



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:44 am GMT

PDB ID : 2FT3  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

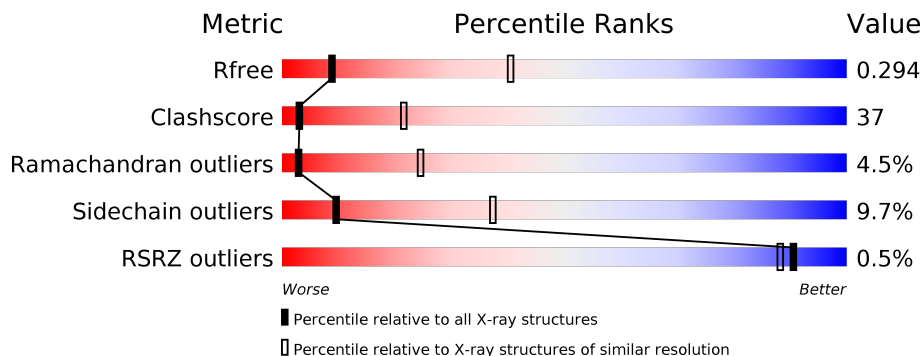
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>32%</div> <div>46%</div> <div>13%</div> <div>•</div> <div>9%</div> </div>
1	B	332	<div> <div>%</div> <div>39%</div> <div>45%</div> <div>6%</div> <div>•</div> <div>9%</div> </div>
1	C	332	<div> <div>%</div> <div>36%</div> <div>48%</div> <div>6%</div> <div>•</div> <div>9%</div> </div>
1	D	332	<div> <div>38%</div> <div>42%</div> <div>10%</div> <div>•</div> <div>8%</div> </div>
1	E	332	<div> <div>%</div> <div>39%</div> <div>40%</div> <div>10%</div> <div>•</div> <div>9%</div> </div>
1	F	332	<div> <div>34%</div> <div>47%</div> <div>9%</div> <div>•</div> <div>8%</div> </div>

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](#)

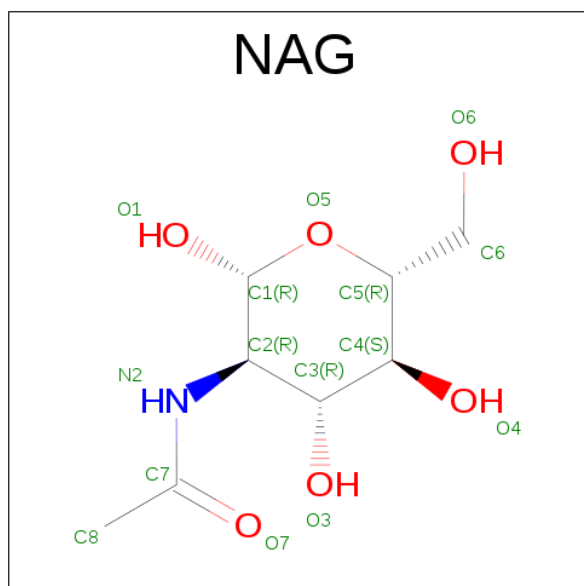
There are 3 unique types of molecules in this entry. The entry contains 14674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

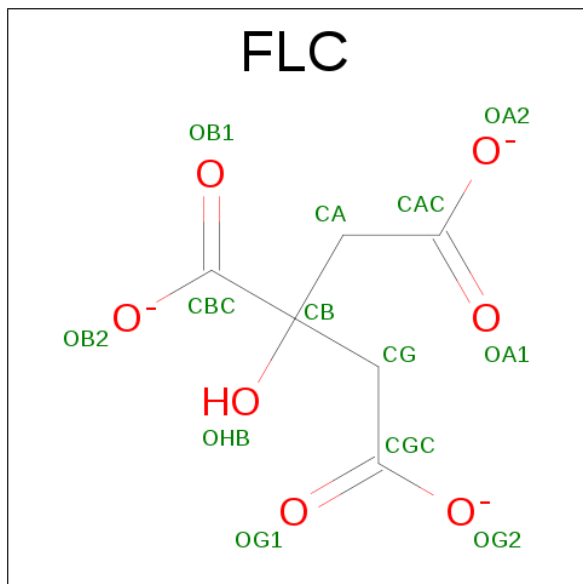
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2416	1545	428	432	11			
1	B	303	Total	C	N	O	S	0	0	0
			2416	1545	428	432	11			
1	C	303	Total	C	N	O	S	0	0	0
			2416	1545	428	432	11			
1	D	304	Total	C	N	O	S	0	0	0
			2420	1547	429	433	11			
1	E	303	Total	C	N	O	S	0	0	0
	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

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: 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 (three-letter code: FLC) (formula:  $C_6H_5O_7^-$ ).

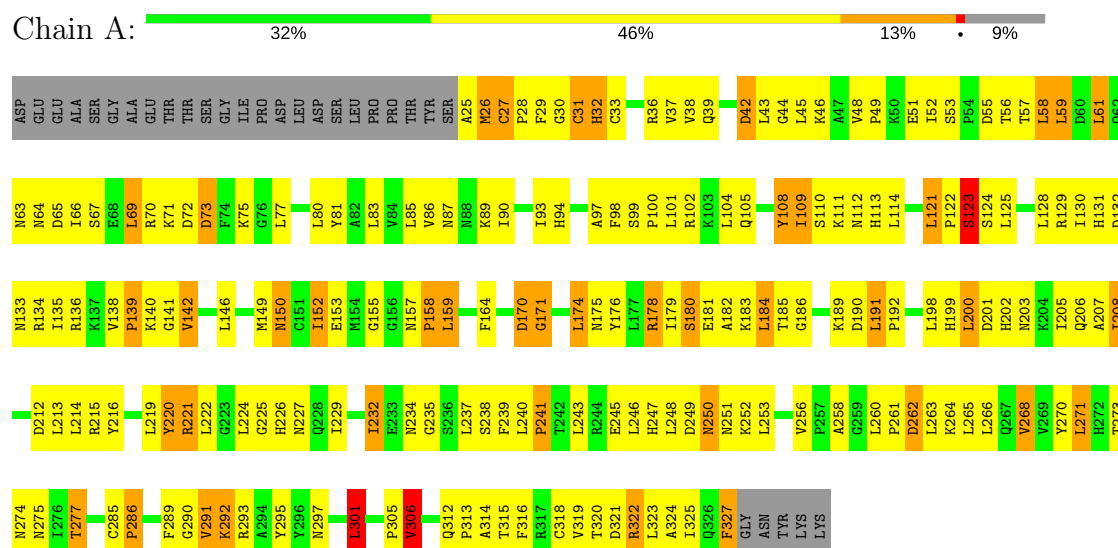


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

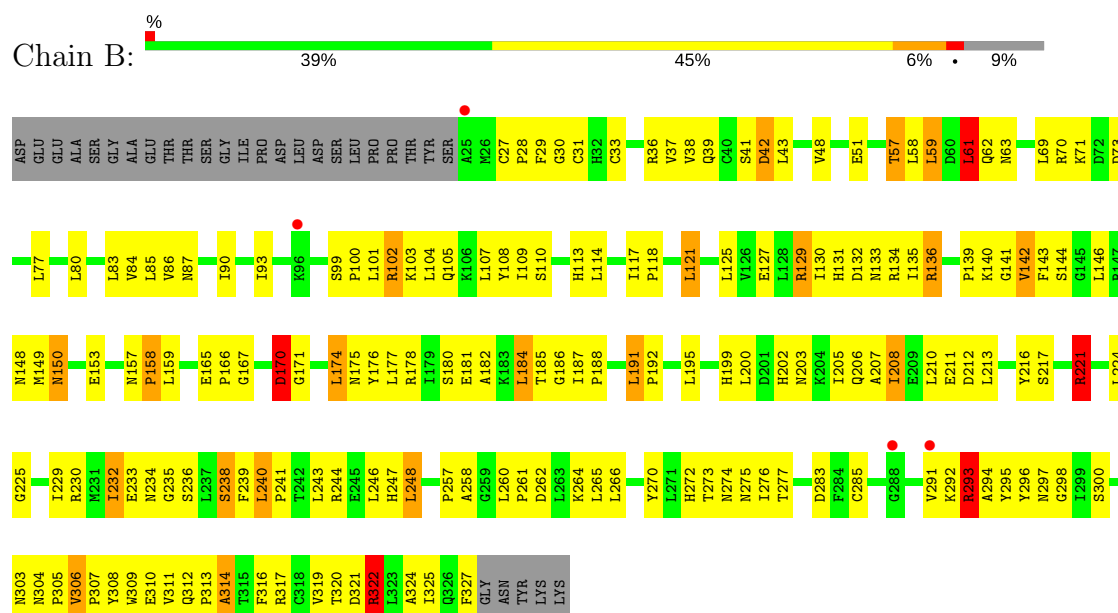
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

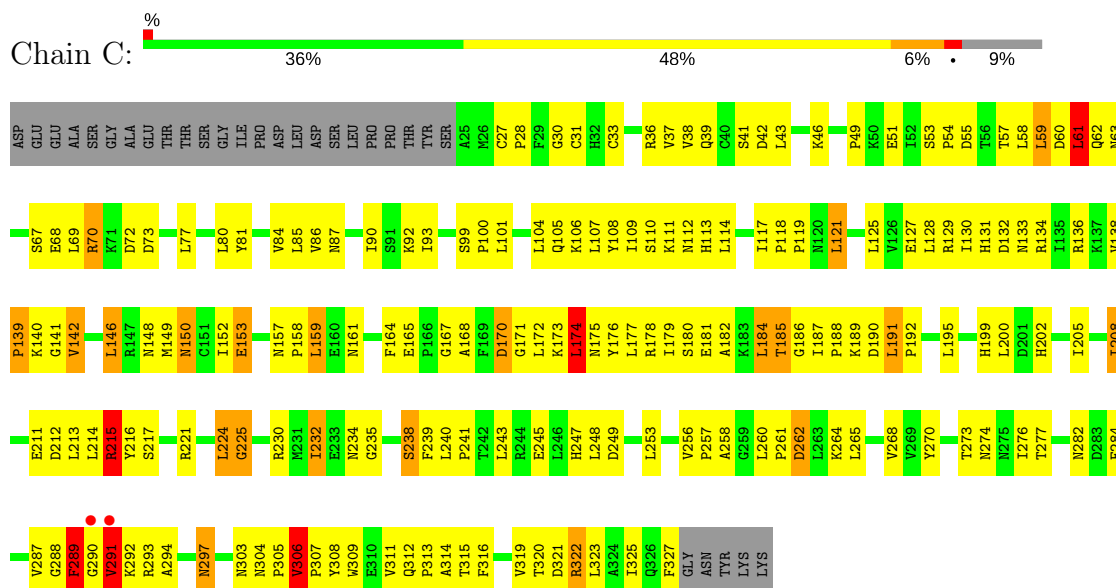
#### • Molecule 1: Biglycan



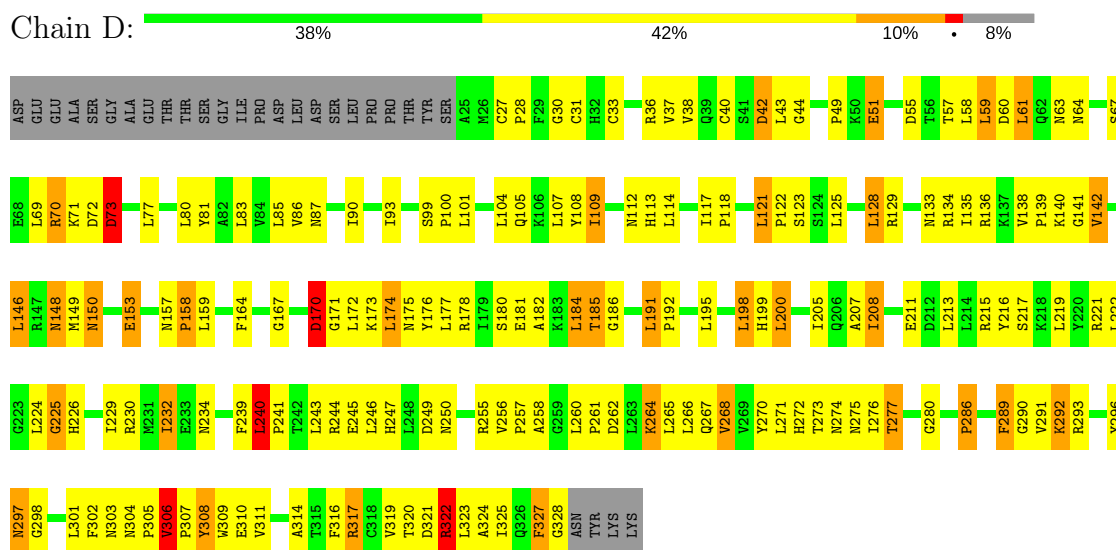
#### • Molecule 1: Biglycan



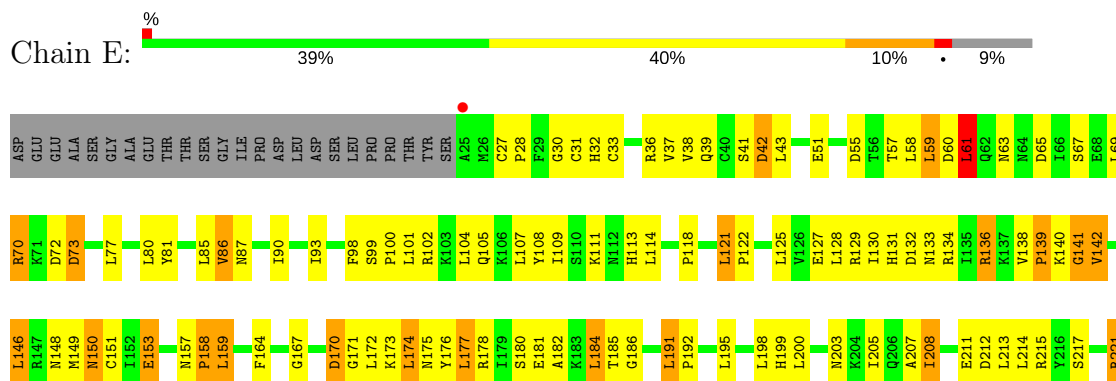
#### • Molecule 1: Biglycan

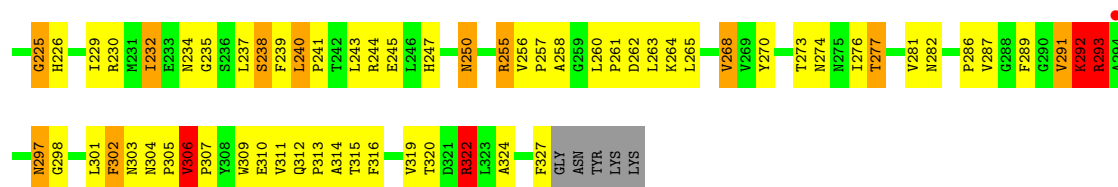


• Molecule 1: Biglycan



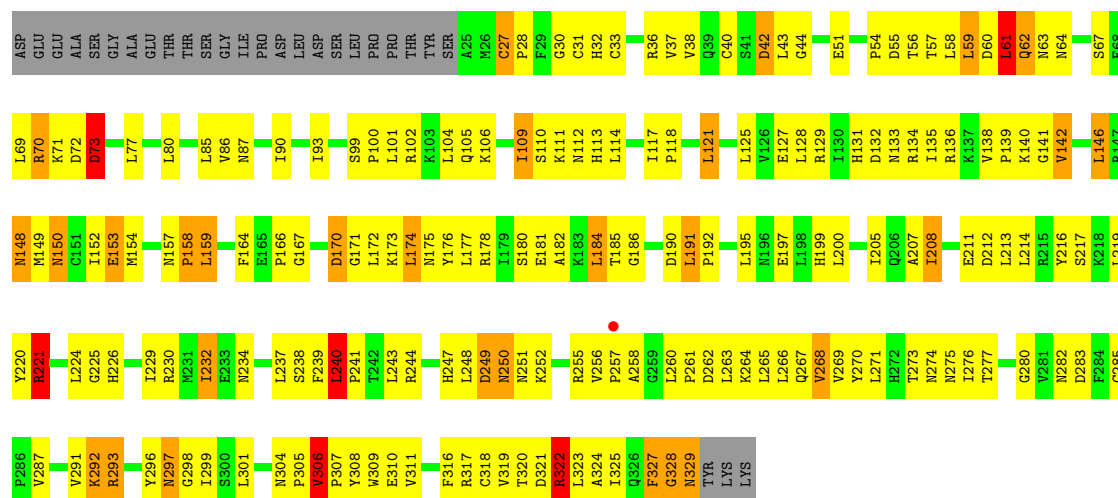
• Molecule 1: Biglycan





• Molecule 1: Biglycan

Chain F: 34% 47% 9% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	206.51Å 119.22Å 140.62Å 90.00° 116.61° 90.00°	Depositor
Resolution (Å)	23.00 – 3.40 22.86 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (23.00-3.40) 96.5 (22.86-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.37Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.258 , 0.291 0.255 , 0.294	Depositor DCC
$R_{free}$ test set	2040 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 29.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.098 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.090 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	14674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

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	1.07	3/2468 (0.1%)	1.23	17/3342 (0.5%)
1	B	1.05	1/2468 (0.0%)	1.23	23/3342 (0.7%)
1	C	1.01	1/2468 (0.0%)	1.28	24/3342 (0.7%)
1	D	1.05	2/2472 (0.1%)	1.29	24/3347 (0.7%)
1	E	1.06	1/2468 (0.0%)	1.36	26/3342 (0.8%)
1	F	1.05	2/2480 (0.1%)	1.25	30/3358 (0.9%)
All	All	1.05	10/14824 (0.1%)	1.27	144/20073 (0.7%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	GLN	CD-NE2	-7.44	1.14	1.32
1	E	151	CYS	CB-SG	-6.55	1.71	1.82
1	F	62	GLN	CD-OE1	-6.31	1.10	1.24
1	A	108	TYR	CE1-CZ	-5.78	1.31	1.38
1	B	291	VAL	CA-CB	5.62	1.66	1.54
1	C	291	VAL	CA-CB	5.38	1.66	1.54
1	A	220	TYR	CE1-CZ	5.23	1.45	1.38
1	D	51	GLU	CG-CD	5.06	1.59	1.51
1	D	308	TYR	CD1-CE1	-5.04	1.31	1.39
1	A	31	CYS	CB-SG	-5.00	1.73	1.81

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	ARG	NE-CZ-NH2	-20.38	110.11	120.30
1	E	244	ARG	NE-CZ-NH2	18.19	129.40	120.30
1	D	317	ARG	NE-CZ-NH2	17.19	128.90	120.30
1	E	244	ARG	NE-CZ-NH1	-15.47	112.56	120.30
1	E	136	ARG	NE-CZ-NH2	-15.26	112.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	317	ARG	NE-CZ-NH1	-15.16	112.72	120.30
1	E	255	ARG	NE-CZ-NH2	14.68	127.64	120.30
1	E	255	ARG	NE-CZ-NH1	-13.86	113.37	120.30
1	C	221	ARG	NE-CZ-NH1	13.23	126.91	120.30
1	E	70	ARG	NE-CZ-NH1	-13.12	113.74	120.30
1	E	136	ARG	NE-CZ-NH1	13.03	126.82	120.30
1	E	70	ARG	NE-CZ-NH2	12.35	126.48	120.30
1	C	215	ARG	NE-CZ-NH1	-12.11	114.24	120.30
1	F	322	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	D	322	ARG	NE-CZ-NH1	-10.85	114.88	120.30
1	B	102	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	C	215	ARG	NE-CZ-NH2	10.68	125.64	120.30
1	F	322	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	B	102	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	F	136	ARG	NE-CZ-NH1	-10.05	115.28	120.30
1	D	322	ARG	NE-CZ-NH2	9.75	125.17	120.30
1	D	230	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	E	244	ARG	CD-NE-CZ	9.39	136.75	123.60
1	D	230	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	322	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	F	244	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	F	249	ASP	CB-CG-OD2	8.36	125.83	118.30
1	C	321	ASP	CB-CG-OD2	8.20	125.68	118.30
1	B	321	ASP	CB-CG-OD2	8.13	125.62	118.30
1	D	317	ARG	CD-NE-CZ	7.96	134.74	123.60
1	F	221	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	C	221	ARG	CG-CD-NE	-7.87	95.28	111.80
1	F	136	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	D	244	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	F	321	ASP	CB-CG-OD2	7.76	125.29	118.30
1	F	42	ASP	CB-CG-OD2	7.74	125.26	118.30
1	B	129	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	136	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	C	190	ASP	CB-CG-OD2	7.44	125.00	118.30
1	E	322	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	F	230	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	D	321	ASP	CB-CG-OD2	7.34	124.91	118.30
1	A	178	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	B	129	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	136	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	E	230	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	A	55	ASP	CB-CG-OD2	7.14	124.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	E	65	ASP	CB-CG-OD2	7.12	124.71	118.30
1	E	255	ARG	CD-NE-CZ	7.07	133.49	123.60
1	B	61	LEU	CA-CB-CG	7.06	131.54	115.30
1	C	262	ASP	CB-CG-OD2	7.02	124.62	118.30
1	E	60	ASP	CB-CG-OD2	6.99	124.59	118.30
1	F	55	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	65	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	321	ASP	CB-CG-OD2	6.89	124.50	118.30
1	C	230	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	E	322	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	C	212	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	215	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	F	221	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	F	70	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	58	LEU	CA-CB-CG	6.71	130.73	115.30
1	B	244	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	E	70	ARG	CD-NE-CZ	6.68	132.96	123.60
1	C	60	ASP	CB-CG-OD2	6.62	124.26	118.30
1	E	215	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	D	42	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	230	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	212	ASP	CB-CG-OD2	6.50	124.15	118.30
1	E	61	LEU	CA-CB-CG	6.50	130.25	115.30
1	C	221	ARG	CD-NE-CZ	6.47	132.66	123.60
1	F	73	ASP	CB-CG-OD2	6.47	124.12	118.30
1	E	136	ARG	CD-NE-CZ	6.44	132.61	123.60
1	F	318	CYS	CA-CB-SG	-6.43	102.43	114.00
1	B	283	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	136	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	42	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	72	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	73	ASP	CB-CG-OD2	6.29	123.96	118.30
1	F	230	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	C	70	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	322	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	E	42	ASP	CB-CG-OD2	6.08	123.78	118.30
1	F	70	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	61	LEU	CA-CB-CG	6.05	129.21	115.30
1	E	72	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	60	ASP	CB-CG-OD2	6.02	123.72	118.30
1	F	244	ARG	NE-CZ-NH2	-5.99	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	ASP	CB-CG-OD2	5.97	123.67	118.30
1	F	283	ASP	CB-CG-OD1	5.92	123.63	118.30
1	F	262	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	61	LEU	CB-CA-C	5.90	121.41	110.20
1	A	178	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	286	PRO	N-CD-CG	-5.84	94.43	103.20
1	E	212	ASP	CB-CG-OD2	5.83	123.54	118.30
1	F	190	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	128	LEU	CB-CG-CD2	5.75	120.78	111.00
1	C	249	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	221	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	F	317	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	42	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	285	CYS	CA-CB-SG	-5.67	103.79	114.00
1	D	70	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	F	285	CYS	CA-CB-SG	-5.63	103.86	114.00
1	D	170	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	55	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	136	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	200	LEU	CA-CB-CG	5.56	128.10	115.30
1	F	255	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	244	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	27	CYS	N-CA-C	5.53	125.93	111.00
1	B	102	ARG	CD-NE-CZ	5.48	131.27	123.60
1	A	136	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	D	200	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	170	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	221	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	E	55	ASP	CB-CG-OD2	5.44	123.20	118.30
1	C	72	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	222	LEU	CB-CG-CD2	5.42	120.21	111.00
1	A	58	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	F	61	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	55	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	255	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	104	LEU	CA-CB-CG	5.26	127.39	115.30
1	F	255	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	E	293	ARG	N-CA-C	5.23	125.11	111.00
1	A	212	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	104	LEU	CA-CB-CG	5.18	127.22	115.30
1	E	230	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	262	ASP	CB-CG-OD2	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	B	248	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	C	174	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	F	27	CYS	N-CA-C	5.14	124.87	111.00
1	F	212	ASP	CB-CG-OD2	5.14	122.92	118.30
1	D	262	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	271	LEU	CA-CB-CG	5.10	127.03	115.30
1	C	136	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	129	ARG	CD-NE-CZ	5.07	130.69	123.60
1	F	166	PRO	N-CD-CG	-5.05	95.62	103.20
1	A	301	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	C	248	LEU	CB-CG-CD2	-5.04	102.44	111.00
1	C	224	LEU	CB-CG-CD1	-5.03	102.46	111.00

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	222	0
1	B	2416	0	2466	163	0
1	C	2416	0	2466	188	0
1	D	2420	0	2469	167	0
1	E	2416	0	2466	173	0
1	F	2428	0	2475	191	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
3	C	13	0	5	3	0
3	D	13	0	5	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	13	0	5	2	0
3	F	13	0	5	2	0
All	All	14674	0	14916	1104	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 37.

All (1104) 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: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: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: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
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:A:232:ILE:HD13	1:A:232:ILE:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD12	1:B:121:LEU:H	1.36	0.89
1:A:232:ILE:HD13	1:A:232:ILE:C	1.93	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:HA2	3:B:2191:FLC:OG2	1.72	0.88
1:C:232:ILE:HD13	1:C:232:ILE:C	1.94	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: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:CD1	1:A:174:LEU:O	2.24	0.85
1:C:174:LEU:O	1:C:174:LEU:HD12	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:D:239:PHE:C	1:D:241:PRO:HD3	2.00	0.83
1:B:211:GLU:N	1:B:211:GLU:OE1	2.12	0.82
1:E:292:LYS:HE2	1:E:292:LYS:N	1.95	0.82
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:LEU:N	1:C:121:LEU:HD12	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:E:316:PHE:O	1:E:319:VAL:HG12	1.82	0.78
1:A:128:LEU:HB3	1:A:149:MET:HE1	1.66	0.78
1:A:290:GLY:O	1:A:291:VAL:HB	1.82	0.77
1:A:33:CYS:HB2	1:A:37:VAL:O	1.85	0.77
3:E:2194:FLC:OB2	3:E:2194:FLC:OG1	2.01	0.77
1:A:33:CYS:HB3	1:A:38:VAL:HA	1.64	0.77
1:D:232:ILE:HD13	1:D:232:ILE:C	2.05	0.77
1:C:192:PRO:O	1:C:195:LEU:HB2	1.85	0.77
1:E:232:ILE:C	1:E:232:ILE:HD13	2.06	0.76
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:113:HIS:CD2	1:A:134:ARG:CZ	2.70	0.75
1:A:198:LEU:HD11	1:A:200:LEU:HD22	1.68	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:B:83:LEU:HD12	1:B:84:VAL:H	1.51	0.75
3:B:2191:FLC:OG2	3:B:2191:FLC:CA	2.35	0.74
3:C:2192:FLC:OHB	3:C:2192:FLC:OA1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:174:LEU:C	1:C:174:LEU:HD12	2.07	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:E:291:VAL:C	1:E:292:LYS:HE2	2.09	0.73
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:B:232:ILE:HD13	1:B:232:ILE:C	2.10	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:182:ALA:HB3	1:E:184:LEU:HD23	1.72	0.71
1:E:28:PRO:HB2	1:E:31:CYS:SG	2.30	0.71
1:A:184:LEU:CD2	1:A:184:LEU:N	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:O	1:E:232:ILE:HD13	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
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:F:273:THR:HG22	1:F:273:THR:O	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ASN:HA	1:E:174:LEU:HB2	1.72	0.69
1:F:28:PRO:HD3	1:F:51:GLU:O	1.92	0.69
1:E:239:PHE:C	1:E:241:PRO:HD3	2.12	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: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: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:150:ASN:HA	1:B:174:LEU:HB2	1.75	0.68
1:F:121:LEU:HD12	1:F:121:LEU:N	2.03	0.68
1:C:167:GLY:O	1:C:170:ASP:HB2	1.94	0.68
1:C:59:LEU:HD13	1:C:61:LEU:HD22	1.76	0.68
1:A:239:PHE:C	1:A:241:PRO:HD2	2.14	0.68
1:A:149:MET:HE3	1:A:152:ILE:CG1	2.24	0.68
1:C:149:MET:O	1:C:150:ASN:HB3	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: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:A:90:ILE:HD12	1:A:112:ASN:OD1	1.93	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
1:E:277:THR:O	1:E:306:VAL:HB	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:186:GLY:HA2	1:B:205:ILE:HG23	1.76	0.66
1:F:293:ARG:NH1	1:F:296:TYR:CZ	2.63	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:C:121:LEU:CD1	1:C:121:LEU:H	1.97	0.65
1:C:59:LEU:HD13	1:C:61:LEU:CD2	2.26	0.65
1:E:139:PRO:HD2	1:E:142:VAL:HG21	1.78	0.65
1:C:51:GLU:HA	1:C:51:GLU:OE2	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: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
1:F:268:VAL:O	1:F:268:VAL:HG22	1.96	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:128:LEU:HB3	1:A:149:MET:CE	2.27	0.64
1:A:174:LEU:C	1:A:174:LEU:CD1	2.66	0.64
1:A:319:VAL:HG22	1:A:320:THR:N	2.11	0.64
1:C:174:LEU:C	1:C:174:LEU:CD1	2.65	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:O	1:F:174:LEU:HD12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:HIS:CD2	1:A:134:ARG:NH2	2.65	0.63
1:A:69:LEU:HB2	1:A:93:ILE:HG23	1.79	0.63
1:D:30:GLY:HA3	1:D:43:LEU:HD22	1.79	0.63
1:B:239:PHE:C	1:B:241:PRO:HD3	2.18	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:CD1	1:A:232:ILE:O	2.43	0.63
1:B:200:LEU:O	1:B:203:ASN:ND2	2.30	0.63
1:C:211:GLU:N	1:C:211:GLU:OE1	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:178:ARG:HE	1:C:180:SER:HB3	1.64	0.63
1:D:273:THR:HG22	1:D:273:THR:O	1.98	0.63
1:A:273:THR:O	1:A:273:THR:HG22	1.99	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
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:114:LEU:HB2	1:B:133:ASN:OD1	1.99	0.62
1:B:69:LEU:HD23	1:B:93:ILE:CG1	2.27	0.62
1:F:264:LYS:C	1:F:265:LEU:HD12	2.19	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:F:329:ASN:HD22	1:F:329:ASN:C	2.02	0.62
1:B:311:VAL:HG11	1:B:327:PHE:HE1	1.63	0.62
1:C:268:VAL:HG22	1:C:268:VAL:O	1.99	0.62
1:D:30:GLY:HA3	1:D:43:LEU:CD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:ILE:HD13	1:F:232:ILE:C	2.20	0.61
1:C:232:ILE:HG21	1:C:257:PRO:HB3	1.81	0.61
1:E:133:ASN:H	1:E:157:ASN:HD21	1.46	0.61
1:A:232:ILE:C	1:A:232:ILE:CD1	2.67	0.61
3:E:2194:FLC:OG1	3:E:2194:FLC:CBC	2.48	0.61
1:E:63:ASN:ND2	1:E:63:ASN:O	2.33	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:F:239:PHE:C	1:F:241:PRO:HD3	2.20	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: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
1:F:239:PHE:O	1:F:241:PRO:HD3	2.00	0.60
1:F:30:GLY:HA3	1:F:43:LEU:HD22	1.81	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:D:174:LEU:C	1:D:174:LEU:HD12	2.22	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:D:128:LEU:HB3	1:D:149:MET:HE1	1.83	0.59
1:E:59:LEU:HD13	1:E:61:LEU:HD22	1.83	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:F:36:ARG:O	1:F:57:THR:HG22	2.01	0.59
1:A:180:SER:OG	1:A:181:GLU:CG	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:86:VAL:HG12	1:A:87:ASN:N	2.17	0.59
1:C:239:PHE:C	1:C:241:PRO:HD3	2.23	0.59
1:E:140:LYS:HG3	1:E:141:GLY:H	1.68	0.59
3:F:2195:FLC:OB2	3:F:2195:FLC:OA1	2.20	0.59
1:A:174:LEU:HD11	1:A:192:PRO:HG2	1.83	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:CG2	1:B:273:THR:O	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: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
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: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:149:MET:HE3	1:A:152:ILE:HG13	1.86	0.58
1:E:51:GLU:HA	1:E:51:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:OE1	1:A:39:GLN:HA	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:B:260:LEU:HB2	1:B:261:PRO:HD3	1.85	0.57
1:C:133:ASN:H	1:C:157:ASN:ND2	2.03	0.57
1:C:36:ARG:O	1:C:57:THR:HG22	2.05	0.57
1:E:121:LEU:HD12	1:E:121:LEU:N	2.13	0.57
1:F:128:LEU:HB3	1:F:149:MET:CE	2.34	0.57
1:A:42:ASP:OD1	1:A:63:ASN:ND2	2.37	0.57
1:F:128:LEU:HB3	1:F:149:MET:HE1	1.85	0.57
1:C:273:THR:HG22	1:C:273:THR:O	2.04	0.57
1:B:108:TYR:HE1	1:B:127:GLU:HG2	1.69	0.57
1:B:33:CYS:CB	1:B:38:VAL:HA	2.35	0.57
1:D:174:LEU:C	1:D:174:LEU:CD1	2.72	0.57
1:F:234:ASN:HB3	1:F:258:ALA:HB3	1.86	0.57
1:A:239:PHE:C	1:A:241:PRO:CD	2.73	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:C:240:LEU:HB3	1:C:243:LEU:HB2	1.86	0.57
1:C:245:GLU:CD	1:C:268:VAL:HG11	2.25	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:HD23	1:C:146:LEU:N	2.20	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: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:128:LEU:HB3	1:E:149:MET:HE1	1.88	0.56
1:E:149:MET:O	1:E:150:ASN:HB3	2.06	0.56
1:A:216:TYR:O	1:A:219:LEU:HG	2.05	0.56
1:B:239:PHE:C	1:B:241:PRO:CD	2.73	0.56
1:C:41:SER:O	1:C:42:ASP:HB2	2.05	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:D:33:CYS:HB3	1:D:38:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:264:LYS:C	1:C:265:LEU:HD12	2.27	0.56
1:F:110:SER:O	1:F:112:ASN:ND2	2.39	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:E:176:TYR:CD2	1:E:176:TYR:C	2.79	0.55
1:A:240:LEU:N	1:A:241:PRO:CD	2.70	0.55
1:A:291:VAL:C	1:A:293:ARG:H	2.10	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:C	1:A:100:PRO:HD2	2.27	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:E:146:LEU:HD23	1:E:146:LEU:N	2.22	0.54
1:E:30:GLY:HA3	1:E:43:LEU:HD22	1.90	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:H82	2:D:807:NAG:H3	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: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
1:B:295:TYR:HB3	1:B:320:THR:HG23	1.90	0.53
1:E:232:ILE:HG21	1:E:257:PRO:HB3	1.89	0.53
1:E:36:ARG:O	1:E:57:THR:HG22	2.07	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:F:276:ILE:CB	1:F:304:ASN:ND2	2.65	0.53
1:A:178:ARG:CZ	1:B:43:LEU:HD23	2.38	0.53
1:A:49:PRO:HG2	1:A:52:ILE:HD11	1.90	0.53
1:A:149:MET:CE	1:A:152:ILE:HG12	2.38	0.53
1:A:240:LEU:O	1:A:241:PRO:C	2.45	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:F:197:GLU:CD	1:F:221:ARG:HD3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:CG1	1:D:164:PHE:CD1	2.92	0.53
1:A:85:LEU:HB2	1:A:109:ILE:CG2	2.38	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:A:98:PHE:O	1:A:101:LEU:HB2	2.09	0.53
1:B:130:ILE:HG12	1:B:130:ILE:O	2.09	0.53
1:B:39:GLN:OE1	1:B:41:SER:OG	2.23	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:245:GLU:CG	1:E:268:VAL:CG1	2.86	0.53
1:E:59:LEU:HD22	1:E:61:LEU:HD22	1.91	0.53
1:A:290:GLY:HA3	1:A:292:LYS:CE	2.39	0.53
1:B:121:LEU:CD1	1:B:121:LEU:H	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
1:C:159:LEU:CD2	1:C:159:LEU:N	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:111:LYS:C	1:F:112:ASN:HD22	2.13	0.52
1:F:264:LYS:O	1:F:293:ARG:HA	2.09	0.52
1:A:206:GLN:O	1:A:207:ALA:HB2	2.09	0.52
1:F:273:THR:CG2	1:F:273:THR:O	2.58	0.52
1:A:291:VAL:C	1:A:293:ARG:N	2.60	0.52
1:B:131:HIS:CD2	1:B:132:ASP:N	2.78	0.52
1:C:307:PRO:O	1:C:308:TYR:C	2.46	0.52
1:D:81:TYR:O	1:D:104:LEU:HD22	2.09	0.52
1:D:264:LYS:C	1:D:265:LEU:HD12	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:F:232:ILE:HD13	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: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:135:ILE:O	1:F:158:PRO:HD2	2.10	0.51
1:F:27:CYS:CB	1:F:28:PRO:CD	2.77	0.51
1:A:70:ARG:O	1:A:71:LYS:C	2.48	0.51
1:C:176:TYR:C	1:C:176:TYR:CD2	2.83	0.51
1:D:199:HIS:N	1:D:199:HIS:CD2	2.77	0.51
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:N	1:A:220:TYR:HD2	2.08	0.51
1:B:107:LEU:HD11	1:B:109:ILE:HG23	1.91	0.51
1:B:62:GLN:HG3	1:B:86:VAL:O	2.10	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: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: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:HD23	1:B:159:LEU:N	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:201:ASP:N	1:A:201:ASP:OD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:E:273:THR:O	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: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:191:LEU:CB	1:C:192:PRO:CD	2.88	0.50
1:C:30:GLY:HA3	1:C:43:LEU:HD22	1.93	0.50
1:D:308:TYR:CE2	1:D:309:TRP:HB3	2.46	0.50
1:E:245:GLU:CD	1:E:268:VAL:HG11	2.32	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
1:D:245:GLU:HG2	1:D:268:VAL:HG13	1.92	0.50
1:E:264:LYS:C	1:E:265:LEU:HD12	2.32	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:149:MET:CE	1:A:152:ILE:CG1	2.89	0.50
1:A:63:ASN:O	1:A:63:ASN:ND2	2.45	0.50
1:C:146:LEU:CD2	1:C:146:LEU:H	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:A:205:ILE:HG13	1:A:227:ASN:OD1	2.12	0.49
1:A:33:CYS:CB	1:A:38:VAL:HA	2.37	0.49
1:B:312:GLN:HG3	1:B:313:PRO:HD2	1.93	0.49
1:B:51:GLU:HA	1:B:51:GLU:OE2	2.12	0.49
1:C:247:HIS:ND1	3:C:2192:FLC:HG2	2.27	0.49
1:F:138:VAL:O	1:F:138:VAL:HG13	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HB2	1:B:248:LEU:HD13	1.93	0.49
1:B:27:CYS:CB	1:B:28:PRO:CD	2.78	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:245:GLU:CD	1:A:268:VAL:HG11	2.32	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:C:199:HIS:N	1:C:199:HIS:CD2	2.80	0.49
1:C:84:VAL:HG13	1:C:86:VAL:HG23	1.95	0.49
1:D:70:ARG:O	1:D:73:ASP:HB2	2.12	0.49
1:F:301:LEU:HB3	1:F:327:PHE:CD2	2.47	0.49
1:F:85:LEU:HB2	1:F:109:ILE:HG22	1.94	0.49
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:138:VAL:CG1	1:C:164:PHE:CD1	2.96	0.49
1:C:240:LEU:O	1:C:241:PRO:C	2.51	0.49
1:C:69:LEU:HD21	1:C:90:ILE:HD13	1.95	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:E:104:LEU:HD12	1:E:122:PRO:HG2	1.95	0.49
1:E:240:LEU:O	1:E:241:PRO:C	2.49	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:86:VAL:HG13	1:A:110:SER:HB2	1.94	0.48
1:A:27:CYS:O	1:B:221:ARG:NH1	2.46	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:B:70:ARG:O	1:B:71:LYS:C	2.51	0.48
1:C:63:ASN:ND2	1:C:63:ASN:O	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:138:VAL:CG1	1:F:164:PHE:HD1	2.25	0.48
1:F:40:CYS:HB2	1:F:61:LEU:HB3	1.94	0.48
1:B:140:LYS:HG3	1:B:141:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LEU:CD2	1:B:184:LEU:N	2.76	0.48
1:D:308:TYR:HD2	1:D:309:TRP:N	2.07	0.48
1:E:239:PHE:O	1:E:241:PRO:HD3	2.12	0.48
1:E:33:CYS:CB	1:E:38:VAL:HA	2.41	0.48
1:D:261:PRO:O	1:D:293:ARG:NH2	2.45	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: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:E:322:ARG:HD3	1:E:322:ARG:C	2.33	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
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:O	1:C:130:ILE:HG12	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:HD13	1:A:174:LEU:O	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: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: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:E:273:THR:HA	1:E:303:ASN:O	2.14	0.47
1:F:139:PRO:HD2	1:F:142:VAL:CG2	2.42	0.47
1:F:69:LEU:HD21	1:F:90:ILE:HD13	1.96	0.47
1:B:264:LYS:C	1:B:265:LEU:HD12	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:O	1:B:150:ASN:HB3	2.14	0.47
1:B:233:GLU:O	1:B:236:SER:OG	2.23	0.47
1:B:48:VAL:HB	1:B:73:ASP:OD2	2.14	0.47
1:A:114:LEU:O	1:A:134:ARG:HB2	2.14	0.47
1:A:27:CYS:CB	1:A:28:PRO:CD	2.85	0.47
1:B:210:LEU:HB3	1:B:211:GLU:OE1	2.14	0.47
1:B:319:VAL:CG2	1:B:320:THR:N	2.78	0.47
1:E:276:ILE:CB	1:E:304:ASN:ND2	2.73	0.47
1:A:201:ASP:O	1:A:202:HIS:HB2	2.15	0.47
1:B:277:THR:HA	1:B:305:PRO:O	2.14	0.47
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: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:D:247:HIS:ND1	3:D:2193:FLC:HA1	2.30	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:F:30:GLY:HA3	1:F:43:LEU:CD2	2.43	0.47
1:B:133:ASN:H	1:B:157:ASN:HD21	1.62	0.47
1:B:225:GLY:HA3	3:B:2191:FLC:OB2	2.15	0.47
1:E:180:SER:O	1:E:181:GLU:C	2.53	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:51:GLU:OE2	1:F:51:GLU:HA	2.14	0.47
1:A:178:ARG:NE	1:A:180:SER:HB3	2.30	0.46
1:A:44:GLY:HA2	1:A:64:ASN:HA	1.96	0.46
1:B:176:TYR:CD2	1:B:176:TYR:C	2.88	0.46
1:F:226:HIS:H	1:F:250:ASN:HB2	1.80	0.46
1:F:199:HIS:O	1:F:200:LEU:HD13	2.15	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: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: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:C:288:GLY:O	1:C:289:PHE:C	2.54	0.46
1:D:311:VAL:HG11	1:D:327:PHE:CE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:180:SER:O	1:B:181:GLU:C	2.54	0.46
1:B:37:VAL:HG13	1:B:58:LEU:HB2	1.97	0.46
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:O	1:B:208:ILE:HG12	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:A:159:LEU:H	1:A:159:LEU:HD23	1.79	0.46
1:B:80:LEU:HB3	1:B:101:LEU:CD2	2.45	0.46
1:B:146:LEU:HG	1:B:146:LEU:H	1.33	0.46
1:D:117:ILE:HB	1:D:142:VAL:HG11	1.98	0.46
1:A:305:PRO:C	1:A:306:VAL:HG12	2.36	0.46
1:B:143:PHE:O	1:B:144:SER:C	2.54	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:C:276:ILE:N	1:C:304:ASN:ND2	2.64	0.46
1:D:297:ASN:HA	1:D:297:ASN:HD22	1.51	0.46
1:D:323:LEU:HD22	1:D:323:LEU:H	1.80	0.46
1:D:51:GLU:HA	1:D:51:GLU:OE2	2.15	0.46
1:E:111:LYS:HG2	1:E:132:ASP:OD1	2.16	0.46
1:E:312:GLN:HG3	1:E:313:PRO:HD2	1.98	0.46
1:F:301:LEU:HA	1:F:301:LEU:HD12	1.79	0.46
1:F:71:LYS:HD2	1:F:72:ASP:OD1	2.15	0.46
1:A:312:GLN:O	1:A:315:THR:HB	2.16	0.45
1:A:94:HIS:O	1:A:97:ALA:HB2	2.16	0.45
1:B:191:LEU:HB2	1:B:216:TYR:OH	2.16	0.45
1:C:105:GLN:O	1:C:125:LEU:HD12	2.16	0.45
1:C:30:GLY:HA3	1:C:43:LEU:CD2	2.45	0.45
1:E:118:PRO:O	1:E:121:LEU:HD11	2.15	0.45
1:F:176:TYR:CD2	1:F:176:TYR:C	2.90	0.45
1:C:240:LEU:HD23	1:C:243:LEU:HD13	1.98	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: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:D:195:LEU:O	1:D:219:LEU:HD23	2.16	0.45
1:D:307:PRO:O	1:D:308:TYR:C	2.54	0.45
1:E:195:LEU:HD12	1:E:195:LEU:HA	1.74	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:ND2	1:F:148:ASN:N	2.64	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:A:57:THR:HG23	1:A:58:LEU:N	2.32	0.45
1:B:247:HIS:CD2	1:B:270:TYR:CD1	3.04	0.45
1:E:293:ARG:C	1:E:293:ARG:HD3	2.36	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:316:PHE:CD2	1:B:325:ILE:HD13	2.51	0.45
1:B:41:SER:O	1:B:42:ASP:HB2	2.16	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:HD22	1:F:148:ASN:N	2.15	0.45
1:A:189:LYS:O	1:A:215:ARG:HD2	2.16	0.45
1:A:25:ALA:C	1:A:26:MET:O	2.54	0.45
1:A:32:HIS:HD2	1:B:176:TYR:HB2	1.82	0.45
1:B:59:LEU:HB2	1:B:80:LEU:HD11	1.98	0.45
1:C:117:ILE:HB	1:C:142:VAL:HG11	1.99	0.45
1:C:268:VAL:HG13	1:C:268:VAL:O	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:D:234:ASN:HB3	1:D:258:ALA:HB3	1.98	0.45
1:E:108:TYR:CD1	1:E:129:ARG:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:86:VAL:HG12	1:C:87:ASN:N	2.31	0.44
3:D:2193:FLC:CGC	3:D:2193:FLC:OA1	2.61	0.44
1:F:219:LEU:C	1:F:220:TYR:HD2	2.20	0.44
1:F:260:LEU:HB2	1:F:261:PRO:HD3	1.99	0.44
1:A:122:PRO:O	1:A:123:SER:C	2.54	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:H	1:C:146:LEU:HD23	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:CD1	1:F:240:LEU:N	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:HG	1:C:128:LEU:O	2.17	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: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:F:54:PRO:C	1:F:56:THR:H	2.21	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: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:C:232:ILE:CD1	1:C:232:ILE:C	2.69	0.44
1:D:70:ARG:O	1:D:71:LYS:C	2.56	0.44
1:F:329:ASN:ND2	1:F:329:ASN:C	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:80:LEU:HD23	1:A:101:LEU:HD21	1.99	0.44
1:A:28:PRO:HD3	1:A:51:GLU:O	2.17	0.44
1:B:70:ARG:O	1:B:73:ASP:HB2	2.18	0.44
1:F:269:VAL:HG12	1:F:299:ILE:HG12	2.00	0.44
1:F:70:ARG:O	1:F: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:A:70:ARG:O	1:A:73:ASP:HB2	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:253:LEU:O	1:A:275:ASN:HB3	2.18	0.43
1:A:83:LEU:CD2	1:A:85:LEU:HD11	2.27	0.43
1:F:102:ARG:HG2	1:F:102:ARG:O	2.17	0.43
1:F:174:LEU:C	1:F:174:LEU:HD12	2.38	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:114:LEU:O	1:E:134:ARG:HB2	2.17	0.43
1:E:69:LEU:HD23	1:E:93:ILE:CG1	2.46	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:D:176:TYR:C	1:D:176:TYR:CD2	2.91	0.43
1:A:256:VAL:HG22	1:A:271:LEU:CD1	2.49	0.43
1:A:29:PHE:CE2	1:B:221:ARG:HG2	2.53	0.43
1:B:159:LEU:HD23	1:B:159:LEU:H	1.82	0.43
1:C:224:LEU:O	1:C:225:GLY:O	2.37	0.43
1:C:41:SER:O	1:C:42:ASP:CB	2.64	0.43
1:D:81:TYR:O	1:D:105:GLN:N	2.50	0.43
1:E:311:VAL:HG13	1:E:311:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ILE:HD11	1:A:213:LEU:HG	2.01	0.43
1:C:292:LYS:HE3	1:C:292:LYS:HB2	1.63	0.43
1:F:220:TYR:N	1:F:220:TYR:CD2	2.85	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:HG22	1:B:325:ILE:O	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:C:111:LYS:C	1:C:112:ASN:HD22	2.22	0.43
1:E:174:LEU:HD12	1:E:174:LEU:C	2.39	0.43
1:E:297:ASN:HA	1:E:297:ASN:HD22	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:235:GLY:O	1:B:238:SER:CB	2.64	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:E:32:HIS:HB2	1:F:176:TYR:CD1	2.54	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:HD22	1:B:184:LEU:N	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:C:253:LEU:HB2	1:C:274:ASN:CG	2.38	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:198:LEU:HD11	1:E:200:LEU:CD2	2.48	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: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
1:A:313:PRO:C	1:A:315:THR:N	2.72	0.42
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:C:245:GLU:CD	1:C:268:VAL:CG1	2.87	0.42
1:D:276:ILE:CB	1:D:304:ASN:ND2	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:LEU:HB3	1:E:240:LEU:HD11	2.00	0.42
1:E:80:LEU:HD23	1:E:101:LEU:CD2	2.49	0.42
1:F:174:LEU:C	1:F:174:LEU:CD1	2.87	0.42
1:C:232:ILE:CG2	1:C:257:PRO:HB3	2.47	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:D:33:CYS:CB	1:D:38:VAL:HA	2.49	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:B:108:TYR:CD1	1:B:129:ARG:HG3	2.54	0.42
1:C:191:LEU:HB3	1:C:192:PRO:HD2	2.02	0.42
1:C:27:CYS:CB	1:C:28:PRO:CD	2.83	0.42
1:D:222:LEU:O	1:D:246:LEU:HD12	2.19	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:E:81:TYR:CE1	1:E:105:GLN:OE1	2.72	0.42
1:A:85:LEU:CB	1:A:109:ILE:HG22	2.44	0.42
1:A:190:ASP:N	1:A:190:ASP:OD2	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:232:ILE:CD1	1:E:232:ILE:C	2.78	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:226:HIS:H	1:D:250:ASN:HB2	1.84	0.42
1:D:69:LEU:HB2	1:D:93:ILE:HG23	2.02	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:129:ARG:CZ	1:F:153:GLU:HG3	2.49	0.42
1:F:86:VAL:HG12	1:F:87:ASN:N	2.34	0.42
1:A:32:HIS:C	1:A:32:HIS:ND1	2.73	0.42
1:A:61:LEU:HD21	1:A:85:LEU:HD21	2.02	0.42
1:C:128:LEU:HB3	1:C:149:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:ARG:C	1:F:324:ALA:H	2.23	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: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:197:GLU:OE1	1:F:221:ARG:HD3	2.20	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:A:203:ASN:HB2	1:A:227:ASN:OD1	2.20	0.42
1:A:66:ILE:HG13	1:A:66:ILE:H	1.51	0.42
1:E:174:LEU:CD1	1:E:174:LEU:C	2.88	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:A:42:ASP:C	1:B:178:ARG:HH12	2.24	0.41
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:HA	1:C:297:ASN:HD22	1.44	0.41
1:E:63:ASN:CG	1:E:63:ASN:O	2.57	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:F:282:ASN:ND2	1:F:287:VAL:HG22	2.35	0.41
1:B:195:LEU:HA	1:B:195:LEU:HD12	1.83	0.41
1:C:208:ILE:HD13	1:C:208:ILE:HG21	1.73	0.41
1:C:260:LEU:HD12	1:C:284:PHE:CE1	2.55	0.41
1:C:245:GLU:CG	1:C:268:VAL:CG1	2.98	0.41
1:D:108:TYR:CD1	1:D:129:ARG:HG3	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:F:263:LEU:O	1:F:265:LEU:N	2.53	0.41
1:A:275:ASN:ND2	2:A:801:NAG:C4	2.75	0.41
1:A:28:PRO:HB2	1:A:31:CYS:SG	2.60	0.41
1:B:130:ILE:HD11	1:B:135:ILE:HD11	2.02	0.41
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:128:LEU:HB3	1:C:149:MET:CE	2.50	0.41
1:C:323:LEU:HD22	1:C:323:LEU:H	1.85	0.41
1:C:53:SER:HA	1:C:54:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:32:HIS:C	1:E:32:HIS:ND1	2.74	0.41
1:F:256:VAL:HG13	1:F:271:LEU:HD11	2.02	0.41
1:A:122:PRO:C	1:A:124:SER:N	2.73	0.41
1:A:139:PRO:CD	1:A:142:VAL:HG21	2.31	0.41
1:A:174:LEU:C	1:A:174:LEU:HD13	2.40	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:149:MET:HE3	1:C:152:ILE:CG1	2.51	0.41
1:C:184:LEU:N	1:C:184:LEU:CD2	2.83	0.41
1:C:62:GLN:O	1:C:63:ASN:HB3	2.21	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:D:207:ALA:HA	1:D:229:ILE:HG23	2.01	0.41
1:D:28:PRO:HB2	1:D:31:CYS:SG	2.61	0.41
1:D:322:ARG:HH22	1:D:328:GLY:C	2.24	0.41
1:E:245:GLU:CG	1:E:268:VAL:HG13	2.50	0.41
1:E:32:HIS:O	1:E:39:GLN:HB3	2.20	0.41
1:F:158:PRO:CG	1:F:158:PRO:O	2.68	0.41
1:F:248:LEU:HA	1:F:248:LEU:HD12	1.65	0.41
1:A:146:LEU:HG	1:A:146:LEU:H	1.51	0.41
1:C:149:MET:HE3	1:C:152:ILE:HD11	2.03	0.41
1:E:121:LEU:CD1	1:E:121:LEU:H	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:HA	1:A:80:LEU:HD12	1.83	0.41
1:B:246:LEU:HD21	1:B:248:LEU:CD2	2.50	0.41
1:C:172:LEU:O	1:C:174:LEU:N	2.53	0.41
1:C:28:PRO:HG3	1:C:49:PRO:HB2	2.03	0.41
1:D:138:VAL:HG11	1:D:164:PHE:CD1	2.56	0.41
1:E:298:GLY:HA2	1:E:324:ALA:O	2.20	0.41
1:A:221:ARG:NH2	1:A:245:GLU:HG3	2.36	0.41
1:A:248:LEU:HA	1:A:248:LEU:HD12	1.73	0.41
1:A:77:LEU:HB3	1:A:80:LEU:HB2	2.01	0.41
1:B:213:LEU:HD13	1:B:240:LEU:CD2	2.41	0.41
1:C:239:PHE:O	1:C:241:PRO:CD	2.68	0.41
1:E:98:PHE:C	1:E:100:PRO:HD2	2.41	0.41
1:E:191:LEU:CB	1:E:192:PRO:CD	2.97	0.41
1:E:225:GLY:O	1:E:226:HIS:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:TYR:N	1:F:220:TYR:HD2	2.18	0.41
1:A:179:ILE:HG21	1:A:179:ILE:HD13	1.54	0.41
1:A:182:ALA:HB3	1:A:184:LEU:HD23	2.01	0.41
1:A:99:SER:N	1:A:100:PRO:CD	2.83	0.41
1:C:69:LEU:CD2	1:C:93:ILE:HG12	2.48	0.41
1:E:268:VAL:HG22	1:E:268:VAL:O	2.18	0.41
1:F:200:LEU:HB2	1:F:224:LEU:HD23	2.03	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:111:LYS:C	1:A:112:ASN:HD22	2.24	0.41
1:B:240:LEU:HB3	1:B:243:LEU:HB2	2.02	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:HG2	1:E:102:ARG:O	2.21	0.41
1:E:130:ILE:HG12	1:E:130:ILE:O	2.21	0.41
1:A:264:LYS:C	1:A:265:LEU:HD12	2.42	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:A:178:ARG:NH2	1:B:43:LEU:HD23	2.35	0.41
1:C:180:SER:O	1:C:181:GLU:C	2.60	0.41
1:C:39:GLN:OE1	1:C:41:SER:OG	2.36	0.41
1:F:62:GLN:HB2	1:F:62:GLN:HE21	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:N	1:A:69:LEU:HD22	2.37	0.40
1:B:63:ASN:ND2	1:B:63:ASN:O	2.55	0.40
1:C:68:GLU:HB3	1:C:92:LYS:HB2	2.03	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ARG:O	1:E:73:ASP:HB2	2.21	0.40
1:F:138:VAL:HA	1:F:139:PRO:HD3	1.77	0.40
1:D:205:ILE:HD13	1:D:205:ILE:HG21	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:D:239:PHE:C	1:D:241:PRO:CD	2.76	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%)	2	22
1	B	301/332 (91%)	225 (75%)	68 (23%)	8 (3%)	6	37
1	C	301/332 (91%)	219 (73%)	68 (23%)	14 (5%)	3	23
1	D	302/332 (91%)	230 (76%)	59 (20%)	13 (4%)	3	26
1	E	301/332 (91%)	229 (76%)	53 (18%)	19 (6%)	1	16
1	F	303/332 (91%)	223 (74%)	67 (22%)	13 (4%)	3	26
All	All	1809/1992 (91%)	1342 (74%)	385 (21%)	82 (4%)	3	24

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
1	C	291	VAL

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Mol	Chain	Res	Type
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
1	F	293	ARG

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Mol	Chain	Res	Type
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 ⓘ

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%)	244 (89%)	29 (11%)	8	33
1	B	273/297 (92%)	253 (93%)	20 (7%)	16	52
1	C	273/297 (92%)	249 (91%)	24 (9%)	12	42
1	D	273/297 (92%)	243 (89%)	30 (11%)	7	31
1	E	273/297 (92%)	245 (90%)	28 (10%)	8	35
1	F	274/297 (92%)	246 (90%)	28 (10%)	8	35
All	All	1639/1782 (92%)	1480 (90%)	159 (10%)	9	37

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

Mol	Chain	Res	Type
1	A	32	HIS
1	A	46	LYS
1	A	59	LEU
1	A	61	LEU
1	A	67	SER
1	A	69	LEU
1	A	73	ASP
1	A	109	ILE
1	A	121	LEU
1	A	123	SER
1	A	142	VAL
1	A	159	LEU
1	A	170	ASP
1	A	174	LEU
1	A	180	SER
1	A	184	LEU
1	A	185	THR
1	A	191	LEU
1	A	208	ILE
1	A	221	ARG
1	A	232	ILE
1	A	250	ASN
1	A	268	VAL
1	A	277	THR
1	A	292	LYS
1	A	297	ASN
1	A	306	VAL
1	A	322	ARG

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Mol	Chain	Res	Type
1	A	327	PHE
1	B	57	THR
1	B	59	LEU
1	B	61	LEU
1	B	121	LEU
1	B	142	VAL
1	B	148	ASN
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	292	LYS
1	B	293	ARG
1	B	297	ASN
1	B	306	VAL
1	B	322	ARG
1	C	46	LYS
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	153	GLU
1	C	159	LEU
1	C	170	ASP
1	C	174	LEU
1	C	184	LEU
1	C	185	THR
1	C	191	LEU
1	C	208	ILE
1	C	215	ARG
1	C	232	ILE
1	C	238	SER
1	C	289	PHE
1	C	291	VAL

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Mol	Chain	Res	Type
1	C	297	ASN
1	C	306	VAL
1	C	322	ARG
1	D	59	LEU
1	D	61	LEU
1	D	67	SER
1	D	73	ASP
1	D	109	ILE
1	D	121	LEU
1	D	123	SER
1	D	142	VAL
1	D	146	LEU
1	D	148	ASN
1	D	153	GLU
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	286	PRO
1	D	292	LYS
1	D	297	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	73	ASP
1	E	121	LEU
1	E	142	VAL
1	E	146	LEU
1	E	148	ASN
1	E	153	GLU

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Mol	Chain	Res	Type
1	E	159	LEU
1	E	170	ASP
1	E	174	LEU
1	E	184	LEU
1	E	185	THR
1	E	191	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	306	VAL
1	E	322	ARG
1	F	59	LEU
1	F	61	LEU
1	F	67	SER
1	F	73	ASP
1	F	109	ILE
1	F	121	LEU
1	F	142	VAL
1	F	146	LEU
1	F	148	ASN
1	F	153	GLU
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	208	ILE
1	F	221	ARG
1	F	232	ILE
1	F	238	SER
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	306	VAL
1	F	322	ARG
1	F	329	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	63	ASN
1	A	105	GLN
1	A	113	HIS
1	A	148	ASN
1	A	206	GLN
1	A	297	ASN
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	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	131	HIS
1	C	148	ASN
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
1	D	113	HIS
1	D	148	ASN

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Mol	Chain	Res	Type
1	D	175	ASN
1	D	199	HIS
1	D	206	GLN
1	D	250	ASN
1	D	297	ASN
1	E	62	GLN
1	E	63	ASN
1	E	78	GLN
1	E	87	ASN
1	E	148	ASN
1	E	175	ASN
1	E	199	HIS
1	E	206	GLN
1	E	297	ASN
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	148	ASN
1	F	161	ASN
1	F	175	ASN
1	F	199	HIS
1	F	206	GLN
1	F	297	ASN
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 ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	2190	-	3,12,12	0.49	0	3,17,17	3.70	1 (33%)
2	NAG	A	801	1	14,14,15	1.18	1 (7%)	15,19,21	1.96	5 (33%)
3	FLC	B	2191	-	3,12,12	0.93	0	3,17,17	0.81	0
2	NAG	B	803	1	14,14,15	1.04	1 (7%)	15,19,21	1.65	3 (20%)
3	FLC	C	2192	-	3,12,12	1.26	0	3,17,17	5.05	2 (66%)
2	NAG	C	805	1	14,14,15	1.30	2 (14%)	15,19,21	1.78	4 (26%)
3	FLC	D	2193	1	3,12,12	1.11	0	3,17,17	3.01	2 (66%)
2	NAG	D	807	1	14,14,15	0.94	0	15,19,21	1.55	3 (20%)
3	FLC	E	2194	-	3,12,12	1.31	1 (33%)	3,17,17	4.00	2 (66%)
2	NAG	E	809	1	14,14,15	1.30	2 (14%)	15,19,21	2.30	4 (26%)
3	FLC	F	2195	-	3,12,12	2.17	2 (66%)	3,17,17	6.08	2 (66%)
2	NAG	F	811	1	14,14,15	1.06	1 (7%)	15,19,21	1.85	5 (33%)

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	A	2190	-	-	0/6/16/16	0/0/0/0
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	FLC	B	2191	-	-	0/6/16/16	0/0/0/0
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	FLC	C	2192	-	-	0/6/16/16	0/0/0/0
2	NAG	C	805	1	-	0/6/23/26	0/1/1/1
3	FLC	D	2193	1	-	0/6/16/16	0/0/0/0
2	NAG	D	807	1	-	0/6/23/26	0/1/1/1
3	FLC	E	2194	-	-	0/6/16/16	0/0/0/0
2	NAG	E	809	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	F	2195	-	-	0/6/16/16	0/0/0/0
2	NAG	F	811	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2194	FLC	CG-CB	-2.00	1.51	1.54
2	C	805	NAG	C1-C2	2.09	1.55	1.52
2	E	809	NAG	C4-C3	2.15	1.57	1.52
3	F	2195	FLC	OHB-CB	2.18	1.46	1.43
2	B	803	NAG	C1-C2	2.21	1.55	1.52
2	F	811	NAG	C1-C2	2.61	1.56	1.52
2	A	801	NAG	C1-C2	2.70	1.56	1.52
2	E	809	NAG	C1-C2	2.88	1.56	1.52
3	F	2195	FLC	CG-CB	2.91	1.59	1.54
2	C	805	NAG	C3-C2	2.98	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2192	FLC	CB-CA-CAC	-7.38	103.42	114.95
3	E	2194	FLC	CB-CG-CGC	-6.31	105.09	114.95
3	A	2190	FLC	CB-CG-CGC	-6.19	105.28	114.95
3	C	2192	FLC	CB-CG-CGC	-4.68	107.63	114.95
3	D	2193	FLC	CB-CG-CGC	-3.83	108.96	114.95
3	D	2193	FLC	CB-CA-CAC	-3.42	109.60	114.95
2	A	801	NAG	O5-C1-C2	-3.35	106.81	111.47
2	B	803	NAG	O4-C4-C5	-3.00	101.73	109.28
2	C	805	NAG	O3-C3-C4	-2.98	103.86	110.36
3	F	2195	FLC	CG-CB-CA	-2.87	102.60	109.75
2	A	801	NAG	C1-O5-C5	-2.51	108.71	112.17
3	E	2194	FLC	CB-CA-CAC	-2.42	111.17	114.95
2	B	803	NAG	C6-C5-C4	-2.40	107.39	113.00
2	F	811	NAG	O3-C3-C4	-2.30	105.34	110.36
2	D	807	NAG	O7-C7-C8	-2.17	118.11	122.06
2	F	811	NAG	O7-C7-C8	-2.15	118.14	122.06
2	A	801	NAG	O6-C6-C5	-2.13	104.17	111.34
2	F	811	NAG	C2-N2-C7	2.29	126.29	122.94
2	D	807	NAG	C1-O5-C5	2.42	115.50	112.17
2	E	809	NAG	C3-C4-C5	2.53	114.67	110.22
2	F	811	NAG	C8-C7-N2	2.58	120.77	116.11
2	C	805	NAG	O4-C4-C5	3.04	116.95	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	805	NAG	C4-C3-C2	3.07	115.52	111.02
2	A	801	NAG	C1-C2-N2	3.15	115.86	110.49
2	B	803	NAG	C3-C4-C5	3.25	115.94	110.22
2	C	805	NAG	C1-O5-C5	3.33	116.75	112.17
2	A	801	NAG	C8-C7-N2	3.36	122.18	116.11
2	D	807	NAG	C8-C7-N2	3.52	122.46	116.11
2	E	809	NAG	C1-C2-N2	4.13	117.54	110.49
2	E	809	NAG	C2-N2-C7	4.40	129.35	122.94
2	E	809	NAG	C1-O5-C5	4.57	118.47	112.17
2	F	811	NAG	C4-C3-C2	4.76	118.00	111.02
3	F	2195	FLC	CB-CG-CGC	10.04	130.64	114.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	809	NAG	O7-C7-N2-C2
2	E	809	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	5	0
3	B	2191	FLC	3	0
3	C	2192	FLC	3	0
3	D	2193	FLC	6	0
2	D	807	NAG	1	0
3	E	2194	FLC	2	0
3	F	2195	FLC	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	303/332 (91%)	0.19	0 100 100	8, 38, 52, 57	0
1	B	303/332 (91%)	0.30	4 (1%) 77 73	8, 38, 53, 70	0
1	C	303/332 (91%)	0.23	2 (0%) 87 85	8, 38, 53, 67	0
1	D	304/332 (91%)	0.18	0 100 100	8, 38, 52, 57	0
1	E	303/332 (91%)	0.21	2 (0%) 87 85	8, 37, 53, 64	0
1	F	305/332 (91%)	0.22	1 (0%) 93 92	6, 38, 52, 58	0
All	All	1821/1992 (91%)	0.22	9 (0%) 90 88	6, 38, 53, 70	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	GLY	3.6
1	B	288	GLY	3.1
1	B	25	ALA	3.0
1	E	25	ALA	2.7
1	E	294	ALA	2.6
1	C	291	VAL	2.4
1	B	291	VAL	2.3
1	B	96	LYS	2.1
1	F	257	PRO	2.0

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FLC	B	2191	13/13	0.90	0.30	1.28	49,53,56,57	0
3	FLC	E	2194	13/13	0.92	0.21	-0.35	36,44,47,48	0
3	FLC	A	2190	13/13	0.94	0.20	-0.70	47,50,53,53	0
3	FLC	F	2195	13/13	0.87	0.21	-0.76	38,42,42,43	0
3	FLC	D	2193	13/13	0.95	0.17	-1.15	38,40,44,45	0
3	FLC	C	2192	13/13	0.94	0.18	-1.25	38,43,46,46	0
2	NAG	E	809	14/15	0.72	0.40	-	59,61,62,62	0
2	NAG	A	801	14/15	0.89	0.24	-	51,53,55,55	0
2	NAG	D	807	14/15	0.89	0.27	-	58,59,61,62	0
2	NAG	B	803	14/15	0.80	0.27	-	46,50,51,51	0
2	NAG	C	805	14/15	0.79	0.30	-	53,56,57,58	0
2	NAG	F	811	14/15	0.89	0.16	-	49,50,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.