



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:06 AM BST

PDB ID : 1FZA
Title : CRYSTAL STRUCTURE OF FIBRINOGEN FRAGMENT D
Authors : Spraggon, G.; Everse, S.J.; Doolittle, R.F.
Deposited on : 1997-08-05
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.13.1

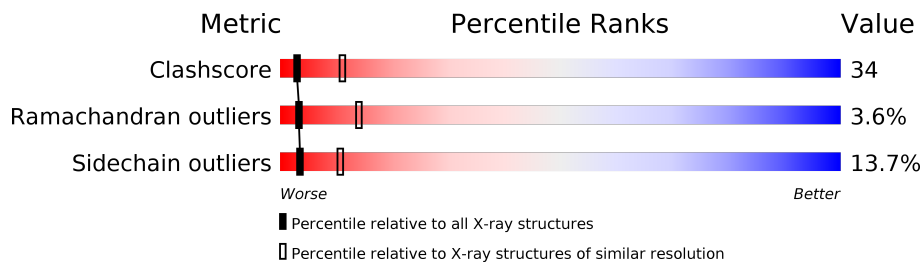
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	39% 41% 16% ..
1	D	87	38% 43% 16% ..
2	B	328	40% 45% 10% 5%
2	E	328	41% 45% 10% 5%
3	C	319	43% 46% 7% ..
3	F	319	42% 47% 7% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11418 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
			Total	C	N	O	S			
1	A	85	697	432	132	130	3	0	0	0
1	D	85	697	432	132	130	3	0	0	0

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	313	2517	1571	444	480	22	0	0	0
2	E	313	2517	1571	444	480	22	0	0	0

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	309	2480	1574	415	478	13	0	0	0
3	F	309	2480	1574	415	478	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	LYS	ILE	conflict	UNP P02679
F	88	LYS	ILE	conflict	UNP P02679

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
4	E	1	14	8	1	5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	C	1	1	1	0	0
5	F	1	1	1	0	0

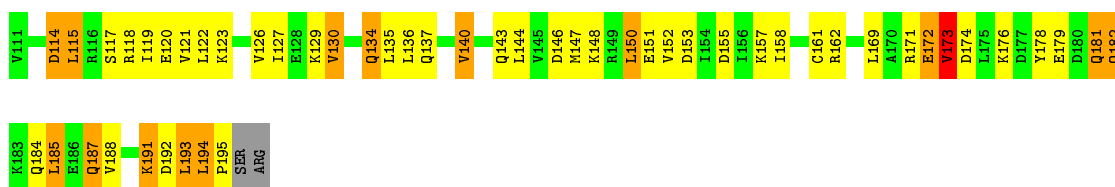
3 Residue-property plots [i](#)

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.

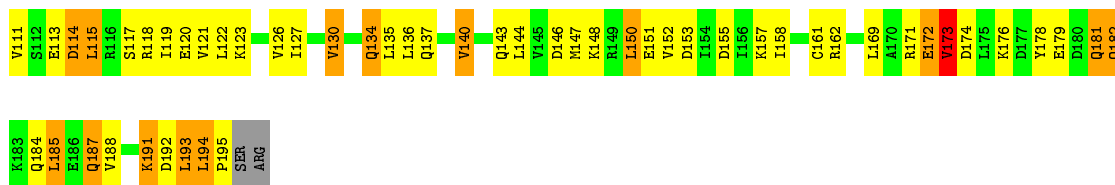
- Molecule 1: FIBRINOGEN

Chain A: 



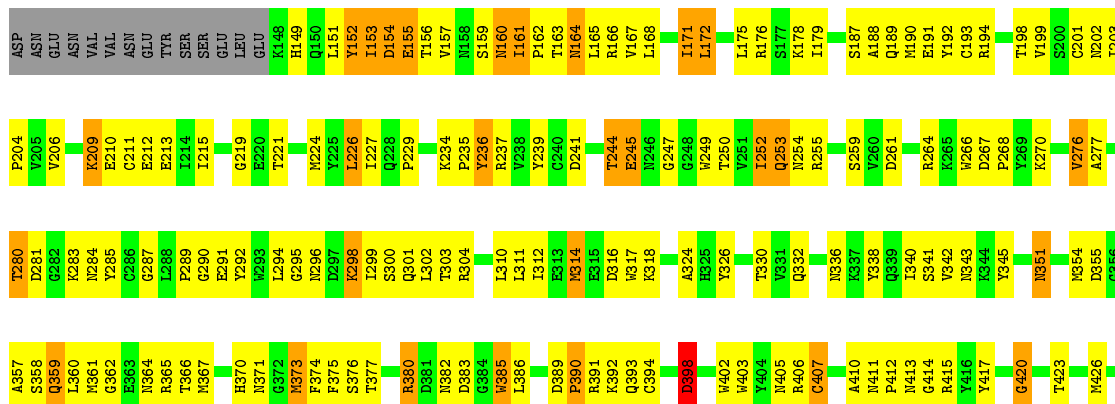
- Molecule 1: FIBRINOGEN

Chain D: 



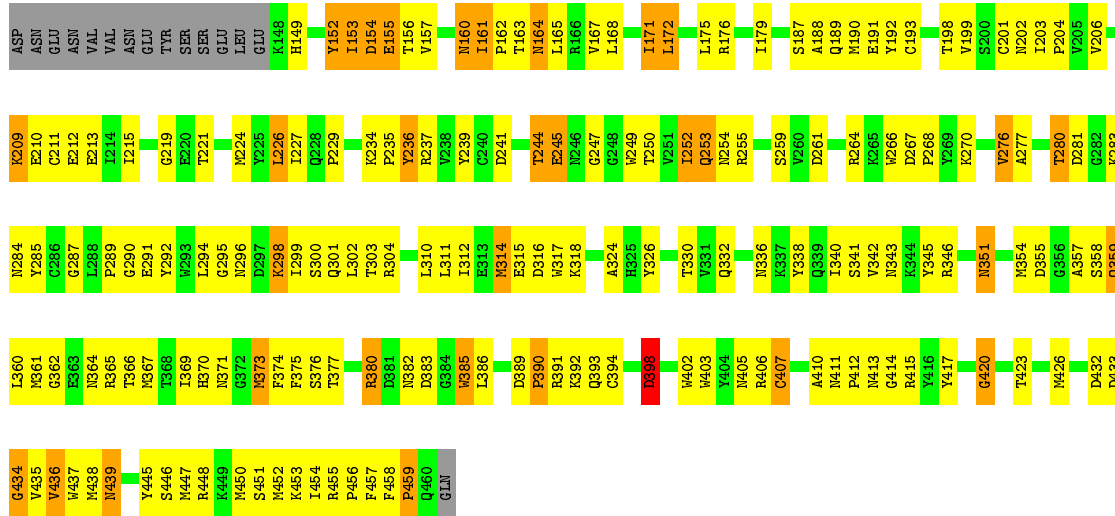
- Molecule 2: FIBRINOGEN

Chain B: 

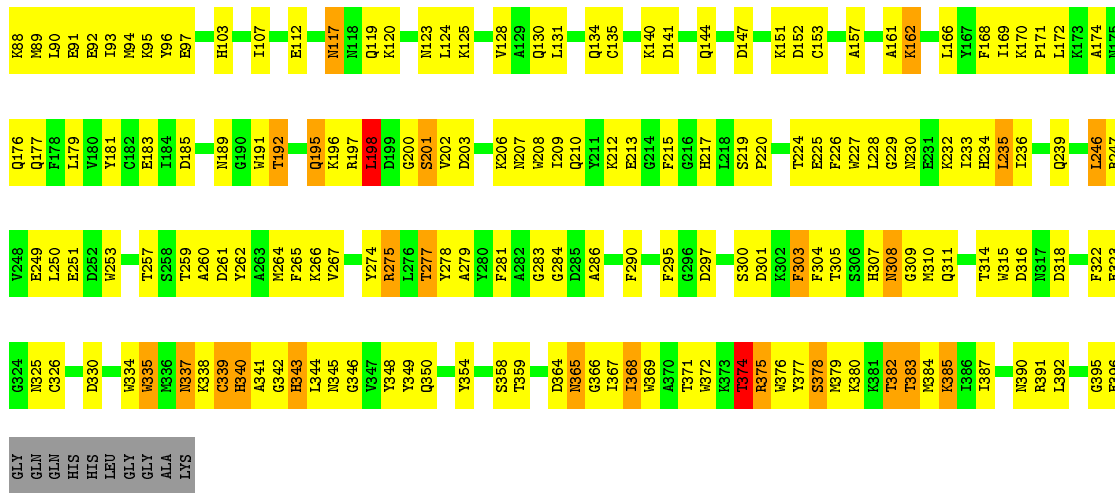




• Molecule 2: FIBRINOGEN



• Molecule 3: FIBRINOGEN



• Molecule 3: FIBRINOGEN



W175	Q176	Q177	F178	L179	W180	Y181	G182	E183	I184	D185	G186	S187	G188	N189	G190	W191	T192	Q195	K196	R197	L198	D199	G200	S201	V202	D203	K206	N207	W208	I209	Q210	Y211	K212	E213	G214	F215	G216	H217	L218	S219	P220	T224	E225	F226	W227	L228	G229	N230	K232	E231	I233	H234	L235	L236	Q239
L246	R247	V248	E249	L250	E251	D252	W253	T257	S258	T259	A260	D261	Y262	A263	M264	F265	K266	V267	Y274	R275	L276	T277	Y278	A279	Y280	F281	A282	G283	G284	D285	A286	F290	F295	G296	D297	D301	K302	F303	F304	T305	S306	H307	N308	G309	M310	Q311	T314	W315	D316	M317	D318				
F322	E323	G324	N325	C326	D330	W334	W335	M336	K338	C339	H340	A341	G342	H343	L344	N345	G346	V347	Y348	Y349	Q350	Y354	S358	T359	D364	N365	G366	I367	I368	W369	A370	T371	W372	K373	T374	R375	W376	Y377	S378	M379	K380	K381	T382	T383	M384	K385	I386	I387	N390	R391	G395				
E396	GLY	GLN	GLN	HIS	HIS	LEU	GLY	ALA	LYS																																														

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.72Å 48.08Å 167.56Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	87.1 (30.00-2.90)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.263 , 0.363	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11418	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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: 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	0.56	0/699	0.75	0/933
1	D	0.56	0/699	0.75	0/933
2	B	0.57	0/2581	0.84	1/3487 (0.0%)
2	E	0.57	0/2581	0.84	1/3487 (0.0%)
3	C	0.51	0/2546	0.71	0/3440
3	F	0.51	0/2546	0.71	0/3440
All	All	0.55	0/11652	0.77	2/15720 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	247	GLY	N-CA-C	-5.09	100.39	113.10
2	B	247	GLY	N-CA-C	-5.07	100.43	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	236	TYR	Sidechain
2	E	236	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	697	0	744	51	0
1	D	697	0	744	50	3
2	B	2517	0	2380	176	4
2	E	2517	0	2380	180	0
3	C	2480	0	2333	180	3
3	F	2480	0	2332	180	4
4	B	14	0	13	2	0
4	E	14	0	13	3	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
All	All	11418	0	10939	764	7

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 34.

All (764) 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)
3:C:396:GLU:HA	3:F:187:SER:N	1.59	1.18
1:A:194:LEU:HB3	1:A:195:PRO:HD3	1.33	1.07
3:C:396:GLU:HA	3:F:186:GLY:C	1.74	1.07
1:D:194:LEU:HB3	1:D:195:PRO:HD3	1.33	1.05
3:C:310:MET:SD	3:C:337:ASN:HB2	1.97	1.05
3:F:310:MET:SD	3:F:337:ASN:HB2	1.97	1.05
2:B:198:THR:HG22	3:C:140:LYS:HB3	1.42	1.01
3:F:219:SER:H	3:F:224:THR:HG21	1.26	1.00
2:E:198:THR:HG22	3:F:140:LYS:HB3	1.42	0.99
2:E:351:ASN:HD21	2:E:354:MET:HG2	1.28	0.98
2:B:298:LYS:H	2:B:298:LYS:HZ1	1.11	0.97
2:B:351:ASN:HD21	2:B:354:MET:HG2	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:SER:H	3:C:224:THR:HG21	1.26	0.96
2:E:358:SER:HA	2:E:365:ARG:HH12	1.33	0.94
3:C:396:GLU:HG3	3:F:186:GLY:HA2	1.47	0.93
2:B:167:VAL:HG23	2:B:168:LEU:HD12	1.51	0.92
2:B:303:THR:HB	2:B:330:THR:HA	1.52	0.91
2:E:303:THR:HB	2:E:330:THR:HA	1.52	0.91
3:C:396:GLU:CA	3:F:187:SER:N	2.33	0.91
2:B:358:SER:HA	2:B:365:ARG:HH12	1.33	0.90
2:E:167:VAL:HG23	2:E:168:LEU:HD12	1.51	0.90
3:F:88:LYS:HB3	3:F:92:GLU:HB2	1.53	0.89
3:C:88:LYS:HB3	3:C:92:GLU:HB2	1.53	0.89
1:D:185:LEU:O	1:D:185:LEU:HD12	1.73	0.88
2:E:235:PRO:HG2	3:F:168:PHE:HE2	1.39	0.87
3:F:209:ILE:HD12	3:F:209:ILE:H	1.39	0.87
3:C:209:ILE:H	3:C:209:ILE:HD12	1.39	0.86
2:B:235:PRO:HG2	3:C:168:PHE:HE2	1.39	0.86
1:A:185:LEU:HD12	1:A:185:LEU:O	1.73	0.86
2:E:370:HIS:O	2:E:373:MET:HB2	1.76	0.86
2:E:439:ASN:H	2:E:439:ASN:HD22	1.24	0.86
3:C:340:HIS:CE1	3:C:364:ASP:HB2	2.11	0.85
3:F:340:HIS:CE1	3:F:364:ASP:HB2	2.11	0.85
1:D:158:ILE:HG23	2:E:189:GLN:HE21	1.41	0.84
2:B:439:ASN:H	2:B:439:ASN:HD22	1.24	0.84
2:B:370:HIS:O	2:B:373:MET:HB2	1.76	0.84
2:B:210:GLU:HG2	2:B:212:GLU:H	1.43	0.84
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.61	0.83
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.41	0.83
2:E:210:GLU:HG2	2:E:212:GLU:H	1.43	0.83
2:E:298:LYS:HZ1	2:E:298:LYS:H	1.27	0.83
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.61	0.82
3:C:396:GLU:HA	3:F:186:GLY:CA	2.09	0.82
3:C:348:TYR:HA	3:C:367:ILE:HD11	1.60	0.81
3:F:348:TYR:HA	3:F:367:ILE:HD11	1.60	0.81
3:C:340:HIS:HE1	3:C:364:ASP:HB2	1.45	0.81
3:F:340:HIS:HE1	3:F:364:ASP:HB2	1.45	0.80
2:E:298:LYS:NZ	2:E:298:LYS:H	1.79	0.80
2:E:276:VAL:HA	2:E:292:TYR:CD2	2.17	0.80
3:F:318:ASP:HB2	3:F:325:ASN:HD22	1.47	0.80
2:B:298:LYS:H	2:B:298:LYS:NZ	1.79	0.79
3:C:318:ASP:HB2	3:C:325:ASN:HD22	1.47	0.79
3:C:260:ALA:HA	3:C:284:GLY:HA3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HA	2:B:292:TYR:CD2	2.17	0.78
2:E:351:ASN:ND2	2:E:354:MET:HG2	1.99	0.77
2:B:351:ASN:ND2	2:B:354:MET:HG2	1.99	0.77
3:F:219:SER:H	3:F:224:THR:CG2	1.97	0.77
3:F:374:THR:HG23	3:F:377:TYR:HB2	1.66	0.77
3:F:260:ALA:HA	3:F:284:GLY:HA3	1.65	0.76
3:C:374:THR:HG23	3:C:377:TYR:HB2	1.66	0.76
1:D:191:LYS:HE3	1:D:191:LYS:HA	1.68	0.76
2:B:152:TYR:HD1	2:B:153:ILE:N	1.84	0.76
2:B:235:PRO:HG2	3:C:168:PHE:CE2	2.21	0.76
2:E:295:GLY:O	2:E:299:ILE:HG13	1.86	0.76
2:B:295:GLY:O	2:B:299:ILE:HG13	1.86	0.75
2:E:235:PRO:HG2	3:F:168:PHE:CE2	2.21	0.75
2:E:152:TYR:HD1	2:E:153:ILE:N	1.84	0.75
3:F:278:TYR:H	3:F:308:ASN:HD21	1.35	0.75
1:A:191:LYS:HA	1:A:191:LYS:HE3	1.68	0.75
3:C:322:PHE:HB2	3:C:338:LYS:HA	1.69	0.75
3:C:219:SER:H	3:C:224:THR:CG2	1.97	0.75
3:C:396:GLU:CG	3:F:186:GLY:HA2	2.16	0.74
2:E:373:MET:HG2	2:E:405:ASN:HB2	1.69	0.74
3:C:219:SER:N	3:C:224:THR:HG21	2.03	0.74
3:F:286:ALA:O	3:F:371:THR:HG23	1.89	0.73
3:C:286:ALA:O	3:C:371:THR:HG23	1.88	0.73
1:A:140:VAL:HG11	2:B:171:ILE:HD11	1.70	0.73
3:F:322:PHE:HB2	3:F:338:LYS:HA	1.69	0.73
3:C:195:GLN:HG2	3:C:384:MET:SD	2.29	0.73
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.24	0.73
3:F:195:GLN:HG2	3:F:384:MET:SD	2.29	0.73
2:E:163:THR:O	2:E:167:VAL:HG22	1.89	0.73
2:B:163:THR:O	2:B:167:VAL:HG22	1.89	0.72
2:B:373:MET:HG2	2:B:405:ASN:HB2	1.70	0.72
2:E:212:GLU:O	2:E:215:ILE:HG22	1.90	0.72
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.72	0.72
2:B:212:GLU:O	2:B:215:ILE:HG22	1.90	0.72
1:D:140:VAL:HG11	2:E:171:ILE:HD11	1.70	0.72
2:E:373:MET:SD	2:E:405:ASN:HB2	2.30	0.72
3:C:278:TYR:H	3:C:308:ASN:HD21	1.35	0.72
2:B:373:MET:SD	2:B:405:ASN:HB2	2.30	0.72
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.24	0.71
2:E:294:LEU:HD23	2:E:299:ILE:HG12	1.72	0.71
2:E:358:SER:HA	2:E:365:ARG:NH1	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:HG3	3:F:186:GLY:CA	2.20	0.71
2:B:358:SER:HA	2:B:365:ARG:NH1	2.06	0.71
3:F:157:ALA:HA	3:F:161:ALA:HB3	1.72	0.71
2:E:357:ALA:HA	2:E:439:ASN:HD21	1.56	0.71
2:E:351:ASN:O	2:E:355:ASP:HB2	1.91	0.70
2:B:294:LEU:HD23	2:B:299:ILE:HG12	1.72	0.70
3:F:219:SER:N	3:F:224:THR:HG21	2.03	0.70
2:B:280:THR:OG1	2:B:283:LYS:HB2	1.92	0.70
2:B:439:ASN:HD22	2:B:439:ASN:N	1.90	0.70
1:A:162:ARG:NH1	2:B:259:SER:HB3	2.07	0.69
2:B:351:ASN:O	2:B:355:ASP:HB2	1.91	0.69
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.56	0.69
2:E:280:THR:OG1	2:E:283:LYS:HB2	1.92	0.69
2:B:199:VAL:O	3:C:141:ASP:HA	1.93	0.69
2:B:420:GLY:HA3	2:B:445:TYR:CE1	2.27	0.69
3:C:396:GLU:HA	3:F:186:GLY:HA2	1.74	0.69
2:E:199:VAL:O	3:F:141:ASP:HA	1.93	0.69
1:D:162:ARG:NH1	2:E:259:SER:HB3	2.07	0.69
2:E:373:MET:CG	2:E:405:ASN:HB2	2.24	0.68
2:E:420:GLY:HA3	2:E:445:TYR:CE1	2.27	0.68
2:B:316:ASP:HB3	2:B:318:LYS:H	1.58	0.68
3:C:250:LEU:HD22	3:C:379:MET:HG3	1.74	0.68
3:F:307:HIS:HE1	3:F:341:ALA:H	1.42	0.68
3:F:250:LEU:HD22	3:F:379:MET:HG3	1.74	0.68
2:E:316:ASP:HB3	2:E:318:LYS:H	1.58	0.68
2:B:314:MET:HE3	2:B:437:TRP:HB2	1.76	0.68
2:E:314:MET:HE3	2:E:437:TRP:HB2	1.75	0.68
3:C:307:HIS:HE1	3:C:341:ALA:H	1.42	0.67
2:E:267:ASP:HB3	2:E:268:PRO:CD	2.25	0.67
3:F:308:ASN:HD22	3:F:309:GLY:H	1.43	0.67
2:B:267:ASP:HB3	2:B:268:PRO:CD	2.25	0.67
2:B:357:ALA:HB3	2:B:360:LEU:HD23	1.76	0.67
3:C:307:HIS:CE1	3:C:341:ALA:H	2.13	0.67
2:E:162:PRO:HA	2:E:165:LEU:HD12	1.77	0.67
2:B:373:MET:CG	2:B:405:ASN:HB2	2.24	0.67
2:E:252:ILE:HB	2:E:452:MET:O	1.94	0.67
2:E:439:ASN:N	2:E:439:ASN:HD22	1.90	0.67
2:B:252:ILE:HB	2:B:452:MET:O	1.94	0.66
3:F:153:CYS:SG	3:F:192:THR:HB	2.36	0.66
1:A:194:LEU:CB	1:A:195:PRO:HD3	2.18	0.66
2:E:357:ALA:HB3	2:E:360:LEU:HD23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:CYS:SG	3:C:192:THR:HB	2.36	0.66
2:B:310:LEU:HD21	2:B:312:ILE:HD11	1.76	0.66
3:F:307:HIS:CE1	3:F:341:ALA:H	2.13	0.66
2:B:162:PRO:HA	2:B:165:LEU:HD12	1.77	0.66
2:E:310:LEU:HD21	2:E:312:ILE:HD11	1.76	0.66
2:B:255:ARG:HA	2:B:291:GLU:HG2	1.78	0.65
2:E:252:ILE:HD13	2:E:454:ILE:HB	1.79	0.65
2:E:255:ARG:HA	2:E:291:GLU:HG2	1.78	0.65
2:B:252:ILE:HD13	2:B:454:ILE:HB	1.79	0.65
3:C:308:ASN:HD22	3:C:309:GLY:H	1.43	0.65
1:A:162:ARG:HH11	2:B:259:SER:HB3	1.62	0.64
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.33	0.64
2:E:390:PRO:HB3	2:E:393:GLN:OE1	1.97	0.64
3:C:396:GLU:CB	3:F:186:GLY:HA2	2.28	0.64
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.33	0.64
1:D:162:ARG:HH11	2:E:259:SER:HB3	1.62	0.64
2:B:390:PRO:HB3	2:B:393:GLN:OE1	1.97	0.64
3:F:92:GLU:O	3:F:95:LYS:HG2	1.98	0.64
3:C:92:GLU:O	3:C:95:LYS:HG2	1.98	0.63
2:E:277:ALA:HA	2:E:289:PRO:HA	1.80	0.63
2:E:202:ASN:ND2	2:E:284:ASN:HB3	2.13	0.63
1:A:193:LEU:HD23	1:A:194:LEU:H	1.63	0.63
3:C:153:CYS:SG	3:C:192:THR:HA	2.38	0.63
1:D:194:LEU:HB3	1:D:195:PRO:CD	2.20	0.63
2:B:202:ASN:ND2	2:B:284:ASN:HB3	2.13	0.63
2:B:277:ALA:HA	2:B:289:PRO:HA	1.80	0.63
3:C:170:LYS:HG2	3:C:174:ALA:HB3	1.81	0.63
1:A:185:LEU:HD12	1:A:185:LEU:C	2.20	0.62
3:F:153:CYS:SG	3:F:192:THR:HA	2.38	0.62
1:D:193:LEU:HD23	1:D:194:LEU:H	1.63	0.62
2:E:417:TYR:OH	2:E:433:ASP:HB2	1.99	0.62
3:F:209:ILE:H	3:F:209:ILE:CD1	2.12	0.62
3:C:209:ILE:H	3:C:209:ILE:CD1	2.12	0.62
3:C:264:MET:HB2	3:C:279:ALA:H	1.65	0.62
3:F:170:LYS:HG2	3:F:174:ALA:HB3	1.81	0.62
2:B:417:TYR:OH	2:B:433:ASP:HB2	1.99	0.62
3:C:396:GLU:HA	3:F:187:SER:H	1.63	0.62
3:F:264:MET:HB2	3:F:279:ALA:H	1.65	0.62
3:F:274:TYR:O	3:F:335:TRP:HZ3	1.83	0.62
3:F:367:ILE:HD12	3:F:367:ILE:H	1.65	0.62
3:C:103:HIS:O	3:C:107:ILE:HD13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:394:CYS:SG	2:E:407:CYS:N	2.74	0.61
3:F:334:TRP:CZ2	3:F:343:HIS:HA	2.36	0.61
3:C:367:ILE:H	3:C:367:ILE:HD12	1.65	0.61
1:D:151:GLU:HG2	1:D:178:TYR:HE2	1.66	0.61
3:C:125:LYS:O	3:C:128:VAL:HG22	2.01	0.61
3:F:88:LYS:HD3	3:F:92:GLU:HB2	1.83	0.61
2:E:380:ARG:HB2	2:E:380:ARG:HH11	1.65	0.61
2:B:380:ARG:HH11	2:B:380:ARG:HB2	1.65	0.60
2:B:394:CYS:SG	2:B:407:CYS:N	2.73	0.60
3:C:274:TYR:O	3:C:335:TRP:HZ3	1.83	0.60
1:A:151:GLU:HG2	1:A:178:TYR:HE2	1.66	0.60
3:C:88:LYS:HA	3:C:91:GLU:HB2	1.84	0.60
3:C:90:LEU:HA	3:C:93:ILE:HB	1.83	0.60
1:D:148:LYS:O	1:D:152:VAL:HG23	2.02	0.60
1:D:185:LEU:C	1:D:185:LEU:HD12	2.19	0.60
1:A:193:LEU:HD23	1:A:194:LEU:N	2.17	0.60
3:F:103:HIS:O	3:F:107:ILE:HD13	2.01	0.60
3:C:334:TRP:CZ2	3:C:343:HIS:HA	2.36	0.60
3:C:88:LYS:HD3	3:C:92:GLU:HB2	1.83	0.60
2:E:314:MET:HE3	2:E:437:TRP:CB	2.32	0.60
3:F:88:LYS:HA	3:F:91:GLU:HB2	1.84	0.60
3:F:90:LEU:HA	3:F:93:ILE:HB	1.83	0.60
3:C:334:TRP:CE2	3:C:343:HIS:HB2	2.38	0.59
3:F:125:LYS:O	3:F:128:VAL:HG22	2.01	0.59
2:E:298:LYS:O	2:E:302:LEU:HG	2.03	0.59
3:F:203:ASP:O	3:F:206:LYS:HE2	2.03	0.59
1:D:194:LEU:CB	1:D:195:PRO:HD3	2.18	0.59
1:A:143:GLN:NE2	3:C:117:ASN:HB3	2.18	0.59
1:A:148:LYS:O	1:A:152:VAL:HG23	2.02	0.59
2:E:303:THR:CB	2:E:330:THR:HA	2.30	0.59
2:E:179:ILE:HG21	3:F:120:LYS:HB3	1.83	0.59
3:F:334:TRP:CE2	3:F:343:HIS:HB2	2.38	0.59
3:C:203:ASP:O	3:C:206:LYS:HE2	2.03	0.59
2:B:303:THR:CB	2:B:330:THR:HA	2.30	0.58
1:D:143:GLN:NE2	3:F:117:ASN:HB3	2.18	0.58
3:F:264:MET:HG3	3:F:279:ALA:HB3	1.85	0.58
2:B:179:ILE:HG21	3:C:120:LYS:HB3	1.83	0.58
1:D:193:LEU:HD23	1:D:194:LEU:N	2.17	0.58
2:E:188:ALA:O	2:E:191:GLU:HB2	2.04	0.58
2:E:453:LYS:O	2:E:454:ILE:HD12	2.04	0.58
2:B:298:LYS:O	2:B:302:LEU:HG	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:MET:HE3	2:B:437:TRP:CB	2.33	0.58
2:E:439:ASN:H	2:E:439:ASN:ND2	2.00	0.58
3:C:396:GLU:C	3:F:187:SER:H	2.06	0.58
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.86	0.58
3:C:396:GLU:C	3:F:187:SER:N	2.57	0.58
1:A:194:LEU:HB3	1:A:195:PRO:CD	2.20	0.58
2:B:439:ASN:H	2:B:439:ASN:ND2	2.00	0.58
2:B:194:ARG:NH2	2:E:191:GLU:OE2	2.37	0.58
2:B:298:LYS:HZ1	2:B:298:LYS:N	1.93	0.57
2:B:453:LYS:O	2:B:454:ILE:HD12	2.04	0.57
2:E:210:GLU:HG2	2:E:211:CYS:N	2.18	0.57
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.02	0.57
2:B:210:GLU:HG2	2:B:211:CYS:N	2.18	0.57
1:D:143:GLN:HE22	3:F:117:ASN:CB	2.18	0.57
1:A:143:GLN:HE22	3:C:117:ASN:CB	2.18	0.57
3:F:172:LEU:O	3:F:172:LEU:HD13	2.05	0.57
3:F:307:HIS:O	3:F:310:MET:HB2	2.05	0.57
2:B:405:ASN:C	2:B:407:CYS:N	2.57	0.57
3:C:172:LEU:O	3:C:172:LEU:HD13	2.05	0.57
3:C:264:MET:HG3	3:C:279:ALA:HB3	1.85	0.57
3:C:367:ILE:HD12	3:C:378:SER:OG	2.05	0.57
3:F:308:ASN:HD22	3:F:309:GLY:N	2.03	0.56
2:E:439:ASN:N	2:E:439:ASN:ND2	2.53	0.56
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.03	0.56
2:B:188:ALA:O	2:B:191:GLU:HB2	2.04	0.56
1:A:153:ASP:O	1:A:157:LYS:HG2	2.05	0.56
3:C:307:HIS:O	3:C:310:MET:HB2	2.05	0.56
2:B:234:LYS:HA	2:B:234:LYS:HE2	1.87	0.56
3:F:367:ILE:HD12	3:F:378:SER:OG	2.05	0.56
2:B:420:GLY:HA2	2:B:446:SER:O	2.06	0.56
3:C:308:ASN:HD22	3:C:309:GLY:N	2.03	0.56
2:E:340:ILE:HG12	2:E:341:SER:N	2.21	0.56
3:F:189:ASN:ND2	3:F:391:ARG:HH21	2.04	0.56
2:B:340:ILE:HG12	2:B:341:SER:N	2.21	0.56
1:D:153:ASP:O	1:D:157:LYS:HG2	2.05	0.56
2:E:405:ASN:C	2:E:407:CYS:N	2.57	0.56
2:E:266:TRP:CE3	2:E:380:ARG:HD2	2.41	0.56
3:C:166:LEU:HB3	3:C:179:LEU:HD11	1.86	0.55
2:B:436:VAL:HG12	2:B:437:TRP:H	1.71	0.55
2:E:436:VAL:HG12	2:E:437:TRP:H	1.71	0.55
3:F:236:ILE:O	3:F:239:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:CA	3:F:186:GLY:HA2	2.36	0.55
3:F:304:PHE:O	3:F:338:LYS:HB3	2.07	0.55
1:A:134:GLN:O	1:A:137:GLN:HG2	2.07	0.55
2:B:211:CYS:SG	2:B:250:THR:HA	2.46	0.55
2:E:234:LYS:HA	2:E:234:LYS:HE2	1.87	0.55
3:C:236:ILE:O	3:C:239:GLN:HG2	2.06	0.55
3:C:189:ASN:ND2	3:C:391:ARG:HH21	2.04	0.55
2:E:211:CYS:SG	2:E:250:THR:HA	2.46	0.55
2:B:266:TRP:CE3	2:B:380:ARG:HD2	2.41	0.55
2:E:367:MET:O	2:E:406:ARG:HB2	2.07	0.55
2:E:420:GLY:HA2	2:E:446:SER:O	2.06	0.55
1:A:147:MET:HG3	2:B:175:LEU:HD22	1.89	0.55
2:B:357:ALA:HA	2:B:439:ASN:ND2	2.21	0.55
2:B:154:ASP:HB2	2:B:157:VAL:HB	1.89	0.54
3:F:209:ILE:N	3:F:209:ILE:HD12	2.17	0.54
3:C:267:VAL:HG13	3:C:274:TYR:O	2.07	0.54
4:B:1:NAG:H5	4:B:1:NAG:N2	2.23	0.54
3:C:169:ILE:O	3:C:177:GLN:HB2	2.08	0.54
3:C:264:MET:O	3:C:278:TYR:HA	2.07	0.54
2:E:154:ASP:HB2	2:E:157:VAL:HB	1.89	0.54
2:E:161:ILE:N	2:E:162:PRO:CD	2.70	0.54
3:F:267:VAL:HG13	3:F:274:TYR:O	2.07	0.54
3:C:304:PHE:O	3:C:338:LYS:HB3	2.07	0.54
1:D:134:GLN:O	1:D:137:GLN:HG2	2.07	0.54
2:B:161:ILE:N	2:B:162:PRO:CD	2.70	0.54
1:D:117:SER:O	1:D:121:VAL:HG22	2.08	0.54
1:D:143:GLN:HE22	3:F:117:ASN:HB3	1.72	0.54
3:F:169:ILE:O	3:F:177:GLN:HB2	2.08	0.54
2:B:367:MET:O	2:B:406:ARG:HB2	2.07	0.54
2:B:439:ASN:ND2	2:B:439:ASN:N	2.53	0.54
3:F:246:LEU:HG	3:F:246:LEU:O	2.06	0.54
3:F:264:MET:O	3:F:278:TYR:HA	2.07	0.54
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.08	0.54
1:A:176:LYS:H	1:A:176:LYS:HD3	1.73	0.54
1:A:143:GLN:HE22	3:C:117:ASN:HB3	1.72	0.54
3:C:228:LEU:O	3:C:232:LYS:HD2	2.08	0.54
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.90	0.54
3:F:228:LEU:O	3:F:232:LYS:HD2	2.08	0.54
2:E:360:LEU:HB3	2:E:364:ASN:HB3	1.91	0.53
3:F:191:TRP:CE2	3:F:387:ILE:HD12	2.43	0.53
3:F:207:ASN:OD1	3:F:209:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:SER:O	1:A:121:VAL:HG22	2.08	0.53
2:B:226:LEU:HD23	2:B:236:TYR:O	2.08	0.53
3:C:310:MET:SD	3:C:337:ASN:CB	2.87	0.53
3:C:337:ASN:C	3:C:339:CYS:N	2.61	0.53
3:C:207:ASN:OD1	3:C:209:ILE:N	2.41	0.53
2:E:255:ARG:HH11	2:E:413:ASN:HA	1.73	0.53
2:B:255:ARG:HH11	2:B:413:ASN:HA	1.73	0.53
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.91	0.53
2:B:360:LEU:HB3	2:B:364:ASN:HB3	1.91	0.53
2:E:226:LEU:HD23	2:E:236:TYR:O	2.08	0.53
2:E:298:LYS:HZ2	2:E:298:LYS:HB2	1.72	0.53
3:C:191:TRP:CE2	3:C:387:ILE:HD12	2.43	0.53
3:C:260:ALA:HB2	3:C:286:ALA:HB3	1.90	0.53
1:D:147:MET:HG3	2:E:175:LEU:HD22	1.90	0.53
2:E:210:GLU:OE2	2:E:212:GLU:HB3	2.08	0.53
4:E:1:NAG:H5	4:E:1:NAG:N2	2.23	0.53
2:B:210:GLU:HG2	2:B:212:GLU:N	2.18	0.52
2:B:359:GLN:H	2:B:359:GLN:HE21	1.57	0.52
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.90	0.52
3:F:88:LYS:HB3	3:F:92:GLU:CB	2.34	0.52
1:A:155:ASP:HB2	1:A:173:VAL:HG11	1.91	0.52
3:C:212:LYS:HG3	3:C:274:TYR:OH	2.09	0.52
1:D:176:LYS:H	1:D:176:LYS:HD3	1.73	0.52
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.91	0.52
1:A:130:VAL:HG23	2:B:161:ILE:HD11	1.92	0.52
2:B:167:VAL:HG23	2:B:168:LEU:H	1.75	0.52
3:C:171:PRO:HD2	3:C:174:ALA:HB2	1.92	0.52
2:E:376:SER:HB3	2:E:382:ASN:H	1.75	0.52
2:E:357:ALA:HA	2:E:439:ASN:ND2	2.21	0.52
2:B:300:SER:HB2	2:B:304:ARG:HH12	1.74	0.52
2:B:376:SER:HB3	2:B:382:ASN:H	1.74	0.52
2:E:254:ASN:O	2:E:291:GLU:HA	2.10	0.52
2:E:300:SER:HB2	2:E:304:ARG:HH12	1.74	0.52
1:D:184:GLN:O	1:D:187:GLN:HB3	2.09	0.52
4:E:1:NAG:HN2	4:E:1:NAG:H5	1.75	0.52
2:E:359:GLN:HE21	2:E:359:GLN:H	1.57	0.52
2:E:376:SER:HB3	2:E:382:ASN:N	2.25	0.52
2:B:312:ILE:HB	2:B:324:ALA:HB3	1.90	0.52
2:B:376:SER:HB3	2:B:382:ASN:N	2.25	0.52
2:B:254:ASN:O	2:B:291:GLU:HA	2.10	0.52
2:E:210:GLU:HG2	2:E:212:GLU:N	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:171:PRO:HD2	3:F:174:ALA:HB2	1.92	0.52
1:A:184:GLN:O	1:A:187:GLN:HB3	2.09	0.52
3:C:246:LEU:O	3:C:246:LEU:HG	2.06	0.52
2:E:167:VAL:HG23	2:E:168:LEU:H	1.75	0.52
1:A:179:GLU:O	1:A:182:GLN:HB2	2.10	0.51
3:C:88:LYS:HB3	3:C:92:GLU:CB	2.34	0.51
2:E:296:ASN:HB3	2:E:338:TYR:CE1	2.45	0.51
3:F:275:ARG:HA	3:F:311:GLN:HA	1.92	0.51
3:C:275:ARG:HA	3:C:311:GLN:HA	1.92	0.51
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.92	0.51
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.10	0.51
3:F:212:LYS:HG3	3:F:274:TYR:OH	2.09	0.51
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.45	0.51
3:C:330:ASP:O	3:C:365:ASN:HB2	2.10	0.51
1:D:130:VAL:HG23	2:E:161:ILE:HD11	1.92	0.51
1:D:179:GLU:O	1:D:182:GLN:HB2	2.10	0.51
2:B:342:VAL:H	2:B:371:ASN:ND2	2.09	0.51
2:B:436:VAL:HG13	2:B:445:TYR:O	2.11	0.51
1:D:155:ASP:HB2	1:D:173:VAL:HG11	1.91	0.51
1:A:172:GLU:O	1:A:173:VAL:HG13	2.11	0.51
3:F:330:ASP:O	3:F:365:ASN:HB2	2.09	0.51
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.10	0.51
2:B:266:TRP:HA	2:B:377:THR:HG21	1.93	0.51
2:E:351:ASN:C	2:E:351:ASN:HD22	2.14	0.51
3:C:305:THR:HB	3:C:341:ALA:HB2	1.93	0.51
3:F:369:TRP:CD1	3:F:371:THR:HG22	2.46	0.51
4:B:1:NAG:H5	4:B:1:NAG:HN2	1.75	0.50
2:B:155:GLU:HB2	3:C:96:TYR:CZ	2.46	0.50
3:C:185:ASP:OD1	3:C:189:ASN:HB2	2.12	0.50
3:C:369:TRP:CD1	3:C:371:THR:HG22	2.46	0.50
1:D:172:GLU:O	1:D:173:VAL:HG13	2.11	0.50
2:E:436:VAL:HG13	2:E:445:TYR:O	2.11	0.50
3:F:119:GLN:HA	3:F:119:GLN:OE1	2.11	0.50
3:F:367:ILE:O	3:F:378:SER:HA	2.11	0.50
2:B:152:TYR:C	2:B:152:TYR:CD1	2.85	0.50
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.80	0.50
3:F:365:ASN:HD22	3:F:365:ASN:N	2.10	0.50
3:F:227:TRP:CZ2	3:F:230:ASN:ND2	2.80	0.50
2:B:311:LEU:HD12	2:B:312:ILE:H	1.77	0.50
2:B:351:ASN:C	2:B:351:ASN:HD22	2.14	0.50
2:E:342:VAL:H	2:E:371:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:368:ILE:HD13	3:F:368:ILE:H	1.77	0.50
3:C:265:PHE:CE1	3:C:267:VAL:HG23	2.47	0.50
2:E:314:MET:CE	2:E:437:TRP:CB	2.90	0.50
2:B:361:MET:O	2:B:364:ASN:HB2	2.12	0.49
3:C:369:TRP:HD1	3:C:372:TRP:HB2	1.76	0.49
3:C:367:ILE:O	3:C:378:SER:HA	2.11	0.49
3:F:334:TRP:HE3	3:F:345:ASN:ND2	2.10	0.49
3:F:337:ASN:C	3:F:339:CYS:N	2.61	0.49
2:B:300:SER:HB2	2:B:304:ARG:NH1	2.27	0.49
2:E:155:GLU:HB2	3:F:96:TYR:CZ	2.46	0.49
2:B:340:ILE:HB	2:B:403:TRP:CE2	2.48	0.49
2:B:314:MET:CE	2:B:437:TRP:CB	2.90	0.49
3:C:368:ILE:HD13	3:C:368:ILE:H	1.77	0.49
3:F:265:PHE:CE1	3:F:267:VAL:HG23	2.47	0.49
3:C:119:GLN:HA	3:C:119:GLN:OE1	2.11	0.49
2:E:361:MET:O	2:E:364:ASN:HB2	2.12	0.49
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.93	0.49
2:B:340:ILE:HG12	2:B:341:SER:H	1.78	0.49
2:E:266:TRP:HA	2:E:377:THR:HG21	1.93	0.49
2:E:311:LEU:HD12	2:E:312:ILE:H	1.77	0.49
2:E:340:ILE:HB	2:E:403:TRP:CE2	2.48	0.49
2:E:412:PRO:HB3	2:E:450:MET:SD	2.53	0.49
3:F:369:TRP:HD1	3:F:372:TRP:HB2	1.76	0.49
3:F:305:THR:HB	3:F:341:ALA:HB2	1.93	0.49
2:E:300:SER:HB2	2:E:304:ARG:NH1	2.27	0.49
2:E:340:ILE:HG12	2:E:341:SER:H	1.78	0.49
3:F:310:MET:SD	3:F:337:ASN:CB	2.87	0.49
2:B:412:PRO:HB3	2:B:450:MET:SD	2.53	0.49
3:C:209:ILE:N	3:C:209:ILE:HD12	2.17	0.49
3:C:253:TRP:HA	3:C:380:LYS:HD2	1.95	0.49
1:D:115:LEU:HA	1:D:118:ARG:HH21	1.78	0.49
3:C:266:LYS:O	3:C:277:THR:HG23	2.13	0.49
3:F:185:ASP:OD1	3:F:189:ASN:HB2	2.12	0.49
1:A:122:LEU:HD12	1:A:123:LYS:NZ	2.28	0.49
3:C:262:TYR:CE2	3:C:281:PHE:HD1	2.31	0.49
3:C:365:ASN:N	3:C:365:ASN:HD22	2.10	0.49
2:E:224:MET:SD	2:E:237:ARG:HB3	2.53	0.49
2:E:276:VAL:O	2:E:290:GLY:N	2.45	0.49
2:B:224:MET:SD	2:B:237:ARG:HB3	2.53	0.48
3:C:262:TYR:CE2	3:C:290:PHE:HB2	2.48	0.48
2:E:283:LYS:HE2	2:E:283:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:266:LYS:O	3:F:277:THR:HG23	2.13	0.48
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.49	0.48
3:C:274:TYR:O	3:C:335:TRP:CZ3	2.65	0.48
2:E:152:TYR:C	2:E:152:TYR:CD1	2.85	0.48
1:A:115:LEU:HA	1:A:118:ARG:HH21	1.78	0.48
2:B:276:VAL:O	2:B:290:GLY:N	2.45	0.48
1:D:122:LEU:HD12	1:D:123:LYS:NZ	2.28	0.48
3:F:201:SER:HG	3:F:225:GLU:HG3	1.78	0.48
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.48	0.48
3:C:201:SER:HG	3:C:225:GLU:HG3	1.78	0.48
3:C:191:TRP:CZ3	3:C:387:ILE:HB	2.48	0.48
3:F:123:ASN:HD22	3:F:123:ASN:N	2.12	0.48
3:F:262:TYR:CE2	3:F:290:PHE:HB2	2.48	0.48
3:C:219:SER:OG	3:C:224:THR:HG22	2.13	0.48
3:C:253:TRP:CD1	3:C:253:TRP:N	2.81	0.48
3:C:208:TRP:HA	3:C:314:THR:HG21	1.95	0.48
3:C:334:TRP:HE3	3:C:345:ASN:ND2	2.10	0.48
3:F:208:TRP:HA	3:F:314:THR:HG21	1.95	0.48
3:F:253:TRP:HA	3:F:380:LYS:HD2	1.95	0.48
3:F:334:TRP:CD1	3:F:343:HIS:HB2	2.49	0.48
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.49	0.48
2:B:283:LYS:HE2	2:B:283:LYS:H	1.78	0.48
2:E:385:TRP:HB3	2:E:392:LYS:HZ2	1.78	0.48
3:F:247:ARG:HD3	3:F:261:ASP:OD1	2.14	0.48
3:F:262:TYR:CE2	3:F:281:PHE:HD1	2.31	0.48
1:A:130:VAL:HG22	1:A:192:ASP:OD2	2.14	0.48
3:C:334:TRP:CD2	3:C:343:HIS:HB2	2.49	0.48
2:E:261:ASP:O	2:E:264:ARG:NE	2.41	0.48
2:E:203:ILE:O	3:F:217:HIS:HA	2.14	0.48
3:F:219:SER:OG	3:F:224:THR:HG22	2.13	0.48
2:B:167:VAL:HG23	2:B:168:LEU:N	2.29	0.47
2:E:285:TYR:HD1	2:E:285:TYR:H	1.62	0.47
2:E:380:ARG:CB	2:E:380:ARG:HH11	2.27	0.47
2:B:294:LEU:CD2	2:B:299:ILE:HG12	2.44	0.47
2:B:385:TRP:HB3	2:B:392:LYS:HZ2	1.78	0.47
3:C:247:ARG:HD3	3:C:261:ASP:OD1	2.14	0.47
3:C:334:TRP:CD1	3:C:343:HIS:HB2	2.49	0.47
3:F:181:TYR:HE1	3:F:220:PRO:O	1.98	0.47
1:D:114:ASP:HB3	3:F:90:LEU:HD21	1.96	0.47
2:B:203:ILE:O	3:C:217:HIS:HA	2.14	0.47
2:B:380:ARG:HH11	2:B:380:ARG:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ASP:HB3	2:B:268:PRO:HD2	1.97	0.47
2:B:455:ARG:HG2	2:B:456:PRO:HD2	1.96	0.47
2:E:455:ARG:HG2	2:E:456:PRO:HD2	1.96	0.47
2:B:411:ASN:O	2:B:435:VAL:HA	2.14	0.47
2:E:187:SER:O	2:E:190:MET:HB2	2.15	0.47
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.63	0.47
2:E:167:VAL:HG23	2:E:168:LEU:N	2.29	0.47
3:F:225:GLU:O	3:F:226:PHE:HB3	2.15	0.47
2:B:300:SER:HB2	2:B:332:GLN:O	2.14	0.47
2:B:326:TYR:N	2:B:326:TYR:CD1	2.83	0.47
3:C:181:TYR:HE1	3:C:220:PRO:O	1.98	0.47
1:D:127:ILE:CD1	1:D:193:LEU:HD13	2.44	0.47
1:D:158:ILE:HG23	2:E:189:GLN:NE2	2.21	0.47
2:E:152:TYR:C	2:E:152:TYR:HD1	2.18	0.47
2:E:215:ILE:HG13	2:E:219:GLY:O	2.15	0.47
2:E:405:ASN:C	2:E:407:CYS:H	2.18	0.47
2:B:362:GLY:O	2:B:366:THR:HG23	2.15	0.47
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.97	0.47
2:E:300:SER:HB2	2:E:332:GLN:O	2.14	0.47
3:F:253:TRP:N	3:F:253:TRP:CD1	2.81	0.47
3:F:334:TRP:CD2	3:F:343:HIS:HB2	2.49	0.47
1:A:114:ASP:HB3	3:C:90:LEU:HD21	1.96	0.47
2:B:410:ALA:HA	2:B:436:VAL:O	2.14	0.47
3:C:197:ARG:NH1	3:C:346:GLY:O	2.48	0.47
3:C:227:TRP:CD1	3:C:229:GLY:HA2	2.50	0.47
3:C:246:LEU:HD22	3:C:265:PHE:CE2	2.50	0.47
1:D:150:LEU:HD22	1:D:150:LEU:HA	1.75	0.47
3:F:151:LYS:HD3	3:F:170:LYS:O	2.15	0.47
3:F:197:ARG:NH1	3:F:346:GLY:O	2.48	0.47
3:C:123:ASN:N	3:C:123:ASN:HD22	2.12	0.47
3:C:225:GLU:O	3:C:226:PHE:HB3	2.15	0.47
1:D:130:VAL:HG22	1:D:192:ASP:OD2	2.14	0.47
3:C:151:LYS:HD3	3:C:170:LYS:O	2.15	0.47
2:E:311:LEU:HD12	2:E:312:ILE:N	2.30	0.47
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.63	0.47
2:B:163:THR:O	2:B:165:LEU:N	2.38	0.46
2:E:411:ASN:O	2:E:435:VAL:HA	2.14	0.46
3:F:246:LEU:HD22	3:F:265:PHE:CE2	2.50	0.46
2:B:311:LEU:HD12	2:B:312:ILE:N	2.30	0.46
2:E:163:THR:O	2:E:165:LEU:N	2.38	0.46
2:E:410:ALA:HA	2:E:436:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:274:TYR:O	3:F:335:TRP:CZ3	2.65	0.46
1:A:127:ILE:CD1	1:A:193:LEU:HD13	2.44	0.46
2:E:402:TRP:CZ3	2:E:412:PRO:HD2	2.51	0.46
3:F:227:TRP:CD1	3:F:229:GLY:HA2	2.50	0.46
2:E:163:THR:C	2:E:165:LEU:H	2.19	0.46
2:E:374:PHE:O	2:E:403:TRP:HA	2.16	0.46
3:F:343:HIS:ND1	3:F:343:HIS:O	2.49	0.46
2:B:152:TYR:HD1	2:B:152:TYR:C	2.18	0.46
2:B:152:TYR:CD1	2:B:153:ILE:N	2.75	0.46
2:B:215:ILE:HG13	2:B:219:GLY:O	2.15	0.46
2:B:405:ASN:C	2:B:407:CYS:H	2.18	0.46
3:C:343:HIS:O	3:C:343:HIS:ND1	2.49	0.46
4:E:1:NAG:C5	4:E:1:NAG:N2	2.78	0.46
3:F:232:LYS:O	3:F:236:ILE:HD12	2.16	0.46
2:B:187:SER:O	2:B:190:MET:HB2	2.15	0.46
2:E:326:TYR:N	2:E:326:TYR:CD1	2.83	0.46
2:E:362:GLY:O	2:E:366:THR:HG23	2.15	0.46
2:E:415:ARG:O	2:E:434:GLY:HA2	2.15	0.46
2:B:163:THR:C	2:B:165:LEU:H	2.19	0.46
2:B:415:ARG:O	2:B:434:GLY:HA2	2.15	0.46
3:F:251:GLU:HG3	3:F:257:THR:HG22	1.97	0.46
3:C:232:LYS:O	3:C:236:ILE:HD12	2.15	0.46
3:C:335:TRP:N	3:C:335:TRP:CD1	2.84	0.46
3:F:88:LYS:CD	3:F:92:GLU:HB2	2.45	0.46
2:B:167:VAL:HG23	2:B:168:LEU:CD1	2.36	0.45
2:B:209:LYS:HG3	2:B:229:PRO:HA	1.98	0.45
2:E:209:LYS:HG3	2:E:229:PRO:HA	1.98	0.45
2:E:383:ASP:OD1	2:E:385:TRP:CE2	2.69	0.45
2:B:280:THR:OG1	2:B:281:ASP:N	2.49	0.45
2:B:383:ASP:OD1	2:B:385:TRP:CE2	2.70	0.45
3:F:250:LEU:HD22	3:F:379:MET:CG	2.45	0.45
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.98	0.45
2:B:261:ASP:O	2:B:264:ARG:NE	2.41	0.45
3:F:335:TRP:CD1	3:F:335:TRP:N	2.84	0.45
2:B:402:TRP:CZ3	2:B:412:PRO:HD2	2.51	0.45
1:D:126:VAL:HG12	1:D:193:LEU:HD12	1.98	0.45
3:F:89:MET:HG3	3:F:90:LEU:H	1.82	0.45
1:A:144:LEU:CD1	2:B:175:LEU:HD21	2.46	0.45
3:C:250:LEU:HD22	3:C:379:MET:CG	2.45	0.45
1:D:152:VAL:O	1:D:155:ASP:HB3	2.17	0.45
1:A:152:VAL:O	1:A:155:ASP:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:PHE:O	2:B:403:TRP:HA	2.16	0.45
3:C:200:GLY:O	3:C:202:VAL:N	2.50	0.45
1:D:144:LEU:CD1	2:E:175:LEU:HD21	2.46	0.45
2:E:267:ASP:HB3	2:E:268:PRO:HD2	1.97	0.45
3:F:172:LEU:H	3:F:239:GLN:HE21	1.65	0.45
1:A:115:LEU:HA	1:A:118:ARG:HE	1.82	0.45
1:A:126:VAL:HG12	1:A:193:LEU:HD12	1.98	0.45
3:C:235:LEU:HD13	3:C:235:LEU:HA	1.77	0.45
3:C:253:TRP:CH2	3:C:350:GLN:HA	2.51	0.45
2:E:244:THR:O	2:E:245:GLU:O	2.35	0.45
2:E:351:ASN:O	2:E:351:ASN:ND2	2.41	0.45
3:F:253:TRP:CH2	3:F:350:GLN:HA	2.51	0.45
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.99	0.44
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.98	0.44
2:E:201:CYS:O	2:E:203:ILE:HD13	2.17	0.44
3:F:200:GLY:O	3:F:202:VAL:N	2.50	0.44
2:B:191:GLU:O	2:B:193:CYS:N	2.50	0.44
1:D:181:GLN:N	1:D:181:GLN:HE21	2.16	0.44
2:E:191:GLU:O	2:E:193:CYS:N	2.50	0.44
2:E:203:ILE:N	2:E:203:ILE:HD13	2.33	0.44
2:B:244:THR:O	2:B:245:GLU:O	2.35	0.44
3:C:89:MET:HG3	3:C:90:LEU:H	1.82	0.44
2:E:294:LEU:CD2	2:E:299:ILE:HG12	2.44	0.44
2:E:280:THR:HG23	2:E:287:GLY:H	1.83	0.44
2:E:229:PRO:CG	2:E:302:LEU:HD21	2.48	0.44
2:E:351:ASN:HD21	2:E:354:MET:H	1.65	0.44
3:F:349:TYR:HB2	3:F:378:SER:CB	2.48	0.44
2:B:201:CYS:O	2:B:203:ILE:HD13	2.17	0.44
3:C:161:ALA:C	3:C:162:LYS:HD3	2.38	0.44
3:C:318:ASP:CG	3:C:325:ASN:HB3	2.38	0.44
2:E:280:THR:OG1	2:E:281:ASP:N	2.49	0.44
3:F:318:ASP:CG	3:F:325:ASN:HB3	2.38	0.44
1:A:135:LEU:C	1:A:135:LEU:HD13	2.38	0.44
2:B:168:LEU:O	2:B:172:LEU:HB2	2.18	0.44
2:B:203:ILE:HD13	2:B:203:ILE:N	2.33	0.44
3:C:131:LEU:O	3:C:134:GLN:N	2.49	0.44
3:C:349:TYR:HB2	3:C:378:SER:HB2	1.99	0.44
2:E:168:LEU:O	2:E:172:LEU:HB2	2.18	0.44
3:F:206:LYS:HB3	3:F:210:GLN:HB2	2.00	0.44
3:C:124:LEU:O	3:C:128:VAL:HG13	2.18	0.44
2:E:172:LEU:HA	2:E:172:LEU:HD13	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:226:LEU:HD23	2:E:236:TYR:C	2.38	0.44
3:F:161:ALA:C	3:F:162:LYS:HD3	2.38	0.44
3:C:349:TYR:HB2	3:C:378:SER:CB	2.47	0.43
3:F:124:LEU:O	3:F:128:VAL:HG13	2.18	0.43
2:B:212:GLU:HG3	2:B:213:GLU:N	2.32	0.43
2:B:229:PRO:CG	2:B:302:LEU:HD21	2.48	0.43
1:D:115:LEU:HA	1:D:118:ARG:HE	1.82	0.43
2:E:167:VAL:HG23	2:E:168:LEU:CD1	2.36	0.43
2:E:360:LEU:HD22	2:E:360:LEU:N	2.33	0.43
3:F:247:ARG:HG2	3:F:385:LYS:HE2	2.00	0.43
1:A:127:ILE:HD13	1:A:193:LEU:HD13	2.00	0.43
1:A:181:GLN:N	1:A:181:GLN:HE21	2.16	0.43
2:B:298:LYS:HB2	2:B:298:LYS:HZ2	1.82	0.43
2:B:359:GLN:N	2:B:359:GLN:HE21	2.17	0.43
1:D:127:ILE:HD13	1:D:193:LEU:HD13	2.00	0.43
3:C:172:LEU:H	3:C:239:GLN:HE21	1.65	0.43
3:C:88:LYS:CD	3:C:92:GLU:HB2	2.45	0.43
1:D:135:LEU:C	1:D:135:LEU:HD13	2.38	0.43
1:A:176:LYS:H	1:A:176:LYS:CD	2.29	0.43
2:B:351:ASN:HD21	2:B:354:MET:H	1.65	0.43
2:B:389:ASP:C	2:B:391:ARG:H	2.22	0.43
2:B:360:LEU:HD22	2:B:360:LEU:N	2.33	0.43
3:C:206:LYS:HB3	3:C:210:GLN:HB2	2.00	0.43
3:C:264:MET:CG	3:C:279:ALA:HB3	2.49	0.43
1:D:188:VAL:HG21	2:E:167:VAL:HG21	1.99	0.43
3:F:235:LEU:HD13	3:F:235:LEU:HA	1.77	0.43
3:C:247:ARG:HG2	3:C:385:LYS:HE2	2.00	0.43
1:D:115:LEU:CA	1:D:118:ARG:HE	2.32	0.43
1:A:157:LYS:HE2	2:B:398:ASP:OD2	2.19	0.43
3:C:301:ASP:O	3:C:305:THR:HG23	2.19	0.43
2:E:168:LEU:HD12	2:E:168:LEU:N	2.34	0.43
2:E:212:GLU:HG3	2:E:213:GLU:N	2.32	0.43
3:F:307:HIS:HE1	3:F:342:GLY:H	1.67	0.43
2:B:156:THR:O	2:B:160:ASN:HB3	2.18	0.43
2:B:226:LEU:HD23	2:B:236:TYR:C	2.38	0.43
2:E:156:THR:O	2:E:160:ASN:HB3	2.18	0.43
3:F:349:TYR:HB2	3:F:378:SER:HB2	1.99	0.43
2:B:386:LEU:O	2:B:386:LEU:HD12	2.19	0.42
3:C:198:LEU:HD23	3:C:225:GLU:HG2	2.01	0.42
2:E:157:VAL:HA	2:E:160:ASN:HB3	2.00	0.42
2:E:332:GLN:HG2	2:E:336:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:423:THR:OG1	2:E:426:MET:HG3	2.19	0.42
3:F:354:TYR:O	3:F:376:TRP:HB3	2.19	0.42
2:E:164:ASN:H	2:E:164:ASN:ND2	2.17	0.42
2:E:359:GLN:HE21	2:E:359:GLN:N	2.17	0.42
2:E:389:ASP:C	2:E:391:ARG:H	2.22	0.42
3:F:369:TRP:NE1	3:F:371:THR:CG2	2.82	0.42
1:A:119:ILE:O	1:A:123:LYS:N	2.52	0.42
2:B:351:ASN:ND2	2:B:354:MET:H	2.18	0.42
2:B:423:THR:OG1	2:B:426:MET:HG3	2.19	0.42
3:C:183:GLU:O	3:C:191:TRP:HB2	2.20	0.42
3:C:234:HIS:CG	3:C:235:LEU:N	2.87	0.42
3:C:303:PHE:HD1	3:C:303:PHE:HA	1.68	0.42
3:C:369:TRP:NE1	3:C:371:THR:CG2	2.82	0.42
3:F:301:ASP:O	3:F:305:THR:HG23	2.19	0.42
1:A:150:LEU:HD22	1:A:150:LEU:HA	1.75	0.42
2:B:157:VAL:HA	2:B:160:ASN:HB3	2.00	0.42
2:B:351:ASN:O	2:B:351:ASN:ND2	2.41	0.42
2:B:375:PHE:CE1	2:B:402:TRP:HA	2.55	0.42
3:C:206:LYS:HE3	3:C:215:PHE:CD2	2.54	0.42
3:C:354:TYR:O	3:C:376:TRP:HB3	2.19	0.42
1:D:191:LYS:HG3	1:D:192:ASP:N	2.35	0.42
2:E:212:GLU:HG2	2:E:458:PHE:HE2	1.85	0.42
3:F:366:GLY:O	3:F:368:ILE:HG23	2.20	0.42
1:A:136:LEU:O	1:A:140:VAL:HG23	2.19	0.42
2:B:212:GLU:HG2	2:B:458:PHE:HE2	1.85	0.42
2:B:414:GLY:HA3	2:B:434:GLY:O	2.19	0.42
2:E:276:VAL:O	2:E:289:PRO:HA	2.20	0.42
1:D:157:LYS:HE2	2:E:398:ASP:OD2	2.19	0.42
3:F:206:LYS:HE3	3:F:215:PHE:CD2	2.54	0.42
3:F:94:MET:HA	3:F:97:GLU:OE2	2.20	0.42
2:B:168:LEU:HD12	2:B:168:LEU:N	2.34	0.42
3:C:247:ARG:HD2	3:C:259:THR:HB	2.02	0.42
3:C:348:TYR:HA	3:C:367:ILE:CD1	2.41	0.42
3:C:366:GLY:O	3:C:368:ILE:HG23	2.20	0.42
1:D:119:ILE:O	1:D:123:LYS:N	2.52	0.42
2:E:204:PRO:HG3	3:F:217:HIS:CD2	2.55	0.42
2:E:227:ILE:HD11	2:E:236:TYR:CE2	2.55	0.42
2:E:375:PHE:CE1	2:E:402:TRP:HA	2.54	0.42
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
3:F:183:GLU:O	3:F:191:TRP:HB2	2.20	0.42
2:B:276:VAL:O	2:B:289:PRO:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:HG2	2:B:336:ASN:HB2	2.01	0.42
3:F:131:LEU:O	3:F:134:GLN:N	2.49	0.42
2:B:168:LEU:HD12	2:B:168:LEU:H	1.85	0.42
2:B:276:VAL:HA	2:B:292:TYR:CE2	2.53	0.42
2:B:280:THR:HG23	2:B:287:GLY:H	1.83	0.42
3:C:196:LYS:HA	3:C:382:THR:O	2.19	0.42
1:D:136:LEU:O	1:D:140:VAL:HG23	2.19	0.42
2:E:414:GLY:HA3	2:E:434:GLY:O	2.19	0.42
2:B:317:TRP:CD1	2:B:420:GLY:N	2.85	0.42
2:E:168:LEU:HD12	2:E:168:LEU:H	1.85	0.42
2:B:164:ASN:ND2	2:B:164:ASN:H	2.17	0.41
3:C:315:TRP:CE2	3:C:316:ASP:HB3	2.55	0.41
3:F:198:LEU:HD23	3:F:225:GLU:HG2	2.00	0.41
3:F:247:ARG:HD2	3:F:259:THR:HB	2.02	0.41
3:F:338:LYS:O	3:F:339:CYS:HB2	2.20	0.41
3:C:168:PHE:HE1	3:C:179:LEU:HB2	1.85	0.41
2:E:276:VAL:HA	2:E:292:TYR:CE2	2.53	0.41
3:F:326:CYS:SG	3:F:339:CYS:N	2.93	0.41
3:F:196:LYS:HA	3:F:382:THR:O	2.19	0.41
1:A:115:LEU:CA	1:A:118:ARG:HE	2.32	0.41
1:A:191:LYS:HG3	1:A:192:ASP:N	2.35	0.41
2:B:370:HIS:CE1	2:B:402:TRP:HE1	2.38	0.41
2:B:204:PRO:HG3	3:C:217:HIS:CD2	2.55	0.41
3:C:93:ILE:HD12	3:C:93:ILE:N	2.36	0.41
3:C:94:MET:HA	3:C:97:GLU:OE2	2.20	0.41
3:F:346:GLY:O	3:F:367:ILE:HG13	2.20	0.41
3:F:295:PHE:CD2	3:F:375:ARG:HD2	2.55	0.41
1:A:176:LYS:N	1:A:176:LYS:HD3	2.35	0.41
2:B:285:TYR:HD1	2:B:285:TYR:H	1.62	0.41
3:C:346:GLY:O	3:C:367:ILE:HG13	2.20	0.41
3:C:295:PHE:CD2	3:C:375:ARG:HD2	2.55	0.41
2:E:386:LEU:O	2:E:386:LEU:HD12	2.19	0.41
3:F:334:TRP:CE2	3:F:343:HIS:HA	2.55	0.41
3:C:307:HIS:HE1	3:C:342:GLY:H	1.67	0.41
3:C:334:TRP:CE2	3:C:343:HIS:HA	2.55	0.41
1:D:114:ASP:HA	1:D:117:SER:HB3	2.03	0.41
3:F:151:LYS:HD3	3:F:151:LYS:HA	1.80	0.41
3:F:315:TRP:CE2	3:F:316:ASP:HB3	2.55	0.41
1:A:129:LYS:HA	1:A:129:LYS:HD3	1.90	0.41
2:B:227:ILE:HD11	2:B:236:TYR:CE2	2.55	0.41
2:E:376:SER:HB3	2:E:382:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:213:GLU:O	3:F:232:LYS:HE3	2.21	0.41
3:F:264:MET:CG	3:F:279:ALA:HB3	2.49	0.41
3:F:93:ILE:N	3:F:93:ILE:HD12	2.36	0.41
1:D:119:ILE:O	1:D:123:LYS:HB2	2.21	0.41
3:F:330:ASP:HA	3:F:365:ASN:HB3	2.03	0.41
2:B:253:GLN:NE2	2:B:451:SER:HA	2.36	0.41
1:D:176:LYS:HD3	1:D:176:LYS:N	2.35	0.41
2:E:351:ASN:ND2	2:E:354:MET:H	2.18	0.41
2:E:253:GLN:NE2	2:E:451:SER:HA	2.36	0.41
3:C:232:LYS:O	3:C:233:ILE:C	2.58	0.41
3:F:168:PHE:HE1	3:F:179:LEU:HB2	1.85	0.41
3:F:234:HIS:CG	3:F:235:LEU:N	2.87	0.41
3:F:305:THR:CB	3:F:341:ALA:HB2	2.51	0.41
2:B:178:LYS:HE2	2:B:178:LYS:HB2	1.85	0.41
3:C:213:GLU:O	3:C:232:LYS:HE3	2.21	0.41
3:C:247:ARG:CD	3:C:259:THR:HB	2.51	0.41
3:C:246:LEU:O	3:C:261:ASP:HA	2.21	0.41
3:C:337:ASN:C	3:C:339:CYS:H	2.24	0.41
3:C:338:LYS:O	3:C:339:CYS:HB2	2.20	0.41
3:C:330:ASP:HA	3:C:365:ASN:HB3	2.03	0.41
3:F:168:PHE:CD1	3:F:179:LEU:HD13	2.56	0.41
3:F:337:ASN:C	3:F:339:CYS:H	2.24	0.41
2:B:276:VAL:HG13	2:B:292:TYR:CE2	2.56	0.41
3:C:326:CYS:SG	3:C:339:CYS:N	2.93	0.41
3:C:305:THR:CB	3:C:341:ALA:HB2	2.51	0.41
3:F:246:LEU:O	3:F:261:ASP:HA	2.21	0.41
3:C:168:PHE:CD1	3:C:179:LEU:HD13	2.56	0.40
2:E:276:VAL:HG13	2:E:292:TYR:CE2	2.56	0.40
1:A:114:ASP:HA	1:A:117:SER:HB3	2.03	0.40
2:B:351:ASN:C	2:B:351:ASN:ND2	2.74	0.40
2:B:376:SER:HB3	2:B:382:ASN:HB2	2.03	0.40
3:C:195:GLN:HA	3:C:226:PHE:O	2.21	0.40
2:E:317:TRP:CD1	2:E:420:GLY:N	2.85	0.40
2:E:351:ASN:C	2:E:351:ASN:ND2	2.74	0.40
3:F:232:LYS:O	3:F:233:ILE:C	2.58	0.40
3:F:247:ARG:CD	3:F:259:THR:HB	2.51	0.40
3:C:191:TRP:CE3	3:C:385:LYS:HE3	2.56	0.40
2:E:239:TYR:CE1	2:E:289:PRO:HD3	2.56	0.40
3:F:307:HIS:NE2	3:F:340:HIS:HA	2.36	0.40
3:C:212:LYS:HE3	3:C:213:GLU:OE2	2.22	0.40
2:E:345:TYR:CG	2:E:346:ARG:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:383:ASP:OD1	2:E:385:TRP:CD2	2.74	0.40
3:F:171:PRO:HD2	3:F:174:ALA:CB	2.51	0.40
3:F:184:ILE:HA	3:F:189:ASN:O	2.21	0.40
3:F:253:TRP:CD1	3:F:380:LYS:HB2	2.57	0.40
3:F:277:THR:HA	3:F:308:ASN:ND2	2.37	0.40
1:A:119:ILE:O	1:A:123:LYS:HB2	2.21	0.40
2:B:383:ASP:OD1	2:B:385:TRP:CD2	2.74	0.40
3:C:253:TRP:CD1	3:C:380:LYS:HB2	2.57	0.40
3:C:277:THR:HA	3:C:308:ASN:ND2	2.37	0.40
2:E:315:GLU:HG2	2:E:316:ASP:O	2.22	0.40
2:E:354:MET:HA	2:E:369:ILE:HG23	2.04	0.40
2:E:402:TRP:CG	2:E:403:TRP:N	2.90	0.40
3:C:392:LEU:HD22	3:F:186:GLY:O	2.20	0.40
3:F:370:ALA:HA	3:F:373:LYS:O	2.21	0.40

All (7) 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:303:PHE:CD2	3:F:277:THR:CG2[2_746]	1.40	0.80
3:C:303:PHE:CE2	3:F:277:THR:CG2[2_746]	1.65	0.55
2:B:159:SER:CB	1:D:114:ASP:OD1[2_545]	1.85	0.35
2:B:162:PRO:CG	1:D:113:GLU:OE1[2_545]	1.93	0.27
3:C:300:SER:CB	3:F:275:ARG:NH1[2_746]	2.06	0.14
2:B:151:LEU:CD2	3:F:102:THR:OG1[2_545]	2.11	0.09
2:B:166:ARG:NE	1:D:111:VAL:CG2[2_545]	2.15	0.05

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	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	2	8
2	B	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	3	12
2	E	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	3	12
3	C	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	4	18
3	F	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	4	18
All	All	1402/1468 (96%)	1118 (80%)	234 (17%)	50 (4%)	3	14

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
2	B	245	GLU
2	B	280	THR
2	B	398	ASP
2	B	420	GLY
3	C	201	SER
3	C	339	CYS
1	D	173	VAL
2	E	245	GLU
2	E	280	THR
2	E	398	ASP
2	E	420	GLY
3	F	201	SER
3	F	339	CYS
2	B	153	ILE
2	B	192	TYR
2	B	276	VAL
2	B	407	CYS
2	B	434	GLY
3	C	198	LEU
3	C	283	GLY
3	C	374	THR
2	E	153	ILE
2	E	192	TYR
2	E	276	VAL
2	E	407	CYS
2	E	434	GLY
3	F	198	LEU
3	F	283	GLY
3	F	374	THR

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	194	LEU
2	B	390	PRO
2	B	459	PRO
3	C	275	ARG
3	C	358	SER
1	D	115	LEU
1	D	194	LEU
2	E	390	PRO
2	E	459	PRO
3	F	275	ARG
3	F	358	SER
1	A	114	ASP
1	D	114	ASP
2	B	244	THR
3	C	176	GLN
2	E	244	THR
3	F	176	GLN
3	C	395	GLY
3	F	395	GLY

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	80/82 (98%)	62 (78%)	18 (22%)	1	2
1	D	80/82 (98%)	62 (78%)	18 (22%)	1	2
2	B	271/286 (95%)	237 (88%)	34 (12%)	4	14
2	E	271/286 (95%)	237 (88%)	34 (12%)	4	14
3	C	261/267 (98%)	229 (88%)	32 (12%)	4	14
3	F	261/267 (98%)	229 (88%)	32 (12%)	4	14
All	All	1224/1270 (96%)	1056 (86%)	168 (14%)	3	11

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	130	VAL
1	A	134	GLN
1	A	140	VAL
1	A	146	ASP
1	A	150	LEU
1	A	161	CYS
1	A	169	LEU
1	A	171	ARG
1	A	172	GLU
1	A	173	VAL
1	A	174	ASP
1	A	181	GLN
1	A	182	GLN
1	A	185	LEU
1	A	187	GLN
1	A	191	LYS
1	A	193	LEU
2	B	149	HIS
2	B	152	TYR
2	B	154	ASP
2	B	155	GLU
2	B	160	ASN
2	B	161	ILE
2	B	164	ASN
2	B	171	ILE
2	B	172	LEU
2	B	176	ARG
2	B	206	VAL
2	B	209	LYS
2	B	221	THR
2	B	226	LEU
2	B	252	ILE
2	B	253	GLN
2	B	298	LYS
2	B	301	GLN
2	B	314	MET
2	B	343	ASN
2	B	351	ASN
2	B	359	GLN
2	B	373	MET
2	B	380	ARG
2	B	385	TRP

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Mol	Chain	Res	Type
2	B	398	ASP
2	B	432	ASP
2	B	436	VAL
2	B	438	MET
2	B	439	ASN
2	B	447	MET
2	B	448	ARG
2	B	457	PHE
2	B	459	PRO
3	C	112	GLU
3	C	117	ASN
3	C	130	GLN
3	C	135	CYS
3	C	144	GLN
3	C	147	ASP
3	C	152	ASP
3	C	162	LYS
3	C	192	THR
3	C	195	GLN
3	C	198	LEU
3	C	235	LEU
3	C	246	LEU
3	C	277	THR
3	C	297	ASP
3	C	303	PHE
3	C	308	ASN
3	C	323	GLU
3	C	335	TRP
3	C	337	ASN
3	C	340	HIS
3	C	343	HIS
3	C	359	THR
3	C	365	ASN
3	C	368	ILE
3	C	374	THR
3	C	375	ARG
3	C	378	SER
3	C	382	THR
3	C	383	THR
3	C	385	LYS
3	C	390	ASN
1	D	120	GLU

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Mol	Chain	Res	Type
1	D	130	VAL
1	D	134	GLN
1	D	140	VAL
1	D	146	ASP
1	D	150	LEU
1	D	161	CYS
1	D	169	LEU
1	D	171	ARG
1	D	172	GLU
1	D	173	VAL
1	D	174	ASP
1	D	181	GLN
1	D	182	GLN
1	D	185	LEU
1	D	187	GLN
1	D	191	LYS
1	D	193	LEU
2	E	149	HIS
2	E	152	TYR
2	E	154	ASP
2	E	155	GLU
2	E	160	ASN
2	E	161	ILE
2	E	164	ASN
2	E	171	ILE
2	E	172	LEU
2	E	176	ARG
2	E	206	VAL
2	E	209	LYS
2	E	221	THR
2	E	226	LEU
2	E	252	ILE
2	E	253	GLN
2	E	298	LYS
2	E	301	GLN
2	E	314	MET
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	373	MET
2	E	380	ARG
2	E	385	TRP

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Mol	Chain	Res	Type
2	E	398	ASP
2	E	432	ASP
2	E	436	VAL
2	E	438	MET
2	E	439	ASN
2	E	447	MET
2	E	448	ARG
2	E	457	PHE
2	E	459	PRO
3	F	112	GLU
3	F	117	ASN
3	F	130	GLN
3	F	135	CYS
3	F	144	GLN
3	F	147	ASP
3	F	152	ASP
3	F	162	LYS
3	F	192	THR
3	F	195	GLN
3	F	198	LEU
3	F	235	LEU
3	F	246	LEU
3	F	277	THR
3	F	297	ASP
3	F	303	PHE
3	F	308	ASN
3	F	323	GLU
3	F	335	TRP
3	F	337	ASN
3	F	340	HIS
3	F	343	HIS
3	F	359	THR
3	F	365	ASN
3	F	368	ILE
3	F	374	THR
3	F	375	ARG
3	F	378	SER
3	F	382	THR
3	F	383	THR
3	F	385	LYS
3	F	390	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	143	GLN
1	A	181	GLN
2	B	160	ASN
2	B	174	ASN
2	B	180	GLN
2	B	189	GLN
2	B	228	GLN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	339	GLN
2	B	343	ASN
2	B	351	ASN
2	B	359	GLN
2	B	371	ASN
2	B	439	ASN
3	C	117	ASN
3	C	123	ASN
3	C	136	GLN
3	C	176	GLN
3	C	189	ASN
3	C	230	ASN
3	C	234	HIS
3	C	239	GLN
3	C	307	HIS
3	C	308	ASN
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	329	GLN
3	C	337	ASN
3	C	361	ASN
3	C	365	ASN
1	D	137	GLN
1	D	143	GLN
1	D	181	GLN
2	E	160	ASN
2	E	174	ASN
2	E	180	GLN
2	E	189	GLN
2	E	228	GLN

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Mol	Chain	Res	Type
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	339	GLN
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	371	ASN
2	E	439	ASN
3	F	117	ASN
3	F	123	ASN
3	F	136	GLN
3	F	176	GLN
3	F	189	ASN
3	F	230	ASN
3	F	234	HIS
3	F	239	GLN
3	F	307	HIS
3	F	308	ASN
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN
3	F	361	ASN
3	F	365	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	NAG	B	1	-	14,14,15	0.57	0	17,19,21	0.70	0
4	NAG	E	1	-	14,14,15	0.56	0	17,19,21	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1	-	-	2/6/23/26	0/1/1/1
4	NAG	E	1	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	2	0
4	E	1	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.