Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:41 PM GMT

PDB ID	:	1Y9E
Title	:	Crystal structure of Bacillus subtilis protein yhfP with NAD bound
Authors	:	Min, T.; Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-12-15
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

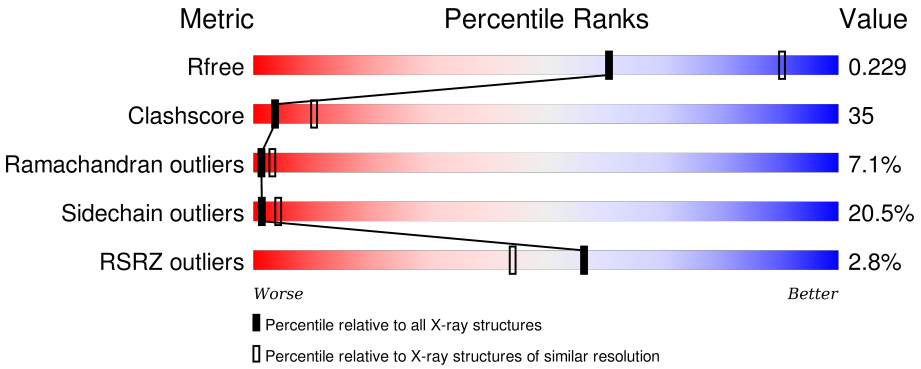
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 >=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 <=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	330	2% 42% 34% 17% 7%
1	B	330	4% 34% 40% 16% 10%
1	C	330	5% 35% 36% 21% 8%
1	D	330	3% 34% 39% 19% 8%
1	E	330	2% 37% 40% 13% 10%

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Mol	Chain	Length	Quality of chain
1	F	330	% 36% 36% 18% 10%

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
2	NAD	E	5255	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14982 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 hypothetical protein yhfP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	Se	0	0	0
			2429	1529	414	481	1	4			
1	B	329	Total	C	N	O	S	Se	0	0	0
			2421	1525	406	485	1	4			
1	C	329	Total	C	N	O	S	Se	0	0	0
			2412	1516	408	483	1	4			
1	D	329	Total	C	N	O	S	Se	0	0	0
			2431	1527	414	485	1	4			
1	E	329	Total	C	N	O	S	Se	0	0	0
			2433	1531	414	483	1	4			
1	F	329	Total	C	N	O	S	Se	0	0	0
			2437	1533	414	485	1	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
A	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
A	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
A	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
B	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
C	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
D	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
E	126	MSE	MET	MODIFIED RESIDUE	UNP O07615

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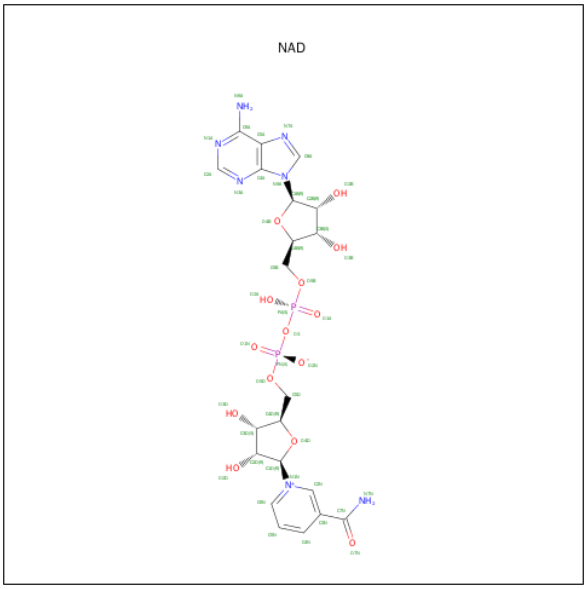
Chain	Residue	Modelled	Actual	Comment	Reference
E	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
E	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
E	288	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	126	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	170	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	278	MSE	MET	MODIFIED RESIDUE	UNP O07615
F	288	MSE	MET	MODIFIED RESIDUE	UNP O07615

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 11 6 5	0	0
2	B	1	Total C N 11 6 5	0	0
2	C	1	Total C N 11 6 5	0	0
2	D	1	Total C N 11 6 5	0	0
2	E	1	Total C N 11 6 5	0	0
2	F	1	Total C N 11 6 5	0	0

- Molecule 3 is water.

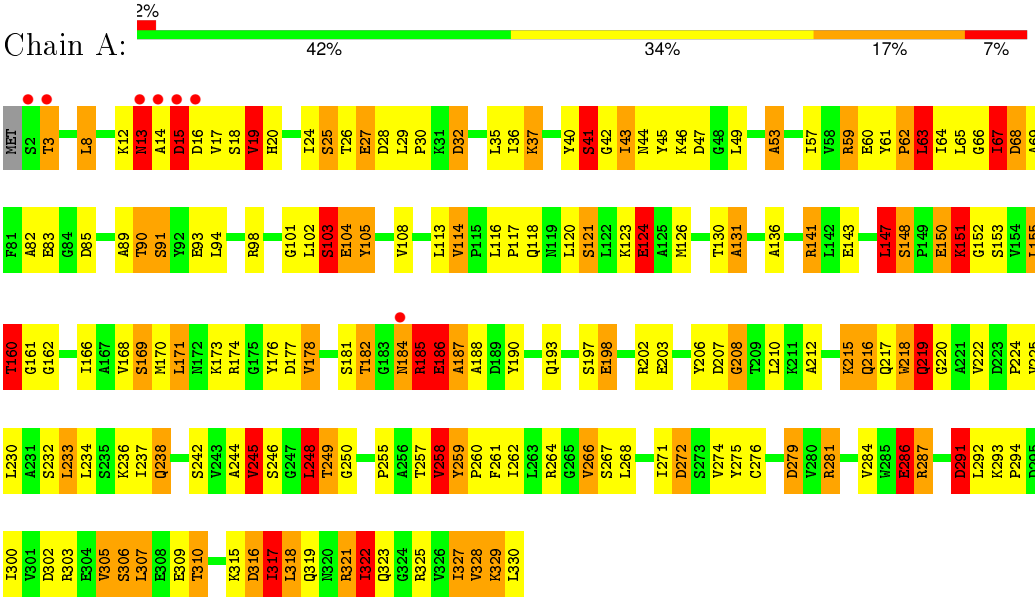
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0
3	B	56	Total O 56 56	0	0
3	C	57	Total O 57 57	0	0
3	D	53	Total O 53 53	0	0
3	E	60	Total O 60 60	0	0
3	F	62	Total O 62 62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

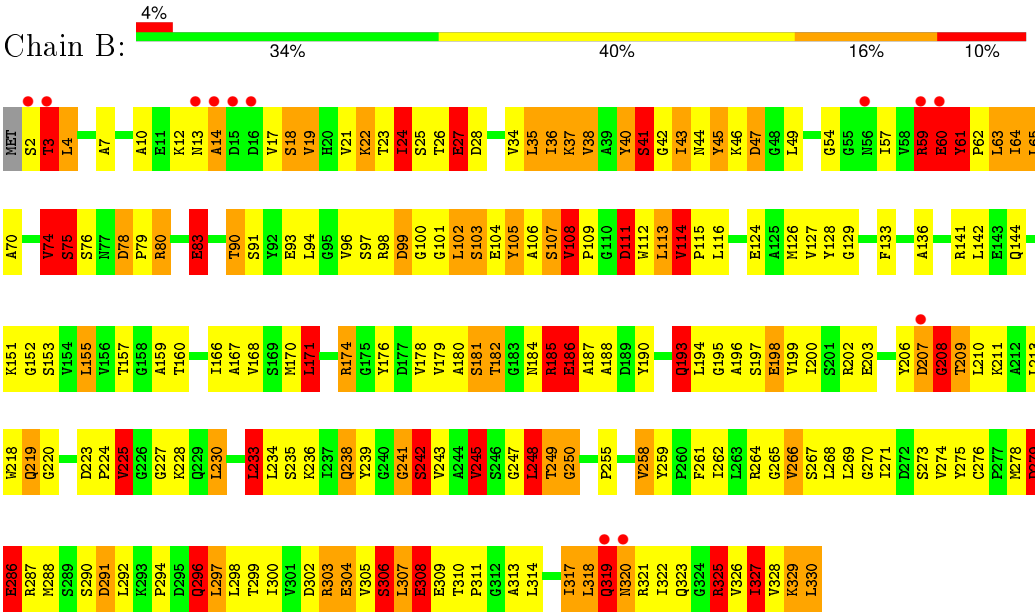
- Molecule 1: hypothetical protein yhfP

Chain A:



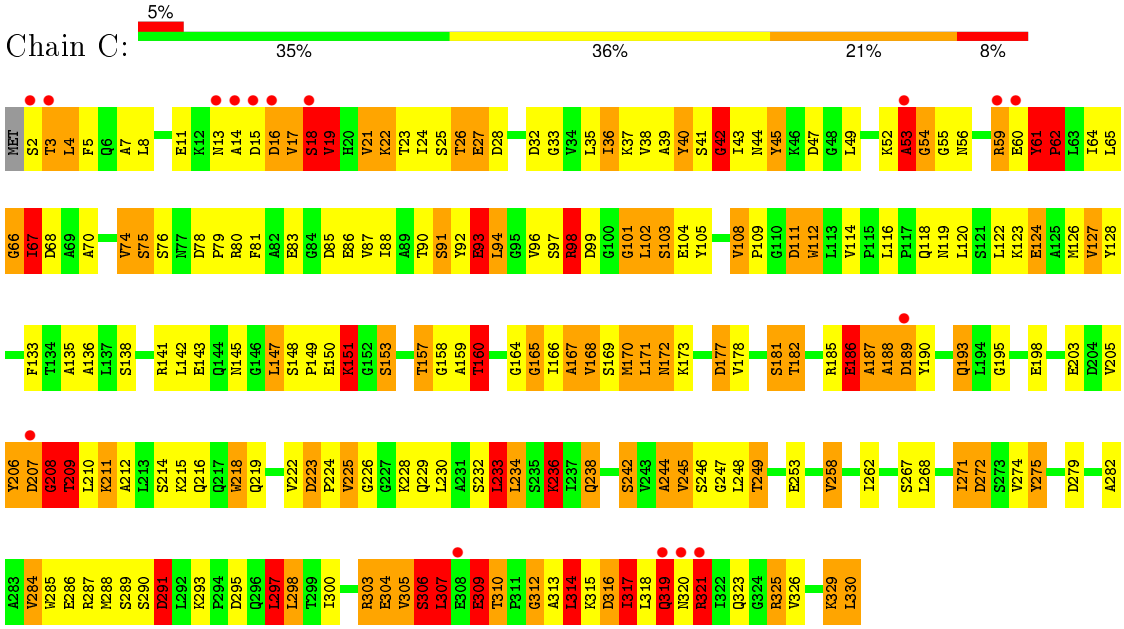
- Molecule 1: hypothetical protein yhfP

Chain B:



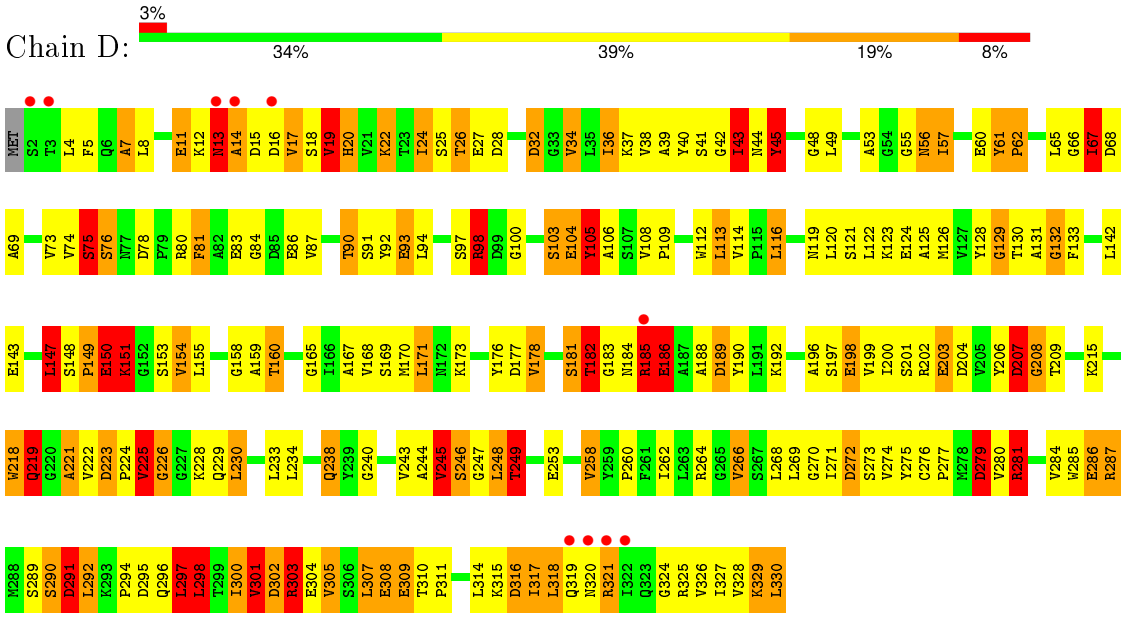
• Molecule 1: hypothetical protein yhfP

Chain C:



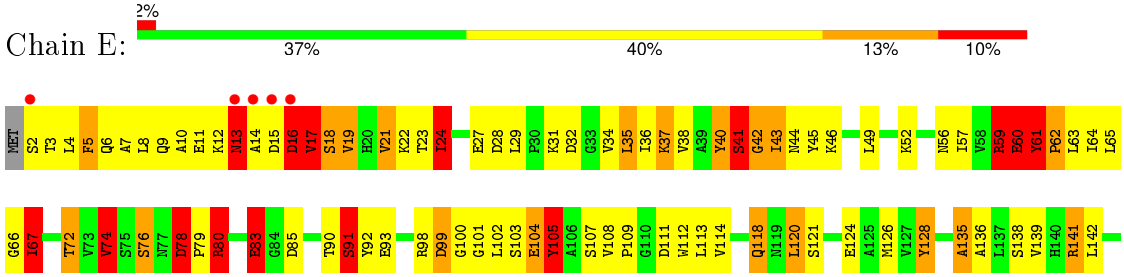
• Molecule 1: hypothetical protein yhfP

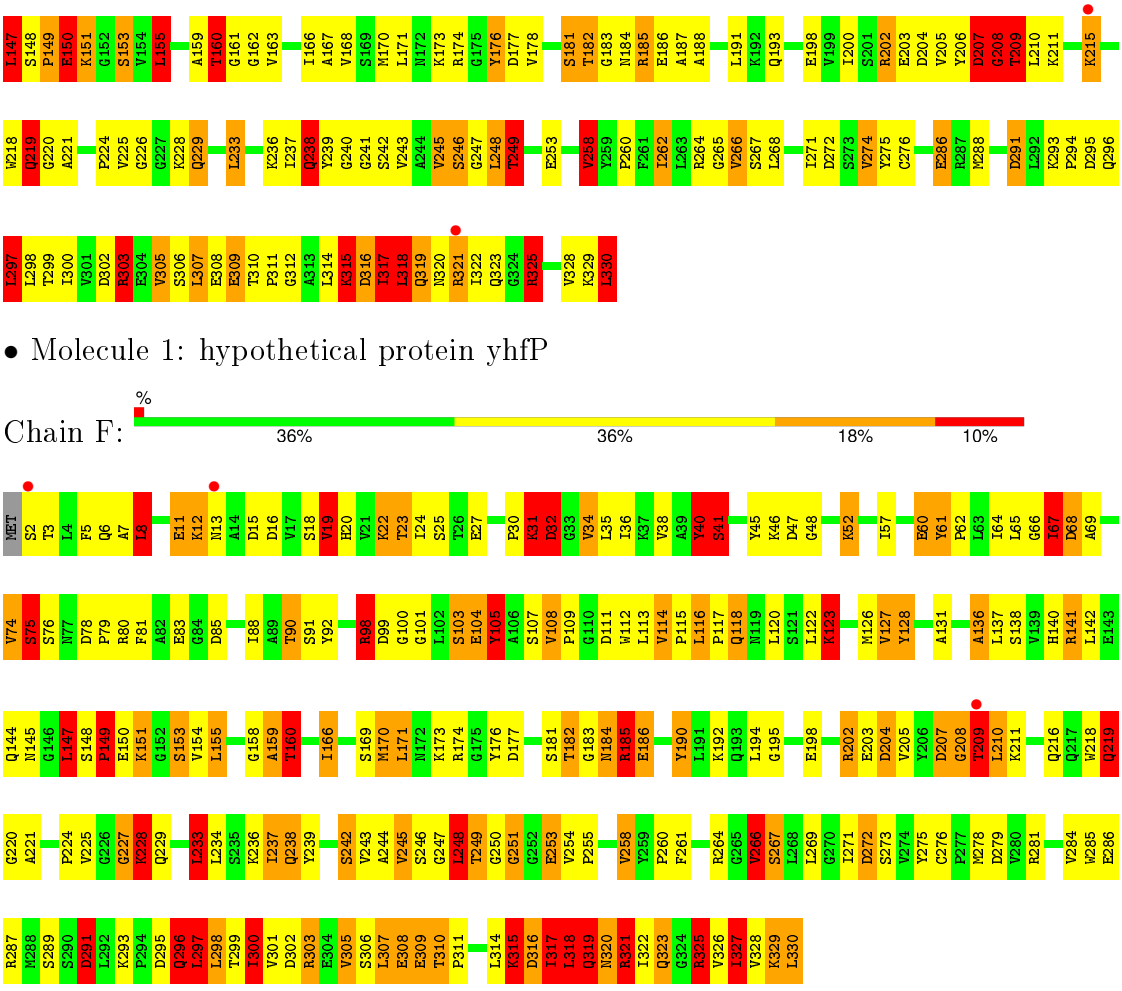
Chain D:



• Molecule 1: hypothetical protein yhfP

Chain E:





- Molecule 1: hypothetical protein yhfP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.27Å 136.92Å 167.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.98-2.80) 94.5 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.233 0.225 , 0.229	Depositor DCC
R_{free} test set	2568 reflections (4.72%)	DCC
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 130775 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14982	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NAD

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	2.12	70/2461 (2.8%)	2.05	88/3333 (2.6%)
1	B	2.16	86/2453 (3.5%)	1.85	60/3325 (1.8%)
1	C	2.09	72/2444 (2.9%)	1.87	55/3315 (1.7%)
1	D	2.18	81/2463 (3.3%)	1.83	56/3335 (1.7%)
1	E	2.20	82/2465 (3.3%)	1.92	70/3338 (2.1%)
1	F	2.22	89/2469 (3.6%)	1.99	85/3343 (2.5%)
All	All	2.16	480/14755 (3.3%)	1.92	414/19989 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
1	C	1	8
1	D	1	5
1	E	0	5
1	F	0	4
All	All	2	40

All (480) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	GLU	CG-CD	18.13	1.79	1.51
1	B	286	GLU	CG-CD	17.69	1.78	1.51
1	E	286	GLU	CD-OE1	16.23	1.43	1.25
1	A	286	GLU	CG-CD	15.81	1.75	1.51
1	E	83	GLU	CG-CD	15.61	1.75	1.51
1	D	286	GLU	CG-CD	15.51	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	209	THR	CA-CB	14.89	1.92	1.53
1	D	225	VAL	CB-CG2	13.93	1.82	1.52
1	A	238	GLN	CG-CD	13.82	1.82	1.51
1	F	186	GLU	CG-CD	13.14	1.71	1.51
1	D	186	GLU	CG-CD	12.47	1.70	1.51
1	D	203	GLU	CG-CD	12.37	1.70	1.51
1	C	207	ASP	CB-CG	12.29	1.77	1.51
1	B	83	GLU	CG-CD	12.22	1.70	1.51
1	E	319	GLN	CG-CD	11.79	1.78	1.51
1	E	59	ARG	CG-CD	11.21	1.79	1.51
1	D	253	GLU	CG-CD	11.12	1.68	1.51
1	D	45	TYR	CE1-CZ	11.04	1.52	1.38
1	F	286	GLU	CG-CD	10.91	1.68	1.51
1	B	215	LYS	CB-CG	10.82	1.81	1.52
1	F	105	TYR	N-CA	10.78	1.68	1.46
1	D	286	GLU	CD-OE2	10.74	1.37	1.25
1	E	286	GLU	CD-OE2	10.62	1.37	1.25
1	D	45	TYR	CE2-CZ	10.53	1.52	1.38
1	B	248	LEU	CG-CD1	10.45	1.90	1.51
1	B	286	GLU	CB-CG	10.44	1.72	1.52
1	E	238	GLN	CD-NE2	10.43	1.58	1.32
1	C	198	GLU	CD-OE1	10.41	1.37	1.25
1	A	298	LEU	CG-CD1	10.33	1.90	1.51
1	F	238	GLN	CD-NE2	10.29	1.58	1.32
1	C	258	VAL	CB-CG2	-9.92	1.32	1.52
1	B	186	GLU	CG-CD	9.90	1.66	1.51
1	A	258	VAL	CB-CG2	-9.82	1.32	1.52
1	C	151	LYS	C-O	9.79	1.42	1.23
1	D	279	ASP	CB-CG	-9.66	1.31	1.51
1	F	329	LYS	CE-NZ	9.61	1.73	1.49
1	C	208	GLY	CA-C	9.60	1.67	1.51
1	B	108	VAL	CB-CG2	-9.57	1.32	1.52
1	A	83	GLU	CG-CD	9.44	1.66	1.51
1	E	128	TYR	CD2-CE2	9.35	1.53	1.39
1	D	258	VAL	CB-CG2	-9.25	1.33	1.52
1	C	245	VAL	CB-CG2	-9.21	1.33	1.52
1	C	27	GLU	CG-CD	9.11	1.65	1.51
1	B	238	GLN	CD-NE2	9.09	1.55	1.32
1	F	315	LYS	CD-CE	9.06	1.74	1.51
1	C	198	GLU	CD-OE2	9.05	1.35	1.25
1	B	207	ASP	CB-CG	8.77	1.70	1.51
1	F	40	TYR	CZ-OH	8.77	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	225	VAL	CB-CG1	-8.76	1.34	1.52
1	F	83	GLU	CD-OE1	8.71	1.35	1.25
1	C	27	GLU	CB-CG	8.62	1.68	1.52
1	E	198	GLU	CD-OE2	8.62	1.35	1.25
1	C	42	GLY	C-O	8.57	1.37	1.23
1	F	329	LYS	CD-CE	8.54	1.72	1.51
1	A	27	GLU	CG-CD	8.54	1.64	1.51
1	B	303	ARG	CB-CG	8.52	1.75	1.52
1	D	198	GLU	CD-OE1	8.51	1.35	1.25
1	B	309	GLU	CD-OE2	8.48	1.34	1.25
1	E	208	GLY	N-CA	8.44	1.58	1.46
1	D	246	SER	N-CA	8.44	1.63	1.46
1	A	151	LYS	C-O	8.43	1.39	1.23
1	B	27	GLU	CG-CD	8.41	1.64	1.51
1	F	228	LYS	CE-NZ	8.38	1.70	1.49
1	A	286	GLU	CD-OE1	8.34	1.34	1.25
1	A	286	GLU	CD-OE2	8.32	1.34	1.25
1	E	160	THR	N-CA	8.30	1.62	1.46
1	B	266	VAL	CB-CG2	-8.29	1.35	1.52
1	E	67	ILE	CA-CB	8.19	1.73	1.54
1	A	123	LYS	CD-CE	8.14	1.71	1.51
1	E	128	TYR	CD1-CE1	8.12	1.51	1.39
1	E	105	TYR	N-CA	8.05	1.62	1.46
1	C	45	TYR	CD2-CE2	8.02	1.51	1.39
1	F	198	GLU	CD-OE2	7.84	1.34	1.25
1	D	73	VAL	CB-CG2	-7.82	1.36	1.52
1	A	89	ALA	CA-CB	7.81	1.68	1.52
1	E	59	ARG	CB-CG	7.80	1.73	1.52
1	C	112	TRP	CB-CG	7.78	1.64	1.50
1	B	106	ALA	CA-CB	7.72	1.68	1.52
1	F	202	ARG	NE-CZ	7.71	1.43	1.33
1	D	151	LYS	C-O	7.71	1.38	1.23
1	D	83	GLU	CD-OE1	7.70	1.34	1.25
1	D	45	TYR	CD2-CE2	7.67	1.50	1.39
1	D	215	LYS	CD-CE	7.63	1.70	1.51
1	A	93	GLU	CG-CD	7.59	1.63	1.51
1	B	285	TRP	CG-CD1	7.57	1.47	1.36
1	E	44	ASN	CB-CG	7.52	1.68	1.51
1	F	151	LYS	C-O	7.49	1.37	1.23
1	F	92	TYR	CD1-CE1	7.48	1.50	1.39
1	F	315	LYS	CE-NZ	7.47	1.67	1.49
1	A	37	LYS	CD-CE	7.44	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	VAL	CB-CG2	7.43	1.68	1.52
1	D	151	LYS	CD-CE	7.43	1.69	1.51
1	E	228	LYS	CD-CE	7.42	1.69	1.51
1	E	176	TYR	CD2-CE2	-7.42	1.28	1.39
1	E	323	GLN	CG-CD	7.41	1.68	1.51
1	F	284	VAL	CB-CG2	-7.40	1.37	1.52
1	D	186	GLU	CB-CG	7.38	1.66	1.52
1	A	83	GLU	CD-OE1	7.38	1.33	1.25
1	A	160	THR	CA-CB	7.36	1.72	1.53
1	B	159	ALA	N-CA	7.34	1.61	1.46
1	A	245	VAL	CB-CG1	-7.33	1.37	1.52
1	B	160	THR	CA-CB	7.32	1.72	1.53
1	D	26	THR	CB-CG2	7.31	1.76	1.52
1	A	45	TYR	CG-CD1	7.31	1.48	1.39
1	C	19	VAL	CB-CG1	7.29	1.68	1.52
1	F	276	CYS	CB-SG	-7.24	1.70	1.82
1	C	249	THR	C-O	7.19	1.37	1.23
1	E	42	GLY	C-O	7.17	1.35	1.23
1	D	13	ASN	CB-CG	7.17	1.67	1.51
1	B	306	SER	CB-OG	7.16	1.51	1.42
1	C	198	GLU	CG-CD	7.16	1.62	1.51
1	B	160	THR	N-CA	7.15	1.60	1.46
1	F	75	SER	N-CA	7.14	1.60	1.46
1	C	304	GLU	CG-CD	7.11	1.62	1.51
1	C	238	GLN	CD-NE2	7.11	1.50	1.32
1	A	37	LYS	CE-NZ	7.08	1.66	1.49
1	F	293	LYS	C-O	7.07	1.36	1.23
1	F	309	GLU	CD-OE1	7.06	1.33	1.25
1	D	83	GLU	CD-OE2	7.05	1.33	1.25
1	F	67	ILE	CA-CB	7.05	1.71	1.54
1	E	62	PRO	N-CA	7.03	1.59	1.47
1	B	59	ARG	CG-CD	7.03	1.69	1.51
1	A	203	GLU	CD-OE1	7.00	1.33	1.25
1	D	190	TYR	CE1-CZ	7.00	1.47	1.38
1	F	170	MSE	SE-CE	-6.99	1.54	1.95
1	C	275	TYR	CD2-CE2	6.99	1.49	1.39
1	F	321	ARG	CG-CD	6.97	1.69	1.51
1	B	198	GLU	CG-CD	6.96	1.62	1.51
1	D	225	VAL	CB-CG1	6.95	1.67	1.52
1	B	3	THR	CB-CG2	6.93	1.75	1.52
1	C	242	SER	CB-OG	-6.92	1.33	1.42
1	B	235	SER	C-O	6.92	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	GLU	CG-CD	6.90	1.62	1.51
1	D	198	GLU	CB-CG	6.88	1.65	1.52
1	B	22	LYS	CB-CG	6.87	1.71	1.52
1	B	303	ARG	CG-CD	6.86	1.69	1.51
1	B	242	SER	CB-OG	-6.86	1.33	1.42
1	A	228	LYS	CE-NZ	6.86	1.66	1.49
1	E	56	ASN	CB-CG	6.85	1.66	1.51
1	D	188	ALA	CA-CB	6.85	1.66	1.52
1	A	41	SER	C-O	6.83	1.36	1.23
1	F	118	GLN	CG-CD	6.83	1.66	1.51
1	F	326	VAL	CB-CG1	-6.83	1.38	1.52
1	B	124	GLU	CD-OE1	6.79	1.33	1.25
1	E	286	GLU	CG-CD	6.78	1.62	1.51
1	C	284	VAL	CB-CG1	-6.78	1.38	1.52
1	A	131	ALA	CA-CB	6.76	1.66	1.52
1	B	24	ILE	CB-CG2	6.74	1.73	1.52
1	F	166	ILE	CB-CG2	6.73	1.73	1.52
1	D	40	TYR	CE1-CZ	6.72	1.47	1.38
1	F	11	GLU	CD-OE1	6.70	1.33	1.25
1	D	92	TYR	CD1-CE1	6.69	1.49	1.39
1	A	190	TYR	CD1-CE1	6.67	1.49	1.39
1	E	141	ARG	CZ-NH1	-6.66	1.24	1.33
1	D	309	GLU	CG-CD	6.65	1.61	1.51
1	B	198	GLU	CD-OE2	6.62	1.32	1.25
1	F	65	LEU	C-O	6.60	1.35	1.23
1	A	160	THR	N-CA	6.59	1.59	1.46
1	A	305	VAL	CB-CG2	-6.59	1.39	1.52
1	A	169	SER	CB-OG	-6.59	1.33	1.42
1	D	45	TYR	CG-CD1	6.58	1.47	1.39
1	F	61	TYR	CD2-CE2	6.56	1.49	1.39
1	F	249	THR	CB-CG2	6.55	1.74	1.52
1	F	103	SER	CB-OG	-6.54	1.33	1.42
1	F	239	TYR	CD2-CE2	6.54	1.49	1.39
1	E	76	SER	CA-CB	6.54	1.62	1.52
1	A	60	GLU	CG-CD	6.53	1.61	1.51
1	C	87	VAL	CB-CG2	-6.52	1.39	1.52
1	A	328	VAL	CA-CB	-6.50	1.41	1.54
1	C	218	TRP	CG-CD1	6.50	1.45	1.36
1	A	63	LEU	N-CA	6.49	1.59	1.46
1	E	118	GLN	CG-CD	6.48	1.66	1.51
1	F	319	GLN	CG-CD	6.46	1.66	1.51
1	D	238	GLN	CD-NE2	6.46	1.49	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	PHE	CD1-CE1	6.45	1.52	1.39
1	E	21	VAL	CA-CB	-6.44	1.41	1.54
1	F	228	LYS	CD-CE	6.44	1.67	1.51
1	F	31	LYS	CB-CG	6.43	1.70	1.52
1	A	131	ALA	CA-C	-6.42	1.36	1.52
1	B	215	LYS	CG-CD	6.42	1.74	1.52
1	D	225	VAL	CA-CB	6.42	1.68	1.54
1	D	143	GLU	CB-CG	-6.38	1.40	1.52
1	E	34	VAL	CB-CG2	-6.38	1.39	1.52
1	E	209	THR	CA-CB	-6.37	1.36	1.53
1	C	190	TYR	CE2-CZ	6.36	1.46	1.38
1	E	246	SER	N-CA	6.34	1.59	1.46
1	C	153	SER	CB-OG	-6.34	1.34	1.42
1	F	203	GLU	CD-OE1	6.34	1.32	1.25
1	B	286	GLU	CD-OE1	6.33	1.32	1.25
1	D	98	ARG	CZ-NH2	6.33	1.41	1.33
1	F	273	SER	CB-OG	6.33	1.50	1.42
1	C	203	GLU	CD-OE2	6.32	1.32	1.25
1	C	53	ALA	CA-CB	6.32	1.65	1.52
1	B	159	ALA	CA-CB	-6.31	1.39	1.52
1	D	150	GLU	CG-CD	6.30	1.61	1.51
1	D	219	GLN	N-CA	6.30	1.58	1.46
1	D	45	TYR	CG-CD2	6.28	1.47	1.39
1	F	238	GLN	CB-CG	-6.28	1.35	1.52
1	C	303	ARG	CA-C	6.27	1.69	1.52
1	B	239	TYR	CD1-CE1	6.26	1.48	1.39
1	F	160	THR	N-CA	6.26	1.58	1.46
1	C	143	GLU	CD-OE1	6.24	1.32	1.25
1	A	118	GLN	CG-CD	6.23	1.65	1.51
1	B	104	GLU	CG-CD	6.23	1.61	1.51
1	F	267	SER	CB-OG	6.22	1.50	1.42
1	E	162	GLY	C-O	6.20	1.33	1.23
1	B	267	SER	CB-OG	-6.18	1.34	1.42
1	D	61	TYR	CD2-CE2	6.17	1.48	1.39
1	B	208	GLY	CA-C	6.17	1.61	1.51
1	A	287	ARG	CZ-NH1	-6.15	1.25	1.33
1	F	160	THR	CA-CB	6.15	1.69	1.53
1	C	83	GLU	CD-OE1	6.15	1.32	1.25
1	A	121	SER	CA-CB	-6.15	1.43	1.52
1	B	265	GLY	C-O	-6.14	1.13	1.23
1	E	168	VAL	CB-CG2	6.14	1.65	1.52
1	F	185	ARG	N-CA	6.14	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	229	GLN	CD-NE2	6.14	1.48	1.32
1	C	45	TYR	CE2-CZ	6.13	1.46	1.38
1	B	207	ASP	C-O	6.13	1.34	1.23
1	B	273	SER	CB-OG	6.12	1.50	1.42
1	E	150	GLU	CG-CD	6.12	1.61	1.51
1	C	40	TYR	CB-CG	-6.11	1.42	1.51
1	E	40	TYR	CD2-CE2	6.10	1.48	1.39
1	D	286	GLU	CB-CG	6.10	1.63	1.52
1	C	286	GLU	CG-CD	6.09	1.61	1.51
1	F	202	ARG	CD-NE	6.08	1.56	1.46
1	A	114	VAL	CB-CG2	6.07	1.65	1.52
1	D	7	ALA	CA-CB	-6.07	1.39	1.52
1	F	123	LYS	CE-NZ	6.07	1.64	1.49
1	D	124	GLU	CD-OE1	6.06	1.32	1.25
1	C	275	TYR	CE2-CZ	6.06	1.46	1.38
1	A	317	ILE	N-CA	6.05	1.58	1.46
1	F	99	ASP	CB-CG	6.04	1.64	1.51
1	D	249	THR	CB-CG2	6.04	1.72	1.52
1	F	325	ARG	CB-CG	6.04	1.68	1.52
1	B	245	VAL	CB-CG1	-6.03	1.40	1.52
1	A	279	ASP	CB-CG	-6.02	1.39	1.51
1	C	124	GLU	CB-CG	6.02	1.63	1.52
1	F	305	VAL	CB-CG2	-6.02	1.40	1.52
1	E	99	ASP	CB-CG	6.01	1.64	1.51
1	E	182	THR	CB-CG2	6.01	1.72	1.52
1	E	177	ASP	C-O	6.00	1.34	1.23
1	D	40	TYR	CD1-CE1	5.99	1.48	1.39
1	B	199	VAL	CB-CG1	-5.98	1.40	1.52
1	F	153	SER	CB-OG	-5.97	1.34	1.42
1	C	232	SER	CB-OG	5.97	1.50	1.42
1	E	60	GLU	CG-CD	5.97	1.60	1.51
1	F	3	THR	N-CA	5.97	1.58	1.46
1	D	106	ALA	CA-CB	-5.96	1.40	1.52
1	A	53	ALA	CA-CB	5.95	1.65	1.52
1	D	93	GLU	CG-CD	5.94	1.60	1.51
1	B	326	VAL	CB-CG1	-5.94	1.40	1.52
1	D	329	LYS	CE-NZ	5.94	1.63	1.49
1	A	19	VAL	CA-CB	5.93	1.67	1.54
1	C	112	TRP	CE3-CZ3	5.93	1.48	1.38
1	B	215	LYS	CD-CE	5.93	1.66	1.51
1	F	296	GLN	C-O	5.92	1.34	1.23
1	A	275	TYR	CE2-CZ	5.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	THR	CB-CG2	5.92	1.71	1.52
1	A	259	TYR	CD1-CE1	-5.91	1.30	1.39
1	A	291	ASP	CB-CG	-5.90	1.39	1.51
1	E	215	LYS	CD-CE	5.90	1.66	1.51
1	E	258	VAL	CB-CG1	-5.89	1.40	1.52
1	C	128	TYR	CD1-CE1	-5.86	1.30	1.39
1	A	143	GLU	C-O	-5.85	1.12	1.23
1	E	31	LYS	CB-CG	5.85	1.68	1.52
1	F	128	TYR	CB-CG	-5.85	1.42	1.51
1	F	5	PHE	CD2-CE2	5.84	1.50	1.39
1	F	192	LYS	CE-NZ	5.84	1.63	1.49
1	A	203	GLU	CD-OE2	5.84	1.32	1.25
1	A	321	ARG	CD-NE	5.84	1.56	1.46
1	B	75	SER	CA-C	5.83	1.68	1.52
1	F	325	ARG	CZ-NH2	5.81	1.40	1.33
1	F	11	GLU	CG-CD	5.79	1.60	1.51
1	D	84	GLY	C-O	-5.79	1.14	1.23
1	C	303	ARG	N-CA	5.78	1.57	1.46
1	E	319	GLN	CB-CG	5.78	1.68	1.52
1	B	105	TYR	CB-CG	-5.77	1.43	1.51
1	B	198	GLU	CB-CG	5.77	1.63	1.52
1	E	21	VAL	CB-CG1	-5.77	1.40	1.52
1	F	209	THR	CB-CG2	5.76	1.71	1.52
1	A	236	LYS	CE-NZ	5.76	1.63	1.49
1	A	121	SER	C-O	5.75	1.34	1.23
1	D	203	GLU	CD-OE1	5.75	1.31	1.25
1	E	151	LYS	C-O	5.75	1.34	1.23
1	A	19	VAL	N-CA	5.74	1.57	1.46
1	C	94	LEU	CG-CD1	5.72	1.73	1.51
1	C	258	VAL	CA-C	5.72	1.67	1.52
1	F	325	ARG	CG-CD	5.72	1.66	1.51
1	C	128	TYR	CD2-CE2	-5.72	1.30	1.39
1	F	253	GLU	CD-OE1	5.71	1.31	1.25
1	F	136	ALA	CA-CB	-5.71	1.40	1.52
1	B	225	VAL	CB-CG1	-5.71	1.40	1.52
1	C	206	TYR	CZ-OH	-5.70	1.28	1.37
1	D	207	ASP	C-O	5.70	1.34	1.23
1	D	40	TYR	CB-CG	-5.70	1.43	1.51
1	E	45	TYR	CD2-CE2	-5.69	1.30	1.39
1	E	203	GLU	CB-CG	-5.69	1.41	1.52
1	D	149	PRO	N-CA	5.69	1.56	1.47
1	D	81	PHE	CB-CG	-5.68	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	208	GLY	C-O	5.67	1.32	1.23
1	C	3	THR	CB-CG2	5.67	1.71	1.52
1	C	160	THR	CA-CB	5.66	1.68	1.53
1	F	45	TYR	CE1-CZ	5.64	1.45	1.38
1	F	76	SER	C-O	5.64	1.34	1.23
1	B	37	LYS	CE-NZ	5.63	1.63	1.49
1	D	321	ARG	CG-CD	5.63	1.66	1.51
1	D	104	GLU	CD-OE1	5.62	1.31	1.25
1	D	215	LYS	CG-CD	5.62	1.71	1.52
1	E	62	PRO	CB-CG	5.61	1.78	1.50
1	E	264	ARG	CG-CD	-5.61	1.38	1.51
1	E	253	GLU	CD-OE1	5.61	1.31	1.25
1	D	16	ASP	CB-CG	5.60	1.63	1.51
1	E	59	ARG	NE-CZ	5.58	1.40	1.33
1	B	133	PHE	CG-CD1	-5.58	1.30	1.38
1	F	83	GLU	CD-OE2	5.58	1.31	1.25
1	E	186	GLU	CB-CG	5.58	1.62	1.52
1	F	275	TYR	CG-CD1	5.57	1.46	1.39
1	A	198	GLU	CD-OE1	5.56	1.31	1.25
1	D	273	SER	CB-OG	5.56	1.49	1.42
1	A	27	GLU	CD-OE2	5.56	1.31	1.25
1	B	309	GLU	CD-OE1	5.56	1.31	1.25
1	D	266	VAL	CB-CG1	-5.55	1.41	1.52
1	A	321	ARG	NE-CZ	5.54	1.40	1.33
1	E	92	TYR	CD1-CE1	5.54	1.47	1.39
1	A	78	ASP	N-CA	-5.54	1.35	1.46
1	D	244	ALA	CA-CB	-5.54	1.40	1.52
1	F	228	LYS	CG-CD	5.54	1.71	1.52
1	B	296	GLN	CG-CD	5.53	1.63	1.51
1	F	154	VAL	CB-CG2	-5.53	1.41	1.52
1	B	45	TYR	CE2-CZ	5.53	1.45	1.38
1	B	174	ARG	C-O	5.53	1.33	1.23
1	D	104	GLU	CG-CD	5.53	1.60	1.51
1	E	17	VAL	CA-CB	5.52	1.66	1.54
1	A	136	ALA	CA-CB	5.52	1.64	1.52
1	B	207	ASP	C-N	5.52	1.43	1.33
1	A	222	VAL	CB-CG2	-5.51	1.41	1.52
1	D	57	ILE	CA-CB	-5.50	1.42	1.54
1	B	249	THR	CB-CG2	5.49	1.70	1.52
1	E	186	GLU	CG-CD	5.48	1.60	1.51
1	C	45	TYR	CD1-CE1	5.48	1.47	1.39
1	E	56	ASN	CG-OD1	5.48	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	161	GLY	C-O	5.47	1.32	1.23
1	D	309	GLU	CD-OE2	5.47	1.31	1.25
1	E	105	TYR	CD1-CE1	-5.46	1.31	1.39
1	A	91	SER	CB-OG	5.46	1.49	1.42
1	C	133	PHE	CD2-CE2	5.46	1.50	1.39
1	B	180	ALA	N-CA	5.45	1.57	1.46
1	B	116	LEU	C-O	-5.45	1.12	1.23
1	E	303	ARG	CG-CD	5.44	1.65	1.51
1	E	226	GLY	N-CA	5.44	1.54	1.46
1	B	114	VAL	CA-CB	5.43	1.66	1.54
1	F	249	THR	N-CA	5.43	1.57	1.46
1	B	308	GLU	CD-OE1	5.42	1.31	1.25
1	E	149	PRO	C-O	-5.41	1.12	1.23
1	B	195	GLY	N-CA	5.41	1.54	1.46
1	C	124	GLU	CD-OE1	5.41	1.31	1.25
1	B	245	VAL	CA-CB	-5.40	1.43	1.54
1	C	87	VAL	CB-CG1	-5.39	1.41	1.52
1	E	167	ALA	CA-CB	-5.38	1.41	1.52
1	E	205	VAL	CB-CG1	-5.38	1.41	1.52
1	F	127	VAL	CB-CG2	-5.37	1.41	1.52
1	A	210	LEU	CG-CD1	5.37	1.71	1.51
1	E	21	VAL	CB-CG2	-5.36	1.41	1.52
1	C	286	GLU	CB-CG	5.36	1.62	1.52
1	C	215	LYS	CD-CE	5.36	1.64	1.51
1	C	62	PRO	CB-CG	5.35	1.76	1.50
1	A	284	VAL	CB-CG2	-5.35	1.41	1.52
1	C	306	SER	CB-OG	-5.35	1.35	1.42
1	C	167	ALA	CA-CB	-5.35	1.41	1.52
1	D	34	VAL	CB-CG2	-5.35	1.41	1.52
1	D	198	GLU	CD-OE2	5.34	1.31	1.25
1	D	328	VAL	CB-CG1	-5.33	1.41	1.52
1	C	275	TYR	CG-CD2	5.33	1.46	1.39
1	D	19	VAL	CB-CG1	-5.32	1.41	1.52
1	B	327	ILE	CA-CB	-5.32	1.42	1.54
1	A	322	ILE	CG1-CD1	5.32	1.87	1.50
1	A	238	GLN	CB-CG	5.32	1.66	1.52
1	E	128	TYR	CG-CD1	5.31	1.46	1.39
1	F	275	TYR	CD2-CE2	5.31	1.47	1.39
1	C	321	ARG	CG-CD	5.30	1.65	1.51
1	E	315	LYS	CD-CE	5.30	1.64	1.51
1	B	202	ARG	CG-CD	5.30	1.65	1.51
1	E	276	CYS	CB-SG	-5.30	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	153	SER	CA-CB	-5.29	1.45	1.52
1	F	149	PRO	C-O	-5.29	1.12	1.23
1	B	210	LEU	CG-CD1	5.29	1.71	1.51
1	F	254	VAL	CA-CB	-5.29	1.43	1.54
1	D	226	GLY	N-CA	5.29	1.53	1.46
1	E	309	GLU	CG-CD	5.29	1.59	1.51
1	B	250	GLY	N-CA	5.29	1.53	1.46
1	D	105	TYR	N-CA	5.29	1.56	1.46
1	B	258	VAL	CB-CG2	-5.29	1.41	1.52
1	C	236	LYS	CE-NZ	5.28	1.62	1.49
1	D	87	VAL	CB-CG2	5.28	1.64	1.52
1	D	190	TYR	CE2-CZ	5.28	1.45	1.38
1	B	196	ALA	CA-CB	-5.28	1.41	1.52
1	F	249	THR	C-O	5.26	1.33	1.23
1	F	279	ASP	CB-CG	5.26	1.62	1.51
1	A	202	ARG	CG-CD	5.26	1.65	1.51
1	B	74	VAL	CB-CG1	-5.26	1.41	1.52
1	A	203	GLU	CB-CG	5.25	1.62	1.52
1	A	275	TYR	CB-CG	-5.25	1.43	1.51
1	F	195	GLY	C-O	-5.25	1.15	1.23
1	E	107	SER	CB-OG	5.24	1.49	1.42
1	B	239	TYR	CG-CD1	5.22	1.46	1.39
1	B	38	VAL	CB-CG2	-5.22	1.41	1.52
1	F	202	ARG	C-O	5.22	1.33	1.23
1	F	207	ASP	C-O	5.22	1.33	1.23
1	B	22	LYS	CA-CB	5.22	1.65	1.53
1	E	5	PHE	C-O	5.22	1.33	1.23
1	E	264	ARG	CZ-NH1	5.21	1.39	1.33
1	A	168	VAL	CA-CB	5.21	1.65	1.54
1	D	298	LEU	CG-CD1	5.21	1.71	1.51
1	E	321	ARG	NE-CZ	5.21	1.39	1.33
1	F	202	ARG	CZ-NH1	5.21	1.39	1.33
1	D	62	PRO	CG-CD	5.20	1.67	1.50
1	E	184	ASN	CG-OD1	-5.20	1.12	1.24
1	B	40	TYR	CE1-CZ	5.20	1.45	1.38
1	C	177	ASP	CA-C	-5.20	1.39	1.52
1	C	282	ALA	C-O	5.20	1.33	1.23
1	B	150	GLU	CB-CG	5.20	1.62	1.52
1	C	96	VAL	CB-CG2	5.20	1.63	1.52
1	A	67	ILE	N-CA	5.20	1.56	1.46
1	F	45	TYR	CB-CG	-5.20	1.43	1.51
1	F	60	GLU	CG-CD	5.18	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	285	TRP	CB-CG	5.17	1.59	1.50
1	F	308	GLU	CD-OE1	5.17	1.31	1.25
1	D	240	GLY	C-O	-5.16	1.15	1.23
1	F	209	THR	CA-C	5.16	1.66	1.52
1	A	82	ALA	CA-CB	-5.15	1.41	1.52
1	C	60	GLU	CG-CD	5.14	1.59	1.51
1	D	28	ASP	CB-CG	5.14	1.62	1.51
1	F	38	VAL	CB-CG1	-5.14	1.42	1.52
1	B	185	ARG	CB-CG	5.14	1.66	1.52
1	E	135	ALA	CA-CB	-5.14	1.41	1.52
1	E	40	TYR	CE1-CZ	5.13	1.45	1.38
1	B	45	TYR	CG-CD1	5.13	1.45	1.39
1	B	241	GLY	C-O	-5.13	1.15	1.23
1	A	202	ARG	NE-CZ	5.12	1.39	1.33
1	D	92	TYR	CE2-CZ	5.12	1.45	1.38
1	B	286	GLU	CD-OE2	5.11	1.31	1.25
1	F	27	GLU	CD-OE2	5.10	1.31	1.25
1	B	62	PRO	N-CA	5.10	1.55	1.47
1	D	301	VAL	CA-CB	5.09	1.65	1.54
1	E	163	VAL	CB-CG2	5.09	1.63	1.52
1	D	39	ALA	N-CA	5.09	1.56	1.46
1	A	266	VAL	CB-CG1	-5.08	1.42	1.52
1	F	266	VAL	CB-CG2	-5.08	1.42	1.52
1	C	19	VAL	CA-CB	5.08	1.65	1.54
1	F	45	TYR	C-O	5.07	1.32	1.23
1	C	96	VAL	CA-CB	5.07	1.65	1.54
1	A	159	ALA	N-CA	5.07	1.56	1.46
1	C	150	GLU	CG-CD	5.06	1.59	1.51
1	D	178	VAL	CB-CG2	-5.06	1.42	1.52
1	B	185	ARG	CG-CD	5.06	1.64	1.51
1	D	303	ARG	CB-CG	5.06	1.66	1.52
1	D	215	LYS	CE-NZ	5.06	1.61	1.49
1	E	174	ARG	CZ-NH1	-5.06	1.26	1.33
1	A	41	SER	CA-CB	-5.06	1.45	1.52
1	C	208	GLY	N-CA	5.06	1.53	1.46
1	E	98	ARG	CZ-NH1	5.06	1.39	1.33
1	A	45	TYR	CD1-CE1	5.05	1.47	1.39
1	E	262	ILE	C-O	-5.05	1.13	1.23
1	E	114	VAL	CB-CG2	-5.05	1.42	1.52
1	E	275	TYR	CG-CD2	5.05	1.45	1.39
1	C	66	GLY	C-O	5.05	1.31	1.23
1	E	153	SER	N-CA	5.05	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	GLY	C-O	5.03	1.31	1.23
1	C	244	ALA	C-O	5.03	1.32	1.23
1	C	329	LYS	CD-CE	5.03	1.63	1.51
1	B	105	TYR	N-CA	5.03	1.56	1.46
1	B	99	ASP	C-O	-5.02	1.13	1.23
1	B	105	TYR	CE2-CZ	5.02	1.45	1.38
1	B	112	TRP	CG-CD1	5.02	1.43	1.36
1	F	116	LEU	N-CA	5.02	1.56	1.46
1	C	86	GLU	CD-OE1	5.01	1.31	1.25
1	B	329	LYS	CE-NZ	5.01	1.61	1.49
1	C	170	MSE	CG-SE	-5.01	1.78	1.95
1	B	47	ASP	CB-CG	-5.00	1.41	1.51

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	TYR	C-N-CD	-21.88	72.47	120.60
1	A	325	ARG	NE-CZ-NH1	-17.28	111.66	120.30
1	F	325	ARG	NE-CZ-NH1	-16.71	111.94	120.30
1	C	207	ASP	CB-CG-OD1	16.28	132.95	118.30
1	C	279	ASP	CB-CG-OD1	-13.84	105.84	118.30
1	F	202	ARG	NE-CZ-NH1	13.77	127.19	120.30
1	D	32	ASP	CB-CG-OD1	-13.53	106.12	118.30
1	E	141	ARG	NE-CZ-NH2	13.12	126.86	120.30
1	E	120	LEU	CB-CG-CD1	-12.86	89.15	111.00
1	A	210	LEU	CB-CG-CD2	-12.45	89.84	111.00
1	B	80	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	E	120	LEU	CA-CB-CG	12.33	143.66	115.30
1	A	61	TYR	C-N-CA	12.21	173.28	122.00
1	A	85	ASP	CB-CG-OD1	-12.10	107.41	118.30
1	E	207	ASP	CB-CG-OD1	11.87	128.99	118.30
1	A	279	ASP	CB-CG-OD1	-11.84	107.64	118.30
1	B	279	ASP	CB-CG-OD1	-11.53	107.92	118.30
1	A	141	ARG	NE-CZ-NH1	-11.46	114.57	120.30
1	B	41	SER	CA-C-N	-11.43	93.34	116.20
1	D	279	ASP	CB-CG-OD1	-11.28	108.15	118.30
1	E	307	LEU	CB-CG-CD1	-11.26	91.87	111.00
1	B	233	LEU	CB-CG-CD1	-11.19	91.98	111.00
1	C	279	ASP	CB-CG-OD2	11.16	128.35	118.30
1	A	321	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	A	298	LEU	CB-CG-CD2	-10.95	92.39	111.00
1	F	300	ILE	CG1-CB-CG2	-10.88	87.46	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	98	ARG	NE-CZ-NH2	10.80	125.70	120.30
1	A	202	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	E	298	LEU	CB-CG-CD1	-10.70	92.82	111.00
1	F	41	SER	N-CA-CB	-10.53	94.71	110.50
1	A	41	SER	N-CA-C	10.48	139.30	111.00
1	C	98	ARG	NE-CZ-NH1	-10.30	115.15	120.30
1	C	248	LEU	CB-CG-CD2	-10.29	93.50	111.00
1	C	85	ASP	CB-CG-OD2	-10.16	109.16	118.30
1	A	41	SER	CA-C-N	-10.11	95.99	116.20
1	C	61	TYR	N-CA-C	10.05	138.13	111.00
1	C	207	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	A	238	GLN	CA-CB-CG	9.81	134.98	113.40
1	C	85	ASP	CB-CG-OD1	9.74	127.07	118.30
1	D	80	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	B	41	SER	CB-CA-C	-9.41	92.22	110.10
1	A	298	LEU	CB-CG-CD1	9.39	126.96	111.00
1	C	102	LEU	CB-CG-CD1	-9.36	95.08	111.00
1	F	141	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	A	248	LEU	CA-CB-CG	-9.31	93.88	115.30
1	D	279	ASP	N-CA-CB	-9.31	93.84	110.60
1	E	59	ARG	CG-CD-NE	9.26	131.25	111.80
1	A	80	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	F	173	LYS	CD-CE-NZ	-9.18	90.59	111.70
1	C	295	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	A	327	ILE	CB-CA-C	-9.12	93.37	111.60
1	F	248	LEU	CB-CG-CD2	-9.11	95.51	111.00
1	A	147	LEU	CA-CB-CG	8.84	135.64	115.30
1	C	245	VAL	CB-CA-C	-8.84	94.61	111.40
1	C	307	LEU	CB-CG-CD1	-8.76	96.11	111.00
1	D	78	ASP	CB-CG-OD2	-8.72	110.46	118.30
1	A	155	LEU	CA-CB-CG	8.71	135.33	115.30
1	B	41	SER	N-CA-C	8.70	134.50	111.00
1	D	189	ASP	CB-CG-OD1	8.70	126.13	118.30
1	F	185	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	F	330	LEU	CA-CB-CG	-8.63	95.45	115.30
1	E	41	SER	N-CA-CB	-8.52	97.73	110.50
1	C	102	LEU	CA-CB-CG	8.51	134.86	115.30
1	F	131	ALA	C-N-CA	-8.50	104.44	122.30
1	F	233	LEU	CB-CG-CD2	-8.45	96.64	111.00
1	B	210	LEU	CA-CB-CG	8.43	134.69	115.30
1	D	223	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	F	174	ARG	NE-CZ-NH2	-8.41	116.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	85	ASP	CB-CG-OD1	8.40	125.86	118.30
1	E	174	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	D	42	GLY	N-CA-C	-8.31	92.32	113.10
1	E	174	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	B	248	LEU	CB-CG-CD1	8.27	125.06	111.00
1	A	325	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	D	78	ASP	CB-CG-OD1	8.19	125.67	118.30
1	D	223	ASP	CB-CG-OD1	8.13	125.61	118.30
1	C	61	TYR	C-N-CD	8.12	145.45	128.40
1	D	189	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	E	207	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	A	63	LEU	CB-CG-CD2	-8.01	97.38	111.00
1	E	41	SER	CA-C-N	-7.96	100.27	116.20
1	D	281	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	E	61	TYR	N-CA-C	7.93	132.40	111.00
1	E	185	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	E	207	ASP	C-N-CA	7.89	138.87	122.30
1	E	204	ASP	CB-CG-OD2	7.84	125.36	118.30
1	F	83	GLU	OE1-CD-OE2	7.84	132.71	123.30
1	B	245	VAL	CB-CA-C	-7.83	96.52	111.40
1	E	141	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	A	85	ASP	CB-CG-OD2	7.75	125.28	118.30
1	F	147	LEU	CA-CB-CG	7.71	133.02	115.30
1	F	41	SER	CA-C-N	-7.69	100.83	116.20
1	C	233	LEU	CA-CB-CG	7.68	132.97	115.30
1	E	41	SER	N-CA-C	7.67	131.71	111.00
1	A	245	VAL	CB-CA-C	-7.57	97.02	111.40
1	A	94	LEU	CB-CG-CD1	-7.55	98.16	111.00
1	C	189	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	148	SER	N-CA-CB	-7.52	99.22	110.50
1	C	291	ASP	CB-CG-OD1	-7.48	111.57	118.30
1	B	171	LEU	CB-CG-CD1	7.45	123.66	111.00
1	E	238	GLN	CG-CD-OE1	-7.42	106.76	121.60
1	A	279	ASP	CB-CG-OD2	7.39	124.95	118.30
1	B	303	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	F	202	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	F	327	ILE	CB-CG1-CD1	-7.35	93.32	113.90
1	E	233	LEU	CA-CB-CG	7.33	132.17	115.30
1	C	116	LEU	CB-CG-CD2	-7.31	98.58	111.00
1	E	202	ARG	CG-CD-NE	-7.26	96.56	111.80
1	B	61	TYR	N-CA-C	7.24	130.56	111.00
1	E	219	GLN	N-CA-CB	7.24	123.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	207	ASP	O-C-N	7.22	135.47	123.20
1	A	177	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	111	ASP	CB-CG-OD2	7.20	124.78	118.30
1	F	325	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	218	TRP	C-N-CA	-7.13	103.87	121.70
1	F	317	ILE	N-CA-C	-7.11	91.82	111.00
1	F	75	SER	CB-CA-C	-7.10	96.61	110.10
1	B	264	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	D	207	ASP	C-N-CA	7.09	137.18	122.30
1	F	233	LEU	CB-CG-CD1	-7.08	98.97	111.00
1	A	43	ILE	CG1-CB-CG2	-7.07	95.84	111.40
1	F	74	VAL	O-C-N	-7.07	111.39	122.70
1	F	238	GLN	CG-CD-OE1	-7.07	107.46	121.60
1	E	286	GLU	CG-CD-OE2	-7.05	104.20	118.30
1	A	291	ASP	N-CA-CB	-7.05	97.91	110.60
1	C	207	ASP	N-CA-C	-7.03	92.02	111.00
1	F	202	ARG	CD-NE-CZ	7.03	133.44	123.60
1	B	330	LEU	CA-CB-CG	-7.02	99.15	115.30
1	F	301	VAL	CB-CA-C	-7.01	98.07	111.40
1	F	298	LEU	CB-CG-CD1	7.00	122.91	111.00
1	B	225	VAL	CG1-CB-CG2	-7.00	99.70	110.90
1	A	93	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	F	41	SER	C-N-CA	6.97	136.93	122.30
1	E	59	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	219	GLN	N-CA-CB	6.95	123.10	110.60
1	B	281	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	59	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	F	258	VAL	N-CA-C	-6.94	92.27	111.00
1	E	113	LEU	CB-CG-CD2	-6.93	99.23	111.00
1	E	246	SER	N-CA-C	6.92	129.69	111.00
1	B	41	SER	C-N-CA	6.92	136.83	122.30
1	C	234	LEU	CB-CG-CD2	-6.91	99.25	111.00
1	F	177	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	E	151	LYS	CD-CE-NZ	-6.88	95.88	111.70
1	D	147	LEU	CA-CB-CG	6.86	131.08	115.30
1	D	321	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	B	105	TYR	N-CA-C	6.81	129.39	111.00
1	E	211	LYS	CB-CA-C	-6.75	96.91	110.40
1	D	62	PRO	N-CA-C	-6.74	94.57	112.10
1	A	169	SER	CB-CA-C	-6.73	97.31	110.10
1	E	291	ASP	CB-CG-OD2	6.73	124.36	118.30
1	D	218	TRP	C-N-CA	-6.73	104.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	LEU	CA-CB-CG	6.72	130.75	115.30
1	B	4	LEU	CA-CB-CG	6.72	130.75	115.30
1	F	75	SER	N-CA-C	6.71	129.11	111.00
1	B	111	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	281	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	F	245	VAL	CB-CA-C	-6.69	98.68	111.40
1	E	309	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	D	275	TYR	CB-CG-CD2	6.68	125.00	121.00
1	D	182	THR	CB-CA-C	-6.67	93.59	111.60
1	C	168	VAL	CB-CA-C	-6.67	98.73	111.40
1	F	11	GLU	CA-CB-CG	-6.67	98.73	113.40
1	C	181	SER	CB-CA-C	-6.63	97.51	110.10
1	F	207	ASP	C-N-CA	-6.62	108.40	122.30
1	B	309	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	B	279	ASP	N-CA-CB	-6.60	98.72	110.60
1	E	295	ASP	CB-CG-OD2	6.58	124.22	118.30
1	F	20	HIS	CB-CA-C	-6.57	97.25	110.40
1	D	132	GLY	N-CA-C	-6.55	96.73	113.10
1	D	269	LEU	CB-CG-CD1	-6.51	99.93	111.00
1	F	209	THR	CA-CB-CG2	6.51	121.51	112.40
1	D	264	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	F	41	SER	N-CA-C	6.49	128.53	111.00
1	A	63	LEU	N-CA-C	6.48	128.51	111.00
1	E	318	LEU	CA-CB-CG	6.48	130.20	115.30
1	D	32	ASP	CB-CG-OD2	6.48	124.13	118.30
1	D	246	SER	N-CA-C	6.48	128.48	111.00
1	E	104	GLU	N-CA-C	-6.47	93.54	111.00
1	B	215	LYS	CA-CB-CG	6.44	127.57	113.40
1	C	177	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	B	41	SER	O-C-N	6.43	134.13	123.20
1	E	83	GLU	OE1-CD-OE2	-6.42	115.59	123.30
1	C	307	LEU	CB-CG-CD2	6.41	121.90	111.00
1	C	40	TYR	CB-CA-C	-6.41	97.59	110.40
1	F	318	LEU	CB-CG-CD2	6.40	121.88	111.00
1	F	68	ASP	CB-CA-C	-6.39	97.63	110.40
1	D	230	LEU	CB-CG-CD1	-6.38	100.15	111.00
1	D	291	ASP	CB-CG-OD2	6.37	124.03	118.30
1	F	74	VAL	CA-C-N	6.36	131.19	117.20
1	B	238	GLN	CG-CD-OE1	-6.36	108.89	121.60
1	D	248	LEU	CB-CG-CD2	-6.34	100.23	111.00
1	D	150	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	E	183	GLY	C-N-CA	-6.33	105.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	104	GLU	O-C-N	-6.32	112.58	122.70
1	C	42	GLY	N-CA-C	-6.31	97.33	113.10
1	D	287	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	D	116	LEU	CB-CG-CD2	-6.24	100.39	111.00
1	D	42	GLY	C-N-CA	6.24	137.30	121.70
1	B	330	LEU	CB-CG-CD2	6.24	121.60	111.00
1	F	151	LYS	CA-C-N	-6.23	103.73	116.20
1	D	94	LEU	CA-CB-CG	-6.23	100.96	115.30
1	F	204	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	182	THR	CB-CA-C	-6.21	94.82	111.60
1	F	242	SER	N-CA-C	6.20	127.74	111.00
1	F	248	LEU	CA-C-N	6.19	130.82	117.20
1	F	104	GLU	C-N-CA	-6.19	106.23	121.70
1	C	329	LYS	CD-CE-NZ	6.18	125.92	111.70
1	C	111	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	A	68	ASP	CB-CA-C	-6.16	98.08	110.40
1	B	317	ILE	CG1-CB-CG2	-6.12	97.95	111.40
1	E	316	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	197	SER	CB-CA-C	-6.10	98.50	110.10
1	C	74	VAL	N-CA-C	-6.10	94.53	111.00
1	C	127	VAL	CB-CA-C	-6.10	99.82	111.40
1	E	238	GLN	CA-CB-CG	6.08	126.78	113.40
1	E	78	ASP	CB-CG-OD1	6.08	123.77	118.30
1	E	147	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	181	SER	N-CA-CB	-6.07	101.39	110.50
1	A	302	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	D	204	ASP	CB-CG-OD2	6.06	123.75	118.30
1	F	131	ALA	N-CA-C	-6.05	94.65	111.00
1	F	38	VAL	CG1-CB-CG2	-6.05	101.22	110.90
1	D	287	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	A	236	LYS	CD-CE-NZ	-6.02	97.86	111.70
1	F	111	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	59	ARG	CB-CG-CD	6.00	127.19	111.60
1	F	147	LEU	CB-CG-CD1	5.99	121.18	111.00
1	A	182	THR	CB-CA-C	-5.98	95.46	111.60
1	F	98	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	102	LEU	CA-CB-CG	-5.96	101.59	115.30
1	A	116	LEU	C-N-CD	5.96	140.91	128.40
1	D	113	LEU	CA-CB-CG	-5.96	101.61	115.30
1	A	15	ASP	CB-CG-OD2	5.95	123.66	118.30
1	F	169	SER	N-CA-C	5.95	127.05	111.00
1	B	207	ASP	CB-CG-OD1	5.94	123.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	43	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	C	36	ILE	CB-CA-C	-5.93	99.75	111.60
1	A	327	ILE	CG1-CB-CG2	-5.92	98.38	111.40
1	A	316	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	182	THR	CB-CA-C	-5.91	95.64	111.60
1	A	32	ASP	CB-CG-OD2	5.91	123.62	118.30
1	F	159	ALA	C-N-CA	-5.91	106.92	121.70
1	F	34	VAL	N-CA-C	-5.90	95.06	111.00
1	C	317	ILE	CB-CA-C	-5.89	99.81	111.60
1	B	113	LEU	CB-CG-CD1	-5.89	100.99	111.00
1	B	83	GLU	C-N-CA	-5.88	109.94	122.30
1	B	286	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	D	151	LYS	CA-C-N	-5.87	104.46	116.20
1	E	302	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	E	210	LEU	CB-CA-C	-5.87	99.05	110.20
1	E	204	ASP	CB-CG-OD1	-5.85	113.03	118.30
1	B	78	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	317	ILE	N-CA-CB	5.85	124.25	110.80
1	B	61	TYR	C-N-CD	5.84	140.67	128.40
1	A	329	LYS	CD-CE-NZ	-5.80	98.35	111.70
1	C	295	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	103	SER	CB-CA-C	-5.80	99.08	110.10
1	F	8	LEU	CA-CB-CG	-5.79	101.99	115.30
1	E	286	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	E	24	ILE	CG1-CB-CG2	-5.79	98.67	111.40
1	E	72	THR	N-CA-C	-5.78	95.40	111.00
1	F	169	SER	CB-CA-C	-5.77	99.14	110.10
1	B	182	THR	N-CA-CB	5.77	121.26	110.30
1	C	209	THR	CB-CA-C	5.76	127.16	111.60
1	B	193	GLN	N-CA-CB	-5.76	100.23	110.60
1	D	286	GLU	N-CA-CB	5.75	120.94	110.60
1	D	198	GLU	N-CA-C	-5.74	95.50	111.00
1	B	319	GLN	CB-CA-C	5.74	121.88	110.40
1	F	137	LEU	CB-CG-CD1	5.74	120.76	111.00
1	A	80	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	D	154	VAL	CB-CA-C	-5.74	100.50	111.40
1	B	186	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	B	243	VAL	CG1-CB-CG2	5.73	120.06	110.90
1	A	141	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	F	264	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	321	ARG	CD-NE-CZ	5.71	131.60	123.60
1	C	4	LEU	CB-CA-C	5.71	121.06	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	C	223	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	E	61	TYR	C-N-CD	5.70	140.36	128.40
1	B	67	ILE	N-CA-CB	5.69	123.89	110.80
1	A	171	LEU	CA-CB-CG	5.69	128.38	115.30
1	F	207	ASP	CA-C-O	5.69	132.04	120.10
1	A	306	SER	CA-CB-OG	-5.68	95.85	111.20
1	E	155	LEU	CB-CG-CD2	5.68	120.65	111.00
1	A	178	VAL	CB-CA-C	5.66	122.16	111.40
1	A	64	ILE	CB-CA-C	-5.66	100.28	111.60
1	F	303	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	151	LYS	CD-CE-NZ	5.65	124.70	111.70
1	F	295	ASP	CB-CG-OD1	5.65	123.39	118.30
1	F	219	GLN	N-CA-CB	5.63	120.74	110.60
1	E	16	ASP	C-N-CA	-5.63	107.63	121.70
1	F	205	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	B	279	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	67	ILE	N-CA-CB	5.61	123.70	110.80
1	A	328	VAL	CB-CA-C	-5.61	100.75	111.40
1	F	308	GLU	N-CA-CB	-5.60	100.52	110.60
1	B	308	GLU	N-CA-CB	5.60	120.68	110.60
1	E	208	GLY	CA-C-N	-5.58	104.92	117.20
1	F	225	VAL	CB-CA-C	-5.58	100.80	111.40
1	E	142	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	15	ASP	N-CA-C	5.56	126.01	111.00
1	A	233	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	E	67	ILE	N-CA-CB	5.55	123.57	110.80
1	A	19	VAL	N-CA-C	5.54	125.97	111.00
1	A	98	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	131	ALA	N-CA-C	-5.53	96.06	111.00
1	E	264	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	A	218	TRP	N-CA-C	5.53	125.93	111.00
1	C	247	GLY	C-N-CA	5.52	135.51	121.70
1	C	248	LEU	CB-CA-C	-5.52	99.71	110.20
1	E	207	ASP	O-C-N	5.52	132.58	123.20
1	E	236	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	F	67	ILE	N-CA-CB	5.50	123.44	110.80
1	A	68	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	F	177	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	185	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	271	ILE	CA-CB-CG1	-5.47	100.61	111.00
1	B	105	TYR	CB-CG-CD1	-5.47	117.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	3	THR	CB-CA-C	-5.47	96.84	111.60
1	E	307	LEU	CB-CG-CD2	5.46	120.29	111.00
1	F	171	LEU	C-N-CA	-5.46	108.05	121.70
1	F	104	GLU	CA-C-N	5.46	129.20	117.20
1	A	159	ALA	CA-C-N	5.46	129.20	117.20
1	A	287	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	A	177	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	37	LYS	CD-CE-NZ	5.45	124.24	111.70
1	B	213	LEU	CB-CG-CD2	5.45	120.26	111.00
1	F	207	ASP	CB-CG-OD2	5.44	123.20	118.30
1	E	155	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	149	PRO	O-C-N	-5.43	114.01	122.70
1	F	22	LYS	CA-CB-CG	5.43	125.34	113.40
1	D	245	VAL	CB-CA-C	-5.42	101.11	111.40
1	D	316	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	E	316	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	8	LEU	CA-CB-CG	-5.41	102.86	115.30
1	B	249	THR	C-N-CA	-5.41	110.94	122.30
1	A	19	VAL	CB-CA-C	-5.39	101.16	111.40
1	F	225	VAL	C-N-CA	-5.39	110.99	122.30
1	D	218	TRP	O-C-N	-5.38	114.09	122.70
1	F	182	THR	CB-CA-C	-5.38	97.08	111.60
1	B	80	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	F	122	LEU	CB-CG-CD1	-5.37	101.86	111.00
1	F	248	LEU	CB-CG-CD1	5.36	120.12	111.00
1	B	266	VAL	CB-CA-C	5.35	121.57	111.40
1	A	219	GLN	CB-CG-CD	5.33	125.47	111.60
1	E	246	SER	CA-C-N	5.33	126.87	116.20
1	A	16	ASP	N-CA-C	5.32	125.38	111.00
1	E	182	THR	N-CA-CB	5.32	120.41	110.30
1	E	105	TYR	N-CA-CB	5.31	120.15	110.60
1	D	65	LEU	C-N-CA	-5.30	111.17	122.30
1	D	230	LEU	CA-CB-CG	5.30	127.49	115.30
1	F	291	ASP	N-CA-CB	-5.30	101.07	110.60
1	A	182	THR	OG1-CB-CG2	5.28	122.14	110.00
1	A	215	LYS	CA-CB-CG	5.28	125.01	113.40
1	B	65	LEU	CB-CG-CD1	5.26	119.95	111.00
1	A	83	GLU	CA-CB-CG	5.26	124.97	113.40
1	B	249	THR	O-C-N	-5.26	114.26	123.20
1	F	105	TYR	N-CA-CB	5.26	120.06	110.60
1	E	178	VAL	CB-CA-C	-5.24	101.44	111.40
1	E	325	ARG	NE-CZ-NH2	5.24	122.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	46	LYS	CD-CE-NZ	-5.24	99.64	111.70
1	C	33	GLY	N-CA-C	5.23	126.18	113.10
1	B	236	LYS	CD-CE-NZ	-5.22	99.69	111.70
1	A	78	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	F	27	GLU	CB-CA-C	-5.21	99.97	110.40
1	B	223	ASP	C-N-CD	-5.21	109.13	120.60
1	B	75	SER	N-CA-C	5.21	125.06	111.00
1	D	119	ASN	N-CA-CB	-5.20	101.23	110.60
1	A	113	LEU	CA-CB-CG	-5.20	103.34	115.30
1	A	131	ALA	CA-C-O	-5.19	109.19	120.10
1	C	102	LEU	CB-CA-C	-5.19	100.35	110.20
1	C	149	PRO	CA-C-N	5.18	128.59	117.20
1	B	107	SER	N-CA-CB	-5.17	102.74	110.50
1	D	43	ILE	N-CA-C	5.17	124.96	111.00
1	D	275	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	C	193	GLN	CA-CB-CG	5.16	124.76	113.40
1	D	219	GLN	CB-CA-C	-5.16	100.07	110.40
1	F	160	THR	N-CA-CB	5.16	120.10	110.30
1	F	74	VAL	N-CA-CB	-5.14	100.19	111.50
1	C	304	GLU	CA-CB-CG	5.13	124.69	113.40
1	F	316	ASP	CB-CA-C	-5.13	100.14	110.40
1	D	40	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	E	245	VAL	C-N-CA	-5.12	108.90	121.70
1	D	67	ILE	N-CA-CB	5.12	122.58	110.80
1	F	141	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	124	GLU	N-CA-CB	5.12	119.81	110.60
1	C	314	LEU	CA-CB-CG	5.11	127.06	115.30
1	C	74	VAL	CB-CA-C	-5.11	101.69	111.40
1	E	274	VAL	CA-CB-CG1	-5.11	103.23	110.90
1	A	219	GLN	N-CA-CB	5.11	119.80	110.60
1	D	279	ASP	OD1-CG-OD2	5.10	132.99	123.30
1	B	278	MSE	CG-SE-CE	-5.09	87.70	98.90
1	A	219	GLN	CA-CB-CG	-5.09	102.20	113.40
1	D	219	GLN	CB-CG-CD	5.09	124.83	111.60
1	E	330	LEU	CA-CB-CG	-5.08	103.61	115.30
1	A	291	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	221	ALA	N-CA-C	-5.08	97.28	111.00
1	C	93	GLU	OE1-CD-OE2	-5.08	117.21	123.30
1	A	159	ALA	C-N-CA	-5.07	109.02	121.70
1	A	233	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	C	298	LEU	CB-CG-CD2	5.05	119.58	111.00
1	E	80	ARG	CG-CD-NE	5.05	122.40	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	GLU	N-CA-C	-5.04	97.39	111.00
1	C	165	GLY	N-CA-C	-5.04	100.50	113.10
1	B	194	LEU	CA-CB-CG	5.02	126.85	115.30
1	E	74	VAL	CB-CA-C	-5.01	101.87	111.40
1	F	318	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	325	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	E	219	GLN	CB-CA-C	-5.01	100.38	110.40
1	E	321	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	C	45	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	D	292	LEU	CB-CG-CD1	5.00	119.50	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	43	ILE	CA
1	D	43	ILE	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ASN	Peptide
1	A	131	ALA	Peptide
1	A	150	GLU	Peptide
1	A	184	ASN	Peptide
1	A	186	GLU	Peptide
1	A	208	GLY	Peptide
1	A	41	SER	Mainchain,Peptide
1	A	62	PRO	Peptide
1	B	13	ASN	Peptide
1	B	2	SER	Peptide
1	B	209	THR	Peptide
1	B	250	GLY	Peptide
1	B	290	SER	Peptide
1	B	40	TYR	Peptide
1	B	41	SER	Peptide
1	B	60	GLU	Peptide
1	B	61	TYR	Peptide
1	C	186	GLU	Peptide
1	C	208	GLY	Peptide
1	C	209	THR	Peptide
1	C	316	ASP	Peptide
1	C	319	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	C	42	GLY	Peptide
1	C	52	LYS	Peptide
1	C	61	TYR	Peptide
1	D	131	ALA	Peptide
1	D	247	GLY	Peptide
1	D	284	VAL	Peptide
1	D	301	VAL	Peptide
1	D	61	TYR	Peptide
1	E	13	ASN	Peptide
1	E	249	THR	Peptide
1	E	40	TYR	Peptide
1	E	41	SER	Peptide
1	E	60	GLU	Peptide
1	F	15	ASP	Peptide
1	F	209	THR	Peptide
1	F	251	GLY	Peptide
1	F	40	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2429	0	2454	160	0
1	B	2421	0	2425	168	0
1	C	2412	0	2405	206	0
1	D	2431	0	2444	169	0
1	E	2433	0	2458	165	0
1	F	2437	0	2460	186	0
2	A	11	0	4	5	0
2	B	11	0	4	5	0
2	C	11	0	4	4	0
2	D	11	0	4	0	0
2	E	11	0	4	0	0
2	F	11	0	4	5	0
3	A	65	0	0	1	0
3	B	56	0	0	3	0
3	C	57	0	0	5	0
3	D	53	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	60	0	0	7	0
3	F	62	0	0	8	0
All	All	14982	0	14670	1037	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 35.

All (1037) 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:3:THR:CG2	1:B:3:THR:CB	1.75	1.60
1:A:24:ILE:CG1	1:A:24:ILE:CD1	1.81	1.58
1:D:26:THR:CB	1:D:26:THR:CG2	1.76	1.57
1:B:303:ARG:CB	1:B:303:ARG:CG	1.75	1.57
1:B:215:LYS:CB	1:B:215:LYS:CG	1.81	1.57
1:F:67:ILE:CD1	1:F:67:ILE:CG1	1.78	1.56
1:F:322:ILE:CG1	1:F:322:ILE:CD1	1.75	1.56
1:E:59:ARG:CG	1:E:59:ARG:CD	1.80	1.55
1:F:315:LYS:NZ	1:F:315:LYS:CE	1.67	1.55
1:D:225:VAL:CB	1:D:225:VAL:CG2	1.82	1.55
1:F:228:LYS:NZ	1:F:228:LYS:CE	1.70	1.54
1:C:207:ASP:CG	1:C:207:ASP:CB	1.77	1.53
1:E:83:GLU:CG	1:E:83:GLU:CD	1.75	1.53
1:F:329:LYS:NZ	1:F:329:LYS:CE	1.73	1.52
1:F:105:TYR:CA	1:F:105:TYR:N	1.67	1.52
1:A:286:GLU:CG	1:A:286:GLU:CD	1.75	1.52
1:A:322:ILE:CG1	1:A:322:ILE:CD1	1.87	1.51
1:D:286:GLU:CG	1:D:286:GLU:CD	1.75	1.51
1:B:286:GLU:CD	1:B:286:GLU:CG	1.78	1.50
1:E:319:GLN:CG	1:E:319:GLN:CD	1.78	1.50
1:A:298:LEU:CG	1:A:298:LEU:CD1	1.90	1.50
1:B:248:LEU:CD1	1:B:248:LEU:CG	1.90	1.49
1:D:198:GLU:CD	1:D:198:GLU:CG	1.79	1.48
1:E:207:ASP:CG	1:E:208:GLY:H	1.05	1.46
1:C:62:PRO:CG	1:C:62:PRO:CB	1.76	1.46
1:A:238:GLN:CG	1:A:238:GLN:CD	1.82	1.45
1:F:209:THR:CA	1:F:209:THR:CB	1.92	1.45
1:F:278:MSE:SE	1:F:278:MSE:CE	2.15	1.44
1:E:62:PRO:CG	1:E:62:PRO:CB	1.78	1.43
1:B:207:ASP:O	1:B:209:THR:HG23	1.14	1.26
1:E:41:SER:OG	1:E:42:GLY:N	1.62	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ASP:CG	1:E:208:GLY:N	1.91	1.21
1:C:8:LEU:CD1	1:C:310:THR:HG21	1.72	1.19
1:A:317:ILE:O	1:A:319:GLN:N	1.74	1.18
1:C:21:VAL:O	1:C:21:VAL:HG12	1.44	1.14
1:E:249:THR:CG2	1:E:249:THR:O	1.96	1.14
1:C:74:VAL:O	1:C:75:SER:HB3	1.37	1.13
1:A:218:TRP:O	1:A:219:GLN:HB3	1.34	1.11
1:F:11:GLU:HG3	1:F:12:LYS:H	1.08	1.10
1:A:218:TRP:O	1:A:219:GLN:CB	1.93	1.10
1:C:74:VAL:O	1:C:75:SER:CB	1.98	1.10
1:C:8:LEU:HD13	1:C:310:THR:HG21	1.19	1.09
1:C:21:VAL:CG1	1:C:21:VAL:O	2.00	1.08
1:D:218:TRP:O	1:D:219:GLN:CB	1.97	1.08
1:D:149:PRO:O	1:D:150:GLU:HB3	1.54	1.07
1:B:151:LYS:O	1:B:238:GLN:NE2	1.87	1.07
1:C:159:ALA:O	1:C:160:THR:HB	1.45	1.07
1:D:151:LYS:O	1:D:238:GLN:NE2	1.89	1.06
1:A:80:ARG:CG	1:A:80:ARG:HH11	1.60	1.06
1:B:142:LEU:CD2	1:B:242:SER:HB3	1.86	1.06
1:F:11:GLU:HG3	1:F:12:LYS:N	1.63	1.05
1:B:207:ASP:O	1:B:209:THR:CG2	2.03	1.05
1:C:157:THR:CG2	1:C:224:PRO:HD2	1.85	1.05
1:C:244:ALA:HB1	1:C:271:ILE:HD12	1.33	1.04
1:C:157:THR:HG21	1:C:223:ASP:OD1	1.58	1.03
1:E:41:SER:HB2	1:E:328:VAL:H	1.22	1.03
1:C:305:VAL:CG1	1:C:306:SER:H	1.69	1.03
1:C:43:ILE:CG2	1:C:317:ILE:HD11	1.88	1.03
1:E:13:ASN:N	1:E:13:ASN:HD22	1.54	1.02
1:D:218:TRP:O	1:D:219:GLN:HB2	1.60	1.02
1:B:218:TRP:O	1:B:219:GLN:HB3	1.59	1.01
1:C:305:VAL:HG13	1:C:306:SER:H	1.25	1.01
1:F:41:SER:HB2	1:F:328:VAL:H	1.21	1.01
1:C:157:THR:HG22	1:C:224:PRO:HD2	1.03	1.01
1:B:218:TRP:O	1:B:219:GLN:CB	2.08	1.00
1:F:244:ALA:HB1	1:F:271:ILE:HD11	1.43	1.00
1:A:80:ARG:NH1	1:A:80:ARG:HG3	1.51	1.00
1:A:151:LYS:O	1:A:238:GLN:NE2	1.95	0.99
1:D:49:LEU:HB2	1:D:57:ILE:HD12	1.41	0.99
1:C:157:THR:HG22	1:C:224:PRO:CD	1.93	0.98
1:A:103:SER:HB2	1:A:104:GLU:O	1.64	0.98
1:F:185:ARG:O	1:F:186:GLU:HB2	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ARG:HG3	1:D:98:ARG:HH11	1.26	0.98
1:A:66:GLY:HA3	1:A:101:GLY:H	1.29	0.97
1:C:244:ALA:HB1	1:C:271:ILE:CD1	1.92	0.97
1:E:90:THR:HG22	1:E:91:SER:OG	1.65	0.97
1:C:8:LEU:CD1	1:C:310:THR:CG2	2.42	0.96
1:E:249:THR:HG22	1:E:249:THR:O	1.64	0.96
1:C:317:ILE:O	1:C:318:LEU:HB2	1.62	0.96
1:A:41:SER:OG	1:A:42:GLY:HA2	1.66	0.95
1:D:207:ASP:CG	1:D:208:GLY:H	1.69	0.95
1:F:8:LEU:HD13	1:F:310:THR:CG2	1.97	0.95
1:A:151:LYS:O	1:A:238:GLN:CD	2.06	0.94
1:A:41:SER:OG	1:A:42:GLY:N	1.99	0.94
1:F:8:LEU:HD13	1:F:310:THR:HG22	1.48	0.94
1:F:41:SER:HB3	1:F:327:ILE:HG22	1.49	0.93
1:A:41:SER:OG	1:A:42:GLY:CA	2.15	0.93
1:D:32:ASP:OD1	1:D:32:ASP:N	1.98	0.92
1:B:304:GLU:HG2	1:B:327:ILE:HG22	1.50	0.92
1:F:104:GLU:C	1:F:105:TYR:CA	2.38	0.91
1:F:151:LYS:O	1:F:238:GLN:NE2	2.03	0.91
1:D:297:LEU:O	1:D:300:ILE:HG22	1.69	0.91
1:D:24:ILE:HG22	1:D:25:SER:H	1.35	0.91
1:B:41:SER:HB3	1:B:42:GLY:CA	1.66	0.91
1:B:19:VAL:HG12	1:B:19:VAL:O	1.71	0.90
1:F:105:TYR:N	1:F:105:TYR:HA	1.85	0.90
1:E:159:ALA:O	1:E:160:THR:HB	1.69	0.90
1:C:305:VAL:CG1	1:C:306:SER:N	2.31	0.90
1:C:90:THR:HG22	1:C:91:SER:OG	1.72	0.89
1:E:219:GLN:HA	1:E:238:GLN:HG3	1.53	0.89
1:E:151:LYS:O	1:E:238:GLN:NE2	2.05	0.89
1:A:166:ILE:HG13	1:A:300:ILE:HD13	1.54	0.89
1:A:296:GLN:HB2	1:A:299:THR:HG23	1.54	0.89
1:B:141:ARG:HE	2:B:2255:NAD:H2A	1.36	0.89
1:E:319:GLN:HE21	1:E:321:ARG:HD3	1.36	0.88
1:F:11:GLU:CG	1:F:12:LYS:N	2.35	0.88
1:F:183:GLY:H	1:F:202:ARG:HH11	1.16	0.88
1:C:313:ALA:C	1:C:315:LYS:H	1.71	0.88
1:C:185:ARG:O	1:C:186:GLU:HB2	1.71	0.88
1:C:43:ILE:HG22	1:C:317:ILE:HD11	1.55	0.88
1:C:304:GLU:OE2	1:C:329:LYS:HE3	1.73	0.87
1:E:80:ARG:HG3	1:E:80:ARG:HH11	1.37	0.87
1:A:182:THR:O	1:A:182:THR:HG23	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:ALA:HB1	1:F:271:ILE:CD1	2.04	0.87
1:A:296:GLN:HB2	1:A:299:THR:CG2	2.03	0.87
1:F:159:ALA:O	1:F:160:THR:HB	1.75	0.87
1:C:126:MSE:O	1:C:325:ARG:NH1	2.06	0.87
1:A:151:LYS:O	1:A:238:GLN:OE1	1.93	0.87
1:C:172:ASN:C	1:C:172:ASN:HD22	1.77	0.87
1:D:55:GLY:O	1:D:56:ASN:HB2	1.74	0.86
1:B:41:SER:OG	1:B:328:VAL:N	2.08	0.86
1:B:141:ARG:NE	2:B:2255:NAD:H2A	1.89	0.86
1:E:41:SER:OG	1:E:42:GLY:CA	2.24	0.86
1:F:296:GLN:HB3	1:F:299:THR:HB	1.55	0.86
1:A:162:GLY:O	1:A:166:ILE:HD12	1.76	0.85
1:A:245:VAL:CG2	1:A:268:LEU:HD11	2.06	0.85
1:B:142:LEU:HD23	1:B:242:SER:HB3	1.57	0.85
1:B:185:ARG:O	1:B:187:ALA:N	2.08	0.85
1:A:41:SER:HG	1:A:42:GLY:HA2	1.42	0.84
1:E:149:PRO:O	1:E:150:GLU:HB3	1.78	0.84
1:F:228:LYS:HG2	3:F:6313:HOH:O	1.78	0.84
1:A:182:THR:O	1:A:182:THR:CG2	2.25	0.84
1:D:8:LEU:HD13	1:D:310:THR:HG22	1.59	0.84
1:E:181:SER:HB2	1:E:200:ILE:HG13	1.60	0.83
1:D:55:GLY:O	1:D:56:ASN:CB	2.24	0.83
1:F:227:GLY:HA3	1:F:251:GLY:HA3	1.58	0.82
1:C:11:GLU:H	1:C:18:SER:HB2	1.44	0.82
1:B:317:ILE:HD13	1:B:322:ILE:HD12	1.61	0.82
1:E:13:ASN:HD22	1:E:13:ASN:H	1.21	0.82
1:B:206:TYR:CE1	1:B:209:THR:HA	2.14	0.81
1:D:149:PRO:O	1:D:150:GLU:CB	2.27	0.81
1:A:80:ARG:HH11	1:A:80:ARG:HG3	0.69	0.81
1:D:248:LEU:O	1:D:248:LEU:HD23	1.81	0.81
1:E:319:GLN:NE2	1:E:321:ARG:HD3	1.95	0.81
1:E:207:ASP:O	1:E:209:THR:HG23	1.79	0.81
1:E:319:GLN:HE21	1:E:321:ARG:CD	1.94	0.81
1:D:108:VAL:HG11	1:D:113:LEU:HD21	1.61	0.80
1:C:8:LEU:HD11	1:C:310:THR:CG2	2.12	0.80
1:F:18:SER:O	1:F:19:VAL:HB	1.81	0.80
1:E:218:TRP:O	1:E:219:GLN:CB	2.26	0.80
1:F:305:VAL:CG2	1:F:309:GLU:HB2	2.12	0.80
1:B:3:THR:CG2	1:B:3:THR:HB	2.08	0.80
1:A:46:LYS:HG3	1:A:57:ILE:HD13	1.64	0.80
1:E:13:ASN:ND2	1:E:13:ASN:N	2.26	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:GLU:O	1:F:105:TYR:CA	2.29	0.79
1:C:313:ALA:C	1:C:315:LYS:N	2.30	0.79
1:B:193:GLN:HG2	1:B:299:THR:HG21	1.64	0.79
1:E:2:SER:N	1:E:27:GLU:OE2	2.15	0.79
1:B:7:ALA:HB1	1:B:64:ILE:HD13	1.64	0.79
1:D:207:ASP:CG	1:D:208:GLY:N	2.30	0.79
1:C:138:SER:HA	1:C:271:ILE:HD13	1.62	0.79
1:D:24:ILE:HG22	1:D:25:SER:N	1.97	0.79
1:D:307:LEU:O	1:D:310:THR:HB	1.82	0.79
1:F:272:ASP:H	2:F:6255:NAD:H62A	1.30	0.79
1:F:209:THR:HG22	1:F:228:LYS:HE3	1.63	0.79
1:A:141:ARG:HE	2:A:1255:NAD:H2A	1.47	0.79
1:E:83:GLU:CD	1:E:83:GLU:H	1.86	0.78
1:F:31:LYS:O	1:F:32:ASP:HB3	1.81	0.78
1:B:41:SER:HB3	1:B:42:GLY:HA2	1.63	0.78
1:A:245:VAL:HG22	1:A:268:LEU:HD11	1.66	0.78
1:A:298:LEU:HG	1:A:298:LEU:CD1	2.10	0.78
1:D:225:VAL:CG1	1:D:225:VAL:O	2.30	0.78
1:A:8:LEU:HD13	1:A:310:THR:HG22	1.66	0.78
1:F:209:THR:CG2	1:F:228:LYS:HE3	2.13	0.78
1:C:316:ASP:O	1:C:319:GLN:N	2.17	0.77
1:B:184:ASN:O	1:B:185:ARG:O	2.02	0.77
1:D:225:VAL:O	1:D:225:VAL:HG13	1.85	0.77
1:C:313:ALA:O	1:C:315:LYS:N	2.17	0.77
1:A:185:ARG:O	1:A:186:GLU:O	2.02	0.77
1:A:225:VAL:HG13	1:A:249:THR:HG22	1.67	0.77
1:F:41:SER:CB	1:F:327:ILE:HG22	2.15	0.76
1:B:64:ILE:HB	1:B:99:ASP:HB3	1.67	0.76
1:D:223:ASP:OD2	1:D:230:LEU:HD13	1.86	0.76
1:A:46:LYS:HG3	1:A:57:ILE:CD1	2.16	0.76
1:C:287:ARG:NE	1:C:291:ASP:OD2	2.17	0.76
1:F:66:GLY:HA3	1:F:101:GLY:H	1.51	0.76
1:A:225:VAL:O	1:A:225:VAL:HG12	1.86	0.76
1:E:7:ALA:HB1	1:E:64:ILE:HD13	1.68	0.76
1:B:136:ALA:HB2	1:B:170:MSE:SE	2.34	0.76
1:F:216:GLN:HE21	1:F:238:GLN:HG2	1.49	0.75
1:F:218:TRP:O	1:F:219:GLN:HB3	1.87	0.75
1:D:207:ASP:C	1:D:209:THR:H	1.90	0.75
1:D:103:SER:OG	1:D:105:TYR:O	2.04	0.75
1:F:218:TRP:O	1:F:219:GLN:CB	2.30	0.75
1:B:166:ILE:HG13	1:B:300:ILE:HD13	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ASN:ND2	1:F:185:ARG:O	2.19	0.75
1:C:305:VAL:HG12	1:C:306:SER:N	2.02	0.74
1:E:13:ASN:O	1:E:15:ASP:N	2.20	0.74
1:C:40:TYR:OH	1:C:329:LYS:NZ	2.19	0.74
1:A:242:SER:HB3	1:A:267:SER:OG	1.87	0.74
1:D:317:ILE:O	1:D:318:LEU:CB	2.35	0.74
1:E:18:SER:O	1:E:19:VAL:HB	1.85	0.74
1:F:6:GLN:HE22	1:F:23:THR:HB	1.53	0.74
1:D:18:SER:O	1:D:19:VAL:HB	1.87	0.74
1:B:271:ILE:N	1:B:271:ILE:HD13	2.00	0.74
1:B:61:TYR:O	1:B:61:TYR:HD2	1.70	0.74
1:E:16:ASP:O	1:E:17:VAL:HB	1.88	0.74
1:E:249:THR:HG23	1:E:249:THR:O	1.84	0.74
1:A:158:GLY:O	1:A:159:ALA:O	2.06	0.74
1:D:207:ASP:OD2	1:D:208:GLY:N	2.20	0.73
1:D:308:GLU:O	1:D:311:PRO:HD2	1.88	0.73
1:E:19:VAL:O	1:E:19:VAL:HG12	1.86	0.73
1:E:90:THR:CG2	1:E:91:SER:OG	2.34	0.73
1:F:315:LYS:HA	1:F:315:LYS:HE3	1.70	0.73
1:C:329:LYS:C	1:C:330:LEU:HD23	2.08	0.73
1:B:27:GLU:OE2	1:B:27:GLU:HA	1.88	0.73
1:F:300:ILE:O	1:F:300:ILE:HG13	1.86	0.73
1:E:16:ASP:O	1:E:17:VAL:CB	2.31	0.73
1:E:218:TRP:O	1:E:219:GLN:HB2	1.89	0.73
1:F:35:LEU:C	1:F:36:ILE:HD12	2.09	0.73
1:F:136:ALA:HA	1:F:170:MSE:HE1	1.70	0.73
1:E:7:ALA:CB	1:E:64:ILE:HD13	2.18	0.72
1:B:7:ALA:CB	1:B:64:ILE:HD13	2.19	0.72
1:C:147:LEU:HD22	1:C:219:GLN:OE1	1.89	0.72
1:C:159:ALA:O	1:C:160:THR:CB	2.25	0.72
1:C:151:LYS:O	1:C:238:GLN:NE2	2.22	0.72
1:B:197:SER:O	1:B:198:GLU:HG3	1.89	0.72
1:A:152:GLY:HA3	1:A:238:GLN:OE1	1.89	0.72
1:B:61:TYR:CD2	1:B:61:TYR:O	2.42	0.72
1:A:219:GLN:H	1:A:238:GLN:H	1.36	0.72
1:F:41:SER:HB2	1:F:328:VAL:N	2.00	0.72
1:B:166:ILE:HG13	1:B:300:ILE:CD1	2.20	0.72
1:B:308:GLU:O	1:B:311:PRO:HD2	1.89	0.72
1:A:246:SER:HA	1:D:262:ILE:HG22	1.72	0.71
1:D:49:LEU:CB	1:D:57:ILE:HD12	2.17	0.71
1:B:44:ASN:O	1:B:47:ASP:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:ALA:O	1:F:160:THR:CB	2.35	0.71
1:E:220:GLY:HA2	1:E:237:ILE:HD12	1.71	0.71
1:E:207:ASP:OD1	1:E:208:GLY:N	2.16	0.71
1:C:316:ASP:O	1:C:319:GLN:HG2	1.91	0.71
1:C:185:ARG:O	1:C:186:GLU:CB	2.39	0.71
1:D:86:GLU:HG2	1:D:122:LEU:HD11	1.73	0.71
1:D:24:ILE:CG2	1:D:25:SER:H	2.03	0.70
1:D:8:LEU:HD13	1:D:310:THR:CG2	2.20	0.70
1:B:206:TYR:HE1	1:B:209:THR:HA	1.53	0.70
1:C:44:ASN:ND2	1:C:68:ASP:OD2	2.23	0.70
1:E:11:GLU:O	1:E:17:VAL:HA	1.92	0.70
1:A:206:TYR:CD1	1:A:232:SER:HB2	2.26	0.70
1:B:68:ASP:HB3	1:B:126:MSE:SE	2.41	0.70
1:C:242:SER:HB3	1:C:267:SER:OG	1.91	0.70
1:C:141:ARG:HE	2:C:3255:NAD:H2A	1.55	0.70
1:C:207:ASP:O	1:C:209:THR:HG23	1.90	0.70
1:B:41:SER:CB	1:B:42:GLY:CA	2.48	0.70
1:B:19:VAL:CG1	1:B:19:VAL:O	2.39	0.70
1:E:219:GLN:CA	1:E:238:GLN:HG3	2.20	0.70
1:A:272:ASP:H	2:A:1255:NAD:H62A	1.39	0.70
1:B:152:GLY:O	1:B:219:GLN:NE2	2.25	0.70
1:F:183:GLY:N	1:F:202:ARG:HH11	1.89	0.70
1:F:41:SER:CB	1:F:328:VAL:H	2.03	0.69
1:D:108:VAL:CG1	1:D:113:LEU:HD21	2.22	0.69
1:D:67:ILE:O	1:D:90:THR:HA	1.93	0.69
1:B:318:LEU:O	1:B:320:ASN:N	2.25	0.69
1:C:206:TYR:CZ	1:C:209:THR:HG22	2.27	0.69
1:F:36:ILE:O	1:F:105:TYR:HA	1.93	0.69
1:D:150:GLU:OE1	1:D:151:LYS:HD2	1.92	0.69
1:A:141:ARG:NE	2:A:1255:NAD:H2A	2.08	0.69
1:D:303:ARG:HG2	1:D:304:GLU:H	1.56	0.68
1:B:153:SER:O	1:B:218:TRP:O	2.11	0.68
1:E:173:LYS:HD3	1:E:293:LYS:O	1.93	0.68
1:B:181:SER:HB2	1:B:200:ILE:HG13	1.74	0.68
1:A:296:GLN:CB	1:A:299:THR:HG23	2.24	0.68
1:F:141:ARG:HE	2:F:6255:NAD:H2A	1.57	0.68
1:C:120:LEU:HG	1:C:289:SER:HB2	1.76	0.68
1:A:59:ARG:NE	1:A:59:ARG:HA	2.08	0.68
1:C:329:LYS:O	1:C:330:LEU:HD23	1.94	0.68
1:F:209:THR:HA	1:F:209:THR:CB	2.16	0.68
1:D:303:ARG:HG2	1:D:304:GLU:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:SER:HA	1:C:271:ILE:CD1	2.24	0.68
1:E:207:ASP:C	1:E:209:THR:H	1.95	0.68
1:F:330:LEU:H	1:F:330:LEU:HD12	1.60	0.67
1:D:201:SER:HB2	1:D:203:GLU:OE1	1.94	0.67
1:F:307:LEU:O	1:F:310:THR:HB	1.95	0.67
1:F:36:ILE:N	1:F:36:ILE:HD12	2.08	0.67
1:B:270:GLY:C	1:B:271:ILE:HD13	2.14	0.67
1:B:174:ARG:NH1	1:B:174:ARG:HB3	2.09	0.67
1:A:141:ARG:HE	2:A:1255:NAD:C2A	2.08	0.67
1:D:296:GLN:N	1:D:296:GLN:OE1	2.19	0.67
1:D:36:ILE:HG12	1:D:108:VAL:HG12	1.77	0.66
1:A:13:ASN:O	1:A:15:ASP:N	2.27	0.66
1:E:322:ILE:HG13	3:E:5269:HOH:O	1.94	0.66
1:C:37:LYS:HD2	3:C:3307:HOH:O	1.95	0.66
1:E:207:ASP:OD1	1:E:208:GLY:CA	2.43	0.66
1:D:126:MSE:O	1:D:325:ARG:NH1	2.16	0.66
1:A:298:LEU:CD1	1:A:298:LEU:H	2.07	0.66
1:B:230:LEU:HA	1:B:233:LEU:HD23	1.75	0.66
1:D:316:ASP:O	1:D:319:GLN:O	2.13	0.66
1:D:181:SER:HB2	1:D:200:ILE:HG13	1.76	0.66
1:F:120:LEU:HG	1:F:289:SER:CB	2.26	0.66
1:F:209:THR:HB	1:F:210:LEU:HD23	1.78	0.66
1:F:310:THR:HG22	1:F:311:PRO:HD3	1.78	0.66
1:F:6:GLN:N	1:F:104:GLU:OE1	2.26	0.65
1:B:181:SER:HB2	1:B:200:ILE:CG1	2.26	0.65
1:D:74:VAL:HG12	1:D:74:VAL:O	1.95	0.65
1:F:321:ARG:HD2	1:F:321:ARG:O	1.96	0.65
1:F:208:GLY:O	1:F:209:THR:O	2.15	0.65
1:F:98:ARG:NH2	1:F:107:SER:O	2.28	0.65
1:C:68:ASP:HB3	1:C:126:MSE:SE	2.47	0.65
1:C:230:LEU:HA	1:C:233:LEU:HD13	1.79	0.64
1:C:43:ILE:HD12	1:C:326:VAL:HG12	1.78	0.64
1:B:27:GLU:O	1:B:27:GLU:OE2	2.15	0.64
1:E:317:ILE:O	1:E:318:LEU:HB2	1.97	0.64
1:D:142:LEU:HB3	1:D:147:LEU:HG	1.77	0.64
1:C:317:ILE:O	1:C:318:LEU:CB	2.35	0.64
1:A:298:LEU:H	1:A:298:LEU:HD12	1.62	0.64
1:D:98:ARG:NH1	1:D:98:ARG:HG3	2.06	0.64
1:D:260:PRO:O	1:D:266:VAL:HG13	1.97	0.64
1:F:208:GLY:O	1:F:209:THR:C	2.35	0.64
1:D:8:LEU:CD1	1:D:310:THR:HG22	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ASN:OD1	1:F:141:ARG:NH2	2.27	0.64
1:E:9:GLN:O	1:E:19:VAL:HA	1.97	0.64
1:F:233:LEU:C	1:F:233:LEU:HD23	2.17	0.64
1:D:49:LEU:HB2	1:D:57:ILE:CD1	2.23	0.64
1:C:26:THR:HB	3:C:3297:HOH:O	1.98	0.64
1:C:65:LEU:O	1:C:102:LEU:HD12	1.97	0.64
1:E:126:MSE:O	1:E:325:ARG:NH1	2.31	0.63
1:E:159:ALA:O	1:E:160:THR:CB	2.40	0.63
1:D:90:THR:CG2	1:D:91:SER:OG	2.46	0.63
1:C:19:VAL:O	1:C:19:VAL:CG1	2.46	0.63
1:F:209:THR:HG22	3:F:6313:HOH:O	1.97	0.63
1:C:206:TYR:CE1	1:C:209:THR:HG22	2.33	0.63
1:D:74:VAL:O	1:D:75:SER:CB	2.45	0.63
1:E:224:PRO:O	1:E:247:GLY:HA3	1.97	0.63
1:C:305:VAL:HG12	1:C:306:SER:H	1.58	0.63
1:B:142:LEU:HD22	1:B:242:SER:HB3	1.77	0.63
1:F:330:LEU:N	1:F:330:LEU:HD12	2.13	0.63
1:B:83:GLU:H	1:B:83:GLU:CD	2.02	0.63
1:E:229:GLN:HG2	1:E:229:GLN:O	1.98	0.63
1:D:98:ARG:HH11	1:D:98:ARG:CG	2.05	0.62
1:F:233:LEU:C	1:F:233:LEU:CD2	2.67	0.62
1:A:130:THR:HG22	1:A:130:THR:O	1.99	0.62
1:C:65:LEU:C	1:C:102:LEU:HD12	2.20	0.62
1:C:41:SER:OG	1:C:42:GLY:N	2.29	0.62
1:C:219:GLN:HA	1:C:238:GLN:HG3	1.82	0.62
1:A:66:GLY:CA	1:A:101:GLY:H	2.08	0.62
1:B:304:GLU:HG2	1:B:327:ILE:CG2	2.27	0.62
1:E:21:VAL:HG12	1:E:21:VAL:O	2.00	0.62
1:A:219:GLN:N	1:A:238:GLN:H	1.97	0.62
1:F:305:VAL:HG22	1:F:309:GLU:HB2	1.82	0.62
1:C:272:ASP:H	2:C:3255:NAD:H62A	1.48	0.62
1:F:120:LEU:HG	1:F:289:SER:HB3	1.81	0.62
1:B:66:GLY:HA3	1:B:100:GLY:HA3	1.81	0.61
1:D:207:ASP:O	1:D:209:THR:N	2.23	0.61
1:D:120:LEU:HG	1:D:289:SER:HB3	1.81	0.61
1:E:61:TYR:O	1:E:61:TYR:HD2	1.83	0.61
1:A:44:ASN:O	1:A:47:ASP:HB2	2.00	0.61
1:B:80:ARG:HD3	1:C:275:TYR:HB3	1.81	0.61
1:C:40:TYR:OH	1:C:329:LYS:HE2	2.00	0.61
1:B:307:LEU:O	1:B:310:THR:OG1	2.09	0.61
1:D:43:ILE:HG22	1:D:43:ILE:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ILE:O	1:C:90:THR:HA	2.00	0.61
1:F:316:ASP:C	1:F:317:ILE:O	2.38	0.61
1:A:317:ILE:HA	1:A:322:ILE:HG12	1.82	0.61
1:A:193:GLN:O	1:A:296:GLN:HG3	2.01	0.61
1:E:272:ASP:OD1	1:E:274:VAL:HG23	2.01	0.61
1:F:61:TYR:HB3	1:F:62:PRO:HA	1.82	0.61
1:E:316:ASP:C	1:E:317:ILE:O	2.36	0.60
1:B:24:ILE:HB	1:B:28:ASP:OD1	2.01	0.60
1:C:8:LEU:HD11	1:C:310:THR:HG22	1.81	0.60
1:E:78:ASP:OD1	1:E:80:ARG:HG3	2.02	0.60
1:C:207:ASP:O	1:C:209:THR:N	2.26	0.60
1:A:41:SER:CB	1:A:42:GLY:CA	2.79	0.60
1:D:68:ASP:HB3	1:D:126:MSE:SE	2.51	0.60
1:D:302:ASP:OD1	1:D:302:ASP:C	2.40	0.60
1:A:158:GLY:C	1:A:159:ALA:O	2.36	0.60
1:A:18:SER:OG	1:A:20:HIS:NE2	2.35	0.60
1:E:64:ILE:HG13	1:E:99:ASP:OD1	2.01	0.60
1:C:7:ALA:CB	1:C:64:ILE:HD13	2.32	0.60
1:E:305:VAL:HG13	1:E:309:GLU:HB2	1.84	0.60
1:E:35:LEU:HD13	1:E:74:VAL:CG2	2.32	0.60
1:B:45:TYR:CE1	1:B:318:LEU:HD23	2.37	0.59
1:D:182:THR:HG22	1:D:183:GLY:H	1.68	0.59
1:C:127:VAL:O	1:C:127:VAL:HG12	2.01	0.59
1:E:32:ASP:OD1	1:E:32:ASP:N	2.35	0.59
1:C:141:ARG:NE	2:C:3255:NAD:H2A	2.17	0.59
1:D:37:LYS:HG3	3:D:4273:HOH:O	2.02	0.59
1:B:35:LEU:HD13	1:B:74:VAL:HG13	1.84	0.59
1:F:74:VAL:O	1:F:75:SER:HB2	2.02	0.59
1:C:216:GLN:HE21	1:C:238:GLN:HB3	1.68	0.59
1:A:66:GLY:HA3	1:A:101:GLY:N	2.10	0.59
1:B:83:GLU:N	1:B:83:GLU:CD	2.55	0.59
1:C:151:LYS:HB3	1:C:219:GLN:CD	2.22	0.59
1:A:327:ILE:HG22	1:A:328:VAL:N	2.15	0.59
1:B:197:SER:C	1:B:198:GLU:HG3	2.23	0.59
1:E:67:ILE:O	1:E:90:THR:HA	2.02	0.59
1:C:312:GLY:O	1:C:315:LYS:CB	2.51	0.59
1:F:305:VAL:HG22	1:F:306:SER:N	2.15	0.59
1:D:26:THR:C	1:D:26:THR:CG2	2.70	0.59
1:A:147:LEU:HD22	1:A:219:GLN:OE1	2.03	0.59
1:E:38:VAL:H	1:E:105:TYR:H	1.50	0.59
1:E:303:ARG:HG3	1:E:305:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:ASP:HB3	1:F:126:MSE:HE1	1.85	0.58
1:F:147:LEU:HD22	1:F:219:GLN:OE1	2.04	0.58
1:B:317:ILE:CD1	1:B:322:ILE:HD12	2.32	0.58
1:C:120:LEU:HG	1:C:289:SER:CB	2.33	0.58
1:B:248:LEU:CD1	1:B:248:LEU:CD2	2.80	0.58
1:C:305:VAL:HG13	1:C:306:SER:N	2.04	0.58
1:C:43:ILE:HD12	1:C:326:VAL:CG1	2.32	0.58
1:B:69:ALA:C	1:B:126:MSE:HE3	2.23	0.58
1:D:171:LEU:HD12	1:D:176:TYR:CD1	2.38	0.58
1:B:27:GLU:OE2	1:B:27:GLU:CA	2.51	0.58
1:D:301:VAL:HG13	3:D:4296:HOH:O	2.02	0.58
1:E:41:SER:HG	1:E:42:GLY:H	1.42	0.58
1:C:138:SER:CA	1:C:271:ILE:HD13	2.34	0.58
1:F:66:GLY:HA3	1:F:101:GLY:N	2.19	0.58
1:E:9:GLN:HG3	1:E:10:ALA:N	2.18	0.58
1:F:224:PRO:O	1:F:247:GLY:HA3	2.03	0.58
1:E:37:LYS:HG3	3:E:5261:HOH:O	2.03	0.58
1:D:305:VAL:HG22	1:D:309:GLU:HB2	1.86	0.58
1:F:116:LEU:HD12	1:F:117:PRO:HD2	1.85	0.58
1:D:170:MSE:HG2	1:D:292:LEU:HB3	1.86	0.58
1:B:10:ALA:HA	1:B:19:VAL:HA	1.85	0.57
1:F:183:GLY:H	1:F:202:ARG:NH1	1.96	0.57
1:B:166:ILE:CG2	1:B:170:MSE:HE3	2.34	0.57
1:A:159:ALA:O	1:A:160:THR:HB	2.04	0.57
1:F:136:ALA:CA	1:F:170:MSE:HE1	2.33	0.57
1:C:91:SER:O	1:C:92:TYR:C	2.42	0.57
1:E:303:ARG:HH11	1:E:303:ARG:HB3	1.69	0.57
1:F:220:GLY:HA2	1:F:242:SER:O	2.04	0.57
1:F:148:SER:O	1:F:150:GLU:N	2.37	0.57
1:B:43:ILE:HD12	1:B:313:ALA:HB1	1.86	0.57
1:F:227:GLY:HA2	1:F:253:GLU:O	2.04	0.57
1:C:319:GLN:HG3	1:C:321:ARG:HG2	1.87	0.57
1:E:219:GLN:H	1:E:238:GLN:H	1.52	0.57
1:B:292:LEU:O	1:B:294:PRO:HD3	2.04	0.57
1:B:38:VAL:HG12	1:B:330:LEU:HD13	1.86	0.57
1:E:219:GLN:N	1:E:238:GLN:HG3	2.19	0.57
1:F:296:GLN:O	1:F:298:LEU:N	2.38	0.57
1:D:45:TYR:O	1:D:48:GLY:N	2.38	0.57
1:D:182:THR:O	1:D:201:SER:HA	2.05	0.57
1:B:190:TYR:O	1:B:193:GLN:HB3	2.05	0.57
1:E:36:ILE:O	1:E:105:TYR:HA	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ILE:HG12	1:B:300:ILE:O	2.04	0.57
1:F:88:ILE:HB	1:F:114:VAL:HG13	1.87	0.57
1:C:49:LEU:HD23	1:C:318:LEU:HD21	1.86	0.56
1:C:148:SER:O	1:C:151:LYS:HB2	2.05	0.56
1:C:40:TYR:OH	1:C:329:LYS:CE	2.53	0.56
1:E:43:ILE:HG22	1:E:43:ILE:O	2.05	0.56
1:D:26:THR:HB	1:D:26:THR:CG2	2.16	0.56
1:B:220:GLY:HA2	1:B:242:SER:O	2.05	0.56
1:E:316:ASP:HB3	3:E:5269:HOH:O	2.05	0.56
1:A:207:ASP:O	1:A:208:GLY:C	2.38	0.56
1:C:206:TYR:CE1	1:C:209:THR:HA	2.41	0.56
1:C:207:ASP:C	1:C:209:THR:H	2.09	0.56
1:E:41:SER:OG	1:E:42:GLY:HA2	2.04	0.56
1:B:203:GLU:O	1:B:207:ASP:HB2	2.05	0.56
1:C:119:ASN:O	1:C:120:LEU:HD23	2.04	0.56
1:A:41:SER:HA	1:A:328:VAL:HB	1.87	0.56
1:C:19:VAL:O	1:C:19:VAL:HG12	2.05	0.56
1:A:305:VAL:HG22	1:A:309:GLU:HG3	1.87	0.56
1:B:34:VAL:O	1:B:107:SER:HA	2.06	0.56
1:C:164:GLY:O	1:C:168:VAL:HG23	2.05	0.56
1:F:90:THR:HG23	1:F:91:SER:OG	2.06	0.56
1:F:302:ASP:HB2	1:F:323:GLN:O	2.04	0.56
1:E:240:GLY:HA2	1:E:265:GLY:O	2.06	0.56
1:B:111:ASP:OD1	1:B:111:ASP:N	2.35	0.56
1:C:44:ASN:ND2	1:C:325:ARG:HH21	2.03	0.56
1:F:317:ILE:O	1:F:318:LEU:HB2	2.06	0.56
1:F:155:LEU:O	1:F:221:ALA:HA	2.05	0.56
1:C:316:ASP:N	1:C:316:ASP:OD2	2.39	0.56
1:B:296:GLN:O	1:B:298:LEU:N	2.37	0.56
1:F:207:ASP:O	1:F:208:GLY:C	2.44	0.55
1:B:142:LEU:HD23	1:B:242:SER:CB	2.34	0.55
1:A:8:LEU:HD11	1:A:19:VAL:HG12	1.87	0.55
1:C:245:VAL:CG2	1:C:268:LEU:HD11	2.37	0.55
1:D:90:THR:HG23	1:D:91:SER:OG	2.05	0.55
1:B:90:THR:O	1:B:91:SER:HB2	2.06	0.55
1:A:25:SER:O	1:A:26:THR:C	2.42	0.55
1:C:4:LEU:HA	1:C:24:ILE:O	2.06	0.55
1:B:38:VAL:CG1	1:B:330:LEU:HD13	2.36	0.55
1:F:149:PRO:HA	1:F:176:TYR:CD2	2.41	0.55
1:D:38:VAL:HG12	1:D:330:LEU:HD13	1.88	0.55
1:C:142:LEU:HD23	1:C:242:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HB2	1:A:57:ILE:HD12	1.89	0.55
1:A:261:PHE:CZ	1:D:268:LEU:HD23	2.42	0.55
1:D:177:ASP:OD1	1:E:118:GLN:NE2	2.39	0.55
1:F:138:SER:OG	1:F:271:ILE:HD13	2.06	0.55
1:F:31:LYS:O	1:F:32:ASP:CB	2.52	0.55
1:C:136:ALA:HB2	1:C:170:MSE:HE1	1.89	0.55
1:C:253:GLU:OE1	1:C:253:GLU:HA	2.07	0.55
1:E:6:GLN:NE2	1:E:23:THR:OG1	2.39	0.54
1:E:7:ALA:HA	1:E:103:SER:HA	1.89	0.54
1:C:66:GLY:HA3	1:C:101:GLY:H	1.72	0.54
1:C:245:VAL:HG22	1:C:268:LEU:HD11	1.88	0.54
1:D:34:VAL:HG13	1:D:76:SER:HB2	1.89	0.54
1:F:227:GLY:CA	1:F:251:GLY:HA3	2.32	0.54
1:B:219:GLN:H	1:B:238:GLN:H	1.53	0.54
1:C:172:ASN:C	1:C:172:ASN:ND2	2.54	0.54
1:F:296:GLN:CD	1:F:296:GLN:H	2.10	0.54
1:F:227:GLY:O	1:F:228:LYS:C	2.44	0.54
1:D:202:ARG:O	1:D:206:TYR:O	2.25	0.54
1:E:297:LEU:O	1:E:300:ILE:HG22	2.07	0.54
1:C:173:LYS:HD3	1:C:293:LYS:O	2.07	0.54
1:D:249:THR:HB	3:D:4290:HOH:O	2.07	0.54
1:C:44:ASN:HD21	1:C:325:ARG:NH2	2.05	0.54
1:D:104:GLU:O	1:D:105:TYR:HB2	2.08	0.54
1:F:319:GLN:HG3	1:F:319:GLN:O	2.08	0.54
1:A:262:ILE:HD11	1:D:248:LEU:HD12	1.89	0.54
1:F:104:GLU:O	1:F:105:TYR:O	2.24	0.54
1:C:312:GLY:O	1:C:315:LYS:HB2	2.08	0.54
1:A:117:PRO:HG2	1:A:120:LEU:HD12	1.90	0.54
1:C:25:SER:O	1:C:28:ASP:N	2.29	0.54
1:B:141:ARG:HE	2:B:2255:NAD:C2A	2.16	0.54
1:A:130:THR:O	1:A:130:THR:CG2	2.55	0.54
1:E:46:LYS:HG3	1:E:57:ILE:CD1	2.38	0.54
1:E:128:TYR:OH	1:E:293:LYS:HA	2.08	0.54
1:A:3:THR:O	1:A:25:SER:HB2	2.08	0.54
1:F:41:SER:HB2	1:F:328:VAL:HB	1.90	0.53
1:B:166:ILE:CG1	1:B:300:ILE:HD13	2.36	0.53
1:E:120:LEU:HD21	1:E:128:TYR:HE1	1.72	0.53
1:B:18:SER:O	1:B:19:VAL:HB	2.08	0.53
1:E:61:TYR:CD2	1:E:61:TYR:O	2.61	0.53
1:A:32:ASP:N	1:A:32:ASP:OD1	2.39	0.53
1:B:127:VAL:O	1:B:325:ARG:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ASP:OD2	1:C:207:ASP:CB	2.51	0.53
1:F:16:ASP:HB2	3:F:6272:HOH:O	2.07	0.53
1:A:225:VAL:CG1	1:A:225:VAL:O	2.54	0.53
1:D:90:THR:HG22	1:D:91:SER:OG	2.08	0.53
1:A:248:LEU:HD23	1:D:258:VAL:HG11	1.89	0.53
1:E:78:ASP:OD2	1:E:80:ARG:NH1	2.42	0.53
1:F:281:ARG:HD3	3:F:6285:HOH:O	2.08	0.53
1:A:29:LEU:O	1:A:30:PRO:C	2.45	0.53
1:D:233:LEU:C	1:D:233:LEU:HD23	2.27	0.53
1:C:7:ALA:HB1	1:C:64:ILE:HD13	1.91	0.53
1:B:7:ALA:HA	1:B:103:SER:HB2	1.91	0.53
1:B:25:SER:O	1:B:26:THR:C	2.47	0.53
1:D:7:ALA:HB1	1:D:103:SER:HB2	1.89	0.53
1:C:153:SER:HB3	1:C:177:ASP:HB2	1.91	0.53
1:E:138:SER:OG	1:E:271:ILE:HG13	2.09	0.53
1:A:296:GLN:H	1:A:296:GLN:CD	2.12	0.53
1:F:320:ASN:CG	1:F:320:ASN:O	2.47	0.53
1:F:11:GLU:HG2	3:F:6310:HOH:O	2.09	0.53
1:A:272:ASP:N	2:A:1255:NAD:H62A	2.07	0.53
1:B:98:ARG:CZ	1:B:109:PRO:HD3	2.39	0.53
1:E:308:GLU:OE2	1:E:308:GLU:HA	2.09	0.52
1:F:140:HIS:O	1:F:144:GLN:HG3	2.10	0.52
1:A:316:ASP:O	1:A:317:ILE:O	2.28	0.52
1:C:173:LYS:O	1:C:173:LYS:HG3	2.08	0.52
1:F:209:THR:CA	1:F:210:LEU:HD23	2.39	0.52
1:D:8:LEU:HD12	1:D:311:PRO:HD3	1.90	0.52
1:A:148:SER:HB3	1:A:151:LYS:HD3	1.91	0.52
1:A:153:SER:O	1:A:218:TRP:O	2.28	0.52
1:E:103:SER:O	1:E:330:LEU:HD22	2.09	0.52
1:D:225:VAL:HG22	1:D:249:THR:OG1	2.09	0.52
1:F:216:GLN:NE2	1:F:238:GLN:HG2	2.21	0.52
1:A:244:ALA:HB1	1:A:271:ILE:CD1	2.39	0.52
1:F:325:ARG:HH11	1:F:325:ARG:HB3	1.73	0.52
1:F:308:GLU:OE1	1:F:308:GLU:HA	2.10	0.52
1:A:147:LEU:HD22	1:A:219:GLN:CD	2.30	0.52
1:F:296:GLN:OE1	1:F:296:GLN:N	2.33	0.52
1:B:306:SER:O	1:B:310:THR:HG23	2.10	0.52
1:E:12:LYS:HD2	1:E:61:TYR:CD1	2.44	0.52
1:F:34:VAL:HG12	1:F:36:ILE:HD11	1.92	0.52
1:D:37:LYS:H	1:D:74:VAL:HG23	1.75	0.52
1:A:261:PHE:HB3	1:D:270:GLY:HA2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:GLY:HA3	1:E:100:GLY:HA3	1.91	0.52
1:B:43:ILE:HD12	1:B:313:ALA:CB	2.39	0.51
1:C:211:LYS:O	1:C:212:ALA:C	2.47	0.51
1:A:173:LYS:HE2	1:A:293:LYS:O	2.10	0.51
1:A:316:ASP:OD2	1:A:321:ARG:HD3	2.10	0.51
1:E:219:GLN:O	1:E:241:GLY:HA3	2.10	0.51
1:C:123:LYS:O	1:C:124:GLU:C	2.46	0.51
1:E:66:GLY:HA3	1:E:101:GLY:H	1.75	0.51
1:F:153:SER:O	1:F:218:TRP:O	2.28	0.51
1:B:275:TYR:CE2	1:C:79:PRO:HG2	2.45	0.51
1:B:259:TYR:CE1	1:E:248:LEU:HD23	2.46	0.51
1:E:319:GLN:O	1:E:321:ARG:N	2.43	0.51
1:C:142:LEU:O	1:C:147:LEU:HB2	2.11	0.51
1:A:245:VAL:CG2	1:A:268:LEU:CD1	2.83	0.51
1:A:272:ASP:OD2	1:A:274:VAL:N	2.41	0.51
1:C:40:TYR:CZ	1:C:329:LYS:HE2	2.46	0.51
1:D:44:ASN:O	1:D:45:TYR:C	2.49	0.51
1:F:278:MSE:HB2	1:F:278:MSE:CE	2.41	0.51
1:A:287:ARG:HB3	1:A:292:LEU:HD12	1.91	0.51
1:F:227:GLY:O	1:F:229:GLN:N	2.43	0.51
1:C:171:LEU:HB3	1:C:178:VAL:HG22	1.92	0.51
1:B:216:GLN:HG2	1:B:238:GLN:HA	1.92	0.51
1:F:219:GLN:HA	1:F:238:GLN:HB2	1.92	0.51
1:D:221:ALA:HB3	1:D:243:VAL:HG13	1.92	0.51
1:A:63:LEU:HD23	1:A:63:LEU:C	2.31	0.51
1:C:53:ALA:O	1:C:54:GLY:C	2.48	0.51
1:A:206:TYR:CD1	1:A:232:SER:CB	2.94	0.51
1:A:3:THR:HG23	1:A:26:THR:HG21	1.93	0.51
1:A:36:ILE:O	1:A:105:TYR:HA	2.10	0.51
1:F:36:ILE:N	1:F:36:ILE:CD1	2.74	0.50
1:A:225:VAL:O	1:A:226:GLY:O	2.29	0.50
1:B:310:THR:OG1	1:B:311:PRO:HD3	2.10	0.50
1:D:38:VAL:CG1	1:D:330:LEU:HD13	2.41	0.50
1:A:68:ASP:HB3	1:A:126:MSE:SE	2.61	0.50
1:F:68:ASP:CB	1:F:126:MSE:HE1	2.41	0.50
1:C:49:LEU:HD23	1:C:318:LEU:CD2	2.42	0.50
1:A:287:ARG:NE	1:A:291:ASP:OD1	2.42	0.50
1:A:307:LEU:O	1:A:310:THR:HB	2.12	0.50
1:E:76:SER:OG	1:E:78:ASP:O	2.29	0.50
1:F:325:ARG:NH1	1:F:325:ARG:HB3	2.27	0.50
1:F:147:LEU:HD13	1:F:176:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:ARG:NH1	1:E:80:ARG:HG3	2.14	0.50
1:C:11:GLU:N	1:C:18:SER:HB2	2.19	0.50
1:A:206:TYR:HB2	1:A:232:SER:HB3	1.93	0.50
1:C:141:ARG:HE	2:C:3255:NAD:C2A	2.21	0.50
1:F:220:GLY:CA	1:F:242:SER:O	2.60	0.50
1:C:88:ILE:HG21	1:C:285:TRP:CZ2	2.47	0.50
1:E:260:PRO:O	1:E:266:VAL:HG13	2.12	0.50
1:A:245:VAL:HG21	1:A:268:LEU:HD11	1.93	0.50
1:E:202:ARG:HG3	3:E:5303:HOH:O	2.12	0.50
1:A:255:PRO:HG2	1:A:255:PRO:O	2.12	0.50
1:A:49:LEU:HD23	1:A:318:LEU:HD21	1.92	0.50
1:C:305:VAL:HG13	1:C:309:GLU:HB3	1.93	0.50
1:A:157:THR:OG1	1:A:224:PRO:HD2	2.12	0.50
1:F:138:SER:O	1:F:142:LEU:HG	2.12	0.49
1:D:17:VAL:CG2	1:D:53:ALA:HB2	2.42	0.49
1:E:61:TYR:HB2	3:E:5270:HOH:O	2.11	0.49
1:E:294:PRO:O	1:E:297:LEU:HB2	2.12	0.49
1:B:59:ARG:HG3	1:B:97:SER:HB3	1.92	0.49
1:D:308:GLU:C	1:D:310:THR:H	2.15	0.49
1:D:81:PHE:CZ	1:D:113:LEU:HB2	2.47	0.49
1:D:292:LEU:O	1:D:294:PRO:HD3	2.12	0.49
1:D:207:ASP:C	1:D:209:THR:N	2.61	0.49
1:D:170:MSE:O	1:D:173:LYS:HB3	2.11	0.49
1:F:209:THR:HB	1:F:210:LEU:CD2	2.42	0.49
1:E:153:SER:O	1:E:218:TRP:O	2.31	0.49
1:B:185:ARG:NE	1:B:185:ARG:HA	2.26	0.49
1:D:287:ARG:NE	1:D:291:ASP:OD2	2.45	0.49
1:F:209:THR:CA	1:F:209:THR:HB	2.21	0.49
1:A:245:VAL:HG22	1:A:268:LEU:CD1	2.38	0.49
1:D:43:ILE:N	1:D:43:ILE:HD12	2.28	0.49
1:D:246:SER:HB3	1:D:271:ILE:HB	1.93	0.49
1:C:284:VAL:O	1:C:288:MSE:HG3	2.12	0.49
1:D:185:ARG:O	1:D:186:GLU:HB2	2.13	0.49
1:F:260:PRO:O	1:F:266:VAL:HG13	2.12	0.49
1:F:278:MSE:HB2	1:F:278:MSE:HE2	1.94	0.49
1:C:138:SER:O	1:C:142:LEU:HD12	2.13	0.49
1:A:329:LYS:O	1:A:330:LEU:HG	2.12	0.49
1:B:41:SER:HG	1:B:328:VAL:N	2.10	0.49
1:F:19:VAL:O	1:F:19:VAL:HG12	2.12	0.49
1:F:216:GLN:NE2	1:F:238:GLN:HA	2.28	0.49
1:D:165:GLY:O	1:D:168:VAL:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:LEU:CD2	3:F:6313:HOH:O	2.61	0.49
1:C:219:GLN:HG2	1:C:219:GLN:O	2.13	0.49
1:A:296:GLN:CA	1:A:299:THR:HG23	2.43	0.49
1:E:93:GLU:HB2	1:E:112:TRP:CH2	2.47	0.49
1:C:127:VAL:O	1:C:127:VAL:CG1	2.61	0.49
1:F:272:ASP:O	2:F:6255:NAD:N6A	2.46	0.49
1:D:192:LYS:HD3	1:D:196:ALA:O	2.13	0.49
1:C:5:PHE:HB2	1:C:104:GLU:CG	2.43	0.48
1:C:44:ASN:HD21	1:C:325:ARG:HH21	1.60	0.48
1:B:261:PHE:CZ	1:E:268:LEU:HD23	2.48	0.48
1:A:317:ILE:CD1	1:A:318:LEU:H	2.26	0.48
1:B:219:GLN:HA	1:B:238:GLN:HB2	1.94	0.48
1:B:259:TYR:CE1	1:E:248:LEU:CD2	2.96	0.48
1:B:23:THR:HG22	1:B:23:THR:O	2.13	0.48
1:A:24:ILE:CD1	1:A:24:ILE:CB	2.82	0.48
1:D:308:GLU:C	1:D:310:THR:N	2.66	0.48
1:C:65:LEU:O	1:C:102:LEU:HB2	2.13	0.48
1:C:222:VAL:O	1:C:224:PRO:HD3	2.14	0.48
1:D:12:LYS:HG2	1:D:12:LYS:O	2.13	0.48
1:C:157:THR:HG23	1:C:158:GLY:N	2.28	0.48
1:F:141:ARG:HE	2:F:6255:NAD:C2A	2.24	0.48
1:D:147:LEU:HD13	1:D:176:TYR:CE2	2.49	0.48
1:D:245:VAL:HG22	1:D:268:LEU:HD11	1.95	0.48
1:F:40:TYR:CZ	1:F:123:LYS:HB2	2.49	0.48
1:C:157:THR:HG23	1:C:225:VAL:HB	1.96	0.48
1:A:327:ILE:HG21	1:A:327:ILE:HD13	1.31	0.48
1:F:120:LEU:HG	1:F:289:SER:HB2	1.95	0.48
1:B:49:LEU:HA	1:B:49:LEU:HD23	1.65	0.48
1:C:316:ASP:C	1:C:317:ILE:O	2.52	0.48
1:C:43:ILE:HG23	1:C:317:ILE:HD11	1.84	0.48
1:D:245:VAL:O	1:D:246:SER:CB	2.62	0.48
1:E:246:SER:HB3	1:E:271:ILE:HB	1.96	0.48
1:B:93:GLU:HB3	1:B:97:SER:OG	2.14	0.48
1:C:101:GLY:O	1:C:102:LEU:C	2.51	0.48
1:D:270:GLY:O	1:D:271:ILE:HD13	2.14	0.48
1:F:184:ASN:ND2	1:F:184:ASN:C	2.66	0.47
1:A:166:ILE:CG2	1:A:170:MSE:HE3	2.44	0.47
1:F:297:LEU:O	1:F:300:ILE:HG22	2.14	0.47
1:F:69:ALA:HB2	1:F:101:GLY:HA3	1.95	0.47
1:F:242:SER:HB3	1:F:267:SER:OG	2.13	0.47
1:F:114:VAL:HA	1:F:115:PRO:HD3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:GLU:HB3	1:D:97:SER:HB3	1.96	0.47
1:E:135:ALA:O	1:E:139:VAL:HG23	2.14	0.47
1:A:317:ILE:HD13	1:A:318:LEU:H	1.79	0.47
1:B:220:GLY:CA	1:B:242:SER:O	2.62	0.47
1:C:43:ILE:CG2	1:C:317:ILE:CD1	2.76	0.47
1:E:64:ILE:HG21	1:E:103:SER:HB2	1.97	0.47
1:F:209:THR:CB	1:F:210:LEU:HD23	2.45	0.47
1:C:39:ALA:O	1:C:40:TYR:CD1	2.67	0.47
1:A:159:ALA:O	1:A:160:THR:CB	2.57	0.47
1:D:91:SER:HB3	1:D:274:VAL:HA	1.96	0.47
1:D:74:VAL:O	1:D:75:SER:HB2	2.13	0.47
1:E:170:MSE:HE1	1:E:288:MSE:HE3	1.96	0.47
1:B:41:SER:CB	1:B:42:GLY:HA2	2.35	0.47
1:F:237:ILE:HD13	1:F:243:VAL:CG2	2.44	0.47
1:B:43:ILE:HD13	1:B:314:LEU:HD23	1.96	0.47
1:B:63:LEU:HD12	1:B:98:ARG:N	2.29	0.47
1:C:225:VAL:HA	1:C:249:THR:HB	1.97	0.47
1:E:308:GLU:O	1:E:311:PRO:HD2	2.14	0.47
1:E:159:ALA:HB1	1:E:191:LEU:HD21	1.97	0.47
1:A:185:ARG:O	1:A:186:GLU:C	2.49	0.47
1:B:94:LEU:HD21	1:B:108:VAL:HB	1.97	0.47
1:D:178:VAL:HA	3:D:4261:HOH:O	2.14	0.47
1:A:25:SER:O	1:A:28:ASP:N	2.44	0.47
1:A:120:LEU:HA	1:A:124:GLU:OE1	2.15	0.47
1:C:225:VAL:O	1:C:225:VAL:HG12	2.15	0.47
1:B:174:ARG:CZ	1:B:174:ARG:HB3	2.45	0.47
1:C:103:SER:O	1:C:104:GLU:C	2.53	0.47
1:B:217:GLN:O	1:B:218:TRP:CG	2.67	0.47
1:B:66:GLY:HA3	1:B:101:GLY:H	1.80	0.47
1:D:129:GLY:O	1:D:130:THR:C	2.53	0.47
1:C:38:VAL:N	3:C:3307:HOH:O	2.47	0.47
1:C:142:LEU:HB3	1:C:147:LEU:HG	1.97	0.46
1:C:45:TYR:HA	1:C:317:ILE:CG2	2.45	0.46
1:F:233:LEU:O	1:F:234:LEU:C	2.51	0.46
1:A:47:ASP:OD2	1:A:67:ILE:HG23	2.15	0.46
1:E:303:ARG:CB	1:E:303:ARG:HH11	2.27	0.46
1:E:5:PHE:HB2	1:E:104:GLU:HG3	1.97	0.46
1:F:6:GLN:NE2	1:F:23:THR:HB	2.26	0.46
1:D:182:THR:CG2	1:D:184:ASN:H	2.28	0.46
1:F:136:ALA:N	1:F:170:MSE:HE1	2.31	0.46
1:D:121:SER:O	1:D:122:LEU:C	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:C	1:B:63:LEU:HD23	2.36	0.46
1:C:210:LEU:O	1:C:211:LYS:HB2	2.16	0.46
1:C:214:SER:HB2	1:C:236:LYS:HG3	1.98	0.46
1:B:157:THR:OG1	1:B:224:PRO:HD2	2.15	0.46
1:B:70:ALA:N	1:B:126:MSE:HE3	2.31	0.46
1:F:317:ILE:H	1:F:317:ILE:HG13	1.52	0.46
1:B:34:VAL:HG13	1:B:76:SER:HB2	1.96	0.46
1:D:13:ASN:O	1:D:14:ALA:HB3	2.15	0.46
1:E:241:GLY:O	1:E:266:VAL:HA	2.16	0.46
1:A:13:ASN:N	1:A:13:ASN:HD22	2.13	0.46
1:E:316:ASP:N	1:E:316:ASP:OD2	2.48	0.46
1:D:245:VAL:O	1:D:246:SER:OG	2.30	0.46
1:C:16:ASP:N	1:C:16:ASP:OD1	2.48	0.46
1:F:296:GLN:HB2	1:F:297:LEU:H	1.40	0.46
1:F:185:ARG:O	1:F:186:GLU:CB	2.36	0.46
1:F:233:LEU:O	1:F:233:LEU:HD23	2.16	0.46
1:F:48:GLY:HA3	1:F:317:ILE:HD11	1.98	0.46
1:F:190:TYR:CE2	1:F:194:LEU:HD11	2.51	0.46
1:C:55:GLY:O	1:C:56:ASN:HB2	2.14	0.46
1:E:78:ASP:HA	1:E:79:PRO:HD3	1.43	0.46
1:A:248:LEU:O	1:A:250:GLY:N	2.46	0.46
1:E:24:ILE:HD13	1:E:24:ILE:HG23	1.51	0.46
1:B:303:ARG:HG2	3:B:2301:HOH:O	2.15	0.46
1:C:267:SER:HB3	3:F:6308:HOH:O	2.16	0.46
1:D:207:ASP:OD2	1:D:208:GLY:CA	2.64	0.46
1:F:307:LEU:HD23	1:F:307:LEU:HA	1.58	0.46
1:D:24:ILE:CG2	1:D:25:SER:N	2.64	0.46
1:F:40:TYR:CE1	1:F:123:LYS:HB2	2.50	0.46
1:A:184:ASN:O	1:A:187:ALA:HB2	2.16	0.46
1:D:158:GLY:O	1:D:160:THR:N	2.43	0.46
1:D:279:ASP:HB3	1:D:280:VAL:H	1.46	0.46
1:D:26:THR:HG22	1:D:27:GLU:N	2.31	0.46
1:B:207:ASP:HB3	1:B:208:GLY:H	1.33	0.46
1:B:304:GLU:OE2	1:B:329:LYS:HB2	2.15	0.46
1:D:314:LEU:O	1:D:317:ILE:HD13	2.16	0.46
1:A:121:SER:N	1:A:124:GLU:OE1	2.42	0.46
1:C:167:ALA:O	1:C:171:LEU:HD22	2.16	0.46
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.76	0.46
1:D:219:GLN:H	1:D:238:GLN:H	1.64	0.46
1:F:158:GLY:C	1:F:159:ALA:O	2.51	0.46
1:C:253:GLU:OE1	1:C:253:GLU:CA	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LYS:HG3	1:E:57:ILE:HD13	1.97	0.46
1:D:160:THR:HB	3:D:4262:HOH:O	2.16	0.46
1:D:125:ALA:O	1:D:128:TYR:HB2	2.15	0.46
1:E:121:SER:OG	1:E:124:GLU:HG3	2.14	0.46
1:D:11:GLU:OE2	1:D:22:LYS:HE3	2.15	0.46
1:C:313:ALA:O	1:C:314:LEU:C	2.53	0.45
1:D:8:LEU:HD21	1:D:19:VAL:HG13	1.97	0.45
1:D:326:VAL:HA	3:D:4296:HOH:O	2.17	0.45
1:C:206:TYR:HE1	1:C:209:THR:HA	1.82	0.45
1:A:41:SER:CB	1:A:126:MSE:HB3	2.45	0.45
1:E:147:LEU:CD2	1:E:219:GLN:OE1	2.64	0.45
1:F:209:THR:C	1:F:210:LEU:HD23	2.36	0.45
1:B:296:GLN:O	1:B:297:LEU:CB	2.64	0.45
1:A:46:LYS:HG3	1:A:57:ILE:HD11	1.96	0.45
1:B:69:ALA:HB2	1:B:101:GLY:HA3	1.98	0.45
1:E:329:LYS:HE3	3:E:5315:HOH:O	2.16	0.45
1:F:48:GLY:HA3	1:F:317:ILE:CD1	2.47	0.45
1:E:109:PRO:HD2	1:E:112:TRP:CE3	2.52	0.45
1:D:98:ARG:NH1	1:D:98:ARG:CG	2.71	0.45
1:B:102:LEU:CD2	1:B:328:VAL:HG21	2.47	0.45
1:D:223:ASP:OD2	1:D:226:GLY:CA	2.65	0.45
1:D:167:ALA:O	1:D:171:LEU:HB2	2.16	0.45
1:D:298:LEU:HG	1:D:298:LEU:H	1.39	0.45
1:C:181:SER:OG	1:C:205:VAL:CG2	2.65	0.45
1:A:317:ILE:HD12	1:A:317:ILE:N	2.32	0.45
1:C:45:TYR:CE2	1:C:49:LEU:HD21	2.52	0.45
1:A:296:GLN:HB2	1:A:299:THR:HG21	1.90	0.45
1:A:296:GLN:CB	1:A:299:THR:CG2	2.84	0.45
1:F:47:ASP:O	1:F:48:GLY:C	2.55	0.45
1:B:274:VAL:HG12	1:B:275:TYR:CD2	2.52	0.45
1:C:165:GLY:HA3	1:C:300:ILE:HD11	1.98	0.45
1:B:303:ARG:CB	1:B:303:ARG:CD	2.87	0.45
1:F:104:GLU:O	1:F:105:TYR:C	2.55	0.45
1:F:219:GLN:H	1:F:238:GLN:H	1.65	0.45
1:B:63:LEU:O	1:B:63:LEU:HD23	2.17	0.45
1:B:302:ASP:HB2	1:B:323:GLN:O	2.17	0.45
1:E:8:LEU:HD22	1:E:310:THR:OG1	2.16	0.45
1:C:14:ALA:C	1:C:15:ASP:OD1	2.55	0.45
1:C:22:LYS:HB3	1:C:23:THR:H	1.37	0.45
1:C:147:LEU:HD22	1:C:219:GLN:CD	2.37	0.45
2:B:2255:NAD:H8A	1:E:239:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:PRO:HG2	1:F:112:TRP:CE3	2.52	0.45
1:D:18:SER:O	1:D:19:VAL:CB	2.60	0.44
1:B:108:VAL:HG22	1:B:113:LEU:HD21	1.98	0.44
1:A:261:PHE:HB3	1:D:270:GLY:CA	2.47	0.44
1:F:123:LYS:O	1:F:127:VAL:HG23	2.17	0.44
1:D:222:VAL:O	1:D:224:PRO:HD3	2.18	0.44
1:E:319:GLN:NE2	1:E:321:ARG:CD	2.66	0.44
1:F:184:ASN:HD22	1:F:184:ASN:C	2.18	0.44
1:D:307:LEU:O	1:D:310:THR:CB	2.62	0.44
1:A:91:SER:HB3	1:A:274:VAL:O	2.17	0.44
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.81	0.44
1:C:91:SER:HB3	1:C:274:VAL:HA	1.98	0.44
1:C:44:ASN:ND2	1:C:325:ARG:NH2	2.64	0.44
1:F:66:GLY:CA	1:F:101:GLY:H	2.25	0.44
1:B:90:THR:HB	3:B:2257:HOH:O	2.17	0.44
1:C:138:SER:OG	1:C:271:ILE:HD13	2.18	0.44
1:D:182:THR:HG22	1:D:183:GLY:N	2.32	0.44
1:F:66:GLY:HA3	1:F:100:GLY:HA3	1.99	0.44
1:C:25:SER:O	1:C:28:ASP:HB2	2.18	0.44
1:E:102:LEU:CD2	1:E:328:VAL:HG21	2.47	0.44
1:F:57:ILE:HA	1:F:57:ILE:HD13	1.82	0.44
1:B:128:TYR:CD1	1:B:288:MSE:HE2	2.53	0.44
1:E:319:GLN:HE21	1:E:321:ARG:HD2	1.79	0.44
1:C:218:TRP:O	1:C:238:GLN:HG2	2.17	0.44
1:E:266:VAL:HG23	1:E:267:SER:N	2.33	0.44
1:E:16:ASP:O	1:E:17:VAL:HG23	2.17	0.44
1:E:35:LEU:HD13	1:E:74:VAL:HG21	1.99	0.44
1:C:64:ILE:HG21	1:C:103:SER:HB2	1.99	0.44
1:C:123:LYS:HE3	1:C:304:GLU:OE1	2.17	0.44
1:A:59:ARG:NE	1:A:59:ARG:CA	2.78	0.44
1:D:199:VAL:C	1:D:200:ILE:HG23	2.39	0.44
1:C:166:ILE:O	1:C:169:SER:HB2	2.18	0.44
1:C:216:GLN:NE2	1:C:238:GLN:HB3	2.32	0.44
2:B:2255:NAD:H8A	1:E:239:TYR:CE2	2.53	0.44
1:A:306:SER:O	1:A:307:LEU:C	2.55	0.44
1:E:311:PRO:O	1:E:312:GLY:C	2.55	0.44
1:B:57:ILE:HG22	1:B:96:VAL:HG13	2.00	0.44
1:C:225:VAL:HG22	1:C:249:THR:HG21	2.00	0.43
1:A:41:SER:HB3	1:A:126:MSE:HB3	2.00	0.43
1:C:39:ALA:C	1:C:40:TYR:CD1	2.91	0.43
1:F:141:ARG:NE	2:F:6255:NAD:C2A	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:GLY:C	1:E:209:THR:OG1	2.51	0.43
1:A:216:GLN:NE2	1:A:238:GLN:HA	2.34	0.43
1:C:244:ALA:HB1	1:C:271:ILE:HD11	1.90	0.43
1:C:44:ASN:O	1:C:47:ASP:HB2	2.18	0.43
1:F:166:ILE:HD12	1:F:166:ILE:HG23	1.58	0.43
1:D:5:PHE:CD1	1:D:5:PHE:C	2.92	0.43
1:F:52:LYS:HD3	1:F:315:LYS:HZ1	1.82	0.43
1:C:307:LEU:O	1:C:310:THR:HB	2.18	0.43
1:A:40:TYR:CB	1:A:126:MSE:HG3	2.48	0.43
1:D:69:ALA:O	1:D:126:MSE:HE3	2.18	0.43
1:F:317:ILE:O	1:F:319:GLN:N	2.49	0.43
1:E:35:LEU:HD22	1:E:36:ILE:H	1.83	0.43
1:E:102:LEU:HD21	1:E:328:VAL:HG21	1.99	0.43
1:B:219:GLN:N	1:B:238:GLN:HG3	2.33	0.43
1:B:219:GLN:O	1:B:241:GLY:HA3	2.18	0.43
1:C:223:ASP:HA	1:C:224:PRO:HD2	1.78	0.43
1:C:238:GLN:HG2	1:C:238:GLN:H	1.45	0.43
1:D:203:GLU:HA	1:D:206:TYR:O	2.19	0.43
1:D:206:TYR:CG	1:D:207:ASP:N	2.85	0.43
1:B:25:SER:O	1:B:28:ASP:HB2	2.18	0.43
1:E:43:ILE:HD11	1:E:314:LEU:HG	2.00	0.43
1:A:169:SER:HB3	1:A:294:PRO:CB	2.49	0.43
1:F:145:ASN:ND2	1:F:269:LEU:HD11	2.33	0.43
1:B:303:ARG:CA	1:B:303:ARG:CG	2.82	0.43
1:E:66:GLY:HA3	1:E:101:GLY:N	2.32	0.43
1:A:37:LYS:HD2	1:A:105:TYR:CZ	2.53	0.43
1:C:135:ALA:O	1:C:138:SER:HB2	2.19	0.43
1:E:16:ASP:O	1:E:17:VAL:CG2	2.66	0.43
1:F:74:VAL:O	1:F:75:SER:CB	2.55	0.43
1:D:276:CYS:HA	1:D:277:PRO:HD3	1.87	0.43
1:C:81:PHE:CD1	1:C:81:PHE:N	2.87	0.43
1:C:233:LEU:O	1:C:234:LEU:C	2.56	0.43
1:B:224:PRO:O	1:B:247:GLY:HA3	2.18	0.43
1:D:26:THR:CA	1:D:26:THR:CG2	2.83	0.43
1:B:248:LEU:CD1	1:B:248:LEU:H	2.32	0.43
1:A:147:LEU:HD13	1:A:176:TYR:CE2	2.54	0.43
1:C:5:PHE:HB2	1:C:104:GLU:HG3	2.00	0.43
1:E:219:GLN:N	1:E:238:GLN:CG	2.81	0.43
1:C:66:GLY:CA	1:C:101:GLY:H	2.31	0.43
1:B:217:GLN:O	1:B:218:TRP:CD1	2.72	0.43
1:A:166:ILE:CG1	1:A:300:ILE:HD13	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:CE1	1:D:268:LEU:HD23	2.53	0.43
1:E:155:LEU:O	1:E:221:ALA:HA	2.18	0.43
1:E:258:VAL:HG13	1:E:262:ILE:HG12	2.00	0.43
1:B:78:ASP:HA	1:B:79:PRO:HD2	1.84	0.43
1:B:45:TYR:CE1	1:B:318:LEU:CD2	3.01	0.43
1:B:36:ILE:O	1:B:36:ILE:HG22	2.18	0.43
1:F:6:GLN:O	1:F:104:GLU:HG3	2.18	0.42
1:C:157:THR:CG2	1:C:225:VAL:HB	2.49	0.42
1:E:147:LEU:HD22	1:E:219:GLN:OE1	2.19	0.42
1:D:305:VAL:HG22	1:D:309:GLU:CB	2.49	0.42
1:C:78:ASP:O	1:C:80:ARG:N	2.52	0.42
1:D:66:GLY:HA3	1:D:100:GLY:HA3	2.01	0.42
1:B:225:VAL:HG12	1:B:249:THR:O	2.18	0.42
1:E:120:LEU:HD21	1:E:128:TYR:CE1	2.53	0.42
1:B:245:VAL:HG22	1:B:268:LEU:HD11	2.01	0.42
1:E:208:GLY:C	1:E:209:THR:HG1	2.23	0.42
1:A:287:ARG:NH2	1:A:291:ASP:OD1	2.52	0.42
1:C:124:GLU:HG2	1:C:297:LEU:HD13	2.01	0.42
1:C:172:ASN:OD1	1:C:195:GLY:HA2	2.20	0.42
1:A:220:GLY:HA2	1:A:242:SER:O	2.19	0.42
1:B:167:ALA:O	1:B:171:LEU:HB2	2.20	0.42
1:D:248:LEU:C	1:D:249:THR:O	2.54	0.42
1:E:206:TYR:CE1	1:E:209:THR:HA	2.54	0.42
1:B:155:LEU:HD23	1:B:179:VAL:HG12	2.02	0.42
1:B:37:LYS:HG3	3:B:2268:HOH:O	2.19	0.42
1:F:183:GLY:HA2	3:F:6283:HOH:O	2.18	0.42
1:C:127:VAL:HG11	1:C:297:LEU:HD22	2.01	0.42
1:D:69:ALA:C	1:D:126:MSE:HE3	2.39	0.42
1:B:129:GLY:HA3	1:B:325:ARG:HH21	1.84	0.42
1:E:93:GLU:HB2	1:E:112:TRP:HH2	1.84	0.42
1:D:248:LEU:HD23	1:D:248:LEU:C	2.32	0.42
1:F:229:GLN:HG2	1:F:229:GLN:O	2.19	0.42
1:C:312:GLY:O	1:C:315:LYS:HB3	2.20	0.42
1:D:7:ALA:CB	1:D:103:SER:HB2	2.49	0.42
1:C:228:LYS:O	1:C:229:GLN:C	2.56	0.42
1:A:260:PRO:HA	1:A:264:ARG:HB2	2.00	0.42
1:B:147:LEU:HD13	1:B:176:TYR:CE2	2.53	0.42
1:E:141:ARG:HH11	1:E:141:ARG:HD2	1.56	0.42
1:C:317:ILE:HG21	1:C:317:ILE:HD13	1.60	0.42
1:C:36:ILE:HD12	1:C:108:VAL:HG13	2.02	0.42
1:B:262:ILE:O	1:E:272:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:SER:HB2	1:D:177:ASP:HB2	2.02	0.42
1:A:120:LEU:HA	1:A:120:LEU:HD23	1.91	0.42
1:D:168:VAL:O	1:D:169:SER:C	2.57	0.42
1:E:83:GLU:N	1:E:83:GLU:CD	2.64	0.42
1:B:208:GLY:O	1:B:209:THR:O	2.37	0.42
1:D:148:SER:HB3	1:D:151:LYS:CD	2.50	0.42
1:D:329:LYS:O	1:D:330:LEU:HG	2.19	0.42
1:E:221:ALA:HB3	1:E:243:VAL:HG13	2.02	0.42
1:F:314:LEU:HD23	1:F:314:LEU:HA	1.92	0.42
1:B:44:ASN:ND2	1:B:67:ILE:HD11	2.34	0.42
1:E:306:SER:OG	1:E:308:GLU:HB2	2.20	0.42
1:E:315:LYS:HD2	1:E:319:GLN:OE1	2.20	0.42
1:F:307:LEU:C	1:F:307:LEU:HD22	2.40	0.42
1:A:170:MSE:HG2	1:A:292:LEU:O	2.20	0.42
1:C:36:ILE:HG22	1:C:37:LYS:N	2.35	0.42
1:D:154:VAL:HB	3:D:4261:HOH:O	2.20	0.42
1:E:258:VAL:O	1:E:258:VAL:HG13	2.20	0.42
1:B:114:VAL:HA	1:B:115:PRO:HD3	1.81	0.42
1:A:234:LEU:HA	1:A:237:ILE:HD12	2.02	0.42
1:F:147:LEU:HD22	1:F:219:GLN:CD	2.40	0.41
1:D:303:ARG:CG	1:D:304:GLU:N	2.80	0.41
1:F:7:ALA:HB1	1:F:64:ILE:HD13	2.02	0.41
1:F:248:LEU:O	1:F:249:THR:C	2.58	0.41
1:C:319:GLN:O	1:C:321:ARG:N	2.53	0.41
1:C:36:ILE:CD1	1:C:108:VAL:HG13	2.50	0.41
1:E:42:GLY:HA2	1:E:325:ARG:HH22	1.84	0.41
1:F:298:LEU:HA	1:F:298:LEU:HD23	1.92	0.41
1:F:233:LEU:HD21	1:F:237:ILE:HD11	2.02	0.41
1:B:258:VAL:HG11	1:E:248:LEU:HB3	2.02	0.41
1:D:290:SER:OG	1:D:291:ASP:N	2.53	0.41
1:A:257:THR:HB	1:A:259:TYR:CD2	2.54	0.41
1:F:287:ARG:NE	1:F:291:ASP:OD2	2.53	0.41
1:C:21:VAL:O	1:C:21:VAL:HG13	2.08	0.41
1:B:41:SER:CB	1:B:328:VAL:H	2.29	0.41
1:A:59:ARG:HA	1:A:59:ARG:HE	1.81	0.41
1:C:14:ALA:HB1	3:C:3282:HOH:O	2.19	0.41
1:E:262:ILE:HD13	1:E:262:ILE:HG21	1.88	0.41
1:C:59:ARG:HB2	3:C:3292:HOH:O	2.19	0.41
1:C:109:PRO:HD2	1:C:112:TRP:CE3	2.56	0.41
1:D:281:ARG:HD3	3:D:4268:HOH:O	2.20	0.41
1:E:29:LEU:HA	1:E:29:LEU:HD23	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.81	0.41
1:F:258:VAL:O	1:F:261:PHE:HB2	2.20	0.41
1:B:3:THR:CG2	1:B:3:THR:CA	2.87	0.41
1:D:182:THR:HB	1:D:184:ASN:H	1.86	0.41
1:A:212:ALA:HB1	1:A:259:TYR:CD2	2.56	0.41
1:C:262:ILE:HD13	1:C:262:ILE:HG21	1.80	0.41
1:E:13:ASN:C	1:E:15:ASP:N	2.74	0.41
1:B:101:GLY:C	1:B:103:SER:N	2.73	0.41
1:B:101:GLY:C	1:B:103:SER:H	2.24	0.41
1:E:322:ILE:HD13	1:E:322:ILE:HG21	1.89	0.41
1:C:114:VAL:HG21	1:C:285:TRP:CD1	2.56	0.41
1:E:104:GLU:CG	1:E:104:GLU:O	2.69	0.41
1:C:93:GLU:O	1:C:94:LEU:C	2.59	0.41
1:D:132:GLY:O	1:D:133:PHE:C	2.57	0.41
1:A:238:GLN:CB	1:A:238:GLN:CD	2.82	0.41
1:A:287:ARG:HB3	1:A:292:LEU:CD1	2.50	0.41
1:D:109:PRO:HG2	1:D:112:TRP:CD2	2.56	0.41
1:C:98:ARG:HG3	1:C:99:ASP:N	2.35	0.41
1:A:152:GLY:CA	1:A:238:GLN:OE1	2.66	0.41
1:B:206:TYR:CD1	1:B:209:THR:HA	2.52	0.41
1:C:8:LEU:O	1:C:64:ILE:HA	2.21	0.41
1:C:8:LEU:HD23	1:C:8:LEU:C	2.41	0.41
1:F:78:ASP:HA	1:F:79:PRO:HD3	1.94	0.41
1:F:78:ASP:OD2	1:F:80:ARG:NH2	2.50	0.41
1:B:228:LYS:HA	1:B:255:PRO:HD2	2.02	0.41
1:A:318:LEU:HA	1:A:318:LEU:HD23	1.76	0.41
1:B:151:LYS:HB2	1:B:219:GLN:OE1	2.20	0.41
1:B:34:VAL:O	1:B:36:ILE:HD12	2.21	0.41
1:C:111:ASP:N	1:C:111:ASP:OD1	2.53	0.41
1:C:70:ALA:HB1	1:C:122:LEU:HD23	2.02	0.41
1:E:149:PRO:HA	1:E:176:TYR:CD2	2.55	0.40
1:D:171:LEU:HB3	1:D:178:VAL:CG2	2.51	0.40
1:C:66:GLY:HA3	1:C:101:GLY:N	2.34	0.40
1:E:308:GLU:H	1:E:308:GLU:HG2	1.67	0.40
1:A:63:LEU:O	1:A:63:LEU:HD23	2.21	0.40
1:C:181:SER:OG	1:C:205:VAL:HG21	2.21	0.40
1:B:168:VAL:HG13	1:B:178:VAL:HG11	2.02	0.40
1:E:187:ALA:O	1:E:188:ALA:C	2.60	0.40
1:C:219:GLN:HA	1:C:238:GLN:CG	2.50	0.40
1:B:327:ILE:HG21	1:B:327:ILE:HD13	1.45	0.40
1:E:148:SER:HA	1:E:149:PRO:HD3	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:SER:HB2	1:D:20:HIS:NE2	2.35	0.40
1:B:166:ILE:CG1	1:B:300:ILE:CD1	2.95	0.40
1:F:81:PHE:CZ	1:F:113:LEU:HB2	2.56	0.40
1:F:41:SER:HB2	1:F:328:VAL:O	2.22	0.40
1:B:187:ALA:O	1:B:188:ALA:C	2.59	0.40
1:A:174:ARG:HD2	3:A:1263:HOH:O	2.21	0.40
1:B:12:LYS:HD3	1:B:14:ALA:O	2.22	0.40
1:B:287:ARG:NE	1:B:291:ASP:OD2	2.45	0.40
1:A:262:ILE:O	1:D:272:ASP:HB2	2.21	0.40
1:A:69:ALA:HB2	1:A:101:GLY:HA3	2.03	0.40
1:A:102:LEU:CD2	1:A:328:VAL:HG21	2.51	0.40
1:A:8:LEU:HD11	1:A:19:VAL:CG1	2.51	0.40
1:B:67:ILE:HG22	1:B:94:LEU:O	2.21	0.40
1:E:136:ALA:HB2	1:E:170:MSE:HE1	2.04	0.40
1:F:7:ALA:HA	1:F:103:SER:HB2	2.04	0.40
1:E:319:GLN:HG2	3:E:5309:HOH:O	2.21	0.40
1:A:328:VAL:HG12	1:A:329:LYS:N	2.35	0.40
1:D:53:ALA:C	1:D:55:GLY:H	2.25	0.40
1:F:305:VAL:CG2	1:F:306:SER:N	2.83	0.40
1:F:108:VAL:HG23	1:F:109:PRO:HD2	2.03	0.40
1:C:187:ALA:O	1:C:188:ALA:C	2.60	0.40
1:A:90:THR:CG2	1:A:281:ARG:NH1	2.85	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	327/330 (99%)	268 (82%)	38 (12%)	21 (6%)	2	4
1	B	327/330 (99%)	264 (81%)	37 (11%)	26 (8%)	1	2
1	C	327/330 (99%)	251 (77%)	43 (13%)	33 (10%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	327/330 (99%)	257 (79%)	43 (13%)	27 (8%)	1 2
1	E	327/330 (99%)	274 (84%)	37 (11%)	16 (5%)	3 8
1	F	327/330 (99%)	269 (82%)	41 (12%)	17 (5%)	2 7
All	All	1962/1980 (99%)	1583 (81%)	239 (12%)	140 (7%)	1 3

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	A	41	SER
1	A	62	PRO
1	A	105	TYR
1	A	159	ALA
1	A	185	ARG
1	A	186	GLU
1	A	219	GLN
1	A	258	VAL
1	A	317	ILE
1	A	318	LEU
1	B	3	THR
1	B	14	ALA
1	B	22	LYS
1	B	41	SER
1	B	59	ARG
1	B	67	ILE
1	B	75	SER
1	B	105	TYR
1	B	185	ARG
1	B	186	GLU
1	B	227	GLY
1	B	279	ASP
1	B	291	ASP
1	B	296	GLN
1	B	318	LEU
1	B	319	GLN
1	C	21	VAL
1	C	22	LYS
1	C	103	SER
1	C	186	GLU
1	C	208	GLY
1	C	209	THR

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Mol	Chain	Res	Type
1	C	291	ASP
1	C	297	LEU
1	C	303	ARG
1	C	309	GLU
1	C	317	ILE
1	C	320	ASN
1	D	62	PRO
1	D	129	GLY
1	D	207	ASP
1	D	208	GLY
1	D	219	GLN
1	D	279	ASP
1	D	291	ASP
1	D	297	LEU
1	D	302	ASP
1	D	318	LEU
1	D	320	ASN
1	E	14	ALA
1	E	150	GLU
1	E	208	GLY
1	E	219	GLN
1	E	296	GLN
1	F	32	ASP
1	F	105	TYR
1	F	209	THR
1	F	219	GLN
1	F	291	ASP
1	F	296	GLN
1	F	320	ASN
1	A	17	VAL
1	A	187	ALA
1	A	188	ALA
1	A	226	GLY
1	B	17	VAL
1	B	208	GLY
1	B	219	GLN
1	B	320	ASN
1	C	53	ALA
1	C	54	GLY
1	C	312	GLY
1	C	314	LEU
1	D	150	GLU

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Mol	Chain	Res	Type
1	D	159	ALA
1	D	245	VAL
1	E	41	SER
1	F	19	VAL
1	F	250	GLY
1	A	27	GLU
1	A	53	ALA
1	A	279	ASP
1	A	291	ASP
1	B	321	ARG
1	C	26	THR
1	C	75	SER
1	C	91	SER
1	C	105	TYR
1	C	160	THR
1	C	226	GLY
1	C	290	SER
1	D	13	ASN
1	D	19	VAL
1	D	56	ASN
1	D	185	ARG
1	D	285	TRP
1	E	111	ASP
1	E	160	THR
1	F	228	LYS
1	F	297	LEU
1	C	17	VAL
1	C	18	SER
1	C	101	GLY
1	C	188	ALA
1	D	14	ALA
1	D	290	SER
1	E	91	SER
1	E	297	LEU
1	F	204	ASP
1	A	19	VAL
1	B	19	VAL
1	B	61	TYR
1	C	62	PRO
1	C	187	ALA
1	D	17	VAL
1	D	75	SER

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Mol	Chain	Res	Type
1	D	105	TYR
1	D	324	GLY
1	E	17	VAL
1	E	207	ASP
1	E	209	THR
1	F	75	SER
1	C	61	TYR
1	E	105	TYR
1	F	149	PRO
1	F	227	GLY
1	B	21	VAL
1	D	43	ILE
1	D	67	ILE
1	E	19	VAL
1	F	317	ILE
1	A	67	ILE
1	B	54	GLY
1	B	149	PRO
1	C	19	VAL
1	C	305	VAL
1	C	67	ILE
1	E	317	ILE
1	F	30	PRO

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	259/258 (100%)	207 (80%)	52 (20%)	1 4
1	B	257/258 (100%)	203 (79%)	54 (21%)	1 4
1	C	255/258 (99%)	210 (82%)	45 (18%)	2 7
1	D	259/258 (100%)	204 (79%)	55 (21%)	1 4
1	E	260/258 (101%)	202 (78%)	58 (22%)	1 3
1	F	261/258 (101%)	207 (79%)	54 (21%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1551/1548 (100%)	1233 (80%)	318 (20%)	1 4

All (318) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	12	LYS
1	A	13	ASN
1	A	15	ASP
1	A	25	SER
1	A	35	LEU
1	A	41	SER
1	A	43	ILE
1	A	59	ARG
1	A	63	LEU
1	A	65	LEU
1	A	67	ILE
1	A	78	ASP
1	A	80	ARG
1	A	90	THR
1	A	103	SER
1	A	108	VAL
1	A	114	VAL
1	A	124	GLU
1	A	147	LEU
1	A	150	GLU
1	A	151	LYS
1	A	155	LEU
1	A	160	THR
1	A	171	LEU
1	A	178	VAL
1	A	185	ARG
1	A	198	GLU
1	A	215	LYS
1	A	216	GLN
1	A	217	GLN
1	A	230	LEU
1	A	233	LEU
1	A	245	VAL
1	A	248	LEU
1	A	249	THR
1	A	258	VAL

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Mol	Chain	Res	Type
1	A	266	VAL
1	A	272	ASP
1	A	276	CYS
1	A	286	GLU
1	A	296	GLN
1	A	297	LEU
1	A	298	LEU
1	A	299	THR
1	A	303	ARG
1	A	307	LEU
1	A	310	THR
1	A	315	LYS
1	A	317	ILE
1	A	322	ILE
1	A	323	GLN
1	B	3	THR
1	B	4	LEU
1	B	18	SER
1	B	24	ILE
1	B	27	GLU
1	B	35	LEU
1	B	36	ILE
1	B	43	ILE
1	B	46	LYS
1	B	60	GLU
1	B	61	TYR
1	B	63	LEU
1	B	64	ILE
1	B	65	LEU
1	B	67	ILE
1	B	74	VAL
1	B	75	SER
1	B	83	GLU
1	B	90	THR
1	B	103	SER
1	B	108	VAL
1	B	111	ASP
1	B	114	VAL
1	B	144	GLN
1	B	147	LEU
1	B	155	LEU
1	B	171	LEU

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Mol	Chain	Res	Type
1	B	181	SER
1	B	182	THR
1	B	185	ARG
1	B	186	GLU
1	B	193	GLN
1	B	211	LYS
1	B	215	LYS
1	B	225	VAL
1	B	230	LEU
1	B	233	LEU
1	B	242	SER
1	B	245	VAL
1	B	248	LEU
1	B	266	VAL
1	B	269	LEU
1	B	276	CYS
1	B	279	ASP
1	B	286	GLU
1	B	297	LEU
1	B	304	GLU
1	B	305	VAL
1	B	306	SER
1	B	307	LEU
1	B	308	GLU
1	B	319	GLN
1	B	325	ARG
1	B	327	ILE
1	C	2	SER
1	C	3	THR
1	C	13	ASN
1	C	16	ASP
1	C	17	VAL
1	C	18	SER
1	C	27	GLU
1	C	32	ASP
1	C	35	LEU
1	C	59	ARG
1	C	61	TYR
1	C	67	ILE
1	C	76	SER
1	C	93	GLU
1	C	97	SER

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Mol	Chain	Res	Type
1	C	98	ARG
1	C	108	VAL
1	C	118	GLN
1	C	147	LEU
1	C	151	LYS
1	C	157	THR
1	C	160	THR
1	C	171	LEU
1	C	172	ASN
1	C	182	THR
1	C	189	ASP
1	C	193	GLN
1	C	211	LYS
1	C	233	LEU
1	C	236	LYS
1	C	246	SER
1	C	258	VAL
1	C	272	ASP
1	C	297	LEU
1	C	298	LEU
1	C	306	SER
1	C	307	LEU
1	C	309	GLU
1	C	310	THR
1	C	314	LEU
1	C	319	GLN
1	C	321	ARG
1	C	323	GLN
1	C	325	ARG
1	C	330	LEU
1	D	4	LEU
1	D	11	GLU
1	D	13	ASN
1	D	15	ASP
1	D	20	HIS
1	D	22	LYS
1	D	24	ILE
1	D	36	ILE
1	D	41	SER
1	D	45	TYR
1	D	60	GLU
1	D	67	ILE

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Mol	Chain	Res	Type
1	D	75	SER
1	D	76	SER
1	D	90	THR
1	D	98	ARG
1	D	103	SER
1	D	114	VAL
1	D	116	LEU
1	D	123	LYS
1	D	147	LEU
1	D	150	GLU
1	D	151	LYS
1	D	155	LEU
1	D	160	THR
1	D	171	LEU
1	D	181	SER
1	D	182	THR
1	D	185	ARG
1	D	186	GLU
1	D	189	ASP
1	D	197	SER
1	D	207	ASP
1	D	219	GLN
1	D	225	VAL
1	D	228	LYS
1	D	229	GLN
1	D	234	LEU
1	D	245	VAL
1	D	249	THR
1	D	272	ASP
1	D	281	ARG
1	D	295	ASP
1	D	297	LEU
1	D	298	LEU
1	D	300	ILE
1	D	303	ARG
1	D	305	VAL
1	D	307	LEU
1	D	308	GLU
1	D	315	LYS
1	D	317	ILE
1	D	321	ARG
1	D	327	ILE

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Mol	Chain	Res	Type
1	D	330	LEU
1	E	3	THR
1	E	4	LEU
1	E	13	ASN
1	E	16	ASP
1	E	18	SER
1	E	22	LYS
1	E	24	ILE
1	E	28	ASP
1	E	35	LEU
1	E	37	LYS
1	E	41	SER
1	E	43	ILE
1	E	52	LYS
1	E	59	ARG
1	E	60	GLU
1	E	61	TYR
1	E	63	LEU
1	E	65	LEU
1	E	67	ILE
1	E	72	THR
1	E	74	VAL
1	E	78	ASP
1	E	80	ARG
1	E	83	GLU
1	E	85	ASP
1	E	91	SER
1	E	108	VAL
1	E	147	LEU
1	E	155	LEU
1	E	166	ILE
1	E	171	LEU
1	E	181	SER
1	E	182	THR
1	E	185	ARG
1	E	193	GLN
1	E	215	LYS
1	E	219	GLN
1	E	233	LEU
1	E	238	GLN
1	E	242	SER
1	E	245	VAL

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Mol	Chain	Res	Type
1	E	248	LEU
1	E	249	THR
1	E	258	VAL
1	E	266	VAL
1	E	286	GLU
1	E	291	ASP
1	E	297	LEU
1	E	299	THR
1	E	303	ARG
1	E	305	VAL
1	E	307	LEU
1	E	315	LYS
1	E	317	ILE
1	E	318	LEU
1	E	320	ASN
1	E	325	ARG
1	E	330	LEU
1	F	2	SER
1	F	8	LEU
1	F	12	LYS
1	F	13	ASN
1	F	19	VAL
1	F	22	LYS
1	F	23	THR
1	F	24	ILE
1	F	25	SER
1	F	31	LYS
1	F	32	ASP
1	F	41	SER
1	F	52	LYS
1	F	60	GLU
1	F	67	ILE
1	F	90	THR
1	F	98	ARG
1	F	108	VAL
1	F	114	VAL
1	F	118	GLN
1	F	123	LYS
1	F	128	TYR
1	F	147	LEU
1	F	155	LEU
1	F	160	THR

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Mol	Chain	Res	Type
1	F	171	LEU
1	F	181	SER
1	F	182	THR
1	F	184	ASN
1	F	185	ARG
1	F	190	TYR
1	F	210	LEU
1	F	211	LYS
1	F	233	LEU
1	F	236	LYS
1	F	237	ILE
1	F	245	VAL
1	F	246	SER
1	F	248	LEU
1	F	255	PRO
1	F	266	VAL
1	F	272	ASP
1	F	297	LEU
1	F	300	ILE
1	F	303	ARG
1	F	307	LEU
1	F	310	THR
1	F	315	LYS
1	F	318	LEU
1	F	319	GLN
1	F	321	ARG
1	F	323	GLN
1	F	325	ARG
1	F	327	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	13	ASN
1	A	216	GLN
1	A	217	GLN
1	A	323	GLN
1	B	9	GLN
1	B	193	GLN
1	B	216	GLN
1	B	320	ASN

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Mol	Chain	Res	Type
1	C	44	ASN
1	C	77	ASN
1	C	193	GLN
1	C	216	GLN
1	C	238	GLN
1	C	323	GLN
1	D	9	GLN
1	D	44	ASN
1	D	119	ASN
1	E	6	GLN
1	E	13	ASN
1	E	216	GLN
1	E	238	GLN
1	E	319	GLN
1	F	6	GLN
1	F	184	ASN
1	F	216	GLN
1	F	238	GLN
1	F	323	GLN

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

6 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	$\#\|Z\| > 2$
2	NAD	A	1255	-	9,12,48	1.80	2 (22%)	6,17,73	4.91	3 (50%)
2	NAD	B	2255	-	9,12,48	1.40	3 (33%)	6,17,73	2.56	3 (50%)
2	NAD	C	3255	-	9,12,48	2.92	4 (44%)	6,17,73	2.28	3 (50%)
2	NAD	D	4255	-	9,12,48	2.09	4 (44%)	6,17,73	6.81	2 (33%)
2	NAD	E	5255	-	9,12,48	3.96	5 (55%)	6,17,73	5.51	4 (66%)
2	NAD	F	6255	-	9,12,48	2.94	4 (44%)	6,17,73	6.23	4 (66%)

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
2	NAD	A	1255	-	-	0/0/0/62	0/2/2/5
2	NAD	B	2255	-	-	0/0/0/62	0/2/2/5
2	NAD	C	3255	-	-	0/0/0/62	0/2/2/5
2	NAD	D	4255	-	-	0/0/0/62	0/2/2/5
2	NAD	E	5255	-	-	0/0/0/62	0/2/2/5
2	NAD	F	6255	-	-	0/0/0/62	0/2/2/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4255	NAD	C6A-N6A	-2.72	1.26	1.34
2	B	2255	NAD	C6A-N6A	-2.40	1.27	1.34
2	C	3255	NAD	C4A-N3A	-2.11	1.32	1.35
2	B	2255	NAD	C2A-N3A	2.04	1.35	1.32
2	B	2255	NAD	C8A-N7A	2.06	1.38	1.34
2	E	5255	NAD	C6A-N1A	2.35	1.49	1.37
2	C	3255	NAD	C8A-N7A	2.49	1.39	1.34
2	A	1255	NAD	C2A-N1A	2.49	1.38	1.33
2	D	4255	NAD	C8A-N7A	2.73	1.39	1.34
2	E	5255	NAD	C4A-N3A	3.10	1.40	1.35
2	D	4255	NAD	C2A-N1A	3.22	1.40	1.33
2	F	6255	NAD	C4A-N3A	3.26	1.40	1.35
2	D	4255	NAD	C2A-N3A	3.48	1.38	1.32
2	E	5255	NAD	C2A-N1A	3.57	1.40	1.33
2	F	6255	NAD	C8A-N7A	3.93	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5255	NAD	C8A-N7A	4.04	1.42	1.34
2	A	1255	NAD	C2A-N3A	4.10	1.39	1.32
2	C	3255	NAD	C2A-N1A	4.19	1.41	1.33
2	F	6255	NAD	C2A-N1A	4.54	1.42	1.33
2	F	6255	NAD	C2A-N3A	5.14	1.41	1.32
2	C	3255	NAD	C2A-N3A	6.24	1.43	1.32
2	E	5255	NAD	C2A-N3A	9.72	1.49	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4255	NAD	N3A-C2A-N1A	-16.43	116.31	128.89
2	F	6255	NAD	N3A-C2A-N1A	-14.12	118.08	128.89
2	E	5255	NAD	N3A-C2A-N1A	-11.22	120.31	128.89
2	A	1255	NAD	N3A-C2A-N1A	-7.62	123.06	128.89
2	E	5255	NAD	C2A-N1A-C6A	-6.05	107.95	118.77
2	B	2255	NAD	N3A-C2A-N1A	-3.74	126.03	128.89
2	C	3255	NAD	C2A-N1A-C6A	-3.72	112.12	118.77
2	B	2255	NAD	C2A-N1A-C6A	-3.69	112.17	118.77
2	E	5255	NAD	C4A-C5A-N7A	-3.04	106.68	109.48
2	C	3255	NAD	N3A-C2A-N1A	-2.37	127.08	128.89
2	D	4255	NAD	N6A-C6A-N1A	-2.22	114.43	119.20
2	F	6255	NAD	C2A-N1A-C6A	2.15	122.61	118.77
2	C	3255	NAD	C4A-C5A-N7A	2.20	111.50	109.48
2	B	2255	NAD	C4A-C5A-N7A	2.43	111.72	109.48
2	E	5255	NAD	N6A-C6A-N1A	2.98	125.59	119.20
2	F	6255	NAD	C4A-C5A-N7A	3.62	112.81	109.48
2	F	6255	NAD	N6A-C6A-N1A	3.77	127.29	119.20
2	A	1255	NAD	N6A-C6A-N1A	4.79	129.49	119.20
2	A	1255	NAD	C4A-C5A-N7A	7.47	116.35	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1255	NAD	5	0
2	B	2255	NAD	5	0
2	C	3255	NAD	4	0
2	F	6255	NAD	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	325/330 (98%)	-0.24	7 (2%)	65	54	18, 18, 18, 18	0
1	B	325/330 (98%)	-0.18	12 (3%)	45	33	18, 18, 18, 18	0
1	C	325/330 (98%)	-0.03	16 (4%)	33	22	18, 18, 18, 18	0
1	D	325/330 (98%)	-0.12	10 (3%)	52	40	18, 18, 18, 18	0
1	E	325/330 (98%)	-0.27	7 (2%)	65	54	18, 18, 18, 18	0
1	F	325/330 (98%)	-0.25	3 (0%)	85	79	18, 18, 18, 18	0
All	All	1950/1980 (98%)	-0.18	55 (2%)	56	44	18, 18, 18, 18	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	13	ASN	4.9
1	C	14	ALA	4.7
1	C	2	SER	4.4
1	D	13	ASN	3.7
1	A	2	SER	3.5
1	B	16	ASP	3.5
1	D	16	ASP	3.4
1	E	13	ASN	3.3
1	B	3	THR	3.2
1	E	16	ASP	3.2
1	F	209	THR	3.2
1	C	15	ASP	3.1
1	B	13	ASN	3.0
1	B	320	ASN	3.0
1	B	319	GLN	2.9
1	A	13	ASN	2.9
1	C	53	ALA	2.9
1	D	321	ARG	2.9
1	F	2	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	14	ALA	2.9
1	B	207	ASP	2.8
1	E	15	ASP	2.8
1	D	319	GLN	2.8
1	C	321	ARG	2.8
1	D	2	SER	2.8
1	A	15	ASP	2.8
1	C	16	ASP	2.8
1	A	14	ALA	2.7
1	C	320	ASN	2.7
1	C	60	GLU	2.7
1	E	321	ARG	2.7
1	E	2	SER	2.7
1	A	16	ASP	2.6
1	B	2	SER	2.6
1	B	14	ALA	2.5
1	D	185	ARG	2.5
1	C	319	GLN	2.5
1	A	3	THR	2.5
1	F	13	ASN	2.5
1	C	308	GLU	2.4
1	C	18	SER	2.4
1	D	320	ASN	2.4
1	D	322	ILE	2.4
1	B	59	ARG	2.3
1	A	184	ASN	2.3
1	C	3	THR	2.3
1	B	15	ASP	2.2
1	C	59	ARG	2.2
1	C	207	ASP	2.2
1	D	3	THR	2.1
1	E	215	LYS	2.1
1	C	189	ASP	2.1
1	E	14	ALA	2.1
1	B	60	GLU	2.0
1	B	56	ASN	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^{th} 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^2)	Q<0.9
2	NAD	E	5255	11/44	0.78	0.26	3.40	17,17,17,17	0
2	NAD	D	4255	11/44	0.91	0.18	1.82	17,17,17,17	0
2	NAD	F	6255	11/44	0.87	0.20	1.33	17,17,17,17	0
2	NAD	C	3255	11/44	0.92	0.18	1.24	17,17,17,17	0
2	NAD	A	1255	11/44	0.89	0.20	1.06	17,17,17,17	0
2	NAD	B	2255	11/44	0.90	0.18	0.60	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.