



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:14 PM UTC

PDB ID : 1FZA / pdb_00001fza
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

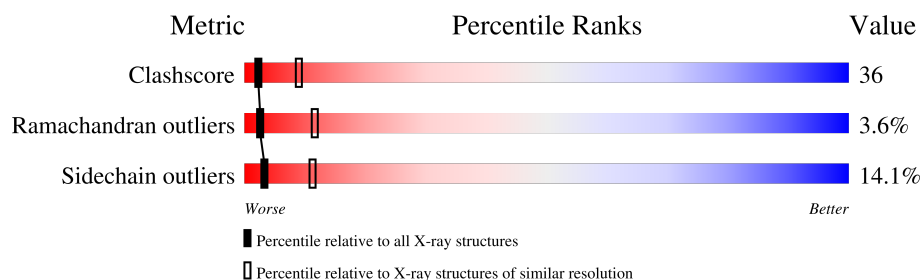
1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	39% 40% 17% ..
1	D	87	38% 41% 17% ..
2	B	328	36% 43% 15% • 5%
2	E	328	36% 43% 15% • 5%
3	C	319	40% 47% 8% • •
3	F	319	39% 49% 8% • •

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
1	A	85	Total	C	N	O	S	0	0	0
			697	432	132	130	3			
1	D	85	Total	C	N	O	S	0	0	0
			697	432	132	130	3			

- Molecule 2 is a protein called FIBRINOGEN.

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

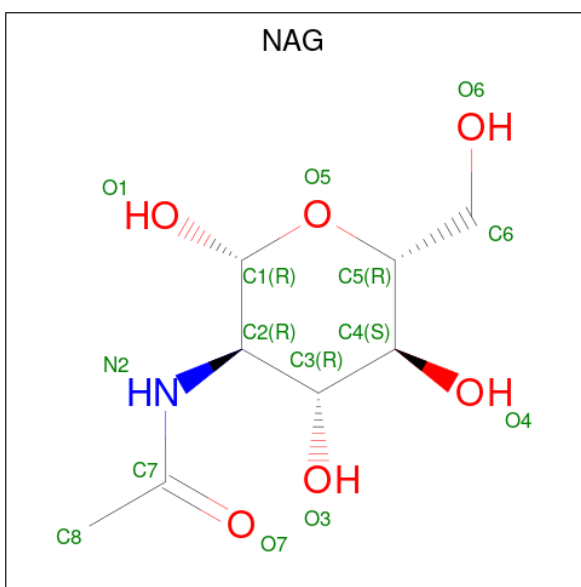
- Molecule 3 is a protein called FIBRINOGEN.

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

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

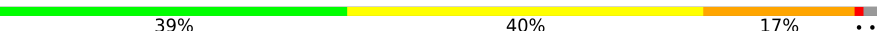
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

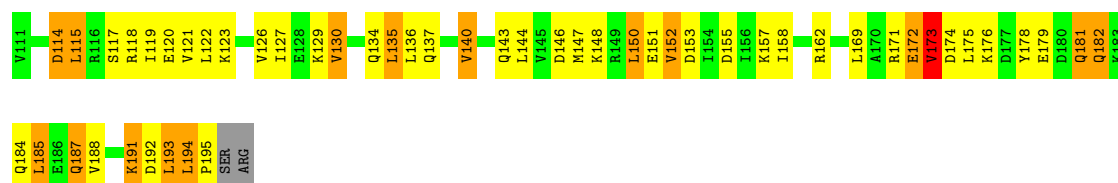
3 Residue-property plots

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

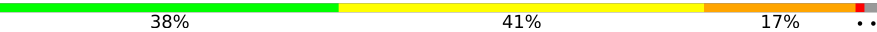
Note EDS was not executed.

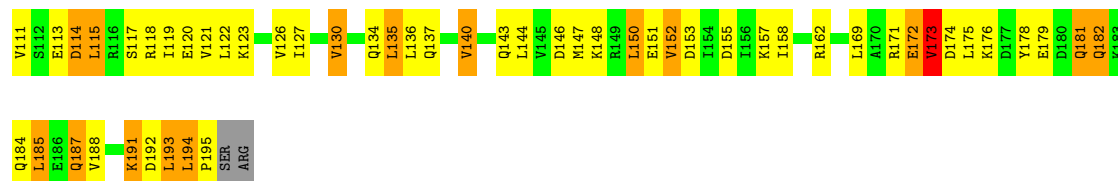
• Molecule 1: FIBRINOGEN

Chain A: 



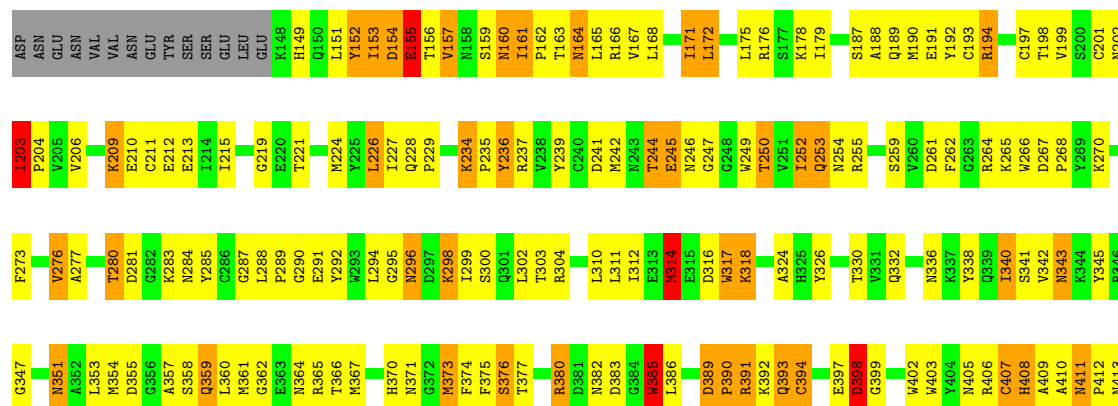
• Molecule 1: FIBRINOGEN

Chain D: 



• Molecule 2: FIBRINOGEN

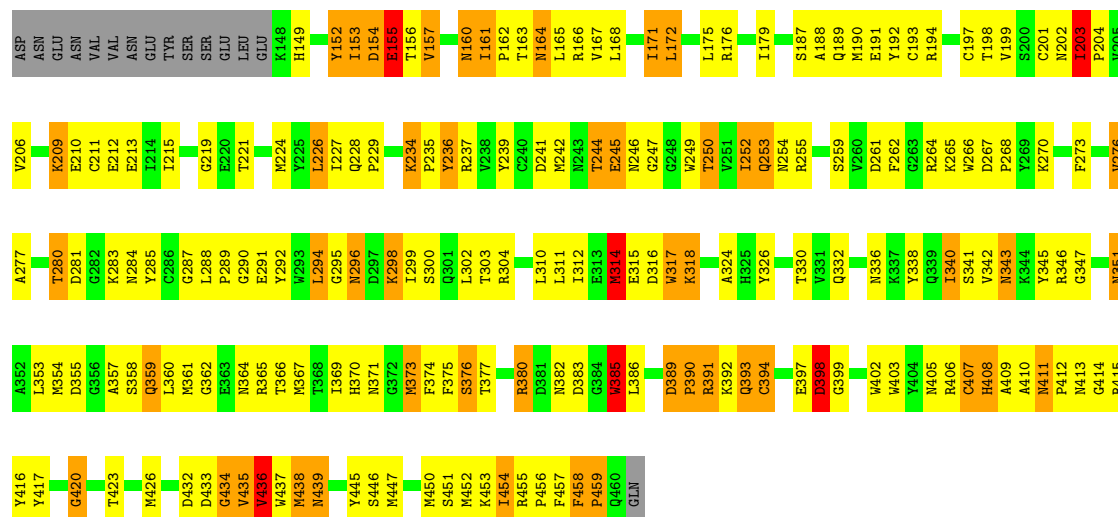
Chain B: 





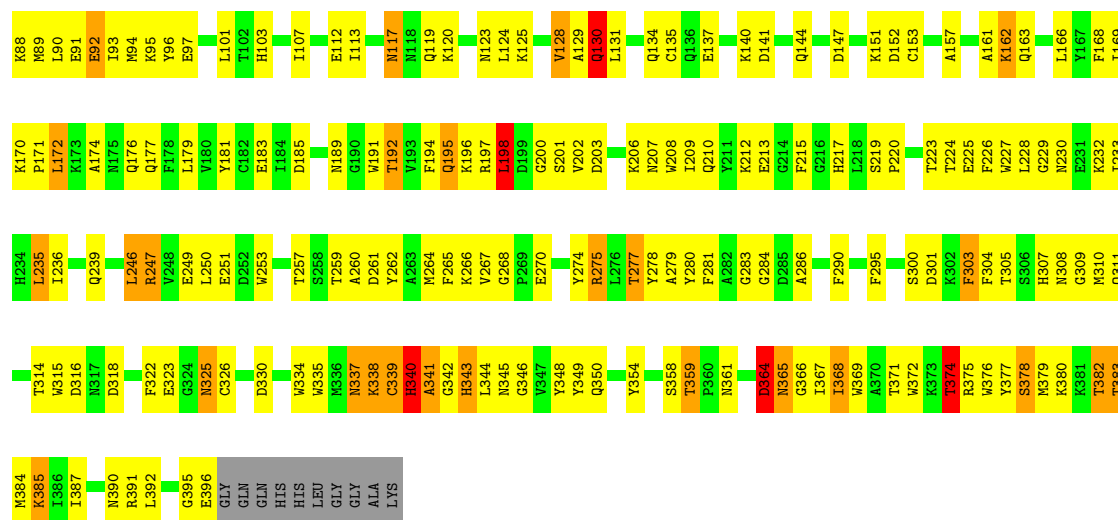
• Molecule 2: FIBRINOGEN

Chain E: 36% 43% 15% • 5%



• Molecule 3: FIBRINOGEN

Chain C: 40% 47% 8% • •



• Molecule 3: FIBRINOGEN

Chain F: 39% 49% 8% • •



T382	T383	K384	K385	T386	I387	N390	R391	G395	E396	GLY	GLN	GLN	HIS	HIS	HIS	LEU	LEU	GLY	GLY	ALA	ALA	LYS																																			
M310	Q311	T314	W315	D316	K317	D318	F322	E323	G324	N325	C326	D330	W334	W335	K336	N337	K338	C339	H340	A341	G342	H343	L344	N345	G346	V347	Y348	Y349	Q350	Y354	S358	T359	F360	N361	K364	N365	G366	I367	I368	W369	A370	T371	W372	K373	T374	R375	W376	Y377	S378	M379	K380	K381					
L169	K170	P171	L172	K173	A174	W175	Q176	Q177	F178	L179	W180	Y181	G182	E183	I184	D185	G186	S187	G188	N189	G190	W191	T192	W193	F194	Q195	K196	R197	L198	D199	G200	S201	V202	D203	K206	N207	W208	I209	Q210	Y211	K212	E213	G214	F215	G216	G217	L218	S219	P220	T223	T224	E225	F226	W227	L228	G229	N230
E231	K232	I233	H234	L235	I236	Q239	L246	R247	V248	E249	L250	E251	W253	T257	S258	T259	A260	D261	Y262	A263	M264	F265	K266	V267	G268	P269	E270	Y274	R275	L276	T277	Y278	A279	Y280	F281	A282	G283	G284	D285	A286	F290	F295	D301	K302	F303	F304	T305	S306	H307	N308	G309						

4 Data and refinement statistics

Xtriage (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.	Xtriage
Total number of atoms	11418	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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	0.69	0/699	1.02	1/933 (0.1%)
1	D	0.68	0/699	1.02	1/933 (0.1%)
2	B	0.71	1/2581 (0.0%)	1.28	36/3487 (1.0%)
2	E	0.72	1/2581 (0.0%)	1.28	36/3487 (1.0%)
3	C	0.60	0/2546	1.07	18/3440 (0.5%)
3	F	0.60	0/2546	1.07	17/3440 (0.5%)
All	All	0.66	2/11652 (0.0%)	1.16	109/15720 (0.7%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	314	MET	SD-CE	-7.20	1.61	1.79
2	E	314	MET	SD-CE	-7.19	1.61	1.79

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	155	GLU	N-CA-C	-10.63	98.84	112.23
2	E	155	GLU	N-CA-C	-10.63	98.84	112.23
2	E	296	ASN	N-CA-C	10.28	123.45	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	ASN	N-CA-C	10.28	123.44	111.11
2	B	203	ILE	N-CA-C	10.17	120.05	108.05
2	E	203	ILE	N-CA-C	10.15	120.03	108.05
2	B	408	HIS	N-CA-C	9.42	122.46	108.14
2	E	408	HIS	N-CA-C	9.41	122.45	108.14
2	E	436	VAL	N-CA-C	9.13	124.05	108.90
2	B	436	VAL	N-CA-C	9.13	124.05	108.90
3	C	364	ASP	N-CA-C	-8.32	100.93	112.25
3	F	364	ASP	N-CA-C	-8.31	100.95	112.25
2	E	247	GLY	N-CA-C	-7.78	100.39	112.45
2	B	353	LEU	N-CA-C	7.76	120.72	111.33
2	B	247	GLY	N-CA-C	-7.76	100.43	112.45
2	E	353	LEU	N-CA-C	7.75	120.71	111.33
2	E	394	CYS	N-CA-C	7.72	120.67	111.33
2	B	394	CYS	N-CA-C	7.70	120.65	111.33
2	E	409	ALA	N-CA-C	-7.66	103.78	113.43
2	B	409	ALA	N-CA-C	-7.62	103.83	113.43
2	E	317	TRP	N-CA-C	-7.62	103.57	113.17
2	B	317	TRP	N-CA-C	-7.60	103.59	113.17
3	C	270	GLU	N-CA-C	-7.58	102.99	111.71
3	F	270	GLU	N-CA-C	-7.56	103.02	111.71
2	B	391	ARG	N-CA-C	-7.29	103.64	112.54
3	C	268	GLY	CA-C-N	7.29	127.72	119.92
3	C	268	GLY	C-N-CA	7.29	127.72	119.92
2	E	391	ARG	N-CA-C	-7.28	103.66	112.54
3	F	268	GLY	CA-C-N	7.25	127.67	119.92
3	F	268	GLY	C-N-CA	7.25	127.67	119.92
2	B	234	LYS	CA-C-N	7.18	127.62	119.93
2	B	234	LYS	C-N-CA	7.18	127.62	119.93
2	E	234	LYS	CA-C-N	7.17	127.60	119.93
2	E	234	LYS	C-N-CA	7.17	127.60	119.93
2	E	197	CYS	N-CA-C	-6.90	101.23	110.55
2	B	197	CYS	N-CA-C	-6.89	101.25	110.55
2	B	194	ARG	N-CA-C	-6.84	104.80	113.01
2	E	194	ARG	N-CA-C	-6.83	104.81	113.01
2	E	458	PHE	CA-C-N	6.63	128.13	119.84
2	E	458	PHE	C-N-CA	6.63	128.13	119.84
2	B	458	PHE	CA-C-N	6.62	128.12	119.84
2	B	458	PHE	C-N-CA	6.62	128.12	119.84
2	B	318	LYS	N-CA-C	-6.62	105.34	113.41
2	E	318	LYS	N-CA-C	-6.59	105.38	113.41
3	F	325	ASN	N-CA-C	6.35	119.25	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	137	GLU	CA-C-N	6.34	127.22	120.11
3	C	137	GLU	C-N-CA	6.34	127.22	120.11
3	C	325	ASN	N-CA-C	6.34	119.24	108.90
3	F	129	ALA	N-CA-C	-6.34	104.37	111.28
3	F	137	GLU	CA-C-N	6.32	127.19	120.11
3	F	137	GLU	C-N-CA	6.32	127.19	120.11
3	C	129	ALA	N-CA-C	-6.31	104.40	111.28
2	E	385	TRP	N-CA-C	6.18	118.08	109.31
3	C	340	HIS	N-CA-C	6.16	117.60	108.60
3	F	340	HIS	N-CA-C	6.16	117.59	108.60
2	B	385	TRP	N-CA-C	6.15	118.04	109.31
2	B	347	GLY	N-CA-C	6.08	118.83	110.56
2	E	347	GLY	N-CA-C	6.08	118.82	110.56
2	B	411	ASN	CA-C-N	6.04	125.72	119.56
2	B	411	ASN	C-N-CA	6.04	125.72	119.56
3	C	223	THR	N-CA-C	-6.02	103.18	110.88
3	F	223	THR	N-CA-C	-6.00	103.20	110.88
2	E	411	ASN	CA-C-N	6.00	125.68	119.56
2	E	411	ASN	C-N-CA	6.00	125.68	119.56
3	F	341	ALA	N-CA-C	-5.94	105.78	114.39
3	C	341	ALA	N-CA-C	-5.93	105.78	114.39
2	E	246	ASN	N-CA-C	-5.88	106.27	113.50
2	B	246	ASN	N-CA-C	-5.86	106.29	113.50
2	E	288	LEU	CA-C-N	5.86	127.16	119.84
2	E	288	LEU	C-N-CA	5.86	127.16	119.84
3	C	280	TYR	N-CA-C	5.84	118.29	109.23
2	B	288	LEU	CA-C-N	5.83	127.13	119.84
2	B	288	LEU	C-N-CA	5.83	127.13	119.84
3	F	280	TYR	N-CA-C	5.81	118.23	109.23
1	A	152	VAL	CB-CA-C	-5.74	104.63	111.81
1	D	152	VAL	CB-CA-C	-5.71	104.67	111.81
2	E	393	GLN	N-CA-C	-5.68	98.70	110.80
2	B	393	GLN	N-CA-C	-5.66	98.74	110.80
2	B	416	TYR	N-CA-C	5.66	118.40	108.56
2	E	416	TYR	N-CA-C	5.64	118.37	108.56
2	B	389	ASP	CA-C-N	5.56	126.79	119.84
2	B	389	ASP	C-N-CA	5.56	126.79	119.84
2	E	273	PHE	N-CA-C	5.56	115.88	108.38
2	E	389	ASP	CA-C-N	5.55	126.78	119.84
2	E	389	ASP	C-N-CA	5.55	126.78	119.84
2	B	273	PHE	N-CA-C	5.54	115.86	108.38
2	B	262	PHE	N-CA-C	-5.50	106.34	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	262	PHE	N-CA-C	-5.50	106.34	113.16
3	C	130	GLN	N-CA-C	-5.49	104.53	111.11
3	F	130	GLN	N-CA-C	-5.48	104.53	111.11
2	E	343	ASN	N-CA-C	5.36	122.21	110.80
3	F	338	LYS	N-CA-C	-5.36	104.83	111.90
2	B	343	ASN	N-CA-C	5.33	122.16	110.80
3	C	338	LYS	N-CA-C	-5.33	104.87	111.90
2	E	228	GLN	CA-C-N	5.30	124.91	119.56
2	E	228	GLN	C-N-CA	5.30	124.91	119.56
3	F	163	GLN	N-CA-C	5.28	118.03	109.06
3	C	163	GLN	N-CA-C	5.27	118.01	109.06
2	B	228	GLN	CA-C-N	5.26	124.87	119.56
2	B	228	GLN	C-N-CA	5.26	124.87	119.56
3	F	247	ARG	N-CA-C	-5.18	102.81	110.48
3	C	247	ARG	N-CA-C	-5.17	102.83	110.48
2	E	265	LYS	N-CA-C	5.12	117.42	110.35
2	B	265	LYS	N-CA-C	5.10	117.39	110.35
3	C	101	LEU	N-CA-C	-5.10	105.18	111.40
2	E	250	THR	N-CA-C	-5.07	100.81	108.67
3	F	101	LEU	N-CA-C	-5.07	105.22	111.40
2	B	250	THR	N-CA-C	-5.06	100.82	108.67
3	C	92	GLU	N-CA-C	-5.00	107.03	113.23

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 ⓘ

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	53	0
1	D	697	0	744	52	3
2	B	2517	0	2380	186	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2517	0	2380	191	0
3	C	2480	0	2333	188	3
3	F	2480	0	2332	191	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	805	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 36.

All (805) 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
3:C:396:GLU:HA	3:F:186:GLY:C	1.74	1.12
1:A:194:LEU:HB3	1:A:195:PRO:HD3	1.33	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:351:ASN:HD21	2:B:354:MET:HG2	1.28	0.97
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:B:314:MET:HE1	2:B:437:TRP:CB	2.02	0.90
2:E:167:VAL:HG23	2:E:168:LEU:HD12	1.51	0.90
2:E:314:MET:HE1	2:E:437:TRP:CB	2.02	0.89
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:HD12	1:D:185:LEU:O	1.73	0.88
2:E:235:PRO:HG2	3:F:168:PHE:HE2	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:298:LYS:HZ1	2:E:298:LYS:H	1.23	0.86
2:E:314:MET:HE1	2:E:437:TRP:CG	2.11	0.86
1:A:185:LEU:O	1:A:185:LEU:HD12	1.73	0.86
2:B:314:MET:HE1	2:B:437:TRP:CG	2.11	0.86
2:E:370:HIS:O	2:E:373:MET:HB2	1.76	0.86
2:E:439:ASN:HD22	2:E:439:ASN:H	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:298:LYS:HZ1	2:B:298:LYS:H	1.22	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: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:H	2:E:298:LYS:NZ	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:A:191:LYS:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:162:ARG:NH1	2:E:259:SER:HB3	2.07	0.69
2:E:199:VAL:O	3:F:141:ASP:HA	1.93	0.69
2:E:317:TRP:CD1	2:E:420:GLY:H	2.11	0.69
2:B:317:TRP:CD1	2:B:420:GLY:H	2.11	0.68
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
3:C:307:HIS:HE1	3:C:341:ALA:H	1.42	0.67
1:A:185:LEU:HD12	1:A:185:LEU:C	2.20	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:HD22	2:E:439:ASN:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HD12	1:D:185:LEU:C	2.19	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
3:C:396:GLU:CB	3:F:186:GLY:HA2	2.28	0.64
2:E:390:PRO:HB3	2:E:393:GLN:OE1	1.97	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:202:ASN:ND2	2:E:284:ASN:HB3	2.13	0.63
2:E:277:ALA:HA	2:E:289:PRO:HA	1.80	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
3:C:396:GLU:C	3:F:187:SER:H	2.06	0.63
3:C:396:GLU:C	3:F:187:SER:N	2.57	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:H	3:F:367:ILE:HD12	1.65	0.62
3:C:103:HIS:O	3:C:107:ILE:HD13	2.01	0.61
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:HD12	3:C:367:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:405:ASN:C	2:E:407:CYS:N	2.57	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:88:LYS:HD3	3:C:92:GLU:HB2	1.83	0.60
3:C:334:TRP:CZ2	3:C:343:HIS:HA	2.36	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:B:405:ASN:C	2:B:407:CYS:N	2.57	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:194:PHE:CZ	3:F:384:MET:HE2	2.38	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
3:C:335:TRP:CD1	3:C:335:TRP:H	2.20	0.58
3:F:335:TRP:H	3:F:335:TRP:CD1	2.20	0.58
3:C:194:PHE:CZ	3:C:384:MET:HE2	2.38	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
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.86	0.58
1:A:194:LEU:HB3	1:A:195:PRO:CD	2.20	0.58
2:B:194:ARG:NH2	2:E:191:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:H	2:B:439:ASN:ND2	2.00	0.58
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
2:B:190:MET:HE1	3:C:130:GLN:HB3	1.86	0.57
3:F:172:LEU:HD13	3:F:172:LEU:O	2.05	0.57
3:F:307:HIS:O	3:F:310:MET:HB2	2.05	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
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.03	0.56
2:E:190:MET:HE1	3:F:130:GLN:HB3	1.86	0.56
2:E:439:ASN:N	2:E:439:ASN:ND2	2.53	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
2:E:314:MET:HE1	2:E:437:TRP:HB2	1.83	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:F:337:ASN:C	3:F:339:CYS:N	2.61	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:266:TRP:CE3	2:E:380:ARG:HD2	2.41	0.56
2:E:351:ASN:C	2:E:351:ASN:HD22	2.14	0.55
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
3:C:396:GLU:CA	3:F:186:GLY:HA2	2.36	0.55
2:B:314:MET:HE1	2:B:437:TRP:HB2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:ASN:HD22	2:B:351:ASN:C	2.14	0.55
2:E:234:LYS:HE2	2:E:234:LYS:HA	1.87	0.55
3:C:189:ASN:ND2	3:C:391:ARG:HH21	2.04	0.55
3:C:236:ILE:O	3:C:239:GLN:HG2	2.06	0.55
2:E:211:CYS:SG	2:E:250:THR:HA	2.46	0.55
2:B:152:TYR:CD1	2:B:152:TYR:C	2.85	0.55
2:B:266:TRP:CE3	2:B:380:ARG:HD2	2.41	0.55
2:B:314:MET:HE3	2:B:447:MET:HE3	1.89	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:HD12	3:F:209:ILE:N	2.17	0.54
2:E:152:TYR:CD1	2:E:152:TYR:C	2.85	0.54
2:E:314:MET:HE3	2:E:447:MET:HE3	1.89	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:N	2:B:439:ASN:ND2	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:143:GLN:HE22	3:C:117:ASN:HB3	1.72	0.54
1:A:176:LYS:H	1:A:176:LYS:HD3	1.73	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
3:C:337:ASN:C	3:C:339:CYS:N	2.61	0.53
2:E:360:LEU:HB3	2:E:364:ASN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:88:LYS:HB3	3:F:92:GLU:CB	2.34	0.52
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.90	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:357:ALA:HA	2:E:439:ASN:ND2	2.21	0.52
2:E:376:SER:HB3	2:E:382:ASN:H	1.75	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:H5	4:E:1:NAG:HN2	1.75	0.52
2:E:359:GLN:H	2:E:359:GLN:HE21	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:152:TYR:HD1	2:E:152:TYR:C	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:210:GLU:HG2	2:E:212:GLU:N	2.18	0.52
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:195:GLN:OE1	3:C:382:THR:HG22	2.10	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: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:E:298:LYS:HZ2	2:E:298:LYS:HB2	1.74	0.51
2:B:298:LYS:HB2	2:B:298:LYS:HZ2	1.75	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
2:E:163:THR:C	2:E:165:LEU:H	2.19	0.51
2:E:405:ASN:C	2:E:407:CYS:H	2.18	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:B:152:TYR:HD1	2:B:152:TYR:C	2.18	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
2:B:163:THR:C	2:B:165:LEU:H	2.19	0.50
2:B:405:ASN:C	2:B:407:CYS:H	2.18	0.50
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:OE1	3:F:119:GLN:HA	2.11	0.50
3:F:367:ILE:O	3:F:378:SER:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.80	0.50
3:F:365:ASN:N	3:F:365:ASN:HD22	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:E:342:VAL:H	2:E:371:ASN:ND2	2.09	0.50
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:385:TRP:HB3	2:E:392:LYS:HZ2	1.76	0.50
2:B:361:MET:O	2:B:364:ASN:HB2	2.12	0.49
3:C:367:ILE:O	3:C:378:SER:HA	2.11	0.49
3:C:369:TRP:HD1	3:C:372:TRP:HB2	1.76	0.49
3:F:334:TRP:HE3	3:F:345:ASN:ND2	2.10	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
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:OE1	3:C:119:GLN:HA	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:B:385:TRP:HB3	2:B:392:LYS:HZ2	1.77	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:HD12	3:C:209:ILE:N	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:HD22	3:C:365:ASN:N	2.10	0.49
2:E:224:MET:SD	2:E:237:ARG:HB3	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:276:VAL:O	2:E:290:GLY:N	2.45	0.49
1:A:135:LEU:HD13	1:A:135:LEU:C	2.38	0.48
2:B:224:MET:SD	2:B:237:ARG:HB3	2.53	0.48
3:C:161:ALA:C	3:C:162:LYS:HD3	2.38	0.48
3:C:318:ASP:CG	3:C:325:ASN:HB3	2.38	0.48
2:E:439:ASN:H	2:E:439:ASN:ND2	2.00	0.48
3:F:318:ASP:CG	3:F:325:ASN:HB3	2.38	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
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
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
2:E:226:LEU:HD23	2:E:236:TYR:C	2.38	0.48
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.48	0.48
3:C:191:TRP:CZ3	3:C:387:ILE:HB	2.48	0.48
3:F:123:ASN:N	3:F:123:ASN:HD22	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
2:E:317:TRP:NE1	2:E:420:GLY:H	2.12	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
1:D:135:LEU:HD13	1:D:135:LEU:C	2.38	0.48
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.49	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
2:B:283:LYS:HE2	2:B:283:LYS:H	1.78	0.48
2:B:317:TRP:NE1	2:B:420:GLY:H	2.12	0.48
2:B:389:ASP:C	2:B:391:ARG:H	2.22	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
3:F:161:ALA:C	3:F:162:LYS:HD3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	2:E:380:ARG:CB	2.27	0.47
2:B:294:LEU:CD2	2:B:299:ILE:HG12	2.44	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
1:D:114:ASP:HB3	3:F:90:LEU:HD21	1.96	0.47
3:F:181:TYR:HE1	3:F:220:PRO:O	1.98	0.47
2:B:203:ILE:O	3:C:217:HIS:HA	2.14	0.47
2:B:226:LEU:HD23	2:B:236:TYR:C	2.38	0.47
2:B:380:ARG:HH11	2:B:380:ARG:CB	2.27	0.47
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
2:E:389:ASP:C	2:E:391:ARG:H	2.22	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:CD1	2:B:326:TYR:N	2.83	0.47
2:B:362:GLY:O	2:B:366:THR:HG23	2.15	0.47
3:C:181:TYR:HE1	3:C:220:PRO:O	1.98	0.47
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.97	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:215:ILE:HG13	2:E:219:GLY:O	2.15	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:HA	1:D:150:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:374:PHE:O	2:E:403:TRP:HA	2.16	0.46
3:F:343:HIS:O	3:F:343:HIS:ND1	2.49	0.46
2:B:215:ILE:HG13	2:B:219:GLY:O	2.15	0.46
3:C:343:HIS:O	3:C:343:HIS:ND1	2.49	0.46
4:E:1:NAG:N2	4:E:1:NAG:C5	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:415:ARG:O	2:B:434:GLY:HA2	2.15	0.46
3:C:194:PHE:HZ	3:C:384:MET:HE2	1.78	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:CD1	3:C:335:TRP:N	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
3:C:232:LYS:O	3:C:233:ILE:C	2.58	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:E:408:HIS:O	2:E:438:MET:HE2	2.17	0.45
3:F:194:PHE:HZ	3:F:384:MET:HE2	1.78	0.45
3:F:337:ASN:C	3:F:339:CYS:H	2.24	0.45
2:B:383:ASP:OD1	2:B:385:TRP:CE2	2.70	0.45
2:B:408:HIS:O	2:B:438:MET:HE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:337:ASN:C	3:C:339:CYS:H	2.24	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
2:B:314:MET:HE1	2:B:437:TRP:HB3	1.95	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
3:F:232:LYS:O	3:F:233:ILE:C	2.58	0.45
1:A:144:LEU:CD1	2:B:175:LEU:HD21	2.46	0.45
2:B:351:ASN:ND2	2:B:351:ASN:C	2.74	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
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:ND2	2:E:351:ASN:O	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:117:SER:C	1:D:119:ILE:H	2.25	0.44
1:D:181:GLN:HE21	1:D:181:GLN:N	2.16	0.44
2:E:191:GLU:O	2:E:193:CYS:N	2.50	0.44
2:E:203:ILE:HD13	2:E:203:ILE:N	2.33	0.44
1:A:175:LEU:O	1:A:176:LYS:C	2.60	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:229:PRO:CG	2:E:302:LEU:HD21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:280:THR:HG23	2:E:287:GLY:H	1.83	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
2:E:280:THR:OG1	2:E:281:ASP:N	2.49	0.44
2:B:163:THR:C	2:B:165:LEU:N	2.76	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
3:C:337:ASN:O	3:C:338:LYS:C	2.60	0.44
1:D:175:LEU:O	1:D:176:LYS:C	2.60	0.44
2:E:163:THR:C	2:E:165:LEU:N	2.76	0.44
2:E:172:LEU:HD13	2:E:172:LEU:HA	1.83	0.44
2:E:351:ASN:ND2	2:E:351:ASN:C	2.74	0.44
3:F:337:ASN:O	3:F:338:LYS:C	2.60	0.44
1:A:117:SER:C	1:A:119:ILE:H	2.25	0.43
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:N	2:E:360:LEU:HD22	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:HE21	1:A:181:GLN:N	2.16	0.43
2:B:359:GLN:HE21	2:B:359:GLN:N	2.17	0.43
1:D:127:ILE:HD13	1:D:193:LEU:HD13	2.00	0.43
3:C:88:LYS:CD	3:C:92:GLU:HB2	2.45	0.43
3:C:172:LEU:H	3:C:239:GLN:HE21	1.65	0.43
2:E:165:LEU:O	2:E:166:ARG:C	2.61	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:360:LEU:N	2:B:360:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD12	2:B:386:LEU:O	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
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
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: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:ND2	2:B:351:ASN:O	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
3:C:274:TYR:O	3:C:275:ARG:C	2.63	0.42
2:B:414:GLY:HA3	2:B:434:GLY:O	2.19	0.42
1:D:157:LYS:HE2	2:E:398:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:276:VAL:O	2:E:289:PRO:HA	2.20	0.42
3:F:94:MET:HA	3:F:97:GLU:OE2	2.20	0.42
3:F:206:LYS:HE3	3:F:215:PHE:CD2	2.54	0.42
2:B:168:LEU:HD12	2:B:168:LEU:N	2.34	0.42
2:B:317:TRP:CG	2:B:420:GLY:H	2.37	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:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
2:E:375:PHE:CE1	2:E:402:TRP:HA	2.54	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
2:B:332:GLN:HG2	2:B:336:ASN:HB2	2.01	0.42
2:B:397:GLU:C	2:B:399:GLY:N	2.78	0.42
3:F:131:LEU:O	3:F:134:GLN:N	2.49	0.42
3:F:359:THR:C	3:F:361:ASN:H	2.27	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
3:F:337:ASN:O	3:F:337:ASN:CG	2.63	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
3:F:219:SER:HG	3:F:224:THR:HG22	1.85	0.42
2:B:160:ASN:ND2	2:B:160:ASN:C	2.78	0.41
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:C:337:ASN:O	3:C:337:ASN:CG	2.63	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
2:B:165:LEU:O	2:B:166:ARG:C	2.61	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:196:LYS:HA	3:F:382:THR:O	2.19	0.41
3:F:326:CYS:SG	3:F:339:CYS:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:CA	1:A:118:ARG:HE	2.32	0.41
2:B:204:PRO:HG3	3:C:217:HIS:CD2	2.55	0.41
2:B:370:HIS:CE1	2:B:402:TRP:HE1	2.38	0.41
3:C:93:ILE:N	3:C:93:ILE:HD12	2.36	0.41
3:C:94:MET:HA	3:C:97:GLU:OE2	2.20	0.41
3:F:295:PHE:CD2	3:F:375:ARG:HD2	2.55	0.41
3:F:346:GLY:O	3:F:367:ILE:HG13	2.20	0.41
1:A:176:LYS:HD3	1:A:176:LYS:N	2.35	0.41
2:B:285:TYR:H	2:B:285:TYR:HD1	1.62	0.41
3:C:295:PHE:CD2	3:C:375:ARG:HD2	2.55	0.41
3:C:346:GLY:O	3:C:367:ILE:HG13	2.20	0.41
2:E:386:LEU:HD12	2:E:386:LEU:O	2.19	0.41
3:F:334:TRP:CE2	3:F:343:HIS:HA	2.55	0.41
3:C:117:ASN:C	3:C:119:GLN:N	2.78	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
2:E:317:TRP:CG	2:E:420:GLY:H	2.37	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:HD3	1:A:129:LYS:HA	1.90	0.41
2:B:227:ILE:HD11	2:B:236:TYR:CE2	2.55	0.41
3:C:359:THR:C	3:C:361:ASN:H	2.27	0.41
3:C:396:GLU:HG3	3:F:185:ASP:C	2.46	0.41
2:E:376:SER:HB3	2:E:382:ASN:HB2	2.03	0.41
3:F:93:ILE:N	3:F:93:ILE:HD12	2.36	0.41
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:274:TYR:O	3:F:275:ARG:C	2.63	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:211:CYS:O	2:B:242:MET:HE1	2.21	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:160:ASN:ND2	2:E:160:ASN:C	2.78	0.41
2:E:253:GLN:NE2	2:E:451:SER:HA	2.36	0.41
2:E:351:ASN:ND2	2:E:354:MET:H	2.18	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:246:LEU:O	3:C:261:ASP:HA	2.21	0.41
3:C:247:ARG:CD	3:C:259:THR:HB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:330:ASP:HA	3:C:365:ASN:HB3	2.03	0.41
3:C:338:LYS:O	3:C:339:CYS:HB2	2.20	0.41
2:E:211:CYS:O	2:E:242:MET:HE1	2.21	0.41
2:E:397:GLU:C	2:E:399:GLY:N	2.78	0.41
3:F:168:PHE:HE1	3:F:179:LEU:HB2	1.85	0.41
3:F:168:PHE:CD1	3:F:179:LEU:HD13	2.56	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
3:F:370:ALA:C	3:F:372:TRP:N	2.78	0.41
2:B:276:VAL:HG13	2:B:292:TYR:CE2	2.56	0.41
3:C:305:THR:CB	3:C:341:ALA:HB2	2.51	0.41
3:C:326:CYS:SG	3:C:339:CYS:N	2.93	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: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
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
1:A:191:LYS:HG3	1:A:192:ASP:N	2.35	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
2:E:383:ASP:OD1	2:E:385:TRP:CD2	2.74	0.40
3:F:96:TYR:C	3:F:98:ALA:H	2.30	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
3:C:392:LEU:HD22	3:F:186:GLY:O	2.20	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	2	7
1	D	83/87 (95%)	64 (77%)	15 (18%)	4 (5%)	2	7
2	B	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	2	10
2	E	311/328 (95%)	252 (81%)	47 (15%)	12 (4%)	2	10
3	C	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	3	15
3	F	307/319 (96%)	243 (79%)	55 (18%)	9 (3%)	3	15
All	All	1402/1468 (96%)	1118 (80%)	234 (17%)	50 (4%)	2	11

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	C	395	GLY
3	F	395	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	80/82 (98%)	63 (79%)	17 (21%)	1	4
1	D	80/82 (98%)	63 (79%)	17 (21%)	1	4
2	B	271/286 (95%)	234 (86%)	37 (14%)	3	12
2	E	271/286 (95%)	233 (86%)	38 (14%)	3	11
3	C	261/267 (98%)	229 (88%)	32 (12%)	4	15
3	F	261/267 (98%)	229 (88%)	32 (12%)	4	15
All	All	1224/1270 (96%)	1051 (86%)	173 (14%)	3	11

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	A	130	VAL
1	A	135	LEU
1	A	140	VAL
1	A	146	ASP
1	A	150	LEU
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

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Mol	Chain	Res	Type
1	A	193	LEU
2	B	149	HIS
2	B	152	TYR
2	B	154	ASP
2	B	155	GLU
2	B	157	VAL
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	203	ILE
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	314	MET
2	B	340	ILE
2	B	343	ASN
2	B	351	ASN
2	B	359	GLN
2	B	373	MET
2	B	376	SER
2	B	380	ARG
2	B	385	TRP
2	B	398	ASP
2	B	432	ASP
2	B	435	VAL
2	B	436	VAL
2	B	438	MET
2	B	439	ASN
2	B	454	ILE
2	B	457	PHE
2	B	459	PRO
3	C	112	GLU
3	C	113	ILE
3	C	117	ASN
3	C	128	VAL

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Mol	Chain	Res	Type
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	172	LEU
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	303	PHE
3	C	323	GLU
3	C	337	ASN
3	C	340	HIS
3	C	343	HIS
3	C	359	THR
3	C	364	ASP
3	C	365	ASN
3	C	368	ILE
3	C	374	THR
3	C	378	SER
3	C	382	THR
3	C	383	THR
3	C	385	LYS
3	C	390	ASN
1	D	120	GLU
1	D	130	VAL
1	D	135	LEU
1	D	140	VAL
1	D	146	ASP
1	D	150	LEU
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

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Mol	Chain	Res	Type
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	157	VAL
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	203	ILE
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	294	LEU
2	E	298	LYS
2	E	314	MET
2	E	340	ILE
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	373	MET
2	E	376	SER
2	E	380	ARG
2	E	385	TRP
2	E	398	ASP
2	E	432	ASP
2	E	435	VAL
2	E	436	VAL
2	E	438	MET
2	E	439	ASN
2	E	454	ILE
2	E	457	PHE
2	E	459	PRO
3	F	112	GLU

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Mol	Chain	Res	Type
3	F	113	ILE
3	F	117	ASN
3	F	128	VAL
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	172	LEU
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	303	PHE
3	F	323	GLU
3	F	337	ASN
3	F	340	HIS
3	F	343	HIS
3	F	359	THR
3	F	364	ASP
3	F	365	ASN
3	F	368	ILE
3	F	374	THR
3	F	378	SER
3	F	382	THR
3	F	383	THR
3	F	385	LYS
3	F	390	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	137	GLN
1	A	143	GLN
1	A	181	GLN
2	B	158	ASN
2	B	160	ASN
2	B	180	GLN

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Mol	Chain	Res	Type
2	B	189	GLN
2	B	228	GLN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	336	ASN
2	B	339	GLN
2	B	343	ASN
2	B	359	GLN
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	131	GLN
1	D	132	HIS
1	D	137	GLN
1	D	143	GLN
1	D	181	GLN
2	E	158	ASN
2	E	160	ASN
2	E	180	GLN
2	E	189	GLN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	336	ASN
2	E	339	GLN

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Mol	Chain	Res	Type
2	E	343	ASN
2	E	351	ASN
2	E	359	GLN
2	E	413	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	337	ASN
3	F	361	ASN
3	F	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	E	1	-	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
4	NAG	B	1	-	14,14,15	0.58	0	17,19,21	0.73	1 (5%)

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	E	1	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C2-N2-C7	-2.11	120.08	122.90
4	E	1	NAG	C2-N2-C7	-2.09	120.09	122.90

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	E	1	NAG	3	0
4	B	1	NAG	2	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.