



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:35 PM UTC

PDB ID : 2FT3 / pdb_00002ft3
Title : Crystal structure of the biglycan dimer core protein
Authors : Scott, P.G.; Dodd, C.M.; Bergmann, E.M.
Deposited on : 2006-01-23
Resolution : 3.40 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

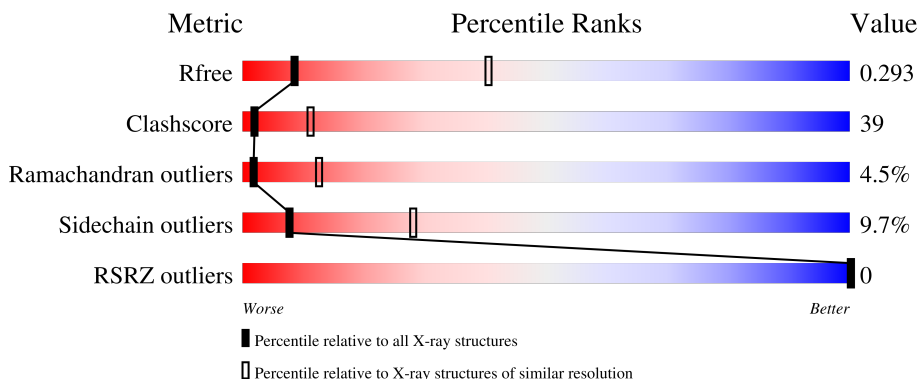
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	332	
1	B	332	
1	C	332	
1	D	332	
1	E	332	

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Mol	Chain	Length	Quality of chain
1	F	332	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	D	2193	-	-	X	-

2 Entry composition [i](#)

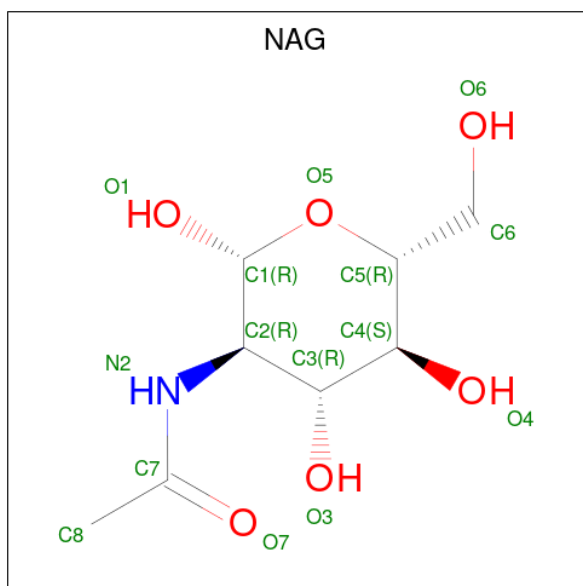
There are 3 unique types of molecules in this entry. The entry contains 14674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Biglycan.

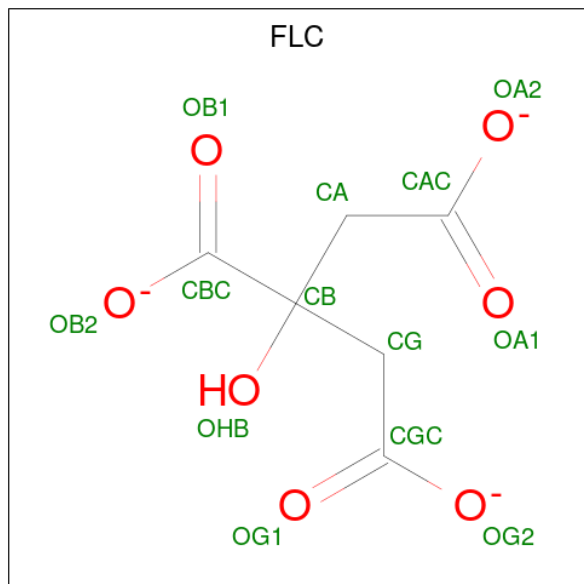
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	B	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	C	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	D	304	Total 2420	C 1547	N 429	O 433	S 11	0	0	0
1	E	303	Total 2416	C 1545	N 428	O 432	S 11	0	0	0
1	F	305	Total 2428	C 1551	N 431	O 435	S 11	0	0	0

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



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

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



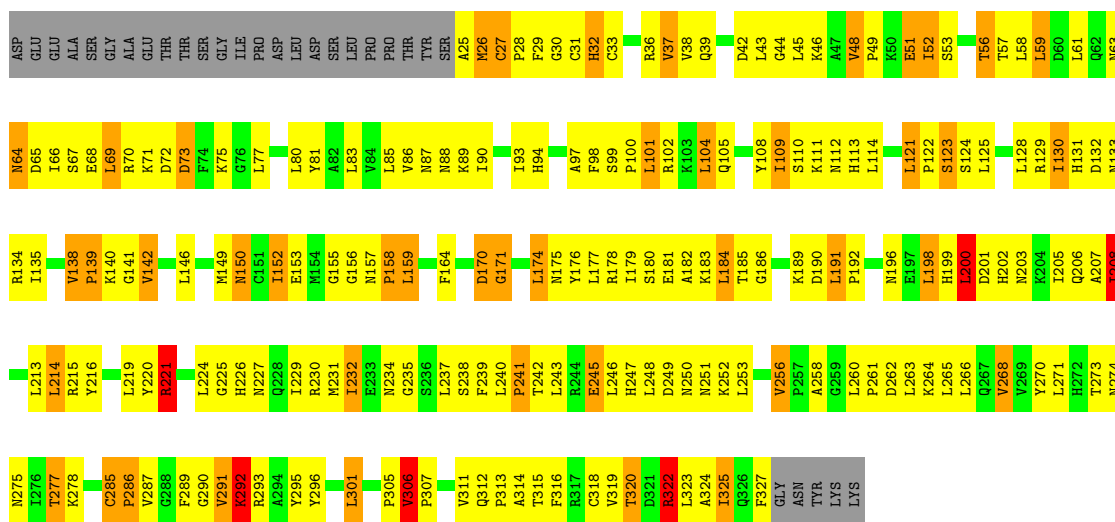
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			13	6 7		
3	B	1	Total	C O	0	0
			13	6 7		
3	C	1	Total	C O	0	0
			13	6 7		
3	D	1	Total	C O	0	0
			13	6 7		
3	E	1	Total	C O	0	0
			13	6 7		
3	F	1	Total	C O	0	0
			13	6 7		

3 Residue-property plots

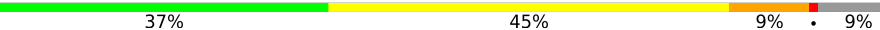
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

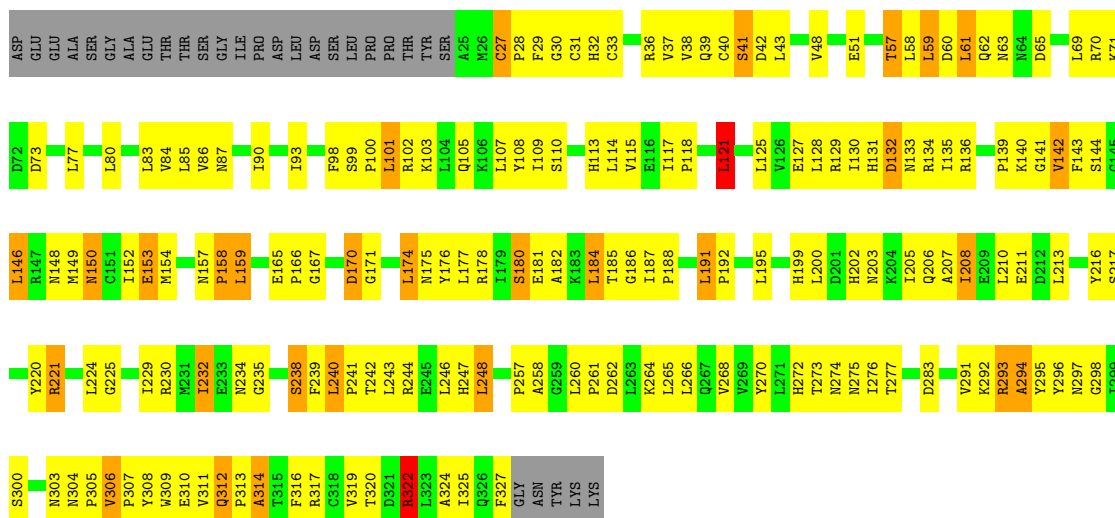
- Molecule 1: Biglycan

Chain A: 

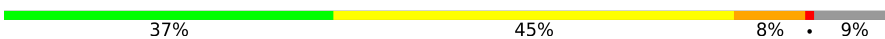


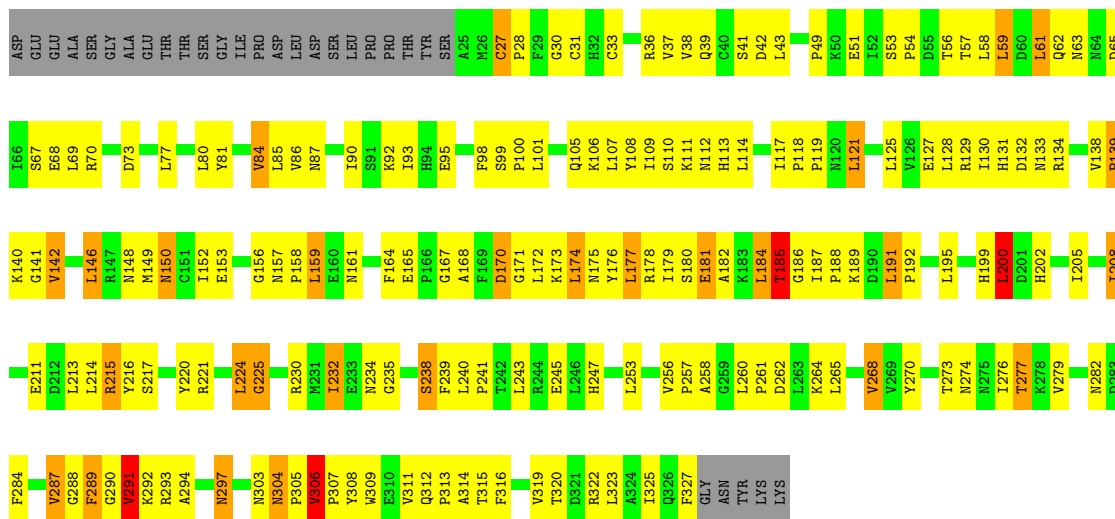
- Molecule 1: Biglycan

Chain B: 



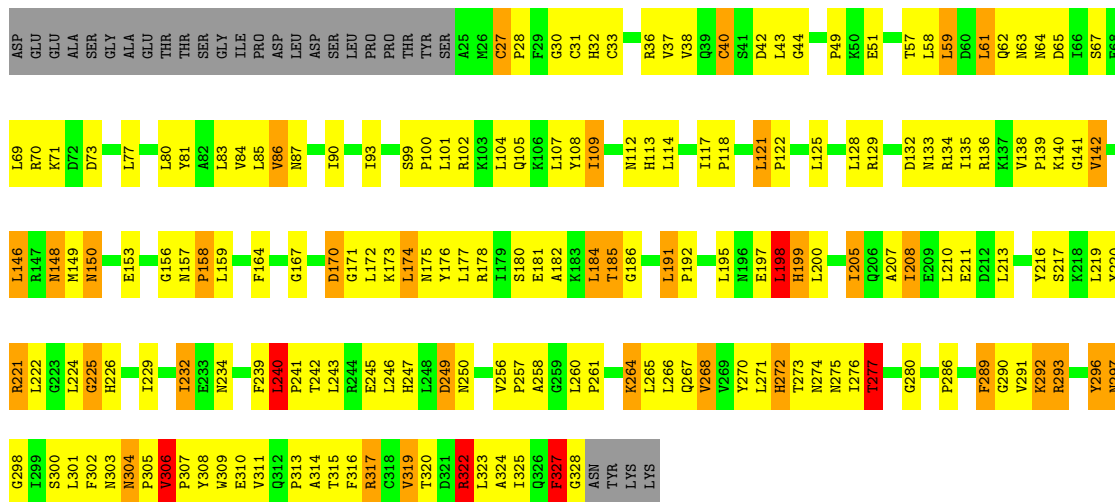
- Molecule 1: Biglycan

Chain C:  37% 45% 8% 9%

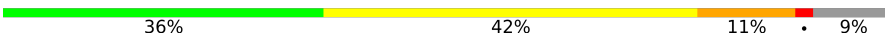


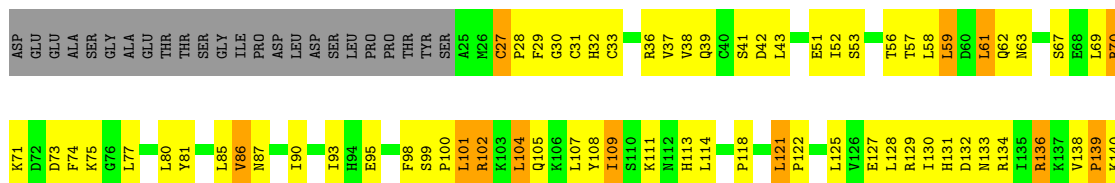
- Molecule 1: Biglycan

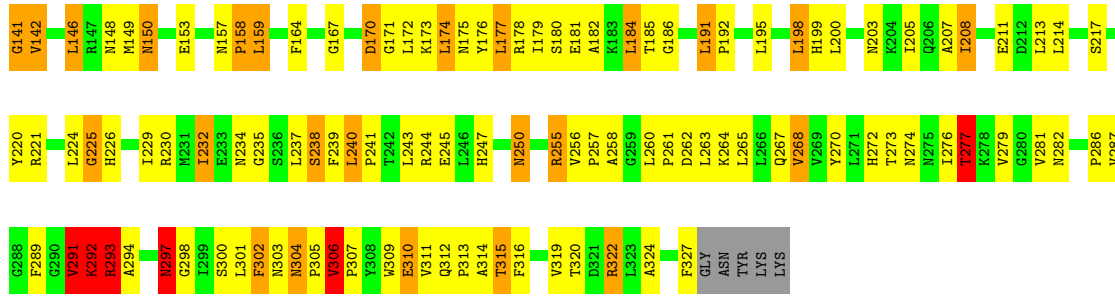
Chain D:  37% 42% 11% 8%



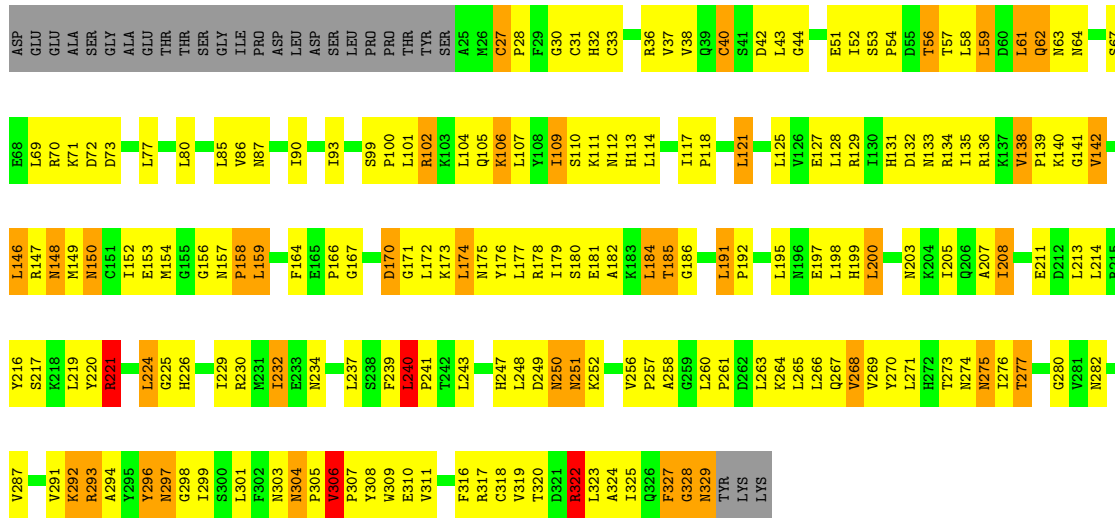
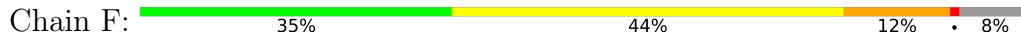
- Molecule 1: Biglycan

Chain E:  36% 42% 11% 9%





• Molecule 1: Biglycan



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.51Å 119.22Å 140.62Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	23.00 – 3.40 23.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (23.00-3.40) 96.5 (23.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.37Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.291 (Not available) , 0.293	Depositor DCC
R_{free} test set	2040 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.098 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-1$ 0.090 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-1$	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14674	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: FLC, 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	1.39	11/2468 (0.4%)	1.49	21/3342 (0.6%)
1	B	1.32	8/2468 (0.3%)	1.47	20/3342 (0.6%)
1	C	1.29	7/2468 (0.3%)	1.46	23/3342 (0.7%)
1	D	1.34	12/2472 (0.5%)	1.45	25/3347 (0.7%)
1	E	1.32	11/2468 (0.4%)	1.50	31/3342 (0.9%)
1	F	1.36	14/2480 (0.6%)	1.42	16/3358 (0.5%)
All	All	1.34	63/14824 (0.4%)	1.47	136/20073 (0.7%)

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	GLN	CD-NE2	-9.05	1.14	1.33
1	B	291	VAL	CA-CB	8.89	1.66	1.54
1	C	291	VAL	CA-CB	8.53	1.66	1.54
1	A	64	ASN	CA-C	-7.37	1.46	1.53
1	D	205	ILE	CA-CB	7.31	1.63	1.54
1	E	291	VAL	CA-CB	7.28	1.64	1.54
1	F	296	TYR	CA-C	-7.25	1.43	1.52
1	D	296	TYR	CA-C	-7.15	1.43	1.52
1	F	62	GLN	CD-OE1	-7.10	1.10	1.23
1	E	277	THR	CA-C	6.86	1.60	1.52
1	D	32	HIS	CA-C	-6.54	1.44	1.52
1	C	291	VAL	CA-C	6.46	1.60	1.52
1	B	115	VAL	CA-CB	6.40	1.61	1.54
1	F	107	LEU	CA-C	-6.21	1.45	1.53
1	E	291	VAL	CA-C	6.16	1.60	1.52
1	D	199	HIS	CA-C	-6.07	1.45	1.52
1	E	62	GLN	CD-NE2	-6.05	1.20	1.33
1	C	279	VAL	CA-CB	6.01	1.60	1.53
1	B	154	MET	CA-C	-5.98	1.45	1.52
1	F	294	ALA	CA-CB	-5.91	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	LEU	CA-C	5.88	1.59	1.53
1	F	147	ARG	CA-C	-5.86	1.45	1.52
1	F	203	ASN	CA-C	-5.85	1.47	1.53
1	F	277	THR	CA-C	5.84	1.59	1.52
1	D	62	GLN	CD-NE2	-5.83	1.21	1.33
1	A	320	THR	CA-CB	-5.79	1.43	1.53
1	A	208	ILE	CA-CB	5.77	1.60	1.53
1	F	138	VAL	CA-CB	-5.72	1.47	1.54
1	F	185	THR	CA-C	5.68	1.60	1.52
1	E	293	ARG	CA-C	5.67	1.60	1.52
1	F	106	LYS	CA-C	5.67	1.59	1.52
1	A	278	LYS	CA-C	5.66	1.59	1.52
1	A	296	TYR	CA-C	-5.65	1.45	1.52
1	E	293	ARG	N-CA	5.63	1.53	1.46
1	E	267	GLN	CA-C	-5.61	1.45	1.52
1	A	196	ASN	CA-C	-5.60	1.45	1.52
1	B	244	ARG	NE-CZ	5.58	1.39	1.33
1	D	300	SER	CA-C	5.55	1.59	1.52
1	C	221	ARG	CD-NE	-5.51	1.38	1.46
1	B	180	SER	C-O	-5.51	1.16	1.23
1	A	104	LEU	CA-C	5.42	1.59	1.52
1	D	327	PHE	CA-C	5.41	1.60	1.52
1	E	179	ILE	CA-CB	-5.40	1.47	1.54
1	E	279	VAL	CA-CB	5.31	1.59	1.53
1	B	294	ALA	N-CA	5.31	1.52	1.46
1	D	293	ARG	N-CA	5.30	1.52	1.45
1	C	177	LEU	CA-C	-5.27	1.45	1.52
1	F	303	ASN	CA-C	-5.25	1.46	1.53
1	E	297	ASN	N-CA	-5.24	1.39	1.46
1	F	179	ILE	CA-CB	-5.22	1.47	1.54
1	D	84	VAL	CA-C	5.21	1.59	1.52
1	A	285	CYS	CA-C	-5.21	1.46	1.53
1	C	221	ARG	NE-CZ	-5.20	1.27	1.33
1	B	65	ASP	CA-C	-5.20	1.46	1.53
1	D	277	THR	CA-C	5.16	1.58	1.52
1	E	315	THR	CA-CB	5.16	1.61	1.53
1	D	62	GLN	CD-OE1	-5.09	1.13	1.23
1	D	292	LYS	CA-C	5.09	1.59	1.52
1	C	277	THR	CA-C	5.08	1.58	1.52
1	A	256	VAL	CA-C	5.06	1.58	1.52
1	F	251	ASN	CA-C	-5.05	1.48	1.53
1	A	307	PRO	CA-C	-5.03	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLU	CA-C	-5.03	1.46	1.52

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	CYS	N-CA-C	12.81	124.87	110.13
1	A	27	CYS	N-CA-C	11.86	125.93	110.40
1	D	27	CYS	N-CA-C	11.59	123.46	110.13
1	E	244	ARG	NE-CZ-NH2	11.33	129.40	119.20
1	C	27	CYS	N-CA-C	10.84	122.60	110.13
1	D	317	ARG	NE-CZ-NH2	10.77	128.90	119.20
1	B	322	ARG	N-CA-C	-10.71	99.74	113.12
1	E	27	CYS	N-CA-C	10.45	122.15	110.13
1	A	292	LYS	N-CA-C	-10.21	99.92	112.38
1	C	221	ARG	NE-CZ-NH2	-10.10	110.11	119.20
1	A	322	ARG	N-CA-C	-9.89	99.33	111.40
1	B	27	CYS	N-CA-C	9.65	121.22	110.13
1	E	255	ARG	NE-CZ-NH2	9.38	127.64	119.20
1	E	244	ARG	NE-CZ-NH1	-8.94	112.56	121.50
1	E	244	ARG	CD-NE-CZ	8.82	136.75	124.40
1	D	317	ARG	NE-CZ-NH1	-8.78	112.72	121.50
1	F	322	ARG	N-CA-C	-8.73	100.32	112.45
1	E	255	ARG	NE-CZ-NH1	-8.13	113.37	121.50
1	E	70	ARG	NE-CZ-NH2	8.08	126.48	119.20
1	B	230	ARG	N-CA-C	-7.79	103.38	113.12
1	E	70	ARG	NE-CZ-NH1	-7.76	113.74	121.50
1	C	221	ARG	CG-CD-NE	-7.60	95.28	112.00
1	B	40	CYS	CA-C-N	-7.50	112.06	122.93
1	B	40	CYS	C-N-CA	-7.50	112.06	122.93
1	D	317	ARG	CD-NE-CZ	7.39	134.74	124.40
1	D	322	ARG	N-CA-C	-7.38	102.20	112.45
1	A	156	GLY	N-CA-C	-7.36	104.71	115.30
1	A	311	VAL	N-CA-C	7.36	117.29	106.85
1	C	215	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	E	136	ARG	NE-CZ-NH2	-7.26	112.67	119.20
1	C	215	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	E	220	TYR	N-CA-C	-7.01	104.71	113.55
1	B	101	LEU	N-CA-C	7.01	119.48	110.65
1	E	29	PHE	N-CA-C	6.79	118.36	110.97
1	E	293	ARG	N-CA-C	6.72	125.11	110.80
1	C	230	ARG	N-CA-C	-6.70	103.77	112.68
1	C	322	ARG	N-CA-C	-6.66	103.20	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	322	ARG	NE-CZ-NH2	6.64	125.17	119.20
1	D	322	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	E	322	ARG	N-CA-C	-6.61	104.86	113.12
1	A	231	MET	N-CA-C	6.52	120.87	107.37
1	B	61	LEU	CB-CA-C	6.50	121.41	111.85
1	B	132	ASP	CB-CA-C	-6.50	102.32	111.80
1	E	255	ARG	CD-NE-CZ	6.49	133.49	124.40
1	A	101	LEU	N-CA-C	6.26	119.60	112.97
1	F	317	ARG	N-CA-C	6.25	118.09	111.28
1	F	102	ARG	N-CA-C	6.24	120.45	112.34
1	F	136	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	D	102	ARG	N-CA-C	6.20	120.40	112.34
1	A	177	LEU	CA-C-N	-6.16	114.09	122.77
1	A	177	LEU	C-N-CA	-6.16	114.09	122.77
1	E	294	ALA	CA-C-N	-6.14	113.00	122.09
1	E	294	ALA	C-N-CA	-6.14	113.00	122.09
1	E	70	ARG	CD-NE-CZ	6.11	132.96	124.40
1	D	319	VAL	CB-CA-C	-6.06	104.92	111.59
1	E	95	GLU	N-CA-C	6.06	117.56	111.07
1	A	230	ARG	N-CA-C	-6.00	105.99	113.55
1	E	102	ARG	N-CA-C	5.96	120.09	112.34
1	C	322	ARG	NE-CZ-NH2	5.95	124.56	119.20
1	D	86	VAL	CB-CA-C	-5.95	102.34	111.08
1	C	221	ARG	CD-NE-CZ	5.90	132.66	124.40
1	E	136	ARG	CD-NE-CZ	5.87	132.61	124.40
1	A	286	PRO	N-CD-CG	-5.84	94.43	103.20
1	B	32	HIS	N-CA-C	-5.83	100.39	109.72
1	F	156	GLY	N-CA-C	-5.82	106.92	115.30
1	D	40	CYS	CB-CA-C	-5.81	103.11	111.70
1	C	185	THR	N-CA-C	-5.79	106.56	113.97
1	B	312	GLN	N-CA-C	5.78	116.25	109.60
1	A	221	ARG	N-CA-C	5.77	119.00	110.46
1	A	52	ILE	N-CA-C	5.74	116.83	106.61
1	C	287	VAL	N-CA-C	5.73	115.86	110.30
1	C	95	GLU	N-CA-C	5.73	117.20	111.07
1	D	132	ASP	CB-CA-C	-5.72	103.61	111.73
1	A	242	THR	N-CA-C	5.71	120.37	113.17
1	C	200	LEU	N-CA-C	-5.67	103.97	112.54
1	E	101	LEU	N-CA-C	5.67	119.32	111.55
1	D	242	THR	N-CA-C	5.65	119.17	112.72
1	C	220	TYR	N-CA-C	-5.65	105.16	112.68
1	F	221	ARG	NE-CZ-NH2	5.64	124.28	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ASP	CA-C-N	-5.60	115.53	123.03
1	B	60	ASP	C-N-CA	-5.60	115.53	123.03
1	D	156	GLY	N-CA-C	-5.60	106.28	114.90
1	F	136	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	A	200	LEU	N-CA-C	-5.59	105.38	113.21
1	B	41	SER	N-CA-C	5.58	118.58	109.59
1	A	65	ASP	N-CA-C	5.58	119.73	111.87
1	D	65	ASP	N-CA-C	5.57	119.65	112.41
1	C	27	CYS	CA-C-N	5.57	125.57	119.89
1	C	27	CYS	C-N-CA	5.57	125.57	119.89
1	F	275	ASN	N-CA-C	-5.55	104.27	111.71
1	F	40	CYS	CA-C-N	-5.54	114.90	122.93
1	F	40	CYS	C-N-CA	-5.54	114.90	122.93
1	A	196	ASN	N-CA-C	-5.53	106.58	113.55
1	B	220	TYR	N-CA-C	-5.50	106.62	113.55
1	D	84	VAL	N-CA-C	5.48	115.48	107.37
1	C	156	GLY	N-CA-C	-5.46	107.43	115.30
1	B	121	LEU	N-CA-C	-5.46	102.55	110.08
1	D	210	LEU	N-CA-C	5.42	116.87	110.97
1	A	138	VAL	N-CA-C	5.41	112.91	107.55
1	C	84	VAL	N-CA-C	5.41	114.54	106.85
1	C	221	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	D	249	ASP	N-CA-C	5.41	117.86	110.55
1	E	310	GLU	N-CA-C	-5.38	106.76	113.38
1	F	106	LYS	N-CA-C	5.37	117.71	109.07
1	E	322	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	E	224	LEU	N-CA-C	-5.34	104.75	113.19
1	E	230	ARG	N-CA-C	-5.33	105.58	112.68
1	E	136	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	A	208	ILE	N-CA-C	5.30	115.99	107.98
1	F	230	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	E	255	ARG	CB-CG-CD	5.29	123.46	111.30
1	B	294	ALA	CA-C-N	-5.27	114.79	122.65
1	B	294	ALA	C-N-CA	-5.27	114.79	122.65
1	A	325	ILE	N-CA-C	5.27	113.96	106.53
1	D	327	PHE	N-CA-C	5.26	122.00	110.80
1	D	198	LEU	CA-C-N	-5.25	114.41	122.87
1	D	198	LEU	C-N-CA	-5.25	114.41	122.87
1	B	283	ASP	N-CA-C	-5.24	106.03	112.90
1	A	287	VAL	N-CA-C	5.22	115.43	110.42
1	D	136	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	E	230	ARG	NE-CZ-NH2	5.21	123.89	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	56	THR	N-CA-C	5.21	117.86	110.10
1	F	318	CYS	CA-CB-SG	-5.21	102.43	114.40
1	C	65	ASP	N-CA-C	5.15	118.67	111.56
1	B	153	GLU	CA-C-N	-5.15	114.40	122.49
1	B	153	GLU	C-N-CA	-5.15	114.40	122.49
1	E	27	CYS	CA-C-N	5.08	125.07	119.89
1	E	27	CYS	C-N-CA	5.08	125.07	119.89
1	C	224	LEU	N-CA-C	-5.08	105.17	113.19
1	D	293	ARG	N-CA-C	5.07	117.94	110.59
1	C	56	THR	N-CA-C	5.06	117.56	109.96
1	F	166	PRO	N-CD-CG	-5.05	95.62	103.20
1	C	230	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	136	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	D	272	HIS	N-CA-C	5.02	117.01	110.43
1	F	224	LEU	N-CA-C	-5.02	104.96	112.54

There are no chirality outliers.

There are no planarity outliers.

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	2416	0	2466	229	0
1	B	2416	0	2466	169	0
1	C	2416	0	2466	190	0
1	D	2420	0	2469	175	0
1	E	2416	0	2466	181	0
1	F	2428	0	2475	200	0
2	A	14	0	13	5	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	13	0	5	0	0
3	B	13	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	13	0	5	3	0
3	D	13	0	5	7	0
3	E	13	0	5	2	0
3	F	13	0	5	2	0
All	All	14674	0	14916	1144	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 39.

All (1144) 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)
1:D:225:GLY:CA	3:D:2193:FLC:OB2	1.87	1.23
1:B:153:GLU:OE1	1:B:178:ARG:HD3	1.39	1.21
1:D:225:GLY:HA3	3:D:2193:FLC:OB2	1.00	1.15
1:E:27:CYS:HB2	1:E:28:PRO:HD2	1.33	1.10
1:C:121:LEU:HD12	1:C:121:LEU:H	1.15	1.09
1:A:93:ILE:HD11	1:A:114:LEU:HD21	1.32	1.09
1:E:153:GLU:OE1	1:E:178:ARG:HD3	1.54	1.05
1:A:83:LEU:HD21	1:A:85:LEU:HD11	1.38	1.04
1:F:121:LEU:HD12	1:F:121:LEU:H	1.20	1.01
1:C:276:ILE:HB	1:C:304:ASN:HD22	1.24	1.01
1:C:276:ILE:HB	1:C:304:ASN:ND2	1.75	1.00
1:C:27:CYS:HB2	1:C:28:PRO:HD2	1.44	1.00
1:A:180:SER:OG	1:A:181:GLU:HG3	1.61	0.99
1:B:293:ARG:HD3	1:B:294:ALA:H	1.24	0.99
1:F:27:CYS:HB2	1:F:28:PRO:HD2	1.45	0.99
1:E:176:TYR:CD2	1:E:177:LEU:N	2.30	0.99
1:A:139:PRO:HD2	1:A:142:VAL:HG21	1.45	0.98
1:B:276:ILE:HB	1:B:304:ASN:HD22	1.28	0.98
1:A:77:LEU:HD23	1:A:80:LEU:HD22	1.44	0.97
1:F:276:ILE:HB	1:F:304:ASN:ND2	1.80	0.97
1:A:174:LEU:HD12	1:A:174:LEU:O	1.65	0.97
1:A:121:LEU:HD12	1:A:121:LEU:H	1.30	0.96
1:A:128:LEU:HB3	1:A:149:MET:HE1	1.44	0.96
1:F:276:ILE:HB	1:F:304:ASN:HD22	1.29	0.96
1:D:290:GLY:HA3	1:D:292:LYS:HE3	1.49	0.95
1:D:276:ILE:HB	1:D:304:ASN:HD22	1.29	0.95
1:A:232:ILE:C	1:A:232:ILE:HD13	1.93	0.94
1:B:276:ILE:HB	1:B:304:ASN:ND2	1.83	0.93
1:D:27:CYS:HB2	1:D:28:PRO:HD2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:CYS:HB2	1:B:28:PRO:HD2	1.50	0.93
1:E:121:LEU:HD12	1:E:121:LEU:H	1.33	0.93
3:D:2193:FLC:OG1	3:D:2193:FLC:OA1	1.87	0.92
1:A:198:LEU:HD11	1:A:200:LEU:CD2	2.00	0.92
1:C:232:ILE:C	1:C:232:ILE:HD13	1.94	0.92
1:A:232:ILE:HD13	1:A:232:ILE:O	1.69	0.91
1:B:121:LEU:HD12	1:B:121:LEU:H	1.36	0.89
1:D:174:LEU:O	1:D:174:LEU:HD12	1.73	0.89
1:A:93:ILE:CD1	1:A:114:LEU:HD21	2.02	0.89
1:B:69:LEU:HD23	1:B:93:ILE:HG12	1.53	0.89
3:B:2191:FLC:OG2	3:B:2191:FLC:HA2	1.72	0.88
1:C:316:PHE:O	1:C:319:VAL:HG12	1.73	0.88
1:D:239:PHE:O	1:D:241:PRO:HD3	1.74	0.88
1:A:240:LEU:HD23	1:A:243:LEU:HD22	1.54	0.87
1:D:239:PHE:C	1:D:241:PRO:HD3	2.00	0.87
1:D:276:ILE:HB	1:D:304:ASN:ND2	1.89	0.87
1:E:27:CYS:HB2	1:E:28:PRO:CD	2.03	0.87
1:C:63:ASN:HA	1:C:87:ASN:O	1.75	0.86
1:D:225:GLY:HA3	3:D:2193:FLC:CBC	2.03	0.86
1:F:264:LYS:O	1:F:265:LEU:HD12	1.76	0.86
1:C:153:GLU:OE1	1:C:178:ARG:HD3	1.75	0.86
1:D:153:GLU:OE1	1:D:178:ARG:HD3	1.76	0.86
1:F:176:TYR:CD2	1:F:177:LEU:N	2.44	0.85
1:C:235:GLY:O	1:C:238:SER:HB3	1.76	0.85
1:A:174:LEU:O	1:A:174:LEU:CD1	2.24	0.85
1:C:174:LEU:HD12	1:C:174:LEU:O	1.75	0.85
1:E:276:ILE:HB	1:E:304:ASN:HD22	1.41	0.85
1:D:240:LEU:HD23	1:D:243:LEU:HD22	1.59	0.85
1:D:178:ARG:HE	1:D:180:SER:HB3	1.39	0.85
1:C:28:PRO:HB2	1:C:31:CYS:SG	2.17	0.85
1:E:276:ILE:HB	1:E:304:ASN:ND2	1.92	0.84
1:F:27:CYS:HB2	1:F:28:PRO:CD	2.05	0.84
1:B:27:CYS:HB2	1:B:28:PRO:CD	2.07	0.84
1:C:290:GLY:O	1:C:291:VAL:HB	1.76	0.83
1:E:28:PRO:HD3	1:E:51:GLU:O	1.78	0.83
1:A:27:CYS:HB2	1:A:28:PRO:HD2	1.60	0.83
1:D:27:CYS:HB2	1:D:28:PRO:CD	2.08	0.83
1:B:213:LEU:HD13	1:B:240:LEU:HD21	1.59	0.83
1:B:85:LEU:HB2	1:B:109:ILE:HG22	1.61	0.83
1:B:211:GLU:N	1:B:211:GLU:OE1	2.12	0.82
1:E:292:LYS:N	1:E:292:LYS:HE2	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ILE:C	1:D:232:ILE:HD13	2.05	0.81
1:A:198:LEU:HD11	1:A:200:LEU:HD21	1.61	0.81
1:D:121:LEU:HD12	1:D:121:LEU:H	1.46	0.81
1:C:27:CYS:HB2	1:C:28:PRO:CD	2.10	0.81
1:D:167:GLY:O	1:D:170:ASP:HB2	1.80	0.81
1:E:232:ILE:HD13	1:E:232:ILE:C	2.06	0.81
1:C:121:LEU:HD12	1:C:121:LEU:N	1.97	0.80
1:D:232:ILE:HD13	1:D:232:ILE:O	1.82	0.80
1:B:83:LEU:HD12	1:B:84:VAL:N	1.96	0.80
1:D:139:PRO:HD2	1:D:142:VAL:HG21	1.62	0.80
1:C:232:ILE:HD13	1:C:232:ILE:O	1.80	0.79
1:D:176:TYR:CD2	1:D:177:LEU:N	2.50	0.79
1:D:239:PHE:O	1:D:241:PRO:CD	2.29	0.79
1:C:159:LEU:N	1:C:159:LEU:HD23	1.98	0.79
1:A:83:LEU:HD21	1:A:85:LEU:CD1	2.13	0.79
1:E:186:GLY:HA2	1:E:205:ILE:HG23	1.65	0.79
1:F:63:ASN:HA	1:F:87:ASN:O	1.83	0.79
1:F:316:PHE:O	1:F:319:VAL:HG12	1.82	0.79
1:B:316:PHE:O	1:B:319:VAL:HG12	1.83	0.78
1:C:174:LEU:HD12	1:C:174:LEU:C	2.07	0.78
1:E:316:PHE:O	1:E:319:VAL:HG12	1.82	0.78
1:A:33:CYS:HB2	1:A:37:VAL:O	1.85	0.77
1:A:290:GLY:O	1:A:291:VAL:HB	1.82	0.77
1:E:128:LEU:HB3	1:E:149:MET:HE1	1.66	0.77
3:E:2194:FLC:OG1	3:E:2194:FLC:OB2	2.01	0.77
1:A:33:CYS:HB3	1:A:38:VAL:HA	1.64	0.77
1:E:291:VAL:C	1:E:292:LYS:HE2	2.09	0.77
1:B:232:ILE:HD13	1:B:232:ILE:C	2.10	0.77
1:C:192:PRO:O	1:C:195:LEU:HB2	1.85	0.77
1:D:308:TYR:CD2	1:D:309:TRP:N	2.54	0.76
1:A:45:LEU:H	1:A:64:ASN:HB3	1.50	0.76
1:F:139:PRO:HD2	1:F:142:VAL:HG21	1.67	0.76
1:B:176:TYR:CD2	1:B:177:LEU:N	2.55	0.75
1:C:176:TYR:CD2	1:C:177:LEU:N	2.54	0.75
1:F:267:GLN:O	1:F:297:ASN:N	2.17	0.75
1:A:27:CYS:HB2	1:A:28:PRO:CD	2.16	0.75
1:E:63:ASN:HA	1:E:87:ASN:O	1.85	0.75
1:A:63:ASN:HA	1:A:87:ASN:O	1.87	0.75
1:A:59:LEU:HD13	1:A:61:LEU:HD22	1.67	0.75
1:A:69:LEU:HD23	1:A:93:ILE:HG12	1.69	0.75
1:A:113:HIS:CD2	1:A:134:ARG:CZ	2.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD11	1:A:200:LEU:HD22	1.68	0.75
1:B:83:LEU:HD12	1:B:84:VAL:H	1.51	0.75
1:D:128:LEU:HB3	1:D:149:MET:HE1	1.69	0.75
3:B:2191:FLC:OG2	3:B:2191:FLC:CA	2.35	0.74
3:C:2192:FLC:OA1	3:C:2192:FLC:OHB	1.99	0.74
1:A:186:GLY:HA2	1:A:205:ILE:HG23	1.68	0.74
1:F:182:ALA:HB3	1:F:184:LEU:HD23	1.69	0.74
1:B:273:THR:HG22	1:B:273:THR:O	1.86	0.74
1:A:178:ARG:HG3	1:A:199:HIS:HB2	1.70	0.74
1:E:114:LEU:HB2	1:E:133:ASN:OD1	1.86	0.74
1:B:63:ASN:HA	1:B:87:ASN:O	1.88	0.74
1:E:239:PHE:C	1:E:241:PRO:HD3	2.12	0.74
1:A:85:LEU:HB2	1:A:109:ILE:HG22	1.69	0.74
1:C:85:LEU:HB2	1:C:109:ILE:HG22	1.68	0.74
1:F:128:LEU:HB3	1:F:149:MET:HE1	1.70	0.73
1:F:186:GLY:HA2	1:F:205:ILE:HG23	1.70	0.73
1:D:114:LEU:HB2	1:D:133:ASN:OD1	1.89	0.73
1:D:266:LEU:HD23	1:D:296:TYR:HE1	1.53	0.73
1:A:239:PHE:C	1:A:241:PRO:HD2	2.14	0.72
1:E:286:PRO:HG2	1:E:293:ARG:HG3	1.70	0.72
1:D:186:GLY:HA2	1:D:205:ILE:HG23	1.70	0.72
1:F:191:LEU:HB3	1:F:192:PRO:CD	2.19	0.72
1:C:128:LEU:HB3	1:C:149:MET:HE1	1.70	0.72
1:F:247:HIS:HA	1:F:270:TYR:HB2	1.71	0.72
1:D:307:PRO:HG2	1:D:310:GLU:HB2	1.69	0.71
1:F:114:LEU:HB2	1:F:133:ASN:OD1	1.89	0.71
1:A:239:PHE:O	1:A:241:PRO:HD2	1.90	0.71
1:F:213:LEU:HD13	1:F:240:LEU:HD21	1.71	0.71
1:E:28:PRO:HB2	1:E:31:CYS:SG	2.30	0.71
1:E:182:ALA:HB3	1:E:184:LEU:HD23	1.72	0.71
1:A:184:LEU:N	1:A:184:LEU:CD2	2.52	0.71
1:F:153:GLU:OE1	1:F:178:ARG:HD3	1.91	0.71
1:D:28:PRO:HD3	1:D:51:GLU:O	1.90	0.71
1:C:277:THR:O	1:C:306:VAL:HB	1.90	0.71
1:E:133:ASN:H	1:E:157:ASN:ND2	1.88	0.71
1:D:104:LEU:HD12	1:D:122:PRO:HG2	1.73	0.70
1:D:150:ASN:HA	1:D:174:LEU:HB2	1.71	0.70
1:E:232:ILE:HD13	1:E:232:ILE:O	1.91	0.70
1:A:319:VAL:HG11	1:A:325:ILE:HD11	1.73	0.70
1:E:69:LEU:HD23	1:E:93:ILE:HG12	1.73	0.70
1:B:102:ARG:HH21	1:B:103:LYS:HE3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:PHE:O	1:D:319:VAL:HG12	1.91	0.70
1:E:178:ARG:HE	1:E:180:SER:HB3	1.57	0.70
1:B:235:GLY:O	1:B:238:SER:HB3	1.92	0.70
1:C:199:HIS:O	1:C:200:LEU:HD13	1.90	0.70
1:D:247:HIS:HA	1:D:270:TYR:HB2	1.71	0.70
1:E:245:GLU:HG2	1:E:268:VAL:CG1	2.22	0.70
1:B:293:ARG:CD	1:B:294:ALA:H	2.01	0.70
1:D:182:ALA:HB3	1:D:184:LEU:HD23	1.73	0.70
1:E:150:ASN:HA	1:E:174:LEU:HB2	1.72	0.69
1:C:174:LEU:C	1:C:174:LEU:CD1	2.65	0.69
1:F:28:PRO:HD3	1:F:51:GLU:O	1.92	0.69
1:F:167:GLY:O	1:F:170:ASP:HB2	1.91	0.69
1:F:307:PRO:HG2	1:F:310:GLU:HB2	1.74	0.69
1:B:319:VAL:HG11	1:B:325:ILE:HD11	1.74	0.69
1:D:69:LEU:HD23	1:D:93:ILE:HG12	1.74	0.69
1:F:273:THR:HG22	1:F:273:THR:O	1.91	0.69
1:A:150:ASN:HA	1:A:174:LEU:HB2	1.74	0.69
1:A:139:PRO:HD2	1:A:142:VAL:CG2	2.20	0.69
1:C:247:HIS:HA	1:C:270:TYR:HB2	1.75	0.69
1:C:319:VAL:HG22	1:C:320:THR:N	2.07	0.68
1:C:225:GLY:HA3	3:C:2192:FLC:OB2	1.94	0.68
1:B:128:LEU:HB3	1:B:149:MET:HE1	1.76	0.68
1:E:192:PRO:O	1:E:195:LEU:HB2	1.93	0.68
1:C:139:PRO:HD2	1:C:142:VAL:HG21	1.76	0.68
1:A:121:LEU:H	1:A:121:LEU:CD1	2.05	0.68
1:B:239:PHE:C	1:B:241:PRO:HD3	2.18	0.68
1:B:150:ASN:HA	1:B:174:LEU:HB2	1.75	0.68
1:A:174:LEU:CD1	1:A:174:LEU:C	2.66	0.68
1:F:121:LEU:HD12	1:F:121:LEU:N	2.03	0.68
1:C:59:LEU:HD13	1:C:61:LEU:HD22	1.76	0.68
1:C:167:GLY:O	1:C:170:ASP:HB2	1.94	0.68
1:A:51:GLU:OE2	1:A:51:GLU:HA	1.92	0.67
1:E:198:LEU:HD11	1:E:200:LEU:HD21	1.76	0.67
1:F:150:ASN:HB2	1:F:175:ASN:ND2	2.09	0.67
1:A:90:ILE:HD12	1:A:112:ASN:OD1	1.93	0.67
1:A:191:LEU:HB3	1:A:192:PRO:CD	2.25	0.67
1:A:240:LEU:CD2	1:A:243:LEU:HD22	2.24	0.67
1:D:213:LEU:HD13	1:D:240:LEU:HD21	1.76	0.67
1:C:277:THR:HA	1:C:305:PRO:O	1.95	0.67
1:C:69:LEU:HD23	1:C:93:ILE:HG12	1.75	0.67
1:D:311:VAL:HG11	1:D:327:PHE:HE1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:THR:O	1:E:306:VAL:HB	1.94	0.67
1:F:264:LYS:C	1:F:265:LEU:HD12	2.19	0.67
1:E:176:TYR:HD2	1:E:177:LEU:N	1.93	0.67
1:A:114:LEU:HB2	1:A:133:ASN:OD1	1.95	0.67
1:A:275:ASN:ND2	2:A:801:NAG:H61	2.10	0.67
1:B:239:PHE:O	1:B:241:PRO:HD2	1.94	0.67
1:C:240:LEU:HD23	1:C:243:LEU:HD22	1.75	0.67
1:D:277:THR:HA	1:D:305:PRO:O	1.94	0.67
1:F:329:ASN:C	1:F:329:ASN:HD22	2.02	0.67
1:E:277:THR:HA	1:E:305:PRO:O	1.95	0.67
1:D:178:ARG:NE	1:D:180:SER:HB3	2.09	0.67
1:D:86:VAL:HG12	1:D:87:ASN:N	2.09	0.66
1:E:273:THR:HG22	1:E:273:THR:O	1.95	0.66
1:B:293:ARG:HD3	1:B:294:ALA:N	2.07	0.66
1:C:191:LEU:HB3	1:C:192:PRO:CD	2.25	0.66
1:F:232:ILE:C	1:F:232:ILE:HD13	2.20	0.66
1:B:186:GLY:HA2	1:B:205:ILE:HG23	1.76	0.66
1:C:149:MET:O	1:C:150:ASN:HB3	1.94	0.66
1:F:293:ARG:NH1	1:F:296:TYR:CZ	2.63	0.66
1:A:232:ILE:C	1:A:232:ILE:CD1	2.67	0.66
1:F:277:THR:HA	1:F:305:PRO:O	1.95	0.66
1:A:153:GLU:OE1	1:A:178:ARG:HD2	1.96	0.66
1:B:178:ARG:HE	1:B:180:SER:HB3	1.61	0.66
1:F:239:PHE:C	1:F:241:PRO:HD3	2.20	0.66
1:C:59:LEU:HD13	1:C:61:LEU:CD2	2.26	0.65
1:C:121:LEU:H	1:C:121:LEU:CD1	1.97	0.65
1:E:139:PRO:HD2	1:E:142:VAL:HG21	1.78	0.65
1:C:51:GLU:OE2	1:C:51:GLU:HA	1.95	0.65
1:D:63:ASN:HA	1:D:87:ASN:O	1.96	0.65
1:E:213:LEU:HD13	1:E:240:LEU:HD21	1.77	0.65
1:F:121:LEU:H	1:F:121:LEU:CD1	1.99	0.65
1:C:113:HIS:CD2	1:C:134:ARG:CZ	2.80	0.65
1:A:30:GLY:HA3	1:A:43:LEU:HD22	1.78	0.65
1:A:149:MET:HE3	1:A:152:ILE:CG1	2.26	0.65
1:B:272:HIS:HD2	1:B:300:SER:OG	1.79	0.65
1:D:150:ASN:HB2	1:D:175:ASN:ND2	2.12	0.65
1:D:240:LEU:HB3	1:D:243:LEU:HB2	1.79	0.65
1:B:308:TYR:CZ	1:B:322:ARG:NH1	2.65	0.65
1:C:109:ILE:HD12	1:C:114:LEU:HD11	1.78	0.65
1:C:282:ASN:HD22	1:C:287:VAL:HG22	1.61	0.65
1:A:140:LYS:HG3	1:A:141:GLY:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:VAL:HG22	1:F:268:VAL:O	1.96	0.65
1:D:174:LEU:HD12	1:D:174:LEU:C	2.22	0.65
1:F:180:SER:OG	1:F:181:GLU:HG3	1.97	0.65
1:A:290:GLY:O	1:A:291:VAL:CB	2.44	0.64
1:B:129:ARG:NH2	1:B:153:GLU:HG3	2.12	0.64
1:A:319:VAL:HG22	1:A:320:THR:N	2.11	0.64
1:F:178:ARG:NE	1:F:180:SER:HB3	2.12	0.64
1:D:133:ASN:H	1:D:157:ASN:ND2	1.96	0.64
1:F:308:TYR:CE1	1:F:309:TRP:HE3	2.15	0.64
1:A:198:LEU:CD1	1:A:200:LEU:HD22	2.27	0.64
1:C:253:LEU:HB2	1:C:274:ASN:OD1	1.97	0.64
1:A:275:ASN:ND2	2:A:801:NAG:C6	2.61	0.64
1:E:33:CYS:HB3	1:E:38:VAL:HA	1.78	0.64
1:F:174:LEU:HD12	1:F:174:LEU:O	1.98	0.64
1:B:80:LEU:HD23	1:B:101:LEU:HD21	1.80	0.64
1:D:149:MET:O	1:D:150:ASN:HB3	1.98	0.64
1:E:167:GLY:O	1:E:170:ASP:HB2	1.98	0.64
1:F:308:TYR:CE1	1:F:309:TRP:CE3	2.86	0.64
1:F:80:LEU:HD23	1:F:101:LEU:HD21	1.80	0.64
1:A:69:LEU:HB2	1:A:93:ILE:HG23	1.79	0.63
1:A:113:HIS:CD2	1:A:134:ARG:NH2	2.65	0.63
1:D:30:GLY:HA3	1:D:43:LEU:HD22	1.79	0.63
1:B:277:THR:O	1:B:306:VAL:HB	1.99	0.63
1:B:59:LEU:HD13	1:B:61:LEU:CD2	2.28	0.63
1:F:37:VAL:HG13	1:F:58:LEU:HB2	1.80	0.63
1:A:232:ILE:O	1:A:232:ILE:CD1	2.43	0.63
1:B:200:LEU:O	1:B:203:ASN:ND2	2.30	0.63
1:C:211:GLU:OE1	1:C:211:GLU:N	2.30	0.63
1:C:276:ILE:CB	1:C:304:ASN:ND2	2.55	0.63
1:F:150:ASN:HA	1:F:174:LEU:HB2	1.80	0.63
1:C:239:PHE:C	1:C:241:PRO:HD3	2.23	0.63
1:C:178:ARG:HE	1:C:180:SER:HB3	1.64	0.63
1:D:273:THR:O	1:D:273:THR:HG22	1.98	0.63
1:B:192:PRO:O	1:B:195:LEU:HB2	1.98	0.63
1:C:178:ARG:NE	1:C:180:SER:HB3	2.14	0.63
1:C:261:PRO:O	1:C:293:ARG:NH2	2.31	0.62
1:E:99:SER:N	1:E:100:PRO:HD2	2.13	0.62
1:A:81:TYR:O	1:A:104:LEU:HD22	1.98	0.62
1:B:99:SER:N	1:B:100:PRO:HD2	2.14	0.62
1:B:319:VAL:HG22	1:B:320:THR:N	2.14	0.62
1:A:184:LEU:N	1:A:184:LEU:HD22	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:THR:HA	1:A:305:PRO:O	1.99	0.62
1:C:186:GLY:HA2	1:C:205:ILE:HG23	1.81	0.62
1:A:275:ASN:HD22	2:A:801:NAG:H4	1.63	0.62
1:F:261:PRO:O	1:F:293:ARG:NH2	2.31	0.62
1:B:69:LEU:HD23	1:B:93:ILE:CG1	2.27	0.62
1:B:114:LEU:HB2	1:B:133:ASN:OD1	1.99	0.62
1:D:319:VAL:HG22	1:D:320:THR:N	2.12	0.62
1:A:104:LEU:HD12	1:A:122:PRO:HG2	1.81	0.62
1:A:273:THR:HG22	1:A:273:THR:O	1.99	0.62
1:B:311:VAL:HG11	1:B:327:PHE:HE1	1.63	0.62
1:C:268:VAL:O	1:C:268:VAL:HG22	1.99	0.62
1:D:30:GLY:HA3	1:D:43:LEU:CD2	2.29	0.62
1:D:174:LEU:C	1:D:174:LEU:CD1	2.72	0.61
1:A:239:PHE:C	1:A:241:PRO:CD	2.73	0.61
1:C:232:ILE:HG21	1:C:257:PRO:HB3	1.81	0.61
1:C:245:GLU:CD	1:C:268:VAL:HG11	2.25	0.61
1:E:133:ASN:H	1:E:157:ASN:HD21	1.46	0.61
1:E:63:ASN:ND2	1:E:63:ASN:O	2.33	0.61
3:E:2194:FLC:OG1	3:E:2194:FLC:CBC	2.48	0.61
1:C:311:VAL:O	1:C:311:VAL:HG13	2.01	0.61
1:D:37:VAL:HG13	1:D:58:LEU:HB2	1.83	0.61
1:A:316:PHE:CD2	1:A:325:ILE:HD13	2.35	0.61
1:B:239:PHE:C	1:B:241:PRO:CD	2.73	0.61
1:A:149:MET:HE3	1:A:152:ILE:HG13	1.83	0.61
1:B:150:ASN:HB2	1:B:175:ASN:ND2	2.15	0.61
1:C:150:ASN:HB2	1:C:175:ASN:ND2	2.15	0.61
1:C:276:ILE:H	1:C:304:ASN:ND2	1.99	0.61
1:B:59:LEU:HD13	1:B:61:LEU:HD22	1.81	0.61
1:A:122:PRO:O	1:A:124:SER:N	2.34	0.60
1:D:240:LEU:CD2	1:D:243:LEU:HD22	2.30	0.60
1:E:59:LEU:HD13	1:E:61:LEU:CD2	2.31	0.60
1:C:260:LEU:HB2	1:C:261:PRO:HD3	1.84	0.60
1:E:240:LEU:HB3	1:E:243:LEU:HB2	1.83	0.60
1:F:178:ARG:HG3	1:F:199:HIS:HB2	1.83	0.60
1:C:264:LYS:C	1:C:265:LEU:HD12	2.27	0.60
1:F:63:ASN:O	1:F:63:ASN:ND2	2.35	0.60
1:B:232:ILE:HD13	1:B:232:ILE:O	2.01	0.60
1:A:153:GLU:OE1	1:A:178:ARG:CD	2.49	0.60
1:D:301:LEU:HB3	1:D:327:PHE:CD2	2.36	0.60
1:F:319:VAL:HG11	1:F:325:ILE:HD11	1.82	0.60
1:E:150:ASN:HB2	1:E:175:ASN:ND2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:GLY:HA3	1:F:43:LEU:HD22	1.81	0.60
1:F:239:PHE:O	1:F:241:PRO:HD3	2.00	0.60
1:F:33:CYS:HB2	1:F:37:VAL:O	2.02	0.60
1:F:44:GLY:HA2	1:F:64:ASN:HA	1.83	0.60
1:C:131:HIS:CD2	1:C:132:ASP:H	2.20	0.60
1:E:176:TYR:CD2	1:E:176:TYR:C	2.79	0.60
1:A:291:VAL:C	1:A:293:ARG:H	2.10	0.60
1:F:266:LEU:HD23	1:F:296:TYR:HE1	1.67	0.60
1:D:85:LEU:HB2	1:D:109:ILE:HG22	1.83	0.60
1:B:247:HIS:HA	1:B:270:TYR:HB2	1.84	0.59
1:E:59:LEU:HD13	1:E:61:LEU:HD22	1.83	0.59
1:F:36:ARG:O	1:F:57:THR:HG22	2.01	0.59
1:F:149:MET:O	1:F:150:ASN:HB3	2.02	0.59
1:F:240:LEU:HD23	1:F:243:LEU:HD22	1.83	0.59
1:A:180:SER:OG	1:A:181:GLU:CG	2.44	0.59
1:D:139:PRO:HD2	1:D:142:VAL:CG2	2.32	0.59
1:D:192:PRO:O	1:D:195:LEU:HB2	2.02	0.59
1:F:178:ARG:HE	1:F:180:SER:HB3	1.67	0.59
1:F:323:LEU:HD22	1:F:323:LEU:H	1.66	0.59
1:B:208:ILE:HG23	1:B:232:ILE:HB	1.84	0.59
1:A:37:VAL:HG13	1:A:58:LEU:HB2	1.85	0.59
1:E:140:LYS:HG3	1:E:141:GLY:H	1.68	0.59
3:F:2195:FLC:OA1	3:F:2195:FLC:OB2	2.20	0.59
1:A:98:PHE:C	1:A:100:PRO:HD2	2.27	0.59
1:A:174:LEU:HD11	1:A:192:PRO:HG2	1.83	0.59
1:C:232:ILE:C	1:C:232:ILE:CD1	2.69	0.59
1:D:113:HIS:CD2	1:D:134:ARG:CZ	2.86	0.59
1:F:28:PRO:HB2	1:F:31:CYS:SG	2.43	0.59
1:A:42:ASP:HA	1:A:63:ASN:HD22	1.66	0.59
1:B:33:CYS:HB3	1:B:38:VAL:HA	1.84	0.59
1:C:28:PRO:HD3	1:C:51:GLU:O	2.03	0.59
1:F:59:LEU:HD13	1:F:61:LEU:HD22	1.84	0.59
1:C:262:ASP:O	1:C:264:LYS:HD2	2.03	0.59
1:E:319:VAL:HG22	1:E:320:THR:N	2.17	0.59
1:E:262:ASP:O	1:E:264:LYS:HD2	2.02	0.58
1:B:273:THR:O	1:B:273:THR:CG2	2.52	0.58
1:E:174:LEU:HD12	1:E:174:LEU:O	2.02	0.58
1:E:311:VAL:HG11	1:E:327:PHE:HE1	1.67	0.58
1:F:197:GLU:CD	1:F:221:ARG:HD3	2.28	0.58
1:C:77:LEU:HD23	1:C:80:LEU:HD22	1.83	0.58
1:D:128:LEU:HB3	1:D:149:MET:CE	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2195:FLC:OB2	3:F:2195:FLC:CAC	2.51	0.58
1:A:184:LEU:HD23	1:A:184:LEU:H	1.66	0.58
1:C:99:SER:N	1:C:100:PRO:HD2	2.18	0.58
1:D:264:LYS:O	1:D:265:LEU:HD12	2.04	0.58
1:C:150:ASN:HA	1:C:174:LEU:HB2	1.85	0.58
1:F:138:VAL:CG1	1:F:164:PHE:CD1	2.87	0.58
1:A:240:LEU:O	1:A:241:PRO:C	2.45	0.58
1:B:109:ILE:HD12	1:B:114:LEU:HD11	1.85	0.58
1:D:140:LYS:HG3	1:D:141:GLY:H	1.69	0.58
1:A:86:VAL:HG12	1:A:87:ASN:N	2.17	0.58
1:E:51:GLU:OE2	1:E:51:GLU:HA	2.02	0.58
1:A:131:HIS:HA	1:A:155:GLY:O	2.04	0.58
1:A:207:ALA:HA	1:A:229:ILE:HG23	1.85	0.58
1:C:159:LEU:HD23	1:C:159:LEU:H	1.66	0.58
1:D:99:SER:N	1:D:100:PRO:HD2	2.18	0.58
1:D:90:ILE:HD12	1:D:112:ASN:OD1	2.04	0.57
1:F:33:CYS:HB3	1:F:38:VAL:HA	1.85	0.57
1:A:39:GLN:HA	1:A:39:GLN:OE1	2.05	0.57
1:E:80:LEU:HD23	1:E:101:LEU:HD21	1.86	0.57
1:F:99:SER:N	1:F:100:PRO:HD2	2.19	0.57
1:A:128:LEU:HB3	1:A:149:MET:CE	2.27	0.57
1:B:260:LEU:HB2	1:B:261:PRO:HD3	1.85	0.57
1:C:36:ARG:O	1:C:57:THR:HG22	2.05	0.57
1:C:133:ASN:H	1:C:157:ASN:ND2	2.03	0.57
1:E:121:LEU:HD12	1:E:121:LEU:N	2.13	0.57
1:A:42:ASP:OD1	1:A:63:ASN:ND2	2.37	0.57
1:B:33:CYS:CB	1:B:38:VAL:HA	2.35	0.57
1:B:108:TYR:HE1	1:B:127:GLU:HG2	1.69	0.57
1:F:234:ASN:HB3	1:F:258:ALA:HB3	1.86	0.57
1:C:273:THR:HG22	1:C:273:THR:O	2.04	0.57
1:E:178:ARG:NE	1:E:180:SER:HB3	2.18	0.57
1:F:276:ILE:H	1:F:304:ASN:ND2	2.03	0.57
1:A:234:ASN:HB3	1:A:258:ALA:HB3	1.86	0.57
1:C:118:PRO:O	1:C:121:LEU:HD11	2.05	0.57
1:E:247:HIS:HA	1:E:270:TYR:HB2	1.87	0.57
1:F:111:LYS:C	1:F:112:ASN:HD22	2.13	0.57
1:C:240:LEU:HB3	1:C:243:LEU:HB2	1.86	0.57
1:A:208:ILE:HG23	1:A:232:ILE:HB	1.86	0.56
1:D:63:ASN:O	1:D:63:ASN:ND2	2.37	0.56
1:B:239:PHE:O	1:B:241:PRO:CD	2.52	0.56
1:C:146:LEU:N	1:C:146:LEU:HD23	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:PRO:O	1:C:308:TYR:C	2.46	0.56
1:C:308:TYR:O	1:C:311:VAL:HG12	2.05	0.56
1:D:27:CYS:CB	1:D:28:PRO:CD	2.78	0.56
1:D:59:LEU:HD13	1:D:61:LEU:HD22	1.87	0.56
1:D:264:LYS:C	1:D:265:LEU:HD12	2.30	0.56
1:C:129:ARG:CZ	1:C:153:GLU:HG3	2.35	0.56
1:C:185:THR:O	1:C:205:ILE:HA	2.06	0.56
1:E:149:MET:O	1:E:150:ASN:HB3	2.06	0.56
1:A:291:VAL:C	1:A:293:ARG:N	2.60	0.56
1:A:216:TYR:O	1:A:219:LEU:HG	2.05	0.56
1:C:41:SER:O	1:C:42:ASP:HB2	2.05	0.56
1:F:128:LEU:CB	1:F:149:MET:HE1	2.35	0.56
1:F:133:ASN:H	1:F:157:ASN:ND2	2.03	0.56
1:A:150:ASN:O	1:A:176:TYR:N	2.37	0.56
1:F:140:LYS:HG3	1:F:141:GLY:H	1.70	0.56
1:A:70:ARG:O	1:A:71:LYS:C	2.48	0.56
1:C:176:TYR:CD2	1:C:176:TYR:C	2.83	0.56
1:D:33:CYS:HB3	1:D:38:VAL:HA	1.86	0.56
1:F:319:VAL:HG22	1:F:320:THR:N	2.20	0.56
1:A:36:ARG:O	1:A:57:THR:HG22	2.06	0.56
1:B:139:PRO:HD2	1:B:142:VAL:HG21	1.88	0.56
1:B:232:ILE:HG21	1:B:257:PRO:HB3	1.88	0.56
1:C:264:LYS:O	1:C:265:LEU:HD12	2.06	0.56
1:B:129:ARG:CZ	1:B:153:GLU:HG3	2.36	0.56
1:F:110:SER:O	1:F:112:ASN:ND2	2.39	0.56
1:F:128:LEU:HB3	1:F:149:MET:CE	2.34	0.56
1:E:191:LEU:HB3	1:E:192:PRO:CD	2.36	0.56
1:F:311:VAL:HG11	1:F:327:PHE:HE1	1.71	0.56
1:F:322:ARG:HH12	1:F:329:ASN:HB3	1.70	0.56
1:A:191:LEU:HB3	1:A:192:PRO:HD2	1.89	0.55
1:C:131:HIS:CD2	1:C:132:ASP:N	2.74	0.55
1:F:192:PRO:O	1:F:195:LEU:HB2	2.05	0.55
1:D:211:GLU:N	1:D:211:GLU:OE1	2.37	0.55
1:E:260:LEU:HB2	1:E:261:PRO:HD3	1.87	0.55
1:C:311:VAL:HG11	1:C:327:PHE:HE1	1.70	0.55
1:E:235:GLY:O	1:E:238:SER:HB3	2.05	0.55
1:A:237:LEU:O	1:A:263:LEU:HD21	2.06	0.55
1:A:240:LEU:N	1:A:241:PRO:CD	2.70	0.55
1:D:239:PHE:C	1:D:241:PRO:CD	2.76	0.55
1:D:44:GLY:HA2	1:D:64:ASN:HA	1.88	0.55
1:F:149:MET:HB2	1:F:172:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:HIS:HA	1:A:270:TYR:HB2	1.88	0.55
1:B:262:ASP:O	1:B:264:LYS:HD2	2.06	0.55
1:C:33:CYS:HB2	1:C:37:VAL:O	2.05	0.55
1:D:239:PHE:O	1:D:241:PRO:HD2	2.04	0.55
1:D:266:LEU:HD23	1:D:296:TYR:CE1	2.39	0.55
1:E:245:GLU:CD	1:E:268:VAL:HG11	2.32	0.55
1:A:316:PHE:O	1:A:319:VAL:HG12	2.07	0.55
1:D:80:LEU:HD23	1:D:101:LEU:HD21	1.89	0.55
1:D:191:LEU:HB3	1:D:192:PRO:CD	2.36	0.55
1:E:85:LEU:HB2	1:E:109:ILE:HG22	1.89	0.55
1:A:159:LEU:HD23	1:A:159:LEU:N	2.22	0.55
1:B:69:LEU:CD2	1:B:93:ILE:HG12	2.33	0.55
1:C:234:ASN:HB3	1:C:258:ALA:HB3	1.89	0.55
1:D:128:LEU:CB	1:D:149:MET:HE1	2.37	0.55
1:C:256:VAL:HG13	1:C:257:PRO:HD2	1.89	0.54
1:D:245:GLU:HG2	1:D:268:VAL:CG1	2.37	0.54
1:E:105:GLN:HA	1:E:125:LEU:HA	1.89	0.54
1:F:191:LEU:CB	1:F:192:PRO:CD	2.85	0.54
1:F:322:ARG:NH1	1:F:329:ASN:HB3	2.22	0.54
1:D:178:ARG:HG3	1:D:199:HIS:HB2	1.88	0.54
1:D:83:LEU:HD21	1:D:85:LEU:HD11	1.88	0.54
1:D:232:ILE:C	1:D:232:ILE:CD1	2.79	0.54
1:E:146:LEU:N	1:E:146:LEU:HD23	2.22	0.54
1:E:30:GLY:HA3	1:E:43:LEU:HD22	1.90	0.54
1:E:264:LYS:C	1:E:265:LEU:HD12	2.32	0.54
1:A:245:GLU:CD	1:A:268:VAL:HG11	2.32	0.54
1:C:133:ASN:H	1:C:157:ASN:HD21	1.54	0.54
1:D:59:LEU:HD13	1:D:61:LEU:CD2	2.38	0.54
1:E:27:CYS:CB	1:E:28:PRO:CD	2.75	0.54
1:F:237:LEU:O	1:F:263:LEU:HD21	2.08	0.54
1:B:182:ALA:HB3	1:B:184:LEU:HD23	1.89	0.54
1:D:216:TYR:O	1:D:219:LEU:HG	2.07	0.54
2:D:807:NAG:H3	2:D:807:NAG:H82	1.90	0.54
1:D:42:ASP:HA	1:D:63:ASN:HD22	1.73	0.54
1:E:276:ILE:H	1:E:304:ASN:ND2	2.06	0.54
1:F:105:GLN:O	1:F:125:LEU:HD12	2.08	0.54
1:C:140:LYS:HG3	1:C:141:GLY:H	1.73	0.54
1:C:240:LEU:O	1:C:241:PRO:C	2.51	0.54
1:D:256:VAL:HG13	1:D:271:LEU:HD11	1.89	0.54
1:E:282:ASN:HD22	1:E:287:VAL:HG22	1.73	0.54
1:F:77:LEU:HD23	1:F:80:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:HB3	1:B:320:THR:HG23	1.90	0.53
1:E:36:ARG:O	1:E:57:THR:HG22	2.07	0.53
1:E:232:ILE:HG21	1:E:257:PRO:HB3	1.89	0.53
1:F:146:LEU:N	1:F:146:LEU:HD23	2.22	0.53
1:A:213:LEU:HB3	1:A:240:LEU:HD11	1.91	0.53
1:B:206:GLN:O	1:B:207:ALA:HB2	2.07	0.53
1:C:182:ALA:HB3	1:C:184:LEU:HD23	1.90	0.53
1:D:277:THR:O	1:D:306:VAL:HB	2.08	0.53
1:E:128:LEU:CB	1:E:149:MET:HE1	2.37	0.53
1:E:240:LEU:O	1:E:241:PRO:C	2.49	0.53
1:F:276:ILE:CB	1:F:304:ASN:ND2	2.65	0.53
1:A:49:PRO:HG2	1:A:52:ILE:HD11	1.90	0.53
1:A:178:ARG:CZ	1:B:43:LEU:HD23	2.38	0.53
1:A:149:MET:CE	1:A:152:ILE:HG12	2.38	0.53
1:B:70:ARG:O	1:B:71:LYS:C	2.51	0.53
1:B:105:GLN:HA	1:B:125:LEU:HA	1.91	0.53
1:D:180:SER:OG	1:D:181:GLU:HG3	2.09	0.53
1:C:235:GLY:O	1:C:238:SER:CB	2.52	0.53
1:F:322:ARG:HH22	1:F:329:ASN:N	2.07	0.53
1:B:199:HIS:O	1:B:200:LEU:HD13	2.09	0.53
1:D:198:LEU:HD11	1:D:200:LEU:HD21	1.90	0.53
1:A:240:LEU:HB3	1:A:243:LEU:HB2	1.90	0.53
1:C:189:LYS:O	1:C:215:ARG:HD3	2.09	0.53
1:D:138:VAL:CG1	1:D:164:PHE:CD1	2.92	0.53
1:E:322:ARG:HD3	1:E:322:ARG:C	2.33	0.53
1:A:85:LEU:HB2	1:A:109:ILE:CG2	2.38	0.53
1:A:98:PHE:O	1:A:101:LEU:HB2	2.09	0.53
1:A:179:ILE:HG22	1:A:179:ILE:O	2.07	0.53
1:A:295:TYR:HB3	1:A:318:CYS:O	2.09	0.53
1:B:39:GLN:OE1	1:B:41:SER:OG	2.23	0.53
1:B:130:ILE:HG12	1:B:130:ILE:O	2.09	0.53
1:C:114:LEU:HB2	1:C:133:ASN:OD1	2.09	0.53
1:D:33:CYS:HB2	1:D:37:VAL:O	2.09	0.53
1:E:59:LEU:HD22	1:E:61:LEU:HD22	1.91	0.53
1:E:245:GLU:CG	1:E:268:VAL:CG1	2.86	0.53
1:A:290:GLY:HA3	1:A:292:LYS:CE	2.39	0.53
1:B:121:LEU:H	1:B:121:LEU:CD1	2.15	0.53
1:D:174:LEU:O	1:D:174:LEU:CD1	2.53	0.53
1:D:308:TYR:O	1:D:311:VAL:HG12	2.09	0.53
1:F:277:THR:O	1:F:306:VAL:HB	2.09	0.53
1:A:81:TYR:CE1	1:A:105:GLN:OE1	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:N	1:C:159:LEU:CD2	2.71	0.52
1:F:159:LEU:HD23	1:F:159:LEU:N	2.24	0.52
1:F:264:LYS:HA	1:F:293:ARG:HD2	1.92	0.52
1:F:101:LEU:HB3	1:F:104:LEU:HB2	1.91	0.52
1:B:131:HIS:CD2	1:B:132:ASP:H	2.28	0.52
1:B:207:ALA:HA	1:B:229:ILE:HG23	1.91	0.52
1:E:108:TYR:HE1	1:E:127:GLU:HG2	1.75	0.52
1:F:176:TYR:HD2	1:F:177:LEU:N	2.03	0.52
1:B:69:LEU:HD21	1:B:90:ILE:HD13	1.92	0.52
1:D:213:LEU:HB3	1:D:240:LEU:HD11	1.91	0.52
1:F:264:LYS:O	1:F:293:ARG:HA	2.09	0.52
1:B:264:LYS:C	1:B:265:LEU:HD12	2.35	0.52
1:A:206:GLN:O	1:A:207:ALA:HB2	2.09	0.52
1:F:273:THR:O	1:F:273:THR:CG2	2.58	0.52
1:B:131:HIS:CD2	1:B:132:ASP:N	2.78	0.52
1:D:81:TYR:O	1:D:104:LEU:HD22	2.09	0.52
1:E:42:ASP:HA	1:E:63:ASN:HD22	1.74	0.52
1:B:167:GLY:O	1:B:170:ASP:HB2	2.09	0.52
1:C:106:LYS:HG2	1:C:127:GLU:HB3	1.90	0.52
1:C:213:LEU:HD13	1:C:240:LEU:HD21	1.92	0.52
1:C:276:ILE:CB	1:C:304:ASN:HD22	2.09	0.52
1:D:289:PHE:HD1	1:F:307:PRO:HD3	1.75	0.52
1:E:159:LEU:N	1:E:159:LEU:HD23	2.25	0.52
1:F:232:ILE:HD13	1:F:232:ILE:O	2.09	0.52
1:A:319:VAL:CG2	1:A:320:THR:N	2.72	0.52
1:B:59:LEU:HD22	1:B:61:LEU:HD22	1.92	0.52
1:D:133:ASN:H	1:D:157:ASN:HD21	1.58	0.52
1:A:262:ASP:O	1:A:264:LYS:HD2	2.10	0.51
1:A:323:LEU:HD22	1:A:323:LEU:H	1.75	0.51
1:C:37:VAL:HG13	1:C:58:LEU:HB2	1.92	0.51
1:D:36:ARG:O	1:D:57:THR:HG22	2.10	0.51
1:A:30:GLY:HA3	1:A:43:LEU:CD2	2.40	0.51
1:A:48:VAL:HG13	1:A:61:LEU:HD11	1.91	0.51
1:A:56:THR:HG22	1:A:80:LEU:HD13	1.92	0.51
1:E:180:SER:O	1:E:181:GLU:C	2.53	0.51
1:A:135:ILE:O	1:A:158:PRO:HD2	2.11	0.51
1:C:282:ASN:ND2	1:C:287:VAL:HG22	2.24	0.51
1:F:27:CYS:CB	1:F:28:PRO:CD	2.77	0.51
1:F:135:ILE:O	1:F:158:PRO:HD2	2.10	0.51
1:B:176:TYR:CD2	1:B:176:TYR:C	2.88	0.51
1:D:199:HIS:N	1:D:199:HIS:CD2	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LEU:CD2	1:E:146:LEU:H	2.20	0.51
1:A:164:PHE:HZ	1:A:179:ILE:HD13	1.75	0.51
1:A:220:TYR:HD2	1:A:220:TYR:N	2.08	0.51
1:B:62:GLN:HG3	1:B:86:VAL:O	2.10	0.51
1:B:107:LEU:HD11	1:B:109:ILE:HG23	1.91	0.51
1:D:146:LEU:HD23	1:D:146:LEU:N	2.26	0.51
1:D:298:GLY:HA2	1:D:324:ALA:O	2.10	0.51
1:B:30:GLY:HA3	1:B:43:LEU:HD22	1.92	0.51
1:F:131:HIS:O	1:F:133:ASN:ND2	2.44	0.51
1:C:42:ASP:HA	1:C:63:ASN:HD22	1.75	0.51
1:C:288:GLY:O	1:C:289:PHE:C	2.54	0.51
1:F:138:VAL:HG11	1:F:164:PHE:CD1	2.45	0.51
1:F:191:LEU:HB3	1:F:192:PRO:HD2	1.90	0.51
1:B:180:SER:O	1:B:181:GLU:C	2.54	0.51
1:E:200:LEU:O	1:E:203:ASN:ND2	2.44	0.51
1:E:208:ILE:HG23	1:E:232:ILE:HB	1.93	0.51
1:F:113:HIS:CD2	1:F:134:ARG:CZ	2.94	0.51
1:B:159:LEU:N	1:B:159:LEU:HD23	2.26	0.51
1:D:264:LYS:HA	1:D:293:ARG:HB3	1.92	0.51
1:E:240:LEU:HD23	1:E:243:LEU:HD13	1.92	0.51
1:E:322:ARG:HD3	1:E:322:ARG:O	2.11	0.51
1:F:232:ILE:HG21	1:F:257:PRO:HB3	1.93	0.51
1:A:149:MET:CE	1:A:152:ILE:CG1	2.89	0.50
1:A:201:ASP:OD1	1:A:201:ASP:N	2.38	0.50
1:A:305:PRO:C	1:A:306:VAL:HG12	2.36	0.50
1:B:143:PHE:O	1:B:144:SER:C	2.54	0.50
1:D:81:TYR:CE1	1:D:105:GLN:OE1	2.63	0.50
1:F:133:ASN:H	1:F:157:ASN:HD21	1.59	0.50
1:D:319:VAL:HG11	1:D:325:ILE:HD11	1.93	0.50
1:E:273:THR:O	1:E:273:THR:CG2	2.60	0.50
1:A:72:ASP:OD2	1:A:75:LYS:HD2	2.11	0.50
1:A:81:TYR:HE1	1:A:105:GLN:OE1	1.94	0.50
1:F:176:TYR:CD2	1:F:176:TYR:C	2.90	0.50
1:A:198:LEU:CD1	1:A:200:LEU:CD2	2.81	0.50
1:B:311:VAL:HG11	1:B:327:PHE:CE1	2.45	0.50
1:C:30:GLY:HA3	1:C:43:LEU:HD22	1.93	0.50
1:C:191:LEU:CB	1:C:192:PRO:CD	2.88	0.50
1:D:308:TYR:CE2	1:D:309:TRP:HB3	2.46	0.50
1:E:234:ASN:HB3	1:E:258:ALA:HB3	1.92	0.50
1:E:264:LYS:O	1:E:265:LEU:HD12	2.12	0.50
1:B:133:ASN:H	1:B:157:ASN:ND2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLU:HG2	1:D:268:VAL:HG13	1.92	0.50
1:D:307:PRO:O	1:D:308:TYR:C	2.54	0.50
1:A:104:LEU:CD1	1:A:125:LEU:HD13	2.42	0.50
1:A:213:LEU:HD13	1:A:240:LEU:HD21	1.93	0.50
1:B:213:LEU:HB3	1:B:240:LEU:HD11	1.94	0.50
1:E:199:HIS:N	1:E:199:HIS:CD2	2.79	0.50
1:F:105:GLN:HA	1:F:125:LEU:HA	1.93	0.50
1:B:234:ASN:HB3	1:B:258:ALA:HB3	1.93	0.50
1:A:63:ASN:ND2	1:A:63:ASN:O	2.45	0.50
1:C:146:LEU:H	1:C:146:LEU:CD2	2.20	0.50
1:C:319:VAL:CG2	1:C:320:THR:N	2.74	0.50
1:D:105:GLN:HA	1:D:125:LEU:HA	1.93	0.50
1:D:264:LYS:HA	1:D:293:ARG:CB	2.42	0.50
1:E:128:LEU:HB3	1:E:149:MET:CE	2.41	0.50
1:E:293:ARG:HD3	1:E:293:ARG:C	2.36	0.50
1:A:33:CYS:CB	1:A:38:VAL:HA	2.37	0.49
1:A:205:ILE:HG13	1:A:227:ASN:OD1	2.12	0.49
1:B:51:GLU:HA	1:B:51:GLU:OE2	2.12	0.49
1:B:312:GLN:HG3	1:B:313:PRO:HD2	1.93	0.49
1:C:247:HIS:ND1	3:C:2192:FLC:HG2	2.27	0.49
1:F:59:LEU:HD13	1:F:61:LEU:CD2	2.42	0.49
1:F:69:LEU:HD23	1:F:93:ILE:HG12	1.93	0.49
1:A:275:ASN:HD22	2:A:801:NAG:C4	2.26	0.49
1:A:25:ALA:C	1:A:26:MET:O	2.54	0.49
1:C:178:ARG:HG3	1:C:199:HIS:HB2	1.92	0.49
1:D:260:LEU:HB2	1:D:261:PRO:HD3	1.94	0.49
1:B:27:CYS:CB	1:B:28:PRO:CD	2.78	0.49
1:B:224:LEU:HB2	1:B:248:LEU:HD13	1.93	0.49
1:C:111:LYS:O	1:C:112:ASN:ND2	2.46	0.49
1:C:312:GLN:HG3	1:C:313:PRO:HD2	1.94	0.49
1:A:99:SER:N	1:A:100:PRO:HD2	2.27	0.49
1:C:110:SER:O	1:C:112:ASN:ND2	2.45	0.49
1:C:113:HIS:HA	1:C:134:ARG:HD2	1.95	0.49
1:F:138:VAL:O	1:F:138:VAL:HG13	2.12	0.49
1:F:219:LEU:C	1:F:220:TYR:HD2	2.20	0.49
1:A:122:PRO:O	1:A:123:SER:C	2.54	0.49
1:C:84:VAL:HG13	1:C:86:VAL:HG23	1.95	0.49
1:C:199:HIS:CD2	1:C:199:HIS:N	2.80	0.49
1:D:70:ARG:O	1:D:73:ASP:HB2	2.12	0.49
1:F:85:LEU:HB2	1:F:109:ILE:HG22	1.94	0.49
1:F:301:LEU:HB3	1:F:327:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:O	1:A:26:MET:O	2.30	0.49
1:B:136:ARG:HG3	1:B:158:PRO:HG2	1.93	0.49
1:B:295:TYR:CB	1:B:320:THR:HG23	2.43	0.49
1:E:113:HIS:HA	1:E:134:ARG:HD2	1.94	0.49
1:F:33:CYS:CB	1:F:38:VAL:HA	2.42	0.49
1:C:69:LEU:HD21	1:C:90:ILE:HD13	1.95	0.49
1:C:138:VAL:CG1	1:C:164:PHE:CD1	2.96	0.49
1:D:301:LEU:O	1:D:304:ASN:HB2	2.13	0.49
1:F:211:GLU:OE1	1:F:211:GLU:N	2.42	0.49
1:D:70:ARG:O	1:D:71:LYS:C	2.56	0.49
1:E:104:LEU:HD12	1:E:122:PRO:HG2	1.95	0.49
1:F:261:PRO:HA	1:F:293:ARG:NH2	2.27	0.49
1:A:178:ARG:CG	1:A:199:HIS:HB2	2.41	0.49
1:B:33:CYS:HB2	1:B:37:VAL:O	2.13	0.49
1:C:59:LEU:HD22	1:C:61:LEU:HD22	1.94	0.49
1:A:27:CYS:O	1:B:221:ARG:NH1	2.46	0.48
1:A:86:VAL:HG13	1:A:110:SER:HB2	1.94	0.48
1:E:37:VAL:HG13	1:E:58:LEU:HB2	1.95	0.48
1:F:260:LEU:HD22	1:F:266:LEU:CD2	2.44	0.48
1:A:33:CYS:CB	1:A:37:VAL:O	2.58	0.48
1:C:63:ASN:O	1:C:63:ASN:ND2	2.47	0.48
1:C:81:TYR:O	1:C:105:GLN:N	2.44	0.48
1:D:135:ILE:O	1:D:158:PRO:HD2	2.13	0.48
1:F:40:CYS:HB2	1:F:61:LEU:HB3	1.94	0.48
1:F:54:PRO:C	1:F:56:THR:H	2.21	0.48
1:F:138:VAL:CG1	1:F:164:PHE:HD1	2.25	0.48
1:F:329:ASN:C	1:F:329:ASN:ND2	2.69	0.48
1:B:140:LYS:HG3	1:B:141:GLY:H	1.78	0.48
1:B:184:LEU:N	1:B:184:LEU:CD2	2.76	0.48
1:D:308:TYR:HD2	1:D:309:TRP:N	2.07	0.48
1:E:33:CYS:CB	1:E:38:VAL:HA	2.41	0.48
1:E:239:PHE:O	1:E:241:PRO:HD3	2.12	0.48
1:D:261:PRO:O	1:D:293:ARG:NH2	2.45	0.48
1:F:174:LEU:HD12	1:F:174:LEU:C	2.38	0.48
1:B:191:LEU:HB3	1:B:192:PRO:CD	2.43	0.48
1:C:325:ILE:HG22	1:C:327:PHE:HB2	1.94	0.48
1:D:176:TYR:CD2	1:D:176:TYR:C	2.91	0.48
1:E:133:ASN:HB2	1:E:157:ASN:HD21	1.78	0.48
1:E:178:ARG:HG3	1:E:199:HIS:HB2	1.94	0.48
1:F:308:TYR:CD1	1:F:309:TRP:CE3	3.01	0.48
1:D:264:LYS:O	1:D:293:ARG:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ARG:HG3	1:E:158:PRO:HG2	1.95	0.48
1:B:28:PRO:HB2	1:B:31:CYS:SG	2.53	0.48
1:C:273:THR:HA	1:C:303:ASN:O	2.13	0.48
1:B:274:ASN:HB3	1:B:275:ASN:H	1.53	0.48
1:C:130:ILE:HG12	1:C:130:ILE:O	2.14	0.48
1:E:291:VAL:O	1:E:292:LYS:HG3	2.13	0.48
1:F:216:TYR:O	1:F:219:LEU:HG	2.14	0.48
1:A:225:GLY:HA2	1:A:249:ASP:O	2.14	0.47
1:B:117:ILE:HB	1:B:142:VAL:HG11	1.96	0.47
1:E:138:VAL:CG1	1:E:164:PHE:CD1	2.97	0.47
1:E:281:VAL:HA	1:E:315:THR:OG1	2.13	0.47
1:A:174:LEU:O	1:A:174:LEU:HD13	2.09	0.47
1:A:290:GLY:HA3	1:A:292:LYS:HE3	1.95	0.47
1:B:80:LEU:HD23	1:B:101:LEU:CD2	2.44	0.47
1:C:33:CYS:CB	1:C:38:VAL:HA	2.44	0.47
1:C:111:LYS:C	1:C:112:ASN:HD22	2.22	0.47
1:E:174:LEU:HD12	1:E:174:LEU:C	2.39	0.47
1:A:191:LEU:CB	1:A:192:PRO:CD	2.88	0.47
1:D:77:LEU:HD23	1:D:80:LEU:HD22	1.97	0.47
1:E:282:ASN:ND2	1:E:287:VAL:HG22	2.28	0.47
1:F:174:LEU:C	1:F:174:LEU:CD1	2.87	0.47
1:F:180:SER:CB	1:F:181:GLU:HG3	2.44	0.47
1:C:33:CYS:HB3	1:C:38:VAL:HA	1.95	0.47
1:C:245:GLU:CD	1:C:268:VAL:CG1	2.87	0.47
1:C:253:LEU:HB2	1:C:274:ASN:CG	2.38	0.47
1:E:273:THR:HA	1:E:303:ASN:O	2.14	0.47
1:F:69:LEU:HD21	1:F:90:ILE:HD13	1.96	0.47
1:F:139:PRO:HD2	1:F:142:VAL:CG2	2.42	0.47
1:D:319:VAL:CG2	1:D:320:THR:N	2.77	0.47
1:E:307:PRO:HB2	1:E:309:TRP:CD2	2.49	0.47
1:A:220:TYR:N	1:A:220:TYR:CD2	2.82	0.47
1:A:291:VAL:H	1:A:292:LYS:HD2	1.80	0.47
1:A:319:VAL:HG22	1:A:320:THR:H	1.79	0.47
1:B:48:VAL:HB	1:B:73:ASP:OD2	2.14	0.47
1:B:149:MET:O	1:B:150:ASN:HB3	2.14	0.47
1:A:27:CYS:CB	1:A:28:PRO:CD	2.85	0.47
1:A:114:LEU:O	1:A:134:ARG:HB2	2.14	0.47
1:A:201:ASP:O	1:A:202:HIS:HB2	2.15	0.47
1:B:210:LEU:HB3	1:B:211:GLU:OE1	2.14	0.47
1:B:277:THR:HA	1:B:305:PRO:O	2.14	0.47
1:B:319:VAL:CG2	1:B:320:THR:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ILE:HG23	1:D:232:ILE:HB	1.97	0.47
1:D:273:THR:O	1:D:273:THR:CG2	2.63	0.47
1:E:211:GLU:OE1	1:E:211:GLU:N	2.41	0.47
1:E:276:ILE:CB	1:E:304:ASN:ND2	2.73	0.47
1:F:195:LEU:O	1:F:219:LEU:HD23	2.14	0.47
1:F:131:HIS:CD2	1:F:132:ASP:H	2.32	0.47
1:F:192:PRO:HD2	1:F:195:LEU:HD22	1.96	0.47
1:F:282:ASN:HD22	1:F:287:VAL:HG22	1.79	0.47
1:A:128:LEU:CB	1:A:149:MET:HE1	2.32	0.47
1:D:247:HIS:ND1	3:D:2193:FCL:HA1	2.30	0.47
1:F:30:GLY:HA3	1:F:43:LEU:CD2	2.43	0.47
1:F:266:LEU:HD23	1:F:296:TYR:CE1	2.50	0.47
1:F:293:ARG:NH1	1:F:296:TYR:CE2	2.83	0.47
1:A:32:HIS:ND1	1:A:32:HIS:C	2.73	0.47
1:A:313:PRO:C	1:A:315:THR:N	2.72	0.47
1:B:133:ASN:H	1:B:157:ASN:HD21	1.62	0.47
1:B:225:GLY:HA3	3:B:2191:FCL:OB2	2.15	0.47
1:F:51:GLU:OE2	1:F:51:GLU:HA	2.14	0.47
1:F:240:LEU:HB3	1:F:243:LEU:HB2	1.97	0.47
1:F:292:LYS:HD2	1:F:293:ARG:H	1.80	0.47
1:F:322:ARG:C	1:F:324:ALA:H	2.23	0.47
1:A:44:GLY:HA2	1:A:64:ASN:HA	1.96	0.46
1:A:174:LEU:C	1:A:174:LEU:HD13	2.40	0.46
1:A:178:ARG:NE	1:A:180:SER:HB3	2.30	0.46
1:E:174:LEU:C	1:E:174:LEU:CD1	2.88	0.46
1:F:226:HIS:H	1:F:250:ASN:HB2	1.80	0.46
1:A:42:ASP:C	1:B:178:ARG:HH12	2.24	0.46
1:F:42:ASP:HA	1:F:63:ASN:HD22	1.79	0.46
1:F:80:LEU:HD23	1:F:101:LEU:CD2	2.45	0.46
1:F:199:HIS:O	1:F:200:LEU:HD13	2.15	0.46
1:A:105:GLN:HA	1:A:125:LEU:HA	1.96	0.46
1:D:261:PRO:HA	1:D:293:ARG:NH2	2.31	0.46
1:E:63:ASN:O	1:E:63:ASN:CG	2.57	0.46
1:F:80:LEU:HB3	1:F:101:LEU:CD2	2.46	0.46
1:F:111:LYS:O	1:F:112:ASN:ND2	2.47	0.46
1:F:213:LEU:HB3	1:F:240:LEU:HD11	1.95	0.46
1:D:311:VAL:HG11	1:D:327:PHE:CE1	2.47	0.46
1:E:131:HIS:CD2	1:E:132:ASP:N	2.84	0.46
1:E:138:VAL:HA	1:E:139:PRO:HD3	1.77	0.46
1:E:207:ALA:HA	1:E:229:ILE:HG23	1.97	0.46
1:B:37:VAL:HG13	1:B:58:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:GLY:HA3	1:E:43:LEU:CD2	2.44	0.46
1:A:32:HIS:HB2	1:B:176:TYR:CD1	2.50	0.46
1:A:93:ILE:CD1	1:A:114:LEU:CD2	2.87	0.46
1:B:181:GLU:HA	1:B:202:HIS:O	2.16	0.46
1:B:208:ILE:HG12	1:B:208:ILE:O	2.15	0.46
1:C:245:GLU:HG2	1:C:268:VAL:CG1	2.45	0.46
1:D:276:ILE:H	1:D:304:ASN:ND2	2.14	0.46
1:E:32:HIS:ND1	1:E:32:HIS:C	2.74	0.46
1:A:122:PRO:C	1:A:124:SER:N	2.73	0.46
1:A:159:LEU:HD23	1:A:159:LEU:H	1.79	0.46
1:B:80:LEU:HB3	1:B:101:LEU:CD2	2.45	0.46
1:B:146:LEU:H	1:B:146:LEU:HG	1.33	0.46
1:D:117:ILE:HB	1:D:142:VAL:HG11	1.98	0.46
1:D:322:ARG:HH22	1:D:328:GLY:C	2.24	0.46
1:B:69:LEU:HD23	1:B:93:ILE:CD1	2.45	0.46
1:E:129:ARG:CZ	1:E:153:GLU:HG3	2.46	0.46
1:F:298:GLY:HA2	1:F:324:ALA:O	2.16	0.46
1:A:111:LYS:C	1:A:112:ASN:HD22	2.24	0.46
1:C:276:ILE:N	1:C:304:ASN:ND2	2.64	0.46
1:D:297:ASN:HD22	1:D:297:ASN:HA	1.51	0.46
1:D:323:LEU:HD22	1:D:323:LEU:H	1.80	0.46
1:E:98:PHE:C	1:E:100:PRO:HD2	2.41	0.46
1:E:111:LYS:HG2	1:E:132:ASP:OD1	2.16	0.46
1:E:225:GLY:O	1:E:226:HIS:C	2.57	0.46
1:E:312:GLN:HG3	1:E:313:PRO:HD2	1.98	0.46
1:F:71:LYS:HD2	1:F:72:ASP:OD1	2.15	0.46
1:F:301:LEU:HD12	1:F:301:LEU:HA	1.79	0.46
1:A:94:HIS:O	1:A:97:ALA:HB2	2.16	0.45
1:A:312:GLN:O	1:A:315:THR:HB	2.16	0.45
1:B:191:LEU:HB2	1:B:216:TYR:OH	2.16	0.45
1:C:30:GLY:HA3	1:C:43:LEU:CD2	2.45	0.45
1:C:105:GLN:O	1:C:125:LEU:HD12	2.16	0.45
1:E:118:PRO:O	1:E:121:LEU:HD11	2.15	0.45
1:A:140:LYS:C	1:A:142:VAL:H	2.24	0.45
1:C:240:LEU:HD23	1:C:243:LEU:HD13	1.98	0.45
1:D:51:GLU:OE2	1:D:51:GLU:HA	2.15	0.45
1:D:118:PRO:O	1:D:121:LEU:HD11	2.16	0.45
1:D:274:ASN:HB3	1:D:275:ASN:H	1.65	0.45
1:D:291:VAL:HG13	1:D:292:LYS:N	2.30	0.45
1:A:264:LYS:C	1:A:265:LEU:HD12	2.42	0.45
1:B:178:ARG:HG3	1:B:199:HIS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:SER:O	1:C:181:GLU:C	2.60	0.45
1:D:195:LEU:O	1:D:219:LEU:HD23	2.16	0.45
1:E:195:LEU:HD12	1:E:195:LEU:HA	1.74	0.45
1:E:232:ILE:C	1:E:232:ILE:CD1	2.78	0.45
1:E:307:PRO:HB2	1:E:309:TRP:CE3	2.52	0.45
1:C:138:VAL:HA	1:C:139:PRO:HD3	1.69	0.45
1:C:164:PHE:HZ	1:C:179:ILE:HD13	1.81	0.45
1:E:109:ILE:HD12	1:E:114:LEU:HD11	1.98	0.45
1:F:148:ASN:N	1:F:148:ASN:ND2	2.64	0.45
1:A:57:THR:HG23	1:A:58:LEU:N	2.32	0.45
1:A:250:ASN:ND2	1:A:273:THR:HB	2.32	0.45
1:A:273:THR:O	1:A:273:THR:CG2	2.64	0.45
1:B:247:HIS:CD2	1:B:270:TYR:CD1	3.04	0.45
1:F:323:LEU:HD22	1:F:323:LEU:N	2.32	0.45
1:A:170:ASP:O	1:A:171:GLY:O	2.34	0.45
1:B:41:SER:O	1:B:42:ASP:HB2	2.16	0.45
1:B:316:PHE:CD2	1:B:325:ILE:HD13	2.51	0.45
1:C:105:GLN:HA	1:C:125:LEU:HA	1.99	0.45
1:F:308:TYR:CD1	1:F:309:TRP:HE3	2.34	0.45
1:A:235:GLY:O	1:A:238:SER:HB3	2.16	0.45
1:B:266:LEU:HD23	1:B:296:TYR:HE1	1.82	0.45
1:B:312:GLN:HG2	1:B:314:ALA:HB3	1.99	0.45
1:B:36:ARG:O	1:B:57:THR:HG22	2.17	0.45
1:D:185:THR:O	1:D:205:ILE:HA	2.17	0.45
1:D:232:ILE:HG21	1:D:257:PRO:HB3	1.98	0.45
1:F:148:ASN:N	1:F:148:ASN:HD22	2.15	0.45
1:A:32:HIS:HD2	1:B:176:TYR:HB2	1.82	0.45
1:A:189:LYS:O	1:A:215:ARG:HD2	2.16	0.45
1:B:59:LEU:HB2	1:B:80:LEU:HD11	1.98	0.45
1:B:242:THR:O	1:B:243:LEU:C	2.60	0.45
1:C:117:ILE:HB	1:C:142:VAL:HG11	1.99	0.45
1:C:268:VAL:O	1:C:268:VAL:HG13	2.17	0.45
1:D:107:LEU:O	1:D:107:LEU:HG	2.16	0.45
1:D:311:VAL:O	1:D:311:VAL:HG13	2.16	0.45
1:F:174:LEU:HD11	1:F:192:PRO:HG2	1.98	0.45
1:A:133:ASN:HB2	1:A:157:ASN:HD21	1.81	0.45
1:A:150:ASN:O	1:A:176:TYR:HB3	2.16	0.45
1:A:319:VAL:CG2	1:A:320:THR:H	2.30	0.45
1:B:232:ILE:CG2	1:B:257:PRO:HB3	2.46	0.45
1:C:98:PHE:C	1:C:100:PRO:HD2	2.42	0.45
1:D:234:ASN:HB3	1:D:258:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:TYR:CD1	1:E:129:ARG:HG3	2.52	0.45
1:E:149:MET:HB2	1:E:172:LEU:HD11	1.99	0.45
1:F:109:ILE:HD12	1:F:114:LEU:HD11	1.98	0.45
1:F:225:GLY:HA2	1:F:249:ASP:O	2.16	0.45
1:A:64:ASN:C	1:A:88:ASN:OD1	2.60	0.44
1:A:245:GLU:CD	1:A:268:VAL:CG1	2.91	0.44
1:C:86:VAL:HG12	1:C:87:ASN:N	2.31	0.44
1:C:129:ARG:NH2	1:C:153:GLU:HG3	2.31	0.44
1:C:181:GLU:HA	1:C:202:HIS:O	2.17	0.44
1:D:240:LEU:O	1:D:241:PRO:C	2.58	0.44
3:D:2193:FLC:OA1	3:D:2193:FLC:CGC	2.61	0.44
1:E:272:HIS:HD1	1:E:300:SER:CB	2.30	0.44
1:F:260:LEU:HB2	1:F:261:PRO:HD3	1.99	0.44
1:A:322:ARG:O	1:A:324:ALA:N	2.50	0.44
1:C:139:PRO:HA	1:C:165:GLU:OE2	2.17	0.44
1:C:146:LEU:HD23	1:C:146:LEU:H	1.81	0.44
1:C:180:SER:OG	1:C:181:GLU:HG3	2.17	0.44
1:C:319:VAL:HG11	1:C:325:ILE:HD11	1.99	0.44
1:E:131:HIS:CD2	1:E:132:ASP:H	2.35	0.44
1:F:240:LEU:N	1:F:240:LEU:CD1	2.80	0.44
1:A:149:MET:O	1:A:150:ASN:HB3	2.18	0.44
1:B:273:THR:HA	1:B:303:ASN:O	2.17	0.44
1:C:128:LEU:O	1:C:128:LEU:HG	2.17	0.44
1:C:149:MET:HE3	1:C:152:ILE:CG1	2.47	0.44
1:D:267:GLN:O	1:D:297:ASN:N	2.42	0.44
1:D:286:PRO:HG3	1:D:293:ARG:HD3	1.99	0.44
1:E:52:ILE:O	1:E:53:SER:C	2.61	0.44
1:E:59:LEU:HA	1:E:59:LEU:HD23	1.76	0.44
1:F:274:ASN:HB3	1:F:275:ASN:H	1.66	0.44
1:A:53:SER:O	1:A:56:THR:HB	2.15	0.44
1:B:99:SER:N	1:B:100:PRO:CD	2.80	0.44
1:C:149:MET:HB2	1:C:172:LEU:HD11	2.00	0.44
1:C:191:LEU:HB2	1:C:216:TYR:OH	2.18	0.44
1:E:69:LEU:HD21	1:E:90:ILE:HD13	1.99	0.44
1:F:180:SER:OG	1:F:181:GLU:CG	2.64	0.44
1:A:68:GLU:C	1:A:69:LEU:HD22	2.42	0.44
1:A:89:LYS:HB2	1:A:89:LYS:HE3	1.65	0.44
1:B:113:HIS:CD2	1:B:134:ARG:CZ	3.01	0.44
1:B:276:ILE:CB	1:B:304:ASN:ND2	2.68	0.44
1:C:138:VAL:HG13	1:C:138:VAL:O	2.16	0.44
1:C:224:LEU:O	1:C:225:GLY:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LEU:HD23	1:E:80:LEU:HD22	2.00	0.44
1:F:131:HIS:CD2	1:F:132:ASP:N	2.86	0.44
1:C:110:SER:HB3	1:C:131:HIS:HB3	1.99	0.44
1:A:226:HIS:H	1:A:250:ASN:HB2	1.82	0.44
1:A:260:LEU:HD22	1:A:266:LEU:CD2	2.48	0.44
1:B:77:LEU:HD23	1:B:80:LEU:HD22	2.00	0.44
1:D:240:LEU:HD23	1:D:243:LEU:HD13	1.99	0.44
1:D:291:VAL:CG1	1:D:292:LYS:N	2.80	0.44
1:E:39:GLN:OE1	1:E:41:SER:OG	2.33	0.44
1:A:28:PRO:HD3	1:A:51:GLU:O	2.17	0.44
1:A:80:LEU:HD23	1:A:101:LEU:HD21	1.99	0.44
1:B:70:ARG:O	1:B:73:ASP:HB2	2.18	0.44
1:F:70:ARG:O	1:F:73:ASP:HB2	2.18	0.44
1:F:269:VAL:HG12	1:F:299:ILE:HG12	2.00	0.44
1:A:70:ARG:O	1:A:73:ASP:HB2	2.18	0.44
1:A:138:VAL:HA	1:A:139:PRO:HD3	1.75	0.44
1:A:251:ASN:HB2	1:A:274:ASN:OD1	2.18	0.44
1:B:110:SER:HB3	1:B:131:HIS:HB3	1.99	0.44
1:B:139:PRO:HA	1:B:165:GLU:OE2	2.18	0.44
1:D:105:GLN:O	1:D:125:LEU:HD12	2.18	0.44
1:E:198:LEU:HG	1:E:200:LEU:CD2	2.48	0.44
1:A:83:LEU:CD2	1:A:85:LEU:HD11	2.27	0.43
1:A:170:ASP:O	1:A:171:GLY:C	2.61	0.43
1:A:253:LEU:O	1:A:275:ASN:HB3	2.18	0.43
1:F:102:ARG:O	1:F:102:ARG:HG2	2.17	0.43
1:A:129:ARG:CZ	1:A:153:GLU:HG3	2.48	0.43
1:A:159:LEU:O	1:A:183:LYS:HB2	2.18	0.43
1:C:80:LEU:HD23	1:C:101:LEU:HD21	2.00	0.43
1:D:306:VAL:HG13	1:D:306:VAL:O	2.18	0.43
1:E:69:LEU:HD23	1:E:93:ILE:CG1	2.46	0.43
1:E:114:LEU:O	1:E:134:ARG:HB2	2.17	0.43
1:A:312:GLN:HG2	1:A:314:ALA:HB3	2.00	0.43
1:C:113:HIS:CD2	1:C:134:ARG:NH2	2.86	0.43
1:C:260:LEU:N	1:C:261:PRO:CD	2.81	0.43
1:C:312:GLN:HG3	1:C:313:PRO:CD	2.47	0.43
1:D:149:MET:O	1:D:150:ASN:CB	2.64	0.43
1:E:301:LEU:C	1:E:302:PHE:O	2.59	0.43
1:A:29:PHE:CE2	1:B:221:ARG:HG2	2.53	0.43
1:A:256:VAL:HG22	1:A:271:LEU:CD1	2.49	0.43
1:B:159:LEU:HD23	1:B:159:LEU:H	1.82	0.43
1:C:41:SER:O	1:C:42:ASP:CB	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:O	1:C:225:GLY:O	2.37	0.43
1:D:81:TYR:O	1:D:105:GLN:N	2.50	0.43
1:E:311:VAL:O	1:E:311:VAL:HG13	2.18	0.43
1:A:208:ILE:HD11	1:A:213:LEU:HG	2.01	0.43
1:C:292:LYS:HB2	1:C:292:LYS:HE3	1.63	0.43
1:F:220:TYR:N	1:F:220:TYR:CD2	2.85	0.43
1:C:110:SER:O	1:C:111:LYS:C	2.59	0.43
1:C:239:PHE:C	1:C:241:PRO:CD	2.90	0.43
1:D:148:ASN:N	1:D:148:ASN:ND2	2.66	0.43
1:D:273:THR:HA	1:D:303:ASN:O	2.19	0.43
1:E:129:ARG:NH2	1:E:153:GLU:HG3	2.33	0.43
1:B:325:ILE:O	1:B:325:ILE:HG22	2.19	0.43
1:C:106:LYS:HD3	1:C:108:TYR:OH	2.18	0.43
1:C:192:PRO:HD2	1:C:195:LEU:HD22	2.00	0.43
1:C:208:ILE:HG23	1:C:232:ILE:HB	2.00	0.43
1:D:105:GLN:C	1:D:125:LEU:HD12	2.44	0.43
1:E:297:ASN:HD22	1:E:297:ASN:HA	1.43	0.43
1:F:104:LEU:CD1	1:F:125:LEU:HD13	2.49	0.43
1:A:108:TYR:HA	1:A:129:ARG:HB2	2.01	0.43
1:B:83:LEU:HD12	1:B:83:LEU:C	2.37	0.43
1:B:235:GLY:O	1:B:238:SER:CB	2.64	0.43
1:E:32:HIS:HB2	1:F:176:TYR:CD1	2.54	0.43
1:E:105:GLN:C	1:E:125:LEU:HD12	2.44	0.43
1:E:105:GLN:O	1:E:125:LEU:HD12	2.19	0.43
1:E:305:PRO:O	1:E:305:PRO:HG2	2.19	0.43
1:F:90:ILE:O	1:F:113:HIS:HB2	2.19	0.43
1:A:150:ASN:HB2	1:A:175:ASN:ND2	2.34	0.42
1:A:246:LEU:HD21	1:A:248:LEU:HD22	2.01	0.42
1:B:184:LEU:N	1:B:184:LEU:HD22	2.34	0.42
1:B:187:ILE:HA	1:B:188:PRO:HD3	1.90	0.42
1:C:118:PRO:HA	1:C:119:PRO:HD3	1.89	0.42
1:D:80:LEU:HB3	1:D:101:LEU:CD2	2.49	0.42
1:D:117:ILE:HA	1:D:118:PRO:HD3	1.91	0.42
1:D:149:MET:HB2	1:D:172:LEU:HD11	2.01	0.42
1:E:33:CYS:HB2	1:E:37:VAL:O	2.18	0.42
1:E:86:VAL:HG12	1:E:87:ASN:N	2.34	0.42
1:E:198:LEU:HD11	1:E:200:LEU:CD2	2.48	0.42
1:F:118:PRO:O	1:F:121:LEU:HD11	2.19	0.42
1:A:153:GLU:OE1	1:A:178:ARG:HD3	2.18	0.42
1:A:216:TYR:HB3	1:A:219:LEU:HD11	2.01	0.42
1:A:260:LEU:HB2	1:A:261:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:CD2	1:A:325:ILE:CD1	3.02	0.42
1:B:178:ARG:NE	1:B:180:SER:HB3	2.31	0.42
1:D:276:ILE:CB	1:D:304:ASN:ND2	2.70	0.42
1:E:80:LEU:HD23	1:E:101:LEU:CD2	2.49	0.42
1:E:213:LEU:HB3	1:E:240:LEU:HD11	2.00	0.42
1:F:54:PRO:C	1:F:56:THR:N	2.77	0.42
1:F:261:PRO:C	1:F:293:ARG:NH2	2.77	0.42
1:B:149:MET:HE3	1:B:152:ILE:CG1	2.49	0.42
1:B:174:LEU:C	1:B:174:LEU:HD12	2.44	0.42
1:C:232:ILE:CG2	1:C:257:PRO:HB3	2.47	0.42
1:D:33:CYS:CB	1:D:38:VAL:HA	2.49	0.42
1:D:226:HIS:CE1	3:D:2193:FLC:OG2	2.72	0.42
1:D:272:HIS:CG	1:D:302:PHE:CZ	3.07	0.42
1:E:107:LEU:HD23	1:E:128:LEU:HD13	2.01	0.42
1:F:69:LEU:HB2	1:F:93:ILE:HG23	2.01	0.42
1:A:213:LEU:O	1:A:214:LEU:C	2.62	0.42
1:B:108:TYR:CD1	1:B:129:ARG:HG3	2.54	0.42
1:C:27:CYS:CB	1:C:28:PRO:CD	2.83	0.42
1:C:191:LEU:HB3	1:C:192:PRO:HD2	2.02	0.42
1:D:222:LEU:O	1:D:246:LEU:HD12	2.19	0.42
1:E:81:TYR:CE1	1:E:105:GLN:OE1	2.72	0.42
1:E:274:ASN:N	1:E:304:ASN:OD1	2.50	0.42
1:E:307:PRO:HG2	1:E:310:GLU:HB2	2.02	0.42
1:F:105:GLN:C	1:F:125:LEU:HD12	2.43	0.42
1:A:85:LEU:CB	1:A:109:ILE:HG22	2.44	0.42
1:A:190:ASP:OD2	1:A:190:ASP:N	2.32	0.42
1:A:301:LEU:HB3	1:A:327:PHE:CD2	2.54	0.42
1:C:69:LEU:HD23	1:C:93:ILE:CG1	2.44	0.42
1:E:70:ARG:O	1:E:71:LYS:C	2.63	0.42
1:E:245:GLU:HG2	1:E:268:VAL:HG13	1.98	0.42
1:F:199:HIS:CD2	1:F:199:HIS:N	2.87	0.42
1:F:226:HIS:HA	1:F:250:ASN:HB3	2.01	0.42
1:B:59:LEU:HD23	1:B:59:LEU:HA	1.60	0.42
1:C:312:GLN:O	1:C:315:THR:HB	2.19	0.42
1:D:69:LEU:HB2	1:D:93:ILE:HG23	2.02	0.42
1:D:226:HIS:H	1:D:250:ASN:HB2	1.84	0.42
1:A:285:CYS:HA	1:A:286:PRO:HD3	1.77	0.42
1:C:140:LYS:HA	1:C:168:ALA:HA	2.01	0.42
1:E:319:VAL:CG2	1:E:320:THR:N	2.82	0.42
1:F:86:VAL:HG12	1:F:87:ASN:N	2.34	0.42
1:F:129:ARG:CZ	1:F:153:GLU:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD21	1:A:85:LEU:HD21	2.02	0.42
1:D:114:LEU:O	1:D:134:ARG:HB2	2.19	0.42
1:D:191:LEU:HB3	1:D:192:PRO:HD2	2.02	0.42
1:E:101:LEU:HB3	1:E:104:LEU:HB2	2.02	0.42
1:E:176:TYR:CD1	1:F:32:HIS:HB2	2.54	0.42
1:E:239:PHE:O	1:E:241:PRO:CD	2.67	0.42
1:A:111:LYS:HA	1:A:132:ASP:HB3	2.02	0.42
1:A:224:LEU:HB2	1:A:248:LEU:CD1	2.50	0.42
1:B:165:GLU:HA	1:B:166:PRO:HD2	1.79	0.42
1:D:224:LEU:O	1:D:225:GLY:O	2.37	0.42
1:D:313:PRO:C	1:D:315:THR:N	2.77	0.42
1:E:176:TYR:CG	1:E:177:LEU:N	2.82	0.42
1:E:256:VAL:HG13	1:E:257:PRO:HD2	2.02	0.42
1:F:59:LEU:HA	1:F:59:LEU:HD23	1.80	0.42
1:F:93:ILE:HD11	1:F:114:LEU:HD21	2.01	0.42
1:F:197:GLU:OE1	1:F:221:ARG:HD3	2.20	0.42
1:A:66:ILE:H	1:A:66:ILE:HG13	1.51	0.42
1:A:203:ASN:HB2	1:A:227:ASN:OD1	2.20	0.42
1:F:106:LYS:HG2	1:F:127:GLU:HB3	2.02	0.42
1:F:208:ILE:HG23	1:F:232:ILE:HB	2.02	0.42
1:B:224:LEU:HB2	1:B:248:LEU:CD1	2.50	0.41
1:B:246:LEU:HD21	1:B:248:LEU:HD22	2.02	0.41
1:C:138:VAL:CG1	1:C:164:PHE:HD1	2.32	0.41
1:C:297:ASN:HD22	1:C:297:ASN:HA	1.44	0.41
1:A:260:LEU:HD22	1:A:266:LEU:HD22	2.03	0.41
1:C:187:ILE:HA	1:C:188:PRO:HD3	1.80	0.41
1:E:69:LEU:CD2	1:E:93:ILE:HG12	2.45	0.41
1:E:113:HIS:O	1:E:114:LEU:C	2.63	0.41
1:F:282:ASN:ND2	1:F:287:VAL:HG22	2.35	0.41
1:B:195:LEU:HD12	1:B:195:LEU:HA	1.83	0.41
1:C:208:ILE:HD13	1:C:208:ILE:HG21	1.73	0.41
1:C:245:GLU:CG	1:C:268:VAL:CG1	2.98	0.41
1:C:260:LEU:HD12	1:C:284:PHE:CE1	2.55	0.41
1:D:28:PRO:HG2	1:D:49:PRO:HG2	2.02	0.41
1:D:40:CYS:HB2	1:D:61:LEU:HB3	2.02	0.41
1:D:108:TYR:CD1	1:D:129:ARG:HG3	2.55	0.41
1:F:263:LEU:O	1:F:265:LEU:N	2.53	0.41
1:A:28:PRO:HB2	1:A:31:CYS:SG	2.60	0.41
1:A:275:ASN:ND2	2:A:801:NAG:C4	2.75	0.41
1:B:98:PHE:C	1:B:100:PRO:HD2	2.45	0.41
1:B:130:ILE:HD11	1:B:135:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PRO:HG2	1:B:310:GLU:HB2	2.01	0.41
1:B:307:PRO:HB2	1:B:309:TRP:CD2	2.56	0.41
1:C:53:SER:HA	1:C:54:PRO:HD3	1.94	0.41
1:C:323:LEU:H	1:C:323:LEU:HD22	1.85	0.41
1:E:133:ASN:N	1:E:157:ASN:HD21	2.16	0.41
1:E:237:LEU:O	1:E:263:LEU:HD21	2.21	0.41
1:E:301:LEU:O	1:E:302:PHE:O	2.39	0.41
1:F:70:ARG:O	1:F:71:LYS:C	2.63	0.41
1:F:256:VAL:HG13	1:F:271:LEU:HD11	2.02	0.41
1:A:139:PRO:CD	1:A:142:VAL:HG21	2.31	0.41
1:A:251:ASN:HB3	1:A:252:LYS:H	1.64	0.41
1:A:316:PHE:HB3	1:A:319:VAL:CG1	2.50	0.41
1:C:69:LEU:HD23	1:C:93:ILE:CD1	2.50	0.41
1:C:70:ARG:O	1:C:73:ASP:HB2	2.20	0.41
1:C:184:LEU:N	1:C:184:LEU:CD2	2.83	0.41
1:D:28:PRO:HB2	1:D:31:CYS:SG	2.61	0.41
1:D:207:ALA:HA	1:D:229:ILE:HG23	2.01	0.41
1:E:32:HIS:O	1:E:39:GLN:HB3	2.20	0.41
1:E:245:GLU:CG	1:E:268:VAL:HG13	2.50	0.41
1:F:240:LEU:O	1:F:241:PRO:C	2.62	0.41
1:F:248:LEU:HA	1:F:248:LEU:HD12	1.65	0.41
1:A:146:LEU:H	1:A:146:LEU:HG	1.51	0.41
1:D:219:LEU:C	1:D:220:TYR:HD2	2.28	0.41
1:E:121:LEU:H	1:E:121:LEU:CD1	2.16	0.41
1:F:207:ALA:HA	1:F:229:ILE:HG23	2.02	0.41
1:F:251:ASN:HB3	1:F:252:LYS:H	1.64	0.41
1:A:80:LEU:HD12	1:A:80:LEU:HA	1.83	0.41
1:B:246:LEU:HD21	1:B:248:LEU:CD2	2.50	0.41
1:C:28:PRO:HG3	1:C:49:PRO:HB2	2.03	0.41
1:C:172:LEU:O	1:C:174:LEU:N	2.53	0.41
1:D:138:VAL:HG11	1:D:164:PHE:CD1	2.56	0.41
1:D:197:GLU:CD	1:D:221:ARG:HD3	2.46	0.41
1:E:298:GLY:HA2	1:E:324:ALA:O	2.20	0.41
1:F:111:LYS:C	1:F:112:ASN:ND2	2.78	0.41
1:A:77:LEU:HB3	1:A:80:LEU:HB2	2.01	0.41
1:A:221:ARG:NH2	1:A:245:GLU:HG3	2.36	0.41
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.73	0.41
1:B:174:LEU:C	1:B:174:LEU:CD1	2.94	0.41
1:B:213:LEU:HD13	1:B:240:LEU:CD2	2.41	0.41
1:C:62:GLN:O	1:C:63:ASN:HB3	2.21	0.41
1:C:239:PHE:O	1:C:241:PRO:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:LEU:CB	1:E:192:PRO:CD	2.97	0.41
1:F:220:TYR:HD2	1:F:220:TYR:N	2.18	0.41
1:F:322:ARG:C	1:F:324:ALA:N	2.78	0.41
1:A:99:SER:N	1:A:100:PRO:CD	2.83	0.41
1:A:179:ILE:HD13	1:A:179:ILE:HG21	1.54	0.41
1:A:182:ALA:HB3	1:A:184:LEU:HD23	2.01	0.41
1:B:240:LEU:HB3	1:B:243:LEU:HB2	2.02	0.41
1:C:69:LEU:CD2	1:C:93:ILE:HG12	2.48	0.41
1:C:107:LEU:HD23	1:C:128:LEU:HD13	2.02	0.41
1:C:240:LEU:CD2	1:C:243:LEU:HD22	2.48	0.41
1:D:138:VAL:HA	1:D:139:PRO:HD3	1.74	0.41
1:E:102:ARG:O	1:E:102:ARG:HG2	2.21	0.41
1:E:130:ILE:HG12	1:E:130:ILE:O	2.21	0.41
1:E:268:VAL:O	1:E:268:VAL:HG22	2.18	0.41
1:F:52:ILE:O	1:F:53:SER:C	2.63	0.41
1:F:200:LEU:HB2	1:F:224:LEU:HD23	2.03	0.41
1:F:232:ILE:C	1:F:232:ILE:CD1	2.89	0.41
1:F:249:ASP:O	1:F:250:ASN:HB2	2.20	0.41
1:F:327:PHE:O	1:F:328:GLY:O	2.39	0.41
1:A:178:ARG:NH2	1:B:43:LEU:HD23	2.35	0.41
1:B:199:HIS:N	1:B:199:HIS:CD2	2.89	0.41
1:B:298:GLY:HA2	1:B:324:ALA:O	2.21	0.41
1:C:39:GLN:OE1	1:C:41:SER:OG	2.36	0.41
1:E:74:PHE:O	1:E:75:LYS:C	2.62	0.41
1:F:62:GLN:HE21	1:F:62:GLN:HB2	1.56	0.41
1:B:118:PRO:O	1:B:121:LEU:HD11	2.20	0.40
1:B:317:ARG:HH11	1:B:317:ARG:HD3	1.73	0.40
1:D:225:GLY:HA2	1:D:249:ASP:O	2.22	0.40
1:E:104:LEU:HD13	1:E:125:LEU:HD13	2.03	0.40
1:F:117:ILE:HD13	1:F:135:ILE:HD13	2.03	0.40
1:B:307:PRO:HB2	1:B:309:TRP:CE3	2.56	0.40
1:C:161:ASN:HD21	1:C:188:PRO:HG3	1.86	0.40
1:D:182:ALA:HB3	1:D:184:LEU:CD2	2.46	0.40
1:F:148:ASN:O	1:F:149:MET:O	2.39	0.40
1:F:152:ILE:HG22	1:F:154:MET:HG3	2.03	0.40
1:F:224:LEU:HB2	1:F:248:LEU:CD1	2.51	0.40
1:F:319:VAL:CG2	1:F:320:THR:N	2.83	0.40
1:A:69:LEU:HD22	1:A:69:LEU:N	2.37	0.40
1:B:63:ASN:O	1:B:63:ASN:ND2	2.55	0.40
1:C:68:GLU:HB3	1:C:92:LYS:HB2	2.03	0.40
1:E:70:ARG:O	1:E:73:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:PRO:HD2	1:E:142:VAL:CG2	2.49	0.40
1:E:191:LEU:HB3	1:E:192:PRO:HD2	2.01	0.40
1:E:301:LEU:HD12	1:E:301:LEU:HA	1.95	0.40
1:F:138:VAL:HA	1:F:139:PRO:HD3	1.77	0.40
1:D:205:ILE:HG21	1:D:205:ILE:HD13	1.76	0.40
1:E:226:HIS:H	1:E:250:ASN:HB2	1.86	0.40
1:C:111:LYS:HG2	1:C:132:ASP:OD1	2.21	0.40
1:E:81:TYR:O	1:E:104:LEU:HD22	2.21	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	301/332 (91%)	216 (72%)	70 (23%)	15 (5%)	1	10
1	B	301/332 (91%)	225 (75%)	68 (23%)	8 (3%)	4	20
1	C	301/332 (91%)	219 (73%)	68 (23%)	14 (5%)	2	12
1	D	302/332 (91%)	230 (76%)	59 (20%)	13 (4%)	2	13
1	E	301/332 (91%)	229 (76%)	53 (18%)	19 (6%)	1	7
1	F	303/332 (91%)	223 (74%)	67 (22%)	13 (4%)	2	13
All	All	1809/1992 (91%)	1342 (74%)	385 (21%)	82 (4%)	2	12

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	291	VAL
1	B	150	ASN
1	C	150	ASN

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Mol	Chain	Res	Type
1	C	291	VAL
1	C	314	ALA
1	D	150	ASN
1	E	150	ASN
1	E	289	PHE
1	F	150	ASN
1	F	291	VAL
1	A	102	ARG
1	A	123	SER
1	A	150	ASN
1	A	171	GLY
1	A	214	LEU
1	A	289	PHE
1	B	217	SER
1	B	293	ARG
1	B	314	ALA
1	C	217	SER
1	C	225	GLY
1	C	289	PHE
1	D	171	GLY
1	D	173	LYS
1	D	225	GLY
1	D	289	PHE
1	D	314	ALA
1	D	327	PHE
1	E	217	SER
1	E	225	GLY
1	F	171	GLY
1	F	173	LYS
1	F	217	SER
1	F	328	GLY
1	C	158	PRO
1	C	173	LYS
1	C	294	ALA
1	D	158	PRO
1	D	280	GLY
1	E	171	GLY
1	E	177	LEU
1	E	291	VAL
1	E	293	ARG
1	E	314	ALA
1	F	158	PRO

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Mol	Chain	Res	Type
1	F	293	ARG
1	F	327	PHE
1	A	301	LEU
1	B	158	PRO
1	D	217	SER
1	E	173	LYS
1	E	214	LEU
1	E	306	VAL
1	F	214	LEU
1	F	280	GLY
1	A	158	PRO
1	A	306	VAL
1	C	171	GLY
1	C	309	TRP
1	D	240	LEU
1	B	29	PHE
1	B	171	GLY
1	C	214	LEU
1	D	264	LYS
1	D	306	VAL
1	E	86	VAL
1	E	158	PRO
1	E	292	LYS
1	E	302	PHE
1	F	306	VAL
1	A	130	ILE
1	E	240	LEU
1	A	139	PRO
1	A	152	ILE
1	A	241	PRO
1	B	240	LEU
1	C	139	PRO
1	C	306	VAL
1	E	139	PRO
1	E	141	GLY
1	F	240	LEU

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	273/297 (92%)	243 (89%)	30 (11%)	6	22
1	B	273/297 (92%)	251 (92%)	22 (8%)	11	36
1	C	273/297 (92%)	250 (92%)	23 (8%)	10	34
1	D	273/297 (92%)	247 (90%)	26 (10%)	8	29
1	E	273/297 (92%)	244 (89%)	29 (11%)	6	23
1	F	274/297 (92%)	245 (89%)	29 (11%)	6	23
All	All	1639/1782 (92%)	1480 (90%)	159 (10%)	8	28

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	VAL
1	A	46	LYS
1	A	48	VAL
1	A	51	GLU
1	A	56	THR
1	A	59	LEU
1	A	67	SER
1	A	69	LEU
1	A	73	ASP
1	A	109	ILE
1	A	121	LEU
1	A	130	ILE
1	A	142	VAL
1	A	159	LEU
1	A	170	ASP
1	A	174	LEU
1	A	184	LEU
1	A	185	THR
1	A	191	LEU
1	A	198	LEU
1	A	200	LEU
1	A	208	ILE
1	A	221	ARG
1	A	232	ILE
1	A	268	VAL
1	A	277	THR

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Mol	Chain	Res	Type
1	A	292	LYS
1	A	306	VAL
1	A	322	ARG
1	B	57	THR
1	B	59	LEU
1	B	121	LEU
1	B	142	VAL
1	B	146	LEU
1	B	148	ASN
1	B	159	LEU
1	B	170	ASP
1	B	174	LEU
1	B	184	LEU
1	B	185	THR
1	B	191	LEU
1	B	208	ILE
1	B	221	ARG
1	B	232	ILE
1	B	238	SER
1	B	248	LEU
1	B	268	VAL
1	B	292	LYS
1	B	297	ASN
1	B	306	VAL
1	B	322	ARG
1	C	59	LEU
1	C	61	LEU
1	C	67	SER
1	C	121	LEU
1	C	142	VAL
1	C	146	LEU
1	C	148	ASN
1	C	159	LEU
1	C	170	ASP
1	C	174	LEU
1	C	181	GLU
1	C	184	LEU
1	C	185	THR
1	C	191	LEU
1	C	200	LEU
1	C	208	ILE
1	C	232	ILE

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Mol	Chain	Res	Type
1	C	238	SER
1	C	268	VAL
1	C	291	VAL
1	C	297	ASN
1	C	304	ASN
1	C	306	VAL
1	D	59	LEU
1	D	61	LEU
1	D	67	SER
1	D	109	ILE
1	D	121	LEU
1	D	142	VAL
1	D	146	LEU
1	D	148	ASN
1	D	159	LEU
1	D	170	ASP
1	D	174	LEU
1	D	184	LEU
1	D	185	THR
1	D	191	LEU
1	D	198	LEU
1	D	208	ILE
1	D	221	ARG
1	D	232	ILE
1	D	240	LEU
1	D	268	VAL
1	D	277	THR
1	D	297	ASN
1	D	304	ASN
1	D	306	VAL
1	D	317	ARG
1	D	322	ARG
1	E	59	LEU
1	E	61	LEU
1	E	67	SER
1	E	104	LEU
1	E	109	ILE
1	E	121	LEU
1	E	142	VAL
1	E	146	LEU
1	E	148	ASN
1	E	159	LEU

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Mol	Chain	Res	Type
1	E	170	ASP
1	E	174	LEU
1	E	184	LEU
1	E	185	THR
1	E	191	LEU
1	E	198	LEU
1	E	208	ILE
1	E	221	ARG
1	E	232	ILE
1	E	238	SER
1	E	250	ASN
1	E	255	ARG
1	E	268	VAL
1	E	277	THR
1	E	292	LYS
1	E	293	ARG
1	E	297	ASN
1	E	304	ASN
1	E	306	VAL
1	F	56	THR
1	F	59	LEU
1	F	61	LEU
1	F	67	SER
1	F	109	ILE
1	F	121	LEU
1	F	142	VAL
1	F	146	LEU
1	F	148	ASN
1	F	159	LEU
1	F	170	ASP
1	F	174	LEU
1	F	184	LEU
1	F	185	THR
1	F	191	LEU
1	F	198	LEU
1	F	200	LEU
1	F	208	ILE
1	F	221	ARG
1	F	232	ILE
1	F	240	LEU
1	F	250	ASN
1	F	268	VAL

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Mol	Chain	Res	Type
1	F	292	LYS
1	F	297	ASN
1	F	304	ASN
1	F	306	VAL
1	F	322	ARG
1	F	329	ASN

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	62	GLN
1	A	63	ASN
1	A	113	HIS
1	A	148	ASN
1	A	202	HIS
1	A	297	ASN
1	A	312	GLN
1	B	62	GLN
1	B	78	GLN
1	B	105	GLN
1	B	113	HIS
1	B	148	ASN
1	B	175	ASN
1	B	199	HIS
1	B	250	ASN
1	B	272	HIS
1	B	297	ASN
1	C	62	GLN
1	C	63	ASN
1	C	78	GLN
1	C	87	ASN
1	C	113	HIS
1	C	120	ASN
1	C	131	HIS
1	C	175	ASN
1	C	199	HIS
1	C	297	ASN
1	C	304	ASN
1	D	62	GLN
1	D	63	ASN
1	D	78	GLN
1	D	105	GLN

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Mol	Chain	Res	Type
1	D	113	HIS
1	D	120	ASN
1	D	148	ASN
1	D	175	ASN
1	D	199	HIS
1	D	250	ASN
1	D	297	ASN
1	D	312	GLN
1	D	326	GLN
1	E	62	GLN
1	E	63	ASN
1	E	78	GLN
1	E	87	ASN
1	E	148	ASN
1	E	150	ASN
1	E	175	ASN
1	E	199	HIS
1	E	282	ASN
1	E	297	ASN
1	E	326	GLN
1	F	62	GLN
1	F	63	ASN
1	F	78	GLN
1	F	87	ASN
1	F	105	GLN
1	F	113	HIS
1	F	120	ASN
1	F	148	ASN
1	F	161	ASN
1	F	175	ASN
1	F	199	HIS
1	F	206	GLN
1	F	282	ASN
1	F	297	ASN
1	F	312	GLN
1	F	329	ASN

5.3.3 RNA

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](#)

12 ligands 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
3	FLC	F	2195	-	12,12,12	1.81	3 (25%)	17,17,17	3.01	9 (52%)
3	FLC	A	2190	-	12,12,12	1.12	1 (8%)	17,17,17	1.59	3 (17%)
2	NAG	A	801	1	14,14,15	1.22	1 (7%)	17,19,21	1.89	5 (29%)
2	NAG	B	803	1	14,14,15	1.06	1 (7%)	17,19,21	1.65	3 (17%)
2	NAG	F	811	1	14,14,15	1.11	1 (7%)	17,19,21	1.92	6 (35%)
3	FLC	C	2192	-	12,12,12	1.69	2 (16%)	17,17,17	2.91	7 (41%)
3	FLC	B	2191	-	12,12,12	1.31	1 (8%)	17,17,17	1.87	3 (17%)
3	FLC	D	2193	-	12,12,12	1.26	0	17,17,17	2.29	6 (35%)
3	FLC	E	2194	-	12,12,12	2.21	1 (8%)	17,17,17	2.99	8 (47%)
2	NAG	E	809	1	14,14,15	1.33	2 (14%)	17,19,21	2.26	4 (23%)
2	NAG	D	807	1	14,14,15	0.97	0	17,19,21	1.76	5 (29%)
2	NAG	C	805	1	14,14,15	1.36	3 (21%)	17,19,21	1.78	5 (29%)

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
3	FLC	F	2195	-	-	4/16/16/16	-
3	FLC	A	2190	-	-	9/16/16/16	-
2	NAG	A	801	1	-	4/6/23/26	0/1/1/1
2	NAG	B	803	1	-	3/6/23/26	0/1/1/1
2	NAG	F	811	1	-	3/6/23/26	0/1/1/1
3	FLC	C	2192	-	-	8/16/16/16	-
3	FLC	B	2191	-	-	8/16/16/16	-
3	FLC	D	2193	-	-	9/16/16/16	-
3	FLC	E	2194	-	-	5/16/16/16	-
2	NAG	E	809	1	-	3/6/23/26	0/1/1/1
2	NAG	D	807	1	-	5/6/23/26	0/1/1/1
2	NAG	C	805	1	-	3/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2194	FLC	CB-CBC	6.56	1.60	1.53
3	C	2192	FLC	CB-CBC	4.33	1.58	1.53
3	F	2195	FLC	CG-CB	4.12	1.59	1.54
2	C	805	NAG	C3-C2	3.10	1.59	1.52
2	E	809	NAG	C1-C2	2.99	1.56	1.52
2	A	801	NAG	C1-C2	2.80	1.56	1.52
2	F	811	NAG	C1-C2	2.71	1.56	1.52
3	F	2195	FLC	CG-CGC	2.61	1.58	1.50
3	B	2191	FLC	CB-CBC	2.46	1.56	1.53
3	F	2195	FLC	OA1-CAC	2.40	1.29	1.22
2	B	803	NAG	C1-C2	2.30	1.55	1.52
3	A	2190	FLC	OB1-CBC	2.21	1.29	1.22
2	C	805	NAG	C1-C2	2.19	1.55	1.52
2	C	805	NAG	C2-N2	2.14	1.49	1.46
2	E	809	NAG	C4-C3	2.12	1.57	1.52
3	C	2192	FLC	OA2-CAC	-2.08	1.24	1.30

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2192	FLC	OHB-CB-CG	-6.37	94.86	109.38
3	F	2195	FLC	CB-CG-CGC	6.11	130.64	113.92
3	C	2192	FLC	OHB-CB-CBC	5.98	117.44	108.96
3	E	2194	FLC	OHB-CB-CG	-5.97	95.75	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2195	FLC	OB2-CBC-CB	5.87	124.40	113.14
3	E	2194	FLC	OHB-CB-CBC	5.66	116.99	108.96
3	E	2194	FLC	OB2-CBC-CB	5.48	123.66	113.14
3	F	2195	FLC	OB1-CBC-CB	-5.10	112.22	122.09
3	B	2191	FLC	OB2-CBC-CB	5.09	122.91	113.14
3	C	2192	FLC	OB2-CBC-CB	4.83	122.40	113.14
2	E	809	NAG	C2-N2-C7	4.82	129.35	122.90
2	F	811	NAG	C4-C3-C2	4.76	118.00	111.02
2	E	809	NAG	C1-O5-C5	4.69	118.47	112.19
3	D	2193	FLC	OB2-CBC-CB	4.61	121.98	113.14
2	E	809	NAG	C1-C2-N2	4.51	117.54	110.43
3	D	2193	FLC	CG-CB-CBC	4.40	119.77	110.03
3	C	2192	FLC	CB-CA-CAC	-3.84	103.42	113.92
2	D	807	NAG	C8-C7-N2	3.82	122.46	116.12
3	E	2194	FLC	OB2-CBC-OB1	-3.68	112.08	123.86
2	A	801	NAG	C8-C7-N2	3.66	122.18	116.12
2	A	801	NAG	C1-C2-N2	3.44	115.86	110.43
2	C	805	NAG	C1-O5-C5	3.41	116.75	112.19
3	D	2193	FLC	CA-CB-CBC	-3.39	102.53	110.03
3	F	2195	FLC	OHB-CB-CBC	-3.39	104.15	108.96
3	B	2191	FLC	OHB-CB-CBC	3.38	113.75	108.96
3	E	2194	FLC	CB-CG-CGC	-3.23	105.09	113.92
3	B	2191	FLC	OHB-CB-CA	-3.20	102.07	109.38
3	A	2190	FLC	CB-CG-CGC	-3.16	105.28	113.92
2	B	803	NAG	C3-C4-C5	3.15	115.94	110.23
3	F	2195	FLC	CG-CB-CBC	3.13	116.96	110.03
2	D	807	NAG	O5-C5-C6	3.11	113.71	107.66
2	C	805	NAG	O4-C4-C5	3.10	116.95	109.32
2	B	803	NAG	O4-C4-C5	-3.08	101.73	109.32
2	C	805	NAG	C4-C3-C2	3.07	115.52	111.02
3	D	2193	FLC	OHB-CB-CA	3.02	116.27	109.38
2	F	811	NAG	O5-C5-C6	2.98	113.47	107.66
3	A	2190	FLC	OA1-CAC-CA	-2.97	114.55	122.95
3	F	2195	FLC	OHB-CB-CG	2.97	116.14	109.38
3	F	2195	FLC	OG2-CGC-OG1	-2.94	115.78	123.33
2	A	801	NAG	O5-C1-C2	-2.90	106.81	111.29
2	F	811	NAG	C8-C7-N2	2.81	120.77	116.12
2	C	805	NAG	O3-C3-C4	-2.76	103.86	110.38
3	D	2193	FLC	OB1-CBC-CB	-2.71	116.85	122.09
3	C	2192	FLC	CG-CB-CBC	2.69	115.99	110.03
3	F	2195	FLC	CG-CB-CA	-2.62	102.60	109.31
2	A	801	NAG	C1-O5-C5	-2.60	108.71	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2194	FLC	CA-CB-CBC	2.57	115.71	110.03
2	F	811	NAG	C2-N2-C7	2.53	126.29	122.90
2	C	805	NAG	O5-C5-C6	2.50	112.53	107.66
2	D	807	NAG	C1-O5-C5	2.47	115.50	112.19
3	C	2192	FLC	OG1-CGC-CG	-2.47	115.96	122.95
2	E	809	NAG	C3-C4-C5	2.45	114.67	110.23
3	E	2194	FLC	OG1-CGC-CG	-2.45	116.02	122.95
3	D	2193	FLC	OHB-CB-CG	-2.43	103.83	109.38
3	F	2195	FLC	OG2-CGC-CG	2.43	122.05	114.35
3	C	2192	FLC	CB-CG-CGC	-2.30	107.63	113.92
2	B	803	NAG	C6-C5-C4	-2.29	107.39	113.02
2	D	807	NAG	O7-C7-C8	-2.22	118.11	122.05
2	F	811	NAG	O7-C7-C8	-2.20	118.14	122.05
2	F	811	NAG	O3-C3-C4	-2.13	105.34	110.38
3	A	2190	FLC	OA2-CAC-CA	2.12	121.07	114.35
2	A	801	NAG	O6-C6-C5	-2.10	104.17	111.33
2	D	807	NAG	O5-C5-C4	-2.03	105.88	110.83
3	E	2194	FLC	OA1-CAC-CA	-2.03	117.20	122.95

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C8-C7-N2-C2
2	A	801	NAG	O7-C7-N2-C2
2	B	803	NAG	C8-C7-N2-C2
2	B	803	NAG	O7-C7-N2-C2
2	C	805	NAG	C8-C7-N2-C2
2	C	805	NAG	O7-C7-N2-C2
2	E	809	NAG	C8-C7-N2-C2
2	E	809	NAG	O7-C7-N2-C2
2	F	811	NAG	C1-C2-N2-C7
3	A	2190	FLC	CAC-CA-CB-CG
3	A	2190	FLC	CAC-CA-CB-OHB
3	B	2191	FLC	CG-CB-CBC-OB1
3	B	2191	FLC	CG-CB-CBC-OB2
3	B	2191	FLC	OHB-CB-CBC-OB1
3	B	2191	FLC	OHB-CB-CBC-OB2
3	B	2191	FLC	OHB-CB-CG-CGC
3	C	2192	FLC	CAC-CA-CB-CBC
3	C	2192	FLC	CAC-CA-CB-CG
3	C	2192	FLC	CAC-CA-CB-OHB

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Mol	Chain	Res	Type	Atoms
3	C	2192	FLC	CA-CB-CBC-OB1
3	C	2192	FLC	CA-CB-CBC-OB2
3	C	2192	FLC	OHB-CB-CBC-OB1
3	C	2192	FLC	OHB-CB-CBC-OB2
3	D	2193	FLC	CA-CB-CBC-OB1
3	D	2193	FLC	CA-CB-CBC-OB2
3	D	2193	FLC	OHB-CB-CBC-OB1
3	D	2193	FLC	OHB-CB-CBC-OB2
3	D	2193	FLC	CA-CB-CG-CGC
3	D	2193	FLC	CBC-CB-CG-CGC
3	E	2194	FLC	CG-CB-CBC-OB1
3	E	2194	FLC	CG-CB-CBC-OB2
3	E	2194	FLC	OHB-CB-CBC-OB1
3	E	2194	FLC	OHB-CB-CBC-OB2
3	F	2195	FLC	CG-CB-CBC-OB1
3	F	2195	FLC	CG-CB-CBC-OB2
3	F	2195	FLC	OHB-CB-CBC-OB1
3	F	2195	FLC	OHB-CB-CBC-OB2
2	D	807	NAG	C8-C7-N2-C2
2	D	807	NAG	O7-C7-N2-C2
2	A	801	NAG	C4-C5-C6-O6
2	F	811	NAG	C8-C7-N2-C2
2	F	811	NAG	O7-C7-N2-C2
2	D	807	NAG	C4-C5-C6-O6
2	C	805	NAG	O5-C5-C6-O6
3	A	2190	FLC	CAC-CA-CB-CBC
3	D	2193	FLC	CAC-CA-CB-CBC
3	D	2193	FLC	OHB-CB-CG-CGC
2	D	807	NAG	O5-C5-C6-O6
2	A	801	NAG	O5-C5-C6-O6
2	B	803	NAG	O5-C5-C6-O6
2	E	809	NAG	O5-C5-C6-O6
3	A	2190	FLC	OHB-CB-CBC-OB2
3	A	2190	FLC	CA-CB-CBC-OB2
3	E	2194	FLC	OHB-CB-CG-CGC
3	B	2191	FLC	CA-CB-CG-CGC
3	A	2190	FLC	CG-CB-CBC-OB2
3	C	2192	FLC	OHB-CB-CG-CGC
3	A	2190	FLC	CG-CB-CBC-OB1
3	B	2191	FLC	CB-CG-CGC-OG2
2	D	807	NAG	C3-C2-N2-C7
3	D	2193	FLC	CAC-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	B	2191	FLC	CB-CG-CGC-OG1
3	A	2190	FLC	OHB-CB-CBC-OB1
3	A	2190	FLC	CA-CB-CBC-OB1

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2195	FLC	2	0
2	A	801	NAG	5	0
3	C	2192	FLC	3	0
3	B	2191	FLC	3	0
3	D	2193	FLC	7	0
3	E	2194	FLC	2	0
2	D	807	NAG	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	303/332 (91%)	-1.71	0 100 100	8, 38, 52, 57	0
1	B	303/332 (91%)	-1.66	0 100 100	8, 38, 53, 70	0
1	C	303/332 (91%)	-1.66	0 100 100	8, 38, 53, 67	0
1	D	304/332 (91%)	-1.68	0 100 100	8, 38, 52, 57	0
1	E	303/332 (91%)	-1.67	0 100 100	8, 37, 53, 64	0
1	F	305/332 (91%)	-1.68	0 100 100	6, 38, 52, 58	0
All	All	1821/1992 (91%)	-1.68	0 100 100	6, 38, 53, 70	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	807	14/15	0.96	0.04	58,59,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	A	801	14/15	0.97	0.05	51,53,55,55	0
2	NAG	C	805	14/15	0.98	0.04	53,56,57,58	0
2	NAG	B	803	14/15	0.98	0.05	46,50,51,51	0
2	NAG	E	809	14/15	0.98	0.04	59,61,62,62	0
2	NAG	F	811	14/15	0.98	0.03	49,50,51,51	0
3	FLC	A	2190	13/13	0.99	0.04	47,50,53,53	0
3	FLC	B	2191	13/13	0.99	0.06	49,53,56,57	0
3	FLC	C	2192	13/13	0.99	0.03	38,43,46,46	0
3	FLC	F	2195	13/13	0.99	0.04	38,42,42,43	0
3	FLC	E	2194	13/13	1.00	0.04	36,44,47,48	0
3	FLC	D	2193	13/13	1.00	0.02	38,40,44,45	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.