Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:31 PM GMT

PDB ID	:	1FZG
Title	:	CRYSTAL STRUCTURE OF FRAGMENT D FROM HUMAN FIBRINOGEN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
Authors	:	Everse, S.J.; Spraggon, G.; Veerapandian, L.; Doolittle, R.F.
Deposited on	:	1999-01-01
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

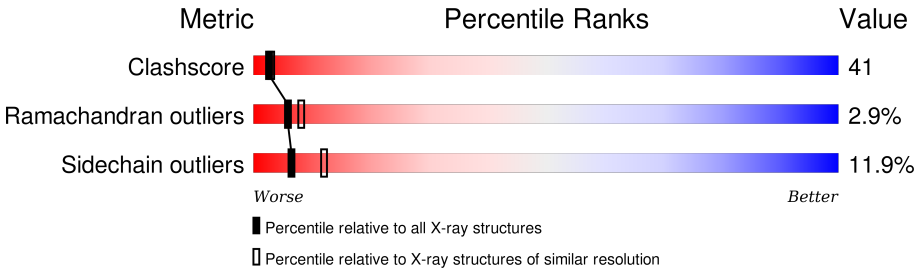
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	20% 34% 21% • 23%
1	D	87	20% 28% 10% 5% 38%
2	B	328	40% 36% 13% • 8%
2	E	328	43% 35% 10% • 10%
3	C	319	49% 33% 8% • 8%
3	F	319	41% 36% 9% • 11%
4	M	4	50% 25% 25%

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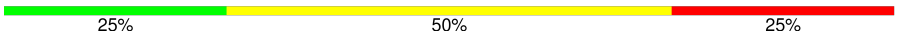
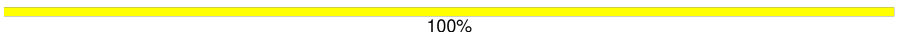
Mol	Chain	Length	Quality of chain
4	N	4	
4	S	4	
4	T	4	

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
5	NAG	B	470	-	-	X	-
5	NAG	E	470	-	-	X	-
5	NAG	E	471	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10713 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 FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			546	337	103	103	3			
1	D	54	Total	C	N	O	S	0	0	0
			440	269	84	84	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2427	1515	429	461	22			
2	E	296	Total	C	N	O	S	0	0	0
			2376	1484	420	450	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2342	1485	396	450	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	S	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	T	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	M	4	Total	C	N	O	0	0	0
			31	19	9	3			
4	N	4	Total	C	N	O	0	0	0
			31	19	9	3			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	C	2	Total	Ca	0	0
			2	2		
6	F	2	Total	Ca	0	0
			2	2		
6	E	2	Total	Ca	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	31	Total	O	0	0
			31	31		
7	C	20	Total	O	0	0
			20	20		
7	D	3	Total	O	0	0
			3	3		
7	E	29	Total	O	0	0
			29	29		
7	F	23	Total	O	0	0
			23	23		

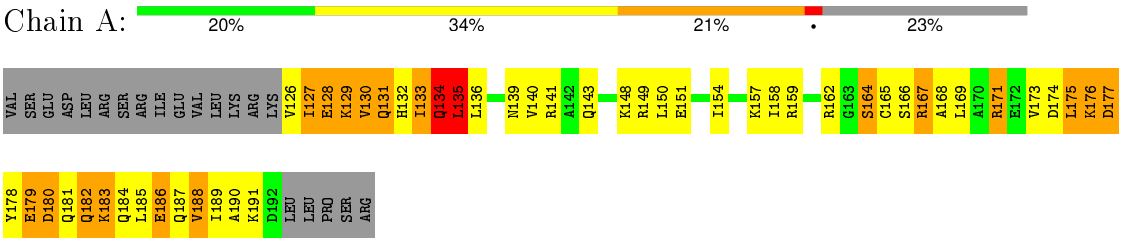
3 Residue-property plots (i)

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

Note EDS was not executed.

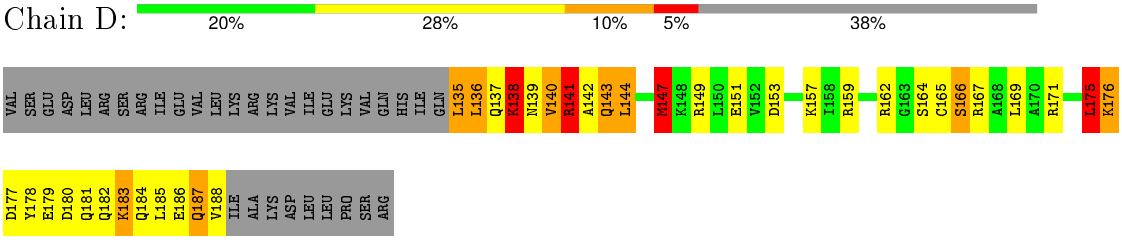
- Molecule 1: FIBRINOGEN

Chain A:



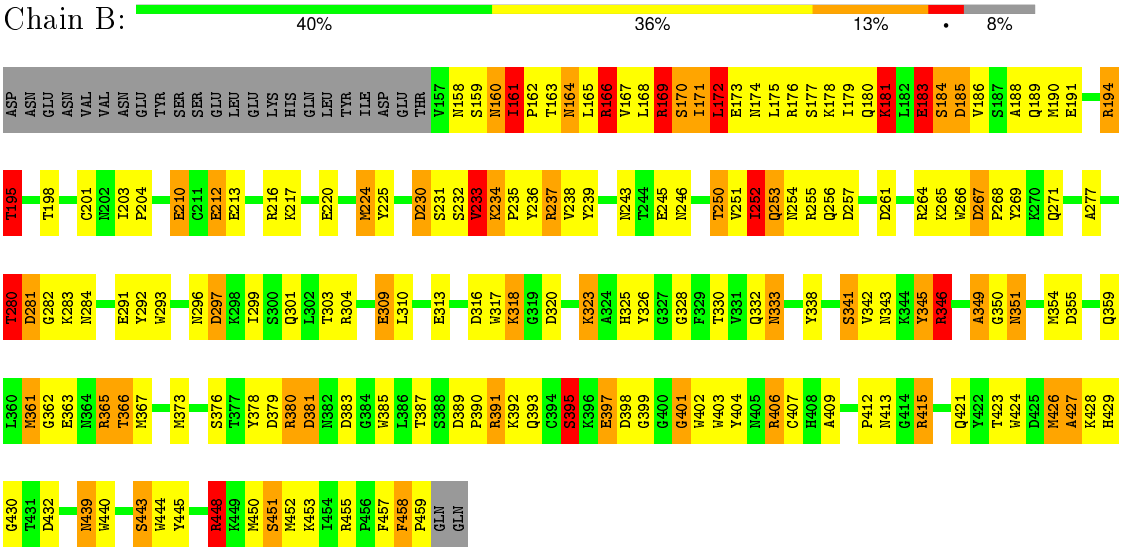
- Molecule 1: FIBRINOGEN

Chain D:



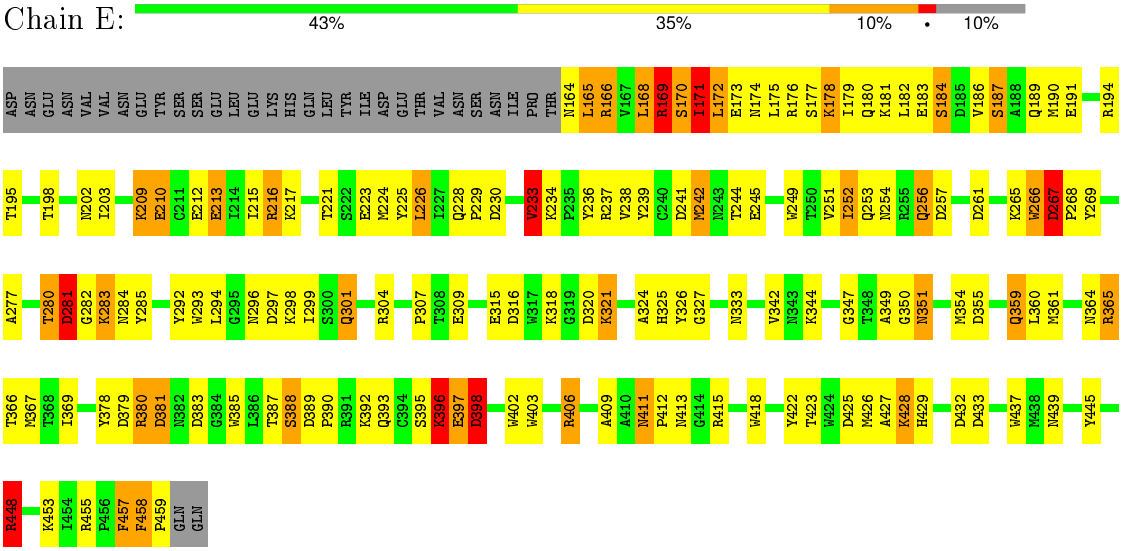
- Molecule 2: FIBRINOGEN

Chain B:



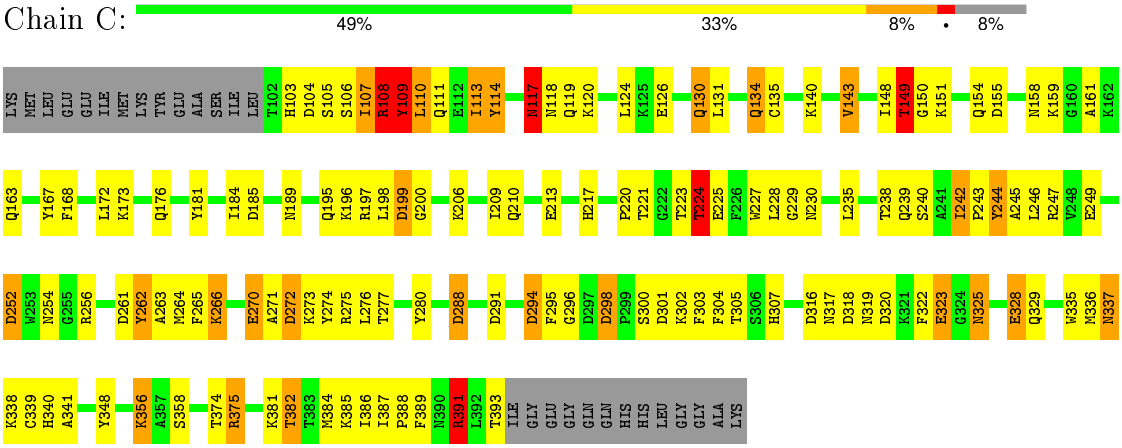
- Molecule 2: FIBRINOGEN

Chain E:



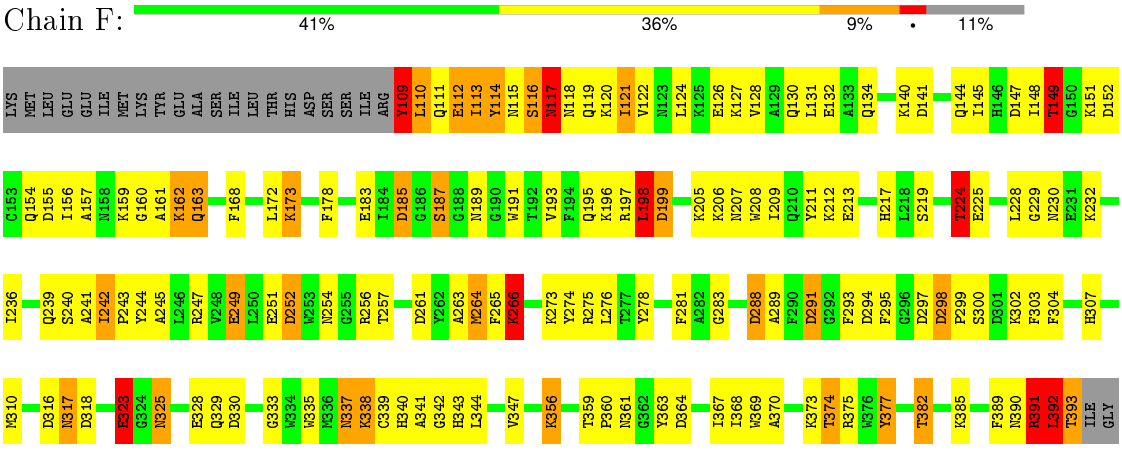
- Molecule 3: FIBRINOGEN

Chain C:



- Molecule 3: FIBRINOGEN

Chain F:



GLU GLY GLN GLN HIS HIS LEU GLY GLY ALA LYS

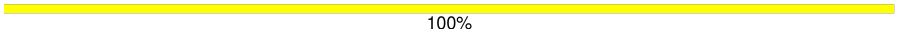
- Molecule 4: FIBRINOGEN

Chain S:

G1 H2 R3 P4

- Molecule 4: FIBRINOGEN

Chain T:



G1 H2 R3 P4

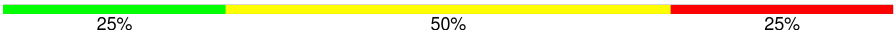
- Molecule 4: FIBRINOGEN

Chain M:

G1 H2 R3 P4

- Molecule 4: FIBRINOGEN

Chain N:



G1 H2 R3 P4

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.80Å 149.40Å 234.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10713	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.72	0/547	2.37	20/730 (2.7%)
1	D	0.73	0/440	2.68	21/586 (3.6%)
2	B	0.95	2/2489 (0.1%)	2.25	110/3363 (3.3%)
2	E	0.86	1/2437 (0.0%)	2.24	92/3290 (2.8%)
3	C	0.86	2/2407 (0.1%)	2.02	71/3256 (2.2%)
3	F	0.77	1/2351 (0.0%)	1.89	57/3180 (1.8%)
4	M	1.13	0/32	4.00	3/42 (7.1%)
4	N	0.84	0/32	4.64	2/42 (4.8%)
4	S	1.04	0/32	4.51	4/42 (9.5%)
4	T	0.83	0/32	1.68	0/42
All	All	0.85	6/10799 (0.1%)	2.18	380/14573 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	GLY	N-CA	8.02	1.58	1.46
2	E	350	GLY	N-CA	7.45	1.57	1.46
3	C	229	GLY	N-CA	7.23	1.56	1.46
3	F	229	GLY	N-CA	6.59	1.55	1.46
2	B	395	SER	CB-OG	-5.82	1.34	1.42
2	B	350	GLY	N-CA	5.39	1.54	1.46

All (380) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	448	ARG	CD-NE-CZ	35.69	173.56	123.60
1	D	162	ARG	CD-NE-CZ	34.21	171.49	123.60
4	N	3	ARG	CD-NE-CZ	27.48	162.08	123.60
2	E	455	ARG	NE-CZ-NH2	-23.33	108.63	120.30
1	A	159	ARG	NE-CZ-NH1	22.89	131.74	120.30
4	M	3	ARG	NE-CZ-NH1	-21.62	109.49	120.30
1	A	159	ARG	NE-CZ-NH2	-20.05	110.28	120.30
4	S	3	ARG	NE-CZ-NH2	-19.55	110.53	120.30
2	E	455	ARG	NE-CZ-NH1	19.12	129.86	120.30
3	C	298	ASP	CB-CG-OD2	-18.24	101.88	118.30
3	C	375	ARG	NE-CZ-NH1	-17.41	111.60	120.30
1	A	159	ARG	CD-NE-CZ	16.96	147.34	123.60
1	D	167	ARG	NE-CZ-NH1	16.33	128.47	120.30
2	E	406	ARG	NE-CZ-NH2	-15.81	112.39	120.30
3	C	228	LEU	CA-C-N	15.45	147.09	116.20
2	B	346	ARG	NE-CZ-NH1	14.91	127.75	120.30
4	S	3	ARG	NE-CZ-NH1	14.87	127.73	120.30
2	B	316	ASP	CB-CG-OD2	-14.75	105.03	118.30
2	B	455	ARG	NE-CZ-NH1	14.34	127.47	120.30
3	F	375	ARG	NE-CZ-NH1	14.28	127.44	120.30
2	B	264	ARG	NE-CZ-NH2	-14.19	113.20	120.30
2	B	166	ARG	NE-CZ-NH1	14.09	127.34	120.30
2	B	194	ARG	NE-CZ-NH1	13.93	127.27	120.30
2	E	406	ARG	NE-CZ-NH1	13.88	127.24	120.30
2	E	349	ALA	CA-C-N	13.87	143.95	116.20
3	F	228	LEU	CA-C-N	13.70	143.59	116.20
1	D	149	ARG	CD-NE-CZ	13.43	142.40	123.60
2	B	349	ALA	CA-C-N	13.10	142.41	116.20
3	F	197	ARG	NE-CZ-NH2	-12.92	113.84	120.30
2	B	194	ARG	NE-CZ-NH2	-12.88	113.86	120.30
3	C	348	TYR	CB-CG-CD2	-12.77	113.34	121.00
2	B	448	ARG	NE-CZ-NH1	12.52	126.56	120.30
2	B	316	ASP	CB-CG-OD1	12.42	129.48	118.30
2	B	448	ARG	CD-NE-CZ	12.39	140.94	123.60
2	B	212	GLU	OE1-CD-OE2	12.38	138.16	123.30
2	E	257	ASP	CB-CG-OD2	12.20	129.28	118.30
3	C	375	ARG	NH1-CZ-NH2	12.05	132.65	119.40
3	C	348	TYR	CB-CG-CD1	11.97	128.18	121.00
3	C	391	ARG	NE-CZ-NH2	-11.85	114.37	120.30
2	E	349	ALA	O-C-N	-11.68	103.35	123.20
2	E	237	ARG	NE-CZ-NH2	-11.60	114.50	120.30
4	S	3	ARG	CA-CB-CG	11.45	138.59	113.40
2	B	320	ASP	CB-CG-OD2	11.39	128.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	181	TYR	CB-CG-CD2	-11.38	114.17	121.00
2	B	237	ARG	NE-CZ-NH1	-11.17	114.72	120.30
1	D	159	ARG	NE-CZ-NH2	11.09	125.84	120.30
3	C	199	ASP	CB-CG-OD1	11.04	128.24	118.30
2	E	216	ARG	CD-NE-CZ	11.03	139.04	123.60
3	C	275	ARG	NE-CZ-NH2	-10.92	114.84	120.30
2	E	365	ARG	CD-NE-CZ	10.89	138.84	123.60
3	F	375	ARG	NE-CZ-NH2	-10.84	114.88	120.30
2	B	267	ASP	CB-CG-OD2	-10.81	108.57	118.30
2	E	448	ARG	NE-CZ-NH1	10.78	125.69	120.30
2	B	304	ARG	CD-NE-CZ	10.73	138.62	123.60
2	E	194	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	A	171	ARG	NE-CZ-NH1	10.49	125.54	120.30
2	E	415	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	E	432	ASP	CB-CG-OD1	10.45	127.71	118.30
2	B	406	ARG	NE-CZ-NH1	10.36	125.48	120.30
2	B	448	ARG	NE-CZ-NH2	-10.28	115.16	120.30
2	B	269	TYR	CB-CG-CD1	-10.26	114.84	121.00
2	B	252	ILE	CA-CB-CG2	10.26	131.41	110.90
2	E	252	ILE	CA-CB-CG2	10.26	131.41	110.90
3	F	363	TYR	CB-CG-CD1	-10.22	114.87	121.00
3	C	108	ARG	NE-CZ-NH2	-10.13	115.23	120.30
2	B	355	ASP	CB-CG-OD1	9.94	127.25	118.30
3	F	323	GLU	OE1-CD-OE2	-9.90	111.42	123.30
2	E	261	ASP	CB-CG-OD1	9.88	127.19	118.30
3	C	181	TYR	CB-CG-CD1	9.87	126.92	121.00
3	C	262	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	D	167	ARG	NE-CZ-NH2	-9.70	115.45	120.30
3	F	363	TYR	CB-CG-CD2	9.66	126.80	121.00
4	M	3	ARG	NE-CZ-NH2	9.64	125.12	120.30
2	E	297	ASP	CB-CG-OD2	-9.33	109.91	118.30
2	B	225	TYR	CB-CG-CD2	9.32	126.59	121.00
2	B	216	ARG	CD-NE-CZ	9.28	136.59	123.60
1	A	167	ARG	CD-NE-CZ	9.26	136.56	123.60
2	B	166	ARG	CD-NE-CZ	9.17	136.44	123.60
2	B	225	TYR	CB-CG-CD1	-9.16	115.50	121.00
3	F	316	ASP	CB-CG-OD1	9.15	126.53	118.30
2	B	280	THR	CA-CB-CG2	-9.13	99.62	112.40
3	C	375	ARG	NE-CZ-NH2	-9.11	115.75	120.30
3	C	108	ARG	NE-CZ-NH1	9.10	124.85	120.30
3	C	199	ASP	CA-C-N	9.03	134.27	116.20
1	A	165	CYS	CA-CB-SG	-9.00	97.80	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	ARG	CD-NE-CZ	8.96	136.15	123.60
2	E	297	ASP	CB-CG-OD1	8.87	126.28	118.30
2	B	406	ARG	NE-CZ-NH2	-8.83	115.89	120.30
3	C	294	ASP	CB-CG-OD2	-8.77	110.40	118.30
3	C	199	ASP	CB-CG-OD2	-8.70	110.47	118.30
3	C	228	LEU	O-C-N	-8.66	108.47	123.20
2	B	409	ALA	N-CA-CB	8.63	122.18	110.10
3	C	298	ASP	CB-CG-OD1	8.62	126.05	118.30
3	F	155	ASP	CB-CG-OD2	8.56	126.01	118.30
2	E	396	LYS	N-CA-CB	8.56	126.01	110.60
2	E	245	GLU	OE1-CD-OE2	8.55	133.57	123.30
1	D	141	ARG	CD-NE-CZ	8.54	135.55	123.60
1	D	141	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	167	ARG	NE-CZ-NH1	8.51	124.56	120.30
3	C	117	ASN	CB-CA-C	8.48	127.36	110.40
3	F	247	ARG	NE-CZ-NH1	-8.43	116.08	120.30
2	B	313	GLU	OE1-CD-OE2	-8.35	113.28	123.30
2	B	426	MET	CG-SD-CE	-8.32	86.89	100.20
3	C	262	TYR	CB-CG-CD2	8.28	125.97	121.00
2	E	411	ASN	CA-CB-CG	8.27	131.59	113.40
2	B	391	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	E	316	ASP	CB-CG-OD1	8.18	125.66	118.30
2	B	359	GLN	CA-CB-CG	8.18	131.39	113.40
3	C	134	GLN	OE1-CD-NE2	8.14	140.63	121.90
3	C	288	ASP	CB-CG-OD2	8.13	125.61	118.30
2	E	210	GLU	OE1-CD-OE2	-8.10	113.58	123.30
3	F	288	ASP	CB-CG-OD1	8.09	125.58	118.30
3	C	126	GLU	CA-CB-CG	8.07	131.15	113.40
2	E	269	TYR	CB-CG-CD2	8.05	125.83	121.00
3	C	134	GLN	CG-CD-OE1	-8.04	105.52	121.60
1	A	149	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	A	180	ASP	CB-CG-OD1	8.03	125.53	118.30
3	F	298	ASP	CB-CG-OD1	8.03	125.53	118.30
2	B	445	TYR	CB-CG-CD2	7.98	125.79	121.00
3	C	337	ASN	O-C-N	-7.97	109.94	122.70
1	A	149	ARG	CD-NE-CZ	7.97	134.76	123.60
1	D	162	ARG	NE-CZ-NH1	7.95	124.28	120.30
3	F	185	ASP	CB-CG-OD2	7.95	125.45	118.30
1	A	171	ARG	NE-CZ-NH2	-7.87	116.36	120.30
3	F	228	LEU	O-C-N	-7.86	109.83	123.20
2	B	269	TYR	CB-CG-CD2	7.86	125.71	121.00
2	E	398	ASP	CB-CG-OD1	7.85	125.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	365	ARG	NE-CZ-NH1	7.84	124.22	120.30
3	C	111	GLN	CA-CB-CG	7.83	130.62	113.40
2	E	395	SER	CA-C-O	-7.73	103.87	120.10
3	F	252	ASP	CB-CG-OD2	-7.73	111.35	118.30
2	B	349	ALA	O-C-N	-7.67	110.17	123.20
1	D	153	ASP	CB-CG-OD1	7.66	125.20	118.30
2	E	354	MET	CG-SD-CE	-7.66	87.95	100.20
2	B	176	ARG	NE-CZ-NH1	-7.58	116.51	120.30
3	F	391	ARG	NE-CZ-NH1	-7.54	116.53	120.30
3	F	298	ASP	CB-CG-OD2	-7.53	111.52	118.30
3	C	228	LEU	CA-C-O	-7.50	104.34	120.10
2	E	257	ASP	OD1-CG-OD2	-7.46	109.14	123.30
3	C	247	ARG	CD-NE-CZ	7.39	133.94	123.60
3	F	318	ASP	CB-CG-OD1	7.36	124.92	118.30
2	B	220	GLU	CG-CD-OE2	-7.33	103.65	118.30
2	B	318	LYS	CB-CA-C	7.32	125.05	110.40
2	B	452	MET	CG-SD-CE	7.32	111.92	100.20
3	C	244	TYR	CB-CG-CD1	-7.32	116.61	121.00
2	E	355	ASP	CB-CG-OD2	7.31	124.88	118.30
3	C	224	THR	N-CA-CB	-7.24	96.55	110.30
3	C	199	ASP	C-N-CA	-7.24	107.10	122.30
3	F	141	ASP	CB-CG-OD2	-7.23	111.79	118.30
2	B	166	ARG	NE-CZ-NH2	-7.22	116.69	120.30
3	C	337	ASN	CA-C-N	7.21	133.06	117.20
1	D	162	ARG	CG-CD-NE	7.20	126.92	111.80
2	E	395	SER	CA-C-N	7.19	133.01	117.20
3	F	141	ASP	CB-CG-OD1	7.14	124.73	118.30
2	E	169	ARG	CD-NE-CZ	7.13	133.58	123.60
3	C	272	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	177	ASP	CB-CG-OD1	-7.06	111.94	118.30
2	B	415	ARG	NE-CZ-NH1	-7.04	116.78	120.30
2	B	213	GLU	CG-CD-OE1	7.01	132.33	118.30
1	D	135	LEU	CB-CA-C	7.00	123.50	110.20
1	D	149	ARG	NE-CZ-NH2	-6.99	116.81	120.30
2	B	313	GLU	CG-CD-OE1	6.98	132.26	118.30
3	F	252	ASP	CB-CG-OD1	6.97	124.57	118.30
2	E	166	ARG	CD-NE-CZ	6.96	133.34	123.60
1	A	164	SER	N-CA-CB	-6.91	100.13	110.50
2	E	261	ASP	CB-CG-OD2	-6.89	112.10	118.30
3	C	301	ASP	CB-CG-OD1	-6.89	112.10	118.30
2	E	380	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	B	455	ARG	NE-CZ-NH2	-6.85	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	261	ASP	CB-CG-OD1	6.82	124.44	118.30
3	F	318	ASP	OD1-CG-OD2	-6.82	110.34	123.30
3	C	185	ASP	CB-CG-OD1	6.81	124.43	118.30
3	C	391	ARG	NH1-CZ-NH2	6.80	126.88	119.40
2	B	267	ASP	CA-CB-CG	-6.78	98.47	113.40
3	F	318	ASP	CB-CG-OD2	6.78	124.41	118.30
2	E	415	ARG	NH1-CZ-NH2	6.76	126.84	119.40
2	E	321	LYS	CA-CB-CG	6.75	128.26	113.40
3	F	338	LYS	O-C-N	-6.74	111.92	122.70
2	B	406	ARG	CD-NE-CZ	6.68	132.95	123.60
2	B	399	GLY	N-CA-C	6.67	129.76	113.10
3	C	391	ARG	CG-CD-NE	-6.65	97.83	111.80
2	E	281	ASP	CB-CG-OD1	-6.65	112.31	118.30
3	F	224	THR	N-CA-CB	-6.64	97.68	110.30
2	B	230	ASP	CB-CG-OD2	-6.60	112.36	118.30
2	B	264	ARG	CD-NE-CZ	-6.58	114.38	123.60
2	B	457	PHE	CA-C-N	6.58	131.68	117.20
2	E	191	GLU	CG-CD-OE2	-6.58	105.15	118.30
2	E	267	ASP	CB-CG-OD2	-6.58	112.38	118.30
3	F	228	LEU	CA-C-O	-6.56	106.33	120.10
2	E	269	TYR	CB-CG-CD1	-6.53	117.08	121.00
2	E	304	ARG	NE-CZ-NH1	-6.52	117.04	120.30
2	E	445	TYR	O-C-N	-6.51	112.28	122.70
3	C	185	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	E	349	ALA	C-N-CA	-6.51	108.64	122.30
2	E	213	GLU	CG-CD-OE1	6.50	131.30	118.30
2	B	379	ASP	CB-CG-OD1	6.49	124.14	118.30
2	E	392	LYS	CA-C-O	6.49	133.73	120.10
2	B	169	ARG	N-CA-CB	-6.48	98.93	110.60
3	C	247	ARG	NE-CZ-NH1	-6.47	117.06	120.30
2	B	261	ASP	CB-CG-OD1	6.44	124.10	118.30
2	B	224	MET	CG-SD-CE	-6.44	89.90	100.20
2	B	243	ASN	CA-CB-CG	-6.43	99.25	113.40
2	B	309	GLU	C-N-CA	6.42	137.75	121.70
3	F	197	ARG	NE-CZ-NH1	6.37	123.48	120.30
3	F	205	LYS	CD-CE-NZ	6.37	126.35	111.70
2	B	415	ARG	CD-NE-CZ	-6.36	114.69	123.60
2	E	237	ARG	CD-NE-CZ	6.36	132.51	123.60
3	C	280	TYR	CB-CG-CD2	-6.34	117.19	121.00
3	C	318	ASP	CA-CB-CG	6.34	127.35	113.40
2	E	457	PHE	CB-CG-CD1	-6.34	116.36	120.80
1	A	135	LEU	CB-CG-CD2	6.26	121.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	E	418	TRP	CA-C-N	6.23	128.66	116.20
2	B	421	GLN	CB-CG-CD	6.22	127.79	111.60
3	F	392	LEU	CA-CB-CG	6.19	129.54	115.30
3	F	291	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	157	LYS	O-C-N	-6.17	112.83	122.70
2	B	255	ARG	CD-NE-CZ	6.16	132.23	123.60
3	C	316	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	180	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	186	GLU	OE1-CD-OE2	6.15	130.68	123.30
3	C	143	VAL	CA-CB-CG2	6.14	120.11	110.90
2	B	237	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	B	216	ARG	NE-CZ-NH1	-6.11	117.24	120.30
2	B	349	ALA	CA-C-O	-6.11	107.27	120.10
2	B	257	ASP	CB-CG-OD1	6.09	123.78	118.30
2	E	304	ARG	CD-NE-CZ	6.08	132.11	123.60
3	F	274	TYR	CB-CG-CD1	6.08	124.65	121.00
3	F	199	ASP	CA-C-N	6.06	128.33	116.20
2	B	365	ARG	NE-CZ-NH2	-6.05	117.27	120.30
3	F	347	VAL	CA-CB-CG2	-6.04	101.85	110.90
3	C	375	ARG	CD-NE-CZ	-6.02	115.17	123.60
2	E	433	ASP	CB-CG-OD2	-6.02	112.89	118.30
2	E	181	LYS	CB-CA-C	6.00	122.40	110.40
2	B	253	GLN	CA-CB-CG	5.99	126.58	113.40
2	B	379	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	167	ARG	CA-CB-CG	5.99	126.57	113.40
2	B	380	ARG	CD-NE-CZ	-5.97	115.24	123.60
1	D	175	LEU	CA-CB-CG	5.97	129.03	115.30
2	E	184	SER	N-CA-CB	-5.96	101.55	110.50
2	B	380	ARG	NE-CZ-NH1	-5.96	117.32	120.30
2	B	267	ASP	CB-CG-OD1	5.96	123.66	118.30
3	C	108	ARG	CD-NE-CZ	5.93	131.90	123.60
2	B	292	TYR	CB-CG-CD1	5.92	124.55	121.00
3	F	261	ASP	CB-CG-OD1	5.92	123.63	118.30
2	B	398	ASP	CB-CG-OD2	5.89	123.60	118.30
2	B	346	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	D	165	CYS	CA-CB-SG	-5.89	103.40	114.00
3	F	114	TYR	CB-CG-CD1	5.89	124.53	121.00
3	F	109	TYR	CB-CG-CD1	5.88	124.53	121.00
3	F	275	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	B	341	SER	N-CA-CB	-5.87	101.70	110.50
2	B	349	ALA	C-N-CA	-5.86	110.00	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	252	ASP	CB-CG-OD1	5.82	123.54	118.30
2	E	433	ASP	CB-CG-OD1	5.82	123.54	118.30
2	B	297	ASP	CB-CG-OD1	5.81	123.53	118.30
2	B	271	GLN	CB-CA-C	-5.79	98.81	110.40
3	F	228	LEU	C-N-CA	-5.79	110.15	122.30
2	E	324	ALA	O-C-N	5.79	131.96	122.70
3	F	185	ASP	OD1-CG-OD2	-5.78	112.31	123.30
2	E	233	VAL	CB-CA-C	-5.78	100.42	111.40
2	E	318	LYS	CA-C-O	5.77	132.21	120.10
2	B	233	VAL	CB-CA-C	-5.76	100.45	111.40
2	E	191	GLU	CG-CD-OE1	5.75	129.80	118.30
3	F	183	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	D	171	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	157	LYS	CA-CB-CG	5.74	126.02	113.40
3	C	167	TYR	CB-CG-CD2	-5.73	117.56	121.00
2	E	252	ILE	N-CA-CB	-5.68	97.75	110.80
3	C	149	THR	N-CA-CB	5.67	121.08	110.30
3	F	109	TYR	CA-CB-CG	5.67	124.18	113.40
3	C	275	ARG	CD-NE-CZ	-5.67	115.66	123.60
2	E	169	ARG	CA-CB-CG	5.67	125.88	113.40
3	C	328	GLU	CA-CB-CG	5.65	125.84	113.40
2	E	178	LYS	CA-CB-CG	5.65	125.82	113.40
2	E	277	ALA	N-CA-CB	-5.62	102.23	110.10
2	E	239	TYR	O-C-N	-5.61	113.72	122.70
3	C	270	GLU	OE1-CD-OE2	5.60	130.03	123.30
2	E	282	GLY	C-N-CA	5.60	135.70	121.70
2	B	448	ARG	CB-CG-CD	5.59	126.14	111.60
3	C	135	CYS	N-CA-CB	-5.58	100.55	110.60
4	N	3	ARG	N-CA-CB	5.58	120.64	110.60
3	C	109	TYR	CB-CG-CD1	5.58	124.35	121.00
3	F	377	TYR	CB-CG-CD2	-5.56	117.66	121.00
2	E	266	TRP	N-CA-CB	-5.54	100.64	110.60
3	C	134	GLN	CA-CB-CG	-5.53	101.23	113.40
2	B	185	ASP	CB-CG-OD1	5.53	123.28	118.30
2	E	457	PHE	CA-C-N	5.52	129.34	117.20
2	E	187	SER	N-CA-CB	-5.52	102.22	110.50
3	F	338	LYS	N-CA-C	5.51	125.89	111.00
2	E	359	GLN	CA-CB-CG	5.50	125.51	113.40
2	B	250	THR	CA-CB-CG2	5.50	120.10	112.40
2	E	320	ASP	CB-CG-OD1	5.49	123.24	118.30
2	E	448	ARG	CG-CD-NE	5.49	123.32	111.80
2	B	345	TYR	CZ-CE2-CD2	-5.48	114.86	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	444	TRP	CA-CB-CG	-5.48	103.29	113.70
2	B	445	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	D	147	MET	CG-SD-CE	-5.46	91.46	100.20
2	B	280	THR	OG1-CB-CG2	5.46	122.55	110.00
4	M	3	ARG	NH1-CZ-NH2	5.44	125.39	119.40
2	B	421	GLN	O-C-N	-5.44	114.00	122.70
2	B	236	TYR	CB-CG-CD2	5.44	124.26	121.00
2	E	226	LEU	CB-CA-C	-5.42	99.89	110.20
2	B	195	THR	CA-CB-OG1	5.41	120.36	109.00
2	E	344	LYS	O-C-N	-5.40	114.06	122.70
3	C	320	ASP	CB-CG-OD2	-5.39	113.45	118.30
3	F	249	GLU	N-CA-CB	5.39	120.30	110.60
3	C	224	THR	CA-CB-CG2	5.38	119.93	112.40
1	D	141	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	B	320	ASP	OD1-CG-OD2	-5.38	113.08	123.30
2	E	392	LYS	O-C-N	-5.37	114.11	122.70
2	B	341	SER	CA-CB-OG	-5.35	96.75	111.20
2	B	181	LYS	CA-CB-CG	5.35	125.16	113.40
3	C	110	LEU	CB-CA-C	5.34	120.35	110.20
2	B	213	GLU	CG-CD-OE2	-5.34	107.62	118.30
1	D	135	LEU	CA-C-O	5.33	131.29	120.10
2	B	284	ASN	CB-CA-C	5.32	121.03	110.40
3	F	149	THR	N-CA-CB	5.31	120.40	110.30
2	E	409	ALA	N-CA-CB	5.31	117.53	110.10
3	F	266	LYS	CB-CA-C	5.30	121.01	110.40
3	F	333	GLY	N-CA-C	-5.30	99.84	113.10
2	B	183	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	D	147	MET	N-CA-CB	-5.30	101.06	110.60
2	E	292	TYR	CB-CG-CD2	5.29	124.17	121.00
3	F	294	ASP	CB-CG-OD2	5.28	123.05	118.30
2	E	321	LYS	CD-CE-NZ	5.27	123.82	111.70
3	F	337	ASN	C-N-CA	-5.26	108.55	121.70
3	F	391	ARG	NH1-CZ-NH2	5.25	125.18	119.40
2	E	237	ARG	NH1-CZ-NH2	5.25	125.18	119.40
2	B	166	ARG	N-CA-CB	5.25	120.05	110.60
2	B	440	TRP	O-C-N	-5.24	114.31	122.70
2	E	242	MET	CG-SD-CE	5.24	108.58	100.20
1	D	166	SER	CA-C-N	5.24	128.72	117.20
3	C	228	LEU	C-N-CA	-5.22	111.33	122.30
2	B	277	ALA	N-CA-CB	-5.20	102.82	110.10
3	C	114	TYR	CB-CG-CD1	-5.20	117.88	121.00
2	B	373	MET	CA-CB-CG	5.19	122.13	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	381	ASP	CB-CA-C	-5.19	100.02	110.40
2	E	213	GLU	CG-CD-OE2	-5.18	107.94	118.30
2	B	213	GLU	N-CA-CB	-5.18	101.28	110.60
3	C	197	ARG	CA-CB-CG	5.18	124.79	113.40
3	F	193	VAL	CA-CB-CG1	5.18	118.66	110.90
3	C	199	ASP	CA-C-O	-5.17	109.24	120.10
3	C	229	GLY	O-C-N	-5.17	114.42	122.70
3	C	356	LYS	CA-CB-CG	5.15	124.74	113.40
2	B	252	ILE	N-CA-CB	-5.15	98.95	110.80
2	E	395	SER	C-N-CA	-5.15	108.83	121.70
2	E	194	ARG	CG-CD-NE	-5.13	101.02	111.80
2	E	413	ASN	O-C-N	-5.13	114.48	123.20
2	B	450	MET	CG-SD-CE	5.13	108.40	100.20
2	E	234	LYS	N-CA-CB	-5.13	101.37	110.60
2	B	451	SER	CB-CA-C	-5.12	100.36	110.10
2	B	318	LYS	CA-CB-CG	5.11	124.65	113.40
2	B	455	ARG	CD-NE-CZ	-5.11	116.44	123.60
2	B	406	ARG	CA-C-O	5.11	130.84	120.10
3	F	356	LYS	CB-CA-C	5.11	120.62	110.40
3	F	198	LEU	CB-CA-C	-5.11	100.49	110.20
3	C	135	CYS	CA-CB-SG	-5.11	104.81	114.00
2	E	327	GLY	CA-C-O	-5.10	111.41	120.60
2	E	347	GLY	CA-C-O	5.10	129.78	120.60
3	F	207	ASN	N-CA-CB	-5.10	101.42	110.60
2	B	239	TYR	CB-CG-CD1	-5.09	117.94	121.00
2	B	401	GLY	N-CA-C	-5.09	100.38	113.10
2	E	437	TRP	N-CA-CB	5.08	119.75	110.60
2	E	318	LYS	O-C-N	-5.08	114.56	123.20
2	E	418	TRP	CA-CB-CG	-5.08	104.04	113.70
3	C	271	ALA	N-CA-CB	5.08	117.21	110.10
2	E	381	ASP	CB-CG-OD1	5.08	122.87	118.30
3	C	336	MET	CG-SD-CE	5.07	108.31	100.20
2	B	397	GLU	OE1-CD-OE2	-5.06	117.22	123.30
3	C	176	GLN	CA-CB-CG	5.05	124.51	113.40
2	B	383	ASP	CB-CG-OD1	-5.05	113.75	118.30
3	C	356	LYS	N-CA-CB	5.05	119.69	110.60
2	E	427	ALA	O-C-N	-5.05	114.62	122.70
3	F	149	THR	OG1-CB-CG2	5.04	121.60	110.00
3	F	330	ASP	CB-CG-OD1	5.03	122.83	118.30
2	B	264	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	E	301	GLN	CA-CB-CG	5.01	124.43	113.40
3	F	247	ARG	CA-C-O	-5.01	109.58	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	3	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	427	ALA	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	546	0	573	106	0
1	D	440	0	456	108	0
2	B	2427	0	2295	163	0
2	E	2376	0	2243	214	0
3	C	2342	0	2188	143	6
3	F	2287	0	2136	223	5
4	M	31	0	32	5	0
4	N	31	0	32	9	0
4	S	31	0	32	7	0
4	T	31	0	32	6	0
5	B	28	0	25	10	0
5	E	28	0	25	11	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
7	A	1	0	0	0	0
7	B	31	0	0	10	0
7	C	20	0	0	2	0
7	D	3	0	0	2	0
7	E	29	0	0	8	0
7	F	23	0	0	2	1
All	All	10713	0	10069	841	6

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 41.

All (841) 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)
2:E:172:LEU:HD11	3:F:114:TYR:CD2	1.31	1.59
3:C:104:ASP:HA	3:C:107:ILE:CD1	1.33	1.53
2:E:171:ILE:CG2	2:E:172:LEU:CD2	1.86	1.50
2:E:171:ILE:CG2	2:E:172:LEU:HD23	1.08	1.49
3:F:109:TYR:N	3:F:112:GLU:CB	1.78	1.46
1:A:179:GLU:C	1:A:183:LYS:HE3	1.36	1.44
2:E:378:TYR:CG	2:E:396:LYS:HE2	1.54	1.42
2:E:176:ARG:HB2	3:F:117:ASN:OD1	1.20	1.33
2:B:361:MET:HB2	5:B:470:NAG:C8	1.56	1.33
2:E:172:LEU:CD1	3:F:114:TYR:CD2	2.11	1.31
3:C:265:PHE:O	3:C:266:LYS:HD2	1.16	1.31
5:B:470:NAG:O3	5:B:471:NAG:N2	1.64	1.27
1:D:138:LYS:O	1:D:141:ARG:HB3	1.27	1.27
1:A:180:ASP:HA	1:A:183:LYS:CD	1.62	1.27
1:D:140:VAL:HG12	3:F:114:TYR:CE2	1.70	1.26
1:A:188:VAL:HG22	2:B:165:LEU:CD2	1.66	1.24
1:D:138:LYS:O	1:D:141:ARG:CB	1.85	1.24
3:C:298:ASP:OD1	3:C:300:SER:N	1.70	1.23
2:E:171:ILE:CG2	2:E:172:LEU:H	1.44	1.23
2:B:230:ASP:O	2:B:233:VAL:HG23	1.34	1.21
3:F:109:TYR:N	3:F:112:GLU:CG	2.03	1.21
3:F:149:THR:HG22	3:F:168:PHE:O	1.42	1.20
3:F:217:HIS:O	3:F:224:THR:HG23	1.38	1.20
3:C:103:HIS:O	3:C:106:SER:OG	1.60	1.17
1:D:178:TYR:O	1:D:182:GLN:HG2	1.43	1.17
3:C:265:PHE:O	3:C:266:LYS:CD	1.92	1.17
1:D:179:GLU:HB3	1:D:183:LYS:NZ	1.59	1.17
1:A:128:GLU:O	1:A:131:GLN:NE2	1.78	1.16
5:E:470:NAG:C6	5:E:471:NAG:C1	2.22	1.16
5:E:470:NAG:H62	5:E:471:NAG:O5	1.44	1.16
1:D:188:VAL:HG22	2:E:165:LEU:HD11	1.23	1.15
2:B:165:LEU:HB3	7:B:498:HOH:O	1.42	1.15
2:E:230:ASP:O	2:E:233:VAL:HG23	1.47	1.14
1:A:180:ASP:N	1:A:183:LYS:HE3	1.63	1.14
1:A:180:ASP:CA	1:A:183:LYS:HD2	1.77	1.14
3:F:185:ASP:OD2	3:F:187:SER:HB2	1.43	1.14
2:E:179:ILE:HD12	3:F:117:ASN:HB2	1.30	1.14
1:D:188:VAL:CG2	2:E:165:LEU:HD11	1.77	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:MET:CB	5:B:470:NAG:H82	1.77	1.13
5:E:470:NAG:H62	5:E:471:NAG:C1	1.77	1.12
2:E:176:ARG:CB	3:F:117:ASN:OD1	1.98	1.12
1:A:133:ILE:O	1:A:135:LEU:N	1.82	1.12
2:E:381:ASP:HB2	2:E:393:GLN:HE22	1.13	1.12
1:A:134:GLN:O	1:A:135:LEU:HD22	1.49	1.11
2:E:168:LEU:HB3	7:E:44:HOH:O	1.50	1.10
3:C:104:ASP:HA	3:C:107:ILE:HD13	1.12	1.10
2:E:169:ARG:NH1	2:E:173:GLU:OE2	1.82	1.10
3:C:104:ASP:CA	3:C:107:ILE:CD1	2.28	1.10
1:D:140:VAL:CG1	3:F:114:TYR:HE2	1.63	1.09
2:E:179:ILE:HD12	3:F:117:ASN:CB	1.81	1.09
3:F:109:TYR:N	3:F:112:GLU:HB2	1.63	1.08
2:B:165:LEU:CB	7:B:498:HOH:O	1.99	1.08
1:A:179:GLU:C	1:A:183:LYS:CE	2.20	1.07
2:E:179:ILE:CD1	3:F:117:ASN:O	2.03	1.06
1:D:166:SER:HB3	2:E:195:THR:HG23	1.32	1.06
3:F:109:TYR:N	3:F:112:GLU:HB3	1.68	1.05
2:E:381:ASP:HB2	2:E:393:GLN:NE2	1.69	1.05
1:A:180:ASP:HA	1:A:183:LYS:HD2	1.36	1.05
1:D:179:GLU:C	1:D:183:LYS:HE3	1.77	1.05
3:C:109:TYR:O	3:C:113:ILE:HD13	1.55	1.05
2:E:171:ILE:HG23	2:E:172:LEU:CD2	1.82	1.04
3:C:104:ASP:CA	3:C:107:ILE:HD13	1.87	1.04
2:E:171:ILE:HG21	2:E:172:LEU:HD23	1.08	1.04
1:A:134:GLN:O	1:A:135:LEU:CD2	2.05	1.04
2:E:378:TYR:CD1	2:E:396:LYS:HE2	1.93	1.04
2:E:176:ARG:HA	3:F:117:ASN:HB3	1.04	1.04
2:E:385:TRP:HD1	2:E:406:ARG:NH1	1.55	1.04
3:C:173:LYS:HE2	3:C:238:THR:O	1.57	1.04
2:B:168:LEU:O	2:B:171:ILE:N	1.91	1.04
2:E:176:ARG:HA	3:F:117:ASN:CB	1.87	1.03
3:F:149:THR:CG2	3:F:168:PHE:O	2.06	1.03
3:C:104:ASP:HA	3:C:107:ILE:HD12	1.36	1.03
2:B:230:ASP:O	2:B:233:VAL:CG2	2.06	1.03
2:E:385:TRP:CD1	2:E:406:ARG:NH1	2.27	1.03
1:D:147:MET:SD	3:F:121:ILE:HD11	1.99	1.02
2:E:378:TYR:CD1	2:E:396:LYS:CE	2.43	1.02
1:D:179:GLU:HB3	1:D:183:LYS:CE	1.88	1.02
1:A:188:VAL:HG22	2:B:165:LEU:HD21	1.02	1.02
3:F:217:HIS:O	3:F:224:THR:CG2	2.06	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:381:ASP:CB	2:E:393:GLN:HE22	1.71	1.02
3:C:105:SER:O	3:C:108:ARG:HG3	1.57	1.01
2:E:378:TYR:CG	2:E:396:LYS:CE	2.43	1.01
1:A:188:VAL:CG2	2:B:165:LEU:HD21	1.90	1.01
2:E:171:ILE:CG2	2:E:172:LEU:N	2.16	1.01
2:E:171:ILE:HG22	2:E:172:LEU:H	0.88	1.00
2:E:172:LEU:HD11	3:F:114:TYR:CE2	1.97	1.00
2:B:323:LYS:HE2	7:B:488:HOH:O	1.59	0.99
2:E:209:LYS:HG3	2:E:213:GLU:OE1	1.60	0.99
1:A:180:ASP:CA	1:A:183:LYS:CD	2.35	0.99
1:D:179:GLU:C	1:D:183:LYS:CE	2.31	0.98
2:E:171:ILE:HG22	2:E:172:LEU:N	1.74	0.98
1:A:148:LYS:HE3	1:A:182:GLN:HE22	1.23	0.98
2:E:176:ARG:CA	3:F:117:ASN:HB3	1.93	0.98
3:F:111:GLN:HE21	3:F:112:GLU:HG2	1.29	0.98
3:F:160:GLY:O	3:F:162:LYS:HE2	1.63	0.97
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.47	0.97
2:B:169:ARG:O	2:B:173:GLU:HG2	1.64	0.97
2:B:361:MET:HB2	5:B:470:NAG:H82	0.99	0.97
2:E:385:TRP:CH2	4:N:3:ARG:HD2	2.00	0.97
1:D:188:VAL:CG1	2:E:165:LEU:HD21	1.96	0.96
2:B:160:ASN:C	2:B:162:PRO:HD2	1.86	0.95
1:D:140:VAL:HG12	3:F:114:TYR:HE2	0.80	0.95
3:F:109:TYR:CA	3:F:112:GLU:HG3	1.95	0.95
1:A:179:GLU:O	1:A:183:LYS:CD	2.13	0.95
3:F:298:ASP:OD1	3:F:300:SER:OG	1.85	0.95
2:E:171:ILE:HG22	2:E:172:LEU:HD23	0.97	0.95
3:F:117:ASN:HD22	3:F:118:ASN:N	1.65	0.95
2:B:381:ASP:OD2	7:B:477:HOH:O	1.84	0.95
1:A:133:ILE:C	1:A:135:LEU:H	1.71	0.94
3:C:265:PHE:C	3:C:266:LYS:HD3	1.88	0.93
2:E:171:ILE:HG23	2:E:172:LEU:HD22	1.47	0.93
1:D:179:GLU:CB	1:D:183:LYS:NZ	2.31	0.93
2:E:179:ILE:HD13	3:F:117:ASN:O	1.67	0.93
2:E:190:MET:SD	3:F:134:GLN:NE2	2.42	0.92
1:D:188:VAL:CG2	2:E:165:LEU:HD21	1.98	0.92
1:A:143:GLN:CD	3:C:117:ASN:HD21	1.72	0.92
5:E:470:NAG:H62	5:E:471:NAG:C5	2.00	0.92
3:F:109:TYR:N	3:F:112:GLU:HG3	1.84	0.92
3:C:265:PHE:C	3:C:266:LYS:CD	2.38	0.92
2:E:179:ILE:HD12	3:F:117:ASN:CA	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:171:ILE:HG22	2:E:172:LEU:CD2	1.74	0.91
3:C:217:HIS:O	3:C:224:THR:HG23	1.71	0.91
1:D:135:LEU:O	1:D:138:LYS:N	2.03	0.91
2:E:423:THR:OG1	2:E:425:ASP:OD1	1.87	0.90
1:A:143:GLN:OE1	3:C:117:ASN:ND2	2.02	0.90
3:F:325:ASN:ND2	3:F:328:GLU:H	1.69	0.90
3:F:263:ALA:HB1	3:F:264:MET:HE1	1.54	0.90
1:A:180:ASP:N	1:A:183:LYS:CE	2.31	0.90
1:D:166:SER:HB3	2:E:195:THR:CG2	2.00	0.90
2:E:252:ILE:HD12	2:E:299:ILE:HG12	1.53	0.90
1:A:180:ASP:OD1	1:A:183:LYS:NZ	2.05	0.90
2:B:169:ARG:NH1	2:B:173:GLU:CD	2.24	0.90
3:F:109:TYR:CB	3:F:112:GLU:HG3	2.02	0.90
3:C:307:HIS:HD2	3:C:335:TRP:O	1.53	0.90
1:A:179:GLU:O	1:A:183:LYS:HD2	1.72	0.89
2:B:265:LYS:HE3	2:B:378:TYR:OH	1.70	0.89
1:D:188:VAL:HG22	2:E:165:LEU:CD1	2.02	0.89
1:D:177:ASP:OD2	2:E:178:LYS:NZ	2.06	0.89
2:E:315:GLU:OE2	2:E:448:ARG:NH1	2.06	0.89
1:A:188:VAL:CG2	2:B:165:LEU:CD2	2.47	0.89
2:B:333:ASN:ND2	2:B:333:ASN:H	1.70	0.89
2:E:172:LEU:CD1	3:F:114:TYR:HD2	1.65	0.88
2:E:172:LEU:HD11	3:F:114:TYR:HD2	1.07	0.88
5:E:470:NAG:O6	5:E:471:NAG:H5	1.73	0.88
2:E:385:TRP:HD1	2:E:406:ARG:HH11	1.15	0.88
1:D:175:LEU:O	1:D:178:TYR:N	2.06	0.88
3:C:105:SER:C	3:C:108:ARG:HG3	1.93	0.88
1:D:179:GLU:O	1:D:183:LYS:HD2	1.71	0.88
1:A:148:LYS:HE3	1:A:182:GLN:NE2	1.88	0.88
2:E:183:GLU:OE1	3:F:120:LYS:HD3	1.74	0.88
1:D:179:GLU:CB	1:D:183:LYS:HZ2	1.88	0.87
1:A:143:GLN:CD	3:C:117:ASN:ND2	2.28	0.86
1:D:180:ASP:N	1:D:183:LYS:HZ2	1.72	0.86
2:E:169:ARG:NH1	2:E:173:GLU:CD	2.27	0.86
1:A:180:ASP:HA	1:A:183:LYS:HD3	1.57	0.86
3:F:185:ASP:OD2	3:F:187:SER:CB	2.23	0.86
2:E:396:LYS:O	2:E:398:ASP:N	2.07	0.86
1:A:143:GLN:NE2	3:C:117:ASN:ND2	2.23	0.86
2:E:230:ASP:O	2:E:233:VAL:CG2	2.23	0.86
2:E:168:LEU:O	2:E:170:SER:N	2.09	0.85
1:D:147:MET:SD	3:F:121:ILE:CD1	2.64	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ILE:O	2:B:164:ASN:HB3	1.76	0.85
3:F:116:SER:O	3:F:119:GLN:N	2.09	0.85
2:B:181:LYS:HE2	2:B:185:ASP:OD2	1.76	0.85
2:B:333:ASN:HD22	2:B:333:ASN:H	1.22	0.85
2:E:179:ILE:CD1	3:F:117:ASN:HB2	2.07	0.84
3:F:189:ASN:OD1	3:F:391:ARG:HG3	1.77	0.84
3:C:240:SER:OG	3:C:242:ILE:CD1	2.25	0.84
1:A:181:GLN:HE22	2:B:174:ASN:ND2	1.76	0.84
1:A:186:GLU:O	1:A:189:ILE:N	2.08	0.84
2:E:169:ARG:HH12	2:E:173:GLU:CD	1.81	0.83
3:F:240:SER:OG	3:F:242:ILE:HG13	1.78	0.83
2:B:415:ARG:NE	7:B:495:HOH:O	2.02	0.83
1:A:169:LEU:HD23	1:A:171:ARG:HD2	1.59	0.83
1:D:179:GLU:CA	1:D:183:LYS:HE3	2.09	0.83
2:E:378:TYR:CB	2:E:396:LYS:HE2	2.09	0.82
2:B:169:ARG:HH12	2:B:173:GLU:CD	1.81	0.82
3:C:209:ILE:H	3:C:209:ILE:HD12	1.44	0.82
1:A:134:GLN:C	1:A:135:LEU:HD23	2.01	0.82
3:C:329:GLN:HE22	4:S:3:ARG:HD2	1.42	0.82
2:E:212:GLU:OE2	2:E:216:ARG:HD3	1.80	0.81
1:A:180:ASP:HA	1:A:183:LYS:CE	2.10	0.81
3:C:217:HIS:O	3:C:224:THR:CG2	2.28	0.81
2:E:168:LEU:O	2:E:169:ARG:C	2.20	0.80
2:B:161:ILE:O	2:B:164:ASN:CB	2.28	0.80
2:E:381:ASP:CB	2:E:393:GLN:NE2	2.35	0.80
2:E:378:TYR:CD1	2:E:396:LYS:HE3	2.15	0.79
1:A:134:GLN:HG3	1:A:135:LEU:HD23	1.62	0.79
2:E:168:LEU:O	2:E:171:ILE:N	2.15	0.79
1:A:180:ASP:C	1:A:183:LYS:HD2	2.02	0.79
2:E:176:ARG:HD3	3:F:113:ILE:HG23	1.62	0.79
3:C:296:GLY:O	7:C:408:HOH:O	1.99	0.79
1:A:140:VAL:HG11	2:B:172:LEU:HD21	1.65	0.79
3:F:109:TYR:HB2	3:F:112:GLU:HG3	1.64	0.79
3:C:104:ASP:HA	3:C:107:ILE:HD11	1.60	0.79
2:B:159:SER:HB2	2:B:162:PRO:HG3	1.65	0.79
2:B:179:ILE:O	2:B:183:GLU:HG2	1.83	0.78
3:F:122:VAL:O	3:F:126:GLU:HG2	1.81	0.78
2:E:385:TRP:CZ2	4:N:3:ARG:HD2	2.18	0.78
2:B:385:TRP:CZ3	4:M:3:ARG:NH1	2.51	0.78
1:A:131:GLN:HA	1:A:134:GLN:HG3	1.62	0.78
3:C:206:LYS:HD2	3:C:210:GLN:OE1	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:CA	1:A:183:LYS:CE	2.62	0.78
2:B:166:ARG:NH2	3:C:106:SER:CB	2.46	0.78
1:A:131:GLN:HA	1:A:134:GLN:CG	2.14	0.78
1:D:188:VAL:HG21	2:E:165:LEU:HD21	1.67	0.77
1:A:178:TYR:O	1:A:182:GLN:HG2	1.84	0.77
2:E:458:PHE:HB3	2:E:459:PRO:HD3	1.67	0.77
2:E:172:LEU:HD12	3:F:114:TYR:HA	1.64	0.77
3:F:161:ALA:O	3:F:162:LYS:HE2	1.85	0.77
1:D:140:VAL:N	3:F:114:TYR:OH	2.18	0.77
5:E:470:NAG:C6	5:E:471:NAG:C5	2.62	0.77
2:B:406:ARG:O	4:M:2:HIS:HA	1.84	0.77
3:F:148:ILE:HG22	3:F:156:ILE:HG12	1.67	0.77
2:B:415:ARG:NH2	7:B:495:HOH:O	2.17	0.76
3:F:209:ILE:HD12	3:F:209:ILE:H	1.50	0.76
3:F:117:ASN:ND2	3:F:118:ASN:N	2.34	0.76
2:E:397:GLU:O	2:E:398:ASP:CG	2.24	0.76
3:C:329:GLN:NE2	4:S:3:ARG:HH11	1.83	0.76
3:F:160:GLY:C	3:F:162:LYS:HE2	2.05	0.76
1:A:127:ILE:HD12	1:A:130:VAL:HG23	1.66	0.76
3:C:252:ASP:OD2	3:C:256:ARG:HB2	1.85	0.76
3:F:307:HIS:HD2	3:F:335:TRP:O	1.69	0.76
1:D:188:VAL:HG11	2:E:165:LEU:HD21	1.67	0.75
5:E:470:NAG:O6	5:E:471:NAG:C1	2.33	0.75
2:E:422:TYR:HA	2:E:426:MET:HE1	1.67	0.75
2:E:422:TYR:HA	2:E:426:MET:CE	2.17	0.74
1:D:179:GLU:HB3	1:D:183:LYS:HZ1	1.49	0.74
2:E:171:ILE:HG21	2:E:172:LEU:CD2	1.81	0.74
1:D:140:VAL:CG1	2:E:172:LEU:HD21	2.17	0.74
1:D:179:GLU:HB3	1:D:183:LYS:HE3	1.68	0.74
3:F:178:PHE:CE1	3:F:232:LYS:HG2	2.22	0.74
3:F:110:LEU:HB2	3:F:111:GLN:NE2	2.01	0.74
2:B:161:ILE:N	2:B:162:PRO:HD2	2.00	0.74
2:B:439:ASN:HD22	2:B:439:ASN:H	1.33	0.73
2:B:428:LYS:HG2	2:B:429:HIS:CD2	2.22	0.73
2:E:171:ILE:O	2:E:174:ASN:N	2.22	0.73
1:D:177:ASP:O	1:D:181:GLN:HB2	1.89	0.73
3:F:304:PHE:O	3:F:337:ASN:O	2.05	0.73
1:A:179:GLU:HB2	1:A:183:LYS:HE3	1.69	0.72
3:C:149:THR:HG23	3:C:168:PHE:O	1.88	0.72
2:E:397:GLU:O	2:E:398:ASP:OD1	2.06	0.72
3:C:294:ASP:OD1	7:C:408:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ASP:N	1:D:183:LYS:NZ	2.36	0.72
1:A:134:GLN:C	1:A:135:LEU:CD2	2.57	0.72
1:A:181:GLN:NE2	2:B:174:ASN:ND2	2.37	0.72
3:C:240:SER:OG	3:C:242:ILE:HG13	1.89	0.72
1:A:151:GLU:HG2	1:A:173:VAL:HG13	1.71	0.72
1:D:188:VAL:CG2	2:E:165:LEU:CD1	2.62	0.71
2:E:179:ILE:CD1	3:F:117:ASN:C	2.58	0.71
2:E:172:LEU:HD12	3:F:114:TYR:CD2	2.22	0.71
3:C:104:ASP:CB	3:C:107:ILE:HD13	2.20	0.71
5:B:470:NAG:O3	5:B:471:NAG:C7	2.39	0.71
3:C:307:HIS:HE1	3:C:341:ALA:H	1.39	0.71
1:A:143:GLN:HE22	3:C:117:ASN:ND2	1.86	0.71
1:D:151:GLU:HG3	2:E:182:LEU:HD21	1.71	0.71
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.91	0.71
1:A:179:GLU:O	1:A:183:LYS:CE	2.38	0.71
3:F:244:TYR:H	3:F:266:LYS:HE2	1.57	0.70
2:E:265:LYS:HE3	2:E:378:TYR:OH	1.91	0.70
3:F:310:MET:SD	3:F:337:ASN:HB2	2.31	0.70
1:D:139:ASN:C	1:D:141:ARG:N	2.44	0.70
2:B:171:ILE:O	2:B:174:ASN:HB2	1.90	0.70
2:B:428:LYS:HG2	2:B:429:HIS:NE2	2.07	0.70
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.40	0.70
1:A:134:GLN:O	1:A:135:LEU:HD23	1.90	0.70
2:E:390:PRO:O	2:E:393:GLN:HG3	1.92	0.70
3:C:307:HIS:CD2	3:C:335:TRP:O	2.42	0.69
1:D:140:VAL:HG11	2:E:172:LEU:HD21	1.72	0.69
1:D:175:LEU:H	1:D:175:LEU:CD2	2.05	0.69
5:E:470:NAG:C6	5:E:471:NAG:H5	2.23	0.69
3:C:195:GLN:OE1	3:C:382:THR:HG22	1.92	0.69
1:D:138:LYS:O	1:D:141:ARG:HB2	1.90	0.69
1:A:179:GLU:CA	1:A:183:LYS:HE3	2.21	0.69
3:C:107:ILE:H	3:C:107:ILE:HD12	1.58	0.69
1:A:179:GLU:C	1:A:183:LYS:CD	2.60	0.69
1:A:166:SER:OG	2:B:195:THR:HG23	1.92	0.68
3:F:337:ASN:O	3:F:338:LYS:C	2.31	0.68
3:F:244:TYR:H	3:F:266:LYS:CE	2.06	0.68
1:D:135:LEU:O	1:D:138:LYS:CB	2.42	0.68
1:A:131:GLN:O	1:A:135:LEU:HG	1.94	0.68
1:A:179:GLU:HB2	1:A:183:LYS:CE	2.24	0.68
2:B:393:GLN:O	2:B:397:GLU:HG3	1.94	0.68
3:F:111:GLN:NE2	3:F:112:GLU:HG2	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:MET:HB2	5:B:470:NAG:H81	1.70	0.68
1:D:186:GLU:O	1:D:187:GLN:C	2.31	0.68
3:F:117:ASN:ND2	3:F:118:ASN:H	1.92	0.67
1:D:179:GLU:O	1:D:183:LYS:CD	2.43	0.67
3:F:114:TYR:HD1	3:F:115:ASN:OD1	1.75	0.67
2:E:381:ASP:OD2	2:E:393:GLN:NE2	2.27	0.67
1:A:130:VAL:O	1:A:134:GLN:N	2.25	0.67
3:F:307:HIS:HE1	3:F:341:ALA:H	1.41	0.67
3:F:291:ASP:OD2	3:F:302:LYS:NZ	2.27	0.67
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.94	0.67
2:B:166:ARG:C	2:B:168:LEU:H	1.98	0.67
3:F:151:LYS:HE2	3:F:172:LEU:HD21	1.76	0.67
3:F:161:ALA:O	3:F:162:LYS:CE	2.42	0.67
2:E:169:ARG:N	7:E:44:HOH:O	2.28	0.67
2:B:432:ASP:OD2	2:B:443:SER:HB3	1.95	0.67
3:C:149:THR:HG22	3:C:150:GLY:H	1.59	0.67
1:D:179:GLU:CB	1:D:183:LYS:HE3	2.26	0.66
2:E:171:ILE:HG23	2:E:172:LEU:N	2.07	0.66
3:F:240:SER:OG	3:F:242:ILE:CG1	2.42	0.66
1:D:139:ASN:O	1:D:140:VAL:C	2.33	0.66
2:E:176:ARG:NH1	3:F:113:ILE:HG12	2.10	0.66
2:B:458:PHE:H	2:B:459:PRO:HD2	1.59	0.66
1:D:139:ASN:O	1:D:141:ARG:N	2.28	0.66
3:F:224:THR:HG22	7:F:411:HOH:O	1.95	0.66
1:A:188:VAL:HG22	2:B:165:LEU:CG	2.26	0.66
1:D:157:LYS:HD3	3:F:132:GLU:HG3	1.77	0.66
3:F:240:SER:HG	3:F:242:ILE:HG13	1.61	0.65
2:B:406:ARG:N	2:B:407:CYS:HA	2.11	0.65
2:B:362:GLY:O	2:B:366:THR:HG23	1.96	0.65
3:C:104:ASP:CA	3:C:107:ILE:HD12	2.14	0.65
2:E:423:THR:HG23	2:E:426:MET:HE3	1.78	0.65
3:C:240:SER:OG	3:C:242:ILE:CG1	2.45	0.65
1:D:175:LEU:O	1:D:178:TYR:HB2	1.97	0.65
2:E:168:LEU:O	2:E:171:ILE:HB	1.96	0.65
1:A:130:VAL:HG23	1:A:131:GLN:OE1	1.97	0.65
3:C:195:GLN:HE22	3:C:382:THR:HG21	1.62	0.65
3:C:130:GLN:O	3:C:134:GLN:HG3	1.97	0.65
3:C:304:PHE:O	3:C:337:ASN:O	2.14	0.65
3:F:340:HIS:CE1	4:T:1:GLY:N	2.65	0.65
1:D:166:SER:CB	2:E:195:THR:CG2	2.75	0.64
3:F:111:GLN:CD	3:F:111:GLN:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ARG:CZ	7:B:495:HOH:O	2.38	0.64
3:F:392:LEU:C	3:F:393:THR:OG1	2.33	0.64
1:D:138:LYS:O	1:D:141:ARG:CA	2.46	0.64
2:E:411:ASN:OD1	7:E:11:HOH:O	2.15	0.64
1:D:183:LYS:O	1:D:186:GLU:HB2	1.97	0.64
5:E:470:NAG:H61	7:E:40:HOH:O	1.98	0.64
2:B:332:GLN:O	2:B:338:TYR:HA	1.96	0.64
3:F:196:LYS:HD2	3:F:198:LEU:CD2	2.27	0.64
2:E:176:ARG:HH11	3:F:113:ILE:HG23	1.63	0.64
2:B:439:ASN:H	2:B:439:ASN:ND2	1.95	0.64
2:B:432:ASP:CB	2:B:443:SER:HB2	2.28	0.64
3:F:241:ALA:O	3:F:243:PRO:CD	2.45	0.64
3:F:172:LEU:H	3:F:239:GLN:NE2	1.96	0.63
2:E:176:ARG:HG3	3:F:117:ASN:H	1.62	0.63
3:F:161:ALA:O	3:F:162:LYS:NZ	2.32	0.63
2:E:171:ILE:O	2:E:174:ASN:HB2	1.97	0.63
2:E:176:ARG:NH1	3:F:113:ILE:CG2	2.61	0.63
1:A:179:GLU:CB	1:A:183:LYS:HE3	2.27	0.63
2:E:179:ILE:HD11	3:F:117:ASN:O	1.94	0.63
2:B:168:LEU:O	2:B:170:SER:N	2.31	0.63
2:B:161:ILE:CG1	2:B:164:ASN:OD1	2.46	0.63
2:E:203:ILE:CD1	3:F:145:ILE:HD11	2.29	0.63
2:E:179:ILE:HG21	3:F:120:LYS:HB3	1.80	0.63
2:E:230:ASP:HB3	2:E:233:VAL:HG22	1.81	0.63
3:C:173:LYS:HB3	3:C:235:LEU:HD22	1.79	0.63
2:B:161:ILE:N	2:B:162:PRO:CD	2.62	0.63
1:A:180:ASP:O	1:A:183:LYS:HD2	1.99	0.62
3:C:184:ILE:HA	3:C:189:ASN:O	1.98	0.62
3:C:103:HIS:CE1	3:C:106:SER:HB3	2.34	0.62
1:D:179:GLU:C	1:D:183:LYS:HD2	2.18	0.62
3:F:241:ALA:O	3:F:243:PRO:HD3	1.99	0.62
1:D:138:LYS:O	1:D:141:ARG:N	2.33	0.62
1:D:179:GLU:CB	1:D:183:LYS:CE	2.70	0.62
3:F:263:ALA:CB	3:F:264:MET:HE1	2.29	0.62
3:F:249:GLU:OE1	3:F:385:LYS:NZ	2.33	0.62
3:C:148:ILE:HD12	3:C:161:ALA:HB2	1.82	0.62
3:F:110:LEU:HB2	3:F:111:GLN:HE22	1.63	0.62
2:B:397:GLU:OE1	4:M:3:ARG:NH1	2.33	0.62
3:F:209:ILE:H	3:F:209:ILE:CD1	2.11	0.62
1:D:166:SER:CB	2:E:195:THR:HG23	2.19	0.61
1:A:127:ILE:HB	1:A:130:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LYS:O	2:B:268:PRO:HD2	2.00	0.61
3:F:195:GLN:OE1	3:F:382:THR:CG2	2.48	0.61
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.82	0.61
1:D:143:GLN:O	1:D:147:MET:HB2	1.99	0.61
3:C:209:ILE:H	3:C:209:ILE:CD1	2.12	0.61
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.65	0.61
2:E:378:TYR:CD2	2:E:396:LYS:HE2	2.28	0.61
1:A:143:GLN:NE2	3:C:117:ASN:HD21	1.90	0.61
1:D:179:GLU:C	1:D:183:LYS:CD	2.68	0.61
1:A:179:GLU:O	1:A:183:LYS:CG	2.48	0.61
2:B:158:ASN:O	2:B:160:ASN:ND2	2.33	0.61
2:E:176:ARG:CA	3:F:117:ASN:CB	2.67	0.61
3:C:322:PHE:CZ	4:S:3:ARG:HG2	2.36	0.61
3:F:244:TYR:HB2	3:F:266:LYS:HE2	1.82	0.61
1:D:178:TYR:O	1:D:182:GLN:CG	2.35	0.60
1:A:127:ILE:O	1:A:129:LYS:N	2.34	0.60
3:F:329:GLN:NE2	4:T:3:ARG:HH21	1.99	0.60
3:C:221:THR:O	3:C:223:THR:HG23	2.01	0.60
1:D:180:ASP:HA	1:D:183:LYS:CD	2.31	0.60
3:C:298:ASP:OD1	3:C:300:SER:CA	2.48	0.60
2:E:179:ILE:CD1	3:F:121:ILE:HG13	2.31	0.60
1:A:179:GLU:O	1:A:183:LYS:HG3	2.02	0.60
2:E:236:TYR:CG	2:E:298:LYS:HE2	2.36	0.60
3:F:149:THR:HG23	3:F:168:PHE:O	2.00	0.60
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.15	0.60
2:B:166:ARG:NH2	3:C:106:SER:HB2	2.15	0.60
2:E:169:ARG:O	2:E:170:SER:C	2.40	0.60
1:A:131:GLN:NE2	1:A:132:HIS:N	2.49	0.60
1:A:175:LEU:O	1:A:179:GLU:HG3	2.02	0.60
3:C:323:GLU:CD	3:C:323:GLU:H	2.03	0.60
1:D:175:LEU:H	1:D:175:LEU:HD22	1.66	0.60
2:E:176:ARG:NH1	3:F:113:ILE:HG23	2.16	0.60
2:B:161:ILE:HG12	2:B:164:ASN:HB3	1.84	0.60
2:E:172:LEU:CD1	3:F:114:TYR:CG	2.82	0.60
1:A:131:GLN:NE2	1:A:132:HIS:H	1.99	0.60
1:D:179:GLU:HB2	1:D:183:LYS:HZ2	1.65	0.59
1:A:139:ASN:HB3	3:C:114:TYR:CE2	2.37	0.59
2:E:172:LEU:HD12	3:F:114:TYR:CA	2.32	0.59
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.66	0.59
1:A:134:GLN:HG3	1:A:135:LEU:CD2	2.32	0.59
1:A:133:ILE:C	1:A:135:LEU:N	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:160:GLY:O	3:F:162:LYS:CE	2.43	0.59
3:F:199:ASP:O	3:F:225:GLU:OE2	2.20	0.59
1:A:188:VAL:HG13	2:B:165:LEU:CD2	2.31	0.59
3:F:178:PHE:CZ	3:F:232:LYS:HG2	2.37	0.59
2:B:309:GLU:OE1	2:B:325:HIS:HE1	1.85	0.59
3:F:254:ASN:OD1	3:F:256:ARG:NH2	2.31	0.59
5:B:470:NAG:HO3	5:B:471:NAG:HN2	1.47	0.59
3:C:322:PHE:CZ	4:S:3:ARG:CG	2.86	0.59
2:E:176:ARG:CA	3:F:117:ASN:OD1	2.51	0.58
3:F:219:SER:N	3:F:224:THR:HG21	2.18	0.58
2:E:283:LYS:HG2	2:E:285:TYR:CE1	2.38	0.58
3:F:111:GLN:NE2	3:F:111:GLN:H	2.02	0.58
2:B:175:LEU:O	2:B:179:ILE:HG13	2.03	0.58
2:B:169:ARG:NH1	2:B:173:GLU:OE1	2.35	0.58
3:C:106:SER:C	3:C:108:ARG:N	2.57	0.58
2:E:179:ILE:CD1	3:F:117:ASN:CA	2.76	0.58
1:A:179:GLU:C	1:A:183:LYS:HD2	2.23	0.58
2:B:179:ILE:HG21	3:C:120:LYS:HB3	1.86	0.58
2:B:179:ILE:CD1	3:C:117:ASN:HB2	2.33	0.58
2:B:432:ASP:OD2	2:B:443:SER:CB	2.51	0.58
3:F:263:ALA:C	3:F:264:MET:HE2	2.24	0.58
2:B:217:LYS:HD3	3:C:213:GLU:CD	2.24	0.58
2:E:221:THR:OG1	2:E:223:GLU:OE2	2.22	0.58
1:D:188:VAL:HG21	2:E:165:LEU:CD2	2.33	0.57
2:E:169:ARG:HB3	2:E:169:ARG:HH11	1.69	0.57
2:E:182:LEU:HB3	3:F:124:LEU:HD21	1.85	0.57
3:C:240:SER:HG	3:C:242:ILE:HD12	1.68	0.57
3:F:157:ALA:O	3:F:159:LYS:N	2.38	0.57
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.85	0.57
3:F:189:ASN:OD1	3:F:391:ARG:CG	2.52	0.57
1:A:127:ILE:HD12	1:A:130:VAL:CG2	2.34	0.57
3:F:263:ALA:HB1	3:F:264:MET:CE	2.31	0.57
3:C:172:LEU:H	3:C:239:GLN:NE2	2.03	0.57
1:A:130:VAL:C	1:A:134:GLN:HG2	2.25	0.57
2:B:361:MET:HB2	5:B:470:NAG:C7	2.31	0.57
3:C:249:GLU:OE2	3:C:385:LYS:NZ	2.36	0.57
1:D:188:VAL:CG2	2:E:165:LEU:CD2	2.77	0.57
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.87	0.57
1:D:144:LEU:HD23	2:E:175:LEU:HD21	1.87	0.56
2:E:176:ARG:HH11	3:F:113:ILE:HG12	1.70	0.56
3:F:329:GLN:HE22	4:T:3:ARG:HE	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:309:GLU:OE1	2:E:325:HIS:CE1	2.58	0.56
2:E:428:LYS:HG2	2:E:429:HIS:CD2	2.40	0.56
1:D:169:LEU:H	2:E:189:GLN:HE22	1.53	0.56
3:F:323:GLU:H	3:F:323:GLU:CD	2.08	0.56
3:F:303:PHE:HE2	3:F:304:PHE:CZ	2.24	0.56
3:F:109:TYR:N	3:F:112:GLU:OE1	2.37	0.56
2:E:184:SER:O	2:E:187:SER:HB3	2.06	0.56
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.88	0.56
2:E:381:ASP:CG	2:E:393:GLN:NE2	2.60	0.55
1:A:169:LEU:H	2:B:189:GLN:NE2	2.04	0.55
3:C:338:LYS:N	3:C:339:CYS:HA	2.21	0.55
2:B:395:SER:HB2	2:B:404:TYR:HE2	1.71	0.55
2:B:171:ILE:O	2:B:174:ASN:N	2.38	0.55
2:E:172:LEU:HD12	3:F:114:TYR:CB	2.35	0.55
1:A:175:LEU:H	1:A:175:LEU:CD2	2.19	0.55
3:F:162:LYS:H	3:F:163:GLN:NE2	2.03	0.55
1:D:180:ASP:HA	1:D:183:LYS:HD3	1.89	0.55
1:D:179:GLU:O	1:D:183:LYS:HE3	2.04	0.55
3:F:298:ASP:OD1	3:F:300:SER:N	2.33	0.55
2:B:181:LYS:CE	2:B:185:ASP:OD2	2.52	0.55
2:B:174:ASN:O	2:B:177:SER:N	2.39	0.55
2:E:252:ILE:HD13	2:E:294:LEU:CD2	2.36	0.55
1:A:166:SER:CB	2:B:195:THR:HG23	2.37	0.55
2:B:161:ILE:HG12	2:B:164:ASN:OD1	2.05	0.55
1:D:140:VAL:O	1:D:144:LEU:HB2	2.07	0.55
1:A:188:VAL:HG13	2:B:165:LEU:HD23	1.89	0.55
3:F:161:ALA:C	3:F:162:LYS:HE2	2.27	0.55
1:D:188:VAL:CG1	2:E:165:LEU:CD2	2.79	0.54
1:A:186:GLU:O	1:A:187:GLN:C	2.45	0.54
3:C:105:SER:CA	3:C:108:ARG:HG3	2.36	0.54
2:B:423:THR:OG1	2:B:426:MET:HG3	2.07	0.54
3:F:196:LYS:HD2	3:F:198:LEU:HD23	1.88	0.54
1:A:150:LEU:HD21	3:C:124:LEU:HD23	1.89	0.54
3:F:160:GLY:O	3:F:162:LYS:HG2	2.07	0.54
1:D:141:ARG:CZ	7:D:72:HOH:O	2.56	0.54
1:D:188:VAL:CB	2:E:165:LEU:HD21	2.37	0.54
1:D:183:LYS:O	1:D:185:LEU:N	2.41	0.54
2:B:169:ARG:NH1	2:B:173:GLU:OE2	2.29	0.54
3:F:172:LEU:HB2	3:F:239:GLN:HB2	1.89	0.54
2:E:169:ARG:O	2:E:173:GLU:HG2	2.08	0.54
2:B:169:ARG:HG2	2:B:169:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.42	0.54
3:F:109:TYR:HB2	3:F:112:GLU:CG	2.34	0.53
2:B:169:ARG:HH11	2:B:173:GLU:CD	2.11	0.53
3:F:325:ASN:ND2	3:F:328:GLU:N	2.48	0.53
2:E:309:GLU:OE1	2:E:325:HIS:HE1	1.91	0.53
3:F:273:LYS:HZ2	3:F:317:ASN:HD21	1.56	0.53
3:C:131:LEU:O	3:C:134:GLN:N	2.34	0.53
2:E:307:PRO:HB2	2:E:457:PHE:HB3	1.90	0.53
3:C:245:ALA:HB2	3:C:389:PHE:HD1	1.73	0.53
3:F:116:SER:O	3:F:118:ASN:N	2.42	0.53
2:E:360:LEU:HD13	4:N:2:HIS:HB3	1.91	0.53
2:B:439:ASN:ND2	2:B:439:ASN:N	2.56	0.53
1:D:188:VAL:HG13	2:E:165:LEU:HD21	1.85	0.53
5:B:470:NAG:O3	5:B:471:NAG:C2	2.56	0.53
2:E:388:SER:O	2:E:390:PRO:HD3	2.09	0.53
3:C:196:LYS:HD2	3:C:198:LEU:HD23	1.90	0.53
1:D:180:ASP:N	1:D:183:LYS:CE	2.72	0.53
3:C:240:SER:OG	3:C:242:ILE:HD11	2.08	0.53
3:F:160:GLY:HA2	3:F:162:LYS:HE3	1.91	0.53
1:D:180:ASP:CA	1:D:183:LYS:HD2	2.38	0.53
2:B:166:ARG:C	2:B:168:LEU:N	2.62	0.53
3:C:325:ASN:HD22	3:C:325:ASN:C	2.12	0.53
3:F:109:TYR:CA	3:F:112:GLU:HB2	2.37	0.52
3:C:106:SER:O	3:C:108:ARG:N	2.42	0.52
2:B:190:MET:SD	3:C:134:GLN:NE2	2.82	0.52
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.07	0.52
1:D:135:LEU:O	1:D:138:LYS:HB3	2.09	0.52
2:B:159:SER:HB2	2:B:162:PRO:CG	2.36	0.52
1:A:154:ILE:O	1:A:158:ILE:HG13	2.09	0.52
5:E:470:NAG:O6	5:E:471:NAG:C5	2.52	0.52
2:E:172:LEU:CD2	2:E:172:LEU:H	2.22	0.52
2:B:161:ILE:HG12	2:B:164:ASN:CB	2.40	0.52
3:C:149:THR:CG2	3:C:168:PHE:O	2.56	0.52
1:D:188:VAL:HG21	2:E:165:LEU:CG	2.40	0.52
2:B:361:MET:CB	5:B:470:NAG:C8	2.50	0.52
3:C:322:PHE:CE2	4:S:3:ARG:HG2	2.44	0.52
1:A:140:VAL:CG1	2:B:172:LEU:HD21	2.37	0.52
3:C:104:ASP:HB2	3:C:107:ILE:HD13	1.90	0.52
2:E:333:ASN:H	2:E:333:ASN:ND2	2.06	0.52
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.56	0.52
1:D:188:VAL:HG11	2:E:165:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ILE:HD12	3:C:117:ASN:HB2	1.91	0.52
2:B:180:GLN:HA	2:B:183:GLU:CG	2.39	0.52
3:C:240:SER:OG	3:C:242:ILE:HD12	2.07	0.52
2:E:280:THR:O	2:E:281:ASP:C	2.48	0.52
2:E:174:ASN:O	2:E:177:SER:N	2.43	0.51
3:F:109:TYR:N	3:F:112:GLU:CD	2.63	0.51
2:B:363:GLU:HA	2:B:366:THR:HG23	1.92	0.51
3:F:281:PHE:CE2	3:F:283:GLY:HA2	2.45	0.51
3:F:152:ASP:OD2	3:F:244:TYR:OH	2.21	0.51
2:B:395:SER:HB2	2:B:404:TYR:CE2	2.45	0.51
2:B:165:LEU:HB2	7:B:498:HOH:O	1.83	0.51
7:E:40:HOH:O	4:N:4:PRO:HB3	2.10	0.51
3:C:303:PHE:HE2	3:C:304:PHE:CZ	2.28	0.51
1:A:132:HIS:NE2	3:C:107:ILE:HG22	2.24	0.51
1:D:179:GLU:C	1:D:183:LYS:NZ	2.63	0.51
1:D:180:ASP:H	1:D:183:LYS:HZ2	1.56	0.51
2:B:168:LEU:O	2:B:169:ARG:C	2.48	0.51
2:E:230:ASP:HB3	2:E:233:VAL:CG2	2.40	0.51
3:F:217:HIS:O	3:F:224:THR:HG21	2.04	0.51
3:C:338:LYS:HG2	3:C:338:LYS:O	2.10	0.51
3:C:254:ASN:OD1	3:C:256:ARG:NH2	2.45	0.51
1:A:127:ILE:HD12	1:A:131:GLN:OE1	2.11	0.50
2:E:228:GLN:NE2	2:E:233:VAL:O	2.44	0.50
2:E:388:SER:O	2:E:390:PRO:CD	2.59	0.50
1:D:147:MET:SD	3:F:121:ILE:HD13	2.50	0.50
3:F:110:LEU:N	3:F:112:GLU:HG3	2.26	0.50
2:E:439:ASN:H	2:E:439:ASN:ND2	2.08	0.50
2:B:303:THR:HB	2:B:330:THR:HA	1.93	0.50
2:B:161:ILE:O	2:B:164:ASN:N	2.45	0.50
2:B:238:VAL:HG21	2:B:250:THR:CG2	2.41	0.50
2:E:249:TRP:HB3	2:E:453:LYS:HB3	1.93	0.50
1:A:166:SER:N	2:B:195:THR:O	2.42	0.50
3:C:106:SER:C	3:C:108:ARG:H	2.15	0.50
3:F:325:ASN:HD22	3:F:328:GLU:H	1.54	0.50
2:B:310:LEU:HB3	2:B:326:TYR:HB2	1.93	0.50
3:F:370:ALA:HA	3:F:373:LYS:O	2.12	0.50
1:A:174:ASP:OD2	1:A:177:ASP:HB2	2.12	0.50
2:E:378:TYR:CE1	2:E:396:LYS:CE	2.95	0.49
2:E:171:ILE:HG22	2:E:172:LEU:CG	2.38	0.49
1:A:132:HIS:CD2	3:C:107:ILE:CG2	2.95	0.49
3:F:112:GLU:O	3:F:114:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LYS:HE3	2:B:378:TYR:CZ	2.48	0.49
2:B:166:ARG:NH2	3:C:106:SER:OG	2.46	0.49
1:A:188:VAL:CG1	2:B:165:LEU:HD23	2.42	0.49
3:F:249:GLU:CD	3:F:385:LYS:NZ	2.65	0.49
3:C:154:GLN:O	3:C:158:ASN:N	2.41	0.49
3:F:209:ILE:N	3:F:209:ILE:HD12	2.24	0.49
1:A:176:LYS:HZ2	1:A:176:LYS:HA	1.77	0.49
3:F:224:THR:HG22	7:F:429:HOH:O	2.12	0.49
1:A:143:GLN:HE22	3:C:117:ASN:HD22	1.58	0.49
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.48	0.49
1:D:139:ASN:O	1:D:142:ALA:N	2.46	0.49
3:F:263:ALA:CB	3:F:264:MET:CE	2.89	0.49
2:B:385:TRP:CH2	4:M:3:ARG:NH1	2.74	0.49
2:B:351:ASN:CG	2:B:354:MET:HB2	2.33	0.49
2:B:231:SER:O	2:B:232:SER:C	2.51	0.49
2:E:385:TRP:CE2	4:N:3:ARG:HG3	2.47	0.49
2:E:423:THR:OG1	2:E:426:MET:HG3	2.13	0.49
3:C:337:ASN:O	3:C:338:LYS:C	2.51	0.49
3:F:116:SER:OG	3:F:117:ASN:N	2.46	0.48
3:C:244:TYR:H	3:C:266:LYS:HZ3	1.60	0.48
3:F:124:LEU:O	3:F:128:VAL:HG23	2.13	0.48
3:C:172:LEU:CD1	3:C:239:GLN:HE21	2.25	0.48
1:D:139:ASN:C	1:D:141:ARG:H	2.13	0.48
2:B:174:ASN:O	2:B:178:LYS:N	2.38	0.48
2:E:172:LEU:O	2:E:173:GLU:C	2.50	0.48
1:A:128:GLU:C	1:A:129:LYS:HD3	2.34	0.48
2:E:367:MET:HG3	4:N:2:HIS:HB2	1.95	0.48
1:D:176:LYS:HG3	1:D:180:ASP:OD1	2.12	0.48
2:E:267:ASP:CB	2:E:268:PRO:HD3	2.43	0.48
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.46	0.48
2:B:367:MET:SD	2:B:406:ARG:HG2	2.54	0.48
3:F:172:LEU:HG	3:F:239:GLN:HE21	1.78	0.48
2:E:203:ILE:HD13	3:F:145:ILE:HD11	1.96	0.48
2:E:361:MET:O	2:E:364:ASN:HB2	2.13	0.48
2:E:265:LYS:O	2:E:268:PRO:HD2	2.14	0.48
3:F:160:GLY:C	3:F:162:LYS:CE	2.80	0.48
2:E:251:VAL:HG22	2:E:453:LYS:HG2	1.96	0.48
1:D:180:ASP:CA	1:D:183:LYS:CD	2.91	0.48
1:A:127:ILE:O	1:A:128:GLU:C	2.52	0.48
2:B:161:ILE:O	2:B:164:ASN:HB2	2.12	0.48
2:B:402:TRP:CG	2:B:403:TRP:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:LEU:O	1:D:137:GLN:N	2.47	0.48
1:D:183:LYS:O	1:D:186:GLU:N	2.30	0.48
3:C:243:PRO:HA	3:C:266:LYS:NZ	2.28	0.48
3:F:109:TYR:C	3:F:112:GLU:HB2	2.34	0.47
2:B:191:GLU:CD	2:B:194:ARG:HE	2.16	0.47
3:F:173:LYS:HB3	3:F:173:LYS:NZ	2.28	0.47
3:F:112:GLU:C	3:F:114:TYR:N	2.67	0.47
3:C:263:ALA:HB1	3:C:264:MET:HE2	1.96	0.47
3:F:162:LYS:N	3:F:163:GLN:NE2	2.63	0.47
1:A:187:GLN:O	1:A:189:ILE:N	2.47	0.47
2:B:281:ASP:OD1	2:B:282:GLY:N	2.47	0.47
1:D:144:LEU:HA	1:D:144:LEU:HD23	1.80	0.47
2:B:280:THR:O	2:B:281:ASP:C	2.51	0.47
2:B:376:SER:O	2:B:401:GLY:HA2	2.14	0.47
2:E:252:ILE:CD1	2:E:299:ILE:HG12	2.37	0.47
3:F:178:PHE:CD1	3:F:232:LYS:HG2	2.49	0.47
1:D:179:GLU:C	1:D:183:LYS:HZ2	2.16	0.47
3:C:322:PHE:HE2	3:C:329:GLN:NE2	2.12	0.47
2:B:186:VAL:HG13	3:C:131:LEU:HD22	1.96	0.47
2:E:179:ILE:HG21	3:F:120:LYS:CB	2.44	0.47
2:E:169:ARG:HH11	2:E:173:GLU:CD	2.16	0.47
1:A:131:GLN:N	1:A:134:GLN:HG2	2.30	0.47
2:B:413:ASN:HB2	7:B:483:HOH:O	2.14	0.47
3:F:116:SER:O	3:F:117:ASN:C	2.53	0.47
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.13	0.47
2:E:172:LEU:HD12	3:F:114:TYR:CG	2.50	0.47
2:E:252:ILE:HD13	2:E:294:LEU:HD22	1.95	0.47
3:C:387:ILE:HD11	3:C:391:ARG:HG2	1.97	0.47
3:F:252:ASP:OD2	3:F:256:ARG:HB2	2.14	0.47
7:E:40:HOH:O	4:N:4:PRO:CB	2.63	0.46
2:E:458:PHE:CB	2:E:459:PRO:HD3	2.38	0.46
3:F:160:GLY:O	3:F:161:ALA:C	2.53	0.46
3:F:265:PHE:CE2	3:F:276:LEU:CD1	2.98	0.46
1:D:144:LEU:CD2	2:E:175:LEU:HD21	2.46	0.46
2:E:428:LYS:HE3	2:E:428:LYS:HB2	1.78	0.46
1:D:140:VAL:CG1	3:F:114:TYR:CE2	2.56	0.46
2:B:432:ASP:HB2	2:B:443:SER:HB2	1.95	0.46
1:D:176:LYS:HA	1:D:179:GLU:HB2	1.96	0.46
1:D:186:GLU:O	1:D:188:VAL:N	2.48	0.46
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.16	0.46
1:D:179:GLU:O	1:D:183:LYS:CE	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:H	2:B:189:GLN:HE22	1.61	0.46
2:B:362:GLY:O	2:B:366:THR:CG2	2.63	0.46
3:F:359:THR:HB	3:F:360:PRO:HD2	1.98	0.46
3:F:264:MET:N	3:F:264:MET:HE2	2.31	0.46
2:B:252:ILE:HG13	2:B:299:ILE:HG12	1.97	0.46
1:A:188:VAL:CG2	2:B:165:LEU:HD23	2.41	0.45
3:F:236:ILE:O	3:F:239:GLN:HG2	2.15	0.45
1:D:169:LEU:H	2:E:189:GLN:NE2	2.13	0.45
3:F:374:THR:HG23	3:F:377:TYR:HB2	1.98	0.45
3:C:143:VAL:HB	3:C:220:PRO:CG	2.46	0.45
1:A:143:GLN:NE2	3:C:117:ASN:HD22	2.10	0.45
3:F:252:ASP:OD1	3:F:256:ARG:N	2.47	0.45
2:E:439:ASN:H	2:E:439:ASN:HD22	1.62	0.45
3:F:265:PHE:CE2	3:F:276:LEU:HD11	2.52	0.45
2:B:251:VAL:HG22	2:B:453:LYS:HG2	1.97	0.45
1:D:141:ARG:NH2	7:D:72:HOH:O	2.50	0.45
3:C:104:ASP:C	3:C:106:SER:N	2.70	0.45
3:F:114:TYR:O	3:F:117:ASN:ND2	2.50	0.45
3:C:272:ASP:HB2	3:F:299:PRO:HB2	1.99	0.45
3:F:109:TYR:C	3:F:112:GLU:HG3	2.36	0.45
3:C:173:LYS:HB3	3:C:235:LEU:CD2	2.46	0.45
3:F:303:PHE:CE2	3:F:304:PHE:CZ	3.04	0.45
2:E:385:TRP:CZ2	4:N:3:ARG:CD	2.97	0.45
3:F:343:HIS:O	3:F:367:ILE:HA	2.17	0.45
2:B:389:ASP:O	2:B:392:LYS:N	2.46	0.45
3:C:375:ARG:HD2	3:C:375:ARG:HH11	1.35	0.45
2:E:198:THR:HA	3:F:140:LYS:O	2.17	0.45
2:E:179:ILE:HD12	3:F:117:ASN:C	2.28	0.45
2:E:360:LEU:CD1	4:N:2:HIS:HB3	2.47	0.45
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.82	0.45
2:E:176:ARG:NH1	3:F:113:ILE:HG21	2.32	0.45
3:F:307:HIS:CE1	3:F:342:GLY:H	2.34	0.45
2:E:411:ASN:N	2:E:412:PRO:HD3	2.31	0.45
3:F:127:LYS:O	3:F:130:GLN:N	2.50	0.45
3:C:243:PRO:CB	3:C:264:MET:HG3	2.47	0.44
3:C:155:ASP:O	3:C:159:LYS:HG3	2.17	0.44
3:C:388:PRO:O	3:C:391:ARG:HB2	2.17	0.44
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.64	0.44
1:D:176:LYS:HD3	1:D:179:GLU:OE1	2.16	0.44
1:A:132:HIS:CD2	3:C:107:ILE:HG22	2.52	0.44
2:B:406:ARG:N	2:B:407:CYS:CA	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:157:ALA:C	3:F:159:LYS:N	2.69	0.44
3:C:243:PRO:HB3	3:C:264:MET:HG3	1.98	0.44
3:F:148:ILE:HG21	3:F:156:ILE:HG23	1.98	0.44
3:F:289:ALA:HB3	3:F:369:TRP:CE2	2.52	0.44
1:D:188:VAL:CG2	2:E:165:LEU:CG	2.95	0.44
3:C:173:LYS:CE	3:C:238:THR:O	2.48	0.44
2:B:254:ASN:O	2:B:291:GLU:HA	2.17	0.44
3:F:161:ALA:HB1	3:F:163:GLN:NE2	2.33	0.44
3:F:264:MET:O	3:F:278:TYR:HA	2.16	0.44
3:F:392:LEU:HD23	3:F:392:LEU:N	2.32	0.44
2:B:198:THR:HA	3:C:140:LYS:O	2.18	0.44
2:B:317:TRP:CE2	2:B:448:ARG:HB2	2.52	0.44
3:F:392:LEU:C	3:F:393:THR:HG1	2.18	0.44
3:F:212:LYS:HA	3:F:230:ASN:HB2	1.99	0.44
4:T:2:HIS:CD2	4:T:4:PRO:HG3	2.52	0.44
2:B:266:TRP:CE3	2:B:380:ARG:HG2	2.52	0.44
2:B:328:GLY:O	2:B:342:VAL:HA	2.17	0.44
2:B:245:GLU:O	2:B:246:ASN:HB2	2.18	0.44
2:E:176:ARG:CB	3:F:117:ASN:HB3	2.46	0.44
3:C:105:SER:O	3:C:108:ARG:CG	2.47	0.44
2:E:178:LYS:O	2:E:179:ILE:C	2.56	0.44
1:A:180:ASP:HA	1:A:183:LYS:NZ	2.32	0.44
2:B:458:PHE:N	2:B:459:PRO:HD2	2.26	0.44
3:F:304:PHE:CD1	3:F:338:LYS:HD3	2.53	0.44
2:E:226:LEU:HD12	2:E:226:LEU:HA	1.82	0.44
1:D:183:LYS:C	1:D:185:LEU:H	2.21	0.43
2:E:174:ASN:O	2:E:175:LEU:C	2.56	0.43
3:C:105:SER:HA	3:C:108:ARG:HG3	2.00	0.43
2:E:252:ILE:HD13	2:E:294:LEU:HD23	2.00	0.43
3:C:172:LEU:H	3:C:239:GLN:HE21	1.65	0.43
3:C:143:VAL:HB	3:C:220:PRO:HG2	1.99	0.43
2:E:402:TRP:CG	2:E:403:TRP:N	2.86	0.43
1:A:129:LYS:HD3	1:A:129:LYS:N	2.32	0.43
1:A:131:GLN:CA	1:A:134:GLN:CG	2.92	0.43
2:B:169:ARG:HG2	2:B:169:ARG:NH1	2.33	0.43
2:B:168:LEU:C	2:B:170:SER:N	2.71	0.43
3:C:307:HIS:CE1	3:C:341:ALA:H	2.27	0.43
2:E:172:LEU:CD2	2:E:172:LEU:N	2.81	0.43
2:B:161:ILE:HG12	2:B:164:ASN:CG	2.39	0.43
3:C:150:GLY:HA3	3:C:155:ASP:OD2	2.18	0.43
3:C:198:LEU:HA	3:C:381:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:246:LEU:HA	3:C:386:ILE:HG22	2.01	0.43
2:E:180:GLN:OE1	2:E:180:GLN:HA	2.18	0.43
2:B:345:TYR:CG	2:B:346:ARG:N	2.87	0.43
3:F:109:TYR:CA	3:F:112:GLU:CG	2.69	0.43
2:B:265:LYS:HE3	2:B:378:TYR:HH	1.79	0.43
3:F:338:LYS:N	3:F:339:CYS:HA	2.34	0.43
2:E:236:TYR:CD1	2:E:298:LYS:HE2	2.54	0.43
2:E:215:ILE:HD12	2:E:242:MET:HB3	1.99	0.43
3:F:206:LYS:HB2	3:F:211:TYR:CE2	2.54	0.43
2:E:383:ASP:OD1	2:E:383:ASP:C	2.57	0.43
1:D:176:LYS:O	1:D:177:ASP:C	2.56	0.43
5:E:470:NAG:HO6	5:E:471:NAG:H5	1.80	0.43
3:F:389:PHE:O	3:F:391:ARG:N	2.52	0.43
3:F:390:ASN:OD1	3:F:391:ARG:N	2.52	0.43
3:C:209:ILE:N	3:C:209:ILE:HD12	2.23	0.43
2:B:184:SER:O	2:B:188:ALA:N	2.43	0.43
1:D:135:LEU:O	1:D:138:LYS:CA	2.67	0.42
2:E:171:ILE:HG22	2:E:172:LEU:CB	2.49	0.42
3:F:122:VAL:O	3:F:126:GLU:CG	2.62	0.42
3:F:307:HIS:HE1	3:F:342:GLY:H	1.66	0.42
3:F:392:LEU:O	3:F:393:THR:CB	2.67	0.42
3:F:254:ASN:HB2	3:F:256:ARG:NH2	2.33	0.42
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.16	0.42
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.54	0.42
1:D:176:LYS:C	1:D:178:TYR:N	2.72	0.42
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.20	0.42
2:E:379:ASP:O	2:E:380:ARG:HB2	2.18	0.42
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.18	0.42
1:A:127:ILE:HB	1:A:130:VAL:HG22	2.01	0.42
2:E:217:LYS:HG2	3:F:213:GLU:HG3	2.01	0.42
3:F:148:ILE:CG2	3:F:156:ILE:HG23	2.48	0.42
3:C:172:LEU:HD13	3:C:239:GLN:HE21	1.84	0.42
1:A:175:LEU:H	1:A:175:LEU:HD22	1.82	0.42
2:E:406:ARG:CD	7:E:58:HOH:O	2.68	0.42
2:B:180:GLN:O	2:B:183:GLU:HG3	2.20	0.42
2:B:280:THR:HG22	2:B:281:ASP:N	2.34	0.42
2:E:209:LYS:HB3	2:E:229:PRO:HA	2.01	0.42
3:F:307:HIS:CE1	3:F:341:ALA:H	2.29	0.42
3:C:273:LYS:HD2	3:C:319:ASN:ND2	2.35	0.42
3:C:264:MET:HA	3:C:266:LYS:HE2	2.01	0.42
2:B:161:ILE:HB	2:B:164:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:ALA:O	2:B:428:LYS:C	2.58	0.42
3:C:340:HIS:CE1	4:S:1:GLY:N	2.88	0.42
2:B:201:CYS:HB3	2:B:224:MET:CE	2.50	0.42
3:F:325:ASN:HD22	3:F:325:ASN:C	2.23	0.42
3:C:131:LEU:O	3:C:134:GLN:HB2	2.19	0.42
2:B:166:ARG:HH22	3:C:103:HIS:CD2	2.38	0.42
2:B:180:GLN:HA	2:B:183:GLU:HG3	2.02	0.42
2:B:296:ASN:O	2:B:297:ASP:C	2.56	0.42
2:E:301:GLN:NE2	7:E:62:HOH:O	2.44	0.42
3:C:243:PRO:HA	3:C:266:LYS:HZ1	1.85	0.41
3:F:157:ALA:C	3:F:159:LYS:H	2.23	0.41
3:F:230:ASN:HA	3:F:230:ASN:HD22	1.68	0.41
1:A:183:LYS:C	1:A:185:LEU:H	2.23	0.41
2:B:385:TRP:CZ2	4:M:3:ARG:HG3	2.54	0.41
1:D:188:VAL:HG22	2:E:165:LEU:HD21	1.92	0.41
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.88	0.41
2:B:424:TRP:O	2:B:430:GLY:HA2	2.19	0.41
2:E:169:ARG:O	2:E:171:ILE:N	2.53	0.41
2:E:389:ASP:HA	2:E:390:PRO:HD2	1.76	0.41
3:C:322:PHE:CZ	4:S:3:ARG:HG3	2.55	0.41
3:F:340:HIS:CE1	4:T:1:GLY:H2	2.38	0.41
2:B:282:GLY:O	2:B:283:LYS:HD2	2.21	0.41
3:C:295:PHE:HE2	3:C:305:THR:HG21	1.85	0.41
2:E:224:MET:HG2	2:E:225:TYR:N	2.36	0.41
3:C:270:GLU:HB2	3:C:274:TYR:CZ	2.56	0.41
2:E:367:MET:HB2	2:E:406:ARG:HB3	2.03	0.41
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.19	0.41
3:C:189:ASN:OD1	3:C:391:ARG:HG3	2.21	0.41
3:C:151:LYS:HD3	3:C:172:LEU:HD11	2.02	0.41
1:D:175:LEU:O	1:D:176:LYS:C	2.58	0.41
3:F:154:GLN:OE1	3:F:189:ASN:HA	2.21	0.41
3:F:293:PHE:HB3	3:F:295:PHE:CE2	2.56	0.41
3:C:276:LEU:C	3:C:277:THR:HG23	2.40	0.41
3:F:245:ALA:HB2	3:F:389:PHE:HD1	1.85	0.41
2:E:369:ILE:HD13	2:E:369:ILE:HG21	1.86	0.41
1:A:188:VAL:CB	2:B:165:LEU:HD21	2.49	0.41
2:E:213:GLU:OE2	2:E:217:LYS:HE3	2.21	0.41
3:F:131:LEU:O	3:F:134:GLN:N	2.49	0.41
3:F:172:LEU:H	3:F:239:GLN:HE21	1.66	0.41
3:F:364:ASP:OD1	4:T:1:GLY:HA3	2.21	0.41
2:B:389:ASP:HA	2:B:390:PRO:HD2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MET:HG2	2:E:175:LEU:HD22	2.03	0.40
3:F:208:TRP:HB3	3:F:209:ILE:HD12	2.03	0.40
2:E:182:LEU:O	2:E:186:VAL:HG23	2.21	0.40
3:F:392:LEU:O	3:F:393:THR:OG1	2.35	0.40
2:B:309:GLU:OE1	2:B:325:HIS:CE1	2.68	0.40
3:C:249:GLU:OE2	3:C:385:LYS:HE2	2.20	0.40
2:E:359:GLN:N	2:E:359:GLN:OE1	2.51	0.40
2:B:237:ARG:NE	7:B:494:HOH:O	2.34	0.40
2:E:378:TYR:CD2	2:E:396:LYS:CE	2.98	0.40
1:A:148:LYS:CE	1:A:182:GLN:NE2	2.74	0.40
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.20	0.40
3:C:199:ASP:O	3:C:225:GLU:OE2	2.40	0.40
1:D:137:GLN:O	1:D:138:LYS:C	2.60	0.40
1:D:175:LEU:O	1:D:178:TYR:CB	2.67	0.40
2:B:162:PRO:O	2:B:163:THR:C	2.59	0.40
3:C:249:GLU:OE2	3:C:385:LYS:CE	2.69	0.40
1:A:166:SER:HB3	2:B:195:THR:HG23	2.03	0.40
2:E:179:ILE:HD13	3:F:121:ILE:HG13	2.02	0.40
2:E:182:LEU:CB	3:F:124:LEU:HD21	2.49	0.40
3:C:172:LEU:HD12	3:C:239:GLN:NE2	2.36	0.40
3:C:246:LEU:HB3	3:C:262:TYR:HB2	2.03	0.40
2:B:345:TYR:OH	2:B:349:ALA:O	2.38	0.40
2:E:202:ASN:HB2	2:E:284:ASN:O	2.21	0.40
2:E:241:ASP:OD2	2:E:244:THR:OG1	2.25	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:THR:OG1	3:F:328:GLU:OE2[4_466]	1.16	1.04
3:C:375:ARG:NH2	3:F:361:ASN:OD1[4_466]	1.42	0.78
3:C:375:ARG:N	7:F:426:HOH:O[4_466]	1.52	0.68
3:C:374:THR:OG1	3:F:328:GLU:CD[4_466]	1.80	0.40
3:C:295:PHE:O	3:F:329:GLN:OE1[4_466]	2.01	0.19
3:C:374:THR:CB	3:F:328:GLU:CG[4_466]	2.17	0.03

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	65/87 (75%)	52 (80%)	6 (9%)	7 (11%)	0 0
1	D	52/87 (60%)	39 (75%)	8 (15%)	5 (10%)	1 0
2	B	301/328 (92%)	273 (91%)	19 (6%)	9 (3%)	5 7
2	E	294/328 (90%)	262 (89%)	23 (8%)	9 (3%)	5 7
3	C	290/319 (91%)	265 (91%)	24 (8%)	1 (0%)	46 68
3	F	283/319 (89%)	261 (92%)	16 (6%)	6 (2%)	9 14
4	M	2/4 (50%)	2 (100%)	0	0	100 100
4	N	2/4 (50%)	2 (100%)	0	0	100 100
4	S	2/4 (50%)	2 (100%)	0	0	100 100
4	T	2/4 (50%)	2 (100%)	0	0	100 100
All	All	1293/1484 (87%)	1160 (90%)	96 (7%)	37 (3%)	6 8

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	190	ALA
2	B	169	ARG
2	B	171	ILE
2	B	281	ASP
2	E	169	ARG
2	E	171	ILE
2	E	281	ASP
2	E	283	LYS
2	E	397	GLU
2	E	398	ASP
3	F	112	GLU
1	A	127	ILE
1	A	128	GLU

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Mol	Chain	Res	Type
1	A	191	LYS
2	B	160	ASN
2	E	168	LEU
3	F	116	SER
1	A	184	GLN
2	B	172	LEU
1	D	140	VAL
1	D	184	GLN
1	D	187	GLN
2	E	458	PHE
3	F	117	ASN
3	F	110	LEU
2	B	161	ILE
2	B	256	GLN
2	B	458	PHE
1	D	136	LEU
1	D	138	LYS
2	E	256	GLN
1	A	188	VAL
3	F	113	ILE
3	C	107	ILE
2	B	167	VAL
3	F	121	ILE

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	62/82 (76%)	46 (74%)	16 (26%)	0 1
1	D	50/82 (61%)	40 (80%)	10 (20%)	1 3
2	B	261/286 (91%)	226 (87%)	35 (13%)	5 9
2	E	254/286 (89%)	231 (91%)	23 (9%)	12 22
3	C	246/267 (92%)	223 (91%)	23 (9%)	11 21
3	F	239/267 (90%)	214 (90%)	25 (10%)	8 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	M	3/3 (100%)	3 (100%)	0	100 100
4	N	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	S	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	T	3/3 (100%)	3 (100%)	0	100 100
All	All	1124/1282 (88%)	990 (88%)	134 (12%)	6 12

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	VAL
1	A	129	LYS
1	A	130	VAL
1	A	131	GLN
1	A	133	ILE
1	A	134	GLN
1	A	135	LEU
1	A	136	LEU
1	A	141	ARG
1	A	164	SER
1	A	167	ARG
1	A	175	LEU
1	A	176	LYS
1	A	179	GLU
1	A	182	GLN
1	A	183	LYS
2	B	161	ILE
2	B	164	ASN
2	B	166	ARG
2	B	169	ARG
2	B	170	SER
2	B	172	LEU
2	B	181	LYS
2	B	183	GLU
2	B	184	SER
2	B	195	THR
2	B	210	GLU
2	B	233	VAL
2	B	234	LYS
2	B	252	ILE
2	B	253	GLN
2	B	267	ASP

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Mol	Chain	Res	Type
2	B	280	THR
2	B	301	GLN
2	B	318	LYS
2	B	323	LYS
2	B	333	ASN
2	B	341	SER
2	B	343	ASN
2	B	346	ARG
2	B	351	ASN
2	B	361	MET
2	B	365	ARG
2	B	366	THR
2	B	387	THR
2	B	391	ARG
2	B	395	SER
2	B	439	ASN
2	B	443	SER
2	B	448	ARG
2	B	451	SER
3	C	108	ARG
3	C	109	TYR
3	C	110	LEU
3	C	113	ILE
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	130	GLN
3	C	149	THR
3	C	163	GLN
3	C	224	THR
3	C	242	ILE
3	C	266	LYS
3	C	302	LYS
3	C	317	ASN
3	C	323	GLU
3	C	325	ASN
3	C	328	GLU
3	C	356	LYS
3	C	358	SER
3	C	382	THR
3	C	391	ARG
3	C	393	THR

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Mol	Chain	Res	Type
1	D	136	LEU
1	D	138	LYS
1	D	141	ARG
1	D	143	GLN
1	D	144	LEU
1	D	147	MET
1	D	164	SER
1	D	175	LEU
1	D	176	LYS
1	D	183	LYS
2	E	164	ASN
2	E	165	LEU
2	E	166	ARG
2	E	169	ARG
2	E	170	SER
2	E	171	ILE
2	E	172	LEU
2	E	209	LYS
2	E	233	VAL
2	E	238	VAL
2	E	253	GLN
2	E	267	ASP
2	E	280	THR
2	E	321	LYS
2	E	342	VAL
2	E	351	ASN
2	E	365	ARG
2	E	366	THR
2	E	387	THR
2	E	388	SER
2	E	396	LYS
2	E	428	LYS
2	E	448	ARG
3	F	109	TYR
3	F	117	ASN
3	F	144	GLN
3	F	147	ASP
3	F	149	THR
3	F	162	LYS
3	F	163	GLN
3	F	173	LYS
3	F	187	SER

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Mol	Chain	Res	Type
3	F	198	LEU
3	F	224	THR
3	F	242	ILE
3	F	264	MET
3	F	266	LYS
3	F	297	ASP
3	F	317	ASN
3	F	323	GLU
3	F	325	ASN
3	F	356	LYS
3	F	368	ILE
3	F	374	THR
3	F	382	THR
3	F	391	ARG
3	F	392	LEU
3	F	393	THR
4	S	3	ARG
4	N	3	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
2	B	160	ASN
2	B	174	ASN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	333	ASN
2	B	339	GLN
2	B	351	ASN
2	B	408	HIS
2	B	421	GLN
2	B	439	ASN
3	C	117	ASN
3	C	118	ASN
3	C	130	GLN
3	C	163	GLN
3	C	230	ASN

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Mol	Chain	Res	Type
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	329	GLN
2	E	174	ASN
2	E	189	GLN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	333	ASN
2	E	339	GLN
2	E	351	ASN
2	E	393	GLN
2	E	411	ASN
2	E	429	HIS
2	E	439	ASN
3	F	111	GLN
3	F	136	GLN
3	F	144	GLN
3	F	163	GLN
3	F	176	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	470	2,5	14,14,15	1.19	1 (7%)	15,19,21	4.36	6 (40%)
5	NAG	B	471	5	14,14,15	1.52	2 (14%)	15,19,21	4.06	4 (26%)
5	NAG	E	470	2,5	14,14,15	1.29	1 (7%)	15,19,21	1.84	4 (26%)
5	NAG	E	471	5	14,14,15	1.36	2 (14%)	15,19,21	2.09	4 (26%)

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
5	NAG	B	470	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	471	5	-	0/6/23/26	0/1/1/1
5	NAG	E	470	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	471	5	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	471	NAG	O7-C7	-3.77	1.14	1.23
5	E	470	NAG	O7-C7	-3.73	1.14	1.23
5	B	470	NAG	O7-C7	-3.27	1.15	1.23
5	B	471	NAG	O7-C7	-3.04	1.16	1.23
5	E	471	NAG	C2-N2	2.64	1.51	1.46
5	B	471	NAG	O5-C1	3.65	1.49	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	471	NAG	C1-O5-C5	-13.34	95.31	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	470	NAG	C4-C3-C2	-8.37	98.21	111.23
5	B	470	NAG	O4-C4-C3	-7.65	93.12	110.34
5	E	471	NAG	C1-O5-C5	-5.46	105.32	112.25
5	B	470	NAG	C2-N2-C7	-4.75	116.94	123.04
5	B	470	NAG	C1-O5-C5	-4.36	106.71	112.25
5	E	471	NAG	C3-C2-N2	-2.72	104.03	110.56
5	E	470	NAG	C3-C4-C5	-2.46	105.91	110.20
5	B	471	NAG	O4-C4-C3	-2.21	105.36	110.34
5	E	471	NAG	O5-C5-C6	2.12	111.93	107.35
5	E	470	NAG	C4-C3-C2	2.30	114.81	111.23
5	B	471	NAG	C6-C5-C4	2.64	119.53	113.02
5	E	470	NAG	O7-C7-C8	3.07	127.69	122.06
5	E	471	NAG	C4-C3-C2	3.14	116.11	111.23
5	E	470	NAG	O4-C4-C3	3.74	118.75	110.34
5	B	470	NAG	O3-C3-C2	3.88	116.80	109.11
5	B	471	NAG	C3-C4-C5	6.66	121.81	110.20
5	B	470	NAG	C3-C4-C5	9.75	127.19	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	10	0
5	B	471	NAG	4	0
5	E	470	NAG	11	0
5	E	471	NAG	10	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.