y737 F738 A741 VAL SER VAL SER ASN ASP ALA PRO V750 L751 L752 D753 H754 F755 L756 D757 D758 E761 V762 D763 V764 D765 A766 I767 C768 D769 G770 E771 M772 V773 L774 I775 E780 H781 Q784 V787 D791

S795 T800 L801 S802 Q803 E804 I805 Q806 D807 R810 Q811 Q812 V813 Q814 K815 L816 A817 F818 E819 R823 N827 N835 E836 E841 P844 R845 R848 T849 S854 K855 V859 A865 A866 R867 V868 M869 K872 S873 E876 Q877 T880 K881 E882 V883 I884

S889 V890 K891 E892 V893 G902 V903 D904 P905 L906 L907 G908 P909 E910 M911 R912 E916 V917 G921 R922 T923 E926 A927 F928 A929 K930 A931 Q932 N936 S937 H942 G943 L947 R950 E951 G952 D953 K954 E955 R956 V957 V958 D959 A962 Q967 E970 L971 D972

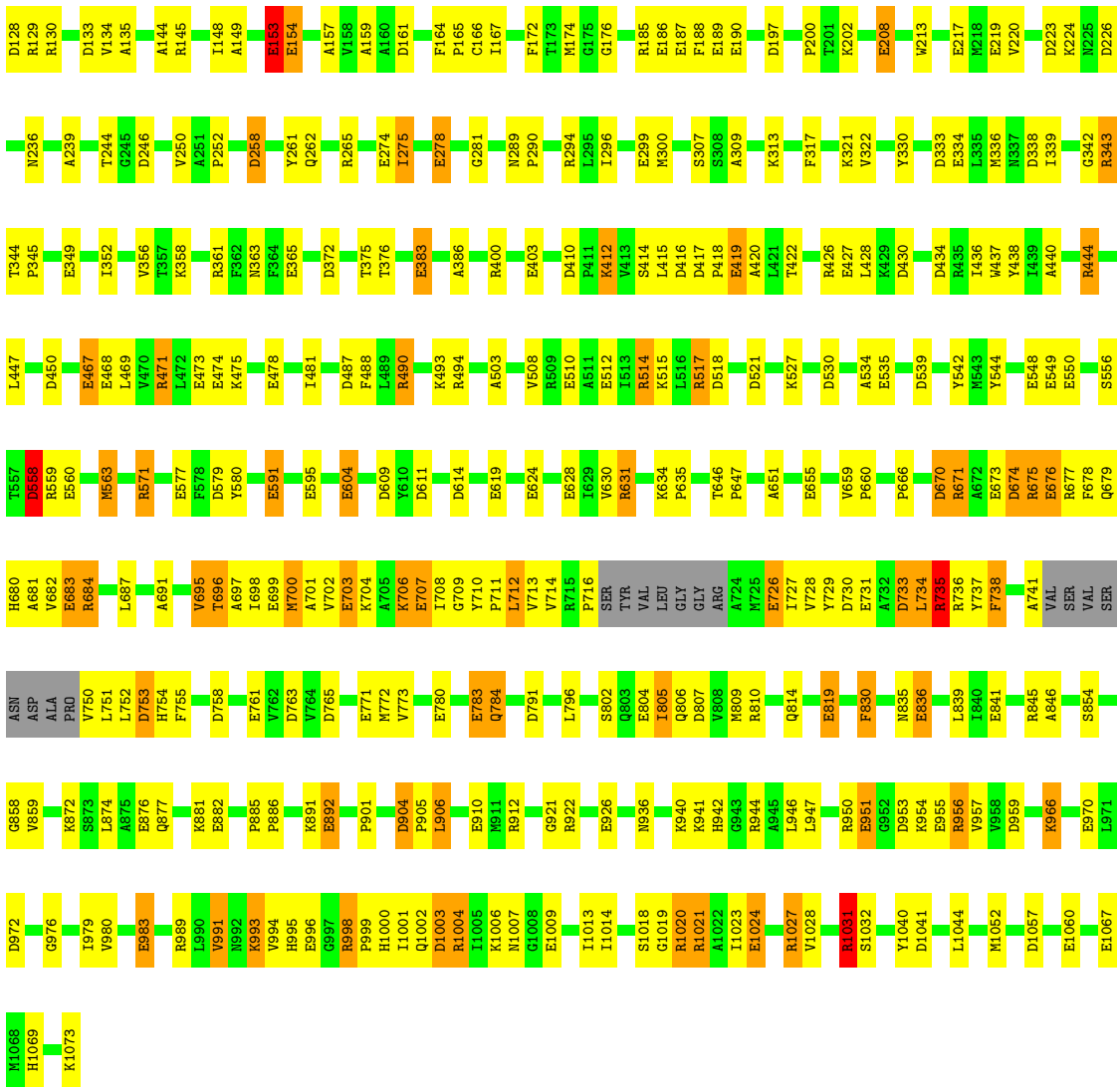
H975 V980 E983 I986 N987 P988 R989 L990 V991 N992 K993 V994 H995 E996 G997 R998 P999 H1000 D1003 N1007 G1008 E1009 I1014 N1015 T1016 T1017 S1018 G1019 R1020 R1021 A1022 I1023 E1024 D1025 S1026 R1027 R1031 Y1036 K1037 D1041 T1042 T1043 L1044 F1048 M1052 A1053 L1054

D1057 E1060 K1061 V1062 I1063 S1064 V1065 Q1066 E1067 M1068 K1073

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

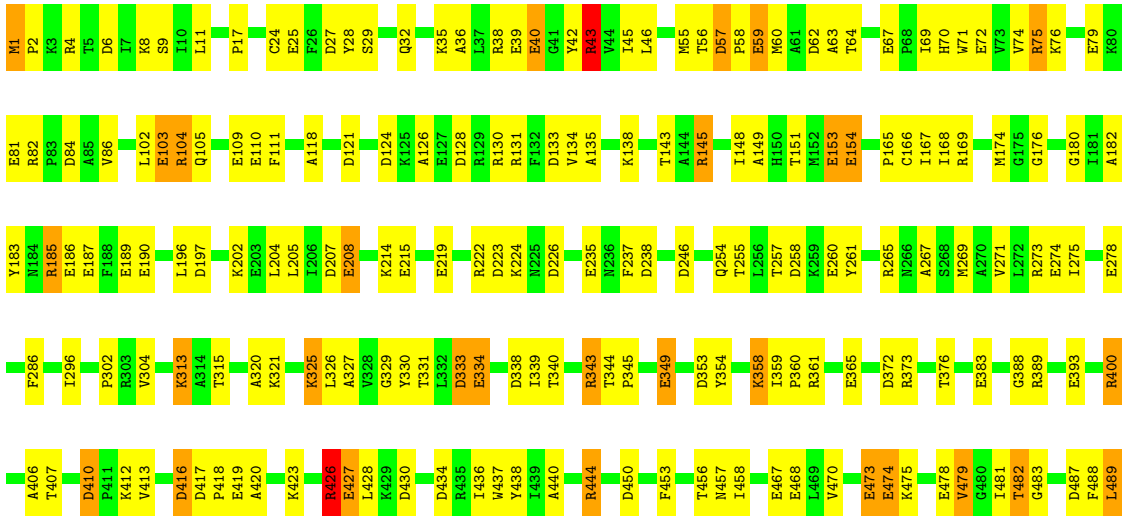
Chain E: 64% 28% 7% •

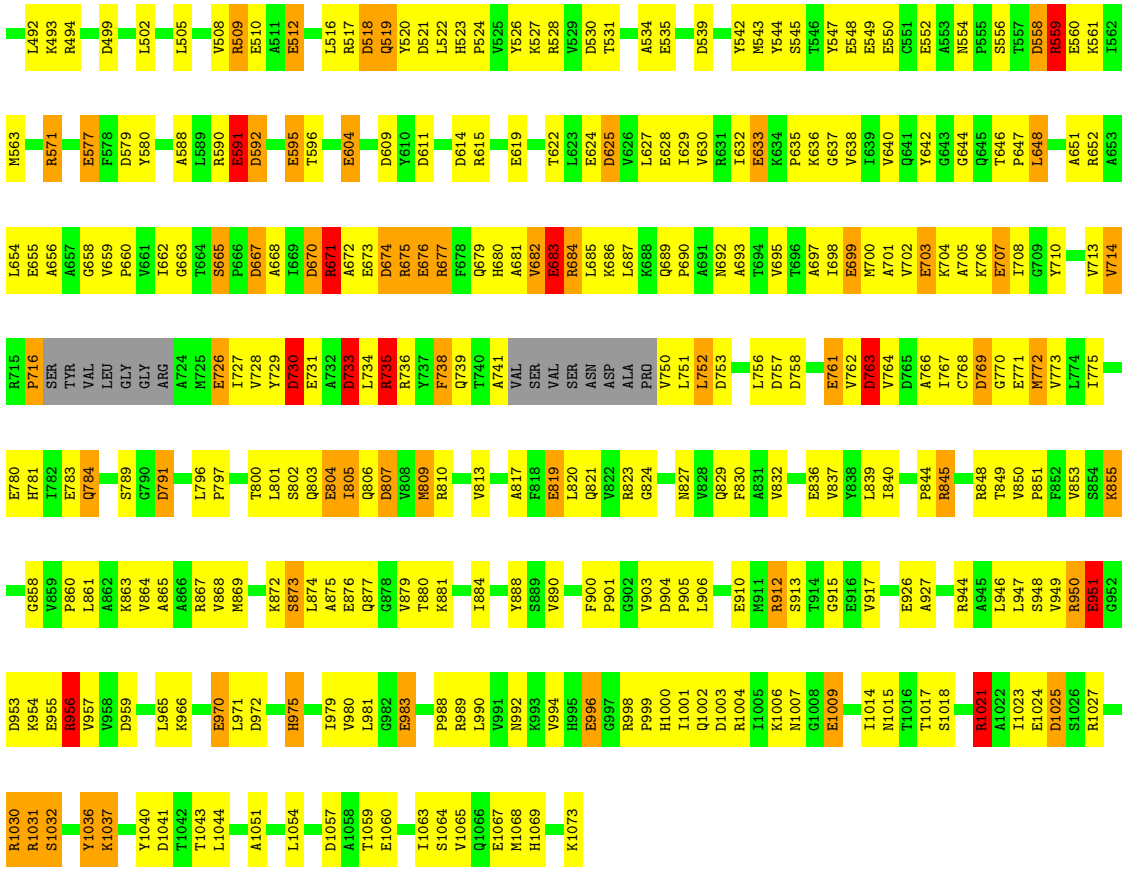
M1 P2 K3 R4 T5 D6 I7 K8 I18 A23 C24 E25 F26 D27 Q32 R38 E39 Y42 R43 L46 T53 E59 M60 A61 D62 E67 E72 K76 E81 R82 P83 D84 E101 L102 E103 R104 E109 E110 M115 D121 K125 A126 E127



- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

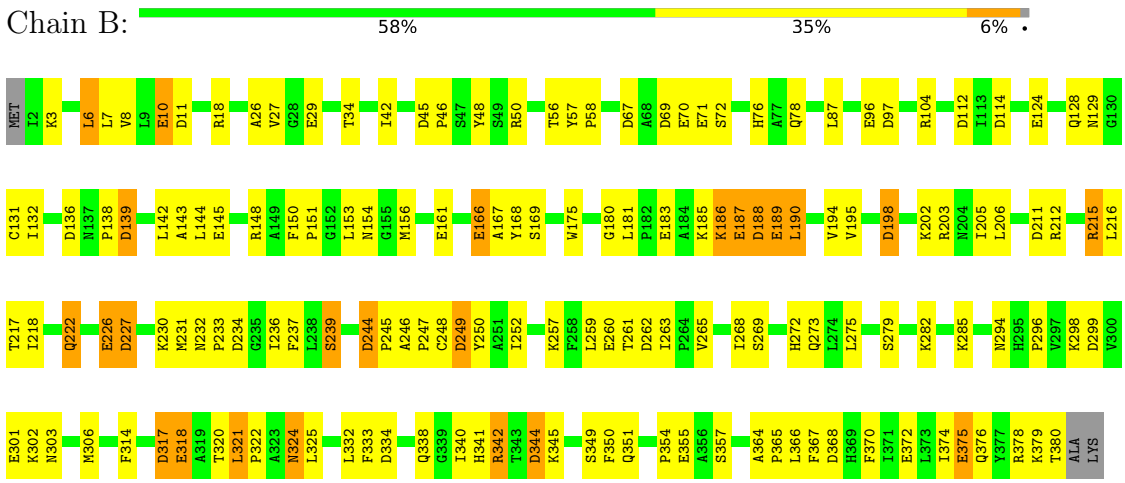
Chain G:





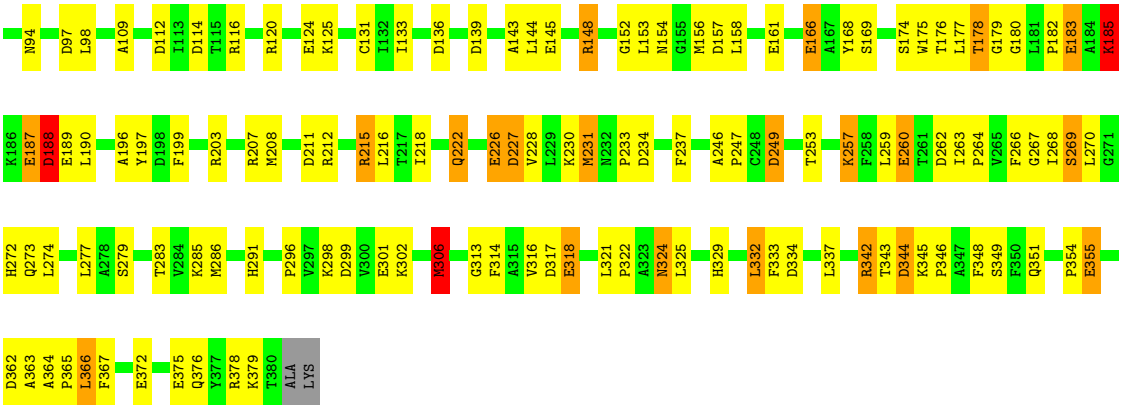
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain B:



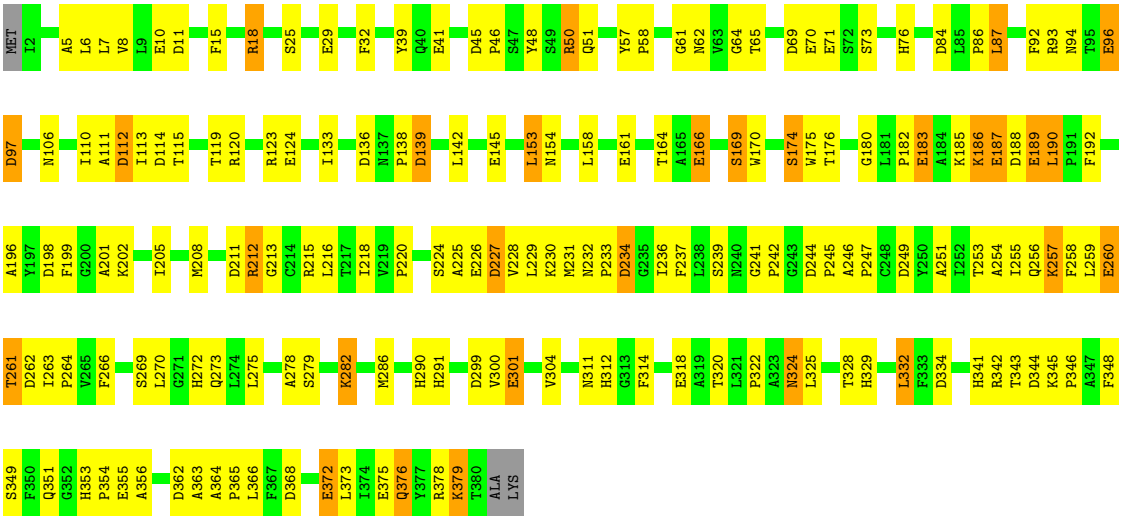
- Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain D:



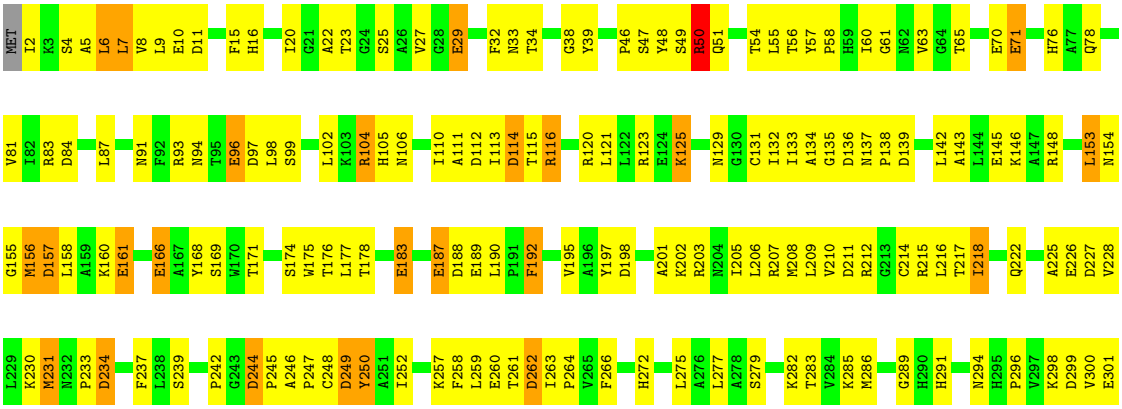
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

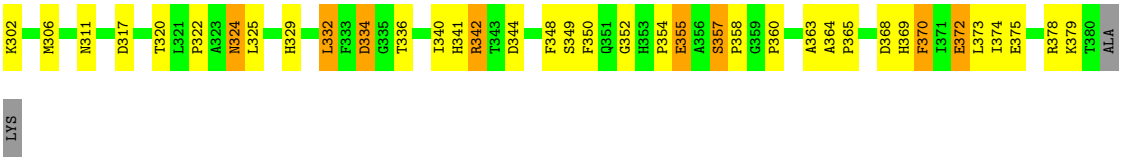
Chain F: 53% 38% 8% •



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 45% 45% 8% •




K302
M306
N311
D317
T320
L321
P322
A323
N324
L325
H329
L332
F333
D334
G335
T336
I340
H341
R342
T343
D344
F348
S349
F350
Q351
G352
H353
P354
E355
A356
S357
P358
G359
P360
A363
A364
P365
D368
H369
F370
I371
E372
L373
I374
E375
R378
K379
T380
ALA
LYS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	152.60Å 164.60Å 332.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (30.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.189 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48668	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NET, MN, ADP, CL, ORN, K

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	1.02	75/8339 (0.9%)	1.40	124/11273 (1.1%)
1	C	1.05	77/8295 (0.9%)	1.45	145/11214 (1.3%)
1	E	1.05	77/8338 (0.9%)	1.40	116/11270 (1.0%)
1	G	1.00	72/8320 (0.9%)	1.44	131/11246 (1.2%)
2	B	0.90	19/2957 (0.6%)	1.29	37/4016 (0.9%)
2	D	0.97	18/2957 (0.6%)	1.36	36/4016 (0.9%)
2	F	0.93	20/2957 (0.7%)	1.35	40/4016 (1.0%)
2	H	0.93	18/2966 (0.6%)	1.36	35/4028 (0.9%)
All	All	1.01	376/45129 (0.8%)	1.40	664/61079 (1.1%)

All (376) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CD-OE2	10.28	1.36	1.25
1	E	1009[A]	GLU	CD-OE2	9.59	1.36	1.25
1	E	1009[B]	GLU	CD-OE2	9.59	1.36	1.25
1	C	955	GLU	CD-OE2	9.24	1.35	1.25
1	C	951	GLU	CD-OE2	8.93	1.35	1.25
1	C	771	GLU	CD-OE2	8.88	1.35	1.25
1	C	72	GLU	CD-OE2	8.71	1.35	1.25
1	E	365	GLU	CD-OE2	8.70	1.35	1.25
1	C	1024	GLU	CD-OE2	8.40	1.34	1.25
1	C	996	GLU	CD-OE2	8.29	1.34	1.25
1	E	655	GLU	CD-OE2	8.24	1.34	1.25
2	H	166	GLU	CD-OE2	7.95	1.34	1.25
1	C	59	GLU	CD-OE2	7.88	1.34	1.25
2	H	183	GLU	CD-OE2	7.81	1.34	1.25
1	C	109	GLU	CD-OE2	7.80	1.34	1.25
1	E	535	GLU	CD-OE2	7.67	1.34	1.25
1	A	838	TYR	CE2-CZ	7.63	1.48	1.38
1	E	983	GLU	CD-OE2	7.60	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	355	GLU	CD-OE2	7.59	1.33	1.25
1	A	512	GLU	CD-OE2	7.58	1.33	1.25
2	D	166	GLU	CD-OE2	7.48	1.33	1.25
1	E	993	LYS	CE-NZ	7.46	1.67	1.49
2	D	189	GLU	CD-OE2	7.43	1.33	1.25
1	E	882	GLU	CD-OE2	7.43	1.33	1.25
1	C	550	GLU	CD-OE2	7.39	1.33	1.25
1	G	683	GLU	CD-OE2	7.37	1.33	1.25
1	G	39	GLU	CD-OE2	7.32	1.33	1.25
1	G	955	GLU	CD-OE2	7.30	1.33	1.25
2	H	70	GLU	CD-OE2	7.27	1.33	1.25
2	D	10	GLU	CD-OE2	7.24	1.33	1.25
1	E	624	GLU	CD-OE2	7.20	1.33	1.25
1	E	468	GLU	CD-OE2	7.17	1.33	1.25
2	B	372	GLU	CD-OE2	7.15	1.33	1.25
1	C	334	GLU	CD-OE2	7.14	1.33	1.25
1	G	478	GLU	CD-OE2	7.13	1.33	1.25
1	G	1024	GLU	CD-OE2	7.13	1.33	1.25
1	A	1009	GLU	CD-OE2	7.12	1.33	1.25
2	F	372	GLU	CD-OE2	7.11	1.33	1.25
2	D	318	GLU	CD-OE2	7.10	1.33	1.25
1	G	703	GLU	CD-OE2	7.10	1.33	1.25
1	A	217	GLU	CD-OE2	7.03	1.33	1.25
1	C	67	GLU	CD-OE2	7.00	1.33	1.25
1	G	876	GLU	CD-OE2	7.00	1.33	1.25
1	G	365	GLU	CD-OE2	7.00	1.33	1.25
1	C	39	GLU	CD-OE2	6.98	1.33	1.25
1	C	217	GLU	CD-OE2	6.98	1.33	1.25
1	A	153	GLU	CD-OE2	6.97	1.33	1.25
1	E	39	GLU	CD-OE2	6.97	1.33	1.25
1	A	955	GLU	CD-OE2	6.93	1.33	1.25
1	G	804	GLU	CD-OE2	6.93	1.33	1.25
1	A	703	GLU	CD-OE2	6.92	1.33	1.25
1	E	403	GLU	CD-OE2	6.92	1.33	1.25
1	G	219	GLU	CD-OE2	6.88	1.33	1.25
1	C	419	GLU	CD-OE2	6.87	1.33	1.25
1	C	219	GLU	CD-OE2	6.85	1.33	1.25
2	B	166	GLU	CD-OE2	6.85	1.33	1.25
2	H	226	GLU	CD-OE2	6.83	1.33	1.25
2	F	189	GLU	CD-OE2	6.83	1.33	1.25
2	H	372	GLU	CD-OE2	6.83	1.33	1.25
1	E	153	GLU	CD-OE2	6.82	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	655	GLU	CD-OE2	6.81	1.33	1.25
2	F	187	GLU	CD-OE2	6.81	1.33	1.25
1	C	683	GLU	CD-OE2	6.81	1.33	1.25
1	G	726	GLU	CD-OE2	6.79	1.33	1.25
1	E	726	GLU	CD-OE2	6.76	1.33	1.25
1	G	110	GLU	CD-OE2	6.76	1.33	1.25
2	D	301	GLU	CD-OE2	6.74	1.33	1.25
1	C	910	GLU	CD-OE2	6.73	1.33	1.25
1	C	731	GLU	CD-OE2	6.72	1.33	1.25
2	F	226	GLU	CD-OE2	6.71	1.33	1.25
1	E	836	GLU	CD-OE2	6.70	1.33	1.25
2	B	96	GLU	CD-OE2	6.69	1.33	1.25
1	E	699	GLU	CD-OE2	6.69	1.33	1.25
1	A	882	GLU	CD-OE2	6.68	1.33	1.25
1	E	996	GLU	CD-OE2	6.65	1.32	1.25
1	E	59	GLU	CD-OE2	6.63	1.32	1.25
1	A	699	GLU	CD-OE2	6.62	1.32	1.25
2	B	145	GLU	CD-OE2	6.62	1.32	1.25
2	D	375	GLU	CD-OE2	6.62	1.32	1.25
2	H	260	GLU	CD-OE2	6.61	1.32	1.25
1	G	676	GLU	CD-OE2	6.59	1.32	1.25
1	C	676	GLU	CD-OE2	6.58	1.32	1.25
1	A	109	GLU	CD-OE2	6.58	1.32	1.25
2	B	70	GLU	CD-OE2	6.58	1.32	1.25
1	E	673	GLU	CD-OE2	6.58	1.32	1.25
2	H	10	GLU	CD-OE2	6.57	1.32	1.25
1	G	699	GLU	CD-OE2	6.57	1.32	1.25
1	G	235	GLU	CD-OE2	6.56	1.32	1.25
1	C	703	GLU	CD-OE2	6.53	1.32	1.25
1	A	655	GLU	CD-OE2	6.53	1.32	1.25
1	C	549	GLU	CD-OE2	6.52	1.32	1.25
1	A	604	GLU	CD-OE2	6.51	1.32	1.25
1	A	591	GLU	CD-OE2	6.51	1.32	1.25
1	A	683	GLU	CD-OE2	6.50	1.32	1.25
1	A	560	GLU	CD-OE2	6.49	1.32	1.25
2	F	301	GLU	CD-OE2	6.48	1.32	1.25
2	H	187	GLU	CD-OE2	6.47	1.32	1.25
1	E	703	GLU	CD-OE2	6.46	1.32	1.25
1	A	841	GLU	CD-OE2	6.43	1.32	1.25
1	C	40	GLU	CD-OE1	-6.43	1.18	1.25
2	F	183	GLU	CD-OE2	6.42	1.32	1.25
2	D	226	GLU	CD-OE2	6.41	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	GLU	CD-OE2	6.41	1.32	1.25
2	F	375	GLU	CD-OE2	6.41	1.32	1.25
1	C	67	GLU	CD-OE1	-6.39	1.18	1.25
1	A	970	GLU	CD-OE2	6.37	1.32	1.25
2	F	145	GLU	CD-OE2	6.37	1.32	1.25
1	G	595	GLU	CD-OE2	6.36	1.32	1.25
1	A	910	GLU	CD-OE2	6.36	1.32	1.25
1	E	550	GLU	CD-OE2	6.35	1.32	1.25
1	G	996	GLU	CD-OE2	6.35	1.32	1.25
2	B	226	GLU	CD-OE2	6.34	1.32	1.25
1	A	25	GLU	CD-OE2	6.34	1.32	1.25
1	A	235	GLU	CD-OE2	6.34	1.32	1.25
2	B	29	GLU	CD-OE2	6.34	1.32	1.25
1	C	278	GLU	CD-OE2	6.33	1.32	1.25
1	A	81	GLU	CD-OE2	6.32	1.32	1.25
1	A	510	GLU	CD-OE2	6.32	1.32	1.25
1	C	72	GLU	CD-OE1	-6.32	1.18	1.25
2	H	145[A]	GLU	CD-OE2	6.32	1.32	1.25
2	H	145[B]	GLU	CD-OE2	6.32	1.32	1.25
1	C	478	GLU	CD-OE2	6.31	1.32	1.25
1	C	761	GLU	CD-OE2	6.30	1.32	1.25
1	A	983	GLU	CD-OE2	6.30	1.32	1.25
1	E	876	GLU	CD-OE2	6.29	1.32	1.25
2	F	29	GLU	CD-OE2	6.29	1.32	1.25
1	G	549	GLU	CD-OE2	6.28	1.32	1.25
1	G	467	GLU	CD-OE2	6.28	1.32	1.25
1	G	473	GLU	CD-OE2	6.28	1.32	1.25
1	A	478	GLU	CD-OE2	6.27	1.32	1.25
1	C	403	GLU	CD-OE2	6.26	1.32	1.25
1	A	365	GLU	CD-OE2	6.26	1.32	1.25
1	E	804	GLU	CD-OE2	6.25	1.32	1.25
1	E	910	GLU	CD-OE2	6.24	1.32	1.25
1	G	40	GLU	CD-OE2	6.24	1.32	1.25
1	E	707	GLU	CD-OE2	6.24	1.32	1.25
1	E	771	GLU	CD-OE2	6.24	1.32	1.25
2	H	96	GLU	CD-OE2	6.24	1.32	1.25
1	E	591	GLU	CD-OE2	6.23	1.32	1.25
1	E	1009[A]	GLU	CD-OE1	-6.22	1.18	1.25
1	E	1009[B]	GLU	CD-OE1	-6.22	1.18	1.25
1	C	560	GLU	CD-OE2	6.22	1.32	1.25
2	B	318	GLU	CD-OE2	6.21	1.32	1.25
2	F	166	GLU	CD-OE2	6.21	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	GLU	CD-OE2	6.21	1.32	1.25
1	C	836	GLU	CD-OE2	6.20	1.32	1.25
1	E	955	GLU	CD-OE2	6.20	1.32	1.25
1	A	427	GLU	CD-OE2	6.20	1.32	1.25
1	A	836	GLU	CD-OE2	6.20	1.32	1.25
1	E	1024	GLU	CD-OE2	6.20	1.32	1.25
1	E	219	GLU	CD-OE2	6.19	1.32	1.25
1	G	560	GLU	CD-OE2	6.18	1.32	1.25
1	G	186	GLU	CD-OE2	6.17	1.32	1.25
1	C	591	GLU	CD-OE2	6.17	1.32	1.25
1	G	1009	GLU	CD-OE2	6.17	1.32	1.25
1	G	154	GLU	CD-OE2	6.16	1.32	1.25
1	C	726	GLU	CD-OE2	6.15	1.32	1.25
2	F	355	GLU	CD-OE2	6.12	1.32	1.25
1	A	467	GLU	CD-OE2	6.12	1.32	1.25
1	A	676	GLU	CD-OE2	6.12	1.32	1.25
1	C	208	GLU	CD-OE2	6.11	1.32	1.25
1	G	187	GLU	CD-OE2	6.10	1.32	1.25
1	G	474	GLU	CD-OE2	6.09	1.32	1.25
1	C	189	GLU	CD-OE2	6.09	1.32	1.25
1	A	916	GLU	CD-OE2	6.09	1.32	1.25
1	A	1024	GLU	CD-OE2	6.07	1.32	1.25
1	A	771	GLU	CD-OE2	6.07	1.32	1.25
1	A	59	GLU	CD-OE2	6.05	1.32	1.25
1	C	512	GLU	CD-OE2	6.05	1.32	1.25
1	G	1067	GLU	CD-OE2	6.05	1.32	1.25
1	E	109	GLU	CD-OE2	6.04	1.32	1.25
1	A	707	GLU	CD-OE2	6.04	1.32	1.25
1	E	892	GLU	CD-OE2	6.04	1.32	1.25
1	E	154	GLU	CD-OE2	6.03	1.32	1.25
2	D	183	GLU	CD-OE2	6.03	1.32	1.25
1	G	25	GLU	CD-OE2	6.03	1.32	1.25
1	C	577	GLU	CD-OE2	6.02	1.32	1.25
1	A	110	GLU	CD-OE2	6.02	1.32	1.25
2	H	71	GLU	CD-OE2	6.02	1.32	1.25
1	E	628	GLU	CD-OE2	6.01	1.32	1.25
1	A	190	GLU	CD-OE2	6.00	1.32	1.25
1	A	72	GLU	CD-OE2	5.99	1.32	1.25
1	G	951	GLU	CD-OE2	5.98	1.32	1.25
1	A	219	GLU	CD-OE2	5.98	1.32	1.25
1	A	673	GLU	CD-OE2	5.96	1.32	1.25
1	E	549	GLU	CD-OE2	5.96	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	109	GLU	CD-OE2	5.95	1.32	1.25
2	B	189	GLU	CD-OE2	5.95	1.32	1.25
1	E	127	GLU	CD-OE2	5.95	1.32	1.25
1	G	707	GLU	CD-OE2	5.95	1.32	1.25
2	F	96	GLU	CD-OE2	5.94	1.32	1.25
2	F	260	GLU	CD-OE2	5.94	1.32	1.25
2	D	372	GLU	CD-OE2	5.92	1.32	1.25
1	G	731	GLU	CD-OE2	5.92	1.32	1.25
1	A	951	GLU	CD-OE2	5.92	1.32	1.25
1	C	187	GLU	CD-OE2	5.92	1.32	1.25
1	E	467	GLU	CD-OE2	5.91	1.32	1.25
1	G	512	GLU	CD-OE2	5.91	1.32	1.25
1	G	190	GLU	CD-OE2	5.91	1.32	1.25
1	E	819	GLU	CD-OE2	5.91	1.32	1.25
1	C	550	GLU	CD-OE1	-5.91	1.19	1.25
1	C	624	GLU	CD-OE2	5.90	1.32	1.25
1	G	591	GLU	CD-OE2	5.90	1.32	1.25
1	G	153	GLU	CD-OE2	5.89	1.32	1.25
2	B	183	GLU	CD-OE2	5.88	1.32	1.25
1	E	419	GLU	CD-OE2	5.88	1.32	1.25
1	E	761	GLU	CD-OE2	5.85	1.32	1.25
1	E	278	GLU	CD-OE2	5.85	1.32	1.25
1	E	474	GLU	CD-OE2	5.84	1.32	1.25
1	C	804	GLU	CD-OE2	5.84	1.32	1.25
1	E	186	GLU	CD-OE2	5.83	1.32	1.25
2	B	124	GLU	CD-OE2	5.83	1.32	1.25
1	E	970	GLU	CD-OE2	5.83	1.32	1.25
2	F	124	GLU	CD-OE2	5.82	1.32	1.25
1	C	186	GLU	CD-OE2	5.82	1.32	1.25
1	G	836	GLU	CD-OE2	5.82	1.32	1.25
1	G	819	GLU	CD-OE2	5.82	1.32	1.25
1	C	699	GLU	CD-OE2	5.81	1.32	1.25
1	C	707	GLU	CD-OE2	5.81	1.32	1.25
2	H	375	GLU	CD-OE2	5.81	1.32	1.25
1	E	619	GLU	CD-OE2	5.80	1.32	1.25
1	E	1067	GLU	CD-OE2	5.80	1.32	1.25
1	G	510	GLU	CD-OE2	5.80	1.32	1.25
1	C	876	GLU	CD-OE2	5.79	1.32	1.25
1	E	187	GLU	CD-OE2	5.78	1.32	1.25
1	C	595	GLU	CD-OE2	5.77	1.31	1.25
1	E	683	GLU	CD-OE2	5.77	1.31	1.25
1	C	349	GLU	CD-OE2	5.76	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	70	GLU	CD-OE2	5.76	1.31	1.25
1	A	468	GLU	CD-OE2	5.75	1.31	1.25
1	G	552	GLU	CD-OE2	5.75	1.31	1.25
1	E	478[A]	GLU	CD-OE2	5.74	1.31	1.25
1	E	478[B]	GLU	CD-OE2	5.74	1.31	1.25
1	E	349	GLU	CD-OE2	5.74	1.31	1.25
1	C	190	GLU	CD-OE2	5.74	1.31	1.25
1	G	535	GLU	CD-OE2	5.73	1.31	1.25
2	B	161	GLU	CD-OE2	5.71	1.31	1.25
1	G	419	GLU	CD-OE2	5.71	1.31	1.25
2	H	189	GLU	CD-OE2	5.71	1.31	1.25
2	D	124	GLU	CD-OE2	5.71	1.31	1.25
1	A	187	GLU	CD-OE2	5.71	1.31	1.25
1	E	731	GLU	CD-OE2	5.70	1.31	1.25
2	D	187	GLU	CD-OE2	5.69	1.31	1.25
1	G	1060	GLU	CD-OE2	5.68	1.31	1.25
1	G	970	GLU	CD-OE2	5.67	1.31	1.25
2	F	318	GLU	CD-OE2	5.67	1.31	1.25
1	A	731	GLU	CD-OE2	5.67	1.31	1.25
2	B	355	GLU	CD-OE2	5.67	1.31	1.25
1	G	577	GLU	CD-OE2	5.66	1.31	1.25
1	G	619	GLU	CD-OE2	5.66	1.31	1.25
1	C	951	GLU	CD-OE1	-5.65	1.19	1.25
1	C	153	GLU	CD-OE2	5.65	1.31	1.25
1	G	103	GLU	CD-OE2	5.65	1.31	1.25
1	A	103	GLU	CD-OE2	5.64	1.31	1.25
1	A	393	GLU	CD-OE2	5.63	1.31	1.25
2	D	145	GLU	CD-OE2	5.62	1.31	1.25
1	E	208	GLU	CD-OE2	5.61	1.31	1.25
1	A	876	GLU	CD-OE2	5.60	1.31	1.25
1	C	882	GLU	CD-OE2	5.60	1.31	1.25
1	C	79	GLU	CD-OE2	5.59	1.31	1.25
1	G	761	GLU	CD-OE2	5.59	1.31	1.25
1	E	190	GLU	CD-OE2	5.59	1.31	1.25
1	C	970	GLU	CD-OE2	5.59	1.31	1.25
1	E	1060	GLU	CD-OE2	5.58	1.31	1.25
1	G	383	GLU	CD-OE2	5.58	1.31	1.25
1	C	892	GLU	CD-OE2	5.58	1.31	1.25
2	B	375	GLU	CD-OE2	5.57	1.31	1.25
1	C	474	GLU	CD-OE2	5.57	1.31	1.25
2	F	10	GLU	CD-OE2	5.57	1.31	1.25
1	A	549	GLU	CD-OE2	5.56	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	GLU	CD-OE2	5.55	1.31	1.25
1	A	548	GLU	CD-OE2	5.53	1.31	1.25
1	G	189	GLU	CD-OE2	5.52	1.31	1.25
1	E	217	GLU	CD-OE2	5.52	1.31	1.25
2	F	161	GLU	CD-OE2	5.52	1.31	1.25
2	D	185	LYS	CE-NZ	-5.52	1.35	1.49
1	A	926	GLU	CD-OE2	5.51	1.31	1.25
1	E	334	GLU	CD-OE2	5.49	1.31	1.25
1	C	819	GLU	CD-OE2	5.49	1.31	1.25
1	C	926	GLU	CD-OE2	5.49	1.31	1.25
2	H	29	GLU	CD-OE2	5.48	1.31	1.25
1	G	427	GLU	CD-OE2	5.47	1.31	1.25
2	D	41	GLU	CD-OE2	5.46	1.31	1.25
1	G	274	GLU	CD-OE2	5.45	1.31	1.25
1	E	72	GLU	CD-OE2	5.45	1.31	1.25
1	A	1060	GLU	CD-OE2	5.43	1.31	1.25
2	B	301	GLU	CD-OE2	5.43	1.31	1.25
1	G	780	GLU	CD-OE2	5.43	1.31	1.25
1	A	804[A]	GLU	CD-OE2	5.43	1.31	1.25
1	A	804[B]	GLU	CD-OE2	5.43	1.31	1.25
1	A	39	GLU	CD-OE2	5.42	1.31	1.25
1	G	208	GLU	CD-OE2	5.42	1.31	1.25
1	G	983	GLU	CD-OE2	5.41	1.31	1.25
2	B	187	GLU	CD-OE2	5.41	1.31	1.25
2	D	71	GLU	CD-OE2	5.41	1.31	1.25
1	C	365	GLU	CD-OE2	5.40	1.31	1.25
1	C	673	GLU	CD-OE2	5.40	1.31	1.25
2	F	71	GLU	CD-OE2	5.39	1.31	1.25
1	G	40	GLU	CD-OE1	-5.39	1.19	1.25
1	A	186	GLU	CD-OE2	5.39	1.31	1.25
1	A	552	GLU	CD-OE2	5.39	1.31	1.25
1	G	783	GLU	CD-OE2	5.38	1.31	1.25
1	E	892	GLU	CD-OE1	-5.38	1.19	1.25
1	G	468	GLU	CD-OE2	5.37	1.31	1.25
2	B	260	GLU	CD-OE2	5.37	1.31	1.25
1	C	468	GLU	CD-OE2	5.36	1.31	1.25
1	E	577	GLU	CD-OE2	5.36	1.31	1.25
1	E	67	GLU	CD-OE2	5.36	1.31	1.25
1	A	633	GLU	CD-OE2	5.36	1.31	1.25
1	E	427	GLU	CD-OE2	5.35	1.31	1.25
1	C	299	GLU	CD-OE2	5.35	1.31	1.25
1	G	67	GLU	CD-OE2	5.34	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	604	GLU	CD-OE2	5.34	1.31	1.25
1	A	550	GLU	CD-OE2	5.34	1.31	1.25
1	C	983	GLU	CD-OE2	5.34	1.31	1.25
1	A	780	GLU	CD-OE2	5.33	1.31	1.25
1	C	535	GLU	CD-OE2	5.33	1.31	1.25
1	A	892	GLU	CD-OE2	5.33	1.31	1.25
1	C	260	GLU	CD-OE2	5.33	1.31	1.25
1	A	383	GLU	CD-OE2	5.30	1.31	1.25
1	G	926	GLU	CD-OE2	5.29	1.31	1.25
1	C	655	GLU	CD-OE2	5.29	1.31	1.25
1	C	467	GLU	CD-OE2	5.29	1.31	1.25
1	E	25	GLU	CD-OE2	5.29	1.31	1.25
1	E	510	GLU	CD-OE2	5.29	1.31	1.25
2	H	355	GLU	CD-OE2	5.28	1.31	1.25
1	E	110	GLU	CD-OE2	5.28	1.31	1.25
1	A	208	GLU	CD-OE2	5.27	1.31	1.25
2	F	41	GLU	CD-OE2	5.27	1.31	1.25
1	C	127	GLU	CD-OE2	5.26	1.31	1.25
2	B	71	GLU	CD-OE2	5.26	1.31	1.25
1	A	1067	GLU	CD-OE2	5.25	1.31	1.25
1	A	334	GLU	CD-OE2	5.25	1.31	1.25
2	D	161	GLU	CD-OE2	5.25	1.31	1.25
1	A	577	GLU	CD-OE2	5.24	1.31	1.25
1	E	512	GLU	CD-OE2	5.24	1.31	1.25
1	E	103	GLU	CD-OE2	5.23	1.31	1.25
1	A	595	GLU	CD-OE2	5.23	1.31	1.25
1	G	215	GLU	CD-OE2	5.23	1.31	1.25
1	G	771	GLU	CD-OE2	5.23	1.31	1.25
1	E	783	GLU	CD-OE2	5.22	1.31	1.25
1	A	203	GLU	CD-OE2	5.22	1.31	1.25
1	G	604	GLU	CD-OE2	5.22	1.31	1.25
1	A	299	GLU	CD-OE2	5.21	1.31	1.25
1	G	624	GLU	CD-OE2	5.21	1.31	1.25
1	A	838	TYR	CD1-CE1	-5.20	1.31	1.39
1	A	474	GLU	CD-OE2	5.20	1.31	1.25
1	E	841	GLU	CD-OE2	5.20	1.31	1.25
2	D	260	GLU	CD-OE2	5.19	1.31	1.25
1	C	841	GLU	CD-OE2	5.18	1.31	1.25
1	C	1060	GLU	CD-OE2	5.17	1.31	1.25
1	C	1067	GLU	CD-OE2	5.16	1.31	1.25
1	E	676	GLU	CD-OE2	5.16	1.31	1.25
1	C	996	GLU	CD-OE1	-5.16	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	393	GLU	CD-OE2	5.16	1.31	1.25
2	B	10	GLU	CD-OE2	5.15	1.31	1.25
1	E	780	GLU	CD-OE2	5.14	1.31	1.25
1	C	427	GLU	CD-OE2	5.13	1.31	1.25
1	C	780	GLU	CD-OE2	5.13	1.31	1.25
1	A	79	GLU	CD-OE2	5.12	1.31	1.25
1	A	260	GLU	CD-OE2	5.11	1.31	1.25
2	H	161	GLU	CD-OE2	5.10	1.31	1.25
1	G	349	GLU	CD-OE2	5.10	1.31	1.25
1	G	633	GLU	CD-OE2	5.08	1.31	1.25
1	C	383	GLU	CD-OE1	-5.07	1.20	1.25
1	C	633	GLU	CD-OE2	5.06	1.31	1.25
1	G	334	GLU	CD-OE2	5.06	1.31	1.25
1	G	910	GLU	CD-OE2	5.06	1.31	1.25
1	E	951	GLU	CD-OE2	5.05	1.31	1.25
1	E	383	GLU	CD-OE1	-5.05	1.20	1.25
1	C	1060	GLU	CD-OE1	-5.04	1.20	1.25
1	A	761	GLU	CD-OE2	5.04	1.31	1.25
1	C	430	ASP	CG-OD2	5.03	1.36	1.25
1	G	278	GLU	CD-OE2	5.02	1.31	1.25
1	A	127	GLU	CD-OE1	-5.02	1.20	1.25
1	E	101	GLU	CD-OE1	-5.01	1.20	1.25

All (664) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	261	TYR	CB-CG-CD2	-14.58	112.25	121.00
1	C	490	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	G	43	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	E	609	ASP	CB-CG-OD2	-10.78	108.60	118.30
1	E	514	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	E	361	ARG	NE-CZ-NH1	10.45	125.52	120.30
1	A	736	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	G	222	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	490	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	C	6	ASP	CB-CG-OD2	-9.48	109.77	118.30
2	D	207	ARG	NE-CZ-NH1	9.46	125.03	120.30
2	H	97	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	G	614	ASP	CB-CG-OD2	-9.37	109.87	118.30
1	C	499	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	E	514	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	A	611	ASP	CB-CG-OD2	-9.20	110.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	261	TYR	CB-CG-CD1	9.17	126.50	121.00
2	D	317	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	611	ASP	CB-CG-OD1	9.05	126.45	118.30
1	G	43	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	C	333	ASP	CB-CG-OD1	8.99	126.40	118.30
1	C	161	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	C	84	ASP	CB-CG-OD1	8.96	126.37	118.30
2	B	211	ASP	CB-CG-OD2	-8.94	110.26	118.30
1	C	121	ASP	CB-CG-OD2	-8.83	110.36	118.30
1	C	460	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	C	518	ASP	CB-CG-OD2	-8.79	110.38	118.30
1	C	514	ARG	NE-CZ-NH2	-8.77	115.91	120.30
1	E	43	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	736	ARG	NE-CZ-NH2	-8.77	115.92	120.30
2	F	120	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	765	ASP	CB-CG-OD1	8.72	126.14	118.30
1	G	84	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	G	972	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	C	338	ASP	CB-CG-OD1	8.66	126.10	118.30
1	A	671	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	C	434	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	E	434	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	E	333	ASP	CB-CG-OD1	8.56	126.00	118.30
1	A	426	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	C	959	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	C	769	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	C	823	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	E	1003	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	G	559	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	C	294	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	333	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	E	490	ARG	NE-CZ-NH1	8.32	124.46	120.30
2	D	378	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	G	810	ARG	NE-CZ-NH1	8.31	124.45	120.30
2	D	317	ASP	CB-CG-OD1	8.26	125.74	118.30
1	C	84	ASP	CB-CG-OD2	-8.26	110.86	118.30
1	G	614	ASP	CB-CG-OD1	8.23	125.71	118.30
1	C	121	ASP	CB-CG-OD1	8.23	125.70	118.30
1	A	490	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	E	1041	ASP	CB-CG-OD2	-8.20	110.92	118.30
2	H	114	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	C	460	ARG	NE-CZ-NH1	8.19	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	791	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	A	6	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	G	642	TYR	CB-CG-CD2	-8.11	116.14	121.00
1	E	471	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	E	333	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	E	609	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	128	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	343	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	B	97	ASP	CB-CG-OD2	-8.04	111.06	118.30
1	C	131	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	G	944	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	A	343	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	G	333	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	E	671	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	C	343	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	E	128	ASP	CB-CG-OD1	7.88	125.39	118.30
1	E	372	ASP	CB-CG-OD1	7.84	125.36	118.30
1	G	197	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	904	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	C	823	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	972	ASP	CB-CG-OD2	-7.80	111.28	118.30
2	B	97	ASP	CB-CG-OD1	7.78	125.30	118.30
1	C	959	ASP	CB-CG-OD1	7.78	125.30	118.30
1	C	499	ASP	CB-CG-OD1	7.75	125.28	118.30
2	B	344	ASP	CB-CG-OD2	-7.71	111.36	118.30
2	H	50	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	A	128	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	C	471	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	E	161	ASP	CB-CG-OD2	-7.67	111.39	118.30
2	H	139	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	38	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	C	133	ASP	CB-CG-OD1	7.64	125.18	118.30
1	C	514	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	C	904	ASP	CB-CG-OD1	7.63	125.16	118.30
1	C	43	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	G	956	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	197	ASP	CB-CG-OD1	7.61	125.14	118.30
2	F	344	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	C	631	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	G	736	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	E	434	ASP	CB-CG-OD1	7.58	125.12	118.30
1	C	867	ARG	NE-CZ-NH2	-7.57	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	517	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	338	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	C	441	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	C	518	ASP	CB-CG-OD1	7.54	125.09	118.30
2	H	139	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	765	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	C	769	ASP	CB-CG-OD1	7.54	125.08	118.30
1	G	75	ARG	NE-CZ-NH2	-7.49	116.55	120.30
2	F	227	ASP	CB-CG-OD2	-7.48	111.57	118.30
2	B	368	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	G	735	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	G	410	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	G	434	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	E	558	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	G	84	ASP	CB-CG-OD1	7.40	124.96	118.30
2	D	139	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	G	972	ASP	CB-CG-OD1	7.39	124.95	118.30
1	G	265	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	C	509	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	609	ASP	CB-CG-OD1	7.33	124.89	118.30
1	G	133	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	C	435	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	D	227	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	C	1057	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	579	ASP	CB-CG-OD1	7.28	124.86	118.30
1	A	670	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	G	104	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	G	426	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	E	197	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	C	912	ARG	NE-CZ-NH2	-7.25	116.68	120.30
2	F	139	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	670	ASP	CB-CG-OD1	7.23	124.81	118.30
1	G	373	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	C	763	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	A	131	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	C	1025	ASP	CB-CG-OD2	-7.22	111.80	118.30
2	F	212	ARG	NE-CZ-NH1	7.21	123.90	120.30
2	H	211	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	416	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	1025	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	104	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	E	1031	ARG	NE-CZ-NH1	7.12	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	614	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	G	559	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	E	765	ASP	CB-CG-OD1	7.10	124.69	118.30
2	D	97	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	E	579	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	A	972	ASP	CB-CG-OD2	-7.08	111.93	118.30
2	D	114	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	E	810	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	959	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	G	75	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	C	579	ASP	CB-CG-OD1	7.04	124.63	118.30
1	C	558	ASP	N-CA-CB	-7.03	97.94	110.60
1	C	730	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	867	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	G	735	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	867	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	B	334	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	E	27	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	400	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	C	733	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	736	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	G	372	ASP	CB-CG-OD2	-6.99	112.01	118.30
2	H	50	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	G	62	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	G	416	ASP	CB-CG-OD2	-6.96	112.03	118.30
2	H	93	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	E	62	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	E	579	ASP	CB-CG-OD1	6.93	124.53	118.30
2	H	249	ASP	CB-CG-OD1	6.92	124.53	118.30
2	F	97	ASP	CB-CG-OD2	-6.92	112.07	118.30
2	D	227	ASP	CB-CG-OD1	6.88	124.49	118.30
1	E	518	ASP	CB-CG-OD1	6.88	124.49	118.30
1	G	791	ASP	CB-CG-OD1	6.88	124.49	118.30
2	B	11	ASP	CB-CG-OD2	-6.86	112.12	118.30
2	F	69	ASP	CB-CG-OD1	6.86	124.48	118.30
2	B	212	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	E	128	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	E	400	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	353	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	807	ASP	CB-CG-OD1	6.83	124.44	118.30
2	H	249	ASP	CB-CG-OD2	-6.82	112.16	118.30
2	B	198	ASP	CB-CG-OD1	6.82	124.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	121	ASP	CB-CG-OD2	-6.82	112.16	118.30
2	F	188	ASP	CB-CG-OD1	6.81	124.43	118.30
1	C	716	PRO	N-CA-CB	6.80	111.47	103.30
1	E	223	ASP	CB-CG-OD1	6.80	124.42	118.30
1	E	487	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	E	416	ASP	CB-CG-OD2	-6.78	112.20	118.30
2	B	344	ASP	CB-CG-OD1	6.74	124.37	118.30
1	E	410	ASP	CB-CG-OD1	6.74	124.37	118.30
1	G	959	ASP	CB-CG-OD2	-6.74	112.24	118.30
2	B	114	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	C	614	ASP	CB-CG-OD1	6.72	124.35	118.30
1	G	333	ASP	CB-CG-OD1	6.72	124.35	118.30
1	G	426	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	E	258	ASP	CB-CG-OD1	6.72	124.35	118.30
2	H	114	ASP	CB-CG-OD1	6.72	124.35	118.30
2	D	334	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	E	953	ASP	CB-CG-OD2	-6.71	112.26	118.30
2	H	342	ARG	NE-CZ-NH2	-6.71	116.94	120.30
2	B	368	ASP	CB-CG-OD1	6.70	124.33	118.30
1	C	530	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	579	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	514	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	133	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	769	ASP	CB-CG-OD2	-6.68	112.29	118.30
2	B	262	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	A	763	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	124	ASP	CB-CG-OD1	6.66	124.29	118.30
2	B	227	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	E	989	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	C	614	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	C	223	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	F	188	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	G	625	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	223	ASP	CB-CG-OD1	6.62	124.26	118.30
2	F	198	ASP	CB-CG-OD1	6.62	124.25	118.30
1	G	625	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	E	1041	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	226	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	124	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	G	223	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	G	558	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	471	ARG	NE-CZ-NH1	6.58	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	539	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	G	57	ASP	CB-CG-OD2	-6.55	112.40	118.30
2	D	344	ASP	CB-CG-OD1	6.55	124.19	118.30
1	G	716	PRO	N-CA-CB	6.55	111.16	103.30
1	A	333	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	G	959	ASP	CB-CG-OD1	6.55	124.19	118.30
1	G	667	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	1021	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	G	807	ASP	CB-CG-OD1	6.54	124.18	118.30
2	D	112	ASP	CB-CG-OD1	6.50	124.15	118.30
2	B	249	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	84	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	736	ARG	NE-CZ-NH2	-6.49	117.06	120.30
2	H	84	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	G	121	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	A	959	ASP	CB-CG-OD1	6.47	124.12	118.30
1	G	521	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	E	372	ASP	CB-CG-OD2	-6.45	112.49	118.30
2	F	227	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	410	ASP	CB-CG-OD1	6.45	124.11	118.30
1	G	389	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	716	PRO	N-CA-CB	6.42	111.01	103.30
1	G	753	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	E	1057	ASP	CB-CG-OD1	6.41	124.06	118.30
1	A	518	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	G	539	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	592	ASP	CB-CG-OD1	6.39	124.05	118.30
1	G	807	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	670	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	D	234	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	410	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	1003	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	G	611	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	294	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	H	334	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	E	763	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	G	131	ARG	NE-CZ-NH1	6.35	123.47	120.30
2	D	334	ASP	CB-CG-OD1	6.34	124.01	118.30
1	E	6	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	459	ASP	CB-CG-OD2	-6.34	112.59	118.30
2	B	198	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	956	ARG	NE-CZ-NH1	6.32	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	953	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	133	ASP	CB-CG-OD1	6.32	123.98	118.30
1	G	1041	ASP	CB-CG-OD1	6.32	123.99	118.30
1	E	197	ASP	CB-CG-OD1	6.31	123.98	118.30
1	G	430	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	E	631	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	G	674	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	C	912	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	E	444	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	H	148	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	G	733	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	C	38	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	G	487	ASP	CB-CG-OD2	-6.28	112.65	118.30
2	F	136	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	G	434	ASP	CB-CG-OD1	6.27	123.94	118.30
2	D	139	ASP	CB-CG-OD1	6.27	123.94	118.30
1	C	128	ASP	CB-CG-OD2	-6.26	112.66	118.30
2	D	136	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	27	ASP	CB-CG-OD1	6.26	123.94	118.30
1	C	430	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	E	27	ASP	CB-CG-OD1	6.25	123.93	118.30
1	E	959	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	161	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	265	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	441	ASP	CB-CG-OD1	6.23	123.91	118.30
1	E	944	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	E	410	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	G	758	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	C	807	ASP	CB-CG-OD1	6.23	123.90	118.30
1	G	258	ASP	CB-CG-OD1	6.22	123.90	118.30
1	G	238	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	353	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	652	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	763	ASP	CB-CG-OD1	6.20	123.88	118.30
1	G	124	ASP	CB-CG-OD1	6.19	123.87	118.30
1	G	592	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	E	972	ASP	CB-CG-OD1	6.18	123.86	118.30
2	H	344	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	62	ASP	CB-CG-OD1	6.18	123.86	118.30
2	B	320	THR	CA-CB-CG2	-6.17	103.76	112.40
1	C	609	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	E	716	PRO	N-CA-CB	6.17	110.70	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	733	ASP	CB-CG-OD1	6.16	123.84	118.30
1	E	830	PHE	CB-CA-C	-6.16	98.08	110.40
1	C	1003	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	128	ASP	CB-CG-OD1	6.15	123.83	118.30
1	G	128	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	258	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	998	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	1021	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	223	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	953	ASP	CB-CG-OD1	6.14	123.82	118.30
1	G	609	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	558	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	1057	ASP	CB-CG-OD1	6.13	123.82	118.30
2	B	211	ASP	CB-CG-OD1	6.13	123.82	118.30
2	H	368	ASP	CB-CG-OD1	6.13	123.81	118.30
1	G	444	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	223	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	E	471	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	G	521	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	459	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	671	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	124	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	222	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	F	249	ASP	CB-CG-OD2	-6.11	112.80	118.30
2	H	334	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	674	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	D	249	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	E	450	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	194	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	F	368	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	330	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	G	499	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	G	609	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	1021	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	197	ASP	CB-CG-OD1	6.07	123.77	118.30
1	E	684	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	542	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	197	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	E	998	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	226	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	G	42	TYR	CB-CG-CD1	-6.03	117.38	121.00
1	A	333	ASP	CB-CG-OD1	6.03	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	487	ASP	CB-CG-OD1	6.03	123.72	118.30
2	H	93	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	D	342	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	G	286	PHE	CB-CA-C	-6.02	98.36	110.40
1	G	949	VAL	CA-CB-CG1	-6.02	101.87	110.90
1	G	677	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	G	757	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	55	MET	CG-SD-CE	-6.00	90.59	100.20
1	E	959	ASP	CB-CG-OD1	6.00	123.70	118.30
2	F	114	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	539	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	G	810	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	G	642	TYR	CB-CG-CD1	5.98	124.59	121.00
1	G	410	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	389	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	757	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	D	262	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	H	262	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	G	670	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	F	97	ASP	CB-CG-OD1	5.94	123.65	118.30
1	C	758	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	E	338	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	C	258	ASP	CB-CG-OD1	5.93	123.64	118.30
1	E	791	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	1041	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	426	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	E	674	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	G	38	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	530	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	E	494	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	E	675	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	G	684	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	441	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	904	ASP	CB-CG-OD1	5.89	123.60	118.30
1	E	1057	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	E	611	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	G	558	ASP	N-CA-CB	-5.87	100.04	110.60
1	A	769	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	758	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	631	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	494	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	57	ASP	CB-CG-OD1	5.84	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	343	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	G	989	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	121	ASP	CB-CG-OD2	-5.83	113.05	118.30
2	D	211	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	677	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	953	ASP	CB-CG-OD1	5.81	123.53	118.30
1	E	807	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	G	169	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	104	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	B	342	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	791	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	416	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	904	ASP	CB-CG-OD2	-5.79	113.09	118.30
2	H	234	ASP	CB-CG-OD1	5.79	123.51	118.30
2	F	139	ASP	CB-CG-OD1	5.78	123.50	118.30
2	H	136	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	F	211	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	226	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	G	579	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	416	ASP	CB-CG-OD1	5.75	123.48	118.30
1	E	258	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	C	197	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	521	ASP	CB-CG-OD2	-5.74	113.13	118.30
2	F	211	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	G	904	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	F	368	ASP	CB-CG-OD1	5.74	123.46	118.30
1	E	1003	ASP	CB-CG-OD1	5.73	123.46	118.30
2	B	334	ASP	CB-CG-OD1	5.71	123.44	118.30
2	H	188	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	E	223	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	434	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	425	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	361	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	G	430	ASP	CB-CG-OD1	5.70	123.43	118.30
2	B	249	ASP	CB-CG-OD1	5.70	123.43	118.30
1	E	611	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	690	PRO	N-CA-CB	5.69	110.13	103.30
1	C	956	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	338	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	E	133	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	G	912	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	E	121	ASP	CB-CG-OD1	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	580	TYR	CB-CG-CD2	-5.68	117.59	121.00
2	B	188	ASP	CB-CG-OD2	-5.67	113.19	118.30
2	B	317	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	972	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	G	674	ASP	CB-CG-OD1	5.67	123.40	118.30
2	B	244	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	131	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	197	ASP	CB-CG-OD1	5.66	123.39	118.30
1	E	763	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	972	ASP	CB-CG-OD1	5.65	123.39	118.30
2	D	136	ASP	CB-CG-OD2	-5.65	113.21	118.30
2	D	84	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	557	THR	CA-CB-CG2	-5.64	104.50	112.40
2	F	18	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	F	249	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	807	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	514	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	227	ASP	CB-CG-OD1	5.63	123.36	118.30
2	B	244	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	C	1003	ASP	CB-CG-OD1	5.62	123.36	118.30
1	G	27	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	730	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	38	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	1041	ASP	CB-CG-OD1	5.61	123.35	118.30
2	B	112	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	372	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	E	1031	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	F	234	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	652	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	D	84	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	667	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	207	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	H	234	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	E	84	ASP	CB-CG-OD1	5.56	123.31	118.30
1	G	338	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	A	592	ASP	CB-CG-OD2	-5.56	113.30	118.30
2	D	67	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	G	450	ASP	CB-CG-OD2	-5.56	113.29	118.30
2	D	344	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	121	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	238	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	736	ARG	NE-CZ-NH1	5.56	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	204	LEU	CB-CA-C	-5.55	99.65	110.20
2	F	18	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	G	953	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	441	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	667	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	B	69	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	G	57	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	944	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	161	ASP	CB-CG-OD2	-5.54	113.32	118.30
2	H	97	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	389	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	42	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	G	400	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	E	6	ASP	CB-CG-OD1	5.50	123.25	118.30
1	G	238	ASP	CB-CG-OD1	5.50	123.25	118.30
1	E	758	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	758	ASP	CB-CG-OD2	-5.50	113.36	118.30
2	B	69	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	579	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	614	ASP	CB-CG-OD1	5.48	123.24	118.30
2	F	334	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	539	ASP	CB-CG-OD1	5.48	123.23	118.30
1	E	730	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	H	11	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	F	11	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	124	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	517	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	D	306	MET	N-CA-CB	5.46	120.44	110.60
1	G	6	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	C	810	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	998	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	F	266	PHE	CB-CG-CD1	5.46	124.62	120.80
2	F	372	GLU	N-CA-CB	-5.46	100.78	110.60
1	E	265	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	674	ASP	CB-CG-OD1	5.45	123.20	118.30
1	G	82	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	G	769	ASP	CB-CG-OD2	-5.45	113.40	118.30
2	D	148	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	D	69	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	C	592	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	G	809	MET	CA-CB-CG	-5.43	104.08	113.30
1	G	416	ASP	CB-CG-OD1	5.42	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	922	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	G	128	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	E	84	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	G	27	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	G	1057	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	E	416	ASP	CB-CG-OD1	5.40	123.16	118.30
2	H	84	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	6	ASP	CB-CG-OD1	5.39	123.16	118.30
2	D	67	ASP	CB-CG-OD1	5.39	123.15	118.30
1	G	670	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	207	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	674	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	459	ASP	CB-CG-OD1	5.38	123.15	118.30
2	B	139	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	C	233	SER	N-CA-CB	5.38	118.56	110.50
1	A	430	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	D	166	GLU	N-CA-CB	5.36	120.25	110.60
2	F	234	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	226	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	238	ASP	CB-CG-OD2	-5.34	113.49	118.30
2	B	212	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	F	10	GLU	CB-CA-C	-5.34	99.72	110.40
1	C	82	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	444	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	H	16	HIS	CA-CB-CG	-5.33	104.54	113.60
2	F	344	ASP	CB-CG-OD1	5.33	123.10	118.30
1	G	121	ASP	CB-CG-OD1	5.32	123.08	118.30
1	E	386	ALA	N-CA-CB	5.31	117.54	110.10
2	H	244	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	956	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	487	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	1016	THR	CA-CB-CG2	-5.30	104.98	112.40
1	C	1027	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	F	262	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	E	530	ASP	CB-CG-OD2	-5.29	113.53	118.30
2	D	262	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	694	THR	N-CA-CB	5.29	120.35	110.30
1	C	542	TYR	CB-CG-CD1	5.29	124.17	121.00
1	G	207	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	726	GLU	N-CA-CB	5.29	120.11	110.60
2	F	84	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	625	ASP	CB-CG-OD1	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1048	PHE	CB-CG-CD1	5.28	124.49	120.80
1	G	730	ASP	CB-CG-OD1	5.28	123.05	118.30
2	B	317	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	G	730	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	G	1036	TYR	CA-CB-CG	-5.26	103.40	113.40
1	C	129	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	130	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	867	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	H	197	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	C	194	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	611	ASP	CB-CG-OD1	5.25	123.02	118.30
2	B	136	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	G	6	ASP	CB-CG-OD1	5.24	123.02	118.30
1	E	735	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	H	112	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	517	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	999	PRO	N-CA-CB	5.22	109.57	103.30
2	F	262	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	592	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	609	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	677	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	1036	TYR	CB-CG-CD2	-5.22	117.87	121.00
2	D	114	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	753	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	765	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	G	207	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	E	261	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	E	450	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	434	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	758	ASP	CB-CG-OD1	5.20	122.98	118.30
2	H	368	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	G	226	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	753	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	E	560	GLU	N-CA-C	-5.20	96.97	111.00
1	A	753	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	A	922	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	E	807	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	848	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	D	211	ASP	CB-CG-OD1	5.19	122.97	118.30
1	E	430	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	E	539	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	F	115	THR	CA-CB-CG2	-5.18	105.15	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ASP	CB-CG-OD1	5.18	122.96	118.30
2	F	114	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	757	ASP	CB-CG-OD1	5.17	122.96	118.30
1	E	904	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	E	129	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	246	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	F	112	ASP	CB-CG-OD1	5.15	122.94	118.30
2	B	67	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	E	161	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	430	ASP	CB-CG-OD1	5.15	122.93	118.30
1	G	223	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	459	ASP	CB-CG-OD1	5.14	122.92	118.30
2	D	97	ASP	CB-CG-OD1	5.14	122.92	118.30
1	E	517	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	730	ASP	CB-CG-OD1	5.12	122.91	118.30
2	B	114	ASP	CB-CG-OD1	5.12	122.91	118.30
2	H	136	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	265	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	H	116	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	124	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	G	667	ASP	CB-CG-OD1	5.11	122.90	118.30
2	B	203	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	E	246	ASP	CB-CG-OD1	5.10	122.89	118.30
1	G	1025	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	487	ASP	CB-CG-OD2	-5.09	113.71	118.30
1	C	521	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	609	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	G	1021	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	590	ARG	NE-CZ-NH1	5.09	122.84	120.30
2	F	136	ASP	CB-CG-OD1	5.09	122.88	118.30
2	D	188	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	E	830	PHE	CB-CG-CD2	-5.09	117.24	120.80
2	H	317	ASP	CB-CG-OD1	5.09	122.88	118.30
1	E	226	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	131	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	G	763	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	E	338	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	207	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	E	38	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	G	733	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	791	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	E	670	ASP	CB-CG-OD2	-5.06	113.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	670	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	238	ASP	CB-CG-OD1	5.05	122.85	118.30
2	D	112	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	343	ARG	CD-NE-CZ	5.05	130.67	123.60
1	C	1041	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	667	ASP	CB-CG-OD1	5.04	122.84	118.30
2	F	362	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	763	ASP	CB-CG-OD1	5.04	122.83	118.30
2	B	262	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	521	ASP	CB-CG-OD1	5.03	122.82	118.30
2	F	45	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	999	PRO	N-CA-CB	5.02	109.33	103.30
1	G	518	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	791	ASP	CB-CG-OD1	5.02	122.82	118.30
1	G	671	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	E	521	ASP	CB-CG-OD1	5.00	122.81	118.30
1	C	133	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	C	57	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

There are no planarity outliers.

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	8189	0	8227	251	0
1	C	8165	0	8199	238	0
1	E	8188	0	8225	212	0
1	G	8178	0	8221	338	0
2	B	2895	0	2861	107	0
2	D	2895	0	2861	99	0
2	F	2895	0	2861	113	0
2	H	2900	0	2863	144	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	1	0
5	F	1	0	0	0	0
5	G	3	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	10	0	0	1	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	34	0	44	2	0
8	A	54	0	24	2	0
8	C	54	0	24	0	0
8	E	54	0	24	4	0
8	G	54	0	24	1	0
9	A	9	0	20	0	0
9	C	9	0	20	0	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	830	0	0	24	0
10	B	230	0	0	5	0
10	C	683	0	0	23	0
10	D	238	0	0	4	0
10	E	884	0	0	21	0
10	F	272	0	0	2	0
10	G	666	0	0	20	0
10	H	184	0	0	3	0
All	All	48668	0	44538	1483	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 17.

All (1483) 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:E:993:LYS:CE	1:E:993:LYS:NZ	1.67	1.55
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.28	1.12
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.30	1.11
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.09
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.31	1.07
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.22	1.06
1:G:559:ARG:HG3	1:G:559:ARG:HH11	1.23	1.04
1:E:1002:GLN:HE22	1:E:1006:LYS:HE3	1.19	1.03
1:G:784:GLN:H	1:G:784:GLN:NE2	1.56	1.01
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.23	1.00
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.46	0.98
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.42	0.98
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.45	0.94
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.48	0.94
2:D:324:ASN:H	2:D:324:ASN:HD22	1.12	0.93
2:H:286:MET:HE2	2:H:289:GLY:HA2	1.49	0.93
1:A:784:GLN:HE21	1:A:784:GLN:H	1.15	0.92
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.85	0.92
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.51	0.92
1:G:784:GLN:HE21	1:G:784:GLN:N	1.67	0.92
1:C:698:ILE:HD12	1:C:698:ILE:H	1.33	0.91
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.49	0.91
1:G:1051:ALA:HA	1:G:1054:LEU:HD12	1.53	0.91
1:A:559:ARG:HG3	1:A:559:ARG:HH11	1.36	0.90
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.85	0.90
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.51	0.90
1:E:784:GLN:H	1:E:784:GLN:NE2	1.70	0.90
1:C:1:MET:HG3	1:C:2:PRO:HD2	1.53	0.90
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.54	0.90
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.53	0.89
2:F:228:VAL:HA	2:F:231:MET:CE	2.02	0.89
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.03	0.89
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.36	0.88
1:G:1001:ILE:HD12	1:G:1002:GLN:N	1.89	0.88
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.04	0.87
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.04	0.87
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.91	0.86
1:A:1027[B]:ARG:HH22	1:A:1031:ARG:HH11	1.24	0.85
1:C:559:ARG:NH1	10:C:4442:HOH:O	2.09	0.85
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.12	0.85
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.59	0.85
2:B:324:ASN:HD22	2:B:324:ASN:N	1.73	0.85
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.11	0.85
1:E:726:GLU:HG2	1:E:727:ILE:H	1.40	0.84
2:F:228:VAL:HA	2:F:231:MET:HE3	1.59	0.84
2:H:324:ASN:HD22	2:H:324:ASN:H	1.25	0.84
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.58	0.84
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.07	0.84
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.13	0.84
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.38	0.83
1:E:646:THR:HB	1:E:647:PRO:HD3	1.60	0.83
1:A:1027[B]:ARG:NH2	1:A:1031:ARG:HH11	1.76	0.83
2:D:259:LEU:HD13	2:D:342:ARG:NH1	1.93	0.83
1:C:998:ARG:CG	1:C:999:PRO:HA	2.08	0.82
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.14	0.82
2:F:324:ASN:H	2:F:324:ASN:HD22	1.25	0.82
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.62	0.82
1:E:1001:ILE:HD12	1:E:1002:GLN:N	1.95	0.82
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.62	0.81
1:G:726:GLU:HG3	1:G:727:ILE:N	1.95	0.81
1:E:702:VAL:HG11	1:E:735:ARG:NH2	1.94	0.81
1:A:726:GLU:HG3	1:A:727:ILE:N	1.95	0.81
1:A:1027[B]:ARG:HH22	1:A:1031:ARG:NH1	1.78	0.81
1:C:726:GLU:HG3	1:C:727:ILE:N	1.96	0.81
1:G:865:ALA:O	1:G:869:MET:HG3	1.81	0.81
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.63	0.81
1:A:873:SER:O	1:A:877:GLN:HG3	1.81	0.80
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.64	0.79
2:B:185:LYS:HD3	2:B:190:LEU:HD21	1.64	0.79
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.98	0.79
1:G:682:VAL:HG11	1:G:689:GLN:NE2	1.98	0.78
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.12	0.78
1:G:860:PRO:HB2	1:G:863:LYS:HG3	1.63	0.78
1:C:883:VAL:O	1:C:884:ILE:HD13	1.83	0.78
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.31	0.78
1:G:682:VAL:HG11	1:G:689:GLN:HE21	1.49	0.78
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.64	0.78
1:A:999:PRO:HD2	1:G:983:GLU:OE2	1.84	0.77
2:B:324:ASN:HD22	2:B:324:ASN:H	1.30	0.77
2:F:254:ALA:O	2:F:257:LYS:HB2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:GLN:HG3	1:C:1054:LEU:HD13	1.67	0.77
1:E:784:GLN:H	1:E:784:GLN:HE21	1.32	0.77
1:G:563:MET:CE	1:G:635:PRO:HG3	2.15	0.77
1:G:994:VAL:HG22	1:G:1000:HIS:CG	2.20	0.77
1:E:558:ASP:HB3	1:E:559[B]:ARG:HG3	1.67	0.77
1:A:784:GLN:H	1:A:784:GLN:NE2	1.82	0.77
1:A:751:LEU:HD12	1:A:751:LEU:H	1.50	0.76
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.21	0.76
2:F:324:ASN:O	2:F:342:ARG:HD2	1.84	0.76
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.65	0.76
1:G:1021:ARG:HG2	1:G:1021:ARG:HH11	1.48	0.76
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.51	0.76
2:B:298:LYS:HE2	2:B:303:ASN:OD1	1.86	0.76
2:H:324:ASN:HD22	2:H:324:ASN:N	1.82	0.76
1:E:772[B]:MET:HE3	10:E:4886:HOH:O	1.84	0.76
1:G:784:GLN:H	1:G:784:GLN:HE21	0.82	0.75
1:G:1063:ILE:HD13	1:G:1068:MET:HG2	1.68	0.75
1:E:698:ILE:O	1:E:702:VAL:HG23	1.85	0.75
10:E:4794:HOH:O	2:F:304:VAL:HB	1.85	0.75
2:H:133:ILE:CD1	2:H:143:ALA:HB2	2.16	0.75
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.21	0.74
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.69	0.74
1:C:675:ARG:H	1:C:675:ARG:CD	1.99	0.74
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.16	0.74
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.68	0.74
1:C:1020:ARG:NH2	1:C:1023:ILE:HG21	2.02	0.74
1:E:1027:ARG:HE	1:E:1031:ARG:HE	1.32	0.74
1:G:509:ARG:HH11	1:G:509:ARG:HB2	1.52	0.74
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.03	0.74
1:A:28:TYR:O	1:A:32:GLN:HG3	1.86	0.74
2:H:46:PRO:O	2:H:242:PRO:HG3	1.88	0.74
2:H:299:ASP:OD1	2:H:302:LYS:HD3	1.88	0.74
1:C:400:ARG:HD3	10:C:4363:HOH:O	1.86	0.73
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.18	0.73
1:E:3:LYS:HB2	1:E:42:TYR:OH	1.87	0.73
1:G:339:ILE:HD12	1:G:530:ASP:HA	1.71	0.73
2:B:324:ASN:ND2	2:B:324:ASN:H	1.86	0.73
1:A:1027[B]:ARG:NH1	10:A:4891:HOH:O	2.21	0.72
1:G:704:LYS:O	1:G:708:ILE:HD12	1.87	0.72
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.71	0.72
2:H:286:MET:CE	2:H:289:GLY:HA2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.69	0.72
1:C:1064:SER:OG	1:C:1067:GLU:HG3	1.88	0.72
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.89	0.72
2:B:156:MET:HA	10:B:4197:HOH:O	1.90	0.72
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.54	0.72
1:A:698:ILE:O	1:A:701:ALA:HB3	1.89	0.72
1:G:1:MET:HB3	10:G:4163:HOH:O	1.89	0.72
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.17	0.72
1:A:1020:ARG:NH2	1:A:1023:ILE:HG21	2.05	0.72
1:C:865:ALA:O	1:C:869:MET:HG3	1.90	0.72
1:G:702:VAL:HG21	1:G:735:ARG:NH2	2.04	0.72
1:G:873:SER:O	1:G:877:GLN:HG3	1.90	0.71
1:G:872:LYS:HG2	1:G:877:GLN:HG2	1.71	0.71
1:A:79:GLU:HB2	1:A:111:PHE:CZ	2.25	0.71
2:D:226:GLU:O	2:D:230:LYS:HG3	1.90	0.71
1:E:135:ALA:HB1	1:E:274:GLU:HG3	1.72	0.71
2:H:275:LEU:HD23	2:H:349:SER:OG	1.91	0.71
2:B:139:ASP:OD2	2:B:142:LEU:HB2	1.91	0.71
1:E:726:GLU:HG2	1:E:727:ILE:N	2.06	0.71
2:B:375:GLU:HA	10:B:4246:HOH:O	1.90	0.70
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.72	0.70
1:G:1:MET:H3	1:G:224:LYS:HE3	1.55	0.70
2:H:34:THR:HA	2:H:56:THR:OG1	1.90	0.70
2:B:259:LEU:O	2:B:345:LYS:HD2	1.91	0.70
1:C:954:LYS:O	1:C:957:VAL:HG12	1.91	0.70
1:C:698:ILE:H	1:C:698:ILE:CD1	2.05	0.70
2:D:324:ASN:HD22	2:D:324:ASN:N	1.83	0.70
1:E:698:ILE:HD12	1:E:698:ILE:H	1.56	0.70
1:G:339:ILE:CD1	1:G:530:ASP:HA	2.22	0.70
1:G:340:THR:O	1:G:343:ARG:HB2	1.91	0.70
1:C:146:SER:CB	1:C:205:LEU:HD11	2.22	0.70
1:E:1021:ARG:HG2	1:E:1021:ARG:HH11	1.56	0.70
1:A:1037:LYS:HA	10:A:4585:HOH:O	1.92	0.70
1:G:130:ARG:O	1:G:134:VAL:HG23	1.92	0.70
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.54	0.70
1:C:890:VAL:HG23	1:C:927:ALA:HB1	1.74	0.70
1:A:751:LEU:HD12	1:A:751:LEU:N	2.07	0.69
1:C:51:PRO:O	1:C:855:LYS:HD3	1.91	0.69
2:D:78:GLN:NE2	10:D:1966:HOH:O	2.25	0.69
1:G:1:MET:HE2	10:G:4316:HOH:O	1.92	0.69
1:A:954:LYS:O	1:A:957:VAL:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.74	0.69
1:C:734:LEU:O	1:C:734:LEU:HD12	1.93	0.69
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.75	0.69
1:C:802:SER:O	1:C:806:GLN:HG3	1.93	0.69
2:F:269:SER:O	2:F:272:HIS:HB3	1.92	0.69
1:G:534:ALA:O	2:H:123:ARG:HD3	1.92	0.69
1:G:559:ARG:HG3	1:G:559:ARG:NH1	1.97	0.69
1:A:1027[B]:ARG:NH2	1:A:1031:ARG:NH1	2.39	0.69
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.23	0.69
2:F:232:ASN:N	2:F:233:PRO:HD3	2.07	0.69
1:G:327:ALA:HB2	10:G:4226:HOH:O	1.92	0.69
1:E:872:LYS:HD3	1:E:877:GLN:HG2	1.75	0.68
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.75	0.68
2:H:71:GLU:C	2:H:203:ARG:HG3	2.13	0.68
1:A:1001:ILE:HD13	1:A:1029:ILE:HG13	1.73	0.68
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.23	0.68
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.75	0.68
1:G:35:LYS:NZ	10:G:4207:HOH:O	2.26	0.68
1:C:363:ASN:HA	1:C:365:GLU:OE2	1.93	0.68
2:D:212:ARG:HG3	2:D:212:ARG:HH11	1.59	0.68
2:F:224:SER:OG	2:F:227:ASP:HB2	1.93	0.68
1:E:679:GLN:O	1:E:683:GLU:HB2	1.92	0.68
1:C:103:GLU:HG3	1:C:104:ARG:N	2.08	0.68
1:A:490:ARG:HD3	10:A:4644:HOH:O	1.93	0.68
1:E:1002:GLN:NE2	1:E:1006:LYS:HE3	2.03	0.68
1:A:726:GLU:HG3	1:A:727:ILE:H	1.59	0.68
1:A:228:CYS:SG	1:A:269:MET:HG2	2.34	0.68
2:B:222:GLN:H	2:B:222:GLN:HE21	1.42	0.68
1:E:1027:ARG:HE	1:E:1031:ARG:NE	1.91	0.68
2:F:186:LYS:NZ	10:F:3117:HOH:O	2.27	0.68
1:G:676:GLU:O	1:G:680:HIS:ND1	2.27	0.67
2:H:153:LEU:HA	2:H:156:MET:HE3	1.75	0.67
1:A:822:VAL:O	1:A:823:ARG:HD3	1.94	0.67
1:E:670:ASP:HB2	10:E:4867:HOH:O	1.94	0.67
1:G:690:PRO:HG3	1:G:756:LEU:HD11	1.76	0.67
1:E:145:ARG:O	1:E:208:GLU:HG2	1.95	0.67
1:E:696:THR:H	1:E:700:MET:HE3	1.60	0.67
1:A:279:THR:HG22	10:A:4322:HOH:O	1.93	0.67
2:B:324:ASN:N	2:B:324:ASN:ND2	2.42	0.67
1:C:677:ARG:O	1:C:680:HIS:HB2	1.95	0.67
2:H:121:LEU:CD1	2:H:125:LYS:HD3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG2	1:A:38:ARG:NH1	1.94	0.67
1:C:890:VAL:HG23	1:C:927:ALA:CB	2.24	0.67
1:G:588:ALA:O	1:G:591:GLU:HB3	1.95	0.67
1:G:802:SER:O	1:G:806:GLN:HG3	1.95	0.67
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.29	0.67
2:B:378:ARG:HG2	2:B:378:ARG:HH11	1.60	0.67
1:G:58:PRO:HD2	1:G:59[A]:GLU:OE2	1.95	0.67
1:G:516:LEU:HD11	1:G:520:TYR:CZ	2.29	0.67
1:G:698:ILE:HD12	1:G:698:ILE:N	2.10	0.67
1:A:1020:ARG:O	1:A:1024:GLU:HG3	1.94	0.67
2:B:268:ILE:HD13	2:B:354:PRO:HD2	1.77	0.67
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.77	0.67
1:A:695:VAL:CG1	1:A:701:ALA:HB2	2.13	0.67
1:G:354:TYR:HB2	1:G:388:GLY:O	1.94	0.67
1:G:803:GLN:N	10:G:4710:HOH:O	2.27	0.67
2:D:222:GLN:H	2:D:222:GLN:HE21	1.43	0.66
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.25	0.66
1:G:875:ALA:HB2	10:G:4718:HOH:O	1.93	0.66
1:A:944:ARG:HD3	1:A:972:ASP:OD1	1.96	0.66
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.77	0.66
1:A:863:LYS:HE2	10:A:4593:HOH:O	1.94	0.66
1:G:1:MET:H3	1:G:1:MET:HE2	1.59	0.66
1:E:998:ARG:CB	1:E:999:PRO:HA	2.26	0.66
1:G:475[B]:LYS:HG2	1:G:488:PHE:CZ	2.30	0.66
2:H:202:LYS:NZ	2:H:355:GLU:OE1	2.27	0.66
2:B:226:GLU:O	2:B:230:LYS:HG3	1.96	0.65
1:E:559[B]:ARG:HD2	1:E:595:GLU:HB2	1.77	0.65
1:E:806:GLN:HA	1:E:809:MET:CE	2.26	0.65
1:G:331:THR:N	1:G:334:GLU:OE1	2.28	0.65
2:H:286:MET:HE2	2:H:289:GLY:CA	2.23	0.65
1:C:784:GLN:H	1:C:784:GLN:HE21	1.44	0.65
1:E:698:ILE:HD12	1:E:698:ILE:N	2.10	0.65
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.79	0.65
2:D:64:GLY:HA3	2:D:94:ASN:OD1	1.96	0.65
1:E:5:THR:O	1:E:8:LYS:NZ	2.29	0.65
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.42	0.65
2:B:6:LEU:HD11	2:B:8:VAL:HG22	1.76	0.65
1:C:954:LYS:HG2	1:C:980:VAL:HG21	1.77	0.65
1:E:417:ASP:OD2	1:E:418:PRO:HD2	1.96	0.65
1:G:946:LEU:C	1:G:947:LEU:HD12	2.17	0.65
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.78	0.65
1:A:693:ALA:O	1:A:752:LEU:HB2	1.97	0.65
1:C:802:SER:OG	1:C:805:ILE:HB	1.97	0.65
1:C:807:ASP:O	1:C:811:GLN:HB2	1.96	0.65
1:E:6:ASP:OD2	1:E:6:ASP:N	2.30	0.65
1:C:693:ALA:CB	1:C:704:LYS:HG3	2.27	0.65
2:F:324:ASN:ND2	2:F:324:ASN:H	1.95	0.65
2:H:7:LEU:HD23	2:H:15:PHE:CD2	2.32	0.65
1:E:922:ARG:NH2	1:E:926:GLU:OE1	2.27	0.65
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.97	0.65
2:B:194:VAL:HB	2:B:216:LEU:HD23	1.79	0.64
1:E:563:MET:CE	1:E:635:PRO:HG3	2.27	0.64
2:F:300:VAL:HG22	2:F:328:THR:O	1.96	0.64
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.30	0.64
1:G:343:ARG:NH1	10:G:4538:HOH:O	2.29	0.64
1:C:1009[A]:GLU:OE2	10:C:4707:HOH:O	2.14	0.64
1:E:998:ARG:HG2	1:E:999:PRO:HA	1.80	0.64
1:A:947:LEU:HA	1:A:1014:ILE:HG23	1.79	0.64
2:D:259:LEU:HD13	2:D:342:ARG:HH12	1.62	0.64
1:G:954:LYS:O	1:G:957:VAL:HG12	1.96	0.64
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.78	0.64
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.79	0.64
2:D:363:ALA:O	2:D:366:LEU:HD12	1.98	0.64
1:A:1037:LYS:HD2	10:A:4879:HOH:O	1.97	0.64
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.33	0.64
2:H:324:ASN:ND2	2:H:324:ASN:H	1.95	0.64
2:D:26:ALA:O	2:D:131:CYS:HA	1.98	0.64
1:E:278:GLU:HG2	10:E:4232:HOH:O	1.97	0.64
2:B:144:LEU:O	2:B:148:ARG:HG3	1.97	0.64
1:E:998:ARG:HA	1:E:999:PRO:C	2.17	0.64
1:A:145:ARG:NH2	1:A:161:ASP:OD2	2.29	0.64
1:C:697:ALA:O	1:C:700:MET:HB3	1.98	0.64
1:E:954:LYS:O	1:E:980:VAL:HG11	1.98	0.64
1:C:676:GLU:O	1:C:680:HIS:ND1	2.31	0.64
1:E:153:GLU:HB3	10:E:4782:HOH:O	1.98	0.64
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.80	0.63
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.80	0.63
1:C:735:ARG:O	1:C:738:PHE:N	2.32	0.63
1:E:998:ARG:CG	1:E:999:PRO:HA	2.27	0.63
2:H:71:GLU:O	2:H:203:ARG:HG3	1.98	0.63
1:A:1001:ILE:CD1	1:A:1029:ILE:HG13	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:ASN:H	2:D:324:ASN:ND2	1.93	0.63
2:F:190:LEU:HD23	2:F:213:GLY:HA2	1.80	0.63
1:G:1:MET:N	10:G:4316:HOH:O	2.31	0.63
1:G:166:CYS:C	1:G:167:ILE:HD12	2.18	0.63
2:H:244:ASP:OD2	2:H:245:PRO:HD2	1.98	0.63
1:G:482:THR:HG22	1:G:483:GLY:N	2.14	0.63
1:A:318:PRO:HG3	1:A:610:TYR:OH	1.98	0.63
1:E:713:VAL:HB	1:E:753:ASP:HB2	1.79	0.63
2:B:8:VAL:HG21	2:B:143:ALA:HB3	1.81	0.62
2:H:218:ILE:N	2:H:218:ILE:HD13	2.14	0.62
1:C:7:ILE:HG23	1:C:84:ASP:HB2	1.81	0.62
1:C:730:ASP:OD2	1:C:733:ASP:HB2	1.99	0.62
1:C:1027:ARG:O	1:C:1031:ARG:HG3	1.99	0.62
2:D:71:GLU:O	2:D:203:ARG:HG3	1.99	0.62
1:G:269:MET:O	1:G:273:ARG:HG3	1.99	0.62
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.29	0.62
1:E:1027:ARG:NE	1:E:1031:ARG:HE	1.98	0.62
2:F:5:ALA:HB3	2:F:110:ILE:HG13	1.81	0.62
1:A:663:GLY:CA	1:A:869:MET:HG2	2.29	0.62
1:E:515:LYS:O	1:E:515:LYS:HD3	2.00	0.62
1:G:561:LYS:HE2	10:G:4461:HOH:O	1.99	0.62
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.81	0.62
1:C:1063:ILE:HD13	1:C:1068:MET:HG2	1.82	0.62
2:D:266:PHE:HA	2:D:348:PHE:O	1.98	0.62
1:C:956:ARG:HB3	1:C:1044:LEU:HD21	1.81	0.62
1:E:696:THR:N	1:E:700:MET:HE3	2.15	0.62
1:G:663:GLY:HA3	1:G:869:MET:HE3	1.82	0.62
1:E:481:ILE:HD12	1:E:508:VAL:HG21	1.81	0.62
1:E:734:LEU:HD12	1:E:734:LEU:O	2.00	0.62
1:E:904:ASP:O	1:E:906:LEU:N	2.31	0.62
1:E:994:VAL:HG23	1:E:1001:ILE:HD11	1.82	0.62
2:F:376:GLN:HA	2:F:379:LYS:HZ2	1.64	0.62
2:H:264:PRO:HB3	2:H:373:LEU:HB3	1.81	0.61
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.18	0.61
2:F:236:ILE:HD11	2:F:263:ILE:HG21	1.82	0.61
2:F:286:MET:HE2	2:F:314:PHE:O	1.99	0.61
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.99	0.61
2:B:6:LEU:HD12	2:B:7:LEU:N	2.16	0.61
1:G:698:ILE:HD12	1:G:698:ILE:H	1.66	0.61
2:H:228:VAL:O	2:H:231:MET:HG3	1.99	0.61
1:A:1021:ARG:HH11	1:A:1021:ARG:CG	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:344:ASP:O	2:D:345:LYS:HG2	2.01	0.61
1:G:1:MET:HB2	1:G:224:LYS:NZ	2.16	0.61
1:A:267:ALA:O	1:A:271:VAL:HG23	2.00	0.61
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.83	0.61
1:C:74:VAL:HG11	1:C:102:LEU:HD11	1.83	0.61
2:F:186:LYS:O	2:F:189:GLU:HB2	2.01	0.61
2:H:187:GLU:HG2	2:H:215:ARG:CD	2.20	0.61
1:C:146:SER:HB2	1:C:205:LEU:CD1	2.31	0.61
2:H:248:CYS:O	2:H:252:ILE:HG13	2.01	0.61
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.36	0.60
2:H:334:ASP:OD2	2:H:336:THR:HG23	2.00	0.60
1:E:695:VAL:HA	1:E:700:MET:HE1	1.82	0.60
1:A:27:ASP:OD2	1:A:53:THR:HB	2.01	0.60
1:A:675:ARG:CD	1:A:675:ARG:H	2.14	0.60
1:G:675:ARG:CD	1:G:675:ARG:H	2.13	0.60
2:H:50:ARG:HG2	2:H:158:LEU:CD1	2.31	0.60
1:A:514:ARG:NE	10:A:4660:HOH:O	2.26	0.60
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.47	0.60
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.84	0.60
1:A:559:ARG:HG3	1:A:559:ARG:NH1	2.05	0.60
2:B:378:ARG:HG2	2:B:378:ARG:NH1	2.16	0.60
1:C:32:GLN:OE1	1:C:320:ALA:HB3	2.01	0.60
1:C:56:THR:OG1	1:C:855:LYS:NZ	2.26	0.60
1:E:185:ARG:O	1:E:189:GLU:HG3	2.01	0.60
2:F:201:ALA:HB2	2:F:239:SER:CB	2.32	0.60
1:G:679:GLN:O	1:G:683:GLU:HB2	2.02	0.60
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.37	0.60
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.83	0.60
2:H:279:SER:O	2:H:322:PRO:HG3	2.02	0.60
1:A:712:LEU:HD23	1:A:752:LEU:HG	1.84	0.60
1:C:936:ASN:HB2	10:C:4085:HOH:O	2.02	0.60
1:G:1021:ARG:HG2	1:G:1021:ARG:NH1	2.17	0.60
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.37	0.60
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.83	0.59
2:B:232:ASN:N	2:B:233:PRO:HD3	2.17	0.59
1:C:711:PRO:HG2	1:C:755:PHE:HD2	1.67	0.59
2:H:195:VAL:HG11	2:H:228:VAL:HG13	1.84	0.59
1:E:46:LEU:HG	1:E:46:LEU:O	2.02	0.59
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.02	0.59
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.65	0.59
2:F:354:PRO:HB3	2:F:363:ALA:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:947:LEU:HD12	1:G:947:LEU:N	2.17	0.59
1:G:950:ARG:NH1	10:G:4728:HOH:O	2.33	0.59
1:A:35:LYS:O	1:A:39:GLU:HG3	2.02	0.59
1:A:222:ARG:CZ	1:A:273:ARG:HG2	2.32	0.59
1:A:358:LYS:HE3	10:A:4174:HOH:O	2.01	0.59
2:B:249:ASP:OD2	2:B:250:TYR:N	2.36	0.59
1:C:930:LYS:HE3	10:C:4170:HOH:O	2.01	0.59
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.29	0.59
2:H:155:GLY:O	2:H:247:PRO:HG3	2.02	0.59
1:A:1001:ILE:HG13	1:A:1002:GLN:H	1.67	0.59
1:G:426:ARG:HD3	1:G:426:ARG:C	2.23	0.59
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.20	0.59
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.84	0.59
1:G:954:LYS:O	1:G:980:VAL:HG11	2.01	0.59
2:B:279:SER:O	2:B:322:PRO:HG3	2.03	0.59
1:C:646:THR:HB	1:C:647:PRO:HD3	1.85	0.59
1:A:737:TYR:CE1	1:A:741:ALA:HB2	2.37	0.59
1:C:24:CYS:HB3	1:C:576:ILE:HD12	1.85	0.59
1:C:337:ASN:HB3	1:C:340:THR:OG1	2.03	0.59
1:C:415:LEU:HB2	10:C:4581:HOH:O	2.02	0.59
1:E:167:ILE:N	1:E:167:ILE:HD12	2.18	0.59
2:F:261:THR:OG1	2:F:263:ILE:HG13	2.02	0.59
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.37	0.59
1:C:1063:ILE:HD13	1:C:1068:MET:CG	2.33	0.59
1:G:436:ILE:HG22	10:G:4327:HOH:O	2.02	0.59
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.84	0.58
2:F:251:ALA:O	2:F:255:ILE:HD12	2.02	0.58
2:H:142:LEU:O	2:H:146:LYS:HG3	2.02	0.58
1:A:770:GLY:HA2	1:A:823:ARG:NH1	2.18	0.58
1:A:998:ARG:CB	1:A:999:PRO:HA	2.33	0.58
2:B:344:ASP:OD2	2:B:344:ASP:N	2.28	0.58
2:D:324:ASN:C	2:D:343:THR:HG23	2.24	0.58
1:G:863:LYS:O	1:G:867:ARG:HG3	2.02	0.58
1:E:854:SER:HA	1:E:859:VAL:O	2.02	0.58
1:G:686:LYS:O	1:G:687:LEU:HD23	2.03	0.58
1:G:701:ALA:O	1:G:705:ALA:N	2.29	0.58
1:G:659:VAL:HG13	1:G:660:PRO:HD2	1.85	0.58
2:D:43:LEU:HD21	2:D:80:LEU:HD13	1.85	0.58
1:A:220:VAL:O	1:A:281:GLY:HA2	2.04	0.58
1:C:75:ARG:HD3	10:C:4173:HOH:O	2.04	0.58
1:E:1:MET:N	10:E:4636:HOH:O	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.30	0.58
2:B:364:ALA:N	2:B:365:PRO:HD2	2.19	0.58
1:C:1063:ILE:HG12	1:C:1064:SER:N	2.18	0.58
1:E:1001:ILE:HD12	1:E:1002:GLN:H	1.69	0.58
1:G:64:THR:O	1:G:1065:VAL:HG23	2.03	0.58
1:G:57:ASP:HB3	1:G:59[A]:GLU:OE2	2.03	0.58
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.19	0.58
1:G:775:ILE:HD11	1:G:813:VAL:HG11	1.86	0.58
1:C:1014:ILE:HD12	1:C:1015:ASN:N	2.18	0.58
2:H:168:TYR:CE2	2:H:218:ILE:HG12	2.39	0.58
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.50	0.57
1:C:197:ASP:OD2	1:C:1037:LYS:NZ	2.30	0.57
1:C:267:ALA:O	1:C:271:VAL:HG23	2.04	0.57
2:D:50:ARG:NH2	10:D:1965:HOH:O	2.37	0.57
1:E:274:GLU:OE2	1:E:274:GLU:HA	2.03	0.57
2:H:171:THR:HG22	2:H:190:LEU:HD12	1.86	0.57
2:H:208:MET:HB3	2:H:212:ARG:NH1	2.19	0.57
1:A:1027[B]:ARG:CZ	1:A:1031:ARG:HD3	2.34	0.57
1:G:1:MET:N	1:G:224:LYS:HE3	2.18	0.57
1:G:28:TYR:CE1	1:G:313:LYS:HE3	2.39	0.57
1:G:646:THR:HB	1:G:647:PRO:HD3	1.87	0.57
1:C:482:THR:HG23	10:C:4408:HOH:O	2.04	0.57
2:D:257:LYS:O	2:D:260:GLU:HB2	2.05	0.57
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.19	0.57
1:C:639:ILE:HD13	1:C:869:MET:HE3	1.85	0.57
2:D:318:GLU:O	2:D:321:LEU:HB2	2.04	0.57
2:H:23:THR:HG23	2:H:134:ALA:O	2.05	0.57
1:A:972:ASP:OD2	1:A:1004[B]:ARG:NH1	2.38	0.57
1:C:1061:LYS:HG2	10:C:4542:HOH:O	2.05	0.57
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.39	0.57
2:B:273:GLN:HE21	2:B:351:GLN:HE22	1.52	0.57
1:G:509:ARG:HB2	1:G:509:ARG:NH1	2.17	0.57
1:G:768:CYS:HB2	1:G:773:VAL:HG22	1.85	0.57
1:A:1001:ILE:HG13	1:A:1002:GLN:N	2.19	0.57
1:C:186:GLU:HB2	10:C:4561:HOH:O	2.02	0.57
1:C:693:ALA:HB2	1:C:708:ILE:HD11	1.87	0.57
1:E:417:ASP:OD2	1:E:419:GLU:HB2	2.05	0.57
1:E:966:LYS:O	1:E:966:LYS:HG3	2.02	0.57
1:G:361:ARG:CZ	1:G:571:ARG:HG2	2.35	0.57
1:A:82:ARG:HG3	1:A:82:ARG:NH1	2.15	0.56
1:C:6:ASP:OD2	1:C:6:ASP:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:ASP:HA	2:F:329:HIS:CD2	2.40	0.56
1:C:686:LYS:O	1:C:687:LEU:HD23	2.04	0.56
1:C:698:ILE:HD12	1:C:698:ILE:N	2.12	0.56
1:C:923:THR:OG1	1:C:926:GLU:HB2	2.05	0.56
1:E:32:GLN:HB3	1:E:321:LYS:HG3	1.87	0.56
1:E:691:ALA:CB	1:E:708:ILE:HG23	2.36	0.56
1:E:809:MET:HG2	1:E:830:PHE:CE2	2.41	0.56
1:G:905:PRO:HB2	1:G:1040:TYR:HH	1.69	0.56
1:E:1021:ARG:HG2	1:E:1021:ARG:NH1	2.21	0.56
2:F:279:SER:HB2	2:F:325:LEU:HD11	1.87	0.56
1:G:797:PRO:HD2	1:G:888:TYR:CD1	2.40	0.56
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.40	0.56
1:C:702:VAL:O	1:C:706:LYS:HD3	2.06	0.56
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.41	0.56
1:C:986:ILE:O	1:C:988:PRO:HD3	2.05	0.56
1:E:954:LYS:HE2	1:E:976:GLY:C	2.26	0.56
2:D:174:SER:O	2:D:182:PRO:HD3	2.05	0.56
2:F:228:VAL:HA	2:F:231:MET:HE2	1.84	0.56
1:E:901:PRO:HD2	5:E:4055:CL:CL	2.43	0.56
1:E:993:LYS:NZ	1:E:993:LYS:CD	2.60	0.56
2:F:261:THR:O	2:F:345:LYS:NZ	2.38	0.56
1:G:79:GLU:HG2	1:G:111:PHE:HE2	1.70	0.56
1:G:679:GLN:NE2	1:G:692:ASN:OD1	2.38	0.56
1:G:784:GLN:NE2	1:G:784:GLN:N	2.39	0.56
1:A:979:ILE:HG12	1:G:990:LEU:HD23	1.88	0.56
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.52	0.56
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.36	0.56
1:G:17:PRO:HG3	1:G:917:VAL:HG13	1.87	0.56
1:G:151:THR:HG21	10:G:4266:HOH:O	2.05	0.56
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.35	0.56
1:E:712:LEU:O	1:E:727:ILE:HA	2.05	0.56
1:E:991:VAL:CG2	1:E:1004:ARG:HE	2.19	0.56
2:B:341:HIS:ND1	2:B:342:ARG:N	2.53	0.56
1:G:412:LYS:HD3	1:G:437:TRP:HB2	1.87	0.56
1:G:710:TYR:HB3	1:G:729:TYR:O	2.06	0.56
1:A:715:ARG:NH2	8:A:4006:ADP:O1A	2.27	0.55
1:C:695:VAL:CG2	1:C:752:LEU:HD22	2.36	0.55
1:G:339:ILE:HD11	1:G:531:THR:HG23	1.88	0.55
1:G:766:ALA:HB2	1:G:775:ILE:HD13	1.87	0.55
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.21	0.55
1:G:695:VAL:CG1	1:G:701:ALA:HB2	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:734:LEU:HD12	1:G:734:LEU:O	2.06	0.55
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.88	0.55
1:A:992:ASN:ND2	1:G:975:HIS:NE2	2.55	0.55
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.67	0.55
1:A:692:ASN:O	1:A:693:ALA:HB2	2.06	0.55
1:A:698:ILE:O	1:A:702:VAL:HG23	2.06	0.55
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.19	0.55
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.36	0.55
1:E:43:ARG:NH2	1:E:81:GLU:OE2	2.31	0.55
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.21	0.55
2:H:46:PRO:HA	2:H:76:HIS:CG	2.41	0.55
2:H:78:GLN:HA	2:H:78:GLN:NE2	2.22	0.55
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.71	0.55
1:G:663:GLY:HA3	1:G:869:MET:CE	2.37	0.55
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.28	0.55
1:G:767:ILE:HA	1:G:824:GLY:O	2.07	0.55
2:H:168:TYR:O	2:H:218:ILE:N	2.31	0.55
2:D:237:PHE:HZ	2:D:268:ILE:HD12	1.68	0.55
1:E:941:LYS:HE2	10:E:4911:HOH:O	2.06	0.55
2:B:272:HIS:ND1	2:B:349:SER:OG	2.36	0.55
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.42	0.54
1:E:556[A]:SER:HB2	1:E:558:ASP:HB2	1.89	0.54
1:C:1007:ASN:HB3	1:C:1009[B]:GLU:OE2	2.06	0.54
1:E:336:MET:HB3	1:E:342:GLY:HA2	1.88	0.54
2:F:212:ARG:HG3	2:F:212:ARG:HH11	1.72	0.54
1:G:738:PHE:HA	1:G:741:ALA:HB3	1.89	0.54
1:C:419:GLU:HG3	10:C:4722:HOH:O	2.07	0.54
1:E:735:ARG:O	1:E:738:PHE:HB2	2.07	0.54
1:G:473:GLU:HG2	1:G:505:LEU:HD11	1.89	0.54
1:G:901:PRO:HD2	5:G:4076:CL:CL	2.44	0.54
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.87	0.54
1:C:712:LEU:HD23	1:C:753:ASP:O	2.08	0.54
1:G:267:ALA:O	1:G:271:VAL:HG23	2.07	0.54
2:H:249:ASP:OD2	2:H:250:TYR:HD2	1.91	0.54
1:C:39:GLU:HG3	10:C:4675:HOH:O	2.07	0.54
1:E:734:LEU:HD12	1:E:734:LEU:C	2.27	0.54
1:G:588:ALA:HB2	1:G:863:LYS:HB3	1.89	0.54
2:H:246:ALA:HB3	2:H:247:PRO:HD3	1.88	0.54
1:A:734:LEU:HD12	1:A:734:LEU:O	2.06	0.54
2:B:325:LEU:HD22	2:B:340:ILE:HB	1.89	0.54
1:A:1001:ILE:HD13	1:A:1029:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:ILE:HD13	1:C:869:MET:CE	2.38	0.54
1:E:344:THR:HB	1:E:345:PRO:HD2	1.90	0.54
2:F:324:ASN:HA	2:F:343:THR:OG1	2.07	0.54
1:G:427:GLU:HG3	1:G:438:TYR:CE1	2.43	0.54
1:G:165:PRO:HA	1:G:182:ALA:O	2.07	0.54
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.38	0.54
2:F:169:SER:HA	2:F:216:LEU:O	2.08	0.54
1:E:891:LYS:HG2	1:E:892:GLU:N	2.23	0.54
1:G:637:GLY:HA3	1:G:662:ILE:HG23	1.89	0.54
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.89	0.54
1:A:689:GLN:HG3	1:A:690:PRO:HD2	1.89	0.53
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.22	0.53
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.37	0.53
2:H:324:ASN:ND2	2:H:324:ASN:N	2.56	0.53
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.23	0.53
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.43	0.53
1:G:900:PHE:O	1:G:903:VAL:HB	2.08	0.53
2:B:296:PRO:HB2	2:B:332:LEU:HB2	1.90	0.53
1:E:802:SER:OG	1:E:805:ILE:HB	2.08	0.53
1:A:165:PRO:HB3	1:A:183:TYR:CD1	2.43	0.53
1:C:1:MET:HG3	1:C:2:PRO:CD	2.30	0.53
1:C:78:ILE:O	1:C:82:ARG:N	2.27	0.53
1:C:426:ARG:HD3	1:C:426:ARG:C	2.28	0.53
1:C:1052:MET:HG3	10:C:4623:HOH:O	2.08	0.53
2:H:259:LEU:HD13	2:H:342:ARG:NH1	2.24	0.53
1:A:315:THR:O	1:A:531:THR:HG22	2.08	0.53
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.74	0.53
1:C:470:VAL:O	1:C:474:GLU:HG3	2.08	0.53
1:C:998:ARG:HA	1:C:999:PRO:C	2.27	0.53
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.38	0.53
2:H:6:LEU:HD12	2:H:7:LEU:N	2.24	0.53
1:A:948:SER:O	1:A:1015:ASN:HA	2.09	0.53
1:A:1000:HIS:O	1:A:1003:ASP:HB2	2.09	0.53
1:C:561:LYS:HE2	10:C:4441:HOH:O	2.07	0.53
2:D:175:TRP:CZ2	2:D:177:LEU:HA	2.44	0.53
2:D:188:ASP:OD2	2:D:188:ASP:N	2.41	0.53
2:H:198:ASP:HB2	2:H:218:ILE:CG2	2.39	0.53
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.31	0.53
2:B:245:PRO:HG3	2:B:273:GLN:OE1	2.09	0.53
1:E:18:ILE:HD12	1:E:23:ALA:HA	1.91	0.53
1:G:640:VAL:HG21	1:G:651:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:GLN:H	1:C:784:GLN:NE2	2.07	0.53
2:D:178:THR:HB	10:D:1683:HOH:O	2.08	0.53
1:A:363:ASN:OD1	1:A:381:VAL:HG21	2.09	0.53
2:B:364:ALA:HB3	2:B:365:PRO:HD3	1.91	0.53
1:E:809:MET:HG2	1:E:830:PHE:CD2	2.44	0.53
2:F:153:LEU:HD23	10:F:2053:HOH:O	2.07	0.53
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.73	0.53
1:A:146:SER:HB3	1:A:207:ASP:OD1	2.09	0.53
1:A:1021:ARG:HH11	1:A:1021:ARG:HG3	1.74	0.53
2:D:324:ASN:O	2:D:343:THR:HG23	2.09	0.53
1:A:663:GLY:HA2	1:A:869:MET:HG2	1.90	0.52
2:B:299:ASP:OD1	2:B:302:LYS:HG3	2.10	0.52
1:C:344:THR:HB	1:C:345:PRO:CD	2.39	0.52
2:D:46:PRO:HA	2:D:76:HIS:CG	2.44	0.52
1:E:922:ARG:HH21	1:E:926:GLU:CD	2.10	0.52
2:H:227:ASP:O	2:H:230:LYS:HB2	2.09	0.52
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.43	0.52
1:C:69:ILE:O	1:C:69:ILE:HG22	2.09	0.52
2:F:225:ALA:HB3	2:F:257:LYS:HG2	1.91	0.52
1:G:592:ASP:OD1	1:G:867:ARG:NE	2.34	0.52
1:G:665:SER:OG	1:G:667:ASP:N	2.43	0.52
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.92	0.52
1:E:144:ALA:HB1	1:E:208:GLU:CG	2.39	0.52
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.91	0.52
2:H:50:ARG:HG2	2:H:158:LEU:HD11	1.91	0.52
1:C:77:ILE:O	1:C:81:GLU:N	2.30	0.52
2:F:236:ILE:CD1	2:F:263:ILE:HG21	2.39	0.52
1:A:693:ALA:HB3	1:A:708:ILE:HD11	1.92	0.52
1:E:59:GLU:HG2	1:E:60:MET:HE2	1.92	0.52
1:E:698:ILE:HG23	1:E:738:PHE:CD2	2.45	0.52
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.39	0.52
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.91	0.52
2:H:160:LYS:HE3	2:H:161:GLU:OE2	2.08	0.52
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.90	0.52
1:G:683:GLU:HA	1:G:683:GLU:OE2	2.09	0.52
1:G:693:ALA:HB2	1:G:708:ILE:CD1	2.29	0.52
2:H:272:HIS:CB	2:H:349:SER:HB2	2.40	0.52
1:G:145:ARG:HB2	1:G:208:GLU:OE1	2.09	0.52
1:G:695:VAL:HG13	1:G:700:MET:HG2	1.92	0.52
1:A:164:PHE:HA	1:A:165:PRO:C	2.30	0.52
1:A:724:ALA:O	1:A:725:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.09	0.52
1:C:298:ILE:HG13	10:C:4272:HOH:O	2.09	0.52
2:D:178:THR:HG22	2:D:179:GLY:N	2.25	0.52
1:A:579:ASP:O	1:A:583:VAL:HG23	2.10	0.52
1:A:730:ASP:OD2	1:A:733:ASP:OD2	2.28	0.52
1:C:503:ALA:HB2	1:C:510:GLU:HA	1.91	0.52
1:C:561:LYS:NZ	10:C:4456:HOH:O	2.42	0.52
1:G:361:ARG:NH2	1:G:571:ARG:HG2	2.25	0.52
1:A:194:ARG:NH2	10:A:4618:HOH:O	2.38	0.52
1:A:692:ASN:HB3	1:A:753:ASP:CG	2.31	0.52
1:C:142:GLU:OE2	1:C:294:ARG:NH2	2.42	0.52
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.92	0.52
2:F:234:ASP:OD1	2:F:378:ARG:HD2	2.09	0.52
2:H:363:ALA:C	2:H:365:PRO:HD2	2.31	0.52
2:B:46:PRO:HA	2:B:76:HIS:CG	2.45	0.51
2:F:62:ASN:OD1	2:F:86:PRO:HG3	2.10	0.51
1:G:185:ARG:O	1:G:185:ARG:HG2	2.10	0.51
1:A:82:ARG:HE	1:A:111:PHE:HB3	1.76	0.51
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.41	0.51
1:C:257:THR:HG22	2:D:63:VAL:HG21	1.92	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.93	0.51
1:E:18:ILE:HD12	1:E:23:ALA:C	2.31	0.51
1:E:755:PHE:CE1	8:E:4047:ADP:C2	2.99	0.51
2:F:272:HIS:HA	2:F:349:SER:OG	2.10	0.51
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.29	0.51
1:E:979:ILE:O	1:E:983:GLU:HG3	2.11	0.51
1:G:761:GLU:HG2	1:G:781:HIS:CE1	2.45	0.51
2:H:135:GLY:O	2:H:138:PRO:HD3	2.11	0.51
7:A:4030:ORN:NE	1:C:892:GLU:OE1	2.43	0.51
2:B:338:GLN:NE2	10:B:4164:HOH:O	2.31	0.51
2:D:168:TYR:O	2:D:218:ILE:N	2.35	0.51
1:G:726:GLU:HG3	1:G:727:ILE:H	1.71	0.51
1:A:795:SER:OG	1:A:797:PRO:O	2.29	0.51
1:A:929:ALA:HB2	1:A:1053:ALA:HB1	1.92	0.51
1:A:1037:LYS:HB2	10:A:4564:HOH:O	2.10	0.51
1:C:693:ALA:HB3	1:C:708:ILE:HD11	1.92	0.51
1:G:32:GLN:OE1	1:G:320:ALA:HB3	2.11	0.51
1:A:698:ILE:HD12	1:A:698:ILE:H	1.76	0.51
1:E:121:ASP:O	1:E:125:LYS:HB2	2.11	0.51
1:G:654:LEU:HB3	1:G:659:VAL:HB	1.91	0.51
1:A:559:ARG:HH11	1:A:559:ARG:CG	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:4051:ORN:NE	1:E:783:GLU:OE1	2.44	0.51
1:C:703:GLU:HA	1:C:703:GLU:OE2	2.11	0.51
1:C:735:ARG:O	1:C:738:PHE:HB2	2.11	0.51
1:E:646:THR:HB	1:E:647:PRO:CD	2.38	0.51
1:C:40:GLU:OE1	1:C:325:LYS:HE2	2.11	0.51
1:E:309:ALA:O	1:E:313:LYS:HG2	2.11	0.51
1:E:698:ILE:H	1:E:698:ILE:CD1	2.22	0.51
1:G:735:ARG:O	1:G:738:PHE:HB2	2.11	0.51
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.91	0.51
2:H:350:PHE:HD2	2:H:354:PRO:HD3	1.76	0.51
1:A:569:PRO:O	1:A:571:ARG:HD2	2.10	0.50
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.76	0.50
1:E:678:PHE:O	1:E:681:ALA:N	2.43	0.50
1:G:167:ILE:HD12	1:G:167:ILE:N	2.26	0.50
1:G:563:MET:HE3	1:G:630:VAL:HG22	1.93	0.50
1:G:1003:ASP:O	1:G:1007:ASN:OD1	2.28	0.50
2:H:277:LEU:HD21	2:H:283:THR:HG23	1.92	0.50
1:A:79:GLU:HA	1:A:111:PHE:CE2	2.46	0.50
1:A:375:THR:HG23	1:A:377:GLN:H	1.75	0.50
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.92	0.50
2:H:47:SER:HB2	2:H:311:ASN:ND2	2.27	0.50
1:A:998:ARG:HA	1:A:999:PRO:C	2.28	0.50
2:B:322:PRO:HG2	2:B:324:ASN:HD21	1.76	0.50
1:C:695:VAL:HG23	1:C:752:LEU:HD22	1.92	0.50
1:C:921:GLY:HA3	1:C:926:GLU:HB3	1.91	0.50
1:E:440:ALA:O	1:E:444:ARG:HG3	2.12	0.50
1:G:625:ASP:O	1:G:629:ILE:HG13	2.11	0.50
1:A:757:ASP:OD2	1:A:833:LYS:NZ	2.45	0.50
2:B:370:PHE:O	2:B:374:ILE:HG13	2.11	0.50
1:C:126:ALA:HB3	1:C:302:PRO:HG3	1.92	0.50
1:C:910:GLU:HB2	10:C:4668:HOH:O	2.11	0.50
1:G:829:GLN:O	1:G:840:ILE:HB	2.10	0.50
2:H:25:SER:HA	2:H:132:ILE:O	2.12	0.50
2:B:364:ALA:N	2:B:365:PRO:CD	2.74	0.50
1:C:644:GLY:O	1:C:647:PRO:HD2	2.12	0.50
1:C:680:HIS:HA	1:C:683:GLU:OE2	2.11	0.50
1:C:998:ARG:HE	1:C:1000:HIS:CE1	2.29	0.50
2:H:322:PRO:CB	2:H:324:ASN:HD21	2.24	0.50
1:A:688:LYS:HD3	1:A:838:TYR:CE1	2.47	0.50
1:C:908:GLY:HA3	10:C:4505:HOH:O	2.11	0.50
2:D:152:GLY:O	2:D:156:MET:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:275:LEU:HD23	2:H:349:SER:CB	2.42	0.50
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.35	0.50
1:C:767:ILE:HD13	1:C:865:ALA:HB2	1.94	0.50
1:C:872:LYS:HG3	1:C:876:GLU:HB3	1.93	0.50
1:C:1036:TYR:C	1:C:1037:LYS:HG2	2.30	0.50
2:F:174:SER:O	2:F:182:PRO:HD3	2.12	0.50
1:G:29:SER:HB3	1:G:304:VAL:HG21	1.92	0.50
1:G:353:ASP:OD1	2:H:116:ARG:HD2	2.12	0.50
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.46	0.50
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.46	0.50
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.38	0.49
2:B:222:GLN:HE21	2:B:222:GLN:N	2.10	0.49
1:C:79:GLU:HB2	1:C:111:PHE:CZ	2.47	0.49
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.47	0.49
1:E:703:GLU:O	1:E:706:LYS:HB2	2.12	0.49
1:G:668:ALA:O	1:G:671:ARG:HB2	2.11	0.49
2:H:298:LYS:O	2:H:329:HIS:HA	2.11	0.49
1:A:115:MET:HG2	1:A:118:ALA:O	2.12	0.49
1:A:692:ASN:HB3	1:A:753:ASP:OD1	2.12	0.49
2:F:257:LYS:O	2:F:260:GLU:HB2	2.12	0.49
2:F:328:THR:HG21	2:F:341:HIS:HB2	1.94	0.49
1:G:11:LEU:O	1:G:86:VAL:HG23	2.12	0.49
1:G:509:ARG:NH1	1:G:512:GLU:HG3	2.27	0.49
2:B:206:LEU:N	2:B:206:LEU:HD23	2.27	0.49
2:B:246:ALA:N	2:B:247:PRO:HD2	2.26	0.49
1:G:315:THR:O	1:G:531:THR:HG22	2.13	0.49
2:H:202:LYS:HZ3	2:H:355:GLU:CG	2.26	0.49
1:A:446:GLY:O	1:E:447:LEU:HD23	2.12	0.49
1:C:1014:ILE:HD12	1:C:1014:ILE:C	2.33	0.49
2:H:208:MET:SD	2:H:355:GLU:HA	2.53	0.49
1:A:1067:GLU:O	1:A:1071:GLN:HG3	2.12	0.49
2:D:98:LEU:HD12	2:D:98:LEU:O	2.13	0.49
2:D:212:ARG:HH11	2:D:212:ARG:CG	2.24	0.49
2:D:316:VAL:HB	2:D:337:LEU:HD23	1.94	0.49
1:E:710:TYR:HB3	1:E:729:TYR:O	2.13	0.49
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.73	0.49
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.47	0.49
1:G:951:GLU:OE1	1:G:954:LYS:HD2	2.13	0.49
1:A:698:ILE:HD12	1:A:698:ILE:N	2.27	0.49
1:A:930:LYS:HE3	10:A:4205:HOH:O	2.12	0.49
2:B:26:ALA:O	2:B:131:CYS:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1064:SER:O	1:G:1068:MET:HG3	2.12	0.49
2:H:50:ARG:HG2	2:H:158:LEU:HD13	1.94	0.49
1:A:1:MET:HB3	1:A:224:LYS:NZ	2.27	0.49
1:A:101:GLU:OE2	1:A:101:GLU:HA	2.12	0.49
1:A:728:VAL:HG11	1:A:734:LEU:HA	1.95	0.49
2:B:185:LYS:CD	2:B:190:LEU:HD21	2.39	0.49
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.47	0.49
1:E:252:PRO:HD3	1:E:352:ILE:HD11	1.94	0.49
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.13	0.49
2:F:364:ALA:N	2:F:365:PRO:HD2	2.27	0.49
1:G:103:GLU:HG3	1:G:104:ARG:N	2.28	0.49
1:G:148:ILE:O	10:G:4640:HOH:O	2.19	0.49
1:G:494:ARG:HG3	1:G:547:TYR:CB	2.43	0.49
1:A:163:GLY:O	1:A:166:CYS:HB3	2.11	0.49
2:B:27:VAL:O	2:B:78:GLN:HG2	2.12	0.49
1:C:956:ARG:HD3	1:C:1044:LEU:HD23	1.95	0.49
1:E:144:ALA:HB1	1:E:208:GLU:HG3	1.94	0.49
1:G:590:ARG:HB2	1:G:596:THR:CG2	2.42	0.49
1:G:864:VAL:O	1:G:868:VAL:HG23	2.13	0.49
1:G:1032:SER:O	1:G:1036:TYR:HD1	1.95	0.49
1:C:713:VAL:HG23	1:C:755:PHE:HB2	1.94	0.49
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.29	0.49
2:D:168:TYR:CZ	2:D:218:ILE:HG21	2.48	0.49
1:E:702:VAL:HG11	1:E:735:ARG:HH22	1.75	0.49
1:E:772[A]:MET:HG3	1:E:874:LEU:HD12	1.95	0.49
1:G:79:GLU:HG2	1:G:111:PHE:CE2	2.47	0.49
2:H:192:PHE:O	2:H:215:ARG:HB3	2.12	0.49
2:H:202:LYS:NZ	2:H:355:GLU:CG	2.76	0.49
1:A:734:LEU:HD11	1:A:738:PHE:HE2	1.76	0.49
1:A:997:GLY:O	1:A:998:ARG:HG3	2.13	0.49
1:C:321:LYS:NZ	1:C:338:ASP:OD1	2.43	0.49
1:E:164:PHE:HD2	1:E:166:CYS:HG	1.57	0.49
1:E:514:ARG:HD3	10:E:4452:HOH:O	2.13	0.49
1:A:167:ILE:HD12	1:A:167:ILE:N	2.28	0.48
1:C:237:PHE:HB3	1:C:248:ILE:O	2.12	0.48
1:C:693:ALA:HB1	1:C:704:LYS:HG3	1.95	0.48
2:D:185:LYS:HB2	2:D:190:LEU:HD11	1.95	0.48
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.78	0.48
1:G:35:LYS:HD2	10:G:4199:HOH:O	2.11	0.48
1:G:70:HIS:ND1	1:G:72:GLU:HB2	2.27	0.48
1:G:890:VAL:HG23	1:G:927:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:ALA:HB2	2:H:106:ASN:HA	1.95	0.48
2:H:324:ASN:O	2:H:342:ARG:HD2	2.13	0.48
1:C:675:ARG:H	1:C:675:ARG:HD3	1.74	0.48
2:F:272:HIS:HA	2:F:349:SER:CB	2.43	0.48
1:G:1:MET:HB2	1:G:224:LYS:CE	2.44	0.48
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.42	0.48
1:A:417:ASP:OD1	1:A:423:LYS:NZ	2.29	0.48
1:A:636:LYS:NZ	10:A:4502:HOH:O	2.30	0.48
1:A:663:GLY:HA3	1:A:869:MET:HG2	1.95	0.48
2:F:133:ILE:CG2	2:F:138:PRO:HB3	2.43	0.48
2:F:341:HIS:CD2	2:F:348:PHE:HB3	2.49	0.48
1:A:704:LYS:O	1:A:707:GLU:HB2	2.13	0.48
1:A:947:LEU:CD1	1:A:947:LEU:N	2.77	0.48
2:F:205:ILE:HG21	2:F:237:PHE:CZ	2.49	0.48
1:G:804:GLU:HB2	10:G:4603:HOH:O	2.14	0.48
1:A:467:GLU:O	1:A:471:ARG:HG2	2.14	0.48
1:A:646:THR:HB	1:A:647:PRO:HD3	1.95	0.48
1:C:668:ALA:O	1:C:671:ARG:HB2	2.14	0.48
1:G:224:LYS:HE2	1:G:329:GLY:O	2.14	0.48
2:H:113:ILE:O	2:H:115:THR:N	2.47	0.48
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.46	0.48
1:A:912:ARG:NH1	10:A:4528:HOH:O	2.47	0.48
1:A:947:LEU:N	1:A:947:LEU:HD12	2.29	0.48
2:B:237:PHE:HE1	2:B:268:ILE:HG13	1.78	0.48
1:C:107:VAL:HG12	1:C:107:VAL:O	2.14	0.48
2:D:20:ILE:HG13	2:D:109:ALA:HB3	1.96	0.48
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.39	0.48
1:G:1:MET:HB2	1:G:224:LYS:HE3	1.95	0.48
1:G:36:ALA:HB1	1:G:325:LYS:HE3	1.96	0.48
1:G:57:ASP:HB2	1:G:60:MET:HG2	1.96	0.48
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.11	0.48
1:C:872:LYS:HG2	1:C:877:GLN:HG2	1.94	0.48
1:E:4:ARG:NH2	1:E:6:ASP:OD1	2.37	0.48
1:E:166:CYS:C	1:E:167:ILE:HD12	2.34	0.48
1:G:412:LYS:HG2	1:G:438:TYR:CE1	2.48	0.48
1:G:417:ASP:OD2	1:G:418:PRO:HD2	2.14	0.48
1:G:695:VAL:HG13	1:G:700:MET:CG	2.42	0.48
1:E:159:ALA:HB2	1:E:188:PHE:CZ	2.49	0.48
1:G:622:THR:OG1	1:G:625:ASP:OD1	2.29	0.48
1:G:637:GLY:HA3	1:G:662:ILE:CG2	2.43	0.48
1:G:695:VAL:HG12	1:G:697:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:ILE:O	2:H:99:SER:OG	2.28	0.48
2:H:296:PRO:HB2	2:H:332:LEU:HB2	1.95	0.48
1:A:361:ARG:HG2	1:A:571:ARG:HG3	1.94	0.48
1:C:28:TYR:CZ	1:C:313:LYS:HE3	2.48	0.48
1:G:994:VAL:HG22	1:G:1000:HIS:CD2	2.49	0.48
2:H:201:ALA:HB2	2:H:239:SER:CB	2.43	0.48
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.41	0.48
2:B:232:ASN:N	2:B:233:PRO:CD	2.77	0.48
1:C:784:GLN:HE22	1:C:1043:THR:HB	1.78	0.48
1:E:467:GLU:O	1:E:471:ARG:HG2	2.14	0.48
1:G:69:ILE:HG22	1:G:69:ILE:O	2.13	0.48
1:G:470:VAL:O	1:G:474:GLU:HG3	2.13	0.48
1:G:681:ALA:O	1:G:685:LEU:HG	2.14	0.48
1:A:715:ARG:HG2	1:A:725:MET:SD	2.53	0.47
1:A:784:GLN:HE21	1:A:784:GLN:N	1.97	0.47
2:B:218:ILE:HD13	2:B:218:ILE:N	2.29	0.47
1:C:773:VAL:HG23	1:C:818:PHE:CZ	2.49	0.47
1:C:892:GLU:HG3	1:C:893:VAL:N	2.27	0.47
2:D:246:ALA:N	2:D:247:PRO:HD2	2.28	0.47
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.49	0.47
1:E:845:ARG:NH1	1:E:846:ALA:O	2.47	0.47
1:A:700:MET:O	1:A:704:LYS:HB2	2.14	0.47
1:E:490:ARG:HD3	10:E:4665:HOH:O	2.13	0.47
1:E:682:VAL:CG1	1:E:687:LEU:HB2	2.44	0.47
2:F:7:LEU:HB3	2:F:15:PHE:HB2	1.96	0.47
2:F:208:MET:O	2:F:212:ARG:HG3	2.13	0.47
2:F:228:VAL:O	2:F:231:MET:HB2	2.14	0.47
1:G:772:MET:HG3	1:G:773:VAL:N	2.30	0.47
1:A:778:ILE:HD11	1:A:810:ARG:HG3	1.96	0.47
2:D:299:ASP:OD1	2:D:302:LYS:HD2	2.13	0.47
1:G:257:THR:OG1	1:G:260:GLU:HG3	2.15	0.47
1:G:853:VAL:HG12	1:G:861:LEU:HD11	1.96	0.47
2:H:175:TRP:CZ2	2:H:177:LEU:HA	2.49	0.47
1:A:577:GLU:OE2	1:A:577:GLU:N	2.37	0.47
1:A:681:ALA:O	1:A:685:LEU:HG	2.13	0.47
1:C:12:ILE:HD11	1:C:37:LEU:HD12	1.95	0.47
1:C:64:THR:O	1:C:1065:VAL:HG23	2.14	0.47
1:C:957:VAL:O	1:C:957:VAL:HG22	2.13	0.47
2:F:286:MET:CE	2:F:312:HIS:ND1	2.77	0.47
1:A:344:THR:HB	1:A:345:PRO:HD2	1.96	0.47
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027[A]:ARG:HD3	10:A:4891:HOH:O	2.14	0.47
2:B:168:TYR:CE2	2:B:218:ILE:HG12	2.49	0.47
2:B:322:PRO:CG	2:B:324:ASN:HD21	2.27	0.47
1:C:670:ASP:HB3	1:C:677:ARG:HH21	1.79	0.47
2:D:2:ILE:HG13	2:D:3:LYS:N	2.30	0.47
2:D:39:TYR:CZ	2:D:61:GLY:HA2	2.49	0.47
1:E:571:ARG:HD3	1:E:571:ARG:N	2.28	0.47
2:F:244:ASP:OD2	2:F:245:PRO:HD2	2.15	0.47
1:G:559:ARG:HH11	1:G:559:ARG:CG	2.12	0.47
1:G:1031:ARG:HE	1:G:1031:ARG:HB3	1.42	0.47
2:H:63:VAL:HG12	2:H:91:ASN:HB2	1.96	0.47
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.49	0.47
2:H:364:ALA:N	2:H:365:PRO:CD	2.78	0.47
1:A:166:CYS:C	1:A:167:ILE:HD12	2.35	0.47
1:A:675:ARG:HG3	1:A:751:LEU:HD21	1.96	0.47
1:C:358:LYS:HE3	10:C:4142:HOH:O	2.13	0.47
1:C:679:GLN:HG2	1:C:683:GLU:OE1	2.15	0.47
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.97	0.47
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.97	0.47
2:F:111:ALA:O	2:F:112:ASP:HB2	2.14	0.47
1:G:145:ARG:HB2	1:G:208:GLU:CD	2.35	0.47
1:G:148:ILE:HD13	1:G:204:LEU:O	2.15	0.47
1:G:330:TYR:HA	1:G:334:GLU:OE1	2.15	0.47
1:G:494:ARG:HG3	1:G:547:TYR:HB2	1.96	0.47
1:G:516:LEU:HD11	1:G:520:TYR:CE2	2.49	0.47
1:G:702:VAL:HG21	1:G:735:ARG:CZ	2.44	0.47
1:G:1004:ARG:O	1:G:1009:GLU:HG3	2.15	0.47
2:H:282:LYS:HB2	2:H:320:THR:HG21	1.97	0.47
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.97	0.47
1:E:59:GLU:HG2	1:E:60:MET:CE	2.44	0.47
1:E:735:ARG:O	1:E:738:PHE:N	2.47	0.47
1:E:1019:GLY:O	1:E:1023:ILE:HG13	2.15	0.47
2:F:272:HIS:HB2	2:F:349:SER:HB2	1.97	0.47
1:G:151:THR:OG1	1:G:154:GLU:HG3	2.15	0.47
1:G:524:PRO:HD2	1:G:628:GLU:OE2	2.15	0.47
1:G:548:GLU:OE1	2:H:114:ASP:HA	2.15	0.47
1:G:699:GLU:OE2	1:G:699:GLU:HA	2.15	0.47
1:G:716:PRO:HA	1:G:750:VAL:HG22	1.95	0.47
2:H:98:LEU:O	2:H:102:LEU:HG	2.15	0.47
1:A:1061:LYS:HG2	1:A:1062:VAL:N	2.28	0.47
2:B:217:THR:HG21	2:B:231:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:SER:O	2:B:272:HIS:HB3	2.15	0.47
1:E:1028:VAL:O	1:E:1032:SER:HB2	2.14	0.47
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.96	0.47
1:A:76:LYS:O	1:A:80:LYS:HB3	2.14	0.47
1:A:796:LEU:HD23	1:A:796:LEU:C	2.35	0.47
2:B:317:ASP:O	2:B:321:LEU:HD13	2.14	0.47
1:C:891:LYS:HG2	1:C:892:GLU:N	2.29	0.47
1:E:503:ALA:HB1	1:E:508:VAL:O	2.14	0.47
1:G:400:ARG:HD3	10:G:4399:HOH:O	2.14	0.47
1:G:527:LYS:HB2	1:G:544:TYR:CZ	2.50	0.47
1:G:695:VAL:HG11	1:G:701:ALA:N	2.30	0.47
2:H:158:LEU:CB	2:H:242:PRO:HB2	2.45	0.47
2:H:207:ARG:NH2	10:H:3959:HOH:O	2.48	0.47
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.96	0.46
1:A:698:ILE:H	1:A:698:ILE:CD1	2.29	0.46
1:A:992:ASN:HB2	1:A:999:PRO:O	2.16	0.46
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.47	0.46
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.49	0.46
2:D:208:MET:SD	2:D:355:GLU:HA	2.55	0.46
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.32	0.46
2:F:353:HIS:N	2:F:353:HIS:CD2	2.83	0.46
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.48	0.46
1:G:681:ALA:HA	1:G:684:ARG:HB3	1.96	0.46
1:G:704:LYS:O	1:G:707:GLU:HB2	2.14	0.46
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.96	0.46
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.15	0.46
1:A:333:ASP:OD1	1:A:333:ASP:N	2.48	0.46
2:D:285:LYS:HB2	2:D:314:PHE:CE1	2.50	0.46
1:E:27:ASP:OD2	1:E:53:THR:HB	2.14	0.46
1:E:154:GLU:O	1:E:157:ALA:HB3	2.16	0.46
1:G:135:ALA:O	1:G:138:LYS:HB3	2.16	0.46
1:G:344:THR:HB	1:G:345:PRO:HD2	1.97	0.46
1:G:730:ASP:H	1:G:733:ASP:HB2	1.80	0.46
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.29	0.46
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.75	0.46
1:A:713:VAL:HG12	1:A:713:VAL:O	2.15	0.46
1:A:714:VAL:HG23	1:A:728:VAL:HG23	1.97	0.46
2:B:186:LYS:O	2:B:189:GLU:HB2	2.15	0.46
1:C:701:ALA:O	1:C:705:ALA:N	2.39	0.46
1:E:698:ILE:N	1:E:698:ILE:CD1	2.79	0.46
2:F:164:THR:O	2:F:220:PRO:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.53	0.46
1:G:9:SER:HA	1:G:43:ARG:O	2.15	0.46
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.79	0.46
2:H:325:LEU:HA	2:H:325:LEU:HD23	1.56	0.46
2:B:237:PHE:CE2	2:B:239:SER:HA	2.49	0.46
1:C:563:MET:CE	1:C:635:PRO:HG3	2.46	0.46
2:H:266:PHE:CD2	2:H:370:PHE:CD2	3.04	0.46
1:A:165:PRO:HA	1:A:182:ALA:O	2.16	0.46
2:B:378:ARG:C	2:B:380:THR:H	2.17	0.46
1:C:873:SER:O	1:C:877:GLN:HG3	2.15	0.46
2:D:34:THR:HA	2:D:56:THR:OG1	2.15	0.46
2:D:71:GLU:C	2:D:203:ARG:HG3	2.35	0.46
2:F:87:LEU:HA	2:F:87:LEU:HD12	1.58	0.46
1:G:358:LYS:HG2	1:G:359:ILE:N	2.27	0.46
2:H:206:LEU:O	2:H:210:VAL:HG23	2.15	0.46
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.46	0.46
1:C:325:LYS:O	1:C:330:TYR:HB2	2.15	0.46
2:F:65:THR:OG1	2:F:96:GLU:O	2.27	0.46
2:F:229:LEU:C	2:F:231:MET:H	2.18	0.46
2:F:290:HIS:HB2	2:F:312:HIS:CD2	2.50	0.46
1:G:1:MET:CB	1:G:224:LYS:NZ	2.79	0.46
1:G:948:SER:O	1:G:1015:ASN:HA	2.16	0.46
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.43	0.46
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.96	0.46
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.16	0.46
1:E:708:ILE:HG22	1:E:754:HIS:HB2	1.97	0.46
1:E:728:VAL:HG13	1:E:733:ASP:CB	2.33	0.46
1:G:29:SER:CB	1:G:304:VAL:HG21	2.46	0.46
1:G:577:GLU:O	1:G:580:TYR:HB3	2.16	0.46
1:A:266:ASN:ND2	10:A:4760:HOH:O	2.46	0.46
1:A:780:GLU:OE2	1:A:798:ALA:HB1	2.15	0.46
2:B:128:GLN:HG3	10:B:4129:HOH:O	2.14	0.46
1:C:775:ILE:HG13	1:C:810:ARG:HG2	1.97	0.46
2:D:272:HIS:HA	2:D:349:SER:CB	2.45	0.46
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.98	0.46
2:F:379:LYS:HB2	2:F:379:LYS:NZ	2.30	0.46
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.51	0.46
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.51	0.46
2:D:12:GLY:HA2	2:D:144:LEU:HD13	1.98	0.46
2:D:156:MET:SD	2:D:158:LEU:HD21	2.55	0.46
1:E:415:LEU:HA	10:E:4432:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:805:ILE:HD13	1:E:805:ILE:HA	1.78	0.46
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.51	0.46
1:G:153:GLU:HG2	1:G:153:GLU:O	2.14	0.46
1:G:561:LYS:HG2	1:G:595:GLU:OE2	2.16	0.46
1:G:563:MET:HB2	1:G:638:VAL:HG22	1.98	0.46
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.51	0.46
1:A:612:THR:HG22	1:A:612:THR:O	2.16	0.46
1:A:772:MET:SD	1:A:880:THR:HG22	2.56	0.46
1:C:942:HIS:CD2	1:C:942:HIS:C	2.89	0.46
2:D:306:MET:HB3	2:D:362:ASP:HB3	1.97	0.46
1:G:24:CYS:HB2	1:G:604:GLU:HB2	1.98	0.46
1:G:656:ALA:C	1:G:658:GLY:H	2.20	0.46
1:G:947:LEU:N	1:G:947:LEU:CD1	2.78	0.46
2:H:225:ALA:HA	2:H:258:PHE:CE1	2.51	0.46
1:A:702:VAL:O	1:A:706:LYS:HD3	2.16	0.45
1:C:648:LEU:HD21	1:C:669:ILE:CG2	2.46	0.45
2:F:228:VAL:HG22	2:F:231:MET:HE1	1.98	0.45
1:G:809:MET:HG2	1:G:837:VAL:HG11	1.98	0.45
2:H:352:GLY:O	2:H:354:PRO:HD3	2.16	0.45
1:A:223:ASP:OD1	1:A:227:ASN:HB2	2.16	0.45
1:A:343:ARG:HD3	1:A:343:ARG:N	2.32	0.45
1:C:994:VAL:HG22	1:C:1000:HIS:CG	2.50	0.45
2:D:269:SER:O	2:D:272:HIS:HB3	2.16	0.45
1:E:426:ARG:C	1:E:426:ARG:HD3	2.36	0.45
1:E:994:VAL:CG2	1:E:1001:ILE:HD11	2.46	0.45
1:G:75:ARG:HD3	10:G:4220:HOH:O	2.16	0.45
2:H:91:ASN:O	2:H:94:ASN:HB3	2.16	0.45
2:H:168:TYR:O	2:H:217:THR:HA	2.16	0.45
1:A:695:VAL:HG13	1:A:697:ALA:O	2.17	0.45
1:A:703:GLU:O	1:A:706:LYS:HB2	2.17	0.45
1:C:890:VAL:HG23	1:C:927:ALA:HB3	1.97	0.45
2:D:324:ASN:O	2:D:342:ARG:HD2	2.17	0.45
1:G:148:ILE:CG2	1:G:149:ALA:N	2.80	0.45
1:G:423[B]:LYS:NZ	10:G:4420:HOH:O	2.48	0.45
1:G:577:GLU:HG2	1:G:848:ARG:O	2.17	0.45
2:B:6:LEU:HD11	2:B:8:VAL:CG2	2.44	0.45
1:C:332:LEU:HB3	1:C:347:SER:HB3	1.99	0.45
1:C:375:THR:HG23	1:C:377:GLN:H	1.81	0.45
1:C:469:LEU:O	1:C:473:GLU:HG3	2.17	0.45
1:E:258:ASP:O	1:E:262:GLN:HG2	2.16	0.45
1:E:773:VAL:HG21	1:E:814:GLN:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:901:PRO:C	1:G:903:VAL:H	2.19	0.45
2:H:27:VAL:HG22	2:H:131:CYS:CB	2.33	0.45
1:A:1020:ARG:HH21	1:A:1023:ILE:HG21	1.80	0.45
2:D:185:LYS:HD3	2:D:190:LEU:HD21	1.98	0.45
2:D:212:ARG:HG3	2:D:212:ARG:NH1	2.29	0.45
1:E:995:HIS:CD2	1:E:995:HIS:H	2.35	0.45
2:F:6:LEU:HD12	2:F:7:LEU:N	2.32	0.45
1:G:45:ILE:HG23	1:G:63:ALA:HB3	1.99	0.45
1:G:632:ILE:HG13	1:G:633:GLU:N	2.31	0.45
1:G:775:ILE:HD13	1:G:775:ILE:HA	1.79	0.45
2:H:264:PRO:HG2	2:H:374:ILE:HA	1.97	0.45
2:B:153:LEU:N	2:B:153:LEU:HD12	2.31	0.45
1:C:9:SER:OG	1:C:83:PRO:HA	2.16	0.45
1:E:696:THR:N	1:E:700:MET:CE	2.79	0.45
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.16	0.45
2:H:190:LEU:HD13	2:H:214:CYS:O	2.16	0.45
1:C:490:ARG:HG3	1:C:522:LEU:HD11	1.99	0.45
1:C:648:LEU:HD13	1:C:845:ARG:HD3	1.99	0.45
1:C:1027:ARG:NH2	10:C:4504:HOH:O	2.48	0.45
2:D:197:TYR:HB3	2:D:199:PHE:CZ	2.51	0.45
2:D:324:ASN:ND2	2:D:324:ASN:N	2.56	0.45
2:D:332:LEU:HD12	2:D:332:LEU:HA	1.66	0.45
1:E:130:ARG:O	1:E:134:VAL:HG23	2.17	0.45
1:G:176:GLY:N	8:G:4062:ADP:O2B	2.46	0.45
1:A:481:ILE:HG22	10:A:4638:HOH:O	2.16	0.45
1:A:993:LYS:HB2	1:A:996:GLU:HG3	1.99	0.45
2:B:153:LEU:N	2:B:153:LEU:CD1	2.79	0.45
2:B:236:ILE:HG13	2:B:263:ILE:HG21	1.98	0.45
1:E:239:ALA:HB2	10:E:4316:HOH:O	2.15	0.45
1:E:1003:ASP:O	1:E:1007:ASN:OD1	2.34	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.79	0.45
2:B:34:THR:HA	2:B:56:THR:OG1	2.17	0.45
1:C:250:VAL:HA	1:C:356:VAL:O	2.17	0.45
1:E:317:PHE:CE1	1:E:322:VAL:HG21	2.52	0.45
2:F:376:GLN:HA	2:F:379:LYS:NZ	2.31	0.45
1:G:214:LYS:NZ	1:G:255:THR:OG1	2.37	0.45
1:C:854:SER:HA	1:C:859:VAL:O	2.17	0.45
1:E:103:GLU:HG3	1:E:104:ARG:N	2.31	0.45
1:E:436:ILE:HG22	1:E:437:TRP:CE3	2.52	0.45
1:E:885:PRO:HA	1:E:886:PRO:HD3	1.78	0.45
1:G:11:LEU:HA	1:G:45:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:752:LEU:HD12	1:G:752:LEU:HA	1.47	0.45
2:H:266:PHE:HD2	2:H:370:PHE:CD2	2.33	0.45
1:A:583:VAL:O	1:A:587:LEU:HG	2.16	0.44
1:C:959:ASP:O	1:C:962:ALA:HB3	2.17	0.44
1:G:773:VAL:HG21	1:G:817:ALA:HB3	1.99	0.44
2:D:286:MET:HG3	2:D:313:GLY:O	2.18	0.44
1:G:770:GLY:HA3	1:G:823:ARG:CZ	2.47	0.44
1:G:965:LEU:HG	1:G:971:LEU:HD11	1.99	0.44
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.48	0.44
1:A:730:ASP:H	1:A:733:ASP:HB2	1.82	0.44
1:C:765:ASP:OD2	1:C:827:ASN:HB2	2.18	0.44
2:D:169:SER:HA	2:D:216:LEU:O	2.16	0.44
2:F:236:ILE:HD12	2:F:263:ILE:CG2	2.48	0.44
2:F:279:SER:O	2:F:322:PRO:HG3	2.17	0.44
2:F:300:VAL:HG22	2:F:328:THR:C	2.38	0.44
1:G:803:GLN:HG3	1:G:807:ASP:OD1	2.17	0.44
1:G:830:PHE:CD1	1:G:837:VAL:CG1	3.01	0.44
1:A:4:ARG:NE	1:A:7:ILE:HD12	2.32	0.44
1:A:1017:THR:HG22	1:A:1018:SER:N	2.32	0.44
2:B:6:LEU:HD23	2:B:138:PRO:HB2	1.98	0.44
1:C:44:VAL:HG22	1:C:61:ALA:HB1	2.00	0.44
2:D:249:ASP:O	2:D:253:THR:HB	2.17	0.44
1:G:407:THR:OG1	1:G:410:ASP:OD1	2.35	0.44
1:G:965:LEU:HA	1:G:965:LEU:HD23	1.80	0.44
2:H:6:LEU:HD11	2:H:8:VAL:HG22	1.95	0.44
2:H:48:TYR:O	2:H:51:GLN:HB2	2.16	0.44
2:H:218:ILE:N	2:H:218:ILE:CD1	2.80	0.44
1:A:482:THR:HB	10:A:4453:HOH:O	2.17	0.44
1:A:734:LEU:CD1	1:A:738:PHE:CE2	2.99	0.44
1:A:946:LEU:C	1:A:947:LEU:HD12	2.38	0.44
2:B:181:LEU:HD23	2:B:181:LEU:HA	1.74	0.44
2:D:279:SER:O	2:D:322:PRO:HG3	2.17	0.44
1:E:375:THR:OG1	1:E:376:THR:N	2.48	0.44
2:F:291:HIS:HD2	2:F:311:ASN:OD1	2.01	0.44
1:G:672:ALA:HB3	1:G:844:PRO:HG3	1.99	0.44
1:G:713:VAL:O	1:G:713:VAL:HG12	2.17	0.44
1:G:981:LEU:CD1	1:G:988:PRO:HG3	2.39	0.44
1:A:185:ARG:O	1:A:188:PHE:HB3	2.17	0.44
1:A:654:LEU:O	1:A:659:VAL:HG23	2.17	0.44
2:B:317:ASP:OD2	2:B:318:GLU:N	2.51	0.44
1:C:994:VAL:HA	1:C:1000:HIS:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1063:ILE:CD1	1:C:1068:MET:HG3	2.46	0.44
2:F:92:PHE:CE1	2:F:93:ARG:HG2	2.53	0.44
1:G:998:ARG:HA	1:G:999:PRO:C	2.31	0.44
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.43	0.44
1:A:130:ARG:HB2	1:A:148:ILE:HG13	1.99	0.44
1:A:1054:LEU:HD23	1:A:1054:LEU:HA	1.83	0.44
2:B:10:GLU:HG3	2:B:129:ASN:HB2	2.00	0.44
1:C:805:ILE:HG22	1:C:806:GLN:N	2.32	0.44
1:E:422:THR:HA	10:E:4063:HOH:O	2.18	0.44
1:E:436:ILE:CG2	1:E:437:TRP:CE3	3.00	0.44
1:E:942:HIS:CD2	1:E:942:HIS:C	2.90	0.44
2:F:32:PHE:CG	2:F:119:THR:HG23	2.52	0.44
2:F:187:GLU:HG2	2:F:215:ARG:HD3	2.00	0.44
1:G:70:HIS:CE1	1:G:72:GLU:HB2	2.53	0.44
1:G:648:LEU:HD13	1:G:845:ARG:HD3	2.00	0.44
1:A:362:PHE:CE1	1:A:380:SER:HB3	2.53	0.44
1:A:947:LEU:HG	1:A:1014:ILE:HG21	1.99	0.44
1:C:74:VAL:CG1	1:C:102:LEU:HD11	2.48	0.44
1:G:534:ALA:HB1	2:H:120:ARG:HG2	1.98	0.44
1:G:830:PHE:CE1	1:G:839:LEU:HD13	2.53	0.44
1:G:906:LEU:HD13	1:G:1030:ARG:CD	2.48	0.44
2:H:348:PHE:CD1	2:H:369:HIS:HD2	2.36	0.44
2:B:8:VAL:CG2	2:B:143:ALA:CB	2.96	0.44
2:B:350:PHE:HB2	2:B:366:LEU:HD23	1.98	0.44
1:E:375:THR:HA	10:E:4307:HOH:O	2.18	0.44
1:E:806:GLN:HA	1:E:809:MET:HE2	1.99	0.44
1:E:819:GLU:HB2	10:E:4897:HOH:O	2.16	0.44
2:F:275:LEU:HD23	2:F:349:SER:OG	2.18	0.44
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.20	0.44
1:G:956:ARG:HB3	1:G:1044:LEU:HD23	2.00	0.44
2:H:33:ASN:HA	2:H:291:HIS:O	2.18	0.44
2:H:234:ASP:OD1	2:H:378:ARG:NH1	2.49	0.44
1:A:695:VAL:CG2	1:A:701:ALA:HA	2.39	0.43
2:B:350:PHE:CB	2:B:366:LEU:CD2	2.96	0.43
1:C:883:VAL:C	1:C:884:ILE:HD13	2.37	0.43
1:E:921:GLY:HA3	1:E:926:GLU:HB3	1.99	0.43
2:H:209:LEU:HA	2:H:209:LEU:HD23	1.84	0.43
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.48	0.43
1:C:237:PHE:CE2	1:C:458:ILE:HD13	2.53	0.43
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.18	0.43
2:D:175:TRP:CH2	2:D:177:LEU:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ILE:HD13	1:E:339:ILE:HG21	1.68	0.43
1:G:71:TRP:CZ3	1:G:105:GLN:HG3	2.52	0.43
1:G:493:LYS:HA	1:G:493:LYS:HD2	1.76	0.43
1:G:627:LEU:HD23	1:G:627:LEU:HA	1.81	0.43
1:G:796:LEU:C	1:G:796:LEU:HD23	2.39	0.43
2:H:341:HIS:CD2	2:H:348:PHE:HB3	2.53	0.43
2:H:373:LEU:HD23	2:H:373:LEU:HA	1.86	0.43
1:A:354:TYR:CD2	1:A:387:ILE:HG23	2.53	0.43
1:C:26:PHE:HB2	10:C:4133:HOH:O	2.18	0.43
1:C:332:LEU:CB	1:C:347:SER:HB3	2.48	0.43
1:C:577:GLU:O	1:C:580:TYR:HB3	2.18	0.43
2:D:263:ILE:HA	2:D:264:PRO:HD3	1.81	0.43
1:E:946:LEU:HB3	1:E:1013:ILE:HG12	2.01	0.43
2:F:236:ILE:HD12	2:F:263:ILE:HG22	2.00	0.43
1:G:867:ARG:HB2	1:G:877:GLN:NE2	2.32	0.43
2:H:205:ILE:HG21	2:H:237:PHE:CZ	2.54	0.43
1:A:1021:ARG:CG	1:A:1021:ARG:NH1	2.80	0.43
2:B:248:CYS:C	2:B:252:ILE:HD12	2.38	0.43
1:C:365:GLU:H	1:C:365:GLU:HG3	1.31	0.43
1:E:202:LYS:O	1:E:202:LYS:HG2	2.19	0.43
1:E:493:LYS:HE2	1:E:517:ARG:HD3	2.00	0.43
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.99	0.43
2:F:324:ASN:ND2	2:F:324:ASN:N	2.64	0.43
1:G:698:ILE:N	1:G:698:ILE:CD1	2.79	0.43
1:G:770:GLY:CA	1:G:823:ARG:CZ	2.97	0.43
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.77	0.43
1:A:588:ALA:HB2	1:A:863:LYS:HG2	2.01	0.43
1:C:213:TRP:HH2	1:C:294:ARG:HD3	1.83	0.43
2:D:363:ALA:C	2:D:365:PRO:HD2	2.39	0.43
1:E:681:ALA:O	1:E:684:ARG:HB3	2.19	0.43
1:E:695:VAL:CG1	1:E:696:THR:N	2.81	0.43
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.41	0.43
1:G:820:LEU:O	1:G:821:GLN:HB2	2.19	0.43
1:G:858:GLY:HA2	1:G:1069:HIS:ND1	2.30	0.43
2:H:157:ASP:HB2	2:H:247:PRO:HB2	1.99	0.43
2:H:322:PRO:HD2	2:H:325:LEU:HD12	2.00	0.43
1:A:820:LEU:O	1:A:821:GLN:HB2	2.17	0.43
2:B:275:LEU:HD12	2:B:275:LEU:O	2.17	0.43
1:C:623:LEU:HD12	1:C:654:LEU:HD23	2.00	0.43
1:C:712:LEU:O	1:C:727:ILE:HA	2.19	0.43
2:D:157:ASP:HA	10:D:1865:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:SER:HB3	2:D:270:LEU:H	1.64	0.43
1:E:244:THR:HG23	8:E:4041:ADP:HO3'	1.84	0.43
2:F:269:SER:OG	2:F:270:LEU:N	2.51	0.43
1:G:40:GLU:HG2	1:G:325:LYS:HE2	2.01	0.43
1:G:148:ILE:HG22	1:G:149:ALA:N	2.33	0.43
1:G:246:ASP:C	1:G:360:PRO:HG3	2.39	0.43
1:G:550:GLU:OE2	2:H:120:ARG:NH2	2.46	0.43
1:G:556:SER:O	1:G:561:LYS:NZ	2.50	0.43
1:A:475:LYS:HE2	1:A:488:PHE:CZ	2.53	0.43
1:A:872:LYS:HB2	10:A:4818:HOH:O	2.19	0.43
1:A:1014:ILE:HG23	1:A:1014:ILE:O	2.18	0.43
2:D:325:LEU:HA	2:D:325:LEU:HD23	1.76	0.43
2:H:210:VAL:HA	2:H:214:CYS:O	2.19	0.43
2:H:234:ASP:HB3	2:H:374:ILE:HG23	2.00	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.79	0.43
1:A:631:ARG:HG2	1:A:632:ILE:HG23	2.00	0.43
1:A:751:LEU:O	1:A:752:LEU:HD12	2.18	0.43
1:A:840:ILE:O	1:A:841:GLU:HB3	2.18	0.43
2:B:367:PHE:O	2:B:370:PHE:HB3	2.19	0.43
1:C:787:VAL:HG13	1:C:907:LEU:HB3	2.00	0.43
2:D:227:ASP:O	2:D:230:LYS:HB2	2.19	0.43
2:D:342:ARG:HD2	2:D:342:ARG:HA	1.75	0.43
1:E:710:TYR:HB3	1:E:711:PRO:HA	2.01	0.43
1:A:223:ASP:CG	1:A:227:ASN:HB2	2.40	0.43
1:A:347:SER:O	2:B:296:PRO:HB3	2.19	0.43
1:A:736:ARG:O	1:A:740:THR:HG23	2.18	0.43
2:B:175:TRP:HA	2:B:180:GLY:O	2.18	0.43
1:C:1064:SER:O	1:C:1068:MET:HG3	2.19	0.43
1:E:697:ALA:O	1:E:700:MET:HB2	2.19	0.43
2:F:202:LYS:NZ	2:F:356:ALA:O	2.45	0.43
2:F:228:VAL:HG22	2:F:231:MET:CE	2.49	0.43
1:G:168:ILE:CG2	1:G:204:LEU:HD22	2.49	0.43
1:G:563:MET:HE2	1:G:635:PRO:HG3	1.96	0.43
1:G:703:GLU:OE2	1:G:703:GLU:HA	2.19	0.43
1:G:772:MET:CE	1:G:880:THR:HA	2.49	0.43
2:H:249:ASP:OD2	2:H:249:ASP:N	2.51	0.43
1:C:127:GLU:HB2	1:C:172:PHE:CZ	2.54	0.43
1:C:150:HIS:ND1	1:C:154:GLU:OE2	2.44	0.43
1:C:340:THR:O	1:C:343:ARG:HB2	2.18	0.43
1:C:492:LEU:O	1:C:495:LYS:HB2	2.19	0.43
1:C:1057:ASP:HB3	1:C:1060:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:246:ALA:N	2:F:247:PRO:HD2	2.33	0.43
1:A:712:LEU:O	1:A:727:ILE:HA	2.19	0.42
1:A:975:HIS:CD2	1:A:975:HIS:C	2.93	0.42
2:D:196:ALA:HA	2:D:237:PHE:O	2.19	0.42
1:E:755:PHE:CD1	8:E:4047:ADP:C2	3.07	0.42
2:H:266:PHE:HA	2:H:348:PHE:O	2.19	0.42
1:A:4:ARG:CD	1:A:7:ILE:HD12	2.48	0.42
1:A:657:ALA:HB1	10:A:4512:HOH:O	2.18	0.42
1:C:44:VAL:N	1:C:62:ASP:OD2	2.44	0.42
1:C:65:TYR:OH	1:C:80:LYS:NZ	2.30	0.42
1:C:183:TYR:HB2	1:C:187:GLU:OE1	2.19	0.42
2:D:212:ARG:CG	2:D:212:ARG:NH1	2.77	0.42
1:E:176:GLY:N	8:E:4041:ADP:O2B	2.38	0.42
1:E:294:ARG:NH1	10:E:4632:HOH:O	2.52	0.42
1:G:257:THR:HG1	1:G:260:GLU:HG3	1.84	0.42
1:G:769:ASP:OD2	1:G:769:ASP:N	2.50	0.42
1:G:801:LEU:HD22	1:G:805:ILE:HG21	2.00	0.42
1:C:165:PRO:HA	1:C:182:ALA:O	2.20	0.42
1:C:169:ARG:HH21	1:C:207:ASP:CG	2.22	0.42
1:C:196:LEU:HA	1:C:196:LEU:HD23	1.80	0.42
1:C:812:GLN:O	1:C:816:LEU:HD12	2.18	0.42
1:E:250:VAL:HA	1:E:356:VAL:O	2.19	0.42
1:E:659:VAL:HG13	1:E:660:PRO:HD2	2.01	0.42
2:F:176:THR:O	2:F:180:GLY:N	2.47	0.42
2:F:263:ILE:HA	2:F:264:PRO:HD3	1.75	0.42
1:G:735:ARG:O	1:G:738:PHE:N	2.52	0.42
1:A:150:HIS:NE2	1:A:203:GLU:HG3	2.34	0.42
1:A:383:GLU:OE2	1:A:604:GLU:OE1	2.38	0.42
1:A:1004[A]:ARG:HD2	1:A:1010:TYR:OH	2.19	0.42
1:C:39:GLU:OE1	1:C:325:LYS:NZ	2.36	0.42
1:C:669:ILE:HA	1:C:844:PRO:HG2	2.02	0.42
1:E:784:GLN:HE21	1:E:784:GLN:N	2.09	0.42
2:F:373:LEU:HA	2:F:373:LEU:HD23	1.79	0.42
1:G:118:ALA:HA	10:G:4550:HOH:O	2.19	0.42
2:H:8:VAL:HG12	2:H:9:LEU:N	2.33	0.42
2:H:175:TRP:CH2	2:H:177:LEU:HA	2.55	0.42
1:A:441:ASP:OD2	1:A:444:ARG:NH1	2.50	0.42
1:A:701:ALA:O	1:A:705:ALA:HB2	2.18	0.42
1:A:773:VAL:HG23	1:A:818:PHE:CE2	2.55	0.42
1:C:693:ALA:N	1:C:708:ILE:HD11	2.35	0.42
2:D:228:VAL:HA	2:D:231:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.85	0.42
1:E:436:ILE:HD12	1:E:436:ILE:HA	1.88	0.42
1:G:74:VAL:HG11	1:G:102:LEU:HD11	2.00	0.42
1:G:205:LEU:HD12	1:G:205:LEU:HA	1.89	0.42
1:G:426:ARG:HD3	1:G:427:GLU:N	2.35	0.42
1:G:453:PHE:CD1	1:G:453:PHE:C	2.92	0.42
1:A:128:ASP:OD2	1:A:131:ARG:HG3	2.20	0.42
1:C:461:TRP:HB2	2:D:90:SER:HB3	2.01	0.42
2:D:187:GLU:HG2	2:D:215:ARG:CD	2.47	0.42
2:D:222:GLN:H	2:D:222:GLN:NE2	2.15	0.42
2:D:298:LYS:O	2:D:329:HIS:HA	2.19	0.42
1:E:1052:MET:HG2	10:E:4939:HOH:O	2.18	0.42
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.54	0.42
1:G:456:THR:O	1:G:457:ASN:HB2	2.19	0.42
1:A:35:LYS:HD2	10:A:4186:HOH:O	2.18	0.42
1:C:734:LEU:HD11	1:C:738:PHE:HE2	1.78	0.42
1:C:932:GLN:HG2	1:C:937:SER:HB3	2.01	0.42
1:C:950:ARG:H	1:C:950:ARG:HG3	1.59	0.42
2:D:264:PRO:HA	2:D:346:PRO:O	2.20	0.42
1:E:82:ARG:HD3	10:E:4592:HOH:O	2.18	0.42
1:E:475:LYS:HE2	1:E:488:PHE:CZ	2.55	0.42
2:H:348:PHE:CE1	2:H:369:HIS:HD2	2.37	0.42
1:A:843:ASN:HA	1:A:844:PRO:HD3	1.83	0.42
1:A:1027[B]:ARG:CZ	1:A:1031:ARG:CD	2.98	0.42
1:C:339:ILE:HD13	1:C:339:ILE:HG21	1.87	0.42
1:C:528:ARG:HG2	1:C:543:MET:HG2	2.02	0.42
1:C:954:LYS:CG	1:C:980:VAL:HG21	2.48	0.42
1:C:990:LEU:HD23	1:E:979:ILE:HG12	2.02	0.42
1:E:4:ARG:HA	10:E:4159:HOH:O	2.19	0.42
2:F:218:ILE:HD13	2:F:218:ILE:N	2.34	0.42
2:F:253:THR:O	2:F:256:GLN:HB2	2.19	0.42
1:G:56:THR:OG1	1:G:855:LYS:NZ	2.45	0.42
1:G:406:ALA:HA	1:G:410:ASP:OD2	2.20	0.42
1:G:890:VAL:HG23	1:G:927:ALA:HB3	2.02	0.42
2:H:29:GLU:HA	2:H:129:ASN:HA	2.01	0.42
2:H:176:THR:HB	10:H:3971:HOH:O	2.19	0.42
1:A:38:ARG:NH1	1:A:38:ARG:CG	2.76	0.42
1:A:70:HIS:ND1	1:A:72:GLU:HB2	2.35	0.42
1:A:167:ILE:HG12	8:A:4000:ADP:C2	2.55	0.42
1:E:59:GLU:CG	1:E:60:MET:CE	2.98	0.42
1:E:630:VAL:O	1:E:634[B]:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:991:VAL:HG23	1:E:1004:ARG:HE	1.84	0.42
2:F:187:GLU:HG2	2:F:215:ARG:HD2	2.00	0.42
2:F:286:MET:HE1	2:F:312:HIS:ND1	2.35	0.42
1:G:196:LEU:HD23	1:G:196:LEU:HA	1.89	0.42
1:G:333:ASP:OD1	1:G:333:ASP:N	2.48	0.42
1:A:339:ILE:HD13	1:A:339:ILE:HG21	1.88	0.42
1:A:507:GLY:HA2	10:A:4692:HOH:O	2.19	0.42
1:A:583:VAL:HG12	1:A:587:LEU:HD11	2.02	0.42
1:C:692:ASN:HA	1:C:752:LEU:O	2.20	0.42
1:C:693:ALA:HB1	1:C:704:LYS:CG	2.50	0.42
1:C:715:ARG:HG2	1:C:725:MET:HE2	2.02	0.42
2:D:116:ARG:O	2:D:120:ARG:HG3	2.20	0.42
2:D:233:PRO:HG2	2:D:263:ILE:HD13	2.02	0.42
1:E:220:VAL:O	1:E:281:GLY:HA2	2.20	0.42
2:F:282:LYS:HB2	2:F:320:THR:HG21	2.02	0.42
1:G:644:GLY:O	1:G:647:PRO:HD2	2.20	0.42
1:G:860:PRO:HB2	1:G:863:LYS:CG	2.42	0.42
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.39	0.42
2:H:65:THR:OG1	2:H:96:GLU:O	2.32	0.42
2:H:357:SER:HA	2:H:358:PRO:HA	1.85	0.42
1:A:343:ARG:HD3	1:A:343:ARG:H	1.84	0.41
2:B:222:GLN:HG3	2:B:250:TYR:CE1	2.54	0.41
1:C:534:ALA:HB2	2:D:116:ARG:NH1	2.35	0.41
1:E:631:ARG:HD3	10:E:4457:HOH:O	2.20	0.41
1:G:561:LYS:O	1:G:636:LYS:N	2.46	0.41
1:A:349:GLU:O	2:B:294:ASN:HB2	2.20	0.41
1:A:680:HIS:N	1:A:680:HIS:ND1	2.66	0.41
1:E:103:GLU:HG2	10:E:4707:HOH:O	2.20	0.41
1:E:164:PHE:HA	1:E:165:PRO:C	2.41	0.41
1:E:709:GLY:O	1:E:754:HIS:ND1	2.53	0.41
2:F:253:THR:O	2:F:257:LYS:HD3	2.20	0.41
1:G:1:MET:N	1:G:224:LYS:CE	2.83	0.41
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.19	0.41
1:G:738:PHE:O	1:G:741:ALA:HB3	2.20	0.41
1:G:791:ASP:OD1	1:G:913:SER:OG	2.31	0.41
1:G:1004:ARG:HA	1:G:1009:GLU:HG3	2.02	0.41
2:H:32:PHE:O	2:H:291:HIS:HB2	2.20	0.41
1:A:479:VAL:CG2	1:A:483:GLY:HA3	2.50	0.41
1:A:784:GLN:HE22	1:A:1043:THR:HB	1.84	0.41
1:A:793:ALA:HA	1:A:891:LYS:O	2.21	0.41
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:CYS:O	2:B:252:ILE:HD12	2.20	0.41
1:E:738:PHE:O	1:E:741:ALA:HB3	2.19	0.41
2:F:236:ILE:CD1	2:F:263:ILE:CG2	2.98	0.41
1:G:698:ILE:H	1:G:698:ILE:CD1	2.31	0.41
1:G:762:VAL:HG12	1:G:763:ASP:N	2.34	0.41
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.76	0.41
1:A:950:ARG:HD3	10:A:4709:HOH:O	2.21	0.41
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.56	0.41
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.41
1:E:1020:ARG:HD3	1:E:1020:ARG:HA	1.95	0.41
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.54	0.41
2:B:296:PRO:HD3	2:B:333:PHE:CZ	2.55	0.41
1:C:11:LEU:HA	1:C:45:ILE:O	2.20	0.41
2:D:296:PRO:HB2	2:D:332:LEU:HB2	2.01	0.41
1:E:1:MET:HB2	1:E:224:LYS:HZ1	1.85	0.41
2:F:196:ALA:HA	2:F:237:PHE:O	2.20	0.41
2:F:232:ASN:N	2:F:233:PRO:CD	2.80	0.41
2:F:255:ILE:CG2	2:F:278:ALA:CB	2.98	0.41
1:G:492:LEU:HD13	1:G:502:LEU:HD22	2.01	0.41
1:G:784:GLN:HE22	1:G:1043:THR:HB	1.86	0.41
1:G:1023:ILE:HG23	1:G:1030:ARG:NH2	2.35	0.41
1:A:770:GLY:HA2	1:A:823:ARG:CZ	2.50	0.41
2:B:72:SER:HB2	10:B:4107:HOH:O	2.19	0.41
1:C:1063:ILE:CD1	1:C:1068:MET:CG	2.99	0.41
1:E:148:ILE:CG2	1:E:149:ALA:N	2.84	0.41
1:E:358:LYS:HE3	10:E:4183:HOH:O	2.21	0.41
1:E:1006:LYS:O	1:E:1006:LYS:HG3	2.19	0.41
2:F:255:ILE:HA	2:F:258:PHE:CD2	2.56	0.41
1:G:489:LEU:HA	1:G:489:LEU:HD23	1.83	0.41
2:H:38:GLY:HA3	2:H:358:PRO:HB3	2.01	0.41
2:B:167:ALA:O	2:B:168:TYR:HB3	2.20	0.41
1:C:772:MET:HE1	1:C:880:THR:O	2.19	0.41
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	2.02	0.41
2:D:32:PHE:O	2:D:291:HIS:HB2	2.19	0.41
1:E:571:ARG:HH11	1:E:571:ARG:HD2	1.65	0.41
1:G:850:VAL:HB	1:G:851:PRO:HD3	2.03	0.41
1:G:1021:ARG:NH1	1:G:1021:ARG:CG	2.84	0.41
2:H:369:HIS:O	2:H:372:GLU:HB2	2.20	0.41
1:A:326:LEU:HA	1:A:326:LEU:HD12	1.85	0.41
1:C:167:ILE:HD12	1:C:167:ILE:N	2.35	0.41
1:C:942:HIS:CD2	1:C:943:GLY:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:991:VAL:HG22	1:C:992:ASN:N	2.36	0.41
2:D:267:GLY:O	2:D:349:SER:HB2	2.21	0.41
1:E:412:LYS:HG2	1:E:438:TYR:CZ	2.56	0.41
1:E:469:LEU:O	1:E:473:GLU:HG3	2.20	0.41
2:F:286:MET:HE1	2:F:312:HIS:O	2.21	0.41
1:G:764:VAL:O	1:G:827:ASN:HA	2.21	0.41
1:G:874:LEU:HB3	1:G:879:VAL:O	2.20	0.41
1:G:915:GLY:HA2	10:G:4181:HOH:O	2.21	0.41
1:G:992:ASN:ND2	1:G:996:GLU:HB3	2.36	0.41
1:A:184:ASN:OD1	1:A:186:GLU:HB2	2.20	0.41
2:B:132:ILE:HG21	2:B:132:ILE:HD13	1.84	0.41
2:B:246:ALA:N	2:B:247:PRO:CD	2.84	0.41
1:C:1:MET:CG	1:C:2:PRO:HD2	2.37	0.41
1:C:48:ASN:O	1:C:66:ILE:HA	2.21	0.41
1:C:174:MET:HB2	6:C:4025:PO4:O1	2.20	0.41
1:C:841:GLU:HB2	10:C:4535:HOH:O	2.21	0.41
1:C:868:VAL:HG23	1:C:877:GLN:NE2	2.35	0.41
1:C:902:GLY:O	1:C:1027:ARG:NH2	2.49	0.41
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.51	0.41
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.35	0.41
1:E:714:VAL:HG13	1:E:752:LEU:HD12	2.03	0.41
2:F:46:PRO:HA	2:F:76:HIS:CG	2.55	0.41
2:F:50:ARG:HG3	2:F:158:LEU:HD13	2.02	0.41
2:F:273:GLN:HE21	2:F:351:GLN:HE22	1.67	0.41
1:G:440:ALA:O	1:G:444:ARG:HG3	2.21	0.41
1:G:517:ARG:HG2	1:G:522:LEU:HD23	2.03	0.41
1:G:518:ASP:OD1	1:G:523:HIS:HE1	2.04	0.41
1:G:872:LYS:HG2	1:G:872:LYS:O	2.19	0.41
1:G:1021:ARG:HD3	1:G:1025:ASP:OD2	2.21	0.41
2:H:5:ALA:HB3	2:H:110:ILE:HG13	2.03	0.41
2:H:54:THR:HA	2:H:81:VAL:HB	2.03	0.41
2:B:8:VAL:HG21	2:B:143:ALA:CB	2.49	0.41
2:B:45:ASP:O	2:B:76:HIS:HB2	2.20	0.41
1:C:426:ARG:HD3	1:C:426:ARG:O	2.21	0.41
1:E:796:LEU:HD23	1:E:796:LEU:C	2.42	0.41
1:G:349:GLU:O	2:H:294:ASN:HB2	2.22	0.41
1:G:412:LYS:HD3	1:G:437:TRP:CB	2.50	0.41
2:H:110:ILE:HG12	2:H:111:ALA:N	2.36	0.41
1:A:1051:ALA:O	1:A:1054:LEU:HB2	2.20	0.40
2:B:202:LYS:HB3	2:B:202:LYS:HE2	1.80	0.40
2:B:222:GLN:HG3	2:B:250:TYR:CD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:PRO:HG2	1:C:916:GLU:OE2	2.22	0.40
1:C:336:MET:HB3	1:C:342:GLY:HA2	2.03	0.40
1:E:213:TRP:CZ2	1:E:289:ASN:HB2	2.56	0.40
2:F:199:PHE:O	2:F:241:GLY:HA3	2.22	0.40
1:G:359:ILE:HD13	1:G:359:ILE:HG21	1.79	0.40
1:A:152:MET:O	1:A:155:ALA:HB3	2.21	0.40
1:A:426:ARG:HD3	1:A:426:ARG:C	2.41	0.40
1:A:539:ASP:HB2	10:A:4472:HOH:O	2.22	0.40
1:A:781:HIS:HE1	1:A:789:SER:HB3	1.85	0.40
2:B:236:ILE:HB	2:B:265:VAL:HG22	2.03	0.40
2:D:30:VAL:HG22	2:D:52:ILE:HB	2.03	0.40
2:D:277:LEU:HD21	2:D:283:THR:HG23	2.03	0.40
1:E:275:ILE:HD12	1:E:275:ILE:HA	1.80	0.40
1:E:534:ALA:O	2:F:123:ARG:HD3	2.20	0.40
1:E:651:ALA:HB1	1:E:666:PRO:HG3	2.02	0.40
2:F:6:LEU:HD11	2:F:8:VAL:CG2	2.51	0.40
1:G:143:THR:HA	1:G:296:ILE:HG23	2.03	0.40
2:H:104:ARG:O	2:H:104:ARG:HG3	2.20	0.40
1:A:475:LYS:HA	10:A:4792:HOH:O	2.21	0.40
1:A:835:ASN:HD22	1:A:835:ASN:HA	1.76	0.40
1:C:503:ALA:CB	1:C:510:GLU:HA	2.51	0.40
1:E:734:LEU:O	1:E:737:TYR:HB3	2.21	0.40
1:G:671:ARG:NH2	1:G:819:GLU:O	2.54	0.40
1:A:868:VAL:HA	1:A:872:LYS:O	2.21	0.40
1:A:1017:THR:CG2	1:A:1018:SER:N	2.84	0.40
2:B:227:ASP:HA	2:B:230:LYS:HD2	2.03	0.40
2:B:296:PRO:CD	2:B:333:PHE:CE1	3.05	0.40
1:C:686:LYS:C	1:C:687:LEU:HD23	2.42	0.40
1:C:928:PHE:HD1	1:C:1053:ALA:HB2	1.87	0.40
2:D:364:ALA:N	2:D:365:PRO:CD	2.85	0.40
2:F:46:PRO:O	2:F:242:PRO:HG3	2.22	0.40
1:C:554:ASN:N	1:C:555:PRO:HD3	2.37	0.40
1:C:987:ASN:ND2	10:C:4516:HOH:O	2.46	0.40
2:D:176:THR:O	2:D:180:GLY:N	2.40	0.40
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.76	0.40
1:G:165:PRO:HB3	1:G:183:TYR:CD1	2.57	0.40
1:G:423[B]:LYS:HE3	1:G:427:GLU:HG2	2.04	0.40
1:G:637:GLY:HA2	1:G:660:PRO:O	2.21	0.40
2:H:25:SER:HB2	2:H:133:ILE:HG12	2.03	0.40
2:H:38:GLY:HA3	2:H:358:PRO:CB	2.52	0.40
2:H:153:LEU:HA	2:H:153:LEU:HD12	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.51	0.40
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.87	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	1058/1073 (99%)	1012 (96%)	42 (4%)	4 (0%)	34	30
1	C	1053/1073 (98%)	996 (95%)	51 (5%)	6 (1%)	25	19
1	E	1058/1073 (99%)	1014 (96%)	44 (4%)	0	100	100
1	G	1056/1073 (98%)	1000 (95%)	50 (5%)	6 (1%)	25	19
2	B	377/382 (99%)	361 (96%)	16 (4%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	377/382 (99%)	358 (95%)	18 (5%)	1 (0%)	41	37
2	H	378/382 (99%)	355 (94%)	23 (6%)	0	100	100
All	All	5734/5820 (98%)	5460 (95%)	257 (4%)	17 (0%)	41	37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	A	975	HIS
1	C	698	ILE
1	A	693	ALA
1	C	758	ASP
1	G	738	PHE
1	G	739	GLN
1	G	873	SER

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Mol	Chain	Res	Type
1	C	975	HIS
1	C	368	ALA
1	C	736	ARG
1	G	519	GLN
1	G	975	HIS
2	F	185	LYS
1	C	2	PRO
1	G	2	PRO
1	A	2	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	871/878 (99%)	808 (93%)	63 (7%)	14 9
1	C	866/878 (99%)	799 (92%)	67 (8%)	13 8
1	E	871/878 (99%)	805 (92%)	66 (8%)	13 8
1	G	869/878 (99%)	791 (91%)	78 (9%)	9 6
2	B	308/310 (99%)	284 (92%)	24 (8%)	12 8
2	D	308/310 (99%)	284 (92%)	24 (8%)	12 8
2	F	308/310 (99%)	279 (91%)	29 (9%)	8 5
2	H	309/310 (100%)	271 (88%)	38 (12%)	4 2
All	All	4710/4752 (99%)	4321 (92%)	389 (8%)	11 7

All (389) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	8	LYS
1	A	38	ARG
1	A	79	GLU
1	A	104	ARG

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Mol	Chain	Res	Type
1	A	137	LYS
1	A	138	LYS
1	A	174	MET
1	A	236	ASN
1	A	275	ILE
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	414	SER
1	A	416	ASP
1	A	426	ARG
1	A	490	ARG
1	A	518	ASP
1	A	542	TYR
1	A	548	GLU
1	A	559	ARG
1	A	560	GLU
1	A	571	ARG
1	A	631	ARG
1	A	671	ARG
1	A	675	ARG
1	A	680	HIS
1	A	684	ARG
1	A	688	LYS
1	A	689	GLN
1	A	695	VAL
1	A	704	LYS
1	A	706	LYS
1	A	712	LEU
1	A	715	ARG
1	A	730	ASP
1	A	733	ASP
1	A	735	ARG
1	A	739	GLN
1	A	753	ASP
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	839	LEU
1	A	891	LYS
1	A	895	LEU
1	A	906	LEU

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Mol	Chain	Res	Type
1	A	912	ARG
1	A	940	LYS
1	A	947	LEU
1	A	950	ARG
1	A	967	GLN
1	A	970	GLU
1	A	992	ASN
1	A	1001	ILE
1	A	1006	LYS
1	A	1018	SER
1	A	1021	ARG
1	A	1026	SER
1	A	1027[A]	ARG
1	A	1027[B]	ARG
1	A	1073	LYS
2	B	3	LYS
2	B	6	LEU
2	B	18	ARG
2	B	50	ARG
2	B	87	LEU
2	B	104	ARG
2	B	154	ASN
2	B	166	GLU
2	B	169	SER
2	B	186	LYS
2	B	188	ASP
2	B	190	LEU
2	B	215	ARG
2	B	222	GLN
2	B	239	SER
2	B	257	LYS
2	B	261	THR
2	B	282	LYS
2	B	306	MET
2	B	321	LEU
2	B	324	ASN
2	B	357	SER
2	B	376	GLN
2	B	379	LYS
1	C	1	MET
1	C	43	ARG
1	C	44	VAL

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Mol	Chain	Res	Type
1	C	55	MET
1	C	103	GLU
1	C	104	ARG
1	C	145	ARG
1	C	174	MET
1	C	185	ARG
1	C	202	LYS
1	C	236	ASN
1	C	321	LYS
1	C	343	ARG
1	C	365	GLU
1	C	412	LYS
1	C	414	SER
1	C	416	ASP
1	C	426	ARG
1	C	542	TYR
1	C	548	GLU
1	C	563	MET
1	C	571	ARG
1	C	591	GLU
1	C	648	LEU
1	C	665	SER
1	C	675	ARG
1	C	684	ARG
1	C	696	THR
1	C	704	LYS
1	C	706	LYS
1	C	712	LEU
1	C	726	GLU
1	C	728	VAL
1	C	733	ASP
1	C	735	ARG
1	C	736	ARG
1	C	751	LEU
1	C	757	ASP
1	C	763	ASP
1	C	772	MET
1	C	784	GLN
1	C	795	SER
1	C	800	THR
1	C	805	ILE
1	C	811	GLN

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Mol	Chain	Res	Type
1	C	814	GLN
1	C	827	ASN
1	C	835	ASN
1	C	849	THR
1	C	855	LYS
1	C	881	LYS
1	C	889	SER
1	C	906	LEU
1	C	910	GLU
1	C	912	ARG
1	C	950	ARG
1	C	951	GLU
1	C	967	GLN
1	C	970	GLU
1	C	998	ARG
1	C	1014	ILE
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1031	ARG
1	C	1037	LYS
1	C	1073	LYS
2	D	6	LEU
2	D	50	ARG
2	D	87	LEU
2	D	125	LYS
2	D	148	ARG
2	D	153	LEU
2	D	154	ASN
2	D	166	GLU
2	D	178	THR
2	D	183	GLU
2	D	185	LYS
2	D	188	ASP
2	D	215	ARG
2	D	222	GLN
2	D	231	MET
2	D	257	LYS
2	D	269	SER
2	D	306	MET
2	D	324	ASN
2	D	332	LEU

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Mol	Chain	Res	Type
2	D	333	PHE
2	D	366	LEU
2	D	376	GLN
2	D	379	LYS
1	E	1	MET
1	E	3	LYS
1	E	5	THR
1	E	46	LEU
1	E	76	LYS
1	E	103	GLU
1	E	104	ARG
1	E	115	MET
1	E	153	GLU
1	E	174	MET
1	E	236	ASN
1	E	275	ILE
1	E	299	GLU
1	E	300	MET
1	E	307	SER
1	E	343	ARG
1	E	363	ASN
1	E	412	LYS
1	E	414	SER
1	E	428	LEU
1	E	542	TYR
1	E	548	GLU
1	E	558	ASP
1	E	563	MET
1	E	571	ARG
1	E	591	GLU
1	E	671	ARG
1	E	675	ARG
1	E	676	GLU
1	E	680	HIS
1	E	695	VAL
1	E	696	THR
1	E	700	MET
1	E	704	LYS
1	E	706	LYS
1	E	707	GLU
1	E	712	LEU
1	E	733	ASP

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Mol	Chain	Res	Type
1	E	734	LEU
1	E	735	ARG
1	E	738	PHE
1	E	750	VAL
1	E	751	LEU
1	E	784	GLN
1	E	805	ILE
1	E	835	ASN
1	E	836	GLU
1	E	839	LEU
1	E	881	LYS
1	E	906	LEU
1	E	912	ARG
1	E	936	ASN
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG
1	E	957	VAL
1	E	966	LYS
1	E	991	VAL
1	E	1004	ARG
1	E	1018	SER
1	E	1020	ARG
1	E	1021	ARG
1	E	1027	ARG
1	E	1031	ARG
1	E	1073	LYS
2	F	18	ARG
2	F	25	SER
2	F	50	ARG
2	F	73	SER
2	F	87	LEU
2	F	97	ASP
2	F	106	ASN
2	F	113	ILE
2	F	153	LEU
2	F	154	ASN
2	F	166	GLU
2	F	169	SER
2	F	174	SER
2	F	175	TRP

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Mol	Chain	Res	Type
2	F	183	GLU
2	F	186	LYS
2	F	190	LEU
2	F	192	PHE
2	F	230	LYS
2	F	257	LYS
2	F	261	THR
2	F	282	LYS
2	F	301	GLU
2	F	324	ASN
2	F	332	LEU
2	F	366	LEU
2	F	372	GLU
2	F	376	GLN
2	F	379	LYS
1	G	1	MET
1	G	4	ARG
1	G	8	LYS
1	G	43	ARG
1	G	46	LEU
1	G	55	MET
1	G	59[A]	GLU
1	G	59[B]	GLU
1	G	76	LYS
1	G	145	ARG
1	G	174	MET
1	G	185	ARG
1	G	202	LYS
1	G	275	ILE
1	G	313	LYS
1	G	321	LYS
1	G	325	LYS
1	G	326	LEU
1	G	343	ARG
1	G	358	LYS
1	G	413	VAL
1	G	416	ASP
1	G	426	ARG
1	G	428	LEU
1	G	479	VAL
1	G	482	THR
1	G	489	LEU

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Mol	Chain	Res	Type
1	G	509	ARG
1	G	519	GLN
1	G	542	TYR
1	G	554	ASN
1	G	558	ASP
1	G	559	ARG
1	G	571	ARG
1	G	591	GLU
1	G	648	LEU
1	G	652	ARG
1	G	665	SER
1	G	671	ARG
1	G	673	GLU
1	G	675	ARG
1	G	682	VAL
1	G	683	GLU
1	G	706	LYS
1	G	714	VAL
1	G	730	ASP
1	G	733	ASP
1	G	735	ARG
1	G	751	LEU
1	G	752	LEU
1	G	763	ASP
1	G	772	MET
1	G	784	GLN
1	G	789	SER
1	G	800	THR
1	G	805	ILE
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	881	LYS
1	G	884	ILE
1	G	912	ARG
1	G	950	ARG
1	G	951	GLU
1	G	956	ARG
1	G	966	LYS
1	G	970	GLU
1	G	1006	LYS
1	G	1014	ILE

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Mol	Chain	Res	Type
1	G	1018	SER
1	G	1021	ARG
1	G	1027	ARG
1	G	1030	ARG
1	G	1031	ARG
1	G	1032	SER
1	G	1037	LYS
1	G	1059	THR
1	G	1073	LYS
2	H	2	ILE
2	H	4	SER
2	H	6	LEU
2	H	7	LEU
2	H	49	SER
2	H	50	ARG
2	H	87	LEU
2	H	104	ARG
2	H	125	LYS
2	H	137	ASN
2	H	153	LEU
2	H	154	ASN
2	H	156	MET
2	H	157	ASP
2	H	166	GLU
2	H	169	SER
2	H	174	SER
2	H	178	THR
2	H	183	GLU
2	H	192	PHE
2	H	216	LEU
2	H	218	ILE
2	H	222	GLN
2	H	231	MET
2	H	250	TYR
2	H	257	LYS
2	H	261	THR
2	H	262	ASP
2	H	263	ILE
2	H	300	VAL
2	H	306	MET
2	H	324	ASN
2	H	332	LEU

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Mol	Chain	Res	Type
2	H	340	ILE
2	H	357	SER
2	H	360	PRO
2	H	370	PHE
2	H	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	457	ASN
1	A	784	GLN
1	A	814	GLN
1	A	834	ASN
1	A	835	ASN
1	A	936	ASN
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1035	GLN
1	A	1071	GLN
2	B	51	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	645	GLN
1	C	679	GLN
1	C	689	GLN
1	C	692	ASN
1	C	784	GLN
1	C	812	GLN
1	C	814	GLN
1	C	835	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS

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Mol	Chain	Res	Type
1	C	1035	GLN
1	C	1071	GLN
2	D	51	GLN
2	D	154	ASN
2	D	222	GLN
2	D	324	ASN
2	D	351	GLN
1	E	266	ASN
1	E	457	ASN
1	E	679	GLN
1	E	689	GLN
1	E	692	ASN
1	E	784	GLN
1	E	803	GLN
1	E	812	GLN
1	E	936	ASN
1	E	942	HIS
1	E	987	ASN
1	E	992	ASN
1	E	995	HIS
1	E	1002	GLN
1	E	1007	ASN
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN
2	F	154	ASN
2	F	351	GLN
1	G	105	GLN
1	G	266	ASN
1	G	523	HIS
1	G	689	GLN
1	G	784	GLN
1	G	803	GLN
1	G	835	ASN
1	G	936	ASN
1	G	942	HIS
1	G	987	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1055	ASN
1	G	1071	GLN

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Mol	Chain	Res	Type
2	H	51	GLN
2	H	78	GLN
2	H	105	HIS
2	H	154	ASN
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 82 ligands modelled in this entry, 60 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ORN	A	4072	-	7,8,8	0.79	0	8,9,9	1.43	1 (12%)
6	PO4	C	4040	-	4,4,4	1.25	0	6,6,6	0.80	0
8	ADP	C	4026	4,3	24,29,29	1.08	3 (12%)	29,45,45	1.15	3 (10%)
9	NET	E	4052	-	8,8,8	0.67	0	10,10,10	0.62	0
6	PO4	A	4005	4,3	4,4,4	2.30	2 (50%)	6,6,6	1.25	0
9	NET	G	4073	-	8,8,8	0.78	0	10,10,10	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ADP	E	4047	4,3	24,29,29	1.23	3 (12%)	29,45,45	1.09	3 (10%)
6	PO4	E	4046	4,3	4,4,4	2.02	2 (50%)	6,6,6	1.06	0
6	PO4	G	4067	4,3	4,4,4	2.31	2 (50%)	6,6,6	1.12	0
8	ADP	C	4020	3	24,29,29	1.20	2 (8%)	29,45,45	1.36	3 (10%)
7	ORN	A	4051	-	6,7,8	1.14	1 (16%)	2,7,9	0.41	0
6	PO4	E	4061	-	4,4,4	2.25	3 (75%)	6,6,6	0.91	0
8	ADP	G	4068	4,3	24,29,29	1.14	4 (16%)	29,45,45	1.27	4 (13%)
8	ADP	A	4000	3	24,29,29	1.12	3 (12%)	29,45,45	1.29	3 (10%)
8	ADP	E	4041	3	24,29,29	1.28	3 (12%)	29,45,45	1.42	5 (17%)
6	PO4	C	4025	4,3	4,4,4	2.35	4 (100%)	6,6,6	1.10	0
8	ADP	G	4062	3	24,29,29	1.08	2 (8%)	29,45,45	1.13	3 (10%)
7	ORN	A	4030	-	6,7,8	1.04	1 (16%)	2,7,9	0.93	0
7	ORN	A	4010	-	7,8,8	1.01	1 (14%)	8,9,9	1.52	2 (25%)
9	NET	C	4031	-	8,8,8	0.55	0	10,10,10	0.50	0
8	ADP	A	4006	4,3	24,29,29	1.09	1 (4%)	29,45,45	1.39	4 (13%)
9	NET	A	4011	-	8,8,8	0.67	0	10,10,10	0.56	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
8	ADP	G	4068	4,3	-	3/12/32/32	0/3/3/3
7	ORN	A	4072	-	-	6/8/8/8	-
8	ADP	A	4000	3	-	0/12/32/32	0/3/3/3
8	ADP	E	4041	3	-	1/12/32/32	0/3/3/3
8	ADP	E	4047	4,3	-	3/12/32/32	0/3/3/3
8	ADP	C	4020	3	-	2/12/32/32	0/3/3/3
8	ADP	G	4062	3	-	0/12/32/32	0/3/3/3
7	ORN	A	4030	-	-	4/5/6/8	-
7	ORN	A	4010	-	-	6/8/8/8	-
9	NET	C	4031	-	-	0/12/12/12	-
8	ADP	C	4026	4,3	-	0/12/32/32	0/3/3/3
7	ORN	A	4051	-	-	3/5/6/8	-
9	NET	E	4052	-	-	3/12/12/12	-
8	ADP	A	4006	4,3	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NET	G	4073	-	-	0/12/12/12	-
9	NET	A	4011	-	-	0/12/12/12	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	4067	PO4	P-O2	-3.65	1.43	1.54
8	G	4068	ADP	O3'-C3'	3.04	1.50	1.43
8	E	4047	ADP	O2'-C2'	3.02	1.50	1.43
8	E	4041	ADP	O2'-C2'	3.01	1.50	1.43
6	E	4046	PO4	P-O2	-2.91	1.45	1.54
8	E	4047	ADP	O3'-C3'	2.88	1.49	1.43
8	C	4020	ADP	O2'-C2'	2.87	1.49	1.43
8	C	4020	ADP	O4'-C1'	-2.87	1.37	1.41
6	A	4005	PO4	P-O4	-2.82	1.46	1.54
8	E	4041	ADP	O4'-C1'	-2.79	1.37	1.41
6	A	4005	PO4	P-O2	-2.67	1.46	1.54
8	C	4026	ADP	O3'-C3'	2.66	1.49	1.43
6	E	4061	PO4	P-O4	-2.51	1.47	1.54
8	C	4026	ADP	O4'-C1'	-2.50	1.37	1.41
8	E	4041	ADP	O3'-C3'	2.50	1.48	1.43
6	C	4025	PO4	P-O1	-2.49	1.45	1.50
8	E	4047	ADP	C2-N1	2.48	1.38	1.33
8	A	4006	ADP	O3'-C3'	2.47	1.48	1.43
6	E	4061	PO4	P-O2	-2.47	1.47	1.54
6	C	4025	PO4	P-O3	-2.46	1.47	1.54
7	A	4030	ORN	O-C	2.39	1.29	1.19
8	C	4026	ADP	O2'-C2'	2.38	1.48	1.43
6	C	4025	PO4	P-O2	-2.36	1.47	1.54
8	A	4000	ADP	C2-N1	2.32	1.38	1.33
8	G	4068	ADP	O4'-C1'	-2.30	1.37	1.41
8	G	4062	ADP	O2'-C2'	2.28	1.48	1.43
8	G	4068	ADP	O2'-C2'	2.23	1.48	1.43
8	A	4000	ADP	O4'-C1'	-2.19	1.38	1.41
8	A	4000	ADP	C2'-C1'	-2.19	1.50	1.53
7	A	4051	ORN	O-C	2.16	1.28	1.19
6	G	4067	PO4	P-O3	-2.09	1.48	1.54
7	A	4010	ORN	O-C	2.09	1.28	1.22
6	E	4061	PO4	P-O3	-2.07	1.48	1.54
6	C	4025	PO4	P-O4	-2.07	1.48	1.54
8	G	4068	ADP	C2-N1	2.06	1.37	1.33
6	E	4046	PO4	P-O3	-2.05	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	4062	ADP	O3'-C3'	2.01	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	4020	ADP	C5-C6-N6	5.01	127.96	120.35
8	A	4000	ADP	C5-C6-N6	4.41	127.06	120.35
8	A	4006	ADP	C5-C6-N6	4.25	126.81	120.35
8	E	4041	ADP	C5-C6-N6	4.24	126.80	120.35
8	G	4068	ADP	C5-C6-N6	3.12	125.09	120.35
8	C	4026	ADP	C5-C6-N6	3.01	124.93	120.35
8	A	4006	ADP	O3'-C3'-C2'	2.83	120.99	111.82
8	C	4020	ADP	N6-C6-N1	-2.67	113.02	118.57
8	E	4041	ADP	C3'-C2'-C1'	2.64	104.95	100.98
7	A	4072	ORN	OXT-C-CA	2.64	122.37	113.38
8	G	4068	ADP	O3'-C3'-C2'	2.63	120.33	111.82
8	A	4000	ADP	C5-C6-N1	-2.58	114.50	120.35
8	G	4068	ADP	O3B-PB-O3A	2.58	113.29	104.64
8	C	4020	ADP	C3'-C2'-C1'	2.56	104.83	100.98
8	E	4041	ADP	O3'-C3'-C2'	2.50	119.91	111.82
8	C	4026	ADP	O2'-C2'-C3'	2.48	119.85	111.82
8	A	4006	ADP	O2'-C2'-C3'	2.46	119.78	111.82
8	G	4062	ADP	O3'-C3'-C2'	2.38	119.53	111.82
8	A	4006	ADP	C3'-C2'-C1'	2.38	104.56	100.98
7	A	4010	ORN	OXT-C-CA	2.35	121.38	113.38
8	A	4000	ADP	C3'-C2'-C1'	2.33	104.49	100.98
7	A	4010	ORN	CB-CA-C	-2.31	104.79	110.30
8	E	4047	ADP	C2'-C3'-C4'	-2.28	98.21	102.64
8	G	4068	ADP	O2'-C2'-C3'	2.25	119.08	111.82
8	G	4062	ADP	C5-C6-N1	-2.20	115.38	120.35
8	E	4041	ADP	O2'-C2'-C3'	2.17	118.83	111.82
8	E	4047	ADP	C5-C6-N1	-2.13	115.52	120.35
8	C	4026	ADP	C2'-C3'-C4'	-2.08	98.59	102.64
8	G	4062	ADP	C4-C5-N7	2.07	111.56	109.40
8	E	4047	ADP	C4-C5-N7	2.01	111.50	109.40
8	E	4041	ADP	C1'-N9-C4	-2.01	123.11	126.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	4010	ORN	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
7	A	4010	ORN	C-CA-CB-CG
7	A	4030	ORN	N-CA-CB-CG
7	A	4030	ORN	C-CA-CB-CG
7	A	4051	ORN	N-CA-CB-CG
7	A	4051	ORN	C-CA-CB-CG
7	A	4072	ORN	N-CA-CB-CG
7	A	4072	ORN	C-CA-CB-CG
8	E	4047	ADP	PA-O3A-PB-O3B
8	G	4068	ADP	C5'-O5'-PA-O3A
7	A	4010	ORN	CA-CB-CG-CD
7	A	4072	ORN	CA-CB-CG-CD
7	A	4051	ORN	CA-CB-CG-CD
7	A	4030	ORN	CA-CB-CG-CD
7	A	4010	ORN	OXT-C-CA-N
7	A	4072	ORN	OXT-C-CA-N
8	A	4006	ADP	PA-O3A-PB-O1B
7	A	4010	ORN	O-C-CA-N
7	A	4072	ORN	O-C-CA-N
7	A	4010	ORN	NE-CD-CG-CB
7	A	4030	ORN	NE-CD-CG-CB
8	E	4041	ADP	PB-O3A-PA-O1A
9	E	4052	NET	C4-C3-N1-C7
8	G	4068	ADP	C5'-O5'-PA-O2A
9	E	4052	NET	C4-C3-N1-C5
7	A	4072	ORN	NE-CD-CG-CB
8	A	4006	ADP	PB-O3A-PA-O2A
8	C	4020	ADP	PB-O3A-PA-O1A
8	E	4047	ADP	PB-O3A-PA-O2A
8	G	4068	ADP	PA-O3A-PB-O1B
9	E	4052	NET	C4-C3-N1-C1
8	C	4020	ADP	PA-O3A-PB-O2B
8	A	4006	ADP	PB-O3A-PA-O1A
8	E	4047	ADP	PA-O3A-PB-O1B

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	4047	ADP	2	0
7	A	4051	ORN	1	0
8	A	4000	ADP	1	0
8	E	4041	ADP	2	0

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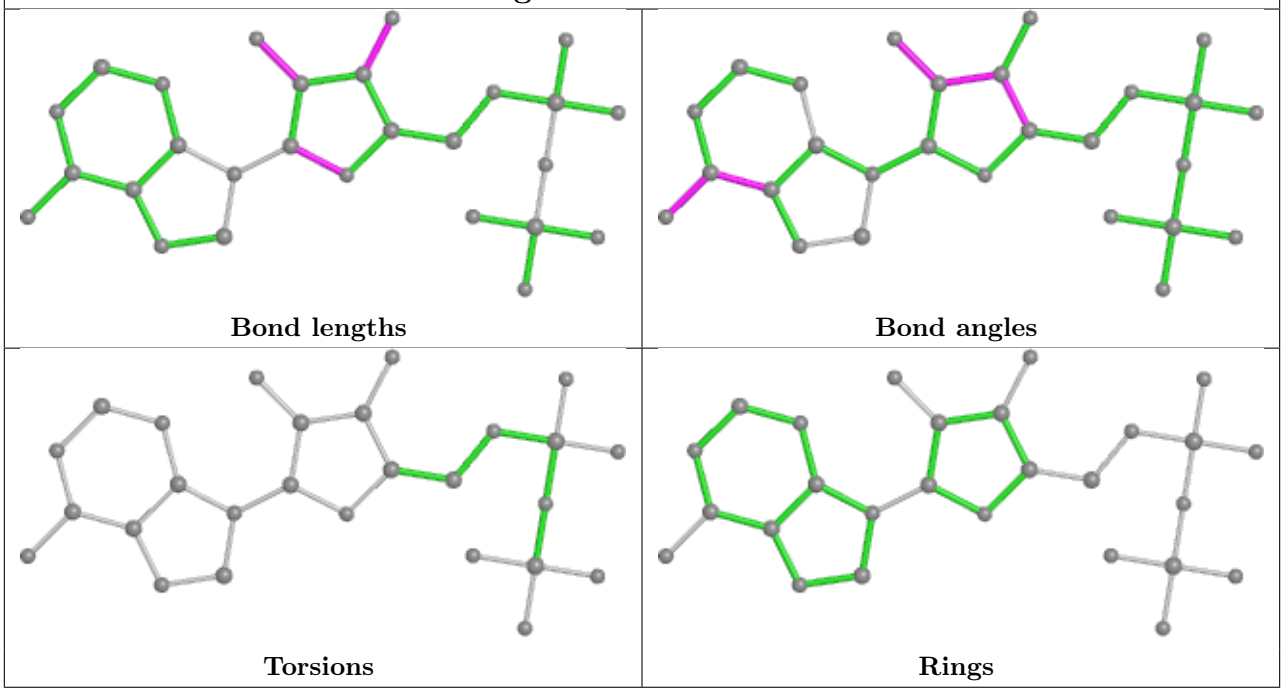
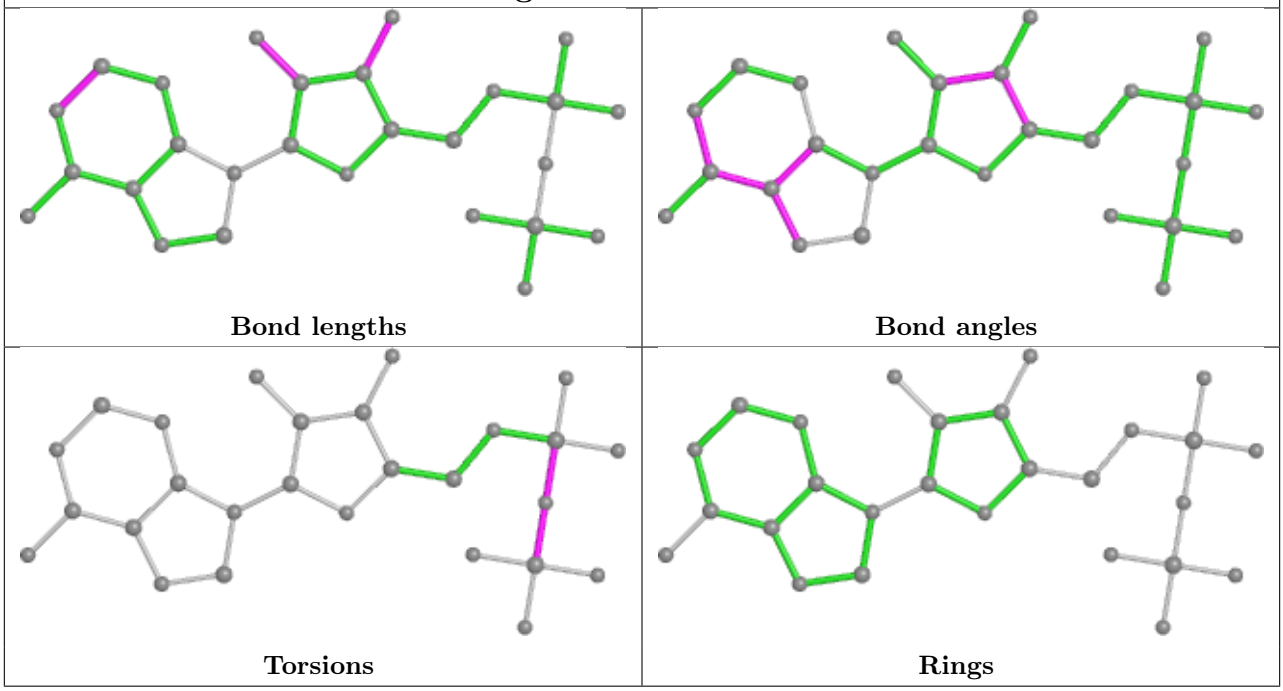
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	4025	PO4	1	0
8	G	4062	ADP	1	0
7	A	4030	ORN	1	0
8	A	4006	ADP	1	0

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

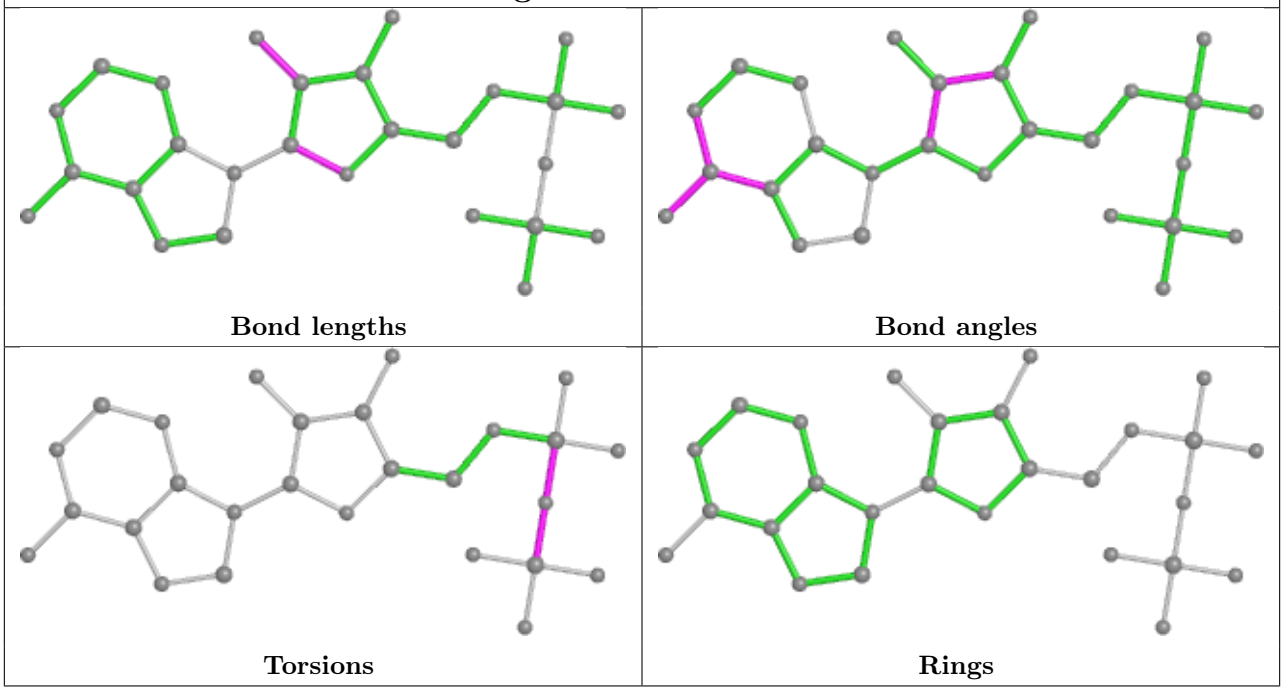
Ligand ADP C 4026



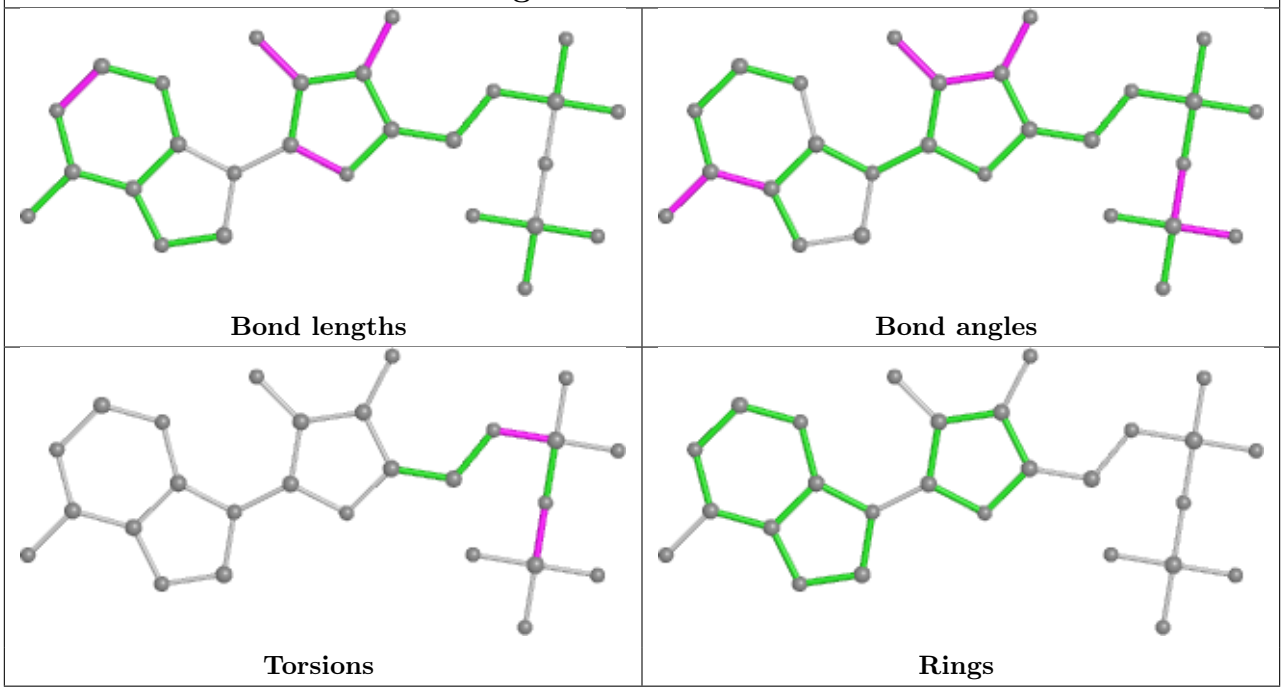
Ligand ADP E 4047



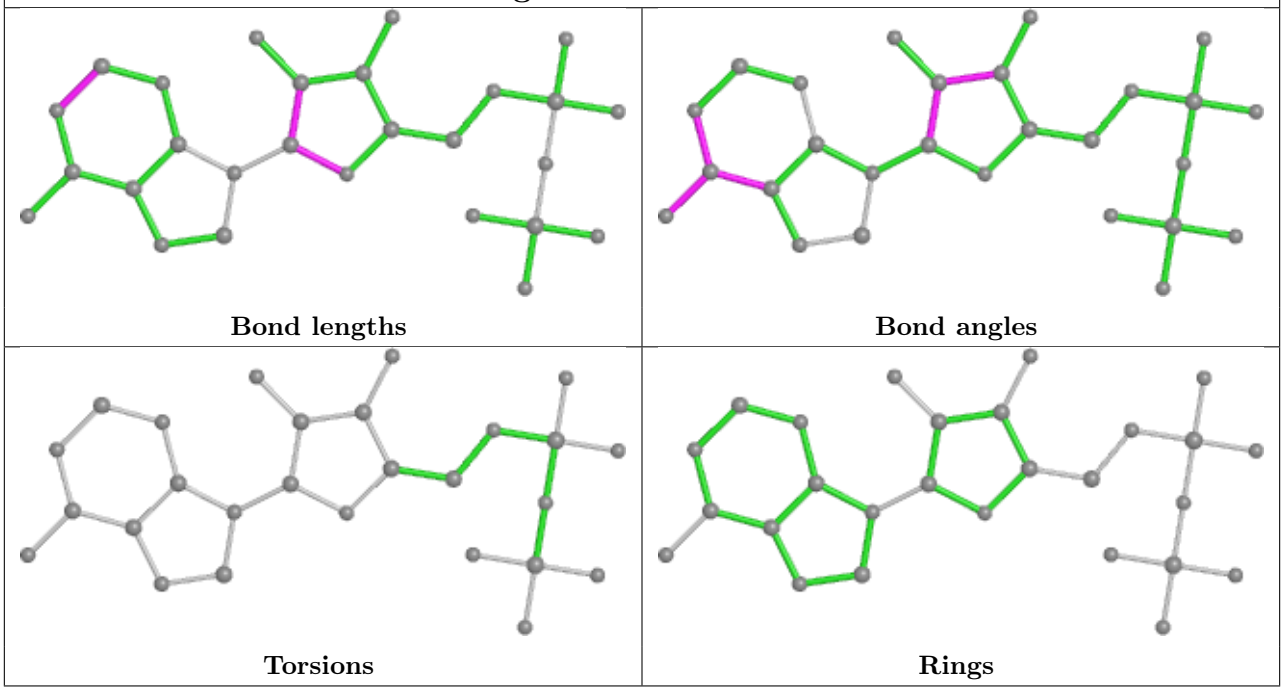
Ligand ADP C 4020



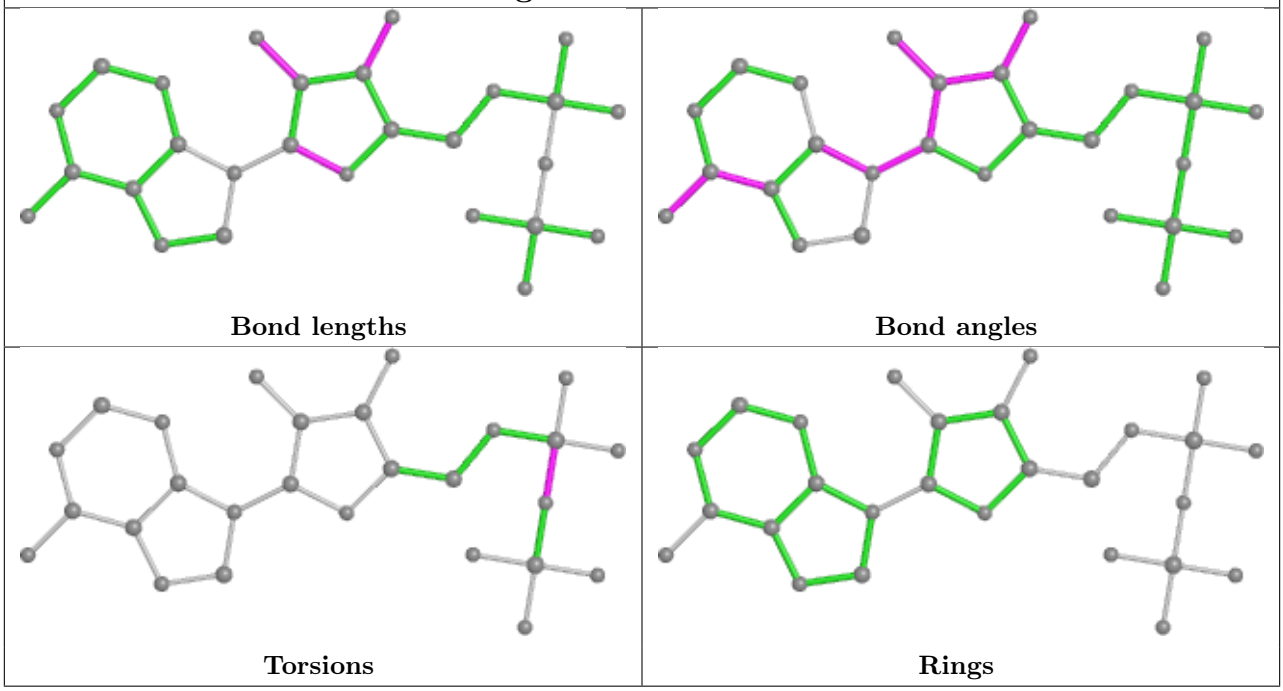
Ligand ADP G 4068



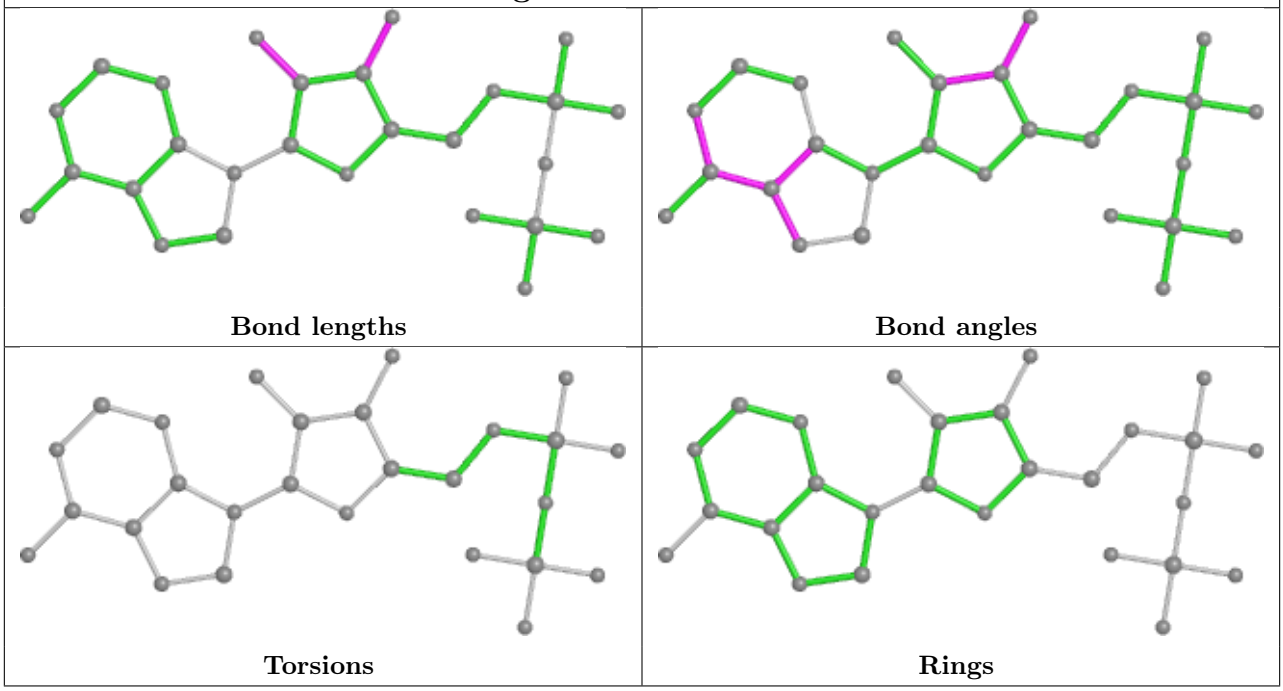
Ligand ADP A 4000



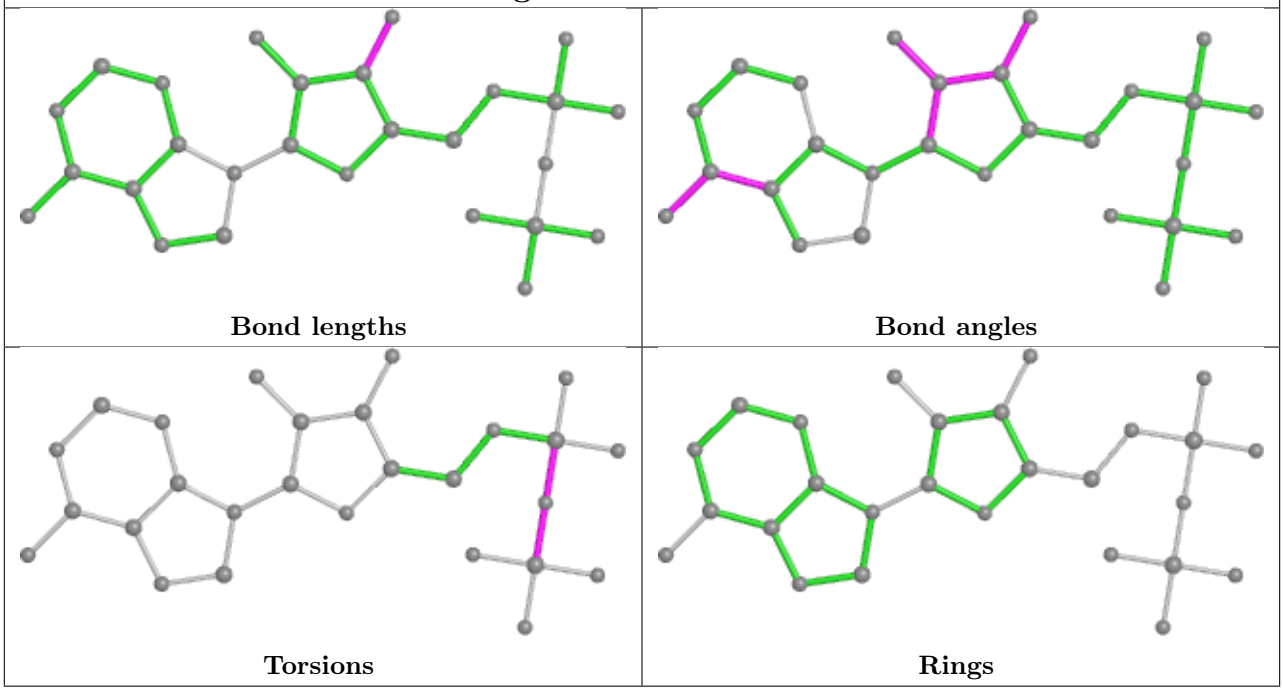
Ligand ADP E 4041



Ligand ADP G 4062



Ligand ADP A 4006



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.