Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 11:07 PM EDT

PDB ID	:	1FZC
Title	:	CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN WITH TWO DIFFERENT BOUND LIGANDS
Authors	:	Everse, S.J.; Spraggon, G.; Veerapandian, L.; Riley, M.; Doolittle, R.F.
Deposited on	:	1998-05-19
Resolution	:	2.30 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:

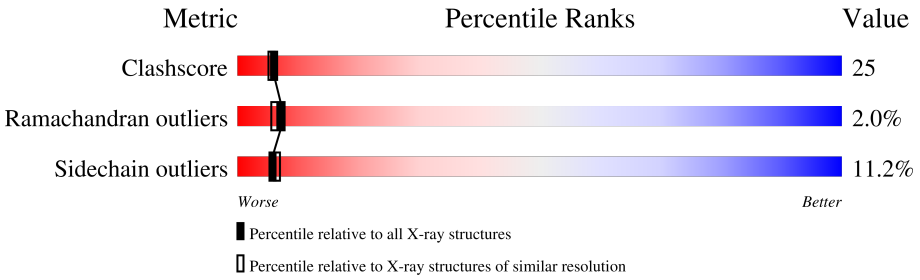
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	44% 32% 8% • 15%
1	D	87	37% 40% 7% • 15%
2	B	328	51% 32% 9% • 6%
2	E	328	52% 31% 9% • 6%
3	C	319	56% 28% 9% • 6%
3	F	319	61% 26% 6% • 6%
4	G	4	50% 25% 25%
4	H	4	75% 25%

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Mol	Chain	Length	Quality of chain
5	I	4	
5	J	4	
6	K	2	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11594 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 FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2473	1544	434	473	22			
2	E	308	Total	C	N	O	S	0	0	0
			2473	1544	434	473	22			

- Molecule 3 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			
3	F	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			

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 a protein called FIBRIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			29	18	7	4			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	H	4	Total C N O 29 18 7 4	0	0	0

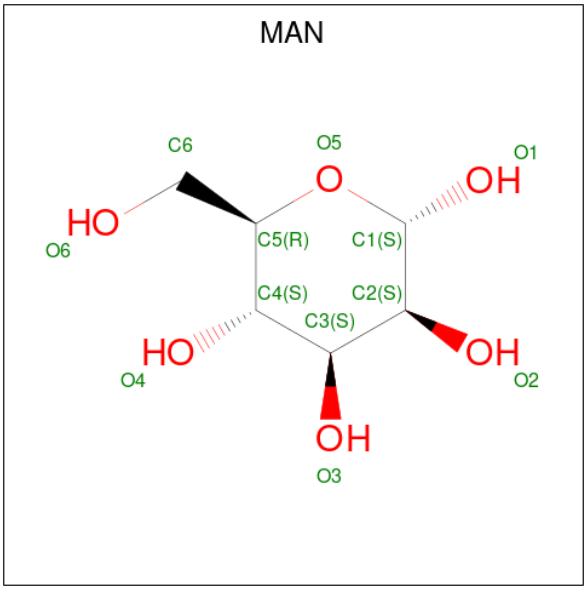
- Molecule 5 is a protein called FIBRIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	I	4	Total C N O 32 19 9 4	0	0	0
5	J	4	Total C N O 32 19 9 4	0	0	0

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	K	2	Total C N O 28 16 2 10	0	0	0

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

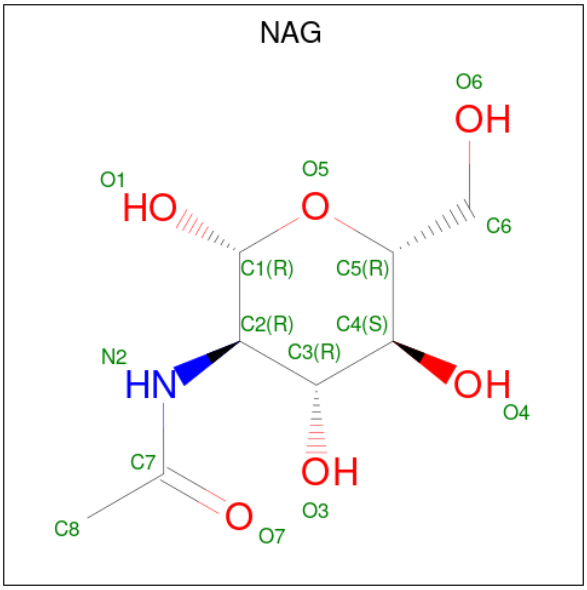


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 11 6 5	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0
8	E	1	Total Ca 1 1	0	0
8	F	1	Total Ca 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	15	Total O 15 15	0	0
10	B	124	Total O 124 124	0	0
10	C	71	Total O 71 71	0	0
10	D	16	Total O 16 16	0	0
10	E	119	Total O 119 119	0	0
10	F	82	Total O 82 82	0	0
10	G	1	Total O 1 1	0	0
10	H	1	Total O 1 1	0	0
10	I	1	Total O 1 1	0	0
10	J	1	Total O 1 1	0	0

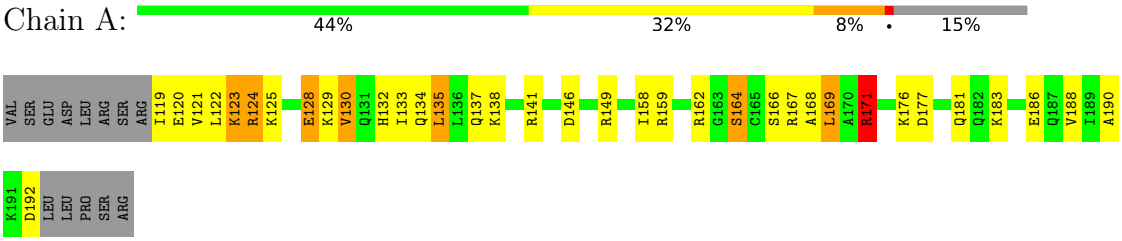
3 Residue-property plots (i)

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.

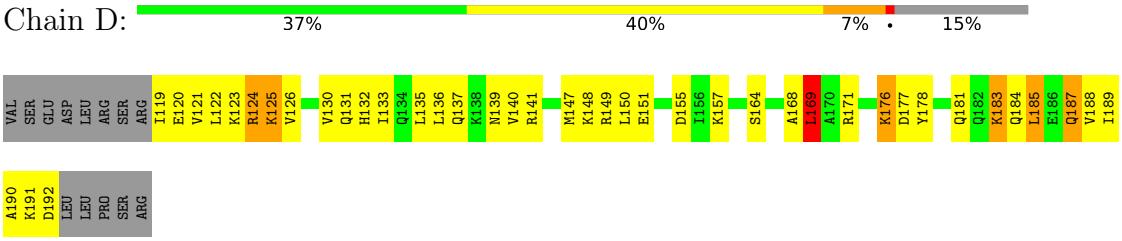
• Molecule 1: FIBRIN

Chain A:



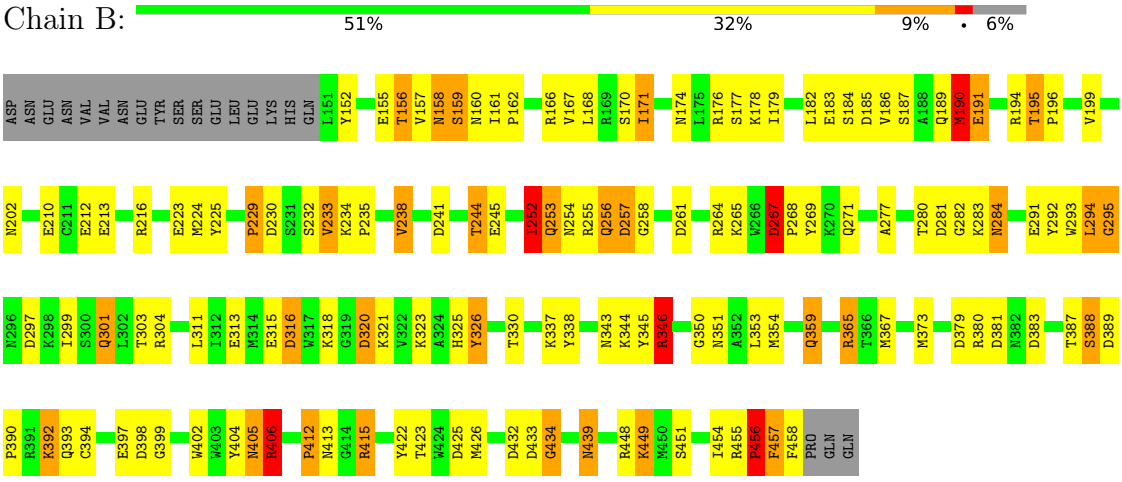
• Molecule 1: FIBRIN

Chain D:



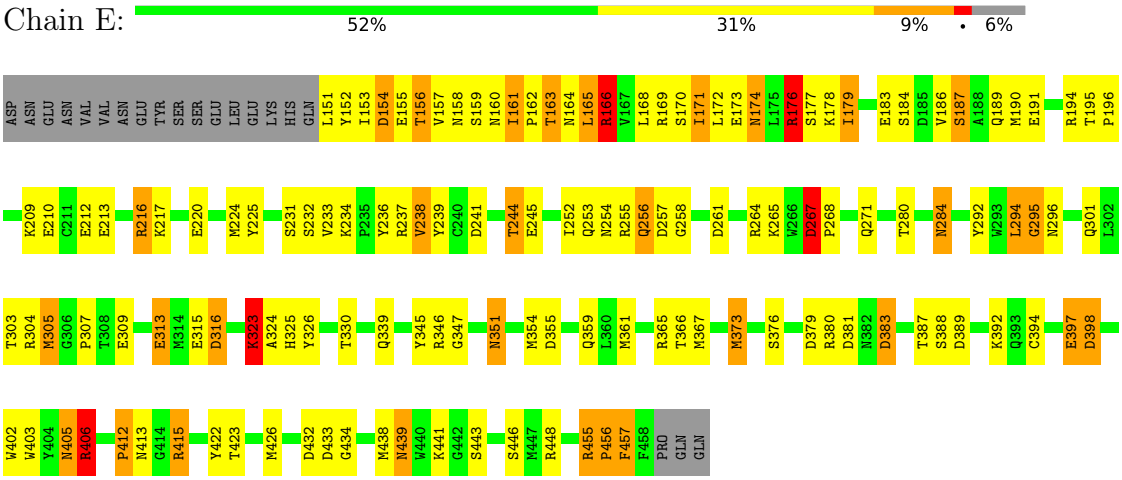
• Molecule 2: FIBRIN

Chain B:



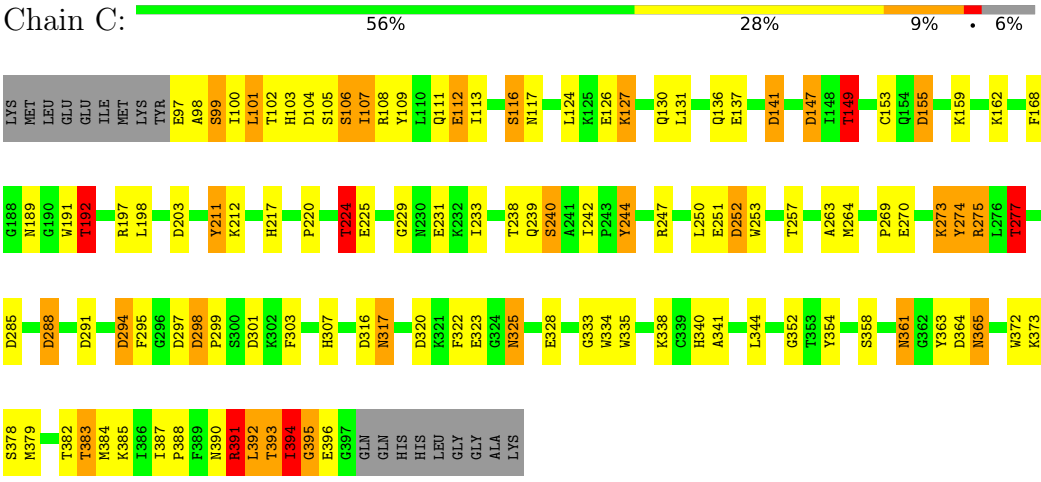
• Molecule 2: FIBRIN

Chain E:



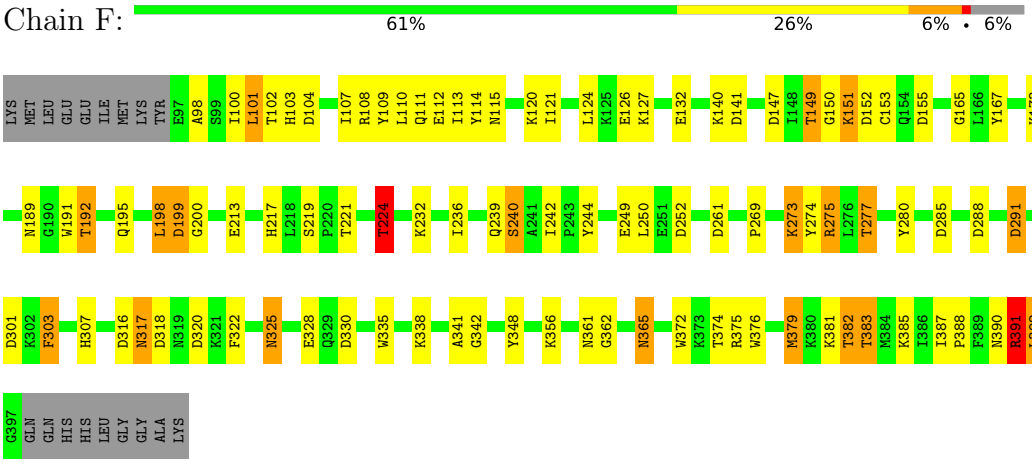
• Molecule 3: FIBRIN

Chain C:



• Molecule 3: FIBRIN

Chain F:



• Molecule 4: FIBRIN

Chain G:

• Molecule 4: FIBRIN

Chain H:

• Molecule 5: FIBRIN

Chain I:

• Molecule 5: FIBRIN

Chain J:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

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	83.44Å 95.60Å 113.64Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (20.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11594	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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, MAN, 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	0.60	0/609	1.86	13/811 (1.6%)
1	D	0.58	0/609	1.62	11/811 (1.4%)
2	B	0.98	3/2535 (0.1%)	1.94	82/3425 (2.4%)
2	E	0.92	3/2535 (0.1%)	1.94	81/3425 (2.4%)
3	C	0.73	1/2469 (0.0%)	1.68	50/3339 (1.5%)
3	F	0.75	1/2469 (0.0%)	1.61	30/3339 (0.9%)
4	G	0.75	0/30	4.32	4/40 (10.0%)
4	H	0.97	0/30	2.53	2/40 (5.0%)
5	I	0.75	0/33	1.89	1/43 (2.3%)
5	J	0.91	0/33	1.42	0/43
All	All	0.83	8/11352 (0.1%)	1.81	274/15316 (1.8%)

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
3	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	GLY	N-CA	12.22	1.64	1.46
2	B	434	GLY	N-CA	11.47	1.63	1.46
2	E	295	GLY	N-CA	11.01	1.62	1.46
2	E	258	GLY	N-CA	10.33	1.61	1.46
2	B	258	GLY	N-CA	7.23	1.56	1.46
3	C	274	TYR	N-CA	6.91	1.60	1.46
2	E	184	SER	CB-OG	-6.05	1.34	1.42
3	F	274	TYR	N-CA	5.11	1.56	1.46

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	3	ARG	NE-CZ-NH2	-23.44	108.58	120.30
1	A	167	ARG	NE-CZ-NH1	18.52	129.56	120.30
2	E	255	ARG	NE-CZ-NH2	15.11	127.86	120.30
2	E	264	ARG	NE-CZ-NH2	-14.71	112.94	120.30
3	C	375	ARG	NE-CZ-NH1	14.15	127.38	120.30
1	A	167	ARG	CD-NE-CZ	13.41	142.38	123.60
1	A	159	ARG	NE-CZ-NH1	13.39	127.00	120.30
2	E	383	ASP	CB-CG-OD2	13.28	130.25	118.30
2	B	255	ARG	NE-CZ-NH1	12.91	126.75	120.30
3	C	197	ARG	NE-CZ-NH2	-12.40	114.10	120.30
2	B	380	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	D	141	ARG	NE-CZ-NH1	11.21	125.91	120.30
2	E	237	ARG	NE-CZ-NH2	11.04	125.82	120.30
2	E	365	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	D	171	ARG	NE-CZ-NH2	-10.94	114.83	120.30
3	F	301	ASP	CB-CG-OD1	10.93	128.13	118.30
2	B	383	ASP	CB-CG-OD2	10.92	128.12	118.30
1	A	146	ASP	CB-CG-OD2	10.81	128.03	118.30
4	H	3	ARG	NE-CZ-NH1	10.79	125.69	120.30
2	E	255	ARG	NE-CZ-NH1	-10.63	114.98	120.30
2	B	338	TYR	CB-CG-CD2	-10.63	114.62	121.00
2	E	365	ARG	NE-CZ-NH2	-10.55	115.03	120.30
3	C	364	ASP	CB-CG-OD1	10.52	127.77	118.30
2	B	297	ASP	CB-CG-OD1	10.52	127.77	118.30
1	D	171	ARG	NE-CZ-NH1	10.40	125.50	120.30
2	E	184	SER	CA-CB-OG	10.38	139.23	111.20
2	E	257	ASP	C-N-CA	-10.14	101.02	122.30
1	A	159	ARG	NE-CZ-NH2	-10.02	115.29	120.30
3	C	252	ASP	CB-CG-OD1	9.93	127.24	118.30
2	B	194	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	D	155	ASP	CB-CG-OD2	9.87	127.19	118.30
2	B	261	ASP	CB-CG-OD1	9.85	127.16	118.30
2	E	304	ARG	CD-NE-CZ	9.84	137.38	123.60
2	E	294	LEU	O-C-N	-9.81	106.52	123.20
2	E	194	ARG	NE-CZ-NH2	-9.73	115.44	120.30
2	B	264	ARG	NE-CZ-NH1	-9.62	115.49	120.30
2	B	433	ASP	C-N-CA	-9.62	102.10	122.30
2	B	338	TYR	CB-CG-CD1	9.62	126.77	121.00
2	E	455	ARG	NE-CZ-NH1	9.61	125.11	120.30
2	E	405	ASN	O-C-N	-9.57	107.38	122.70
2	E	264	ARG	NH1-CZ-NH2	9.54	129.90	119.40
2	E	380	ARG	NE-CZ-NH1	9.54	125.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	252	ILE	CA-CB-CG2	9.48	129.87	110.90
2	B	241	ASP	CB-CG-OD1	9.29	126.66	118.30
3	C	197	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	B	294	LEU	O-C-N	-9.18	107.59	123.20
2	B	304	ARG	NE-CZ-NH2	9.03	124.82	120.30
2	E	241	ASP	CB-CG-OD1	8.91	126.32	118.30
2	B	422	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	A	171	ARG	NE-CZ-NH2	-8.81	115.89	120.30
2	B	380	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	E	365	ARG	CD-NE-CZ	8.79	135.90	123.60
3	C	375	ARG	NE-CZ-NH2	-8.71	115.94	120.30
2	E	294	LEU	CA-C-N	8.67	133.55	116.20
2	B	316	ASP	CB-CG-OD2	-8.65	110.51	118.30
2	B	269	TYR	CB-CG-CD1	-8.54	115.88	121.00
2	E	406	ARG	O-C-N	-8.53	109.05	122.70
2	B	194	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	B	365	ARG	NE-CZ-NH1	8.49	124.55	120.30
2	B	297	ASP	CB-CG-OD2	-8.44	110.70	118.30
2	E	316	ASP	CB-CG-OD2	-8.39	110.75	118.30
5	I	3	ARG	CD-NE-CZ	8.34	135.27	123.60
2	B	294	LEU	CA-C-N	8.32	132.84	116.20
1	D	169	LEU	CA-CB-CG	8.28	134.33	115.30
2	B	267	ASP	CB-CG-OD2	-8.27	110.86	118.30
2	B	381	ASP	CB-CG-OD1	8.26	125.73	118.30
2	B	433	ASP	CB-CG-OD1	8.25	125.72	118.30
2	B	346	ARG	N-CA-CB	8.25	125.45	110.60
2	E	216	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	D	141	ARG	NE-CZ-NH2	-8.19	116.21	120.30
2	E	433	ASP	CB-CA-C	8.12	126.65	110.40
2	E	216	ARG	NE-CZ-NH1	-8.11	116.25	120.30
2	B	456	PRO	CA-C-N	8.05	134.91	117.20
2	E	184	SER	CB-CA-C	8.03	125.36	110.10
2	B	365	ARG	CD-NE-CZ	8.00	134.79	123.60
2	E	346	ARG	NE-CZ-NH2	7.95	124.28	120.30
2	B	422	TYR	CB-CG-CD1	7.93	125.76	121.00
2	B	294	LEU	C-N-CA	-7.92	105.67	122.30
3	C	375	ARG	CD-NE-CZ	7.91	134.68	123.60
2	E	294	LEU	C-N-CA	-7.80	105.92	122.30
3	C	155	ASP	CB-CG-OD2	7.76	125.29	118.30
3	F	320	ASP	CB-CG-OD2	7.73	125.26	118.30
2	B	257	ASP	CA-C-N	7.70	131.59	116.20
2	B	448	ARG	CD-NE-CZ	7.63	134.28	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	257	ASP	CA-C-N	7.62	131.45	116.20
2	E	237	ARG	NE-CZ-NH1	-7.57	116.52	120.30
3	C	225	GLU	OE1-CD-OE2	-7.56	114.23	123.30
2	B	455	ARG	NE-CZ-NH2	-7.55	116.52	120.30
2	B	257	ASP	C-N-CA	-7.51	106.53	122.30
2	B	448	ARG	NE-CZ-NH2	7.50	124.05	120.30
4	G	3	ARG	NH1-CZ-NH2	7.48	127.63	119.40
3	F	348	TYR	CB-CG-CD2	-7.46	116.53	121.00
2	B	432	ASP	CB-CG-OD2	7.37	124.93	118.30
3	C	141	ASP	CB-CG-OD1	7.36	124.93	118.30
2	E	213	GLU	OE1-CD-OE2	-7.34	114.49	123.30
3	F	285	ASP	CB-CG-OD1	7.30	124.87	118.30
2	E	379	ASP	CB-CG-OD1	7.29	124.86	118.30
3	F	252	ASP	CB-CG-OD1	7.24	124.82	118.30
3	F	291	ASP	CB-CG-OD2	-7.22	111.80	118.30
3	F	185	ASP	CB-CG-OD1	7.22	124.80	118.30
2	E	252	ILE	CA-CB-CG2	7.21	125.32	110.90
2	B	433	ASP	O-C-N	-7.21	110.95	123.20
1	D	141	ARG	CD-NE-CZ	7.17	133.64	123.60
1	D	149	ARG	NE-CZ-NH1	7.13	123.86	120.30
3	C	285	ASP	CB-CG-OD1	7.12	124.71	118.30
3	C	301	ASP	CB-CG-OD1	7.10	124.69	118.30
2	E	412	PRO	O-C-N	-7.08	111.38	122.70
3	F	273	LYS	CA-C-N	7.01	132.63	117.20
3	F	297	ASP	CB-CG-OD2	6.97	124.58	118.30
4	G	3	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	E	305	MET	CA-CB-CG	6.97	125.15	113.30
2	B	264	ARG	NH1-CZ-NH2	6.97	127.06	119.40
3	F	199	ASP	CB-CG-OD2	6.90	124.51	118.30
2	E	239	TYR	CB-CG-CD1	-6.90	116.86	121.00
3	F	391	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	141	ARG	NE-CZ-NH2	-6.81	116.89	120.30
2	B	415	ARG	NE-CZ-NH2	-6.77	116.92	120.30
3	C	147	ASP	CB-CG-OD2	-6.76	112.22	118.30
3	C	275	ARG	NE-CZ-NH1	6.75	123.67	120.30
3	C	363	TYR	CB-CG-CD1	-6.71	116.97	121.00
2	B	451	SER	CA-CB-OG	6.68	129.23	111.20
3	F	224	THR	N-CA-CB	-6.65	97.67	110.30
2	B	455	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	E	406	ARG	N-CA-C	6.60	128.83	111.00
2	E	397	GLU	CA-C-N	6.57	131.66	117.20
2	E	166	ARG	NE-CZ-NH1	6.55	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	277	THR	OG1-CB-CG2	-6.55	94.94	110.00
2	E	176	ARG	NE-CZ-NH2	6.54	123.57	120.30
3	C	273	LYS	C-N-CA	-6.53	105.37	121.70
3	C	203	ASP	CB-CG-OD1	6.52	124.17	118.30
2	E	405	ASN	CA-C-N	6.51	131.53	117.20
2	E	415	ARG	NE-CZ-NH2	-6.51	117.04	120.30
2	E	264	ARG	NE-CZ-NH1	-6.48	117.06	120.30
3	F	141	ASP	CB-CG-OD1	6.44	124.09	118.30
3	C	320	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	169	LEU	CB-CG-CD2	6.42	121.91	111.00
2	E	236	TYR	CB-CG-CD2	6.38	124.83	121.00
3	F	221	THR	CA-CB-CG2	-6.38	103.47	112.40
3	F	273	LYS	C-N-CA	-6.37	105.77	121.70
2	E	433	ASP	O-C-N	-6.34	112.42	123.20
2	B	257	ASP	O-C-N	-6.34	112.42	123.20
3	F	165	GLY	O-C-N	-6.34	112.56	122.70
2	B	433	ASP	CA-C-N	6.33	128.85	116.20
2	E	432	ASP	CB-CG-OD1	6.30	123.97	118.30
3	C	185	ASP	CB-CG-OD1	6.29	123.96	118.30
3	C	316	ASP	CB-CG-OD1	6.28	123.95	118.30
3	C	247	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	E	313	GLU	OE1-CD-OE2	-6.24	115.82	123.30
2	E	433	ASP	CA-C-N	6.21	128.63	116.20
1	D	164	SER	CB-CA-C	-6.21	98.31	110.10
1	A	167	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
2	E	261	ASP	CB-CG-OD1	6.20	123.88	118.30
3	C	220	PRO	O-C-N	-6.20	112.78	122.70
3	C	273	LYS	CA-C-N	6.16	130.75	117.20
3	C	320	ASP	CB-CG-OD2	6.14	123.83	118.30
2	E	406	ARG	CD-NE-CZ	6.13	132.19	123.60
2	E	255	ARG	N-CA-CB	6.11	121.61	110.60
2	E	415	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	B	405	ASN	O-C-N	-6.08	112.98	122.70
3	F	330	ASP	CB-CG-OD2	6.07	123.76	118.30
2	B	320	ASP	CB-CG-OD2	6.07	123.76	118.30
3	C	275	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	B	225	TYR	CB-CG-CD1	6.00	124.60	121.00
2	B	185	ASP	CB-CG-OD1	6.00	123.69	118.30
3	C	211	TYR	CB-CG-CD2	-5.97	117.42	121.00
3	C	252	ASP	CB-CG-OD2	-5.96	112.93	118.30
2	E	398	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	135	LEU	CA-CB-CG	5.96	129.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	433	ASP	CB-CA-C	5.95	122.30	110.40
3	F	280	TYR	CB-CG-CD1	5.95	124.57	121.00
1	A	171	ARG	NH1-CZ-NH2	5.95	125.94	119.40
2	E	166	ARG	CD-NE-CZ	5.94	131.91	123.60
3	C	273	LYS	O-C-N	-5.92	113.22	122.70
3	F	316	ASP	CB-CG-OD1	5.92	123.62	118.30
2	E	257	ASP	CB-CG-OD1	5.91	123.62	118.30
2	B	406	ARG	N-CA-C	5.91	126.94	111.00
3	C	320	ASP	OD1-CG-OD2	-5.91	112.08	123.30
2	B	213	GLU	OE1-CD-OE2	-5.90	116.22	123.30
2	B	456	PRO	O-C-N	-5.87	113.31	122.70
2	B	255	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	146	ASP	OD1-CG-OD2	-5.86	112.17	123.30
2	B	265	LYS	O-C-N	5.85	132.06	122.70
3	F	320	ASP	CB-CG-OD1	-5.85	113.04	118.30
2	E	184	SER	N-CA-CB	-5.80	101.79	110.50
3	F	381	LYS	N-CA-CB	5.79	121.03	110.60
2	B	381	ASP	OD1-CG-OD2	-5.79	112.30	123.30
3	C	224	THR	N-CA-CB	-5.78	99.31	110.30
3	C	298	ASP	CB-CG-OD2	5.78	123.50	118.30
4	H	3	ARG	N-CA-CB	5.75	120.96	110.60
2	B	295	GLY	O-C-N	-5.75	113.50	122.70
1	D	171	ARG	CG-CD-NE	5.75	123.87	111.80
2	E	267	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	B	412	PRO	N-CA-C	-5.72	97.22	112.10
3	C	231	GLU	CG-CD-OE1	5.72	129.75	118.30
2	B	264	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	E	316	ASP	CB-CG-OD1	5.70	123.43	118.30
2	E	324	ALA	N-CA-CB	5.69	118.07	110.10
3	C	126	GLU	CB-CG-CD	5.68	129.55	114.20
2	B	223	GLU	CG-CD-OE1	5.67	129.64	118.30
1	A	141	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	C	130	GLN	CG-CD-OE1	5.65	132.90	121.60
3	C	244	TYR	CB-CG-CD1	5.64	124.38	121.00
3	F	379	MET	CG-SD-CE	5.64	109.22	100.20
3	C	285	ASP	CB-CG-OD2	-5.63	113.23	118.30
3	C	379	MET	CA-CB-CG	5.62	122.86	113.30
2	B	415	ARG	NH1-CZ-NH2	5.61	125.57	119.40
2	B	190	MET	N-CA-CB	5.61	120.69	110.60
2	B	415	ARG	NE-CZ-NH1	-5.61	117.50	120.30
3	C	127	LYS	CA-CB-CG	5.59	125.70	113.40
2	B	223	GLU	CG-CD-OE2	-5.57	107.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	295	GLY	O-C-N	-5.57	113.80	122.70
3	F	273	LYS	O-C-N	-5.55	113.83	122.70
1	A	149	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	B	350	GLY	C-N-CA	5.51	135.46	121.70
2	E	237	ARG	CD-NE-CZ	-5.46	115.95	123.60
2	B	337	LYS	CB-CG-CD	5.46	125.80	111.60
2	B	225	TYR	CB-CG-CD2	-5.46	117.72	121.00
2	B	171	ILE	CA-CB-CG2	5.45	121.79	110.90
2	E	292	TYR	CA-CB-CG	5.45	123.75	113.40
4	G	3	ARG	CA-CB-CG	5.43	125.36	113.40
2	B	326	TYR	CB-CG-CD2	-5.42	117.75	121.00
3	F	126	GLU	O-C-N	-5.42	114.04	122.70
3	C	274	TYR	CB-CG-CD2	5.40	124.24	121.00
2	B	269	TYR	CB-CG-CD2	5.38	124.23	121.00
3	C	354	TYR	CB-CG-CD2	-5.36	117.78	121.00
2	E	238	VAL	N-CA-CB	-5.36	99.71	111.50
2	E	376	SER	N-CA-CB	5.36	118.53	110.50
2	B	406	ARG	O-C-N	-5.35	114.14	122.70
3	C	334	TRP	CE3-CZ3-CH2	-5.34	115.33	121.20
2	B	405	ASN	CA-C-N	5.33	128.93	117.20
2	B	318	LYS	CA-CB-CG	5.32	125.10	113.40
2	E	398	ASP	CB-CA-C	5.31	121.01	110.40
2	E	355	ASP	CA-C-N	5.29	126.79	116.20
2	E	379	ASP	OD1-CG-OD2	-5.29	113.25	123.30
2	B	253	GLN	CB-CG-CD	5.29	125.35	111.60
2	E	225	TYR	CB-CG-CD1	5.27	124.16	121.00
2	B	292	TYR	CB-CG-CD2	5.27	124.16	121.00
2	E	339	GLN	O-C-N	-5.25	114.30	122.70
2	E	383	ASP	OD1-CG-OD2	-5.23	113.36	123.30
2	E	397	GLU	OE1-CD-OE2	-5.23	117.03	123.30
3	F	141	ASP	OD1-CG-OD2	-5.22	113.38	123.30
2	B	320	ASP	C-N-CA	5.22	134.74	121.70
2	B	449	LYS	O-C-N	5.20	131.02	122.70
3	C	126	GLU	OE1-CD-OE2	-5.20	117.07	123.30
3	C	395	GLY	N-CA-C	5.19	126.08	113.10
2	E	446	SER	N-CA-CB	-5.19	102.71	110.50
2	E	456	PRO	CA-C-N	5.18	128.60	117.20
2	B	379	ASP	CB-CG-OD2	5.18	122.96	118.30
2	E	213	GLU	CG-CD-OE2	5.17	128.65	118.30
3	C	192	THR	CA-CB-CG2	5.17	119.64	112.40
3	F	375	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	B	238	VAL	N-CA-CB	-5.15	100.16	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	275	ARG	NE-CZ-NH1	-5.15	117.72	120.30
3	C	288	ASP	CB-CG-OD1	5.15	122.94	118.30
3	F	375	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	B	353	LEU	CB-CG-CD1	-5.12	102.30	111.00
2	E	296	ASN	N-CA-CB	5.12	119.81	110.60
3	C	294	ASP	CA-CB-CG	-5.12	102.15	113.40
2	E	381	ASP	CB-CG-OD2	-5.11	113.71	118.30
2	B	399	GLY	N-CA-C	5.08	125.80	113.10
3	F	167	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	E	323	LYS	CB-CA-C	-5.07	100.27	110.40
2	E	176	ARG	CG-CD-NE	5.05	122.41	111.80
3	C	364	ASP	CB-CG-OD2	-5.05	113.75	118.30
3	C	149	THR	N-CA-CB	5.05	119.89	110.30
3	C	238	THR	O-C-N	-5.04	114.64	122.70
2	B	267	ASP	CA-CB-CG	-5.03	102.33	113.40
2	E	412	PRO	CA-C-N	5.03	128.28	117.20
2	B	257	ASP	CB-CG-OD1	5.03	122.83	118.30
2	E	163	THR	N-CA-CB	5.03	119.86	110.30
2	E	347	GLY	C-N-CA	5.03	134.27	121.70
2	B	425	ASP	CB-CG-OD1	5.01	122.81	118.30
3	C	277	THR	CA-CB-CG2	5.00	119.40	112.40
2	E	225	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	274	TYR	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	647	31	0
1	D	608	0	649	58	0
2	B	2473	0	2336	119	0
2	E	2473	0	2335	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2404	0	2249	109	0
3	F	2404	0	2249	135	0
4	G	29	0	32	1	0
4	H	29	0	32	0	0
5	I	32	0	32	0	0
5	J	32	0	32	1	0
6	K	28	0	26	3	0
7	B	11	0	10	2	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	E	14	0	13	2	0
9	J	14	0	13	2	0
10	A	15	0	0	6	0
10	B	124	0	0	18	0
10	C	71	0	0	7	0
10	D	16	0	0	3	0
10	E	119	0	0	6	0
10	F	82	0	0	11	0
10	G	1	0	0	1	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
All	All	11594	0	10655	537	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (537) 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:277:THR:HG21	3:F:303:PHE:CD2	1.37	1.59
3:C:277:THR:CG2	3:F:303:PHE:CE2	1.83	1.42
1:A:135:LEU:HD12	10:A:207:HOH:O	1.27	1.34
2:E:423:THR:H	2:E:426:MET:CE	1.40	1.34
2:E:423:THR:N	2:E:426:MET:CE	1.91	1.33
2:E:373:MET:HE2	2:E:405:ASN:CA	1.62	1.29
2:E:422:TYR:CA	2:E:426:MET:HE3	1.66	1.26
1:D:133:ILE:CD1	2:E:161:ILE:HD13	1.65	1.25
3:C:277:THR:HG21	3:F:303:PHE:CG	1.27	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:GLU:HG3	10:B:590:HOH:O	1.33	1.24
3:C:361:ASN:HB3	10:C:470:HOH:O	1.38	1.22
2:E:373:MET:HE2	2:E:405:ASN:CB	1.72	1.20
3:C:282:ALA:O	3:C:394:ILE:HD12	1.41	1.18
2:E:423:THR:N	2:E:426:MET:HE2	1.52	1.18
2:E:162:PRO:HG3	3:F:103:HIS:CE1	1.79	1.17
2:E:373:MET:HE2	2:E:405:ASN:HA	1.19	1.15
3:C:277:THR:HG22	3:F:303:PHE:CE2	1.36	1.15
3:C:277:THR:CG2	3:F:303:PHE:CD2	2.07	1.14
1:D:133:ILE:HD11	2:E:161:ILE:HD13	1.17	1.13
2:E:373:MET:CE	2:E:405:ASN:HA	1.82	1.09
2:B:326:TYR:CE1	2:B:354:MET:HE3	1.88	1.08
2:E:422:TYR:HA	2:E:426:MET:CE	1.85	1.06
2:E:422:TYR:HA	2:E:426:MET:HE3	1.33	1.06
3:F:98:ALA:HA	3:F:101:LEU:HD12	1.35	1.05
2:E:168:LEU:HA	2:E:171:ILE:HD11	1.37	1.05
2:E:169:ARG:NH2	3:F:109:TYR:HD2	1.54	1.04
3:C:277:THR:CG2	3:F:303:PHE:CG	2.22	1.04
2:B:157:VAL:HG12	3:C:100:ILE:HG22	1.40	1.03
2:E:422:TYR:CA	2:E:426:MET:CE	2.36	1.03
3:F:217:HIS:O	3:F:224:THR:HG23	1.60	1.02
1:D:119:ILE:HD11	1:D:123:LYS:HG3	1.39	1.01
2:E:183:GLU:HG3	3:F:124:LEU:HD13	1.39	1.00
2:B:157:VAL:HG12	3:C:100:ILE:CG2	1.92	0.99
3:F:240:SER:OG	3:F:242:ILE:HD11	1.62	0.99
2:B:244:THR:HG21	2:B:313:GLU:OE2	1.63	0.99
10:E:515:HOH:O	5:J:1:GLY:HA2	1.63	0.98
3:C:103:HIS:O	3:C:107:ILE:HG22	1.64	0.98
2:B:326:TYR:CD1	2:B:354:MET:CE	2.48	0.96
2:B:224:MET:SD	10:B:594:HOH:O	2.23	0.95
2:E:422:TYR:C	2:E:426:MET:CE	2.35	0.95
2:E:165:LEU:HD21	3:F:107:ILE:HD12	1.47	0.95
2:E:169:ARG:O	2:E:173:GLU:HG3	1.66	0.94
6:K:1:NAG:O4	6:K:2:NAG:O5	1.83	0.94
3:C:240:SER:C	3:C:242:ILE:HD12	1.86	0.94
2:B:190:MET:SD	10:C:476:HOH:O	2.26	0.94
2:E:169:ARG:NH2	3:F:109:TYR:CD2	2.31	0.94
2:E:423:THR:H	2:E:426:MET:HE2	0.78	0.93
2:B:326:TYR:HE1	2:B:354:MET:HE3	1.34	0.93
7:B:472:MAN:H2	6:K:2:NAG:O3	1.70	0.92
2:E:422:TYR:CB	2:E:426:MET:HE3	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:VAL:O	1:D:130:VAL:HG23	1.71	0.89
1:D:133:ILE:HD11	2:E:161:ILE:CD1	2.01	0.89
2:B:212:GLU:HG3	2:B:216:ARG:NH1	1.86	0.89
3:C:325:ASN:ND2	3:C:328:GLU:H	1.70	0.89
2:E:373:MET:HE2	2:E:405:ASN:HB2	1.55	0.89
2:E:373:MET:CE	2:E:405:ASN:CB	2.52	0.88
1:D:131:GLN:HG3	1:D:132:HIS:HD2	1.36	0.88
1:D:119:ILE:CD1	1:D:123:LYS:HG3	2.04	0.88
3:F:103:HIS:O	3:F:107:ILE:HG22	1.74	0.88
3:F:114:TYR:HD2	3:F:115:ASN:ND2	1.71	0.87
1:D:133:ILE:CD1	2:E:161:ILE:CD1	2.52	0.87
3:F:98:ALA:HA	3:F:101:LEU:CD1	2.05	0.86
2:B:257:ASP:O	2:B:291:GLU:OE2	1.94	0.86
2:E:169:ARG:HB2	3:F:110:LEU:CD2	2.05	0.86
2:E:326:TYR:HD2	2:E:354:MET:HE2	1.39	0.86
2:E:345:TYR:HB2	2:E:354:MET:CE	2.06	0.86
3:F:217:HIS:O	3:F:224:THR:CG2	2.22	0.86
3:F:240:SER:OG	3:F:242:ILE:CD1	2.23	0.85
2:B:326:TYR:HD1	2:B:354:MET:CE	1.89	0.85
2:B:394:CYS:O	2:B:397:GLU:O	1.94	0.85
2:B:387:THR:HG22	2:B:388:SER:H	1.42	0.84
1:D:119:ILE:HD11	1:D:123:LYS:HE3	1.58	0.84
3:C:149:THR:CG2	3:C:168:PHE:O	2.24	0.84
2:E:326:TYR:CD2	2:E:354:MET:HE2	2.12	0.84
1:D:157:LYS:HE3	3:F:132:GLU:OE2	1.77	0.84
3:F:239:GLN:O	3:F:242:ILE:HD12	1.77	0.83
3:C:240:SER:OG	3:C:242:ILE:HD11	1.78	0.83
2:E:387:THR:HG21	2:E:392:LYS:HB2	1.57	0.83
1:A:119:ILE:HD11	1:A:123:LYS:HD2	1.60	0.83
2:B:412:PRO:HA	10:B:596:HOH:O	1.78	0.83
3:F:391:ARG:O	3:F:395:GLY:HA3	1.77	0.82
2:E:158:ASN:HB2	3:F:100:ILE:HD13	1.62	0.82
2:B:326:TYR:HD1	2:B:354:MET:HE2	1.45	0.81
3:C:217:HIS:O	3:C:224:THR:HG23	1.79	0.81
2:E:345:TYR:HB2	2:E:354:MET:HE3	1.62	0.81
2:E:176:ARG:HE	3:F:120:LYS:NZ	1.80	0.80
2:E:169:ARG:HH21	3:F:109:TYR:HD2	0.82	0.80
2:E:169:ARG:HB2	3:F:110:LEU:HD21	1.64	0.79
1:A:135:LEU:CD1	10:A:203:HOH:O	2.29	0.79
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.62	0.79
2:E:172:LEU:HB3	3:F:113:ILE:CD1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:TYR:CD1	2:B:354:MET:HE2	2.16	0.79
3:F:392:LEU:HG	3:F:393:THR:H	1.47	0.79
2:B:224:MET:HE2	2:B:277:ALA:HB3	1.64	0.79
2:E:224:MET:HG2	10:E:589:HOH:O	1.81	0.78
2:E:422:TYR:HB2	2:E:426:MET:HE3	1.65	0.78
2:E:183:GLU:CG	3:F:124:LEU:HD13	2.13	0.78
2:E:307:PRO:O	2:E:456:PRO:O	2.01	0.78
2:E:224:MET:HE1	10:F:441:HOH:O	1.82	0.78
2:E:168:LEU:O	2:E:171:ILE:HG12	1.83	0.78
2:E:456:PRO:O	2:E:457:PHE:HB3	1.84	0.78
2:E:169:ARG:NE	3:F:110:LEU:HD21	1.99	0.78
3:C:240:SER:O	3:C:242:ILE:HD12	1.84	0.77
2:E:361:MET:HE1	10:E:552:HOH:O	1.84	0.77
3:C:240:SER:O	3:C:242:ILE:CD1	2.32	0.77
3:F:149:THR:HG22	3:F:150:GLY:H	1.49	0.77
2:B:176:ARG:HD3	10:B:583:HOH:O	1.83	0.77
2:B:326:TYR:CE1	2:B:354:MET:CE	2.63	0.77
3:C:149:THR:HG22	3:C:168:PHE:O	1.84	0.77
2:E:158:ASN:CB	3:F:100:ILE:HD13	2.14	0.76
3:F:176:GLN:NE2	10:F:487:HOH:O	2.17	0.76
1:D:177:ASP:O	1:D:181:GLN:HG3	1.85	0.76
3:C:212:LYS:NZ	3:C:270:GLU:OE1	2.17	0.76
2:E:155:GLU:O	2:E:157:VAL:N	2.18	0.76
2:E:158:ASN:CG	3:F:100:ILE:HD13	2.07	0.76
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.67	0.76
2:E:326:TYR:CE2	2:E:354:MET:HE3	2.21	0.75
1:D:126:VAL:HG13	2:E:157:VAL:HG22	1.68	0.75
2:E:394:CYS:O	2:E:397:GLU:O	2.04	0.75
3:F:114:TYR:CD2	3:F:115:ASN:ND2	2.53	0.75
2:B:224:MET:CE	2:B:277:ALA:HB3	2.17	0.74
1:D:123:LYS:HZ3	2:E:151:LEU:N	1.86	0.74
3:C:191:TRP:HH2	3:C:393:THR:HG23	1.53	0.74
2:E:423:THR:N	2:E:426:MET:HE1	1.99	0.74
3:C:340:HIS:O	4:G:1:GLY:N	2.14	0.73
2:B:156:THR:HG22	2:B:160:ASN:ND2	2.03	0.73
3:F:307:HIS:HE1	3:F:341:ALA:H	1.36	0.73
2:B:252:ILE:HG12	2:B:299:ILE:HG12	1.69	0.73
2:E:172:LEU:HB3	3:F:113:ILE:HD12	1.68	0.73
2:E:212:GLU:HG3	2:E:216:ARG:NH1	2.04	0.72
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.90	0.72
3:C:307:HIS:HE1	3:C:341:ALA:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:392:LEU:HG	3:F:393:THR:N	2.05	0.72
2:E:195:THR:HG22	2:E:196:PRO:HD2	1.70	0.71
3:C:391:ARG:O	3:C:395:GLY:HA3	1.91	0.71
2:B:412:PRO:CA	10:B:596:HOH:O	2.37	0.71
1:D:120:GLU:HA	1:D:124:ARG:HB2	1.72	0.71
2:B:252:ILE:HD11	2:B:454:ILE:CD1	2.20	0.71
2:E:163:THR:O	2:E:166:ARG:N	2.23	0.71
2:E:169:ARG:HE	3:F:110:LEU:HD21	1.55	0.71
3:C:149:THR:HG23	3:C:168:PHE:O	1.91	0.71
3:C:217:HIS:O	3:C:224:THR:CG2	2.38	0.71
2:E:326:TYR:HE2	2:E:354:MET:HE3	1.54	0.71
2:E:176:ARG:HE	3:F:120:LYS:HZ2	1.38	0.71
3:F:195:GLN:OE1	3:F:382:THR:CG2	2.38	0.71
2:E:422:TYR:C	2:E:426:MET:HE3	2.06	0.70
2:B:387:THR:HG22	2:B:388:SER:N	2.05	0.70
1:D:131:GLN:HG3	1:D:132:HIS:CD2	2.26	0.70
1:D:151:GLU:HG3	10:D:211:HOH:O	1.91	0.70
2:E:168:LEU:HA	2:E:171:ILE:CD1	2.20	0.70
2:E:179:ILE:HD11	3:F:121:ILE:HG12	1.73	0.70
1:D:136:LEU:HB3	2:E:168:LEU:HD23	1.74	0.69
3:F:239:GLN:O	3:F:242:ILE:CD1	2.40	0.69
2:E:456:PRO:O	2:E:457:PHE:CB	2.41	0.69
3:C:240:SER:C	3:C:242:ILE:CD1	2.60	0.69
2:E:387:THR:HG22	2:E:388:SER:N	2.08	0.68
3:C:189:ASN:OD1	3:C:392:LEU:HB2	1.92	0.68
2:E:323:LYS:HD3	10:E:549:HOH:O	1.94	0.68
3:F:152:ASP:OD2	3:F:244:TYR:OH	2.10	0.68
1:A:135:LEU:HD13	10:A:203:HOH:O	1.94	0.68
3:F:383:THR:HG22	10:F:456:HOH:O	1.93	0.67
3:F:98:ALA:CA	3:F:101:LEU:HD12	2.21	0.67
3:C:153:CYS:SG	3:C:192:THR:HB	2.34	0.67
3:F:100:ILE:O	3:F:102:THR:N	2.25	0.67
2:E:161:ILE:HG21	3:F:103:HIS:ND1	2.10	0.67
2:B:326:TYR:CD1	2:B:354:MET:HE3	2.17	0.67
2:E:162:PRO:HG3	3:F:103:HIS:HE1	1.50	0.67
1:A:120:GLU:HA	1:A:124:ARG:HB2	1.75	0.67
2:B:415:ARG:O	2:B:434:GLY:HA2	1.95	0.67
2:E:438:MET:CE	2:E:443:SER:OG	2.43	0.67
2:B:195:THR:HG22	2:B:196:PRO:HD2	1.77	0.67
1:D:140:VAL:HG23	1:D:185:LEU:HD11	1.77	0.67
2:E:326:TYR:CD2	2:E:354:MET:CE	2.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:MET:HE1	3:C:131:LEU:HA	1.76	0.66
3:C:344:LEU:HD13	3:C:382:THR:HG21	1.78	0.66
2:E:169:ARG:HE	3:F:110:LEU:CD2	2.08	0.66
2:E:161:ILE:CG2	3:F:103:HIS:ND1	2.59	0.66
2:E:326:TYR:CE2	2:E:354:MET:CE	2.79	0.65
3:C:282:ALA:O	3:C:394:ILE:CD1	2.34	0.65
2:E:422:TYR:HA	2:E:426:MET:HE1	1.77	0.65
2:E:439:ASN:HD22	2:E:439:ASN:H	1.45	0.65
3:C:100:ILE:C	3:C:102:THR:H	1.99	0.65
1:A:122:LEU:O	1:A:124:ARG:N	2.29	0.65
2:E:423:THR:N	2:E:426:MET:HE3	2.00	0.65
3:F:151:LYS:HD2	3:F:155:ASP:OD2	1.96	0.65
2:B:412:PRO:O	2:B:413:ASN:HB2	1.96	0.65
2:B:157:VAL:HG12	3:C:100:ILE:HG21	1.76	0.65
3:C:98:ALA:HA	3:C:101:LEU:HD12	1.79	0.65
2:E:172:LEU:CD2	3:F:114:TYR:HA	2.27	0.65
3:F:176:GLN:HG3	10:F:421:HOH:O	1.97	0.65
2:E:195:THR:CG2	2:E:196:PRO:HD2	2.26	0.64
2:E:422:TYR:C	2:E:426:MET:HE1	2.15	0.64
2:E:345:TYR:HB2	2:E:354:MET:HE1	1.78	0.64
3:F:153:CYS:SG	3:F:192:THR:HB	2.38	0.64
3:C:344:LEU:HD13	3:C:382:THR:CG2	2.29	0.64
2:E:373:MET:CE	2:E:405:ASN:HB2	2.25	0.64
3:C:100:ILE:O	3:C:102:THR:N	2.28	0.63
2:E:158:ASN:HB2	3:F:100:ILE:HG21	1.80	0.63
2:E:168:LEU:O	2:E:171:ILE:CG1	2.46	0.63
2:E:164:ASN:O	2:E:168:LEU:HD13	1.99	0.63
2:E:168:LEU:CA	2:E:171:ILE:HD11	2.22	0.63
3:C:153:CYS:HB2	3:C:192:THR:HG22	1.81	0.63
3:C:322:PHE:CE1	3:C:323:GLU:HG2	2.33	0.63
3:F:189:ASN:HD22	3:F:391:ARG:HG3	1.64	0.63
2:B:373:MET:HE2	2:B:404:TYR:O	1.99	0.62
2:E:183:GLU:HB3	10:F:467:HOH:O	1.99	0.62
3:C:104:ASP:O	3:C:107:ILE:CG2	2.48	0.62
2:E:438:MET:HE2	2:E:443:SER:OG	1.99	0.62
2:E:161:ILE:CB	2:E:162:PRO:HD3	2.29	0.62
2:E:315:GLU:OE2	2:E:448:ARG:NH2	2.33	0.62
2:B:252:ILE:CD1	2:B:454:ILE:CD1	2.78	0.61
1:A:164:SER:HB3	3:C:137:GLU:O	2.00	0.61
2:B:315:GLU:HB3	2:B:449:LYS:HB2	1.82	0.61
2:E:179:ILE:HD11	3:F:121:ILE:CG1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:MET:O	2:B:405:ASN:O	2.18	0.61
3:F:100:ILE:C	3:F:102:THR:H	2.04	0.61
2:B:252:ILE:HD11	2:B:454:ILE:HD11	1.82	0.61
2:E:172:LEU:HD22	3:F:114:TYR:HA	1.81	0.61
2:E:309:GLU:OE1	2:E:325:HIS:HE1	1.84	0.61
3:C:307:HIS:HD2	3:C:335:TRP:O	1.82	0.61
2:B:252:ILE:CD1	2:B:454:ILE:HG12	2.31	0.61
2:E:373:MET:CE	2:E:405:ASN:CG	2.70	0.60
2:B:157:VAL:CG1	3:C:100:ILE:CG2	2.76	0.59
1:D:178:TYR:OH	2:E:178:LYS:HD2	2.02	0.59
3:C:269:PRO:O	3:C:273:LYS:O	2.19	0.59
3:C:325:ASN:HD22	3:C:328:GLU:H	1.49	0.59
1:D:126:VAL:CG1	2:E:157:VAL:HG22	2.32	0.59
3:F:273:LYS:NZ	3:F:317:ASN:HD21	2.00	0.59
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.38	0.59
3:C:136:GLN:NE2	10:C:469:HOH:O	2.28	0.59
2:E:405:ASN:O	2:E:406:ARG:C	2.38	0.58
3:F:108:ARG:O	3:F:112:GLU:HG3	2.03	0.58
2:B:157:VAL:CG1	3:C:100:ILE:HG22	2.25	0.58
3:F:269:PRO:O	3:F:273:LYS:O	2.21	0.58
3:F:307:HIS:CE1	3:F:341:ALA:H	2.20	0.58
2:E:294:LEU:O	2:E:295:GLY:C	2.37	0.58
2:E:155:GLU:C	2:E:157:VAL:H	2.05	0.58
3:F:189:ASN:ND2	3:F:391:ARG:HG3	2.19	0.58
3:F:191:TRP:HH2	3:F:393:THR:HG1	1.49	0.58
3:C:103:HIS:O	3:C:107:ILE:CG2	2.46	0.57
3:C:189:ASN:ND2	3:C:391:ARG:HG3	2.19	0.57
3:C:189:ASN:OD1	3:C:392:LEU:HD22	2.04	0.57
3:F:191:TRP:CH2	3:F:393:THR:OG1	2.56	0.57
1:A:122:LEU:O	1:A:125:LYS:N	2.38	0.57
2:B:346:ARG:NE	10:B:593:HOH:O	2.33	0.57
2:E:163:THR:O	2:E:166:ARG:HB2	2.04	0.57
2:E:415:ARG:O	2:E:434:GLY:HA2	2.05	0.57
2:E:422:TYR:CA	2:E:426:MET:HE1	2.31	0.57
3:F:392:LEU:O	3:F:395:GLY:HA3	2.05	0.57
1:D:190:ALA:O	1:D:192:ASP:N	2.33	0.57
2:B:415:ARG:H	2:B:434:GLY:H	1.52	0.57
1:D:147:MET:CE	2:E:179:ILE:HG12	2.35	0.57
2:E:162:PRO:CG	3:F:103:HIS:CE1	2.72	0.57
2:E:412:PRO:O	2:E:413:ASN:HB2	2.05	0.57
2:B:212:GLU:HG3	2:B:216:ARG:HH11	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:387:THR:HG22	2:E:389:ASP:N	2.20	0.56
1:D:147:MET:SD	3:F:121:ILE:HD11	2.45	0.56
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.70	0.56
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.40	0.56
2:B:190:MET:CE	3:C:131:LEU:HA	2.35	0.56
2:B:280:THR:HB	2:B:283:LYS:HG2	1.88	0.56
2:B:456:PRO:O	2:B:457:PHE:HB3	2.06	0.56
1:A:120:GLU:O	1:A:125:LYS:HG2	2.06	0.56
3:C:239:GLN:O	3:C:242:ILE:HD12	2.06	0.56
3:C:382:THR:HG22	3:C:383:THR:N	2.20	0.56
2:E:387:THR:CG2	2:E:388:SER:N	2.69	0.56
2:B:405:ASN:O	2:B:406:ARG:C	2.45	0.55
3:C:322:PHE:CD1	3:C:323:GLU:HG2	2.41	0.55
1:D:133:ILE:HG12	3:F:107:ILE:CD1	2.35	0.55
1:A:171:ARG:NH1	10:A:209:HOH:O	2.28	0.55
3:F:240:SER:C	3:F:242:ILE:HD12	2.27	0.55
1:D:126:VAL:CG2	2:E:157:VAL:HG21	2.36	0.55
2:B:199:VAL:HG23	3:C:141:ASP:HA	1.89	0.55
1:D:133:ILE:HD13	2:E:161:ILE:HD13	1.78	0.55
2:B:229:PRO:HB2	2:B:301:GLN:HE22	1.72	0.54
3:C:298:ASP:CG	3:C:299:PRO:HD2	2.28	0.54
3:F:383:THR:CG2	10:F:456:HOH:O	2.51	0.54
1:D:136:LEU:HD11	3:F:111:GLN:HG2	1.89	0.54
2:B:457:PHE:O	2:B:458:PHE:O	2.25	0.54
1:D:148:LYS:NZ	10:D:213:HOH:O	2.33	0.54
2:E:195:THR:HG22	2:E:196:PRO:CD	2.37	0.54
2:E:254:ASN:HD21	2:E:256:GLN:NE2	2.06	0.54
3:C:251:GLU:HG3	3:C:257:THR:HG22	1.89	0.54
3:C:387:ILE:HG12	3:C:388:PRO:HD2	1.89	0.54
2:E:397:GLU:O	2:E:398:ASP:HB2	2.09	0.53
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.91	0.53
2:E:155:GLU:HG3	2:E:156:THR:H	1.72	0.53
2:E:387:THR:HG21	2:E:392:LYS:CB	2.32	0.53
2:E:438:MET:HE3	2:E:443:SER:OG	2.08	0.53
3:F:392:LEU:O	3:F:395:GLY:N	2.42	0.53
2:B:224:MET:CG	10:B:594:HOH:O	2.56	0.53
3:F:195:GLN:HE22	3:F:382:THR:HG21	1.74	0.53
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.24	0.53
3:C:298:ASP:OD2	3:C:299:PRO:HD2	2.08	0.53
2:E:245:GLU:OE2	2:E:323:LYS:HE3	2.09	0.53
2:E:387:THR:HG22	2:E:389:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLU:OE2	2:B:323:LYS:HE2	2.08	0.52
3:C:104:ASP:O	3:C:107:ILE:HG23	2.09	0.52
2:E:160:ASN:O	2:E:163:THR:N	2.32	0.52
2:E:172:LEU:HB3	3:F:113:ILE:HD11	1.87	0.52
2:E:155:GLU:C	2:E:157:VAL:N	2.62	0.52
2:B:191:GLU:CG	10:B:590:HOH:O	2.16	0.52
2:E:169:ARG:HB2	3:F:110:LEU:HD22	1.86	0.52
2:E:160:ASN:O	2:E:161:ILE:C	2.47	0.52
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.45	0.52
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.09	0.52
2:B:346:ARG:NH2	10:B:593:HOH:O	2.42	0.52
2:B:179:ILE:O	2:B:183:GLU:HG3	2.10	0.52
3:F:325:ASN:ND2	3:F:328:GLU:H	2.07	0.52
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.90	0.52
1:A:188:VAL:HG21	2:B:167:VAL:HG21	1.92	0.51
3:F:149:THR:HG22	3:F:150:GLY:N	2.22	0.51
3:F:261:ASP:OD2	3:F:394:ILE:HG12	2.10	0.51
3:C:108:ARG:O	3:C:112:GLU:HG3	2.10	0.51
3:C:107:ILE:CD1	3:C:111:GLN:OE1	2.58	0.51
3:F:387:ILE:CG1	3:F:388:PRO:HD2	2.41	0.51
2:B:176:ARG:HB2	3:C:117:ASN:HD21	1.74	0.51
3:C:240:SER:O	3:C:242:ILE:HD11	2.08	0.51
3:C:295:PHE:HB3	3:C:375:ARG:NH2	2.25	0.51
2:B:456:PRO:O	2:B:457:PHE:CB	2.56	0.51
2:E:351:ASN:HD21	2:E:354:MET:HG3	1.74	0.51
2:B:212:GLU:CG	2:B:216:ARG:NH1	2.69	0.51
2:B:183:GLU:O	3:C:127:LYS:NZ	2.44	0.51
1:D:136:LEU:HD11	3:F:111:GLN:CG	2.41	0.51
1:D:137:GLN:HB3	1:D:189:ILE:HG12	1.92	0.51
2:B:282:GLY:O	2:B:283:LYS:HD2	2.11	0.51
3:C:277:THR:HG23	10:C:477:HOH:O	2.11	0.51
2:B:295:GLY:HA3	10:B:483:HOH:O	2.12	0.50
3:C:239:GLN:O	3:C:242:ILE:CD1	2.59	0.50
2:E:168:LEU:HD12	2:E:168:LEU:H	1.76	0.50
3:C:275:ARG:HD2	3:F:303:PHE:HE2	1.76	0.50
1:A:166:SER:HB3	2:B:195:THR:HB	1.93	0.50
3:F:318:ASP:C	3:F:318:ASP:OD1	2.50	0.50
2:B:230:ASP:O	2:B:233:VAL:N	2.40	0.50
3:C:361:ASN:ND2	10:C:470:HOH:O	2.28	0.50
1:A:122:LEU:O	1:A:123:LYS:C	2.50	0.49
2:E:309:GLU:OE1	2:E:325:HIS:CE1	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:THR:OG1	2:B:426:MET:CE	2.60	0.49
3:F:379:MET:HE3	3:F:379:MET:HA	1.93	0.49
2:E:153:ILE:C	2:E:155:GLU:H	2.16	0.49
2:B:390:PRO:O	2:B:393:GLN:HG3	2.12	0.49
1:D:178:TYR:OH	2:E:178:LYS:CD	2.60	0.49
2:E:179:ILE:CD1	3:F:121:ILE:HG12	2.42	0.49
2:E:351:ASN:ND2	2:E:354:MET:H	2.10	0.49
2:B:330:THR:HG21	10:B:561:HOH:O	2.13	0.49
3:C:275:ARG:HD2	3:F:303:PHE:CE2	2.48	0.49
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.48	0.49
2:B:186:VAL:O	2:B:190:MET:HG2	2.13	0.49
2:B:412:PRO:CB	10:B:596:HOH:O	2.61	0.49
3:F:356:LYS:HG3	3:F:362:GLY:HA2	1.95	0.49
1:A:169:LEU:H	2:B:189:GLN:NE2	2.11	0.49
3:C:352:GLY:HA2	3:C:378:SER:O	2.13	0.49
1:D:121:VAL:HA	1:D:125:LYS:HG2	1.93	0.49
2:E:183:GLU:HG2	10:F:467:HOH:O	2.13	0.49
9:E:470:NAG:O4	9:J:471:NAG:C1	2.60	0.49
1:A:123:LYS:HB3	1:A:124:ARG:NH2	2.28	0.48
2:B:202:ASN:ND2	2:B:284:ASN:O	2.45	0.48
3:C:106:SER:O	3:C:109:TYR:HB3	2.12	0.48
1:D:151:GLU:OE2	10:D:211:HOH:O	2.20	0.48
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.78	0.48
1:D:147:MET:SD	3:F:121:ILE:CD1	3.01	0.48
2:B:397:GLU:O	2:B:398:ASP:HB2	2.12	0.48
3:F:307:HIS:HD2	3:F:335:TRP:O	1.96	0.48
3:C:192:THR:CG2	10:C:428:HOH:O	2.61	0.48
1:A:128:GLU:O	1:A:132:HIS:HD2	1.96	0.48
2:B:254:ASN:HD21	2:B:256:GLN:NE2	2.11	0.48
3:C:372:TRP:C	3:C:373:LYS:HG2	2.33	0.48
2:E:183:GLU:CG	10:F:467:HOH:O	2.62	0.48
3:F:325:ASN:HD22	3:F:325:ASN:C	2.16	0.48
2:B:359:GLN:H	2:B:359:GLN:HE21	1.62	0.48
3:C:100:ILE:C	3:C:102:THR:N	2.66	0.48
1:D:188:VAL:O	1:D:192:ASP:CG	2.52	0.48
2:B:155:GLU:HG3	2:B:156:THR:N	2.29	0.48
1:A:169:LEU:H	2:B:189:GLN:HE22	1.61	0.48
2:B:157:VAL:CG1	3:C:100:ILE:HG21	2.43	0.47
2:E:244:THR:HG21	2:E:313:GLU:OE2	2.13	0.47
1:A:133:ILE:O	1:A:137:GLN:HG3	2.13	0.47
2:B:182:LEU:HB2	3:C:124:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:MET:HE1	2:E:179:ILE:HG12	1.95	0.47
2:E:161:ILE:HG22	3:F:103:HIS:ND1	2.29	0.47
3:F:322:PHE:CD1	3:F:338:LYS:HD2	2.49	0.47
1:D:123:LYS:HD3	2:E:154:ASP:OD2	2.14	0.47
3:C:273:LYS:NZ	3:C:317:ASN:HD21	2.12	0.47
1:D:176:LYS:HB2	1:D:176:LYS:NZ	2.29	0.47
1:A:177:ASP:O	1:A:181:GLN:HG3	2.15	0.47
2:B:252:ILE:CD1	2:B:454:ILE:HD13	2.44	0.47
3:C:107:ILE:HD11	3:C:111:GLN:OE1	2.15	0.47
1:D:130:VAL:HA	1:D:133:ILE:HD12	1.96	0.47
1:A:129:LYS:HE2	1:A:129:LYS:HA	1.97	0.47
1:D:126:VAL:HG22	2:E:157:VAL:HG21	1.97	0.47
2:E:284:ASN:C	2:E:284:ASN:HD22	2.19	0.47
2:B:159:SER:O	2:B:162:PRO:HD2	2.14	0.46
2:B:387:THR:CG2	2:B:388:SER:H	2.22	0.46
2:E:209:LYS:HD2	2:E:305:MET:CE	2.45	0.46
2:E:367:MET:O	2:E:405:ASN:O	2.33	0.46
3:C:191:TRP:CD2	3:C:385:LYS:HE3	2.50	0.46
1:D:119:ILE:HD11	1:D:123:LYS:CG	2.29	0.46
1:D:183:LYS:O	1:D:184:GLN:C	2.54	0.46
1:D:188:VAL:O	1:D:192:ASP:OD1	2.33	0.46
3:F:100:ILE:HA	10:F:484:HOH:O	2.16	0.46
2:B:293:TRP:CD1	2:B:294:LEU:O	2.69	0.46
1:D:190:ALA:C	1:D:192:ASP:H	2.17	0.46
1:A:130:VAL:O	1:A:134:GLN:HG3	2.15	0.46
2:B:159:SER:C	2:B:162:PRO:HD2	2.36	0.46
2:E:345:TYR:CB	2:E:354:MET:HE1	2.43	0.46
3:F:173:LYS:HB2	3:F:173:LYS:HE3	1.68	0.46
3:F:392:LEU:O	3:F:395:GLY:CA	2.64	0.46
1:D:169:LEU:H	2:E:189:GLN:HE22	1.63	0.46
2:E:295:GLY:HA3	10:E:521:HOH:O	2.16	0.46
2:E:397:GLU:O	2:E:398:ASP:CB	2.63	0.46
2:B:174:ASN:OD1	2:B:178:LYS:HE2	2.16	0.45
1:D:126:VAL:HG21	2:E:157:VAL:HG21	1.98	0.45
2:E:152:TYR:H	2:E:152:TYR:HD1	1.64	0.45
2:E:155:GLU:HG3	2:E:156:THR:N	2.31	0.45
2:E:169:ARG:N	3:F:110:LEU:HD13	2.32	0.45
2:E:402:TRP:CG	2:E:403:TRP:N	2.85	0.45
2:B:267:ASP:N	2:B:268:PRO:CD	2.80	0.45
2:B:284:ASN:C	2:B:284:ASN:HD22	2.20	0.45
2:B:343:ASN:OD1	2:B:344:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:ASP:O	3:C:107:ILE:HG22	2.17	0.45
3:C:365:ASN:HD22	3:C:365:ASN:H	1.65	0.45
2:E:316:ASP:OD2	2:E:441:LYS:NZ	2.38	0.45
3:F:365:ASN:HD22	3:F:365:ASN:H	1.63	0.45
2:B:397:GLU:O	2:B:398:ASP:CB	2.64	0.45
2:E:412:PRO:O	2:E:413:ASN:CB	2.59	0.45
2:E:383:ASP:C	2:E:383:ASP:OD1	2.55	0.45
9:E:470:NAG:H62	9:J:471:NAG:O5	2.17	0.45
3:C:280:TYR:HB3	3:F:275:ARG:NH1	2.32	0.45
1:D:133:ILE:HG12	3:F:107:ILE:HD11	1.97	0.45
3:C:97:GLU:C	3:C:99:SER:H	2.20	0.45
2:E:217:LYS:HB3	3:F:213:GLU:HG3	1.97	0.44
2:E:267:ASP:O	2:E:271:GLN:HG2	2.17	0.44
2:E:373:MET:SD	2:E:405:ASN:HB2	2.57	0.44
3:F:273:LYS:HZ3	3:F:317:ASN:HD21	1.66	0.44
2:B:330:THR:HG23	10:B:586:HOH:O	2.17	0.44
3:F:127:LYS:HB3	3:F:127:LYS:HE2	1.69	0.44
2:B:299:ILE:O	2:B:303:THR:HG23	2.18	0.44
3:F:100:ILE:C	3:F:102:THR:N	2.66	0.44
2:B:155:GLU:HG3	2:B:156:THR:H	1.83	0.44
2:B:190:MET:HE1	3:C:131:LEU:CA	2.46	0.44
3:C:104:ASP:C	3:C:107:ILE:HG22	2.37	0.44
3:C:307:HIS:CE1	3:C:341:ALA:H	2.25	0.44
2:E:174:ASN:O	2:E:177:SER:OG	2.35	0.44
2:B:271:GLN:NE2	10:B:569:HOH:O	2.50	0.44
2:E:373:MET:HE1	2:E:405:ASN:CG	2.38	0.44
3:F:107:ILE:O	3:F:111:GLN:HG3	2.17	0.44
2:B:252:ILE:CD1	2:B:454:ILE:CG1	2.95	0.44
2:E:153:ILE:O	2:E:155:GLU:N	2.51	0.44
3:C:391:ARG:O	3:C:392:LEU:O	2.36	0.44
2:E:158:ASN:OD1	3:F:100:ILE:CD1	2.66	0.44
2:E:212:GLU:CG	2:E:216:ARG:NH1	2.78	0.44
2:B:212:GLU:CG	2:B:216:ARG:HH11	2.31	0.43
2:E:152:TYR:C	2:E:154:ASP:N	2.72	0.43
3:F:232:LYS:O	3:F:236:ILE:HG13	2.18	0.43
3:C:273:LYS:HD3	3:C:273:LYS:HA	1.81	0.43
2:E:169:ARG:HB2	3:F:110:LEU:CD1	2.48	0.43
3:F:322:PHE:HA	3:F:338:LYS:HD3	1.99	0.43
1:D:120:GLU:C	1:D:122:LEU:H	2.22	0.43
2:E:183:GLU:CB	10:F:467:HOH:O	2.64	0.43
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:391:ARG:O	3:F:392:LEU:O	2.36	0.43
1:D:181:GLN:O	1:D:185:LEU:HB2	2.19	0.43
2:E:172:LEU:HD21	3:F:114:TYR:HA	2.00	0.43
2:E:351:ASN:C	2:E:351:ASN:HD22	2.22	0.43
2:E:373:MET:CG	2:E:405:ASN:HB2	2.49	0.43
3:F:103:HIS:O	3:F:107:ILE:N	2.50	0.43
2:B:152:TYR:HD1	2:B:152:TYR:H	1.66	0.43
3:F:392:LEU:O	3:F:393:THR:C	2.57	0.43
2:B:234:LYS:HA	2:B:235:PRO:HD3	1.90	0.43
7:B:472:MAN:H2	6:K:2:NAG:HO3	1.77	0.43
3:C:263:ALA:O	3:C:264:MET:HB2	2.18	0.43
3:C:394:ILE:HG22	3:C:394:ILE:O	2.19	0.43
2:E:162:PRO:CG	3:F:103:HIS:HE1	2.25	0.43
2:E:186:VAL:CG1	3:F:127:LYS:HE2	2.48	0.43
2:E:455:ARG:HG3	2:E:456:PRO:HD2	2.01	0.43
3:F:153:CYS:H	3:F:192:THR:HG22	1.84	0.43
1:A:120:GLU:C	1:A:122:LEU:H	2.23	0.42
3:C:211:TYR:CE2	3:C:333:GLY:HA3	2.54	0.42
2:B:423:THR:OG1	2:B:426:MET:HE2	2.19	0.42
3:F:240:SER:HG	3:F:242:ILE:HD11	1.76	0.42
1:A:122:LEU:C	1:A:124:ARG:N	2.73	0.42
3:C:338:LYS:HG2	10:G:128:HOH:O	2.18	0.42
3:C:322:PHE:CD1	3:C:323:GLU:N	2.87	0.42
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.85	0.42
1:D:176:LYS:HD3	1:D:176:LYS:HA	1.88	0.42
2:E:152:TYR:O	2:E:154:ASP:N	2.52	0.42
3:F:103:HIS:O	3:F:104:ASP:C	2.56	0.42
3:F:219:SER:OG	3:F:224:THR:HB	2.20	0.42
1:A:171:ARG:CZ	10:A:209:HOH:O	2.67	0.42
2:B:157:VAL:O	3:C:103:HIS:HE1	2.03	0.42
2:B:439:ASN:H	2:B:439:ASN:HD22	1.67	0.42
3:C:155:ASP:O	3:C:159:LYS:HG3	2.20	0.42
1:D:187:GLN:O	1:D:188:VAL:C	2.58	0.42
1:A:171:ARG:NH2	10:A:209:HOH:O	2.51	0.42
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.54	0.42
3:C:323:GLU:OE2	10:C:474:HOH:O	2.22	0.42
2:E:159:SER:O	2:E:162:PRO:HD2	2.20	0.42
1:A:119:ILE:HD12	1:A:119:ILE:HA	1.86	0.42
3:C:112:GLU:O	3:C:116:SER:OG	2.37	0.42
2:B:161:ILE:N	2:B:162:PRO:CD	2.83	0.42
2:B:423:THR:OG1	2:B:426:MET:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG23	2:B:189:GLN:HE21	1.85	0.42
2:E:303:THR:HB	2:E:330:THR:HA	2.01	0.42
3:C:108:ARG:HA	3:C:111:GLN:NE2	2.35	0.41
3:C:252:ASP:OD2	3:C:373:LYS:NZ	2.43	0.41
3:C:338:LYS:O	3:C:338:LYS:CG	2.66	0.41
1:D:120:GLU:C	1:D:122:LEU:N	2.74	0.41
2:B:387:THR:HG22	2:B:389:ASP:H	1.85	0.41
1:D:126:VAL:CG2	2:E:157:VAL:CG2	2.98	0.41
2:E:265:LYS:O	2:E:268:PRO:HD2	2.21	0.41
3:F:200:GLY:HA2	10:F:418:HOH:O	2.21	0.41
2:B:346:ARG:CZ	10:B:593:HOH:O	2.67	0.41
2:B:392:LYS:HZ2	2:B:392:LYS:HG2	1.57	0.41
2:E:158:ASN:OD1	3:F:100:ILE:HD13	2.19	0.41
2:B:365:ARG:HD2	10:B:528:HOH:O	2.20	0.41
2:E:176:ARG:HH11	2:E:176:ARG:HD3	1.72	0.41
3:C:344:LEU:HD12	3:C:384:MET:SD	2.61	0.41
3:F:307:HIS:CE1	3:F:342:GLY:H	2.38	0.41
1:A:190:ALA:C	1:A:192:ASP:H	2.24	0.41
2:B:311:LEU:HD11	2:B:323:LYS:HG2	2.03	0.41
2:B:325:HIS:O	2:B:345:TYR:HA	2.21	0.41
3:C:239:GLN:O	3:C:240:SER:C	2.60	0.41
3:F:372:TRP:HZ3	3:F:379:MET:HE2	1.86	0.41
1:A:138:LYS:HA	1:A:138:LYS:HD3	1.94	0.40
2:B:316:ASP:OD1	2:B:316:ASP:C	2.60	0.40
3:C:298:ASP:CG	3:C:299:PRO:CD	2.89	0.40
2:B:158:ASN:HD22	2:B:158:ASN:HA	1.68	0.40
3:C:229:GLY:O	3:C:233:ILE:HG13	2.22	0.40
3:F:104:ASP:C	3:F:107:ILE:HG22	2.41	0.40
2:B:413:ASN:N	10:B:596:HOH:O	2.54	0.40
1:D:133:ILE:CG1	3:F:107:ILE:HD11	2.49	0.40
3:F:249:GLU:HB2	3:F:383:THR:HG23	2.03	0.40
2:B:367:MET:HB2	2:B:406:ARG:HB3	2.04	0.40
2:E:183:GLU:O	2:E:187:SER:HB3	2.21	0.40
2:E:412:PRO:O	10:E:585:HOH:O	2.22	0.40
1:A:128:GLU:O	1:A:132:HIS:CD2	2.75	0.40
2:B:184:SER:CB	10:B:510:HOH:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	72/87 (83%)	67 (93%)	3 (4%)	2 (3%)	5 3
1	D	72/87 (83%)	64 (89%)	6 (8%)	2 (3%)	5 3
2	B	306/328 (93%)	286 (94%)	15 (5%)	5 (2%)	9 9
2	E	306/328 (93%)	281 (92%)	21 (7%)	4 (1%)	12 12
3	C	299/319 (94%)	275 (92%)	17 (6%)	7 (2%)	6 5
3	F	299/319 (94%)	276 (92%)	16 (5%)	7 (2%)	6 5
4	G	2/4 (50%)	2 (100%)	0	0	100 100
4	H	2/4 (50%)	2 (100%)	0	0	100 100
5	I	2/4 (50%)	2 (100%)	0	0	100 100
5	J	2/4 (50%)	2 (100%)	0	0	100 100
All	All	1362/1484 (92%)	1257 (92%)	78 (6%)	27 (2%)	7 6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	240	SER
3	C	392	LEU
2	E	156	THR
3	F	101	LEU
3	F	240	SER
3	F	392	LEU
1	A	123	LYS
2	B	457	PHE
3	C	101	LEU
3	C	396	GLU
1	D	191	LYS
2	E	457	PHE
2	E	154	ASP
3	F	198	LEU

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Mol	Chain	Res	Type
2	B	281	ASP
3	C	253	TRP
1	A	121	VAL
2	B	156	THR
2	B	256	GLN
3	C	391	ARG
1	D	187	GLN
2	E	256	GLN
3	F	199	ASP
3	F	396	GLU
2	B	456	PRO
3	C	394	ILE
3	F	394	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	69/82 (84%)	59 (86%)	10 (14%)	3 3
1	D	69/82 (84%)	62 (90%)	7 (10%)	7 9
2	B	266/286 (93%)	235 (88%)	31 (12%)	5 6
2	E	266/286 (93%)	235 (88%)	31 (12%)	5 6
3	C	252/267 (94%)	220 (87%)	32 (13%)	4 4
3	F	252/267 (94%)	231 (92%)	21 (8%)	11 14
4	G	3/3 (100%)	2 (67%)	1 (33%)	0 0
4	H	3/3 (100%)	3 (100%)	0	100 100
5	I	3/3 (100%)	3 (100%)	0	100 100
5	J	3/3 (100%)	3 (100%)	0	100 100
All	All	1186/1282 (92%)	1053 (89%)	133 (11%)	6 6

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	128	GLU
1	A	130	VAL
1	A	162	ARG
1	A	164	SER
1	A	169	LEU
1	A	171	ARG
1	A	176	LYS
1	A	183	LYS
1	A	186	GLU
2	B	158	ASN
2	B	159	SER
2	B	166	ARG
2	B	168	LEU
2	B	170	SER
2	B	171	ILE
2	B	177	SER
2	B	187	SER
2	B	190	MET
2	B	191	GLU
2	B	195	THR
2	B	210	GLU
2	B	229	PRO
2	B	232	SER
2	B	233	VAL
2	B	238	VAL
2	B	244	THR
2	B	252	ILE
2	B	253	GLN
2	B	267	ASP
2	B	284	ASN
2	B	301	GLN
2	B	320	ASP
2	B	321	LYS
2	B	346	ARG
2	B	351	ASN
2	B	359	GLN
2	B	388	SER
2	B	392	LYS
2	B	406	ARG
2	B	439	ASN
3	C	99	SER
3	C	105	SER

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Mol	Chain	Res	Type
3	C	106	SER
3	C	107	ILE
3	C	112	GLU
3	C	113	ILE
3	C	116	SER
3	C	147	ASP
3	C	149	THR
3	C	162	LYS
3	C	187	SER
3	C	192	THR
3	C	198	LEU
3	C	224	THR
3	C	244	TYR
3	C	250	LEU
3	C	277	THR
3	C	294	ASP
3	C	297	ASP
3	C	303	PHE
3	C	317	ASN
3	C	325	ASN
3	C	358	SER
3	C	361	ASN
3	C	365	ASN
3	C	374	THR
3	C	376	TRP
3	C	383	THR
3	C	390	ASN
3	C	391	ARG
3	C	393	THR
3	C	394	ILE
1	D	124	ARG
1	D	125	LYS
1	D	135	LEU
1	D	169	LEU
1	D	176	LYS
1	D	183	LYS
1	D	185	LEU
2	E	161	ILE
2	E	165	LEU
2	E	166	ARG
2	E	170	SER
2	E	171	ILE

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Mol	Chain	Res	Type
2	E	174	ASN
2	E	176	ARG
2	E	179	ILE
2	E	187	SER
2	E	190	MET
2	E	191	GLU
2	E	210	GLU
2	E	220	GLU
2	E	231	SER
2	E	232	SER
2	E	233	VAL
2	E	234	LYS
2	E	238	VAL
2	E	244	THR
2	E	253	GLN
2	E	267	ASP
2	E	280	THR
2	E	284	ASN
2	E	301	GLN
2	E	323	LYS
2	E	351	ASN
2	E	359	GLN
2	E	366	THR
2	E	373	MET
2	E	406	ARG
2	E	439	ASN
3	F	140	LYS
3	F	147	ASP
3	F	149	THR
3	F	151	LYS
3	F	192	THR
3	F	198	LEU
3	F	224	THR
3	F	250	LEU
3	F	277	THR
3	F	294	ASP
3	F	303	PHE
3	F	317	ASN
3	F	325	ASN
3	F	361	ASN
3	F	365	ASN
3	F	374	THR

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Mol	Chain	Res	Type
3	F	376	TRP
3	F	382	THR
3	F	383	THR
3	F	390	ASN
3	F	391	ARG
4	G	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
2	B	158	ASN
2	B	160	ASN
2	B	189	GLN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	339	GLN
2	B	351	ASN
2	B	359	GLN
2	B	408	HIS
2	B	439	ASN
3	C	103	HIS
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	136	GLN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	325	ASN
3	C	365	ASN
3	C	390	ASN
1	D	132	HIS
1	D	187	GLN
2	E	189	GLN

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Mol	Chain	Res	Type
2	E	253	GLN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	117	ASN
3	F	146	HIS
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	361	ASN
3	F	365	ASN
3	F	390	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)

2 monosaccharides are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	K	1	6,2	14,14,15	1.27	1 (7%)	17,19,21	1.33	3 (17%)
6	NAG	K	2	6	14,14,15	1.31	2 (14%)	17,19,21	1.11	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
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1	NAG	O7-C7	-4.12	1.13	1.23
6	K	2	NAG	O7-C7	-3.72	1.14	1.23
6	K	2	NAG	C2-N2	2.01	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	1	NAG	C3-C4-C5	2.47	114.64	110.24
6	K	1	NAG	C6-C5-C4	-2.39	107.40	113.00
6	K	1	NAG	C1-O5-C5	2.24	115.22	112.19
6	K	2	NAG	C1-O5-C5	2.20	115.17	112.19

There are no chirality outliers.

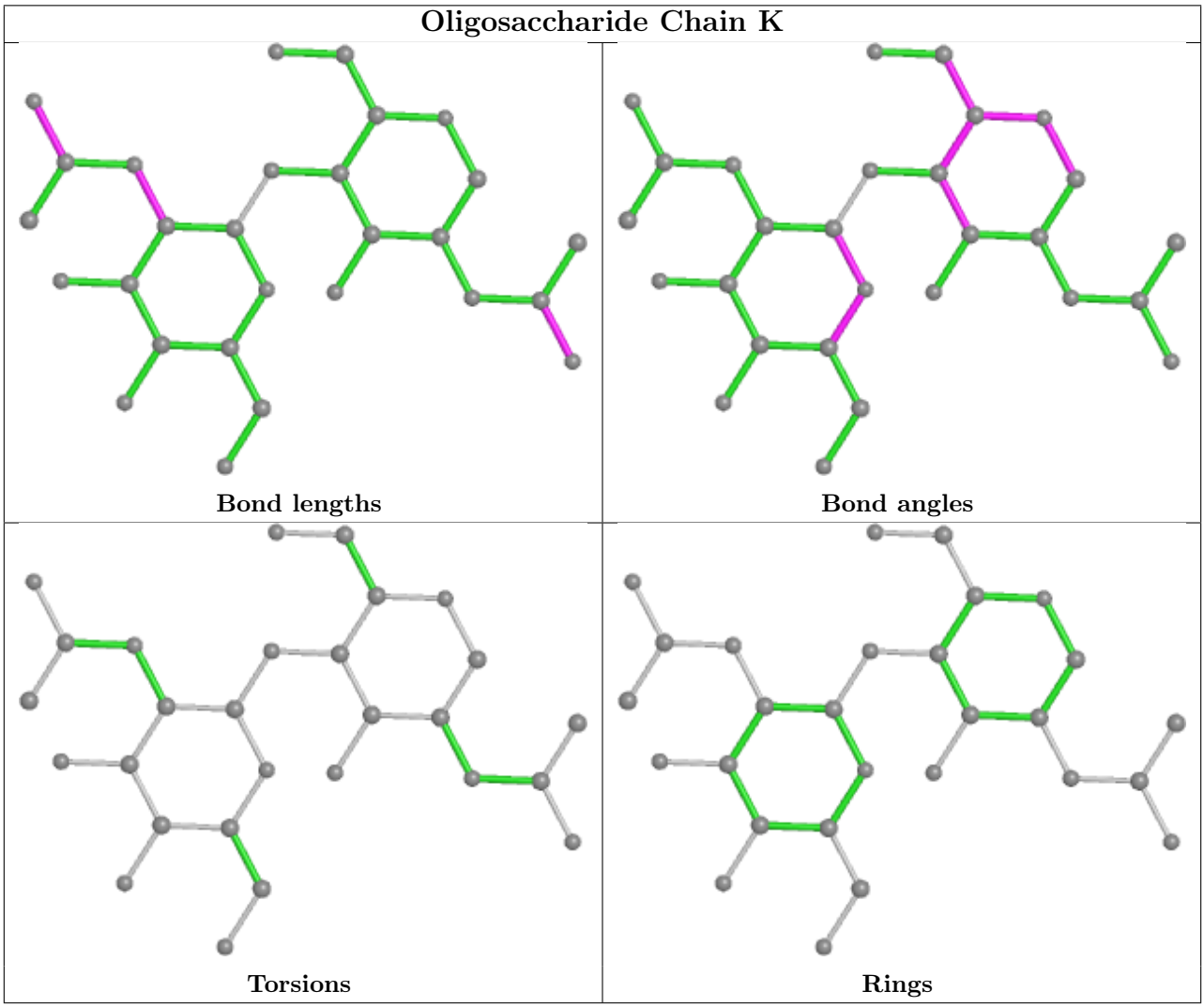
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	3	0
6	K	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
9	NAG	J	471	-	14,14,15	1.28	1 (7%)	17,19,21	1.31	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	B	472	-	11,11,12	1.16	1 (9%)	15,15,17	2.51	4 (26%)
9	NAG	E	470	2	14,14,15	1.25	1 (7%)	17,19,21	1.87	4 (23%)

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
9	NAG	J	471	-	-	2/6/23/26	0/1/1/1
7	MAN	B	472	-	-	0/2/19/22	0/1/1/1
9	NAG	E	470	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	470	NAG	O7-C7	-3.90	1.14	1.23
9	J	471	NAG	O7-C7	-3.62	1.15	1.23
7	B	472	MAN	O5-C1	-3.32	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	472	MAN	O5-C1-C2	6.34	120.55	110.77
7	B	472	MAN	C1-O5-C5	5.83	120.09	112.19
9	E	470	NAG	O5-C1-C2	-4.79	103.72	111.29
9	E	470	NAG	C1-O5-C5	3.66	117.15	112.19
9	J	471	NAG	C1-O5-C5	3.49	116.92	112.19
9	E	470	NAG	O5-C5-C6	-2.41	103.43	107.20
9	E	470	NAG	O3-C3-C2	-2.40	104.50	109.47
7	B	472	MAN	O3-C3-C2	-2.39	105.43	109.99
7	B	472	MAN	C1-C2-C3	2.38	112.60	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	471	NAG	O5-C5-C6-O6
9	J	471	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	471	NAG	2	0
7	B	472	MAN	2	0
9	E	470	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.