



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:54 AM UTC

PDB ID : 1FZB / pdb_00001fzb
Title : CRYSTAL STRUCTURE OF CROSSLINKED FRAGMENT D
Authors : Spraggon, G.; Everse, S.J.; Doolittle, R.F.
Deposited on : 1997-08-05
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

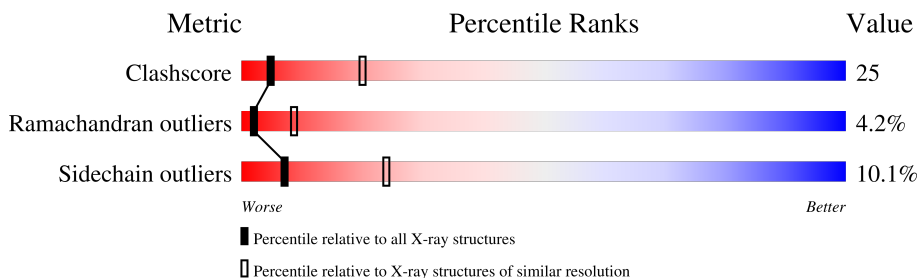
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	87	41% 39% 10% • 7%
1	D	87	41% 40% 9% • 7%
2	B	328	44% 41% 8% • 5%
2	E	328	46% 40% 8% • 5%
3	C	319	51% 36% 9% •
3	F	319	54% 35% 7% • •
4	G	4	50% 25% 25%
4	H	4	25% 25% 25% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11417 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	81	Total	C	N	O	S	0	0	0
			669	413	128	125	3			
1	D	81	Total	C	N	O	S	0	0	0
			669	413	128	125	3			

- Molecule 2 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	0	0	0
			2508	1566	442	478	22			
2	E	312	Total	C	N	O	S	0	0	0
			2508	1566	442	478	22			

- Molecule 3 is a protein called FIBRINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	309	Total	C	N	O	S	0	0	0
			2480	1574	415	478	13			
3	F	311	Total	C	N	O	S	0	0	0
			2493	1581	418	481	13			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called PEPTIDE LIGAND GPRG.

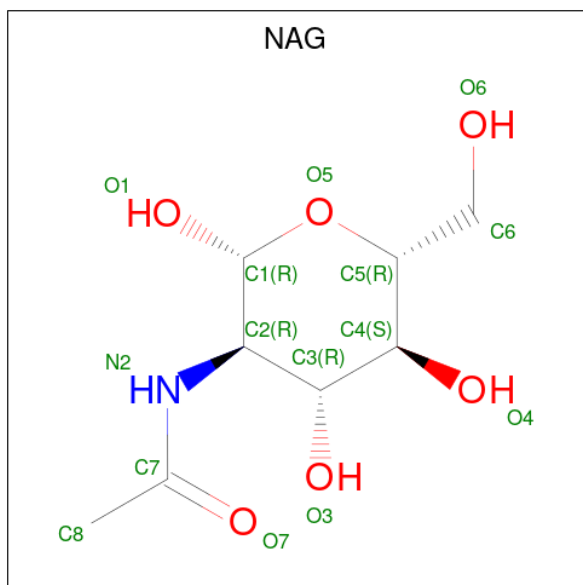
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			30	18	7	5			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			30	18	7	5			

- 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).

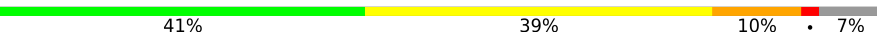
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		

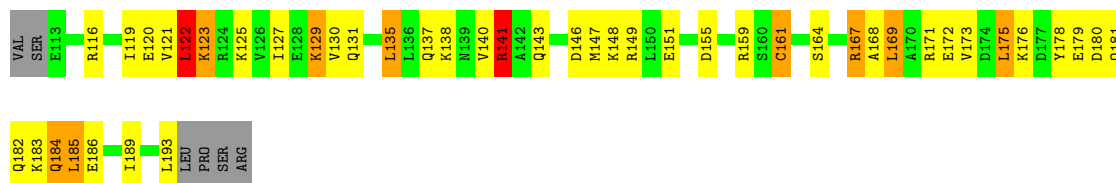
3 Residue-property plots

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

Note EDS was not executed.

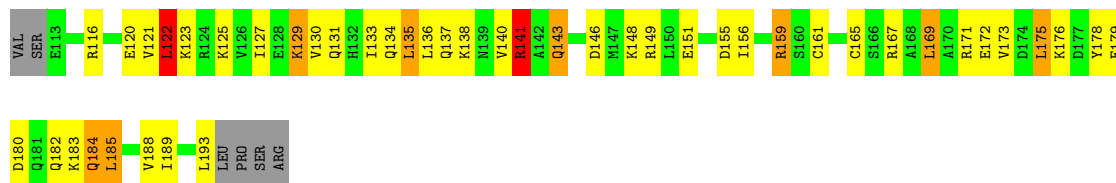
• Molecule 1: FIBRINOGEN

Chain A: 



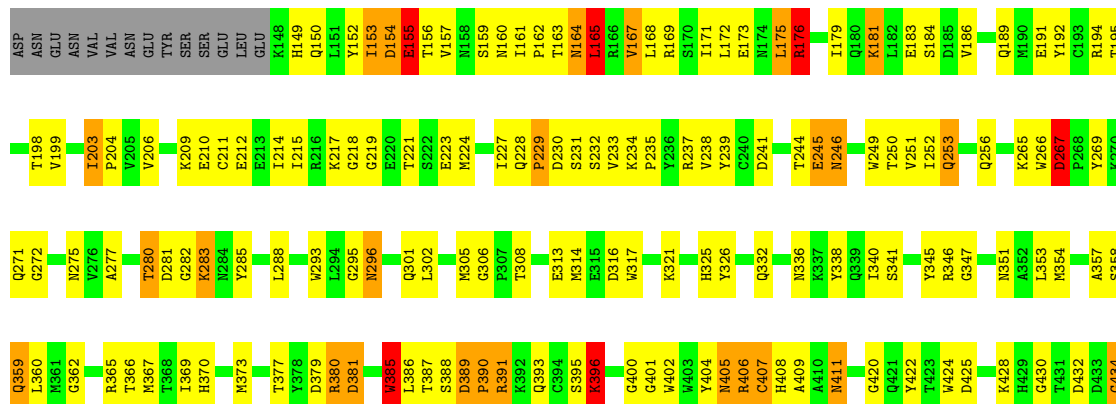
• Molecule 1: FIBRINOGEN

Chain D: 



• Molecule 2: FIBRINOGEN

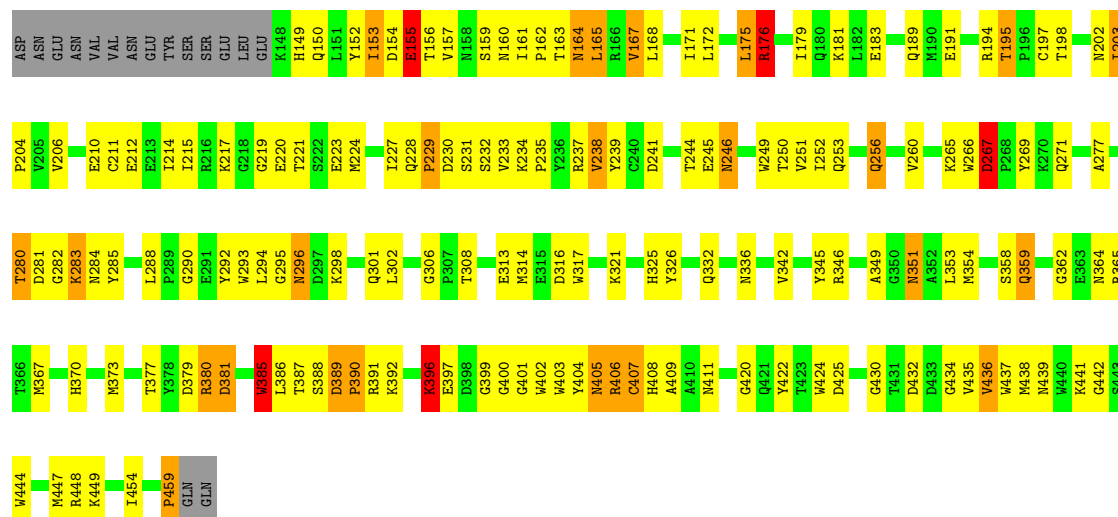
Chain B: 





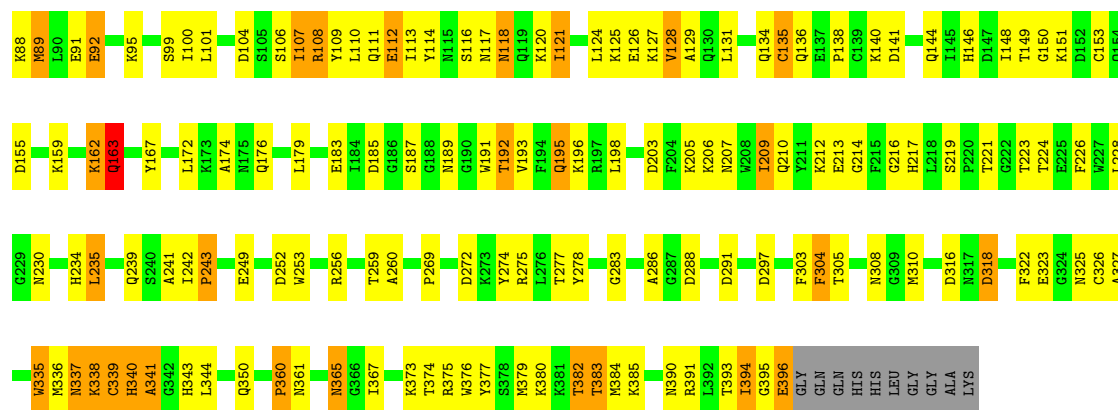
• Molecule 2: FIBRINOGEN

Chain E: 46% 40% 8% 5%



• Molecule 3: FIBRINOGEN

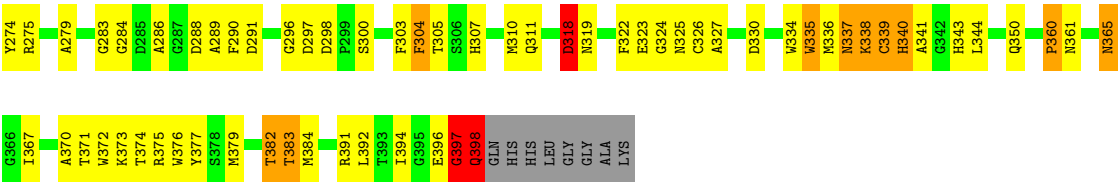
Chain C: 51% 36% 9% 1%



• Molecule 3: FIBRINOGEN

Chain F: 54% 35% 7% 1%

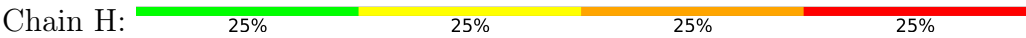




• Molecule 4: PEPTIDE LIGAND GPRG



• Molecule 4: PEPTIDE LIGAND GPRG



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.82Å 95.50Å 113.76Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	88.8 (30.00-2.90)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.241 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11417	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	0.72	1/670 (0.1%)	1.10	4/892 (0.4%)
1	D	0.84	1/670 (0.1%)	1.12	4/892 (0.4%)
2	B	0.79	2/2572 (0.1%)	1.22	39/3475 (1.1%)
2	E	0.82	3/2572 (0.1%)	1.21	34/3475 (1.0%)
3	C	0.72	2/2546 (0.1%)	1.17	19/3440 (0.6%)
3	F	0.70	4/2559 (0.2%)	1.09	20/3457 (0.6%)
4	G	0.60	0/31	0.86	0/40
4	H	0.96	0/31	1.04	0/40
All	All	0.76	13/11651 (0.1%)	1.16	120/15711 (0.8%)

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
2	E	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	459	PRO	C-O	17.55	1.58	1.23
2	B	175	LEU	C-N	-16.50	1.11	1.34
1	D	193	LEU	C-O	15.23	1.54	1.23
2	E	175	LEU	C-N	-15.13	1.13	1.34
2	B	459	PRO	C-O	15.02	1.53	1.23
3	C	396	GLU	C-O	-13.15	0.97	1.23
3	C	396	GLU	CA-C	11.65	1.77	1.52
1	A	193	LEU	C-O	10.70	1.45	1.23
3	F	397	GLY	C-N	-9.89	1.19	1.33
3	F	398	GLN	CA-CB	-8.10	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	398	GLN	CB-CG	-7.64	1.29	1.52
2	E	176	ARG	C-N	-5.61	1.25	1.33
3	F	398	GLN	CA-C	5.23	1.64	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	396	GLU	CA-C-O	-25.65	77.20	120.80
3	F	136	GLN	N-CA-C	-11.49	101.52	114.62
3	C	136	GLN	N-CA-C	-11.48	101.54	114.62
1	D	193	LEU	CA-C-O	-11.40	101.43	120.80
2	E	159	SER	N-CA-C	-10.33	102.84	114.62
2	B	405	ASN	N-CA-C	-10.32	100.31	108.78
2	B	159	SER	N-CA-C	-10.12	103.08	114.62
2	B	406	ARG	N-CA-C	-9.67	97.24	110.68
2	E	203	ILE	N-CA-C	9.24	118.96	108.05
2	E	405	ASN	N-CA-C	-9.02	101.39	108.78
2	E	459	PRO	CA-C-O	-8.96	92.13	119.00
1	A	193	LEU	CA-C-O	-8.84	105.77	120.80
2	B	203	ILE	N-CA-C	8.71	118.33	108.05
3	C	340	HIS	N-CA-C	8.56	120.93	108.86
2	E	406	ARG	N-CA-C	-8.47	98.91	110.68
3	F	340	HIS	N-CA-C	8.28	120.17	108.74
3	F	398	GLN	N-CA-C	8.26	134.13	111.00
2	B	436	VAL	N-CA-C	8.18	122.04	109.12
3	C	341	ALA	N-CA-C	-8.03	105.47	114.62
2	B	272	GLY	N-CA-C	-7.98	104.37	111.95
3	F	228	LEU	N-CA-C	7.91	119.98	111.36
2	E	155	GLU	N-CA-C	-7.86	103.48	113.23
3	C	112	GLU	N-CA-C	-7.85	102.03	111.69
2	E	409	ALA	N-CA-C	-7.76	104.71	114.56
2	E	296	ASN	N-CA-C	7.70	119.67	111.28
2	B	409	ALA	N-CA-C	-7.66	104.84	114.56
2	E	156	THR	N-CA-C	-7.46	103.44	112.54
2	B	459	PRO	CA-C-O	-7.46	96.64	119.00
3	F	242	ILE	CA-C-N	7.32	128.99	119.84
3	F	242	ILE	C-N-CA	7.32	128.99	119.84
2	E	436	VAL	N-CA-C	7.26	120.59	109.12
2	B	156	THR	N-CA-C	-7.21	103.15	112.23
3	C	193	VAL	N-CA-C	7.16	118.25	109.30
2	E	175	LEU	O-C-N	7.09	131.83	122.33
1	A	151	GLU	N-CA-C	-7.00	103.58	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	353	LEU	N-CA-C	6.98	118.68	111.14
2	B	353	LEU	N-CA-C	6.97	118.67	111.14
2	B	167	VAL	O-C-N	6.80	130.74	121.90
3	F	193	VAL	N-CA-C	6.71	117.69	109.30
3	F	112	GLU	N-CA-C	-6.70	103.44	111.69
2	E	285	TYR	N-CA-C	6.70	120.43	109.85
3	F	397	GLY	CA-C-N	-6.67	109.69	121.70
3	F	397	GLY	C-N-CA	-6.67	109.69	121.70
1	D	151	GLU	N-CA-C	-6.66	103.94	111.07
3	C	242	ILE	CA-C-N	6.66	128.16	119.84
3	C	242	ILE	C-N-CA	6.66	128.16	119.84
3	C	338	LYS	N-CA-C	-6.65	102.76	111.74
2	E	400	GLY	N-CA-C	6.64	121.04	112.54
2	B	155	GLU	N-CA-C	-6.64	105.18	113.28
3	F	108	ARG	N-CA-C	-6.60	104.17	111.82
2	E	408	HIS	N-CA-C	6.57	119.39	109.41
2	B	183	GLU	N-CA-C	-6.54	104.07	111.07
3	F	92	GLU	N-CA-C	-6.52	103.68	111.69
3	F	268	GLY	CA-C-N	6.45	126.91	120.52
3	F	268	GLY	C-N-CA	6.45	126.91	120.52
2	B	408	HIS	N-CA-C	6.38	118.64	109.14
3	F	111	GLN	N-CA-C	-6.37	104.97	114.64
3	C	111	GLN	N-CA-C	-6.35	104.99	114.64
2	B	400	GLY	N-CA-C	6.31	120.28	112.14
3	C	92	GLU	N-CA-C	-6.29	103.95	111.69
3	C	393	THR	N-CA-C	-6.28	100.20	109.62
2	E	195	THR	CA-C-N	6.19	126.65	120.52
2	E	195	THR	C-N-CA	6.19	126.65	120.52
2	E	434	GLY	N-CA-C	6.19	127.84	113.18
2	B	385	TRP	N-CA-C	6.10	117.41	108.14
2	E	385	TRP	N-CA-C	6.07	117.37	108.14
2	E	401	GLY	N-CA-C	-6.05	100.92	111.62
2	E	167	VAL	O-C-N	6.01	129.71	121.90
3	C	107	ILE	N-CA-C	-6.00	106.88	111.62
3	C	108	ARG	N-CA-C	-5.99	104.87	111.82
3	C	228	LEU	N-CA-C	5.98	118.76	111.82
3	F	338	LYS	N-CA-C	-5.98	103.66	111.74
2	B	296	ASN	N-CA-C	5.96	118.54	111.33
3	C	163	GLN	N-CA-C	5.91	119.04	109.40
2	B	381	ASP	N-CA-C	5.91	118.58	109.07
2	B	411	ASN	CA-C-N	5.83	125.45	119.56
2	B	411	ASN	C-N-CA	5.83	125.45	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	ASP	N-CA-C	-5.80	106.54	113.21
1	A	141	ARG	N-CA-C	-5.78	104.17	111.11
2	B	396	LYS	N-CA-C	5.78	116.04	108.07
3	C	337	ASN	N-CA-C	-5.77	98.50	110.80
2	B	285	TYR	N-CA-C	5.71	118.87	109.85
3	F	125	LYS	N-CA-C	-5.71	104.26	111.11
2	B	245	GLU	N-CA-C	-5.69	101.75	109.54
1	D	141	ARG	N-CA-C	-5.67	104.30	111.11
3	F	337	ASN	N-CA-C	-5.67	98.72	110.80
2	B	357	ALA	N-CA-C	5.66	117.30	109.15
2	B	194	ARG	N-CA-C	-5.62	105.15	111.28
2	B	175	LEU	O-C-N	5.59	129.82	122.33
2	E	396	LYS	N-CA-C	5.58	115.77	108.07
2	B	434	GLY	N-CA-C	5.53	126.29	113.18
2	E	349	ALA	N-CA-C	5.48	118.18	111.82
2	B	203	ILE	CA-C-N	5.46	125.41	119.78
2	B	203	ILE	C-N-CA	5.46	125.41	119.78
2	E	194	ARG	N-CA-C	-5.45	105.34	111.28
1	D	159	ARG	N-CA-C	-5.43	105.37	111.28
2	E	183	GLU	N-CA-C	-5.42	105.27	111.07
2	E	176	ARG	CA-C-N	5.38	129.77	120.58
2	E	176	ARG	C-N-CA	5.38	129.77	120.58
2	B	401	GLY	N-CA-C	-5.37	103.22	111.64
2	E	203	ILE	CA-C-N	5.36	125.30	119.78
2	E	203	ILE	C-N-CA	5.36	125.30	119.78
2	E	267	ASP	N-CA-C	5.33	120.17	113.25
2	E	381	ASP	N-CA-C	5.33	117.64	109.07
3	F	163	GLN	N-CA-C	5.27	118.15	109.72
2	E	290	GLY	N-CA-C	-5.26	104.54	112.60
3	C	125	LYS	N-CA-C	-5.19	105.62	111.28
2	B	165	LEU	N-CA-C	-5.18	107.98	114.56
2	B	347	GLY	N-CA-C	5.18	118.14	110.63
2	B	267	ASP	N-CA-C	5.17	119.97	113.25
2	B	176	ARG	CA-C-N	5.17	129.42	120.58
2	B	176	ARG	C-N-CA	5.17	129.42	120.58
1	A	123	LYS	N-CA-C	5.11	116.66	111.14
3	C	235	LEU	N-CA-C	5.08	117.47	111.33
2	E	220	GLU	N-CA-C	5.05	120.06	112.94
3	F	398	GLN	CA-C-O	-5.03	112.26	120.80
2	B	305	MET	N-CA-C	-5.02	107.16	113.28
2	B	167	VAL	CA-C-N	-5.01	112.56	120.63
2	B	167	VAL	C-N-CA	-5.01	112.56	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	E	260	VAL	N-CA-C	5.00	115.32	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	292	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	669	0	712	44	0
1	D	669	0	712	54	0
2	B	2508	0	2371	147	0
2	E	2508	0	2372	138	0
3	C	2480	0	2333	133	0
3	F	2493	0	2344	109	0
4	G	30	0	32	0	0
4	H	30	0	32	7	0
5	B	14	0	13	1	0
5	E	14	0	13	6	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
All	All	11417	0	10934	568	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 (568) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:GLU:C	3:C:396:GLU:CA	1.77	1.57
3:C:396:GLU:CA	3:C:396:GLU:O	1.82	1.22
2:E:389:ASP:HB3	2:E:390:PRO:HD2	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:ASP:HB3	2:B:390:PRO:HD2	1.37	1.02
3:C:209:ILE:H	3:C:209:ILE:HD12	1.25	0.98
2:E:380:ARG:HB2	2:E:380:ARG:HH11	1.28	0.98
2:B:380:ARG:HH11	2:B:380:ARG:HB2	1.31	0.96
3:F:209:ILE:HD12	3:F:209:ILE:H	1.29	0.96
2:E:351:ASN:HD21	2:E:354:MET:H	1.09	0.95
2:B:234:LYS:HD3	2:B:235:PRO:HD2	1.46	0.95
2:E:234:LYS:HD3	2:E:235:PRO:HD2	1.47	0.94
3:F:153:CYS:SG	3:F:192:THR:HB	2.07	0.94
1:D:176:LYS:H	1:D:176:LYS:HD2	1.32	0.94
2:E:351:ASN:ND2	2:E:354:MET:H	1.66	0.93
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.53	0.91
1:A:176:LYS:H	1:A:176:LYS:HD2	1.33	0.91
3:F:310:MET:SD	3:F:337:ASN:HB2	2.11	0.90
3:F:322:PHE:HA	3:F:338:LYS:HD2	1.54	0.90
1:D:149:ARG:HH21	2:E:425:ASP:HA	1.35	0.89
3:F:397:GLY:O	3:F:398:GLN:HB2	1.71	0.89
3:C:322:PHE:HB2	3:C:338:LYS:HA	1.52	0.88
2:B:367:MET:HB3	2:B:406:ARG:HB3	1.54	0.88
3:F:322:PHE:HB2	3:F:338:LYS:HA	1.57	0.87
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.55	0.87
2:B:351:ASN:ND2	2:B:354:MET:H	1.73	0.85
2:E:367:MET:HB3	2:E:406:ARG:HB3	1.56	0.85
3:C:322:PHE:HA	3:C:338:LYS:HD2	1.57	0.85
2:B:351:ASN:HD21	2:B:354:MET:H	1.22	0.84
5:E:1:NAG:H3	5:E:1:NAG:O7	1.77	0.83
2:E:359:GLN:H	2:E:359:GLN:HE21	1.26	0.83
1:D:169:LEU:H	2:E:189:GLN:HE22	1.26	0.83
3:C:310:MET:SD	3:C:337:ASN:HB2	2.19	0.82
2:B:198:THR:HG22	3:C:140:LYS:HB2	1.62	0.82
2:B:359:GLN:H	2:B:359:GLN:HE21	1.28	0.81
2:E:364:ASN:HD21	5:E:1:NAG:H5	1.46	0.79
3:F:151:LYS:HB3	3:F:239:GLN:HE22	1.47	0.79
1:A:169:LEU:H	2:B:189:GLN:HE22	1.29	0.79
3:C:151:LYS:HB3	3:C:239:GLN:HE22	1.46	0.78
3:C:209:ILE:H	3:C:209:ILE:CD1	1.96	0.78
3:F:397:GLY:O	3:F:398:GLN:CB	2.27	0.78
3:C:153:CYS:SG	3:C:192:THR:HB	2.24	0.78
1:D:176:LYS:HD2	1:D:176:LYS:N	1.98	0.78
1:A:176:LYS:HD2	1:A:176:LYS:N	1.99	0.77
2:B:359:GLN:H	2:B:359:GLN:NE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LYS:HD3	3:F:100:ILE:HG12	1.64	0.77
1:D:140:VAL:HG12	2:E:172:LEU:HD13	1.66	0.77
1:D:127:ILE:O	1:D:131:GLN:HG2	1.84	0.77
1:D:123:LYS:NZ	2:E:154:ASP:HB2	2.00	0.77
3:F:100:ILE:HG13	3:F:101:LEU:HD22	1.68	0.76
1:D:141:ARG:HA	1:D:141:ARG:HH11	1.50	0.76
1:A:169:LEU:H	2:B:189:GLN:NE2	1.84	0.76
2:E:385:TRP:HE3	2:E:385:TRP:H	1.33	0.76
2:E:351:ASN:C	2:E:351:ASN:HD22	1.93	0.75
2:E:359:GLN:H	2:E:359:GLN:NE2	1.85	0.75
2:E:459:PRO:HG2	2:E:459:PRO:O	1.87	0.75
3:C:100:ILE:HG13	3:C:101:LEU:HD22	1.68	0.75
3:F:326:CYS:HB2	3:F:336:MET:HG3	1.69	0.74
3:C:326:CYS:HB2	3:C:336:MET:HG3	1.69	0.74
2:E:380:ARG:HH11	2:E:380:ARG:CB	2.00	0.74
1:A:141:ARG:HH11	1:A:141:ARG:HA	1.53	0.73
2:B:176:ARG:HG2	3:C:117:ASN:HD21	1.51	0.73
1:D:188:VAL:HG21	2:E:167:VAL:HG21	1.71	0.73
2:B:389:ASP:HB3	2:B:390:PRO:CD	2.17	0.73
2:B:441:LYS:HB2	2:B:447:MET:HE1	1.70	0.72
1:D:133:ILE:HD12	2:E:165:LEU:HD11	1.70	0.72
2:B:396:LYS:HE3	2:B:396:LYS:HA	1.69	0.72
1:A:127:ILE:O	1:A:131:GLN:HG2	1.90	0.72
1:D:123:LYS:HZ2	2:E:154:ASP:HB2	1.53	0.72
2:E:459:PRO:O	2:E:459:PRO:CG	2.38	0.72
2:E:441:LYS:HB2	2:E:447:MET:HE1	1.72	0.72
1:D:140:VAL:HG23	1:D:185:LEU:HD11	1.73	0.71
1:D:135:LEU:HA	1:D:138:LYS:HE2	1.71	0.71
2:B:351:ASN:HD22	2:B:351:ASN:C	1.98	0.71
2:E:266:TRP:HA	2:E:377:THR:HG21	1.73	0.71
3:F:195:GLN:HG2	3:F:384:MET:SD	2.30	0.71
2:B:212:GLU:O	2:B:215:ILE:HG22	1.91	0.70
2:E:211:CYS:SG	2:E:250:THR:HA	2.30	0.70
2:B:385:TRP:HE3	2:B:385:TRP:H	1.39	0.70
2:E:405:ASN:C	2:E:407:CYS:H	1.99	0.70
3:F:335:TRP:H	3:F:335:TRP:CD1	2.08	0.70
1:A:135:LEU:HA	1:A:138:LYS:HE2	1.72	0.70
2:B:176:ARG:CG	3:C:117:ASN:HD21	2.04	0.70
2:B:380:ARG:HH11	2:B:380:ARG:CB	2.03	0.70
2:E:389:ASP:HB3	2:E:390:PRO:CD	2.19	0.69
2:B:266:TRP:HA	2:B:377:THR:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:ASN:C	2:B:407:CYS:H	1.98	0.69
2:E:396:LYS:HE3	2:E:396:LYS:HA	1.73	0.69
3:F:326:CYS:HB3	3:F:336:MET:HE3	1.75	0.69
1:A:140:VAL:HG23	1:A:185:LEU:HD11	1.75	0.69
1:A:168:ALA:HA	2:B:189:GLN:HE22	1.56	0.69
2:B:269:TYR:O	2:B:295:GLY:HA2	1.93	0.69
2:B:157:VAL:HA	2:B:160:ASN:HB3	1.74	0.69
3:F:209:ILE:H	3:F:209:ILE:CD1	2.02	0.69
2:B:171:ILE:HG13	2:B:172:LEU:N	2.08	0.69
3:C:195:GLN:HG2	3:C:384:MET:SD	2.33	0.69
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.74	0.69
2:E:212:GLU:O	2:E:215:ILE:HG22	1.92	0.68
1:A:180:ASP:O	1:A:184:GLN:HG2	1.94	0.68
3:C:396:GLU:O	3:C:396:GLU:N	2.26	0.68
3:C:162:LYS:H	3:C:162:LYS:HD3	1.58	0.68
1:A:149:ARG:HH21	2:B:425:ASP:HA	1.58	0.68
1:D:135:LEU:O	1:D:138:LYS:HG2	1.94	0.68
2:E:210:GLU:OE1	2:E:212:GLU:HB3	1.93	0.68
1:D:149:ARG:NH2	2:E:425:ASP:HA	2.08	0.67
2:E:346:ARG:HG3	2:E:346:ARG:HH11	1.59	0.67
2:E:386:LEU:HD23	2:E:386:LEU:H	1.58	0.66
3:C:221:THR:O	3:C:223:THR:HG23	1.95	0.66
3:F:305:THR:HB	3:F:341:ALA:HB2	1.77	0.66
2:B:210:GLU:OE1	2:B:212:GLU:HB3	1.95	0.66
1:A:135:LEU:O	1:A:138:LYS:HG2	1.96	0.66
2:B:164:ASN:C	2:B:164:ASN:HD22	2.04	0.66
3:C:335:TRP:CD1	3:C:335:TRP:H	2.12	0.66
3:C:395:GLY:O	3:C:396:GLU:HG3	1.96	0.66
2:B:211:CYS:SG	2:B:250:THR:HA	2.36	0.65
1:D:169:LEU:H	2:E:189:GLN:NE2	1.94	0.65
3:C:305:THR:HB	3:C:341:ALA:HB2	1.78	0.64
1:D:143:GLN:HG2	2:E:175:LEU:CD1	2.27	0.64
3:C:326:CYS:SG	3:C:339:CYS:N	2.71	0.64
2:E:164:ASN:C	2:E:164:ASN:HD22	2.06	0.64
2:E:385:TRP:HE3	2:E:385:TRP:N	1.96	0.64
2:E:171:ILE:HG13	2:E:172:LEU:N	2.13	0.63
3:F:339:CYS:HB2	4:H:1:GLY:O	1.98	0.63
1:D:180:ASP:O	1:D:184:GLN:HG2	1.97	0.63
3:F:95:LYS:HZ2	3:F:96:TYR:HE1	1.47	0.63
3:F:162:LYS:HD3	3:F:162:LYS:H	1.63	0.63
2:E:230:ASP:O	2:E:233:VAL:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:176:ARG:HG3	2:E:176:ARG:HH11	1.64	0.62
2:B:172:LEU:HG	3:C:113:ILE:CG2	2.28	0.62
2:B:386:LEU:H	2:B:386:LEU:HD23	1.64	0.62
2:B:346:ARG:HG3	2:B:346:ARG:HH11	1.65	0.62
2:B:169:ARG:HG3	3:C:110:LEU:HD21	1.82	0.62
4:H:1:GLY:H3	4:H:3:ARG:HH21	1.47	0.62
2:E:176:ARG:HG3	2:E:176:ARG:NH1	2.16	0.61
5:E:1:NAG:O7	5:E:1:NAG:C3	2.47	0.61
2:B:229:PRO:HD2	2:B:233:VAL:HG21	1.82	0.61
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.82	0.61
1:D:123:LYS:HE3	2:E:152:TYR:HB3	1.82	0.61
2:E:214:ILE:HD11	2:E:227:ILE:HG22	1.83	0.61
2:E:364:ASN:ND2	5:E:1:NAG:H5	2.13	0.61
3:C:104:ASP:HA	3:C:107:ILE:HD13	1.82	0.61
2:E:351:ASN:HD21	2:E:354:MET:N	1.92	0.61
2:B:172:LEU:O	3:C:113:ILE:HG21	2.00	0.60
1:D:148:LYS:HE3	1:D:175:LEU:HB3	1.83	0.60
3:F:172:LEU:HG	3:F:239:GLN:HE21	1.66	0.60
1:A:137:GLN:O	1:A:141:ARG:HB2	2.02	0.60
2:B:459:PRO:O	2:B:459:PRO:HG2	2.01	0.60
2:E:157:VAL:HA	2:E:160:ASN:HB3	1.82	0.60
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.02	0.60
2:E:326:TYR:CE2	2:E:345:TYR:HB2	2.37	0.60
1:A:148:LYS:HE3	1:A:175:LEU:HB3	1.84	0.59
2:B:405:ASN:C	2:B:407:CYS:N	2.59	0.59
3:C:209:ILE:HD12	3:C:209:ILE:N	2.07	0.59
3:C:396:GLU:C	3:C:396:GLU:HA	2.13	0.59
2:B:230:ASP:HB3	2:B:233:VAL:HG13	1.84	0.59
1:D:169:LEU:HD12	1:D:171:ARG:CG	2.32	0.59
2:B:167:VAL:HG23	2:B:168:LEU:N	2.18	0.59
3:C:365:ASN:HD22	3:C:365:ASN:H	1.49	0.59
3:F:195:GLN:HG2	3:F:384:MET:CG	2.33	0.59
3:F:88:LYS:HB3	3:F:92:GLU:HB2	1.85	0.58
2:E:153:ILE:C	2:E:155:GLU:H	2.12	0.58
3:C:196:LYS:HE3	3:C:383:THR:HB	1.85	0.58
1:A:169:LEU:N	2:B:189:GLN:HE22	2.01	0.58
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.38	0.58
1:D:116:ARG:CZ	3:F:89:MET:HA	2.33	0.58
2:E:438:MET:HA	2:E:442:GLY:HA2	1.86	0.58
2:B:385:TRP:HE3	2:B:385:TRP:N	2.00	0.58
1:D:130:VAL:HG13	1:D:131:GLN:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:HG2	2:E:175:LEU:HD12	1.86	0.57
1:D:184:GLN:HE21	1:D:184:GLN:N	2.02	0.57
1:A:184:GLN:HE21	1:A:184:GLN:N	2.03	0.57
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.04	0.57
3:C:151:LYS:HB3	3:C:239:GLN:NE2	2.18	0.57
2:B:267:ASP:O	2:B:271:GLN:HG2	2.03	0.57
3:F:288:ASP:CG	3:F:291:ASP:HB2	2.30	0.57
3:C:395:GLY:O	3:C:396:GLU:CG	2.53	0.57
2:B:153:ILE:C	2:B:155:GLU:H	2.13	0.57
2:B:459:PRO:O	2:B:459:PRO:CG	2.53	0.57
3:C:326:CYS:HB3	3:C:336:MET:HE3	1.86	0.56
2:E:385:TRP:N	2:E:385:TRP:CE3	2.73	0.56
2:B:161:ILE:HA	2:B:164:ASN:OD1	2.06	0.56
2:B:230:ASP:O	2:B:233:VAL:HG22	2.05	0.56
3:C:277:THR:HG21	3:F:303:PHE:CD2	2.41	0.56
2:E:167:VAL:HG23	2:E:168:LEU:N	2.20	0.56
1:A:179:GLU:HA	1:A:182:GLN:NE2	2.21	0.56
2:B:175:LEU:O	2:B:179:ILE:HG13	2.06	0.56
2:B:206:VAL:HG22	3:C:214:GLY:O	2.06	0.56
1:D:169:LEU:HD12	1:D:171:ARG:HG3	1.86	0.56
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.87	0.56
2:E:405:ASN:C	2:E:407:CYS:N	2.62	0.56
3:F:151:LYS:HB3	3:F:239:GLN:NE2	2.20	0.55
1:A:178:TYR:O	1:A:182:GLN:HG3	2.05	0.55
3:F:264:MET:HB2	3:F:279:ALA:HB2	1.88	0.55
2:B:154:ASP:O	2:B:157:VAL:HB	2.06	0.55
2:B:424:TRP:O	2:B:430:GLY:HA2	2.07	0.55
2:E:267:ASP:O	2:E:271:GLN:HG2	2.06	0.55
1:A:169:LEU:HD12	1:A:171:ARG:CG	2.36	0.55
3:F:149:THR:HG22	3:F:150:GLY:N	2.21	0.55
3:C:395:GLY:C	3:C:396:GLU:HG3	2.31	0.55
1:D:179:GLU:HA	1:D:182:GLN:HE21	1.72	0.55
3:C:274:TYR:O	3:C:335:TRP:HZ3	1.89	0.55
2:B:179:ILE:HD13	3:C:120:LYS:HB2	1.89	0.55
2:E:154:ASP:O	2:E:157:VAL:HB	2.07	0.55
1:A:169:LEU:HD12	1:A:171:ARG:HG3	1.89	0.55
2:B:199:VAL:O	3:C:141:ASP:HA	2.06	0.55
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.07	0.55
2:E:245:GLU:C	2:E:246:ASN:HD22	2.15	0.54
3:F:221:THR:O	3:F:223:THR:HG23	2.07	0.54
2:B:186:VAL:HG11	3:C:127:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:326:TYR:CE2	2:B:345:TYR:HB2	2.42	0.54
2:B:373:MET:HE2	2:B:405:ASN:HA	1.89	0.54
3:C:149:THR:HG22	3:C:150:GLY:N	2.23	0.54
3:C:390:ASN:O	3:C:394:ILE:HG23	2.08	0.54
2:E:229:PRO:HD2	2:E:233:VAL:HG21	1.89	0.54
1:A:122:LEU:HA	1:A:125:LYS:HD2	1.89	0.54
2:B:157:VAL:HG13	2:B:161:ILE:HG12	1.89	0.54
1:D:178:TYR:O	1:D:182:GLN:HG3	2.08	0.54
3:F:365:ASN:HD22	3:F:365:ASN:H	1.54	0.54
1:A:149:ARG:NH2	2:B:425:ASP:HA	2.21	0.54
2:E:228:GLN:HB2	2:E:235:PRO:HB3	1.89	0.54
2:E:230:ASP:HB3	2:E:233:VAL:HG13	1.89	0.53
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.90	0.53
3:C:344:LEU:HB3	3:C:382:THR:HG21	1.89	0.53
2:E:411:ASN:O	2:E:435:VAL:HA	2.08	0.53
1:D:137:GLN:O	1:D:141:ARG:HB2	2.09	0.53
1:D:165:CYS:O	2:E:197:CYS:HB3	2.08	0.53
1:A:125:LYS:O	1:A:129:LYS:HG2	2.09	0.53
2:B:189:GLN:HG3	3:C:131:LEU:HD11	1.91	0.53
3:C:196:LYS:CE	3:C:383:THR:HB	2.39	0.53
3:F:275:ARG:HA	3:F:311:GLN:HA	1.89	0.53
2:B:223:GLU:HA	2:B:239:TYR:CE1	2.44	0.53
3:C:365:ASN:HD22	3:C:365:ASN:N	2.05	0.53
1:D:125:LYS:O	1:D:129:LYS:HG2	2.09	0.53
2:E:239:TYR:HD2	2:E:251:VAL:HG21	1.74	0.53
2:E:294:LEU:O	2:E:298:LYS:HD2	2.08	0.53
3:C:195:GLN:HG2	3:C:384:MET:CG	2.39	0.53
1:D:159:ARG:NH1	1:D:159:ARG:HB3	2.24	0.53
1:D:179:GLU:HA	1:D:182:GLN:NE2	2.23	0.53
1:A:123:LYS:HE3	2:B:152:TYR:CD2	2.43	0.52
1:A:155:ASP:HB2	1:A:171:ARG:HH12	1.73	0.52
2:E:438:MET:HA	2:E:442:GLY:CA	2.39	0.52
1:A:179:GLU:HA	1:A:182:GLN:HE21	1.74	0.52
3:F:123:ASN:O	3:F:126:GLU:HB2	2.09	0.52
3:F:307:HIS:HD2	3:F:335:TRP:O	1.91	0.52
2:B:234:LYS:HD3	2:B:235:PRO:CD	2.31	0.52
2:E:167:VAL:HG23	2:E:168:LEU:H	1.73	0.52
2:B:385:TRP:N	2:B:385:TRP:CE3	2.78	0.52
3:C:108:ARG:HD3	3:C:108:ARG:H	1.74	0.52
3:F:89:MET:C	3:F:91:GLU:H	2.16	0.52
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:380:ARG:HB2	2:E:380:ARG:NH1	2.11	0.51
1:A:149:ARG:NH2	2:B:424:TRP:O	2.41	0.51
3:C:288:ASP:CG	3:C:291:ASP:HB2	2.35	0.51
1:A:181:GLN:HE21	2:B:171:ILE:HG22	1.74	0.51
2:B:167:VAL:HG23	2:B:168:LEU:H	1.74	0.51
2:B:314:MET:HA	2:B:449:LYS:O	2.10	0.51
3:C:88:LYS:HB3	3:C:92:GLU:HB2	1.93	0.51
3:F:116:SER:O	3:F:120:LYS:HG2	2.09	0.51
2:E:314:MET:O	2:E:321:LYS:HG3	2.10	0.51
3:F:219:SER:OG	3:F:224:THR:HG22	2.11	0.51
3:C:304:PHE:O	3:C:337:ASN:O	2.28	0.51
2:B:173:GLU:HG2	3:C:113:ILE:CD1	2.41	0.51
2:B:317:TRP:CD1	2:B:420:GLY:HA3	2.46	0.51
3:C:114:TYR:O	3:C:118:ASN:HB2	2.11	0.51
2:B:157:VAL:HA	2:B:160:ASN:CB	2.41	0.50
3:C:234:HIS:CD2	3:C:269:PRO:HA	2.45	0.50
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.75	0.50
2:E:245:GLU:O	2:E:246:ASN:HB2	2.11	0.50
3:F:104:ASP:HA	3:F:107:ILE:HD13	1.93	0.50
3:F:264:MET:HB2	3:F:279:ALA:CB	2.41	0.50
3:F:322:PHE:CD1	3:F:323:GLU:N	2.79	0.50
1:A:120:GLU:C	1:A:122:LEU:H	2.20	0.50
3:C:340:HIS:ND1	3:C:343:HIS:HB2	2.26	0.50
1:D:120:GLU:C	1:D:122:LEU:H	2.19	0.50
2:B:245:GLU:C	2:B:246:ASN:HD22	2.19	0.50
3:C:89:MET:C	3:C:91:GLU:H	2.19	0.50
2:E:157:VAL:HG13	2:E:161:ILE:HG12	1.94	0.50
2:E:234:LYS:HD3	2:E:235:PRO:CD	2.32	0.50
3:F:365:ASN:HD22	3:F:365:ASN:N	2.08	0.50
3:C:172:LEU:HG	3:C:239:GLN:HE21	1.76	0.50
2:E:175:LEU:O	2:E:179:ILE:HG13	2.12	0.50
2:E:314:MET:HA	2:E:449:LYS:O	2.12	0.50
2:B:169:ARG:HE	3:C:109:TYR:HE2	1.59	0.50
3:F:360:PRO:HG2	3:F:361:ASN:H	1.76	0.50
3:C:259:THR:O	3:C:286:ALA:HB3	2.12	0.50
3:F:196:LYS:CE	3:F:383:THR:HB	2.42	0.50
1:D:143:GLN:HG2	2:E:175:LEU:HD13	1.92	0.50
2:E:161:ILE:HA	2:E:164:ASN:OD1	2.12	0.50
2:B:351:ASN:ND2	2:B:351:ASN:C	2.68	0.49
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.94	0.49
2:B:438:MET:HA	2:B:442:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.77	0.49
1:D:122:LEU:HA	1:D:125:LYS:HD2	1.94	0.49
1:A:161:CYS:HA	3:C:135:CYS:CB	2.42	0.49
3:F:196:LYS:HE3	3:F:383:THR:HB	1.94	0.49
1:A:130:VAL:HG13	1:A:131:GLN:OE1	2.12	0.49
2:B:438:MET:HA	2:B:442:GLY:CA	2.42	0.49
3:C:167:TYR:O	3:C:179:LEU:HD12	2.12	0.49
2:B:230:ASP:C	2:B:232:SER:H	2.21	0.49
2:B:314:MET:O	2:B:321:LYS:HG3	2.13	0.49
2:B:402:TRP:HB3	2:B:404:TYR:CE2	2.48	0.49
3:F:326:CYS:SG	3:F:339:CYS:N	2.86	0.49
2:E:277:ALA:HA	2:E:288:LEU:O	2.12	0.49
3:F:304:PHE:O	3:F:337:ASN:O	2.31	0.49
2:B:164:ASN:C	2:B:164:ASN:ND2	2.71	0.48
3:C:325:ASN:C	3:C:325:ASN:HD22	2.20	0.48
3:C:116:SER:O	3:C:120:LYS:HG2	2.13	0.48
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.77	0.48
3:C:343:HIS:O	3:C:367:ILE:HA	2.12	0.48
2:E:198:THR:HG22	3:F:140:LYS:HB2	1.95	0.48
3:F:374:THR:HG23	3:F:376:TRP:H	1.77	0.48
2:B:358:SER:HA	2:B:365:ARG:CZ	2.43	0.48
3:C:275:ARG:NH1	3:F:300:SER:HB3	2.28	0.48
1:D:135:LEU:HD22	1:D:138:LYS:NZ	2.28	0.48
2:E:358:SER:HA	2:E:365:ARG:CZ	2.43	0.48
1:D:155:ASP:HB2	1:D:171:ARG:HH12	1.78	0.48
2:E:373:MET:HE2	2:E:405:ASN:HA	1.95	0.48
3:C:108:ARG:O	3:C:112:GLU:HG3	2.13	0.48
3:C:219:SER:OG	3:C:224:THR:HG22	2.13	0.48
2:E:230:ASP:C	2:E:232:SER:H	2.22	0.48
3:F:274:TYR:O	3:F:335:TRP:HZ3	1.97	0.48
2:B:275:ASN:OD1	3:C:138:PRO:HB2	2.13	0.48
3:C:239:GLN:C	3:C:241:ALA:H	2.20	0.48
2:B:346:ARG:HG3	2:B:346:ARG:NH1	2.28	0.48
3:C:146:HIS:HB2	3:C:167:TYR:CD2	2.49	0.48
3:C:335:TRP:CD1	3:C:335:TRP:N	2.78	0.48
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.31	0.48
3:C:322:PHE:CD1	3:C:323:GLU:N	2.81	0.48
3:C:322:PHE:CB	3:C:338:LYS:HA	2.35	0.48
2:E:223:GLU:HA	2:E:239:TYR:CE1	2.49	0.48
2:E:325:HIS:O	2:E:345:TYR:HA	2.14	0.48
2:E:373:MET:HE2	2:E:404:TYR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:307:HIS:CE1	3:F:341:ALA:H	2.31	0.48
2:B:209:LYS:HA	2:B:228:GLN:O	2.14	0.47
2:E:269:TYR:O	2:E:295:GLY:HA2	2.14	0.47
3:F:114:TYR:O	3:F:118:ASN:HB2	2.14	0.47
1:A:180:ASP:HA	1:A:183:LYS:HD2	1.97	0.47
2:B:325:HIS:O	2:B:345:TYR:HA	2.15	0.47
3:C:252:ASP:OD2	3:C:256:ARG:HB2	2.14	0.47
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.96	0.47
2:B:179:ILE:HG21	3:C:120:LYS:HB3	1.96	0.47
2:B:245:GLU:O	2:B:246:ASN:HB2	2.15	0.47
2:E:172:LEU:HD23	3:F:110:LEU:HD22	1.95	0.47
2:E:206:VAL:HG22	3:F:214:GLY:O	2.15	0.47
2:E:306:GLY:O	2:E:308:THR:HG23	2.13	0.47
1:A:135:LEU:HD22	1:A:138:LYS:NZ	2.30	0.47
2:E:424:TRP:O	2:E:430:GLY:HA2	2.14	0.47
2:E:439:ASN:HD22	2:E:439:ASN:H	1.63	0.47
3:F:195:GLN:HG2	3:F:384:MET:HG3	1.96	0.47
3:F:108:ARG:H	3:F:108:ARG:HD3	1.79	0.47
2:E:163:THR:C	2:E:165:LEU:H	2.23	0.47
4:H:2:PRO:O	4:H:3:ARG:HB2	2.15	0.47
3:C:303:PHE:C	3:C:305:THR:H	2.22	0.47
2:E:150:GLN:HB3	2:E:152:TYR:CE1	2.50	0.47
2:E:164:ASN:C	2:E:164:ASN:ND2	2.71	0.47
3:C:212:LYS:HG3	3:C:274:TYR:OH	2.15	0.46
1:D:135:LEU:HD13	1:D:138:LYS:HE2	1.97	0.46
2:E:317:TRP:CD1	2:E:420:GLY:HA3	2.50	0.46
1:D:180:ASP:HA	1:D:183:LYS:HD2	1.97	0.46
3:F:189:ASN:CG	3:F:391:ARG:HH21	2.23	0.46
2:B:150:GLN:HB3	2:B:152:TYR:CE1	2.50	0.46
2:B:172:LEU:HG	3:C:113:ILE:HG21	1.96	0.46
3:C:140:LYS:HE2	3:C:140:LYS:HB3	1.84	0.46
2:E:436:VAL:CG1	2:E:437:TRP:N	2.79	0.46
3:C:155:ASP:O	3:C:159:LYS:HG2	2.15	0.46
2:E:367:MET:HE2	2:E:367:MET:HA	1.96	0.46
1:A:159:ARG:NH1	1:A:159:ARG:HB3	2.31	0.46
2:E:316:ASP:HB3	2:E:441:LYS:HE3	1.97	0.46
2:B:214:ILE:HD11	2:B:227:ILE:HG22	1.96	0.46
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.16	0.46
1:A:135:LEU:HD13	1:A:138:LYS:HE2	1.97	0.46
1:A:167:ARG:HB3	2:B:192:TYR:CG	2.50	0.46
1:D:137:GLN:HB2	1:D:189:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:126:GLU:O	3:F:129:ALA:HB3	2.15	0.46
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.81	0.46
2:B:215:ILE:HA	2:B:219:GLY:O	2.16	0.46
2:E:215:ILE:HA	2:E:219:GLY:O	2.16	0.46
1:A:147:MET:SD	3:C:121:ILE:HD11	2.56	0.46
2:B:168:LEU:HD23	3:C:110:LEU:HD13	1.98	0.46
3:F:325:ASN:HD22	3:F:325:ASN:C	2.24	0.46
2:B:316:ASP:HB3	2:B:441:LYS:HE3	1.98	0.45
3:C:124:LEU:O	3:C:128:VAL:HG13	2.16	0.45
2:E:293:TRP:HZ2	2:E:296:ASN:ND2	2.14	0.45
2:B:246:ASN:HD22	2:B:246:ASN:N	2.14	0.45
2:E:351:ASN:ND2	2:E:351:ASN:C	2.65	0.45
2:B:277:ALA:HA	2:B:288:LEU:O	2.16	0.45
3:C:259:THR:O	3:C:286:ALA:CB	2.64	0.45
2:B:176:ARG:NH1	2:B:176:ARG:HG3	2.31	0.45
2:E:157:VAL:HA	2:E:160:ASN:CB	2.46	0.45
2:E:402:TRP:HB3	2:E:404:TYR:CE2	2.51	0.45
3:F:89:MET:C	3:F:91:GLU:N	2.75	0.45
3:F:195:GLN:HE21	3:F:195:GLN:HB2	1.63	0.45
3:F:239:GLN:C	3:F:241:ALA:H	2.25	0.45
2:B:332:GLN:HB3	2:B:336:ASN:HB2	1.99	0.45
2:B:369:ILE:O	2:B:405:ASN:HB2	2.16	0.45
3:C:88:LYS:HA	3:C:91:GLU:OE1	2.16	0.45
2:B:395:SER:HB2	2:B:404:TYR:CE2	2.52	0.45
1:D:156:ILE:O	1:D:159:ARG:HG2	2.16	0.45
2:E:161:ILE:O	2:E:165:LEU:HB2	2.17	0.45
2:E:293:TRP:HZ2	2:E:296:ASN:HD21	1.63	0.45
2:B:411:ASN:O	2:B:435:VAL:HA	2.16	0.45
2:B:424:TRP:CD1	2:B:424:TRP:H	2.35	0.45
5:B:1:NAG:O7	5:B:1:NAG:H3	2.17	0.45
3:F:252:ASP:OD2	3:F:256:ARG:HB2	2.17	0.45
3:F:343:HIS:O	3:F:367:ILE:HA	2.17	0.45
2:B:228:GLN:HB2	2:B:235:PRO:HB3	1.98	0.45
3:C:104:ASP:C	3:C:106:SER:H	2.23	0.45
1:D:123:LYS:HZ1	2:E:154:ASP:HB2	1.80	0.45
2:E:346:ARG:HG3	2:E:346:ARG:NH1	2.26	0.44
2:E:392:LYS:HZ2	2:E:406:ARG:NH1	2.15	0.44
2:E:301:GLN:NE2	2:E:301:GLN:C	2.75	0.44
3:C:344:LEU:HD12	3:C:384:MET:HE3	2.00	0.44
1:D:136:LEU:HB3	2:E:168:LEU:HD11	1.98	0.44
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HD3	2:B:428:LYS:O	2.18	0.44
3:C:206:LYS:HA	3:C:206:LYS:HD3	1.84	0.44
3:F:208:TRP:HB3	3:F:209:ILE:HD12	2.00	0.44
3:F:234:HIS:CD2	3:F:269:PRO:HA	2.52	0.44
3:C:189:ASN:CG	3:C:391:ARG:HH21	2.26	0.44
1:A:182:GLN:O	1:A:186:GLU:HG2	2.17	0.44
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.78	0.44
2:B:293:TRP:HZ2	2:B:296:ASN:HD21	1.65	0.44
3:F:121:ILE:HA	3:F:124:LEU:HB3	1.99	0.44
3:C:207:ASN:HB2	3:C:316:ASP:OD2	2.17	0.44
1:D:140:VAL:HG21	2:E:171:ILE:HD11	2.00	0.44
1:D:155:ASP:HA	1:D:171:ARG:NH1	2.33	0.44
3:F:310:MET:SD	3:F:337:ASN:CB	2.97	0.44
2:B:239:TYR:HD2	2:B:251:VAL:HG21	1.83	0.44
2:E:280:THR:OG1	2:E:281:ASP:N	2.49	0.44
3:F:106:SER:C	3:F:107:ILE:HD12	2.43	0.44
2:B:265:LYS:HB3	2:B:379:ASP:OD2	2.18	0.44
2:B:293:TRP:HZ2	2:B:296:ASN:ND2	2.16	0.44
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.99	0.44
2:E:364:ASN:HD21	5:E:1:NAG:H3	1.82	0.44
3:F:340:HIS:N	4:H:1:GLY:O	2.46	0.44
2:B:367:MET:HE2	2:B:367:MET:HA	1.99	0.43
3:C:162:LYS:HZ3	3:C:163:GLN:HB2	1.82	0.43
2:B:280:THR:OG1	2:B:283:LYS:HB2	2.18	0.43
1:D:159:ARG:CB	1:D:159:ARG:HH11	2.31	0.43
3:F:326:CYS:CB	3:F:336:MET:HE3	2.47	0.43
2:B:161:ILE:HA	2:B:164:ASN:CG	2.43	0.43
3:F:108:ARG:O	3:F:112:GLU:HG3	2.18	0.43
2:E:238:VAL:HG23	2:E:294:LEU:HD11	2.01	0.43
1:A:116:ARG:O	1:A:119:ILE:HG13	2.18	0.43
2:B:380:ARG:HB2	2:B:380:ARG:NH1	2.15	0.43
3:C:106:SER:C	3:C:107:ILE:HD12	2.44	0.43
1:D:185:LEU:HG	2:E:171:ILE:HD13	2.00	0.43
3:F:296:GLY:O	3:F:298:ASP:N	2.52	0.43
3:F:374:THR:C	3:F:376:TRP:H	2.26	0.43
2:B:186:VAL:HG21	3:C:128:VAL:HG12	2.00	0.43
3:C:162:LYS:NZ	3:C:163:GLN:HB2	2.34	0.43
2:E:280:THR:OG1	2:E:283:LYS:HB2	2.18	0.43
3:F:162:LYS:NZ	3:F:163:GLN:HB2	2.33	0.43
2:B:218:GLY:HA3	3:C:210:GLN:HG2	2.01	0.43
3:C:167:TYR:O	3:C:179:LEU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:364:ASN:HD21	5:E:1:NAG:C5	2.23	0.43
3:F:259:THR:O	3:F:286:ALA:HB3	2.19	0.43
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.18	0.43
2:B:386:LEU:O	2:B:388:SER:N	2.46	0.43
3:C:89:MET:C	3:C:91:GLU:N	2.77	0.43
3:C:195:GLN:HG2	3:C:384:MET:HG3	2.00	0.43
3:C:303:PHE:O	3:C:305:THR:N	2.52	0.43
2:B:340:ILE:HG12	2:B:341:SER:N	2.33	0.43
3:C:217:HIS:O	3:C:224:THR:HG23	2.19	0.43
3:C:360:PRO:HG2	3:C:361:ASN:H	1.84	0.43
2:E:358:SER:HA	2:E:365:ARG:NH2	2.34	0.43
2:B:306:GLY:O	2:B:308:THR:HG23	2.20	0.42
2:B:370:HIS:CE1	2:B:402:TRP:HE1	2.37	0.42
3:F:196:LYS:O	3:F:225:GLU:HB2	2.18	0.42
2:B:181:LYS:O	2:B:184:SER:HB3	2.19	0.42
2:B:389:ASP:C	2:B:391:ARG:H	2.27	0.42
1:D:159:ARG:NH1	1:D:159:ARG:CB	2.82	0.42
2:E:386:LEU:O	2:E:388:SER:N	2.47	0.42
3:F:307:HIS:HE1	3:F:341:ALA:H	1.67	0.42
3:F:330:ASP:CG	4:H:3:ARG:HH22	2.26	0.42
2:B:441:LYS:CB	2:B:447:MET:HE1	2.46	0.42
3:C:174:ALA:HB2	3:C:235:LEU:HD13	2.01	0.42
3:C:374:THR:C	3:C:376:TRP:H	2.26	0.42
1:D:136:LEU:HD13	2:E:168:LEU:HD21	2.01	0.42
2:E:217:LYS:HB3	3:F:213:GLU:HG3	2.00	0.42
1:A:164:SER:HB2	3:C:135:CYS:HB3	2.01	0.42
2:B:217:LYS:HB3	3:C:213:GLU:HG3	2.02	0.42
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.77	0.42
3:F:334:TRP:CH2	3:F:344:LEU:HB2	2.54	0.42
2:B:199:VAL:HG23	3:C:141:ASP:HA	2.01	0.42
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.20	0.42
1:D:120:GLU:C	1:D:122:LEU:N	2.78	0.42
2:E:332:GLN:HB3	2:E:336:ASN:HB2	2.01	0.42
1:A:137:GLN:HB2	1:A:189:ILE:HG12	2.01	0.42
1:D:130:VAL:O	1:D:134:GLN:HG3	2.19	0.42
3:F:303:PHE:C	3:F:305:THR:H	2.27	0.42
2:B:253:GLN:HB3	2:B:452:MET:HB2	2.02	0.42
2:B:265:LYS:HB3	2:B:379:ASP:CG	2.45	0.42
3:F:339:CYS:CB	4:H:1:GLY:O	2.67	0.42
3:F:370:ALA:C	3:F:372:TRP:H	2.27	0.42
3:C:303:PHE:C	3:C:305:THR:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:MET:CG	3:C:337:ASN:HB2	2.49	0.42
3:F:104:ASP:C	3:F:106:SER:H	2.28	0.42
3:F:252:ASP:C	3:F:254:ASN:H	2.28	0.42
2:E:317:TRP:HA	2:E:448:ARG:NH1	2.34	0.42
3:F:242:ILE:HG23	3:F:243:PRO:HD2	2.02	0.42
2:E:202:ASN:ND2	2:E:284:ASN:O	2.52	0.41
2:E:402:TRP:CG	2:E:403:TRP:N	2.87	0.41
3:F:259:THR:OG1	3:F:284:GLY:HA2	2.19	0.41
2:B:167:VAL:C	2:B:169:ARG:N	2.78	0.41
3:C:146:HIS:HB2	3:C:167:TYR:CE2	2.55	0.41
2:E:294:LEU:HG	2:E:298:LYS:HD2	2.01	0.41
2:B:359:GLN:NE2	2:B:359:GLN:N	2.60	0.41
3:F:176:GLN:O	3:F:176:GLN:HG2	2.20	0.41
3:F:340:HIS:ND1	3:F:343:HIS:HB2	2.36	0.41
2:B:280:THR:OG1	2:B:281:ASP:N	2.52	0.41
3:C:95:LYS:O	3:C:99:SER:HB2	2.20	0.41
3:C:185:ASP:CG	3:C:187:SER:HG	2.28	0.41
3:F:140:LYS:HE2	3:F:140:LYS:HB3	1.86	0.41
3:F:149:THR:CG2	3:F:150:GLY:N	2.82	0.41
1:A:120:GLU:C	1:A:122:LEU:N	2.79	0.41
2:B:176:ARG:HG3	2:B:176:ARG:HH11	1.85	0.41
3:F:290:PHE:HD1	3:F:290:PHE:HA	1.76	0.41
2:B:302:LEU:HD13	2:B:454:ILE:HD11	2.02	0.41
3:F:307:HIS:HA	3:F:310:MET:HG3	2.02	0.41
2:B:163:THR:C	2:B:165:LEU:H	2.28	0.41
2:B:325:HIS:HB3	2:B:346:ARG:O	2.21	0.41
3:C:230:ASN:HB3	3:C:274:TYR:CG	2.55	0.41
3:C:272:ASP:OD1	3:C:275:ARG:NH1	2.54	0.41
3:C:278:TYR:CE2	3:C:308:ASN:HB2	2.56	0.41
2:E:422:TYR:CE1	2:E:444:TRP:HA	2.56	0.41
3:F:130:GLN:O	3:F:133:ALA:HB3	2.20	0.41
3:F:172:LEU:H	3:F:239:GLN:NE2	2.18	0.41
2:B:167:VAL:CG2	2:B:168:LEU:N	2.84	0.41
2:B:393:GLN:HE21	2:B:393:GLN:HB3	1.69	0.41
1:D:123:LYS:HD3	1:D:123:LYS:HA	1.87	0.41
2:E:246:ASN:HD22	2:E:246:ASN:N	2.19	0.41
3:F:88:LYS:HA	3:F:91:GLU:OE1	2.21	0.41
3:F:229:GLY:O	3:F:230:ASN:C	2.63	0.41
3:F:318:ASP:HB3	3:F:319:ASN:H	1.71	0.41
4:H:1:GLY:H3	4:H:3:ARG:NH2	2.16	0.41
2:B:301:GLN:C	2:B:301:GLN:NE2	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:LEU:HA	2:B:360:LEU:HD23	1.86	0.41
3:C:195:GLN:OE1	3:C:382:THR:CG2	2.68	0.41
2:E:256:GLN:HA	2:E:449:LYS:HG2	2.03	0.41
3:F:226:PHE:CD2	3:F:226:PHE:C	2.98	0.41
2:B:296:ASN:HB3	2:B:338:TYR:CD1	2.56	0.40
2:B:373:MET:HE2	2:B:404:TYR:O	2.21	0.40
2:B:396:LYS:HA	2:B:396:LYS:CE	2.44	0.40
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.56	0.40
2:B:439:ASN:H	2:B:439:ASN:HD22	1.69	0.40
3:C:216:GLY:HA3	3:C:226:PHE:HA	2.03	0.40
2:E:325:HIS:HB3	2:E:346:ARG:O	2.21	0.40
2:B:389:ASP:CB	2:B:390:PRO:HD2	2.28	0.40
3:C:253:TRP:HA	3:C:380:LYS:HD2	2.04	0.40
2:E:342:VAL:HG23	2:E:354:MET:HG2	2.03	0.40
3:F:95:LYS:O	3:F:99:SER:HB2	2.22	0.40
3:F:289:ALA:HA	3:F:371:THR:HG23	2.02	0.40
1:A:119:ILE:O	1:A:122:LEU:HB3	2.22	0.40
2:B:176:ARG:HG2	3:C:117:ASN:ND2	2.29	0.40
3:C:126:GLU:O	3:C:129:ALA:HB3	2.21	0.40
3:C:149:THR:CG2	3:C:150:GLY:N	2.84	0.40
3:C:239:GLN:O	3:C:241:ALA:N	2.54	0.40
3:C:310:MET:SD	3:C:337:ASN:CB	3.02	0.40
3:C:374:THR:C	3:C:376:TRP:N	2.80	0.40
2:E:266:TRP:CE3	2:E:380:ARG:HD2	2.56	0.40
2:E:265:LYS:HB3	2:E:379:ASP:OD2	2.22	0.40
2:E:367:MET:HG3	2:E:406:ARG:HD2	2.03	0.40
2:E:386:LEU:H	2:E:386:LEU:CD2	2.32	0.40
2:E:397:GLU:C	2:E:399:GLY:H	2.29	0.40
3:C:203:ASP:OD2	3:C:205:LYS:HB3	2.22	0.40
3:C:373:LYS:HB2	3:C:379:MET:HE1	2.03	0.40
2:E:241:ASP:HB3	2:E:249:TRP:HB2	2.04	0.40
3:F:373:LYS:HB2	3:F:379:MET:HE1	2.02	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	79/87 (91%)	72 (91%)	5 (6%)	2 (2%)	4	17
1	D	79/87 (91%)	72 (91%)	5 (6%)	2 (2%)	4	17
2	B	310/328 (94%)	263 (85%)	33 (11%)	14 (4%)	2	8
2	E	310/328 (94%)	258 (83%)	39 (13%)	13 (4%)	2	9
3	C	307/319 (96%)	264 (86%)	33 (11%)	10 (3%)	3	13
3	F	309/319 (97%)	257 (83%)	38 (12%)	14 (4%)	2	8
4	G	2/4 (50%)	0	0	2 (100%)	0	0
4	H	2/4 (50%)	0	0	2 (100%)	0	0
All	All	1398/1476 (95%)	1186 (85%)	153 (11%)	59 (4%)	2	9

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	149	HIS
2	B	280	THR
2	B	391	ARG
2	B	407	CYS
3	C	89	MET
3	C	318	ASP
2	E	149	HIS
2	E	280	THR
2	E	391	ARG
2	E	407	CYS
3	F	89	MET
3	F	318	ASP
3	F	339	CYS
1	A	122	LEU
2	B	231	SER
2	B	389	ASP
3	C	283	GLY
3	C	304	PHE
3	C	339	CYS
1	D	122	LEU
2	E	362	GLY
2	E	389	ASP
3	F	283	GLY

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Mol	Chain	Res	Type
3	F	297	ASP
3	F	304	PHE
4	H	2	PRO
2	B	256	GLN
2	B	362	GLY
2	B	387	THR
3	C	198	LEU
3	C	243	PRO
2	E	231	SER
2	E	256	GLN
2	E	387	THR
3	F	243	PRO
3	F	394	ILE
3	F	396	GLU
4	G	2	PRO
3	C	260	ALA
3	C	297	ASP
3	F	198	LEU
3	F	360	PRO
4	G	3	ARG
2	B	434	GLY
3	C	360	PRO
2	E	229	PRO
3	F	397	GLY
2	B	229	PRO
2	B	390	PRO
3	F	260	ALA
2	B	282	GLY
2	E	282	GLY
2	E	390	PRO
1	A	121	VAL
1	D	121	VAL
4	H	3	ARG
2	B	153	ILE
3	F	324	GLY
2	E	153	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	76/82 (93%)	62 (82%)	14 (18%)	1	6
1	D	76/82 (93%)	62 (82%)	14 (18%)	1	6
2	B	270/286 (94%)	246 (91%)	24 (9%)	9	28
2	E	270/286 (94%)	246 (91%)	24 (9%)	9	28
3	C	261/267 (98%)	239 (92%)	22 (8%)	10	31
3	F	262/267 (98%)	239 (91%)	23 (9%)	9	29
4	G	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	H	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1221/1276 (96%)	1098 (90%)	123 (10%)	7	24

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	129	LYS
1	A	135	LEU
1	A	141	ARG
1	A	143	GLN
1	A	146	ASP
1	A	161	CYS
1	A	167	ARG
1	A	169	LEU
1	A	172	GLU
1	A	173	VAL
1	A	175	LEU
1	A	184	GLN
1	A	185	LEU
2	B	155	GLU
2	B	164	ASN
2	B	165	LEU
2	B	176	ARG
2	B	181	LYS
2	B	191	GLU
2	B	195	THR
2	B	221	THR
2	B	224	MET
2	B	238	VAL

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Mol	Chain	Res	Type
2	B	244	THR
2	B	246	ASN
2	B	252	ILE
2	B	253	GLN
2	B	267	ASP
2	B	283	LYS
2	B	313	GLU
2	B	359	GLN
2	B	366	THR
2	B	380	ARG
2	B	381	ASP
2	B	385	TRP
2	B	396	LYS
2	B	432	ASP
3	C	118	ASN
3	C	121	ILE
3	C	128	VAL
3	C	134	GLN
3	C	135	CYS
3	C	144	GLN
3	C	148	ILE
3	C	162	LYS
3	C	163	GLN
3	C	176	GLN
3	C	192	THR
3	C	195	GLN
3	C	209	ILE
3	C	243	PRO
3	C	318	ASP
3	C	335	TRP
3	C	350	GLN
3	C	365	ASN
3	C	375	ARG
3	C	382	THR
3	C	383	THR
3	C	394	ILE
1	D	122	LEU
1	D	129	LYS
1	D	135	LEU
1	D	141	ARG
1	D	143	GLN
1	D	146	ASP

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Mol	Chain	Res	Type
1	D	161	CYS
1	D	167	ARG
1	D	169	LEU
1	D	172	GLU
1	D	173	VAL
1	D	175	LEU
1	D	184	GLN
1	D	185	LEU
2	E	155	GLU
2	E	164	ASN
2	E	165	LEU
2	E	176	ARG
2	E	181	LYS
2	E	191	GLU
2	E	195	THR
2	E	221	THR
2	E	224	MET
2	E	238	VAL
2	E	244	THR
2	E	246	ASN
2	E	252	ILE
2	E	253	GLN
2	E	267	ASP
2	E	283	LYS
2	E	313	GLU
2	E	351	ASN
2	E	359	GLN
2	E	380	ARG
2	E	381	ASP
2	E	385	TRP
2	E	396	LYS
2	E	432	ASP
3	F	118	ASN
3	F	128	VAL
3	F	134	GLN
3	F	135	CYS
3	F	144	GLN
3	F	148	ILE
3	F	162	LYS
3	F	163	GLN
3	F	176	GLN
3	F	192	THR

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Mol	Chain	Res	Type
3	F	195	GLN
3	F	209	ILE
3	F	243	PRO
3	F	254	ASN
3	F	318	ASP
3	F	335	TRP
3	F	350	GLN
3	F	365	ASN
3	F	375	ARG
3	F	382	THR
3	F	383	THR
3	F	392	LEU
3	F	398	GLN
4	G	3	ARG
4	H	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	137	GLN
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
2	B	150	GLN
2	B	180	GLN
2	B	189	GLN
2	B	228	GLN
2	B	246	ASN
2	B	253	GLN
2	B	256	GLN
2	B	296	ASN
2	B	332	GLN
2	B	351	ASN
2	B	359	GLN
2	B	393	GLN
2	B	408	HIS
2	B	439	ASN
3	C	111	GLN
3	C	118	ASN
3	C	130	GLN
3	C	134	GLN

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Mol	Chain	Res	Type
3	C	136	GLN
3	C	176	GLN
3	C	177	GLN
3	C	189	ASN
3	C	230	ASN
3	C	239	GLN
3	C	319	ASN
3	C	325	ASN
3	C	365	ASN
3	C	390	ASN
1	D	132	HIS
1	D	182	GLN
1	D	184	GLN
2	E	158	ASN
2	E	174	ASN
2	E	180	GLN
2	E	189	GLN
2	E	228	GLN
2	E	246	ASN
2	E	253	GLN
2	E	256	GLN
2	E	296	ASN
2	E	301	GLN
2	E	332	GLN
2	E	351	ASN
2	E	359	GLN
2	E	364	ASN
2	E	393	GLN
2	E	408	HIS
2	E	439	ASN
3	F	115	ASN
3	F	117	ASN
3	F	118	ASN
3	F	130	GLN
3	F	134	GLN
3	F	136	GLN
3	F	176	GLN
3	F	177	GLN
3	F	189	ASN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS

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Mol	Chain	Res	Type
3	F	325	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	B	1	-	14,14,15	0.45	0	17,19,21	0.68	0
5	NAG	E	1	-	14,14,15	0.50	0	17,19,21	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1	-	-	3/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C3-C2-N2-C7
5	B	1	NAG	C4-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	NAG	1	0
5	E	1	NAG	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F	1
2	E	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	397:GLY	C	398:GLN	N	1.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	175:LEU	C	176:ARG	N	1.13
1	B	175:LEU	C	176:ARG	N	1.11

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.