



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:47 PM UTC

PDB ID : 1FZF / pdb_00001fzf
Title : CRYSTAL STRUCTURE OF FRAGMENT DOUBLE-D FROM HUMAN FIBRIN WITH THE PEPTIDE LIGAND GLY-HIS-ARG-PRO-AMIDE
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Deposited on : 1998-12-28
Resolution : 2.70 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

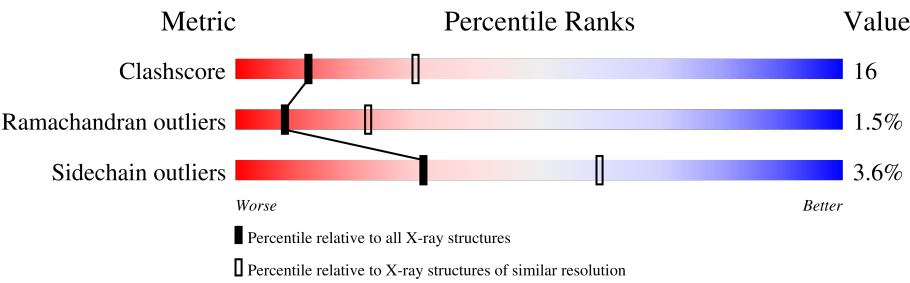
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	46% 29% • 23%
1	D	87	39% 21% • 38%
2	B	328	65% 22% 5% • 8%
2	E	328	61% 24% 5% 10%
3	C	319	62% 26% • 8%
3	F	319	61% 25% • 11%
4	M	4	75% 25%
4	N	4	50% 50%

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Mol	Chain	Length	Quality of chain
4	S	4	 75%25%
4	T	4	 75%25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10581 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			547	337	103	104	3			
1	D	54	Total	C	N	O	S	0	0	0
			441	269	84	85	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1515	429	462	22			
2	E	296	Total	C	N	O	S	0	0	0
			2377	1484	420	451	22			

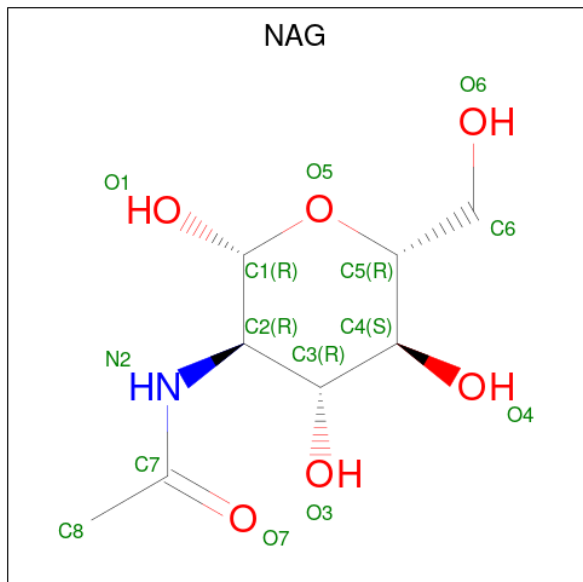
- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2343	1485	396	451	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called FIBRINOGEN.

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

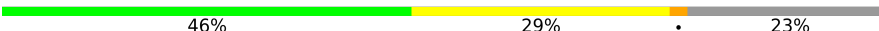
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	2	Total	Ca	0	0
			2	2		
6	E	2	Total	Ca	0	0
			2	2		
6	F	1	Total	Ca	0	0
			1	1		

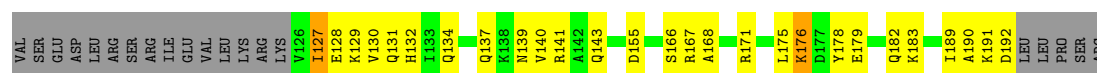
3 Residue-property plots [i](#)

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

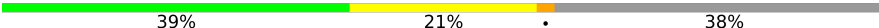
Note EDS was not executed.

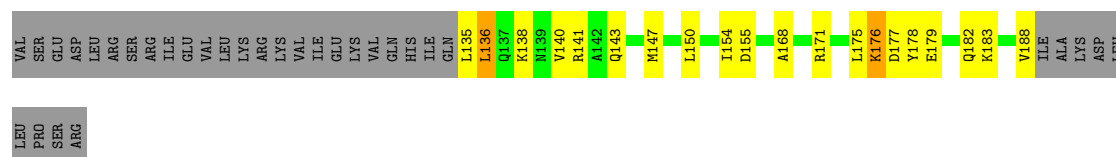
• Molecule 1: FIBRINOGEN

Chain A: 



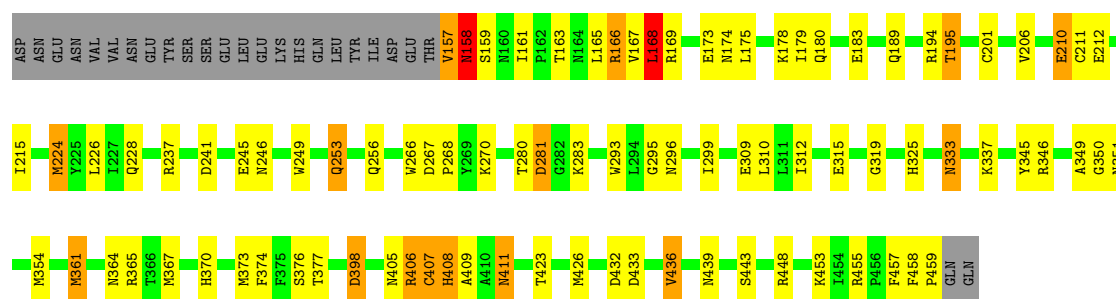
• Molecule 1: FIBRINOGEN

Chain D: 



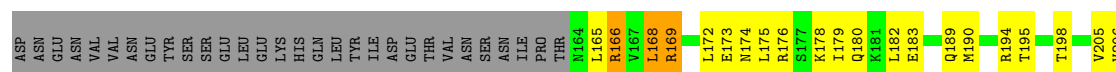
• Molecule 2: FIBRINOGEN

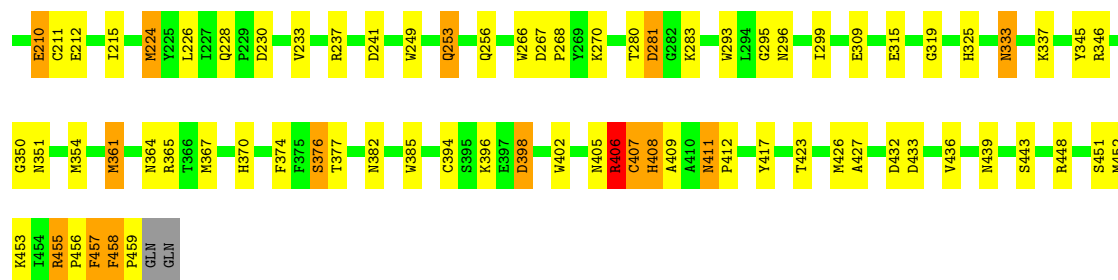
Chain B: 



• Molecule 2: FIBRINOGEN

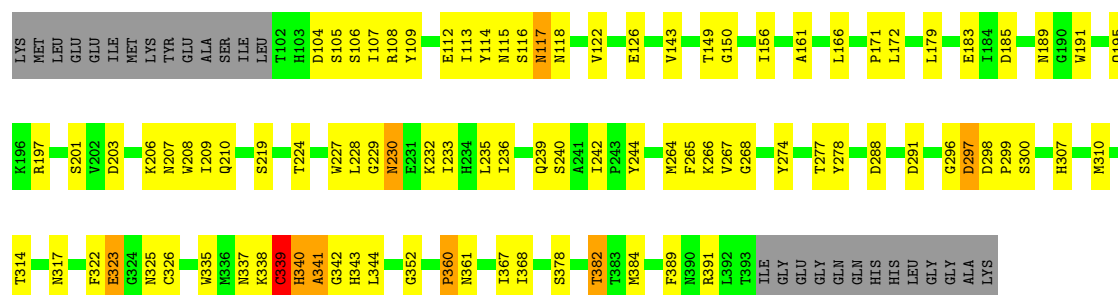
Chain E: 





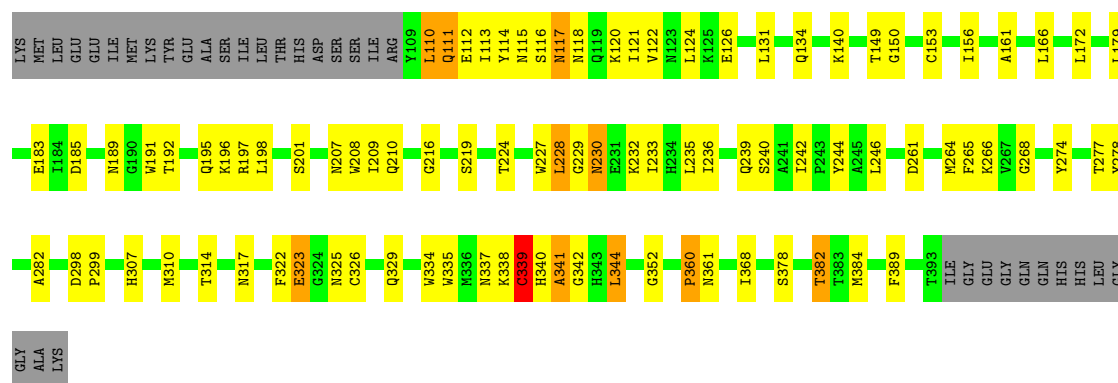
- Molecule 3: FIBRINOGEN

Chain C: 62% 26% 8%



- Molecule 3: FIBRINOGEN

Chain F: 61% 25% 11%



- Molecule 4: FIBRINOGEN

Chain S: 75% 25%



- Molecule 4: FIBRINOGEN

Chain T: 75% 25%



- Molecule 4: FIBRINOGEN

Chain M:  75% 25%



● Molecule 4: FIBRINOGEN

Chain N:  50% 50%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.80Å 149.40Å 234.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	88.5 (30.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.233 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.58	1/548 (0.2%)	1.06	2/731 (0.3%)
1	D	0.40	0/441	0.97	3/587 (0.5%)
2	B	0.47	0/2490	1.04	18/3364 (0.5%)
2	E	0.46	0/2438	1.01	17/3291 (0.5%)
3	C	0.47	0/2408	0.92	7/3257 (0.2%)
3	F	0.49	0/2351	0.94	7/3180 (0.2%)
4	M	0.65	0/32	0.49	0/42
4	N	0.55	0/32	0.65	0/42
4	S	0.50	0/32	0.69	0/42
4	T	0.54	0/32	0.68	0/42
All	All	0.48	1/10804 (0.0%)	0.98	54/14578 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ASP	C-O	-9.35	1.04	1.23

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ASP	CA-C-O	-15.56	94.35	120.80
2	B	157	VAL	N-CA-C	12.78	146.79	111.00
2	B	408	HIS	N-CA-C	8.95	122.48	108.79
3	C	340	HIS	N-CA-C	8.83	121.50	108.60
2	B	406	ARG	N-CA-C	-8.65	99.35	111.81
2	E	408	HIS	N-CA-C	8.59	121.93	108.79
3	F	340	HIS	N-CA-C	8.12	120.46	108.60
2	B	409	ALA	N-CA-C	-7.80	104.25	114.31
2	B	194	ARG	N-CA-C	-7.72	102.80	111.14
2	E	406	ARG	N-CA-C	-7.57	100.91	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	ASN	N-CA-C	-7.50	94.83	110.80
3	C	341	ALA	N-CA-C	-7.43	105.13	114.56
2	E	409	ALA	N-CA-C	-7.37	104.81	114.31
2	B	168	LEU	N-CA-C	-7.17	106.45	114.62
2	E	194	ARG	N-CA-C	-7.08	103.49	111.07
3	C	201	SER	N-CA-C	7.07	118.64	111.07
2	E	166	ARG	N-CA-C	-6.94	104.73	112.57
2	B	157	VAL	CB-CA-C	-6.77	98.54	111.40
2	E	398	ASP	N-CA-C	6.65	120.08	112.57
3	F	228	LEU	N-CA-C	-6.60	101.38	110.35
3	F	341	ALA	N-CA-C	-6.47	106.34	114.56
2	E	211	CYS	N-CA-C	6.36	118.21	111.28
2	E	436	VAL	N-CA-C	6.33	118.77	108.97
2	B	436	VAL	N-CA-C	6.30	118.47	108.89
3	C	228	LEU	N-CA-C	-6.17	101.96	110.35
2	E	206	VAL	N-CA-C	6.10	117.45	109.58
3	F	201	SER	N-CA-C	6.09	117.59	111.07
2	E	411	ASN	CA-C-N	6.03	125.91	119.28
2	E	411	ASN	C-N-CA	6.03	125.91	119.28
2	E	228	GLN	CA-C-N	5.92	125.79	119.28
2	E	228	GLN	C-N-CA	5.92	125.79	119.28
3	F	344	LEU	N-CA-C	5.89	119.72	112.54
2	B	228	GLN	CA-C-N	5.79	125.47	119.56
2	B	228	GLN	C-N-CA	5.79	125.47	119.56
1	A	141	ARG	N-CA-C	-5.68	105.09	111.28
2	B	206	VAL	N-CA-C	5.65	116.89	109.21
1	D	136	LEU	N-CA-C	-5.63	105.13	112.23
2	B	211	CYS	N-CA-C	5.51	118.00	111.33
3	F	339	CYS	N-CA-C	5.30	122.10	110.80
3	C	339	CYS	N-CA-C	5.24	121.95	110.80
2	B	166	ARG	N-CA-C	-5.23	106.75	113.02
1	D	141	ARG	N-CA-C	-5.20	105.61	111.28
2	B	398	ASP	N-CA-C	5.20	119.12	112.26
3	C	344	LEU	N-CA-C	5.18	118.87	112.54
3	C	368	ILE	N-CA-C	5.18	117.22	109.20
1	D	177	ASP	N-CA-C	-5.14	105.11	111.33
3	F	368	ILE	N-CA-C	5.12	117.13	109.20
2	E	455	ARG	CA-C-N	5.08	126.19	119.84
2	E	455	ARG	C-N-CA	5.08	126.19	119.84
2	B	349	ALA	N-CA-C	-5.06	102.02	109.86
2	E	169	ARG	N-CA-C	-5.05	105.66	111.07
2	E	394	CYS	N-CA-C	5.03	116.45	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	ASN	CA-C-N	5.00	124.78	119.28
2	B	411	ASN	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

There are no planarity outliers.

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	547	0	573	24	0
1	D	441	0	458	19	0
2	B	2428	0	2296	67	0
2	E	2377	0	2245	92	0
3	C	2343	0	2188	68	0
3	F	2287	0	2136	83	0
4	M	31	0	32	1	0
4	N	31	0	32	2	0
4	S	31	0	32	1	0
4	T	31	0	32	1	0
5	B	14	0	13	6	0
5	E	14	0	13	3	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
All	All	10581	0	10050	324	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 16.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ARG:HA	3:F:117:ASN:HB3	1.30	1.06
2:E:402:TRP:CH2	2:E:452:MET:HE1	2.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:MET:SD	3:C:337:ASN:HB2	2.16	0.85
3:C:107:ILE:HD12	3:C:107:ILE:H	1.42	0.85
3:F:310:MET:SD	3:F:337:ASN:HB2	2.18	0.84
5:B:470:NAG:H2	5:B:470:NAG:H62	1.61	0.82
3:C:209:ILE:H	3:C:209:ILE:HD12	1.41	0.82
2:B:157:VAL:CG1	2:B:157:VAL:O	2.27	0.81
3:F:209:ILE:HD12	3:F:209:ILE:H	1.44	0.81
2:E:166:ARG:HH22	3:F:110:LEU:HG	1.47	0.78
2:E:189:GLN:HG3	3:F:131:LEU:HD11	1.63	0.78
1:A:131:GLN:HA	1:A:134:GLN:HG2	1.67	0.76
2:E:402:TRP:CZ3	2:E:452:MET:HE1	2.21	0.76
2:E:179:ILE:HG21	3:F:120:LYS:HB3	1.69	0.75
2:E:169:ARG:O	2:E:173:GLU:HG2	1.86	0.74
3:F:307:HIS:HE1	3:F:341:ALA:H	1.35	0.74
3:C:117:ASN:HD22	3:C:118:ASN:N	1.87	0.73
2:E:176:ARG:HA	3:F:117:ASN:CB	2.16	0.73
2:E:182:LEU:HB2	3:F:124:LEU:HD21	1.71	0.72
2:E:333:ASN:ND2	2:E:333:ASN:H	1.87	0.72
1:D:140:VAL:HG12	3:F:114:TYR:CE1	2.24	0.72
2:E:190:MET:HG3	3:F:134:GLN:HE22	1.53	0.72
3:C:322:PHE:HB2	3:C:338:LYS:HA	1.72	0.71
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.39	0.71
2:E:179:ILE:HG21	3:F:120:LYS:CB	2.21	0.71
1:D:188:VAL:HG22	2:E:165:LEU:HD13	1.73	0.70
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.73	0.70
2:B:333:ASN:H	2:B:333:ASN:ND2	1.90	0.70
3:C:149:THR:HG22	3:C:150:GLY:H	1.57	0.70
2:B:364:ASN:ND2	5:B:470:NAG:C1	2.55	0.70
2:B:405:ASN:C	2:B:407:CYS:H	1.98	0.69
2:B:351:ASN:ND2	2:B:354:MET:H	1.90	0.69
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.39	0.68
3:F:360:PRO:HG2	3:F:361:ASN:H	1.57	0.68
2:E:412:PRO:HG2	2:E:452:MET:CE	2.24	0.68
2:B:157:VAL:O	2:B:157:VAL:HG13	1.93	0.68
2:E:364:ASN:HD21	5:E:470:NAG:C1	2.06	0.68
2:E:405:ASN:C	2:E:407:CYS:H	2.01	0.67
2:E:402:TRP:HH2	2:E:452:MET:HE1	1.58	0.67
2:B:166:ARG:C	2:B:168:LEU:H	2.01	0.67
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.75	0.67
3:F:117:ASN:HD22	3:F:118:ASN:N	1.93	0.66
2:E:180:GLN:O	2:E:183:GLU:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:LEU:H	3:C:239:GLN:HE21	1.44	0.65
2:E:351:ASN:ND2	2:E:354:MET:H	1.94	0.65
1:A:131:GLN:CD	1:A:131:GLN:H	2.04	0.65
3:C:307:HIS:HE1	3:C:341:ALA:H	1.45	0.65
3:F:149:THR:HG22	3:F:150:GLY:H	1.61	0.65
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.79	0.65
2:B:364:ASN:HD21	5:B:470:NAG:C1	2.09	0.64
3:C:360:PRO:HG2	3:C:361:ASN:H	1.63	0.64
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.61	0.64
3:C:307:HIS:HD2	3:C:335:TRP:O	1.80	0.64
2:B:180:GLN:O	2:B:183:GLU:HG2	1.98	0.64
3:F:322:PHE:HB2	3:F:338:LYS:HA	1.80	0.63
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.47	0.63
1:D:140:VAL:HG12	3:F:114:TYR:HE1	1.64	0.62
3:F:235:LEU:O	3:F:239:GLN:HB3	2.00	0.62
2:B:367:MET:HB2	2:B:406:ARG:HB3	1.82	0.61
1:D:155:ASP:HA	1:D:171:ARG:NH1	2.16	0.61
3:C:264:MET:O	3:C:278:TYR:HA	2.01	0.61
3:F:307:HIS:HD2	3:F:335:TRP:O	1.82	0.61
2:E:172:LEU:HD13	3:F:114:TYR:HB2	1.83	0.61
2:E:182:LEU:CB	3:F:124:LEU:HD21	2.30	0.60
3:C:104:ASP:HA	3:C:107:ILE:HD13	1.83	0.60
3:C:172:LEU:H	3:C:239:GLN:NE2	2.00	0.60
3:C:235:LEU:O	3:C:239:GLN:HB3	2.02	0.60
2:B:458:PHE:HB3	2:B:459:PRO:HD3	1.82	0.60
1:D:175:LEU:HD23	1:D:175:LEU:H	1.66	0.60
3:F:323:GLU:H	3:F:323:GLU:CD	2.10	0.59
2:B:169:ARG:O	2:B:173:GLU:HG2	2.02	0.59
2:B:210:GLU:OE1	2:B:212:GLU:HB3	2.02	0.59
3:C:240:SER:OG	3:C:242:ILE:HG12	2.02	0.59
2:E:168:LEU:H	2:E:168:LEU:HD22	1.66	0.59
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.03	0.59
3:C:107:ILE:H	3:C:107:ILE:CD1	2.15	0.59
3:F:195:GLN:HB3	3:F:384:MET:HB2	1.84	0.59
2:B:351:ASN:HD22	2:B:351:ASN:C	2.10	0.58
1:A:155:ASP:HA	1:A:171:ARG:NH1	2.18	0.58
5:B:470:NAG:H2	5:B:470:NAG:C6	2.33	0.58
3:C:195:GLN:HB3	3:C:384:MET:HB2	1.85	0.58
3:C:209:ILE:H	3:C:209:ILE:CD1	2.15	0.58
3:F:307:HIS:CE1	3:F:341:ALA:H	2.18	0.58
2:B:201:CYS:O	3:C:143:VAL:HG21	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:H	1:A:175:LEU:HD23	1.69	0.57
2:E:190:MET:CG	3:F:134:GLN:HE22	2.17	0.57
2:E:432:ASP:OD2	2:E:443:SER:HB2	2.04	0.57
3:C:107:ILE:HD12	3:C:107:ILE:N	2.18	0.57
2:E:183:GLU:HA	3:F:124:LEU:CD1	2.35	0.57
2:E:351:ASN:C	2:E:351:ASN:HD22	2.12	0.56
2:B:295:GLY:O	2:B:299:ILE:HG13	2.05	0.56
3:C:149:THR:HG22	3:C:150:GLY:N	2.21	0.56
1:D:147:MET:SD	3:F:121:ILE:HD11	2.46	0.56
1:D:175:LEU:H	1:D:175:LEU:CD2	2.19	0.56
2:E:212:GLU:O	2:E:215:ILE:HG22	2.06	0.56
3:F:172:LEU:H	3:F:239:GLN:NE2	2.04	0.56
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.04	0.55
3:C:323:GLU:H	3:C:323:GLU:CD	2.14	0.55
1:A:129:LYS:HE2	3:C:104:ASP:HB2	1.88	0.55
3:C:108:ARG:O	3:C:112:GLU:HG3	2.07	0.55
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.89	0.55
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.55	0.55
3:F:307:HIS:CE1	3:F:342:GLY:H	2.25	0.55
2:B:361:MET:HE3	2:B:365:ARG:HH21	1.72	0.54
3:F:264:MET:O	3:F:278:TYR:HA	2.07	0.54
3:F:265:PHE:C	3:F:266:LYS:HD2	2.33	0.54
2:E:367:MET:HG3	4:N:2:HIS:HB2	1.90	0.54
3:F:307:HIS:HE1	3:F:342:GLY:H	1.56	0.54
2:E:319:GLY:HA2	2:E:448:ARG:HH22	1.73	0.54
1:A:175:LEU:H	1:A:175:LEU:CD2	2.21	0.54
2:E:325:HIS:HB3	2:E:346:ARG:HG3	1.89	0.54
2:E:333:ASN:H	2:E:333:ASN:HD22	1.53	0.54
3:F:149:THR:HG22	3:F:150:GLY:N	2.23	0.54
3:F:172:LEU:H	3:F:239:GLN:HE21	1.56	0.54
2:E:361:MET:HE3	2:E:365:ARG:HH21	1.72	0.53
2:B:175:LEU:O	2:B:179:ILE:HG12	2.09	0.53
2:E:224:MET:CE	2:E:237:ARG:HD3	2.39	0.53
2:B:224:MET:CE	2:B:237:ARG:HD3	2.38	0.53
2:E:175:LEU:O	2:E:179:ILE:HG12	2.09	0.53
2:E:361:MET:O	2:E:364:ASN:HB2	2.08	0.53
2:B:405:ASN:C	2:B:407:CYS:N	2.65	0.53
3:F:240:SER:OG	3:F:242:ILE:HG12	2.09	0.53
2:B:157:VAL:O	2:B:157:VAL:HG12	2.03	0.53
2:E:337:LYS:HB2	2:E:374:PHE:CD1	2.44	0.53
3:C:326:CYS:SG	3:C:339:CYS:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:219:SER:OG	3:F:224:THR:HG22	2.09	0.52
3:C:391:ARG:HG2	3:C:391:ARG:HH11	1.74	0.52
2:E:350:GLY:HA3	2:E:439:ASN:HB3	1.90	0.52
2:E:190:MET:SD	3:F:134:GLN:NE2	2.82	0.52
1:A:139:ASN:HB3	3:C:114:TYR:CE1	2.44	0.52
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.90	0.52
2:B:319:GLY:HA2	2:B:448:ARG:HH22	1.74	0.52
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.92	0.52
3:F:122:VAL:O	3:F:126:GLU:HG2	2.10	0.52
3:F:232:LYS:O	3:F:236:ILE:HG13	2.10	0.52
2:B:325:HIS:HB3	2:B:346:ARG:HG3	1.90	0.52
3:F:166:LEU:HD13	3:F:179:LEU:HD21	1.92	0.52
2:B:163:THR:C	2:B:165:LEU:H	2.16	0.52
2:B:163:THR:O	2:B:166:ARG:HG2	2.10	0.52
2:B:212:GLU:O	2:B:215:ILE:HG22	2.09	0.52
3:F:268:GLY:O	3:F:274:TYR:HA	2.09	0.51
2:B:423:THR:OG1	2:B:426:MET:HE3	2.11	0.51
2:E:398:ASP:HA	2:E:433:ASP:CB	2.40	0.51
3:F:115:ASN:HA	3:F:118:ASN:HB3	1.92	0.51
3:F:229:GLY:O	3:F:233:ILE:HG13	2.10	0.51
2:B:253:GLN:C	2:B:253:GLN:HE21	2.19	0.51
3:F:242:ILE:O	3:F:242:ILE:HG13	2.10	0.51
3:C:265:PHE:C	3:C:266:LYS:HD2	2.36	0.51
2:B:266:TRP:HA	2:B:377:THR:HG21	1.92	0.50
3:C:166:LEU:HD13	3:C:179:LEU:HD21	1.93	0.50
3:F:156:ILE:HG22	3:F:161:ALA:HB2	1.93	0.50
1:D:154:ILE:HD12	2:E:182:LEU:HD13	1.92	0.50
2:E:405:ASN:C	2:E:407:CYS:N	2.69	0.50
1:D:175:LEU:O	1:D:178:TYR:HB2	2.11	0.50
2:B:309:GLU:HG2	2:B:455:ARG:O	2.12	0.50
2:B:367:MET:HB2	2:B:406:ARG:CB	2.42	0.50
3:C:122:VAL:O	3:C:126:GLU:HG2	2.12	0.50
3:C:113:ILE:O	3:C:116:SER:HB3	2.12	0.50
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.94	0.49
2:E:325:HIS:O	2:E:345:TYR:HA	2.12	0.49
2:E:183:GLU:HA	3:F:124:LEU:HD11	1.95	0.49
3:F:326:CYS:SG	3:F:339:CYS:N	2.85	0.49
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.94	0.49
1:A:128:GLU:O	1:A:132:HIS:HB2	2.12	0.49
1:A:179:GLU:HA	1:A:182:GLN:NE2	2.27	0.49
2:B:337:LYS:HB2	2:B:374:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ASN:OD1	3:C:210:GLN:HG3	2.13	0.49
2:B:432:ASP:OD2	2:B:443:SER:HB2	2.12	0.49
3:C:337:ASN:C	3:C:339:CYS:N	2.69	0.49
2:E:267:ASP:HB2	2:E:268:PRO:HD3	1.94	0.49
3:F:197:ARG:HB2	3:F:382:THR:HB	1.95	0.48
2:B:350:GLY:HA3	2:B:439:ASN:HB3	1.95	0.48
2:B:361:MET:O	2:B:364:ASN:HB2	2.12	0.48
3:C:229:GLY:O	3:C:233:ILE:HG13	2.14	0.48
3:C:197:ARG:HB2	3:C:382:THR:HB	1.94	0.48
3:F:113:ILE:O	3:F:116:SER:HB3	2.13	0.48
3:C:219:SER:OG	3:C:224:THR:HG22	2.14	0.48
3:C:325:ASN:C	3:C:325:ASN:HD22	2.20	0.48
2:E:295:GLY:O	2:E:299:ILE:HG13	2.13	0.48
3:F:111:GLN:CD	3:F:111:GLN:H	2.21	0.48
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.13	0.48
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.29	0.48
5:B:470:NAG:C6	5:B:470:NAG:C2	2.85	0.48
2:B:373:MET:HE2	2:B:405:ASN:HA	1.95	0.47
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.14	0.47
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.11	0.47
3:C:244:TYR:H	3:C:266:LYS:NZ	2.11	0.47
2:E:224:MET:HE2	2:E:237:ARG:HD3	1.96	0.47
2:E:280:THR:HB	2:E:283:LYS:HB2	1.96	0.47
2:B:333:ASN:H	2:B:333:ASN:HD22	1.58	0.47
3:C:268:GLY:O	3:C:274:TYR:HA	2.15	0.47
2:E:412:PRO:CB	2:E:452:MET:HE3	2.44	0.47
2:E:458:PHE:H	2:E:459:PRO:HD2	1.80	0.47
2:B:309:GLU:HB2	2:B:325:HIS:HE1	1.79	0.47
2:B:398:ASP:HA	2:B:433:ASP:CB	2.43	0.47
3:F:337:ASN:C	3:F:339:CYS:N	2.66	0.47
3:F:352:GLY:HA2	3:F:378:SER:O	2.15	0.47
1:A:137:GLN:O	1:A:140:VAL:HG22	2.14	0.46
3:C:156:ILE:HG22	3:C:161:ALA:HB2	1.97	0.46
3:C:352:GLY:HA2	3:C:378:SER:O	2.16	0.46
3:F:298:ASP:OD1	3:F:299:PRO:HD2	2.15	0.46
1:A:175:LEU:HD23	1:A:175:LEU:N	2.31	0.46
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.50	0.46
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.15	0.46
2:E:293:TRP:HZ2	2:E:296:ASN:ND2	2.09	0.46
2:E:364:ASN:ND2	5:E:470:NAG:H2	2.30	0.46
3:F:209:ILE:H	3:F:209:ILE:CD1	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:C	1:A:129:LYS:HD2	2.41	0.46
3:C:340:HIS:ND1	3:C:343:HIS:HB2	2.31	0.46
3:F:208:TRP:HA	3:F:314:THR:HG21	1.97	0.46
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.81	0.46
3:C:298:ASP:OD1	3:C:299:PRO:HD2	2.16	0.46
3:F:156:ILE:HG22	3:F:161:ALA:CB	2.46	0.46
1:D:175:LEU:HD23	1:D:175:LEU:N	2.30	0.45
2:E:183:GLU:HA	3:F:124:LEU:HD13	1.97	0.45
1:A:176:LYS:HB2	1:A:176:LYS:HZ3	1.80	0.45
2:B:280:THR:HB	2:B:283:LYS:HB2	1.99	0.45
3:F:325:ASN:HD22	3:F:325:ASN:C	2.23	0.45
2:B:315:GLU:HG2	2:B:448:ARG:HH21	1.81	0.45
1:D:179:GLU:HA	1:D:182:GLN:HG2	1.98	0.45
2:E:266:TRP:HA	2:E:377:THR:HG21	1.98	0.45
3:F:228:LEU:HG	3:F:232:LYS:HD2	1.98	0.45
3:C:106:SER:HA	3:C:109:TYR:CD2	2.51	0.45
3:F:244:TYR:H	3:F:266:LYS:NZ	2.14	0.45
2:B:325:HIS:O	2:B:345:TYR:HA	2.17	0.45
1:D:176:LYS:HA	1:D:176:LYS:HZ2	1.81	0.45
1:D:179:GLU:HA	1:D:182:GLN:NE2	2.31	0.45
1:D:179:GLU:O	1:D:182:GLN:HG2	2.16	0.45
2:E:230:ASP:O	2:E:233:VAL:HG22	2.17	0.45
2:E:309:GLU:HB2	2:E:325:HIS:HE1	1.82	0.45
3:F:337:ASN:O	3:F:338:LYS:C	2.59	0.45
2:E:179:ILE:HG13	3:F:117:ASN:HB2	1.97	0.45
2:E:412:PRO:HG2	2:E:452:MET:HE3	1.99	0.45
1:A:129:LYS:HD2	1:A:129:LYS:N	2.32	0.45
3:C:105:SER:HB2	3:C:109:TYR:OH	2.17	0.45
3:C:232:LYS:O	3:C:236:ILE:HG13	2.16	0.45
1:A:179:GLU:HA	1:A:182:GLN:HG2	1.99	0.44
2:E:253:GLN:NE2	2:E:451:SER:HA	2.32	0.44
3:F:244:TYR:H	3:F:266:LYS:HZ3	1.65	0.44
3:F:261:ASP:O	3:F:282:ALA:N	2.49	0.44
1:A:166:SER:HB3	2:B:195:THR:HG23	1.98	0.44
2:B:166:ARG:C	2:B:168:LEU:N	2.72	0.44
3:C:185:ASP:OD2	3:C:189:ASN:HB2	2.17	0.44
3:C:391:ARG:HG2	3:C:391:ARG:NH1	2.32	0.44
2:E:253:GLN:HE21	2:E:253:GLN:C	2.25	0.44
2:E:345:TYR:CG	2:E:346:ARG:N	2.85	0.44
1:A:179:GLU:O	1:A:182:GLN:HG2	2.17	0.44
2:B:267:ASP:HB2	2:B:268:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:307:HIS:CE1	3:C:342:GLY:H	2.36	0.44
3:C:115:ASN:HA	3:C:118:ASN:HB3	2.00	0.44
2:E:249:TRP:HB3	2:E:453:LYS:HB3	2.00	0.44
2:E:367:MET:HB2	2:E:406:ARG:CB	2.47	0.44
3:C:208:TRP:HA	3:C:314:THR:HG21	1.99	0.44
2:B:345:TYR:CG	2:B:346:ARG:N	2.85	0.44
3:C:203:ASP:O	3:C:206:LYS:HE2	2.18	0.44
3:C:242:ILE:O	3:C:242:ILE:HG13	2.17	0.44
2:E:423:THR:OG1	2:E:426:MET:HE3	2.17	0.44
3:F:111:GLN:NE2	3:F:112:GLU:HG3	2.33	0.43
2:B:293:TRP:HZ2	2:B:296:ASN:ND2	2.12	0.43
3:C:265:PHE:CZ	3:C:267:VAL:HG23	2.54	0.43
1:D:179:GLU:HB3	1:D:183:LYS:HE3	2.00	0.43
3:C:296:GLY:O	3:C:297:ASP:C	2.61	0.43
3:C:298:ASP:OD2	3:C:300:SER:HB2	2.18	0.43
2:E:293:TRP:CZ2	2:E:296:ASN:ND2	2.86	0.43
2:E:179:ILE:HG21	3:F:120:LYS:HB2	1.96	0.43
3:C:307:HIS:HE1	3:C:342:GLY:H	1.66	0.43
3:F:196:LYS:HD2	3:F:198:LEU:HD21	2.00	0.43
2:B:174:ASN:O	2:B:178:LYS:HG2	2.18	0.43
3:F:153:CYS:SG	3:F:192:THR:HA	2.59	0.43
2:E:376:SER:HB3	2:E:382:ASN:H	1.84	0.42
3:F:185:ASP:OD2	3:F:189:ASN:HB2	2.19	0.42
2:E:166:ARG:NH2	3:F:110:LEU:HG	2.25	0.42
2:B:310:LEU:HD12	2:B:453:LYS:O	2.19	0.42
3:C:209:ILE:HD12	3:C:209:ILE:N	2.21	0.42
2:E:457:PHE:HB3	2:E:458:PHE:H	1.49	0.42
1:A:134:GLN:HA	1:A:137:GLN:NE2	2.35	0.42
2:B:436:VAL:HG11	2:B:443:SER:HA	2.02	0.42
3:C:156:ILE:HG22	3:C:161:ALA:CB	2.50	0.42
3:F:183:GLU:HB3	3:F:191:TRP:HB2	2.02	0.42
1:A:179:GLU:HB3	1:A:183:LYS:HE3	2.01	0.42
2:E:205:VAL:HG23	3:F:216:GLY:C	2.45	0.42
3:C:343:HIS:O	3:C:367:ILE:HA	2.20	0.41
2:E:385:TRP:CH2	4:N:3:ARG:HD2	2.55	0.41
2:E:455:ARG:HA	2:E:456:PRO:HD3	1.83	0.41
1:A:127:ILE:HB	1:A:130:VAL:HG21	2.02	0.41
5:B:470:NAG:H62	5:B:470:NAG:C2	2.37	0.41
3:C:339:CYS:SG	4:S:3:ARG:CZ	3.09	0.41
2:E:333:ASN:ND2	2:E:333:ASN:N	2.61	0.41
2:E:370:HIS:HE1	2:E:408:HIS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LEU:HD21	2:B:312:ILE:HD11	2.02	0.41
2:E:417:TYR:OH	2:E:427:ALA:HA	2.21	0.41
2:E:458:PHE:N	2:E:459:PRO:HD2	2.35	0.41
1:A:127:ILE:HB	1:A:130:VAL:CG2	2.50	0.41
1:D:135:LEU:N	1:D:135:LEU:HD22	2.36	0.41
1:D:150:LEU:HD12	1:D:150:LEU:HA	1.87	0.41
2:E:179:ILE:HD12	3:F:121:ILE:HG12	2.01	0.41
2:E:315:GLU:HG2	2:E:448:ARG:HH21	1.84	0.41
3:F:344:LEU:HD12	3:F:384:MET:SD	2.60	0.41
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.56	0.41
2:B:408:HIS:O	4:M:1:GLY:HA2	2.20	0.41
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.20	0.41
1:D:136:LEU:C	1:D:138:LYS:N	2.77	0.41
2:E:364:ASN:ND2	5:E:470:NAG:C2	2.84	0.41
2:B:158:ASN:ND2	2:B:159:SER:H	2.18	0.41
3:C:183:GLU:HB3	3:C:191:TRP:HB2	2.03	0.41
2:E:198:THR:HG22	3:F:140:LYS:HB2	2.03	0.41
2:E:226:LEU:HD12	2:E:226:LEU:HA	1.91	0.41
2:B:226:LEU:HD12	2:B:226:LEU:HA	1.97	0.41
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.56	0.41
3:F:322:PHE:HE2	3:F:329:GLN:HE22	1.69	0.41
3:F:339:CYS:SG	4:T:3:ARG:CZ	3.09	0.41
2:B:245:GLU:O	2:B:246:ASN:HB2	2.21	0.40
3:C:171:PRO:HA	3:C:239:GLN:NE2	2.36	0.40
3:F:209:ILE:HD12	3:F:209:ILE:N	2.25	0.40
1:A:175:LEU:O	1:A:178:TYR:HB2	2.22	0.40
2:B:280:THR:O	2:B:281:ASP:C	2.63	0.40
2:E:396:LYS:HD2	2:E:396:LYS:HA	1.88	0.40
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.56	0.40
2:B:166:ARG:HD3	2:B:166:ARG:HA	1.80	0.40
2:E:174:ASN:O	2:E:178:LYS:HG2	2.22	0.40
2:E:280:THR:O	2:E:281:ASP:C	2.63	0.40
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.40	0.40
2:B:163:THR:C	2:B:165:LEU:N	2.80	0.40
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.85	0.40

There are no symmetry-related clashes.

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	65/87 (75%)	58 (89%)	3 (5%)	4 (6%)	1	2
1	D	52/87 (60%)	50 (96%)	2 (4%)	0	100	100
2	B	301/328 (92%)	271 (90%)	25 (8%)	5 (2%)	7	19
2	E	294/328 (90%)	267 (91%)	23 (8%)	4 (1%)	9	23
3	C	290/319 (91%)	265 (91%)	22 (8%)	3 (1%)	12	32
3	F	283/319 (89%)	257 (91%)	23 (8%)	3 (1%)	11	29
4	M	2/4 (50%)	2 (100%)	0	0	100	100
4	N	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	S	2/4 (50%)	2 (100%)	0	0	100	100
4	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1293/1484 (87%)	1175 (91%)	99 (8%)	19 (2%)	8	22

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
2	B	407	CYS
3	C	339	CYS
2	E	407	CYS
3	F	110	LEU
2	B	281	ASP
2	E	281	ASP
2	E	458	PHE
3	F	339	CYS
1	A	190	ALA
2	B	256	GLN
2	B	457	PHE
3	C	360	PRO
3	F	360	PRO

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Mol	Chain	Res	Type
3	C	297	ASP
2	B	167	VAL
2	E	256	GLN
1	A	127	ILE
1	A	189	ILE

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	62/82 (76%)	59 (95%)	3 (5%)	23	50
1	D	50/82 (61%)	48 (96%)	2 (4%)	28	56
2	B	261/286 (91%)	251 (96%)	10 (4%)	29	58
2	E	254/286 (89%)	244 (96%)	10 (4%)	28	57
3	C	246/267 (92%)	239 (97%)	7 (3%)	38	68
3	F	239/267 (90%)	230 (96%)	9 (4%)	29	58
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	3 (100%)	0	100	100
4	S	3/3 (100%)	3 (100%)	0	100	100
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	1124/1282 (88%)	1083 (96%)	41 (4%)	31	60

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	167	ARG
1	A	176	LYS
2	B	158	ASN
2	B	161	ILE
2	B	168	LEU
2	B	195	THR
2	B	210	GLU

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Mol	Chain	Res	Type
2	B	224	MET
2	B	253	GLN
2	B	333	ASN
2	B	361	MET
2	B	376	SER
3	C	117	ASN
3	C	230	ASN
3	C	277	THR
3	C	317	ASN
3	C	323	GLU
3	C	382	THR
3	C	389	PHE
1	D	143	GLN
1	D	176	LYS
2	E	168	LEU
2	E	195	THR
2	E	210	GLU
2	E	224	MET
2	E	253	GLN
2	E	333	ASN
2	E	361	MET
2	E	376	SER
2	E	406	ARG
2	E	457	PHE
3	F	111	GLN
3	F	117	ASN
3	F	230	ASN
3	F	246	LEU
3	F	277	THR
3	F	317	ASN
3	F	323	GLU
3	F	382	THR
3	F	389	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	132	HIS
1	A	134	GLN
1	A	143	GLN
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	182	GLN
2	B	160	ASN
2	B	164	ASN
2	B	174	ASN
2	B	189	GLN
2	B	202	ASN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	333	ASN
2	B	351	ASN
2	B	364	ASN
2	B	408	HIS
2	B	439	ASN
3	C	103	HIS
3	C	117	ASN
3	C	123	ASN
3	C	146	HIS
3	C	163	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	329	GLN
1	D	143	GLN
2	E	164	ASN
2	E	174	ASN
2	E	189	GLN
2	E	202	ASN
2	E	253	GLN
2	E	256	GLN
2	E	296	ASN
2	E	301	GLN
2	E	333	ASN
2	E	351	ASN
2	E	364	ASN
2	E	393	GLN
2	E	408	HIS

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Mol	Chain	Res	Type
2	E	439	ASN
3	F	111	GLN
3	F	118	ASN
3	F	123	ASN
3	F	130	GLN
3	F	134	GLN
3	F	136	GLN
3	F	146	HIS
3	F	163	GLN
3	F	176	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN
4	N	2	HIS

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 8 ligands modelled in this entry, 6 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	$\# Z > 2$
5	NAG	E	470	-	14,14,15	0.51	0	17,19,21	0.69	0
5	NAG	B	470	-	14,14,15	0.53	0	17,19,21	0.80	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
5	NAG	E	470	-	-	2/6/23/26	0/1/1/1
5	NAG	B	470	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	470	NAG	C2-N2-C7	-2.17	119.99	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	470	NAG	O5-C5-C6-O6
5	E	470	NAG	O5-C5-C6-O6
5	E	470	NAG	C4-C5-C6-O6
5	B	470	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	470	NAG	3	0
5	B	470	NAG	6	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.