



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:27 PM UTC

PDB ID : 2RDA / pdb_00002rda
Title : Human Thymidylate Synthase Stabilized in Active Conformation by R163K
Mutation: Asymmetry and Reactivity of Cys195
Authors : Gibson, L.M.; Lovelace, L.L.; Lebioda, L.
Deposited on : 2007-09-21
Resolution : 2.67 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

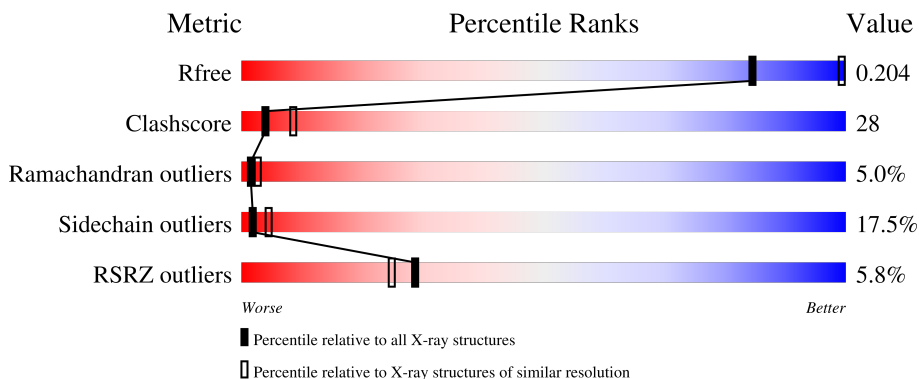
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	
1	C	313	
1	D	313	
1	E	313	

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Mol	Chain	Length	Quality of chain
1	F	313	

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	PO4	C	616	-	X	-	-
2	PO4	E	618	-	-	X	-
2	PO4	E	619	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13834 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2279	1457	399	412	11	0	0	0
1	B	281	2268	1451	395	411	11	0	0	0
1	C	281	2268	1451	395	411	11	0	0	0
1	D	281	2268	1451	395	411	11	0	0	0
1	E	281	2268	1451	395	411	11	0	0	0
1	F	281	2268	1451	395	411	11	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

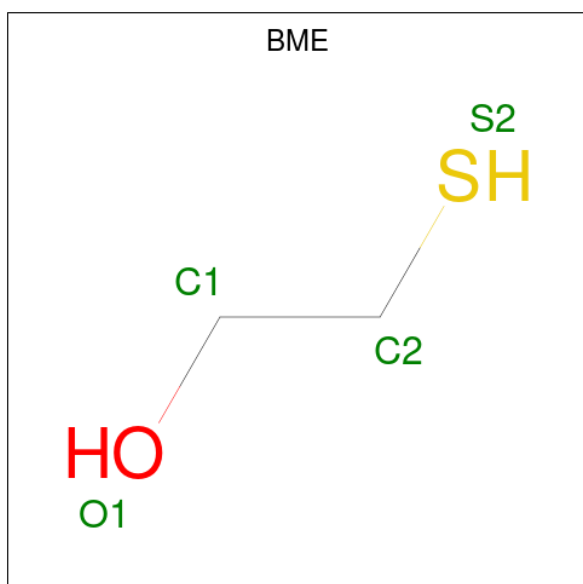
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LYS	ARG	engineered mutation	UNP P04818
B	163	LYS	ARG	engineered mutation	UNP P04818
C	163	LYS	ARG	engineered mutation	UNP P04818
D	163	LYS	ARG	engineered mutation	UNP P04818
E	163	LYS	ARG	engineered mutation	UNP P04818
F	163	LYS	ARG	engineered mutation	UNP P04818

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		

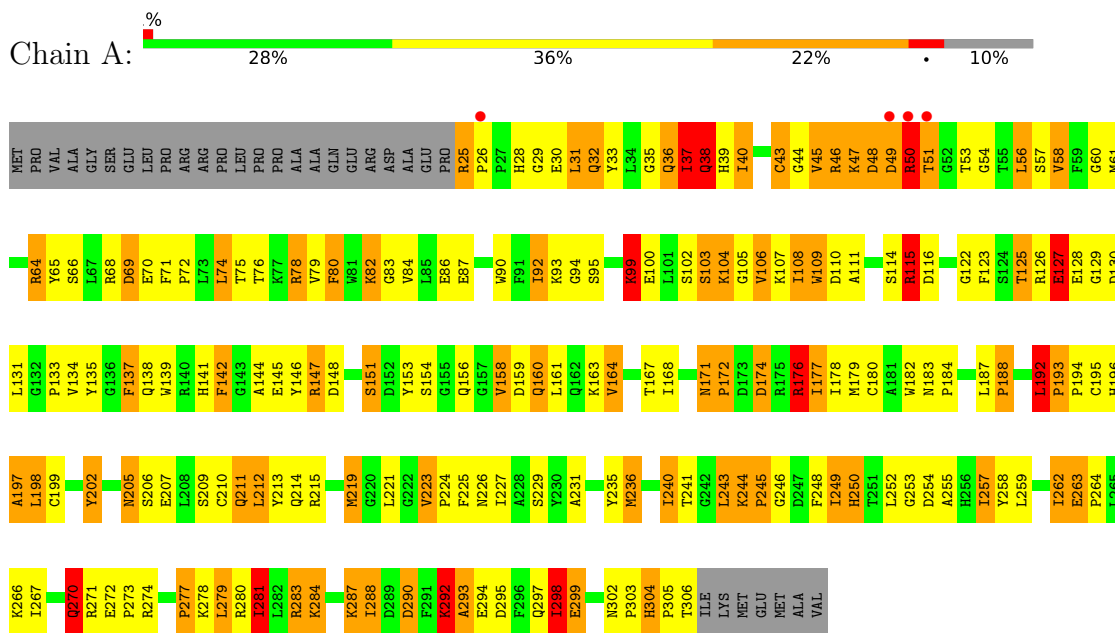
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	52	Total	O	0	0
			52	52		
4	C	30	Total	O	0	0
			30	30		
4	D	23	Total	O	0	0
			23	23		
4	E	9	Total	O	0	0
			9	9		
4	F	6	Total	O	0	0
			6	6		

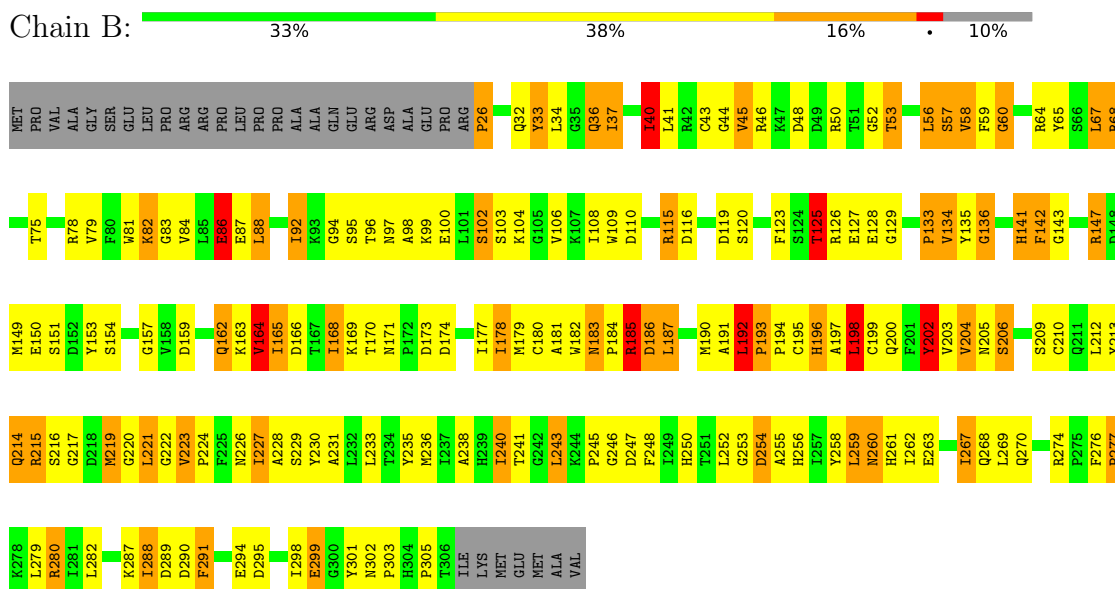
3 Residue-property plots

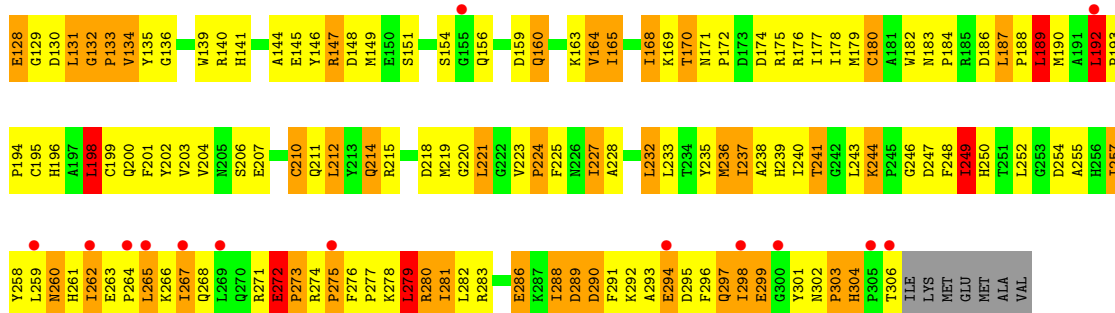
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Thymidylate synthase

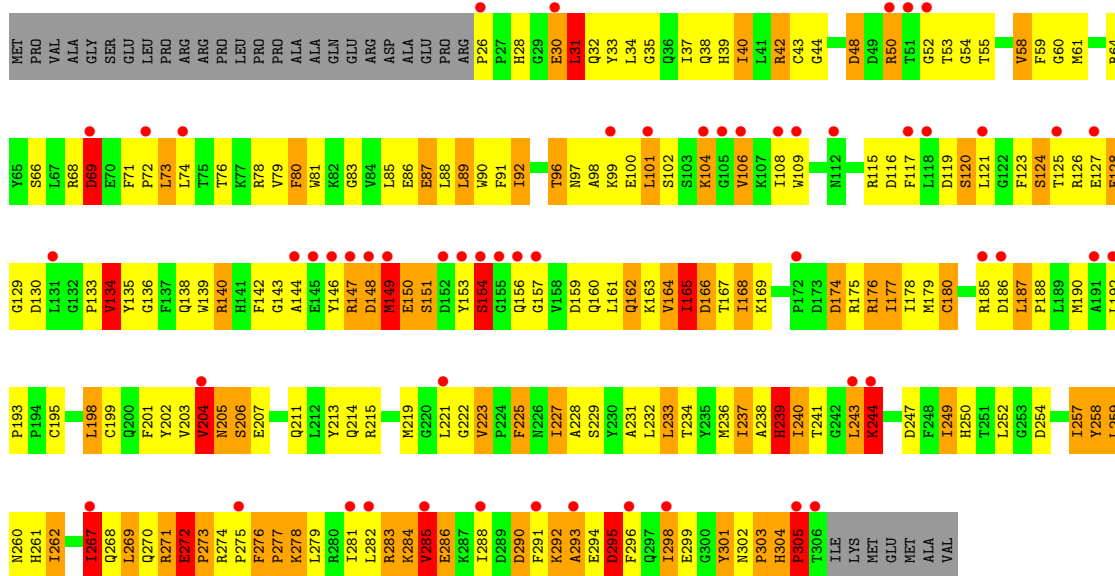
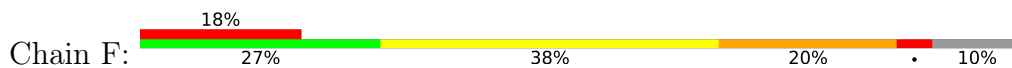


• Molecule 1: Thymidylate synthase





● Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.79Å 123.79Å 284.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.21 – 2.67 107.21 – 2.67	Depositor EDS
% Data completeness (in resolution range)	97.2 (107.21-2.67) 95.2 (107.21-2.67)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.65Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.279 (Not available) , 0.204	Depositor DCC
R_{free} test set	7351 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13834	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BME

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	2.49	138/2339 (5.9%)	2.06	84/3165 (2.7%)
1	B	2.46	119/2328 (5.1%)	2.11	83/3150 (2.6%)
1	C	2.29	86/2328 (3.7%)	2.09	92/3150 (2.9%)
1	D	2.08	73/2328 (3.1%)	1.96	82/3150 (2.6%)
1	E	1.75	32/2328 (1.4%)	1.73	44/3150 (1.4%)
1	F	1.55	17/2328 (0.7%)	1.61	48/3150 (1.5%)
All	All	2.13	465/13979 (3.3%)	1.94	433/18915 (2.3%)

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	1
1	D	0	2
All	All	0	3

All (465) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	84	VAL	CA-CB	-12.96	1.36	1.54
1	F	267	ILE	CA-CB	12.60	1.73	1.54
1	C	302	ASN	N-CA	-12.18	1.35	1.46
1	B	240	ILE	CA-CB	-12.08	1.37	1.54
1	B	178	ILE	N-CA	-10.45	1.34	1.46
1	A	248	PHE	CA-C	10.08	1.64	1.52
1	A	298	ILE	CA-CB	10.00	1.65	1.53
1	B	98	ALA	CA-CB	-9.80	1.37	1.53
1	A	65	TYR	N-CA	9.78	1.57	1.46
1	B	195	CYS	N-CA	-9.70	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	LEU	N-CA	9.66	1.53	1.45
1	A	280	ARG	CA-C	-9.52	1.41	1.52
1	C	92	ILE	CA-CB	-9.29	1.42	1.54
1	C	192	LEU	N-CA	9.29	1.55	1.46
1	A	40	ILE	CA-CB	-9.04	1.41	1.54
1	C	137	PHE	CA-C	9.01	1.64	1.52
1	A	298	ILE	CA-C	-8.86	1.41	1.52
1	A	84	VAL	CA-C	-8.79	1.42	1.52
1	B	165	ILE	N-CA	-8.72	1.35	1.46
1	B	181	ALA	C-O	-8.71	1.11	1.24
1	B	301	TYR	C-O	-8.68	1.13	1.24
1	A	39	HIS	CA-CB	-8.50	1.40	1.53
1	D	197	ALA	CA-CB	-8.40	1.40	1.53
1	C	215	ARG	N-CA	-8.36	1.35	1.46
1	C	223	VAL	CA-CB	-8.36	1.43	1.54
1	C	42	ARG	CG-CD	8.35	1.77	1.52
1	C	167	THR	CA-CB	-8.34	1.40	1.53
1	B	92	ILE	CA-CB	-8.27	1.44	1.54
1	F	227	ILE	CA-CB	-8.24	1.45	1.54
1	B	153	TYR	N-CA	8.17	1.55	1.46
1	D	180	CYS	N-CA	-8.16	1.35	1.45
1	C	264	PRO	CA-C	8.08	1.66	1.52
1	B	203	VAL	C-O	-8.07	1.15	1.24
1	A	245	PRO	C-O	-8.03	1.14	1.23
1	A	227	ILE	CA-CB	-8.01	1.44	1.54
1	A	223	VAL	C-O	-7.98	1.17	1.24
1	D	250	HIS	N-CA	-7.97	1.36	1.46
1	B	150	GLU	CG-CD	7.95	1.72	1.52
1	A	180	CYS	C-O	-7.87	1.14	1.24
1	A	229	SER	CA-C	-7.87	1.41	1.52
1	C	190	MET	CA-C	-7.85	1.43	1.52
1	D	151	SER	CA-C	-7.84	1.42	1.53
1	B	287	LYS	N-CA	-7.84	1.36	1.46
1	B	199	CYS	CA-C	-7.82	1.43	1.52
1	B	86	GLU	N-CA	-7.81	1.36	1.46
1	B	40	ILE	N-CA	-7.78	1.36	1.46
1	A	39	HIS	C-O	-7.74	1.15	1.24
1	E	133	PRO	N-CA	7.72	1.53	1.47
1	A	48	ASP	CA-C	-7.66	1.42	1.52
1	F	285	VAL	N-CA	7.55	1.54	1.46
1	A	80	PHE	C-O	7.53	1.33	1.24
1	B	64	ARG	CZ-NH2	7.52	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	ILE	CG1-CD1	7.52	1.81	1.51
1	A	79	VAL	N-CA	-7.48	1.36	1.46
1	A	249	ILE	CA-CB	-7.46	1.45	1.54
1	C	34	LEU	CA-C	-7.44	1.42	1.52
1	C	37	ILE	N-CA	7.43	1.55	1.46
1	F	204	VAL	CA-CB	7.34	1.64	1.54
1	E	102	SER	N-CA	7.33	1.55	1.46
1	A	178	ILE	C-O	-7.32	1.15	1.23
1	A	305	PRO	CA-C	-7.27	1.43	1.52
1	C	42	ARG	CD-NE	7.25	1.56	1.46
1	B	223	VAL	CA-CB	-7.25	1.44	1.54
1	A	106	VAL	CA-CB	-7.22	1.45	1.54
1	A	178	ILE	N-CA	-7.21	1.38	1.46
1	B	165	ILE	CA-CB	-7.21	1.45	1.54
1	B	238	ALA	CA-CB	-7.21	1.41	1.53
1	B	164	VAL	N-CA	-7.20	1.38	1.46
1	A	43	CYS	C-O	-7.18	1.15	1.23
1	A	197	ALA	CA-CB	-7.16	1.41	1.53
1	E	210	CYS	CA-C	-7.15	1.43	1.52
1	E	133	PRO	CA-C	7.13	1.61	1.53
1	A	174	ASP	CA-C	7.13	1.61	1.52
1	C	198	LEU	CA-CB	-7.13	1.42	1.53
1	B	87	GLU	CA-C	7.12	1.62	1.52
1	D	147	ARG	CA-C	7.10	1.57	1.52
1	D	218	ASP	C-O	7.10	1.32	1.23
1	D	283	ARG	CA-C	-7.10	1.45	1.53
1	C	141	HIS	C-O	7.06	1.30	1.24
1	D	212	LEU	N-CA	-7.04	1.37	1.46
1	E	63	ALA	CA-CB	-7.01	1.41	1.53
1	A	65	TYR	CA-C	-7.00	1.44	1.52
1	C	51	THR	N-CA	6.97	1.54	1.46
1	A	158	VAL	C-O	6.94	1.33	1.24
1	D	92	ILE	CA-CB	-6.94	1.43	1.54
1	C	195	CYS	N-CA	-6.93	1.37	1.46
1	C	206	SER	CA-C	6.88	1.62	1.53
1	D	208	LEU	N-CA	-6.88	1.37	1.46
1	A	32	GLN	CA-CB	-6.87	1.42	1.53
1	A	144	ALA	CA-C	-6.86	1.43	1.52
1	D	88	LEU	N-CA	-6.85	1.38	1.46
1	A	262	ILE	C-O	6.80	1.31	1.24
1	E	107	LYS	CA-C	6.79	1.59	1.53
1	E	204	VAL	CA-CB	6.79	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	GLY	C-O	-6.78	1.14	1.23
1	B	193	PRO	C-O	-6.77	1.19	1.24
1	A	83	GLY	N-CA	6.75	1.54	1.45
1	C	214	GLN	N-CA	-6.74	1.38	1.46
1	A	255	ALA	CA-CB	-6.73	1.44	1.53
1	A	90	TRP	CA-CB	-6.73	1.42	1.53
1	B	40	ILE	CG1-CD1	-6.72	1.25	1.51
1	D	90	TRP	C-O	-6.72	1.16	1.24
1	D	106	VAL	CA-CB	-6.71	1.46	1.54
1	D	59	PHE	C-O	-6.71	1.16	1.24
1	A	161	LEU	C-O	6.70	1.31	1.24
1	B	26	PRO	N-CA	6.70	1.57	1.47
1	D	192	LEU	N-CA	6.70	1.53	1.45
1	A	246	GLY	C-O	6.66	1.32	1.23
1	B	41	LEU	N-CA	6.66	1.54	1.46
1	D	127	GLU	CA-C	6.66	1.61	1.52
1	A	303	PRO	C-O	-6.65	1.15	1.23
1	B	95	SER	C-O	-6.62	1.15	1.23
1	B	150	GLU	CB-CG	6.62	1.72	1.52
1	C	106	VAL	CA-C	-6.61	1.44	1.52
1	B	182	TRP	C-O	6.59	1.31	1.24
1	A	28	HIS	C-O	6.59	1.32	1.23
1	C	87	GLU	C-O	6.59	1.31	1.24
1	C	98	ALA	CA-CB	-6.58	1.41	1.53
1	E	212	LEU	N-CA	-6.58	1.37	1.46
1	B	228	ALA	CA-CB	-6.55	1.43	1.53
1	C	96	THR	N-CA	-6.55	1.38	1.46
1	C	210	CYS	CA-C	-6.55	1.44	1.52
1	A	195	CYS	CA-C	-6.53	1.44	1.52
1	B	64	ARG	CB-CG	6.52	1.72	1.52
1	E	168	ILE	CA-CB	-6.51	1.46	1.54
1	C	267	ILE	CA-CB	6.50	1.61	1.54
1	C	38	GLN	CA-C	-6.49	1.44	1.52
1	C	247	ASP	C-O	6.48	1.32	1.23
1	D	98	ALA	N-CA	6.47	1.53	1.46
1	E	65	TYR	C-O	6.47	1.31	1.24
1	A	297	GLN	CG-CD	6.46	1.68	1.52
1	A	211	GLN	CA-C	-6.46	1.44	1.52
1	B	203	VAL	CA-C	-6.45	1.44	1.52
1	A	142	PHE	C-O	-6.45	1.15	1.23
1	A	229	SER	CA-CB	-6.43	1.43	1.53
1	C	176	ARG	N-CA	-6.42	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	GLN	CG-CD	6.41	1.68	1.52
1	D	214	GLN	C-O	-6.40	1.16	1.24
1	A	179	MET	N-CA	-6.37	1.38	1.46
1	A	194	PRO	CA-C	6.37	1.60	1.52
1	C	256	HIS	CA-C	-6.36	1.44	1.52
1	D	253	GLY	C-O	-6.36	1.15	1.23
1	C	250	HIS	CA-C	-6.35	1.45	1.52
1	C	237	ILE	N-CA	-6.34	1.38	1.46
1	A	26	PRO	CA-C	6.34	1.58	1.52
1	E	279	LEU	N-CA	-6.32	1.38	1.46
1	A	151	SER	CA-C	-6.32	1.44	1.53
1	D	176	ARG	CA-CB	6.32	1.61	1.53
1	A	209	SER	C-O	6.32	1.31	1.23
1	C	139	TRP	CA-C	-6.31	1.44	1.52
1	E	267	ILE	CA-CB	6.30	1.61	1.54
1	A	197	ALA	N-CA	-6.29	1.38	1.46
1	B	294	GLU	CD-OE1	6.28	1.37	1.25
1	D	304	HIS	CA-C	-6.27	1.45	1.53
1	A	40	ILE	N-CA	-6.27	1.38	1.46
1	B	173	ASP	CB-CG	6.27	1.67	1.52
1	E	227	ILE	CA-CB	-6.23	1.47	1.54
1	C	251	THR	CA-C	-6.23	1.45	1.52
1	D	231	ALA	CA-C	6.22	1.60	1.52
1	D	256	HIS	CA-C	6.21	1.60	1.52
1	B	253	GLY	CA-C	6.21	1.60	1.51
1	B	250	HIS	N-CA	-6.20	1.38	1.46
1	B	83	GLY	CA-C	6.19	1.58	1.52
1	B	187	LEU	C-O	-6.18	1.18	1.24
1	C	206	SER	C-O	6.18	1.31	1.23
1	A	193	PRO	C-O	-6.18	1.17	1.24
1	C	84	VAL	N-CA	-6.18	1.38	1.46
1	B	147	ARG	CZ-NH2	6.17	1.41	1.33
1	D	196	HIS	CA-CB	-6.16	1.44	1.52
1	A	254	ASP	CA-C	6.15	1.60	1.52
1	A	92	ILE	CA-CB	-6.14	1.47	1.54
1	A	104	LYS	CE-NZ	6.14	1.67	1.49
1	B	168	ILE	CA-CB	-6.13	1.45	1.54
1	B	294	GLU	CG-CD	6.13	1.67	1.52
1	B	43	CYS	CA-CB	-6.13	1.45	1.54
1	D	190	MET	CA-C	-6.13	1.45	1.52
1	C	87	GLU	CA-C	6.12	1.60	1.52
1	D	85	LEU	C-O	6.12	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	214	GLN	CA-C	-6.11	1.45	1.52
1	B	255	ALA	CA-CB	6.10	1.61	1.53
1	B	88	LEU	N-CA	-6.10	1.39	1.46
1	C	29	GLY	N-CA	6.09	1.53	1.45
1	A	25	ARG	C-N	6.08	1.40	1.33
1	D	79	VAL	CA-CB	6.08	1.62	1.54
1	D	138	GLN	N-CA	6.08	1.54	1.46
1	B	58	VAL	CA-C	6.08	1.59	1.52
1	C	96	THR	CA-CB	-6.07	1.44	1.53
1	D	154	SER	CA-C	6.07	1.60	1.52
1	E	238	ALA	CA-C	6.07	1.60	1.52
1	A	172	PRO	CA-C	6.06	1.61	1.52
1	F	305	PRO	CA-C	6.06	1.61	1.52
1	B	288	ILE	CA-CB	6.05	1.62	1.54
1	C	46	ARG	N-CA	6.05	1.53	1.46
1	B	219	MET	C-O	6.04	1.31	1.24
1	B	41	LEU	C-O	-6.03	1.16	1.24
1	E	225	PHE	C-O	6.03	1.31	1.24
1	B	226	ASN	N-CA	-6.03	1.38	1.46
1	C	183	ASN	CA-C	-6.02	1.45	1.52
1	A	60	GLY	C-O	-6.02	1.15	1.23
1	B	190	MET	C-O	6.02	1.31	1.24
1	C	161	LEU	N-CA	6.02	1.53	1.46
1	F	223	VAL	CA-CB	6.01	1.57	1.54
1	C	241	THR	C-O	-6.00	1.17	1.24
1	D	83	GLY	CA-C	6.00	1.58	1.51
1	A	32	GLN	CG-CD	-6.00	1.37	1.52
1	B	26	PRO	CB-CG	6.00	1.79	1.49
1	D	302	ASN	C-O	-5.99	1.17	1.24
1	A	298	ILE	C-O	-5.98	1.17	1.24
1	A	174	ASP	C-O	5.97	1.31	1.23
1	B	43	CYS	C-O	-5.95	1.16	1.24
1	A	75	THR	CA-C	-5.95	1.45	1.52
1	C	255	ALA	C-O	5.95	1.31	1.24
1	D	149	MET	C-O	-5.95	1.16	1.24
1	A	244	LYS	CA-C	5.93	1.60	1.52
1	D	297	GLN	CA-CB	5.93	1.61	1.53
1	B	87	GLU	C-O	5.93	1.30	1.24
1	A	231	ALA	C-O	5.92	1.31	1.24
1	D	108	ILE	CA-CB	5.90	1.63	1.54
1	C	55	THR	CA-CB	5.89	1.66	1.54
1	D	147	ARG	CZ-NH1	5.89	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	THR	CA-C	-5.88	1.44	1.52
1	B	75	THR	CA-CB	-5.88	1.44	1.53
1	B	203	VAL	C-N	-5.88	1.26	1.33
1	B	290	ASP	CB-CG	5.88	1.66	1.52
1	B	56	LEU	C-O	5.88	1.30	1.23
1	B	133	PRO	CA-C	5.88	1.58	1.52
1	B	142	PHE	CA-C	-5.86	1.45	1.52
1	D	176	ARG	N-CA	5.86	1.52	1.46
1	C	159	ASP	C-O	5.86	1.31	1.23
1	D	185	ARG	C-O	-5.86	1.17	1.24
1	F	231	ALA	N-CA	5.86	1.53	1.46
1	D	59	PHE	N-CA	-5.85	1.38	1.46
1	C	78	ARG	CG-CD	5.85	1.70	1.52
1	A	212	LEU	C-O	5.85	1.31	1.24
1	D	40	ILE	CA-CB	5.85	1.60	1.54
1	F	202	TYR	N-CA	-5.85	1.39	1.46
1	D	150	GLU	CA-CB	-5.83	1.45	1.54
1	D	33	TYR	C-O	-5.82	1.17	1.24
1	B	178	ILE	CG1-CD1	-5.80	1.29	1.51
1	C	178	ILE	N-CA	-5.80	1.39	1.46
1	A	219	MET	N-CA	-5.80	1.38	1.46
1	A	236	MET	N-CA	-5.80	1.39	1.46
1	A	257	ILE	N-CA	-5.80	1.39	1.46
1	B	53	THR	CA-C	5.80	1.59	1.52
1	E	224	PRO	C-O	5.80	1.31	1.24
1	A	70	GLU	CA-C	-5.79	1.45	1.52
1	A	171	ASN	CA-C	-5.79	1.45	1.52
1	A	163	LYS	CD-CE	5.79	1.69	1.52
1	E	102	SER	CA-C	5.79	1.60	1.52
1	A	95	SER	C-O	-5.78	1.16	1.23
1	A	125	THR	CA-CB	5.78	1.63	1.53
1	B	227	ILE	CA-C	5.78	1.60	1.52
1	B	170	THR	CA-CB	-5.77	1.44	1.53
1	D	210	CYS	N-CA	-5.77	1.39	1.46
1	A	127	GLU	CG-CD	5.77	1.66	1.52
1	F	258	TYR	N-CA	5.76	1.53	1.46
1	C	174	ASP	CA-C	5.76	1.60	1.52
1	C	276	PHE	C-O	-5.74	1.16	1.23
1	C	281	ILE	CG1-CD1	5.74	1.74	1.51
1	D	90	TRP	N-CA	-5.72	1.39	1.46
1	D	228	ALA	CA-CB	-5.70	1.44	1.53
1	C	42	ARG	NE-CZ	5.70	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	THR	CA-C	5.70	1.60	1.52
1	B	60	GLY	C-O	-5.70	1.16	1.23
1	D	203	VAL	CA-CB	-5.69	1.47	1.54
1	B	192	LEU	CG-CD2	5.69	1.71	1.52
1	E	298	ILE	N-CA	-5.69	1.39	1.46
1	C	160	GLN	CA-C	-5.68	1.45	1.52
1	A	79	VAL	C-O	5.68	1.31	1.24
1	D	251	THR	CA-C	-5.68	1.46	1.52
1	B	79	VAL	C-O	-5.67	1.17	1.24
1	A	84	VAL	CA-CB	5.67	1.60	1.54
1	C	178	ILE	CA-CB	-5.67	1.47	1.54
1	B	190	MET	CA-C	-5.66	1.45	1.52
1	C	179	MET	N-CA	5.66	1.52	1.46
1	B	109	TRP	CA-C	5.66	1.60	1.52
1	C	199	CYS	CB-SG	-5.66	1.62	1.81
1	A	58	VAL	CA-CB	-5.65	1.49	1.55
1	A	277	PRO	N-CA	-5.65	1.40	1.47
1	B	45	VAL	CA-C	-5.64	1.45	1.52
1	A	280	ARG	C-O	5.64	1.30	1.24
1	B	303	PRO	N-CA	-5.64	1.40	1.46
1	A	31	LEU	CA-C	5.63	1.60	1.52
1	C	198	LEU	N-CA	-5.63	1.39	1.46
1	B	204	VAL	CA-C	5.62	1.59	1.52
1	A	288	ILE	CA-C	5.62	1.59	1.52
1	B	209	SER	CA-C	-5.62	1.46	1.52
1	F	60	GLY	C-O	-5.62	1.16	1.23
1	C	258	TYR	CA-CB	-5.62	1.44	1.53
1	A	109	TRP	C-O	-5.62	1.16	1.24
1	A	58	VAL	N-CA	-5.61	1.39	1.46
1	A	137	PHE	CE1-CZ	5.61	1.55	1.38
1	D	155	GLY	CA-C	5.60	1.59	1.51
1	A	37	ILE	CA-CB	-5.60	1.46	1.54
1	A	61	MET	N-CA	5.59	1.53	1.45
1	A	257	ILE	C-O	-5.58	1.18	1.24
1	B	37	ILE	CA-CB	-5.58	1.47	1.54
1	A	137	PHE	CA-C	-5.58	1.45	1.52
1	E	297	GLN	CA-C	-5.58	1.45	1.52
1	D	275	PRO	C-O	-5.57	1.16	1.24
1	E	64	ARG	CA-C	5.57	1.59	1.52
1	B	295	ASP	C-O	-5.57	1.15	1.24
1	D	224	PRO	C-O	5.57	1.30	1.24
1	D	61	MET	N-CA	5.56	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	TRP	C-O	5.55	1.31	1.24
1	E	193	PRO	CA-C	5.54	1.57	1.52
1	A	164	VAL	C-O	-5.54	1.18	1.24
1	C	213	TYR	CA-C	5.53	1.59	1.52
1	B	84	VAL	N-CA	-5.53	1.39	1.46
1	A	272	GLU	CG-CD	5.53	1.65	1.52
1	C	167	THR	CA-C	-5.52	1.45	1.52
1	A	227	ILE	C-O	5.52	1.30	1.24
1	B	57	SER	C-O	-5.52	1.17	1.23
1	E	139	TRP	N-CA	5.52	1.53	1.46
1	B	291	PHE	CA-C	-5.52	1.45	1.52
1	A	177	ILE	N-CA	-5.52	1.39	1.46
1	B	214	GLN	CA-C	5.52	1.59	1.52
1	E	31	LEU	CA-C	5.51	1.60	1.52
1	C	59	PHE	N-CA	-5.51	1.39	1.46
1	D	133	PRO	CA-C	5.51	1.57	1.52
1	E	303	PRO	C-O	-5.51	1.19	1.24
1	D	199	CYS	CA-C	-5.51	1.45	1.52
1	A	225	PHE	N-CA	5.51	1.53	1.46
1	C	159	ASP	N-CA	-5.51	1.39	1.46
1	F	285	VAL	CA-C	5.51	1.59	1.52
1	A	211	GLN	C-O	5.49	1.30	1.24
1	B	227	ILE	CA-CB	-5.48	1.47	1.54
1	C	192	LEU	CA-C	5.48	1.59	1.52
1	B	305	PRO	N-CA	5.47	1.53	1.46
1	E	97	ASN	CA-C	-5.46	1.46	1.53
1	E	182	TRP	CA-CB	-5.46	1.46	1.53
1	B	116	ASP	CA-C	-5.45	1.45	1.52
1	B	173	ASP	CA-C	-5.45	1.45	1.52
1	A	192	LEU	C-O	5.45	1.30	1.24
1	A	226	ASN	CG-OD1	5.44	1.33	1.23
1	D	231	ALA	C-O	5.43	1.30	1.24
1	A	179	MET	C-O	-5.43	1.17	1.23
1	A	215	ARG	C-N	-5.43	1.26	1.33
1	D	251	THR	C-O	-5.42	1.17	1.24
1	B	147	ARG	CZ-NH1	5.42	1.40	1.32
1	B	141	HIS	N-CA	-5.41	1.39	1.46
1	B	87	GLU	N-CA	-5.41	1.39	1.46
1	C	71	PHE	CA-CB	-5.41	1.44	1.53
1	F	154	SER	CA-C	5.40	1.60	1.52
1	A	281	ILE	CG1-CD1	5.40	1.72	1.51
1	B	159	ASP	C-O	5.40	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	PRO	CA-C	5.39	1.64	1.52
1	A	46	ARG	N-CA	-5.39	1.39	1.46
1	C	210	CYS	C-O	5.39	1.30	1.23
1	B	96	THR	CA-CB	-5.38	1.45	1.53
1	E	189	LEU	CA-C	5.38	1.59	1.52
1	B	150	GLU	CD-OE1	5.37	1.35	1.25
1	B	185	ARG	CG-CD	5.37	1.68	1.52
1	A	69	ASP	CA-C	-5.37	1.44	1.52
1	E	192	LEU	CG-CD2	5.37	1.70	1.52
1	F	238	ALA	N-CA	-5.37	1.39	1.46
1	C	241	THR	CA-CB	5.36	1.67	1.54
1	F	48	ASP	CA-C	5.35	1.59	1.52
1	A	146	TYR	N-CA	-5.34	1.39	1.46
1	C	243	LEU	C-O	-5.34	1.17	1.23
1	A	137	PHE	C-O	-5.34	1.17	1.24
1	C	257	ILE	CA-CB	-5.34	1.45	1.55
1	D	141	HIS	C-O	-5.34	1.19	1.24
1	C	225	PHE	CA-C	5.33	1.59	1.52
1	A	290	ASP	C-O	-5.33	1.16	1.24
1	A	74	LEU	C-O	5.33	1.30	1.23
1	B	65	TYR	C-O	-5.33	1.18	1.24
1	B	134	VAL	CA-C	5.32	1.59	1.52
1	C	49	ASP	C-O	-5.32	1.16	1.24
1	C	208	LEU	N-CA	5.31	1.52	1.46
1	A	257	ILE	CA-CB	-5.30	1.47	1.54
1	D	178	ILE	N-CA	-5.30	1.40	1.46
1	F	160	GLN	CA-C	-5.30	1.45	1.52
1	D	229	SER	CA-CB	-5.30	1.45	1.53
1	D	32	GLN	N-CA	5.29	1.52	1.46
1	A	87	GLU	C-O	5.29	1.30	1.24
1	D	178	ILE	C-O	-5.29	1.18	1.24
1	D	81	TRP	CA-CB	-5.28	1.44	1.53
1	A	292	LYS	CG-CD	5.28	1.68	1.52
1	A	79	VAL	CA-C	5.27	1.59	1.52
1	C	185	ARG	N-CA	5.27	1.52	1.46
1	D	257	ILE	C-O	-5.27	1.18	1.24
1	D	211	GLN	CA-C	-5.26	1.46	1.52
1	C	277	PRO	C-O	-5.26	1.17	1.24
1	C	154	SER	CA-C	-5.26	1.45	1.52
1	B	153	TYR	CA-C	-5.25	1.46	1.52
1	B	186	ASP	CA-C	-5.25	1.45	1.52
1	C	91	PHE	N-CA	5.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	GLY	C-O	-5.25	1.16	1.23
1	A	32	GLN	CA-C	-5.25	1.46	1.52
1	B	277	PRO	CA-CB	-5.25	1.46	1.53
1	A	146	TYR	C-O	5.24	1.30	1.24
1	B	125	THR	N-CA	-5.24	1.39	1.46
1	D	200	GLN	CD-OE1	5.24	1.33	1.23
1	B	180	CYS	N-CA	-5.24	1.39	1.46
1	C	78	ARG	CA-C	5.24	1.60	1.53
1	C	201	PHE	CA-CB	-5.23	1.45	1.53
1	D	218	ASP	CA-C	5.23	1.59	1.52
1	A	188	PRO	C-O	-5.23	1.17	1.24
1	A	287	LYS	CD-CE	5.22	1.68	1.52
1	D	151	SER	N-CA	-5.22	1.39	1.45
1	D	81	TRP	N-CA	-5.22	1.39	1.46
1	B	274	ARG	CZ-NH2	-5.22	1.26	1.33
1	C	200	GLN	C-O	5.21	1.30	1.23
1	B	183	ASN	N-CA	-5.21	1.41	1.46
1	B	151	SER	CA-C	-5.20	1.46	1.53
1	A	160	GLN	C-O	-5.20	1.17	1.24
1	A	214	GLN	N-CA	-5.20	1.39	1.46
1	B	84	VAL	CB-CG2	5.20	1.69	1.52
1	E	228	ALA	CA-CB	-5.19	1.45	1.53
1	A	45	VAL	N-CA	-5.18	1.40	1.46
1	A	50	ARG	N-CA	5.18	1.52	1.46
1	A	205	ASN	CA-C	-5.18	1.45	1.52
1	B	204	VAL	N-CA	-5.18	1.40	1.46
1	D	43	CYS	CA-C	5.18	1.59	1.52
1	A	147	ARG	CZ-NH1	5.17	1.40	1.32
1	B	173	ASP	CG-OD1	5.17	1.35	1.25
1	B	217	GLY	C-O	5.17	1.30	1.23
1	A	36	GLN	N-CA	-5.15	1.40	1.46
1	A	82	LYS	N-CA	-5.14	1.40	1.46
1	F	61	MET	SD-CE	5.13	1.92	1.79
1	C	106	VAL	CA-CB	5.12	1.60	1.54
1	B	228	ALA	CA-C	5.12	1.59	1.52
1	B	267	ILE	N-CA	5.12	1.52	1.46
1	A	207	GLU	N-CA	-5.12	1.39	1.45
1	A	78	ARG	C-O	5.12	1.30	1.23
1	B	220	GLY	C-O	-5.10	1.17	1.23
1	D	163	LYS	CG-CD	5.10	1.67	1.52
1	B	195	CYS	CB-SG	-5.10	1.64	1.81
1	A	43	CYS	CA-CB	-5.09	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	THR	N-CA	-5.09	1.40	1.46
1	C	250	HIS	C-O	-5.09	1.18	1.24
1	B	233	LEU	C-O	-5.08	1.18	1.24
1	C	89	LEU	N-CA	5.07	1.52	1.46
1	D	131	LEU	N-CA	-5.07	1.39	1.46
1	B	68	ARG	CD-NE	5.07	1.53	1.46
1	B	276	PHE	C-O	-5.07	1.17	1.23
1	A	210	CYS	N-CA	-5.06	1.39	1.46
1	D	164	VAL	CA-C	5.06	1.59	1.52
1	A	87	GLU	CA-C	5.05	1.59	1.52
1	C	201	PHE	CD1-CE1	-5.05	1.23	1.38
1	A	221	LEU	CB-CG	5.05	1.63	1.53
1	A	223	VAL	CA-C	5.05	1.58	1.52
1	E	214	GLN	CA-CB	-5.05	1.45	1.53
1	A	225	PHE	C-O	5.05	1.30	1.24
1	B	36	GLN	N-CA	-5.05	1.39	1.46
1	B	150	GLU	CA-CB	5.05	1.61	1.53
1	A	209	SER	CA-CB	-5.04	1.44	1.53
1	E	177	ILE	CA-C	-5.04	1.46	1.52
1	A	180	CYS	N-CA	-5.04	1.40	1.46
1	E	170	THR	CA-C	5.04	1.59	1.52
1	B	243	LEU	CA-C	-5.04	1.46	1.53
1	A	128	GLU	CA-C	5.04	1.58	1.52
1	A	252	LEU	CA-C	5.04	1.58	1.52
1	B	200	GLN	CA-C	-5.04	1.46	1.52
1	B	95	SER	N-CA	5.03	1.52	1.46
1	F	225	PHE	CA-C	5.02	1.59	1.52
1	C	188	PRO	CA-C	5.02	1.59	1.52
1	A	147	ARG	CA-C	-5.01	1.49	1.52
1	B	59	PHE	CB-CG	-5.01	1.39	1.50
1	B	194	PRO	C-O	5.01	1.29	1.23
1	A	243	LEU	CA-C	-5.00	1.46	1.52
1	A	177	ILE	C-O	5.00	1.30	1.24
1	A	38	GLN	N-CA	5.00	1.52	1.46
1	D	71	PHE	N-CA	-5.00	1.39	1.46

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	276	PHE	CA-C-N	13.14	136.27	119.84
1	D	276	PHE	C-N-CA	13.14	136.27	119.84
1	C	263	GLU	CA-C-N	-12.31	107.00	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	GLU	C-N-CA	-12.31	107.00	119.56
1	C	187	LEU	CA-C-N	-12.09	104.73	119.84
1	C	187	LEU	C-N-CA	-12.09	104.73	119.84
1	B	227	ILE	N-CA-C	-11.47	99.14	110.72
1	A	25	ARG	CA-C-N	-11.10	108.95	120.38
1	A	25	ARG	C-N-CA	-11.10	108.95	120.38
1	D	222	GLY	N-CA-C	10.86	125.09	112.50
1	F	304	HIS	CA-C-N	10.83	133.38	119.84
1	F	304	HIS	C-N-CA	10.83	133.38	119.84
1	E	37	ILE	CB-CA-C	-10.62	98.13	112.04
1	D	240	ILE	CB-CA-C	-10.51	96.70	112.05
1	B	241	THR	N-CA-C	-10.34	100.14	113.17
1	B	150	GLU	N-CA-C	-9.89	100.05	113.30
1	C	304	HIS	CA-C-N	-9.55	107.90	119.84
1	C	304	HIS	C-N-CA	-9.55	107.90	119.84
1	E	198	LEU	N-CA-C	9.44	123.42	109.07
1	A	195	CYS	N-CA-C	-9.42	101.34	113.12
1	D	44	GLY	N-CA-C	-9.40	96.91	110.91
1	A	304	HIS	CA-C-N	-9.38	110.74	120.03
1	A	304	HIS	C-N-CA	-9.38	110.74	120.03
1	B	240	ILE	CB-CG1-CD1	-9.34	94.19	113.80
1	A	76	THR	N-CA-C	-9.23	101.71	113.16
1	F	276	PHE	CA-C-N	9.21	131.35	119.84
1	F	276	PHE	C-N-CA	9.21	131.35	119.84
1	D	26	PRO	CA-C-N	-9.15	111.19	120.98
1	D	26	PRO	C-N-CA	-9.15	111.19	120.98
1	C	272	GLU	CA-C-N	-9.08	110.18	119.99
1	C	272	GLU	C-N-CA	-9.08	110.18	119.99
1	E	244	LYS	CA-C-N	9.07	131.18	119.84
1	E	244	LYS	C-N-CA	9.07	131.18	119.84
1	C	193	PRO	CA-C-N	-8.88	111.69	120.21
1	C	193	PRO	C-N-CA	-8.88	111.69	120.21
1	C	293	ALA	N-CA-C	8.51	121.62	111.33
1	D	97	ASN	CB-CA-C	-8.32	97.46	110.78
1	B	26	PRO	CA-C-N	-8.24	111.10	119.92
1	B	26	PRO	C-N-CA	-8.24	111.10	119.92
1	E	272	GLU	CA-C-N	8.21	130.11	119.84
1	E	272	GLU	C-N-CA	8.21	130.11	119.84
1	D	72	PRO	CA-C-N	-8.04	111.90	123.00
1	D	72	PRO	C-N-CA	-8.04	111.90	123.00
1	F	193	PRO	CA-C-N	-8.02	111.64	120.14
1	F	193	PRO	C-N-CA	-8.02	111.64	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	ASN	CA-C-N	-8.00	112.21	120.85
1	C	302	ASN	C-N-CA	-8.00	112.21	120.85
1	D	300	GLY	CA-C-N	-8.00	110.08	121.99
1	D	300	GLY	C-N-CA	-8.00	110.08	121.99
1	F	40	ILE	N-CA-C	-7.89	101.63	110.62
1	D	38	GLN	N-CA-C	-7.71	102.56	110.97
1	C	78	ARG	N-CA-C	-7.71	100.36	110.53
1	B	149	MET	N-CA-C	7.69	121.76	112.38
1	C	181	ALA	N-CA-C	-7.66	103.47	114.12
1	C	32	GLN	N-CA-C	-7.64	102.08	111.40
1	D	141	HIS	N-CA-C	-7.59	101.45	110.41
1	D	215	ARG	N-CA-C	7.56	122.27	112.89
1	B	193	PRO	N-CA-C	-7.50	102.55	110.58
1	C	42	ARG	N-CA-C	-7.50	103.93	113.23
1	A	278	LYS	CB-CG-CD	-7.42	94.23	111.30
1	A	176	ARG	CB-CA-C	-7.42	99.56	111.28
1	D	128	GLU	N-CA-CB	7.42	121.48	109.69
1	B	227	ILE	CB-CA-C	-7.39	102.02	112.22
1	D	94	GLY	N-CA-C	-7.34	104.92	115.27
1	C	65	TYR	N-CA-C	7.34	120.69	108.73
1	D	171	ASN	CA-C-N	7.31	126.94	119.56
1	D	171	ASN	C-N-CA	7.31	126.94	119.56
1	B	195	CYS	CB-CA-C	7.28	121.58	109.56
1	D	75	THR	CA-C-N	-7.26	111.23	122.49
1	D	75	THR	C-N-CA	-7.26	111.23	122.49
1	A	257	ILE	CB-CA-C	-7.26	99.80	110.62
1	D	195	CYS	N-CA-C	7.26	118.98	111.14
1	E	189	LEU	N-CA-C	7.25	126.24	110.80
1	A	171	ASN	CA-C-N	-7.22	110.81	119.84
1	A	171	ASN	C-N-CA	-7.22	110.81	119.84
1	F	285	VAL	N-CA-C	7.20	120.48	108.81
1	E	87	GLU	N-CA-C	7.19	119.74	111.11
1	B	53	THR	CA-C-N	-7.18	110.96	121.30
1	B	53	THR	C-N-CA	-7.18	110.96	121.30
1	D	213	TYR	CA-C-N	-7.18	112.81	122.72
1	D	213	TYR	C-N-CA	-7.18	112.81	122.72
1	A	229	SER	CA-CB-OG	-7.17	96.76	111.10
1	C	29	GLY	N-CA-C	7.13	121.27	112.64
1	D	173	ASP	N-CA-C	7.05	119.99	111.82
1	E	102	SER	N-CA-C	7.03	125.78	110.80
1	E	160	GLN	N-CA-C	-7.02	103.39	112.23
1	B	153	TYR	N-CA-C	-7.01	102.76	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLY	N-CA-C	6.98	124.65	115.36
1	A	299	GLU	N-CA-C	6.98	120.31	109.07
1	D	260	ASN	N-CA-C	6.96	119.71	111.71
1	D	302	ASN	N-CA-C	6.94	122.38	110.02
1	B	299	GLU	N-CA-C	6.94	120.24	109.07
1	E	34	LEU	CA-CB-CG	6.92	140.51	116.30
1	B	43	CYS	CB-CA-C	-6.89	97.97	109.27
1	A	109	TRP	N-CA-C	6.89	121.68	113.28
1	C	183	ASN	CA-C-N	6.84	126.80	119.28
1	C	183	ASN	C-N-CA	6.84	126.80	119.28
1	F	31	LEU	N-CA-C	-6.83	104.68	112.87
1	A	29	GLY	N-CA-C	-6.81	104.32	113.24
1	A	26	PRO	N-CA-C	-6.78	102.42	110.70
1	C	87	GLU	CA-C-N	-6.78	111.39	120.54
1	C	87	GLU	C-N-CA	-6.78	111.39	120.54
1	A	115	ARG	CA-C-N	-6.77	110.54	120.28
1	A	115	ARG	C-N-CA	-6.77	110.54	120.28
1	D	75	THR	N-CA-C	6.77	121.20	113.15
1	C	203	VAL	CB-CA-C	-6.75	100.11	110.50
1	A	284	LYS	CB-CA-C	6.74	121.47	110.22
1	F	38	GLN	N-CA-C	-6.74	103.86	111.14
1	B	238	ALA	N-CA-C	-6.74	103.74	112.23
1	A	145	GLU	N-CA-C	-6.68	99.65	110.20
1	D	297	GLN	CB-CA-C	6.66	121.12	110.19
1	D	69	ASP	N-CA-C	6.66	124.98	110.80
1	B	33	TYR	N-CA-C	-6.58	104.19	111.36
1	C	300	GLY	N-CA-C	-6.58	105.22	115.67
1	B	37	ILE	N-CA-C	6.56	116.72	110.42
1	E	120	SER	N-CA-C	6.55	118.42	111.28
1	B	195	CYS	CA-CB-SG	-6.51	99.44	114.40
1	E	129	GLY	N-CA-C	6.49	123.97	115.47
1	D	226	ASN	N-CA-C	6.49	118.36	111.28
1	E	249	ILE	CB-CA-C	-6.49	101.03	110.63
1	E	38	GLN	N-CA-C	-6.45	104.33	111.82
1	F	290	ASP	N-CA-C	6.45	120.41	112.54
1	C	37	ILE	N-CA-CB	6.44	117.66	110.51
1	C	100	GLU	N-CA-C	-6.44	105.29	113.01
1	C	97	ASN	N-CA-C	6.41	118.73	108.41
1	F	236	MET	N-CA-C	6.41	119.09	111.33
1	D	304	HIS	CA-C-N	6.41	127.85	119.84
1	D	304	HIS	C-N-CA	6.41	127.85	119.84
1	A	253	GLY	N-CA-C	-6.40	98.00	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	SER	CA-CB-OG	-6.40	98.29	111.10
1	D	171	ASN	CB-CA-C	6.40	119.08	111.15
1	A	57	SER	CA-CB-OG	-6.38	98.33	111.10
1	B	58	VAL	N-CA-C	-6.38	98.47	108.81
1	B	196	HIS	CB-CA-C	-6.38	100.12	110.77
1	E	180	CYS	CA-CB-SG	-6.37	99.75	114.40
1	E	134	VAL	CB-CA-C	-6.36	100.86	111.29
1	A	221	LEU	N-CA-C	6.35	118.00	111.14
1	A	94	GLY	CA-C-N	-6.34	108.00	121.32
1	A	94	GLY	C-N-CA	-6.34	108.00	121.32
1	B	247	ASP	CA-C-N	-6.33	114.06	122.99
1	B	247	ASP	C-N-CA	-6.33	114.06	122.99
1	D	147	ARG	CB-CA-C	6.32	120.74	111.65
1	B	104	LYS	CD-CE-NZ	-6.31	91.70	111.90
1	C	257	ILE	CB-CG1-CD1	-6.31	100.56	113.80
1	D	104	LYS	N-CA-C	-6.30	105.17	112.92
1	F	40	ILE	N-CA-CB	6.30	118.34	110.47
1	A	32	GLN	CB-CG-CD	-6.30	101.90	112.60
1	A	270	GLN	CB-CA-C	-6.29	97.16	110.31
1	B	202	TYR	N-CA-CB	-6.29	101.24	111.24
1	E	303	PRO	N-CA-C	6.25	121.12	110.74
1	B	203	VAL	CB-CA-C	-6.25	101.21	110.33
1	E	84	VAL	CA-C-N	-6.25	111.91	120.28
1	E	84	VAL	C-N-CA	-6.25	111.91	120.28
1	F	167	THR	N-CA-C	-6.24	104.93	112.54
1	A	280	ARG	O-C-N	6.23	131.13	123.21
1	C	221	LEU	N-CA-C	6.23	122.96	113.61
1	B	258	TYR	CA-C-O	-6.23	114.77	121.56
1	A	180	CYS	O-C-N	-6.21	115.91	123.30
1	F	299	GLU	N-CA-C	6.20	118.73	108.99
1	A	131	LEU	N-CA-C	-6.20	105.75	113.38
1	A	302	ASN	N-CA-CB	-6.18	103.43	111.09
1	F	295	ASP	N-CA-C	-6.18	105.84	113.19
1	B	240	ILE	N-CA-CB	-6.17	99.61	110.77
1	C	198	LEU	CA-C-N	-6.16	112.93	122.59
1	C	198	LEU	C-N-CA	-6.16	112.93	122.59
1	C	253	GLY	N-CA-C	-6.14	98.63	113.18
1	F	165	ILE	CB-CA-C	-6.13	104.01	112.04
1	C	97	ASN	CB-CA-C	-6.12	100.71	110.81
1	D	175	ARG	N-CA-C	6.12	119.78	112.93
1	C	32	GLN	CB-CA-C	-6.10	100.54	110.79
1	C	78	ARG	NE-CZ-NH2	6.07	124.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	LYS	N-CA-C	-6.07	104.00	111.40
1	F	257	ILE	CB-CA-C	-6.06	102.16	110.77
1	B	162	GLN	N-CA-C	-6.04	104.61	112.23
1	F	273	PRO	N-CA-C	6.03	123.11	112.01
1	B	213	TYR	N-CA-C	-6.02	97.48	108.02
1	A	99	LYS	N-CA-C	-6.01	104.85	111.82
1	D	70	GLU	N-CA-C	6.00	117.03	108.74
1	D	272	GLU	CA-C-N	-6.00	114.09	120.03
1	D	272	GLU	C-N-CA	-6.00	114.09	120.03
1	C	269	LEU	N-CA-C	5.98	120.19	113.01
1	F	203	VAL	CB-CA-C	-5.93	101.67	110.33
1	B	120	SER	CA-C-N	-5.93	113.30	122.49
1	B	120	SER	C-N-CA	-5.93	113.30	122.49
1	D	298	ILE	CA-C-N	-5.93	114.41	122.77
1	D	298	ILE	C-N-CA	-5.93	114.41	122.77
1	E	74	LEU	N-CA-C	5.92	117.53	110.19
1	D	37	ILE	CB-CA-C	-5.92	102.68	112.26
1	B	230	TYR	N-CA-C	-5.91	105.56	112.89
1	B	231	ALA	N-CA-C	-5.90	104.93	111.36
1	C	290	ASP	N-CA-C	5.90	119.22	112.97
1	A	241	THR	N-CA-C	-5.89	104.77	113.61
1	A	95	SER	O-C-N	-5.89	116.13	122.85
1	D	174	ASP	N-CA-C	5.89	119.02	110.42
1	E	119	ASP	N-CA-C	-5.89	105.36	112.54
1	B	240	ILE	CB-CA-C	-5.88	102.73	112.26
1	C	296	PHE	N-CA-C	5.84	118.93	109.40
1	E	201	PHE	N-CA-C	5.84	119.08	109.85
1	C	43	CYS	N-CA-C	5.84	122.36	113.61
1	B	198	LEU	CA-C-N	-5.83	112.66	122.29
1	B	198	LEU	C-N-CA	-5.83	112.66	122.29
1	F	30	GLU	N-CA-C	5.83	122.84	114.39
1	F	238	ALA	N-CA-C	-5.82	105.67	112.89
1	D	78	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	39	HIS	N-CA-C	5.82	118.09	111.11
1	F	267	ILE	CB-CA-C	5.82	119.27	111.94
1	A	38	GLN	N-CA-CB	5.81	118.44	110.01
1	B	229	SER	CA-CB-OG	-5.81	99.48	111.10
1	E	297	GLN	CA-C-N	-5.81	114.97	123.10
1	E	297	GLN	C-N-CA	-5.81	114.97	123.10
1	E	107	LYS	N-CA-C	5.80	117.35	109.11
1	C	263	GLU	CA-C-O	5.80	124.41	118.73
1	F	250	HIS	CA-C-N	-5.80	114.94	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	250	HIS	C-N-CA	-5.80	114.94	123.05
1	C	257	ILE	N-CA-CB	-5.79	101.09	111.92
1	A	305	PRO	CA-C-N	-5.78	111.29	121.70
1	A	305	PRO	C-N-CA	-5.78	111.29	121.70
1	B	94	GLY	N-CA-C	-5.78	107.69	115.21
1	D	169	LYS	N-CA-C	5.78	119.52	112.23
1	C	256	HIS	N-CA-C	5.78	118.19	109.41
1	C	168	ILE	CB-CA-C	-5.78	103.20	112.16
1	B	67	LEU	N-CA-C	-5.77	104.95	113.61
1	B	267	ILE	CB-CA-C	-5.77	104.59	111.81
1	F	71	PHE	CA-C-N	5.76	127.04	119.84
1	F	71	PHE	C-N-CA	5.76	127.04	119.84
1	F	227	ILE	N-CA-C	-5.76	104.71	110.30
1	A	297	GLN	CA-C-N	-5.74	115.41	122.93
1	A	297	GLN	C-N-CA	-5.74	115.41	122.93
1	B	302	ASN	CA-C-N	5.74	125.93	120.31
1	B	302	ASN	C-N-CA	5.74	125.93	120.31
1	E	236	MET	CG-SD-CE	-5.74	88.28	100.90
1	C	302	ASN	N-CA-CB	-5.73	103.58	111.77
1	D	93	LYS	CA-C-N	-5.73	112.86	122.25
1	D	93	LYS	C-N-CA	-5.73	112.86	122.25
1	B	58	VAL	O-C-N	-5.73	116.47	123.00
1	A	174	ASP	CA-C-N	-5.72	114.02	122.83
1	A	174	ASP	C-N-CA	-5.72	114.02	122.83
1	C	74	LEU	N-CA-C	5.72	118.57	110.50
1	C	207	GLU	CB-CA-C	5.72	121.00	109.38
1	B	256	HIS	N-CA-C	5.71	118.53	109.50
1	E	293	ALA	N-CA-C	-5.71	106.02	112.87
1	B	180	CYS	CA-C-N	-5.70	113.66	122.49
1	B	180	CYS	C-N-CA	-5.70	113.66	122.49
1	A	66	SER	CA-C-N	-5.70	113.55	122.49
1	A	66	SER	C-N-CA	-5.70	113.55	122.49
1	C	71	PHE	CA-C-N	-5.68	112.73	119.84
1	C	71	PHE	C-N-CA	-5.68	112.73	119.84
1	D	237	ILE	N-CA-C	-5.68	104.98	110.72
1	C	100	GLU	CA-C-N	-5.68	111.92	122.60
1	C	100	GLU	C-N-CA	-5.68	111.92	122.60
1	C	48	ASP	N-CA-C	5.68	118.21	110.55
1	C	104	LYS	CA-C-N	-5.67	114.80	122.63
1	C	104	LYS	C-N-CA	-5.67	114.80	122.63
1	E	46	ARG	N-CA-C	5.67	117.97	108.73
1	F	186	ASP	N-CA-C	-5.67	106.96	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	VAL	N-CA-CB	5.67	114.32	110.52
1	C	158	VAL	N-CA-C	5.66	116.64	108.48
1	A	138	GLN	N-CA-C	-5.64	105.12	112.23
1	B	248	PHE	CA-C-O	-5.64	114.27	120.36
1	D	88	LEU	N-CA-C	-5.64	105.05	111.14
1	A	240	ILE	CB-CG1-CD1	-5.63	101.97	113.80
1	D	38	GLN	O-C-N	5.63	127.89	122.03
1	C	175	ARG	CB-CG-CD	5.62	124.24	111.30
1	F	293	ALA	N-CA-C	5.62	122.76	110.80
1	D	130	ASP	N-CA-CB	5.61	118.71	110.35
1	A	178	ILE	N-CA-C	5.61	118.21	108.95
1	C	288	ILE	N-CA-C	-5.60	105.26	110.53
1	F	180	CYS	N-CA-C	5.60	117.83	109.59
1	C	84	VAL	CB-CA-C	-5.60	102.11	111.29
1	C	110	ASP	N-CA-C	5.60	117.06	111.07
1	B	78	ARG	CA-C-N	-5.60	114.28	122.68
1	B	78	ARG	C-N-CA	-5.60	114.28	122.68
1	C	241	THR	N-CA-C	-5.59	104.28	113.50
1	D	98	ALA	N-CA-C	5.59	117.84	111.02
1	B	192	LEU	O-C-N	5.57	125.90	121.55
1	A	122	GLY	N-CA-C	-5.57	106.50	115.08
1	D	209	SER	N-CA-C	-5.57	100.95	109.41
1	B	245	PRO	CA-C-O	-5.57	115.00	121.34
1	B	174	ASP	N-CA-C	5.56	117.46	110.24
1	C	281	ILE	N-CA-C	-5.55	102.41	109.58
1	D	59	PHE	CB-CA-C	5.55	118.58	110.26
1	A	195	CYS	CA-C-N	-5.55	115.04	122.42
1	A	195	CYS	C-N-CA	-5.55	115.04	122.42
1	D	221	LEU	N-CA-C	5.55	118.39	111.24
1	D	193	PRO	CA-C-N	-5.53	114.23	119.76
1	D	193	PRO	C-N-CA	-5.53	114.23	119.76
1	C	229	SER	CB-CA-C	-5.52	101.68	110.84
1	B	254	ASP	CA-C-N	-5.52	113.72	121.72
1	B	254	ASP	C-N-CA	-5.52	113.72	121.72
1	D	97	ASN	CA-C-O	-5.51	114.81	120.54
1	A	84	VAL	N-CA-CB	5.50	116.62	110.62
1	B	36	GLN	N-CA-C	-5.50	105.43	111.82
1	C	293	ALA	CA-C-N	5.50	127.65	120.28
1	C	293	ALA	C-N-CA	5.50	127.65	120.28
1	C	298	ILE	CA-C-N	-5.50	114.44	122.19
1	C	298	ILE	C-N-CA	-5.50	114.44	122.19
1	D	90	TRP	N-CA-CB	-5.50	102.10	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASN	CA-C-N	-5.50	113.95	119.56
1	B	171	ASN	C-N-CA	-5.50	113.95	119.56
1	B	157	GLY	N-CA-C	-5.48	102.20	112.22
1	C	249	ILE	CG1-CB-CG2	-5.48	94.27	110.70
1	A	64	ARG	CD-NE-CZ	-5.47	116.74	124.40
1	A	79	VAL	N-CA-CB	-5.47	102.10	110.86
1	F	69	ASP	N-CA-CB	-5.47	107.93	114.17
1	E	183	ASN	CA-C-N	5.45	125.80	119.47
1	E	183	ASN	C-N-CA	5.45	125.80	119.47
1	E	43	CYS	N-CA-C	5.45	119.24	112.59
1	A	274	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	A	270	GLN	CA-C-N	-5.45	113.71	121.50
1	A	270	GLN	C-N-CA	-5.45	113.71	121.50
1	B	53	THR	O-C-N	-5.45	116.59	123.12
1	E	131	LEU	CA-C-N	-5.45	113.32	121.87
1	E	131	LEU	C-N-CA	-5.45	113.32	121.87
1	B	142	PHE	CB-CA-C	-5.44	100.94	109.70
1	B	259	LEU	N-CA-C	5.44	117.64	111.11
1	C	145	GLU	CB-CA-C	-5.43	102.51	110.06
1	A	57	SER	CB-CA-C	-5.43	99.61	110.42
1	D	302	ASN	CA-C-N	-5.43	113.06	119.84
1	D	302	ASN	C-N-CA	-5.43	113.06	119.84
1	D	40	ILE	N-CA-C	5.41	115.51	110.42
1	A	183	ASN	CA-C-N	5.41	125.23	119.28
1	A	183	ASN	C-N-CA	5.41	125.23	119.28
1	C	210	CYS	CA-C-N	-5.41	113.96	122.73
1	C	210	CYS	C-N-CA	-5.41	113.96	122.73
1	D	43	CYS	CA-CB-SG	-5.41	101.96	114.40
1	A	280	ARG	CG-CD-NE	-5.41	100.11	112.00
1	A	58	VAL	O-C-N	-5.39	118.28	122.97
1	D	195	CYS	CA-CB-SG	-5.38	102.02	114.40
1	D	223	VAL	CA-C-N	-5.38	113.49	119.19
1	D	223	VAL	C-N-CA	-5.38	113.49	119.19
1	A	82	LYS	N-CA-C	-5.38	105.50	111.36
1	A	225	PHE	CB-CA-C	-5.35	101.91	110.79
1	A	298	ILE	CA-C-N	-5.34	115.63	123.00
1	A	298	ILE	C-N-CA	-5.34	115.63	123.00
1	C	43	CYS	CA-C-O	-5.34	112.88	119.18
1	E	108	ILE	CA-C-N	-5.33	114.08	122.08
1	E	108	ILE	C-N-CA	-5.33	114.08	122.08
1	C	137	PHE	CA-C-N	5.32	127.41	120.28
1	C	137	PHE	C-N-CA	5.32	127.41	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASP	CA-C-N	-5.32	113.13	120.26
1	C	186	ASP	C-N-CA	-5.32	113.13	120.26
1	F	89	LEU	N-CA-C	-5.30	105.61	111.71
1	F	272	GLU	CA-C-N	5.30	127.19	120.51
1	F	272	GLU	C-N-CA	5.30	127.19	120.51
1	A	122	GLY	CA-C-N	-5.29	114.03	122.66
1	A	122	GLY	C-N-CA	-5.29	114.03	122.66
1	A	45	VAL	N-CA-C	-5.29	100.23	108.86
1	B	40	ILE	CA-CB-CG1	5.29	119.40	110.40
1	B	119	ASP	N-CA-C	-5.29	106.51	113.12
1	F	249	ILE	CA-C-N	-5.28	115.75	122.77
1	F	249	ILE	C-N-CA	-5.28	115.75	122.77
1	A	249	ILE	CG1-CB-CG2	-5.28	94.86	110.70
1	F	249	ILE	N-CA-C	5.28	115.69	107.99
1	B	79	VAL	CA-C-O	-5.27	114.71	121.40
1	B	223	VAL	CA-C-N	-5.27	113.20	119.05
1	B	223	VAL	C-N-CA	-5.27	113.20	119.05
1	E	235	TYR	N-CA-C	5.27	117.71	111.33
1	A	30	GLU	CA-C-N	-5.26	112.70	120.28
1	A	30	GLU	C-N-CA	-5.26	112.70	120.28
1	A	167	THR	CA-C-N	-5.25	113.84	120.56
1	A	167	THR	C-N-CA	-5.25	113.84	120.56
1	C	108	ILE	CA-C-N	-5.25	113.17	122.26
1	C	108	ILE	C-N-CA	-5.25	113.17	122.26
1	B	154	SER	CB-CA-C	5.25	119.20	109.54
1	D	119	ASP	N-CA-C	-5.25	105.16	112.45
1	C	270	GLN	CA-C-N	-5.24	115.49	122.72
1	C	270	GLN	C-N-CA	-5.24	115.49	122.72
1	D	121	LEU	CA-CB-CG	5.23	134.60	116.30
1	C	42	ARG	CA-CB-CG	5.22	124.55	114.10
1	A	168	ILE	N-CA-C	5.22	115.44	110.53
1	C	154	SER	CB-CA-C	-5.22	100.04	110.42
1	C	177	ILE	CB-CA-C	-5.22	104.66	111.81
1	F	160	GLN	N-CA-C	-5.21	105.29	111.69
1	E	104	LYS	N-CA-C	5.20	117.35	111.11
1	C	274	ARG	CA-C-N	5.19	126.33	119.84
1	C	274	ARG	C-N-CA	5.19	126.33	119.84
1	A	250	HIS	CA-C-N	-5.18	115.41	122.93
1	A	250	HIS	C-N-CA	-5.18	115.41	122.93
1	E	96	THR	CB-CA-C	5.18	119.35	110.85
1	F	244	LYS	CA-CB-CG	5.18	124.46	114.10
1	C	219	MET	N-CA-C	-5.17	105.64	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	GLU	N-CA-C	-5.17	106.47	112.89
1	E	106	VAL	CA-C-N	5.17	129.72	122.79
1	E	106	VAL	C-N-CA	5.17	129.72	122.79
1	D	294	GLU	CA-C-N	-5.17	114.38	122.65
1	D	294	GLU	C-N-CA	-5.17	114.38	122.65
1	E	164	VAL	N-CA-C	-5.17	105.35	110.62
1	A	103	SER	N-CA-C	-5.17	106.82	113.23
1	B	203	VAL	CA-C-N	-5.17	114.06	122.33
1	B	203	VAL	C-N-CA	-5.17	114.06	122.33
1	F	26	PRO	CA-C-N	5.16	126.30	119.84
1	F	26	PRO	C-N-CA	5.16	126.30	119.84
1	B	153	TYR	CA-C-N	-5.16	112.84	120.94
1	B	153	TYR	C-N-CA	-5.16	112.84	120.94
1	D	141	HIS	N-CA-CB	-5.15	105.61	111.79
1	D	77	LYS	N-CA-C	-5.14	101.09	108.60
1	F	104	LYS	N-CA-C	-5.14	106.12	114.09
1	B	44	GLY	CA-C-O	-5.13	115.86	121.71
1	A	226	ASN	N-CA-CB	5.12	118.21	110.28
1	F	134	VAL	N-CA-C	5.11	119.98	109.34
1	D	40	ILE	N-CA-CB	5.11	116.43	110.65
1	C	219	MET	O-C-N	5.10	127.53	122.12
1	B	75	THR	CA-C-N	-5.10	112.58	122.06
1	B	75	THR	C-N-CA	-5.10	112.58	122.06
1	E	165	ILE	N-CA-C	-5.10	105.57	110.72
1	B	210	CYS	CB-CA-C	-5.10	99.03	109.38
1	A	229	SER	CB-CA-C	-5.09	102.28	110.74
1	D	210	CYS	CA-C-N	-5.09	113.90	122.29
1	D	210	CYS	C-N-CA	-5.09	113.90	122.29
1	F	154	SER	N-CA-C	5.09	121.63	110.80
1	B	195	CYS	CA-C-N	-5.08	114.41	121.99
1	B	195	CYS	C-N-CA	-5.08	114.41	121.99
1	E	290	ASP	N-CA-CB	-5.08	102.83	111.27
1	F	48	ASP	N-CA-C	5.08	117.40	110.24
1	D	145	GLU	CB-CA-C	-5.07	102.86	110.16
1	F	303	PRO	N-CA-C	5.06	119.03	111.14
1	A	48	ASP	O-C-N	5.05	129.31	122.59
1	D	218	ASP	N-CA-C	5.05	116.71	108.63
1	B	48	ASP	N-CA-C	5.05	118.29	110.17
1	C	44	GLY	N-CA-C	-5.04	105.00	113.02
1	C	296	PHE	CA-C-N	-5.04	115.88	122.99
1	C	296	PHE	C-N-CA	-5.04	115.88	122.99
1	B	143	GLY	N-CA-C	5.04	125.12	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ARG	NE-CZ-NH2	-5.04	114.67	119.20
1	A	209	SER	CA-CB-OG	-5.03	101.03	111.10
1	F	148	ASP	N-CA-C	5.03	116.46	108.96
1	D	234	THR	CA-C-O	-5.03	115.54	120.82
1	D	304	HIS	N-CA-C	-5.03	103.74	110.07
1	C	262	ILE	CA-C-N	-5.01	113.54	120.26
1	C	262	ILE	C-N-CA	-5.01	113.54	120.26
1	A	231	ALA	N-CA-C	-5.01	105.90	111.36
1	C	286	GLU	CB-CA-C	-5.01	100.91	109.03
1	B	57	SER	N-CA-C	-5.01	101.13	108.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	LYS	Peptide
1	D	217	GLY	Peptide
1	D	44	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2279	0	2247	119	0
1	B	2268	0	2235	78	0
1	C	2268	0	2235	106	0
1	D	2268	0	2235	102	0
1	E	2268	0	2235	198	0
1	F	2268	0	2235	170	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	5	0
3	C	4	0	6	3	0
3	E	4	0	6	2	0
4	A	62	0	0	11	0
4	B	52	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	30	0	0	1	0
4	D	23	0	0	3	0
4	E	9	0	0	5	0
4	F	6	0	0	1	0
All	All	13834	0	13434	762	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 28.

All (762) 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:C:42:ARG:CD	1:C:42:ARG:CG	1.77	1.59
1:B:168:ILE:CD1	1:B:168:ILE:CG1	1.81	1.58
1:A:104:LYS:CE	1:A:104:LYS:NZ	1.67	1.54
1:B:26:PRO:CB	1:B:26:PRO:CG	1.79	1.52
1:E:31:LEU:O	1:E:32:GLN:HG2	1.34	1.25
1:F:130:ASP:HB2	1:F:149:MET:HG2	1.23	1.16
1:C:153:TYR:O	1:C:156:GLN:HG3	1.46	1.13
1:A:115:ARG:HG3	1:A:115:ARG:HH11	1.08	1.10
1:E:32:GLN:O	1:E:34:LEU:HD12	1.51	1.10
1:B:115:ARG:HG3	1:B:115:ARG:HH11	0.96	1.08
1:A:109:TRP:CZ3	1:A:192:LEU:HD11	1.91	1.05
1:F:115:ARG:HG2	1:F:128:GLU:HG3	1.37	1.04
1:F:233:LEU:O	1:F:233:LEU:HD12	1.60	1.01
1:C:192:LEU:CD1	1:C:192:LEU:N	2.26	0.99
1:C:257:ILE:HD11	1:C:265:LEU:HD13	1.44	0.99
1:E:30:GLU:OE2	1:E:34:LEU:HG	1.61	0.97
1:E:131:LEU:O	1:E:132:GLY:O	1.81	0.97
1:C:192:LEU:N	1:C:192:LEU:HD12	1.79	0.97
1:F:271:ARG:HH11	1:F:304:HIS:HB3	1.30	0.96
1:B:115:ARG:HG3	1:B:115:ARG:NH1	1.75	0.96
1:A:49:ASP:OD1	1:A:51:THR:OG1	1.83	0.96
1:B:280:ARG:NE	1:B:299:GLU:HG2	1.81	0.95
1:F:204:VAL:O	1:F:207:GLU:HB2	1.65	0.95
1:D:297:GLN:HE21	1:D:299:GLU:HB3	1.30	0.95
1:E:42:ARG:O	4:E:633:HOH:O	1.83	0.95
1:E:261:HIS:HA	1:E:264:PRO:HG2	1.50	0.92
1:A:176:ARG:HG2	1:A:176:ARG:HH11	1.34	0.92
1:E:31:LEU:O	1:E:32:GLN:CG	2.18	0.91
1:E:30:GLU:OE2	1:E:30:GLU:O	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:LYS:HB3	4:D:631:HOH:O	1.71	0.91
1:F:279:LEU:HD12	1:F:298:ILE:HD12	1.53	0.91
1:A:198:LEU:C	1:A:198:LEU:HD12	1.97	0.90
1:A:109:TRP:HZ3	1:A:192:LEU:HD11	1.33	0.89
1:E:97:ASN:OD1	1:E:99:LYS:HB2	1.73	0.89
1:E:160:GLN:HE22	1:E:180:CYS:H	1.19	0.88
1:A:192:LEU:HD22	4:A:666:HOH:O	1.72	0.88
1:E:271:ARG:HD3	1:E:304:HIS:ND1	1.88	0.88
1:A:100:GLU:O	1:A:100:GLU:HG3	1.75	0.87
1:D:47:LYS:HG2	1:D:48:ASP:H	1.39	0.87
1:B:205:ASN:HA	4:B:358:HOH:O	1.75	0.86
1:B:280:ARG:HH11	1:B:280:ARG:CG	1.89	0.86
1:F:72:PRO:HA	1:F:276:PHE:CE1	2.10	0.86
1:B:280:ARG:HE	1:B:299:GLU:HG2	1.41	0.85
1:E:172:PRO:HB3	1:E:203:VAL:HG11	1.57	0.84
1:B:115:ARG:HH11	1:B:115:ARG:CG	1.86	0.84
1:E:30:GLU:HB3	1:E:276:PHE:CZ	2.13	0.84
1:D:33:TYR:OH	1:D:219:MET:O	1.94	0.84
1:E:111:ALA:HA	1:E:115:ARG:NH2	1.91	0.84
1:A:115:ARG:NH2	1:A:126:ARG:O	2.11	0.84
1:A:176:ARG:HG2	1:A:176:ARG:NH1	1.91	0.83
1:F:271:ARG:NH1	1:F:304:HIS:HB3	1.92	0.83
1:E:301:TYR:CZ	1:E:303:PRO:HG3	2.14	0.83
1:E:111:ALA:HA	1:E:115:ARG:HH22	1.46	0.80
1:C:198:LEU:C	1:C:198:LEU:HD12	2.06	0.80
1:D:306:THR:O	1:D:306:THR:HG23	1.81	0.80
1:A:115:ARG:HG3	1:A:115:ARG:NH1	1.86	0.80
1:F:91:PHE:CE1	1:F:135:TYR:HB2	2.15	0.80
1:E:288:ILE:O	4:E:629:HOH:O	2.00	0.80
1:E:30:GLU:HB3	1:E:276:PHE:HZ	1.45	0.80
1:F:81:TRP:CZ2	1:F:85:LEU:HD11	2.17	0.80
1:E:259:LEU:O	1:E:262:ILE:HG12	1.82	0.79
1:A:45:VAL:HG21	1:B:204:VAL:HG21	1.65	0.79
1:A:48:ASP:HB2	4:A:654:HOH:O	1.83	0.78
1:D:76:THR:OG1	1:D:268:GLN:NE2	2.15	0.78
1:A:49:ASP:C	1:A:51:THR:H	1.92	0.78
1:E:44:GLY:O	1:E:56:LEU:HD22	1.83	0.78
1:D:34:LEU:HD22	1:D:269:LEU:HD23	1.65	0.78
1:E:43:CYS:HA	4:E:633:HOH:O	1.84	0.78
1:A:123:PHE:HB3	1:A:126:ARG:HD2	1.64	0.78
1:F:78:ARG:HD2	4:F:316:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:GLY:O	1:F:140:ARG:HG2	1.85	0.76
1:E:291:PHE:CD1	1:E:296:PHE:HZ	2.03	0.76
1:A:299:GLU:O	1:A:299:GLU:HG3	1.85	0.76
1:F:97:ASN:HA	1:F:129:GLY:O	1.86	0.75
1:D:139:TRP:CE2	1:D:179:MET:HE3	2.21	0.75
1:F:130:ASP:HB2	1:F:149:MET:CG	2.12	0.75
1:E:108:ILE:N	1:E:110:ASP:OD2	2.19	0.75
1:A:126:ARG:HG2	1:A:130:ASP:HB3	1.67	0.75
1:C:191:ALA:C	1:C:192:LEU:HD12	2.12	0.75
1:E:192:LEU:HD13	1:E:192:LEU:O	1.87	0.75
1:E:274:ARG:HD2	1:E:304:HIS:CD2	2.22	0.74
1:F:130:ASP:CB	1:F:149:MET:HG2	2.13	0.74
1:D:198:LEU:HD12	1:D:198:LEU:C	2.12	0.74
1:A:109:TRP:HZ3	1:A:192:LEU:CD1	2.00	0.74
1:D:223:VAL:N	1:D:224:PRO:CD	2.50	0.74
1:C:127:GLU:HG2	1:C:149:MET:HE2	1.70	0.74
1:C:126:ARG:HD3	1:C:130:ASP:CG	2.13	0.73
1:F:237:ILE:O	1:F:241:THR:OG1	2.05	0.73
1:C:132:GLY:HA2	1:C:146:TYR:CE2	2.22	0.73
1:D:126:ARG:CD	1:D:130:ASP:HB3	2.18	0.73
1:E:233:LEU:O	1:E:237:ILE:HG13	1.89	0.73
1:E:160:GLN:HE22	1:E:180:CYS:N	1.87	0.73
1:D:126:ARG:HD3	1:D:130:ASP:CG	2.14	0.72
1:E:160:GLN:NE2	1:E:180:CYS:H	1.87	0.72
1:A:193:PRO:O	4:A:666:HOH:O	2.07	0.72
1:E:113:GLY:HA3	1:E:131:LEU:HD23	1.71	0.72
1:F:147:ARG:NH2	1:F:151:SER:OG	2.21	0.72
1:A:115:ARG:HH11	1:A:115:ARG:CG	1.97	0.72
1:F:87:GLU:O	1:F:90:TRP:HB3	1.90	0.71
1:F:239:HIS:O	1:F:241:THR:N	2.23	0.71
1:F:73:LEU:HD11	1:F:79:VAL:HB	1.71	0.71
1:D:147:ARG:HH12	1:D:156:GLN:HE22	1.38	0.71
1:F:100:GLU:O	1:F:100:GLU:HG2	1.91	0.71
1:B:280:ARG:HH11	1:B:280:ARG:HG3	1.54	0.71
1:F:123:PHE:O	1:F:126:ARG:HB3	1.91	0.71
1:D:198:LEU:C	1:D:198:LEU:CD1	2.64	0.70
1:C:259:LEU:O	1:C:262:ILE:HG12	1.91	0.70
1:E:87:GLU:OE1	1:E:91:PHE:CZ	2.45	0.70
1:E:45:VAL:CG2	1:F:204:VAL:HG21	2.21	0.70
1:C:92:ILE:HD11	1:C:236:MET:CE	2.22	0.70
1:D:168:ILE:HD11	1:D:177:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ARG:HH21	1:E:46:ARG:HG3	1.57	0.70
1:E:274:ARG:HD2	1:E:304:HIS:HD2	1.56	0.70
1:A:92:ILE:HD11	1:A:236:MET:HE1	1.73	0.70
1:E:37:ILE:HG23	1:E:257:ILE:HD11	1.73	0.70
1:F:85:LEU:O	1:F:89:LEU:HD12	1.91	0.70
1:C:92:ILE:HD11	1:C:236:MET:HE1	1.74	0.70
1:E:30:GLU:OE2	1:E:34:LEU:CG	2.40	0.70
1:F:92:ILE:O	1:F:140:ARG:NH2	2.24	0.70
1:F:33:TYR:OH	1:F:219:MET:O	2.08	0.69
1:B:123:PHE:HB3	1:B:126:ARG:HD2	1.72	0.69
1:C:99:LYS:O	1:C:103:SER:HB3	1.91	0.69
1:C:92:ILE:HD13	1:C:288:ILE:HG13	1.73	0.69
1:B:185:ARG:HG2	1:B:185:ARG:HH21	1.57	0.69
1:C:257:ILE:CD1	1:C:265:LEU:HD13	2.20	0.69
1:D:34:LEU:HD22	1:D:269:LEU:CD2	2.21	0.69
1:F:48:ASP:OD1	1:F:52:GLY:HA2	1.92	0.69
1:A:240:ILE:CG2	1:A:240:ILE:O	2.41	0.69
1:D:285:VAL:CG1	1:D:290:ASP:HB2	2.23	0.69
1:E:115:ARG:HD2	1:E:116:ASP:H	1.58	0.68
1:D:77:LYS:HG2	1:D:78:ARG:N	2.07	0.68
1:E:218:ASP:OD2	1:E:221:LEU:HD22	1.92	0.68
1:E:257:ILE:O	1:E:257:ILE:CG2	2.40	0.68
1:D:80:PHE:HE1	1:D:82:LYS:HB3	1.58	0.68
1:D:297:GLN:NE2	1:D:299:GLU:HB3	2.06	0.68
1:B:67:LEU:HB2	1:B:246:GLY:O	1.92	0.68
1:D:168:ILE:CD1	1:D:177:ILE:HG21	2.24	0.68
1:E:239:HIS:HD1	1:E:281:ILE:HG13	1.59	0.67
1:E:279:LEU:HD12	1:E:298:ILE:HD13	1.77	0.67
1:C:204:VAL:HG22	1:C:205:ASN:N	2.07	0.67
1:A:160:GLN:OE1	4:A:631:HOH:O	2.12	0.67
1:E:291:PHE:HD1	1:E:296:PHE:CZ	2.13	0.67
1:E:86:GLU:HB3	1:E:106:VAL:HG21	1.76	0.67
1:F:233:LEU:HD12	1:F:233:LEU:C	2.19	0.67
1:F:270:GLN:O	1:F:272:GLU:N	2.27	0.67
1:B:192:LEU:HB2	1:B:193:PRO:CD	2.24	0.67
1:E:79:VAL:O	1:E:81:TRP:N	2.28	0.67
1:E:294:GLU:O	1:E:296:PHE:N	2.28	0.67
1:E:280:ARG:HG2	1:E:299:GLU:OE1	1.95	0.66
1:F:294:GLU:C	1:F:296:PHE:H	2.01	0.66
1:E:98:ALA:HB2	1:E:131:LEU:HD11	1.76	0.66
1:A:198:LEU:C	1:A:198:LEU:CD1	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:SER:HA	1:F:243:LEU:HD22	1.77	0.66
1:F:115:ARG:HG2	1:F:128:GLU:CG	2.20	0.66
1:D:43:CYS:SG	1:D:43:CYS:O	2.53	0.65
1:D:46:ARG:HA	1:D:55:THR:O	1.97	0.65
1:E:257:ILE:O	1:E:257:ILE:HG22	1.97	0.65
1:D:80:PHE:CE1	1:D:82:LYS:HB3	2.31	0.65
1:C:153:TYR:O	1:C:156:GLN:CG	2.35	0.65
1:E:113:GLY:HA3	1:E:131:LEU:CD2	2.26	0.65
1:F:223:VAL:O	1:F:227:ILE:HG13	1.96	0.65
1:D:294:GLU:CD	1:D:294:GLU:H	2.05	0.65
1:D:58:VAL:HG12	1:D:58:VAL:O	1.98	0.64
1:E:192:LEU:HD13	1:E:192:LEU:C	2.21	0.64
1:A:50:ARG:HA	4:A:675:HOH:O	1.98	0.64
1:A:92:ILE:CD1	1:A:236:MET:HE1	2.27	0.64
1:F:88:LEU:HD23	1:F:88:LEU:C	2.21	0.64
1:E:223:VAL:O	1:E:227:ILE:HG13	1.98	0.64
1:C:102:SER:O	1:C:104:LYS:N	2.28	0.64
1:C:192:LEU:CD1	1:C:192:LEU:H	2.07	0.64
1:E:130:ASP:OD2	1:E:149:MET:HB3	1.97	0.64
1:F:88:LEU:CD2	1:F:92:ILE:HD11	2.27	0.64
1:F:274:ARG:HD3	1:F:302:ASN:O	1.96	0.64
1:E:78:ARG:HG3	1:E:79:VAL:H	1.63	0.63
1:A:240:ILE:HD11	1:A:288:ILE:HA	1.80	0.63
1:F:115:ARG:CG	1:F:128:GLU:HG3	2.22	0.63
1:D:77:LYS:HG2	1:D:78:ARG:H	1.63	0.63
1:F:161:LEU:O	1:F:165:ILE:HG12	1.98	0.63
1:F:206:SER:HA	1:F:243:LEU:CD2	2.27	0.63
1:E:132:GLY:HA3	1:E:189:LEU:O	1.98	0.63
1:B:99:LYS:NZ	1:B:128:GLU:HG3	2.14	0.63
1:F:198:LEU:C	1:F:198:LEU:HD23	2.24	0.62
1:A:292:LYS:O	1:A:293:ALA:C	2.41	0.62
1:F:233:LEU:O	1:F:233:LEU:CD1	2.43	0.62
1:E:82:LYS:O	1:E:86:GLU:HB2	1.99	0.62
1:A:46:ARG:C	1:A:48:ASP:H	2.08	0.62
1:E:214:GLN:OE1	1:E:250:HIS:HE1	1.83	0.62
1:E:223:VAL:HB	1:E:224:PRO:HD3	1.82	0.62
1:E:291:PHE:HD1	1:E:296:PHE:HZ	1.46	0.62
1:C:198:LEU:C	1:C:198:LEU:CD1	2.70	0.61
1:E:98:ALA:HB1	1:E:109:TRP:O	1.99	0.61
1:C:174:ASP:OD1	1:C:176:ARG:HB2	2.01	0.61
1:D:147:ARG:NH1	1:D:156:GLN:HE22	1.96	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:C	1:E:261:HIS:H	2.08	0.61
1:D:259:LEU:O	1:D:262:ILE:HG12	2.00	0.61
1:E:37:ILE:HG23	1:E:257:ILE:CD1	2.30	0.61
1:F:148:ASP:OD2	1:F:150:GLU:O	2.18	0.61
1:F:32:GLN:NE2	1:F:64:ARG:O	2.32	0.61
1:F:88:LEU:HD21	1:F:92:ILE:HD11	1.82	0.61
1:F:143:GLY:O	1:F:144:ALA:C	2.39	0.61
1:C:78:ARG:HH11	1:C:78:ARG:CG	2.14	0.61
1:F:301:TYR:C	1:F:303:PRO:HD3	2.26	0.61
1:E:271:ARG:HH11	1:E:304:HIS:CB	2.13	0.61
1:E:254:ASP:OD2	1:F:175:ARG:HD3	2.00	0.60
1:E:302:ASN:N	1:E:303:PRO:HD3	2.16	0.60
1:E:301:TYR:CE2	1:E:303:PRO:HG3	2.37	0.60
1:C:52:GLY:O	4:C:628:HOH:O	2.17	0.60
1:A:32:GLN:O	1:A:36:GLN:HG3	2.02	0.60
1:C:239:HIS:HD1	1:C:281:ILE:HD13	1.66	0.60
1:E:219:MET:HB2	1:E:257:ILE:HG13	1.83	0.60
1:F:80:PHE:HE2	1:F:106:VAL:HG13	1.66	0.60
1:F:279:LEU:HD12	1:F:298:ILE:CD1	2.29	0.60
1:C:87:GLU:O	1:C:88:LEU:C	2.41	0.60
1:D:240:ILE:HG22	1:D:240:ILE:O	2.01	0.60
1:A:176:ARG:HH11	1:A:176:ARG:CG	2.07	0.59
1:A:206:SER:HA	1:A:243:LEU:CD2	2.32	0.59
1:F:301:TYR:O	1:F:303:PRO:HD3	2.01	0.59
1:B:192:LEU:HB2	1:B:193:PRO:HD3	1.84	0.59
1:E:81:TRP:CH2	1:E:232:LEU:HD22	2.37	0.59
1:C:92:ILE:CD1	1:C:236:MET:HE1	2.32	0.59
1:F:97:ASN:OD1	1:F:149:MET:SD	2.61	0.59
1:D:306:THR:O	1:D:306:THR:CG2	2.50	0.59
1:E:46:ARG:HG3	1:E:46:ARG:NH2	2.18	0.59
1:D:100:GLU:HG3	1:D:100:GLU:O	2.01	0.59
1:F:229:SER:O	1:F:232:LEU:HB3	2.02	0.59
1:D:85:LEU:HD11	1:D:296:PHE:CD1	2.38	0.59
1:C:135:TYR:O	1:C:136:GLY:C	2.42	0.59
1:E:211:GLN:HG3	1:E:249:ILE:HB	1.85	0.59
1:F:39:HIS:O	1:F:40:ILE:C	2.43	0.59
1:C:102:SER:C	1:C:104:LYS:H	2.11	0.58
1:E:198:LEU:C	1:E:198:LEU:HD12	2.28	0.58
1:E:240:ILE:HD11	1:E:291:PHE:CE2	2.38	0.58
1:A:147:ARG:HH12	1:A:156:GLN:HE22	1.51	0.58
1:A:292:LYS:O	1:A:294:GLU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ARG:CD	1:E:116:ASP:H	2.17	0.58
1:C:66:SER:O	1:C:67:LEU:HD23	2.04	0.58
1:E:130:ASP:CG	1:E:149:MET:HB3	2.29	0.58
1:F:88:LEU:O	1:F:92:ILE:HG13	2.04	0.58
1:C:257:ILE:HD11	1:C:265:LEU:CD1	2.29	0.57
1:F:97:ASN:HD22	1:F:100:GLU:H	1.52	0.57
1:C:192:LEU:N	1:C:192:LEU:HD13	2.16	0.57
1:C:192:LEU:H	1:C:192:LEU:HD13	1.69	0.57
1:A:176:ARG:HD2	1:B:215:ARG:NH1	2.18	0.57
1:D:252:LEU:HD13	1:D:255:ALA:HB2	1.85	0.57
1:E:128:GLU:O	1:E:149:MET:HE1	2.05	0.57
1:C:214:GLN:OE1	1:C:250:HIS:HE1	1.86	0.56
1:F:259:LEU:O	1:F:262:ILE:HG13	2.05	0.56
1:E:31:LEU:C	1:E:32:GLN:HG2	2.23	0.56
1:F:81:TRP:CE2	1:F:85:LEU:HD11	2.40	0.56
1:F:134:VAL:HG12	1:F:190:MET:HE3	1.87	0.56
1:E:115:ARG:HD2	1:E:116:ASP:N	2.20	0.56
1:A:259:LEU:O	1:A:262:ILE:HG13	2.06	0.56
1:E:88:LEU:HD11	1:E:233:LEU:HB2	1.86	0.56
1:E:124:SER:C	1:E:126:ARG:H	2.14	0.56
1:E:291:PHE:CD1	1:E:296:PHE:CZ	2.86	0.56
1:A:198:LEU:HD12	1:A:198:LEU:O	2.05	0.56
1:E:215:ARG:NH1	1:F:175:ARG:O	2.39	0.56
1:C:263:GLU:O	1:C:264:PRO:C	2.47	0.56
1:D:74:LEU:HD12	1:D:224:PRO:HB3	1.87	0.56
1:E:282:LEU:HD11	1:E:297:GLN:OE1	2.06	0.56
1:E:289:ASP:C	4:E:629:HOH:O	2.49	0.56
1:F:239:HIS:C	1:F:241:THR:H	2.14	0.56
1:F:267:ILE:C	1:F:269:LEU:H	2.14	0.56
1:D:139:TRP:CD2	1:D:179:MET:HE3	2.41	0.55
1:E:135:TYR:O	1:E:136:GLY:C	2.49	0.55
1:A:127:GLU:CD	1:A:127:GLU:H	2.13	0.55
1:F:69:ASP:O	1:F:278:LYS:HG3	2.06	0.55
1:B:164:VAL:HG22	1:B:177:ILE:HG22	1.88	0.55
2:E:618:PO4:O2	3:E:628:BME:H21	2.05	0.55
1:E:33:TYR:O	1:E:34:LEU:C	2.49	0.55
1:E:84:VAL:O	1:E:85:LEU:C	2.40	0.55
1:E:240:ILE:HD11	1:E:291:PHE:HE2	1.70	0.55
1:F:285:VAL:CG1	1:F:290:ASP:HB2	2.37	0.55
1:E:271:ARG:HH11	1:E:304:HIS:HB2	1.71	0.55
1:E:32:GLN:HG3	1:E:64:ARG:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:LEU:O	1:E:132:GLY:C	2.44	0.55
1:E:274:ARG:O	1:E:275:PRO:C	2.48	0.55
1:F:153:TYR:HA	1:F:156:GLN:NE2	2.21	0.55
1:F:207:GLU:OE1	1:F:207:GLU:HA	2.06	0.55
1:C:92:ILE:CD1	1:C:236:MET:CE	2.84	0.55
1:F:244:LYS:HE2	1:F:244:LYS:N	2.22	0.55
1:E:76:THR:HB	1:E:268:GLN:NE2	2.22	0.54
1:F:72:PRO:HA	1:F:276:PHE:CD1	2.41	0.54
1:F:244:LYS:HE2	1:F:244:LYS:H	1.72	0.54
1:A:263:GLU:CB	1:A:264:PRO:HD3	2.37	0.54
4:A:664:HOH:O	1:B:163:LYS:HE2	2.07	0.54
1:E:87:GLU:OE1	1:E:91:PHE:HZ	1.89	0.54
1:F:101:LEU:HA	1:F:104:LYS:HG3	1.88	0.54
1:F:80:PHE:HD2	1:F:83:GLY:HA3	1.71	0.54
1:E:237:ILE:O	1:E:241:THR:OG1	2.26	0.54
1:B:99:LYS:HZ3	1:B:128:GLU:HG3	1.73	0.54
1:D:206:SER:O	1:D:244:LYS:HG3	2.06	0.54
1:E:116:ASP:O	1:E:120:SER:HB3	2.07	0.54
1:C:79:VAL:O	1:C:81:TRP:N	2.38	0.54
1:E:271:ARG:NH1	1:E:304:HIS:HB3	2.22	0.54
1:E:292:LYS:C	1:E:294:GLU:H	2.16	0.54
1:A:171:ASN:O	1:A:172:PRO:C	2.48	0.54
1:A:240:ILE:O	1:A:240:ILE:HG22	2.07	0.54
1:F:37:ILE:HG22	1:F:37:ILE:O	2.08	0.54
1:A:49:ASP:C	1:A:51:THR:N	2.64	0.53
1:C:72:PRO:O	1:C:72:PRO:HG2	2.06	0.53
1:C:127:GLU:CD	1:C:127:GLU:H	2.16	0.53
1:E:263:GLU:N	1:E:264:PRO:HD2	2.23	0.53
1:F:88:LEU:O	1:F:91:PHE:HB2	2.08	0.53
1:D:139:TRP:CE2	1:D:179:MET:CE	2.91	0.53
1:E:30:GLU:O	1:E:34:LEU:HG	2.08	0.53
1:E:194:PRO:O	1:E:215:ARG:NE	2.33	0.53
1:A:176:ARG:NH1	4:A:627:HOH:O	2.40	0.53
1:D:73:LEU:HB3	1:D:277:PRO:HG2	1.90	0.53
1:D:97:ASN:HB3	1:D:100:GLU:HB3	1.90	0.53
1:C:239:HIS:ND1	1:C:281:ILE:HD13	2.22	0.53
1:D:36:GLN:O	1:D:40:ILE:HG13	2.08	0.53
1:E:102:SER:HB3	1:E:106:VAL:O	2.08	0.53
1:E:66:SER:OG	1:E:68:ARG:HG3	2.08	0.53
1:B:221:LEU:HD21	1:B:261:HIS:CE1	2.43	0.53
1:C:103:SER:O	1:C:103:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:LEU:C	1:E:132:GLY:O	2.51	0.53
1:E:175:ARG:NH2	2:E:619:PO4:O2	2.41	0.53
1:F:159:ASP:OD2	1:F:162:GLN:HB2	2.09	0.53
1:A:197:ALA:O	1:A:198:LEU:HB3	2.08	0.53
1:E:232:LEU:O	1:E:236:MET:HG3	2.08	0.53
1:F:72:PRO:CA	1:F:276:PHE:CE1	2.88	0.53
1:F:228:ALA:O	1:F:229:SER:C	2.51	0.53
1:C:204:VAL:CG2	1:C:205:ASN:N	2.71	0.53
1:E:206:SER:HA	1:E:243:LEU:HD22	1.90	0.53
1:F:134:VAL:HG23	1:F:135:TYR:N	2.23	0.53
1:E:60:GLY:O	1:E:61:MET:HG2	2.08	0.53
1:B:259:LEU:O	1:B:262:ILE:HG13	2.09	0.53
1:D:47:LYS:HG2	1:D:48:ASP:N	2.18	0.53
1:D:133:PRO:O	1:D:190:MET:HE2	2.08	0.52
1:E:178:ILE:CG2	1:E:179:MET:N	2.72	0.52
1:E:298:ILE:CG2	1:E:301:TYR:HB2	2.39	0.52
1:A:36:GLN:O	1:A:40:ILE:HG13	2.10	0.52
1:A:102:SER:HB2	1:A:110:ASP:OD1	2.08	0.52
1:A:206:SER:HA	1:A:243:LEU:HD22	1.91	0.52
1:E:290:ASP:N	4:E:629:HOH:O	2.42	0.52
1:A:35:GLY:HA2	1:A:38:GLN:HG3	1.92	0.52
1:B:183:ASN:C	1:B:183:ASN:OD1	2.52	0.52
1:D:198:LEU:HD12	1:D:198:LEU:O	2.09	0.52
1:F:294:GLU:C	1:F:296:PHE:N	2.66	0.52
1:A:306:THR:HB	4:A:671:HOH:O	2.09	0.52
1:C:78:ARG:HH11	1:C:78:ARG:HG2	1.74	0.52
1:E:192:LEU:C	1:E:192:LEU:CD1	2.82	0.52
1:E:303:PRO:O	1:E:304:HIS:C	2.51	0.52
1:F:80:PHE:CD2	1:F:83:GLY:HA3	2.45	0.52
1:F:124:SER:C	1:F:126:ARG:H	2.17	0.52
1:F:225:PHE:O	1:F:228:ALA:HB3	2.10	0.52
1:A:33:TYR:O	1:A:37:ILE:HG13	2.09	0.52
1:A:43:CYS:O	1:A:44:GLY:C	2.49	0.52
1:B:280:ARG:HG3	1:B:280:ARG:NH1	2.23	0.52
1:C:283:ARG:CB	1:C:283:ARG:HH11	2.23	0.52
1:E:90:TRP:NE1	1:E:95:SER:OG	2.43	0.52
1:F:109:TRP:CZ3	1:F:192:LEU:HD21	2.44	0.51
1:C:127:GLU:O	1:C:128:GLU:C	2.53	0.51
1:C:257:ILE:CD1	1:C:265:LEU:CD1	2.86	0.51
1:E:292:LYS:C	1:E:294:GLU:N	2.68	0.51
1:F:292:LYS:O	1:F:295:ASP:OD1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:HIS:O	1:C:142:PHE:C	2.54	0.51
1:F:99:LYS:C	1:F:101:LEU:H	2.17	0.51
1:C:78:ARG:CG	1:C:78:ARG:NH1	2.71	0.51
1:E:67:LEU:HB2	1:E:246:GLY:O	2.10	0.51
1:E:94:GLY:C	1:E:95:SER:O	2.52	0.51
1:F:267:ILE:C	1:F:269:LEU:N	2.68	0.51
1:E:207:GLU:HG2	1:E:244:LYS:HG3	1.92	0.51
1:F:232:LEU:O	1:F:233:LEU:C	2.53	0.51
1:A:115:ARG:O	1:A:116:ASP:C	2.50	0.51
1:B:32:GLN:O	1:B:36:GLN:HG3	2.11	0.51
1:C:223:VAL:HA	1:C:226:ASN:HD22	1.74	0.51
1:C:227:ILE:HD11	1:C:250:HIS:CD2	2.45	0.51
1:F:249:ILE:HD12	1:F:249:ILE:N	2.26	0.51
1:C:227:ILE:HD13	1:C:227:ILE:N	2.25	0.51
1:E:97:ASN:OD1	1:E:99:LYS:CB	2.53	0.51
1:E:102:SER:CA	1:E:106:VAL:O	2.59	0.51
1:A:133:PRO:CB	1:A:137:PHE:CD2	2.94	0.51
1:D:174:ASP:OD1	1:D:176:ARG:HG2	2.10	0.51
1:A:44:GLY:HA2	1:A:58:VAL:HG23	1.93	0.50
1:B:34:LEU:HD22	1:B:269:LEU:HD23	1.93	0.50
1:E:109:TRP:CE3	1:E:131:LEU:HD13	2.46	0.50
1:E:232:LEU:O	1:E:232:LEU:HD12	2.11	0.50
1:F:79:VAL:O	1:F:81:TRP:N	2.44	0.50
1:A:102:SER:O	1:A:107:LYS:NZ	2.32	0.50
1:A:43:CYS:C	1:A:44:GLY:O	2.51	0.50
1:D:257:ILE:HG22	1:D:258:TYR:O	2.11	0.50
1:F:177:ILE:HG21	1:F:201:PHE:HB2	1.93	0.50
1:E:78:ARG:HG3	1:E:79:VAL:N	2.26	0.50
1:E:114:SER:OG	1:E:115:ARG:NE	2.45	0.50
1:E:133:PRO:HB3	1:E:146:TYR:CD1	2.46	0.50
1:F:285:VAL:HG12	1:F:286:GLU:N	2.27	0.50
1:F:80:PHE:O	1:F:83:GLY:N	2.43	0.50
1:F:138:GLN:O	1:F:142:PHE:HB2	2.11	0.50
1:F:279:LEU:CD1	1:F:298:ILE:HD12	2.35	0.50
1:D:274:ARG:HE	1:D:304:HIS:CD2	2.29	0.50
1:F:42:ARG:HH11	1:F:42:ARG:HB2	1.76	0.50
1:A:281:ILE:H	1:A:281:ILE:HD12	1.75	0.50
1:B:88:LEU:O	1:B:92:ILE:HG12	2.11	0.50
1:C:164:VAL:O	1:C:168:ILE:HG13	2.12	0.50
1:D:221:LEU:O	1:D:224:PRO:HD2	2.12	0.50
1:D:282:LEU:HD12	1:D:294:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TYR:CD1	1:B:279:LEU:HD23	2.47	0.50
1:E:32:GLN:C	1:E:34:LEU:HD12	2.33	0.50
1:E:66:SER:HA	1:E:247:ASP:OD1	2.12	0.50
1:F:30:GLU:C	1:F:32:GLN:N	2.68	0.50
1:A:141:HIS:O	1:A:142:PHE:C	2.55	0.49
1:A:279:LEU:CD1	1:A:298:ILE:HD13	2.42	0.49
1:B:168:ILE:CD1	1:B:168:ILE:CB	2.79	0.49
1:F:174:ASP:OD1	1:F:176:ARG:HD2	2.12	0.49
1:A:86:GLU:HG2	1:A:104:LYS:HB2	1.94	0.49
1:C:204:VAL:HG22	1:C:205:ASN:H	1.76	0.49
1:D:192:LEU:HD13	4:D:637:HOH:O	2.11	0.49
1:A:56:LEU:HD13	1:A:259:LEU:CD2	2.42	0.49
1:B:40:ILE:HG22	1:B:40:ILE:O	2.13	0.49
1:E:102:SER:CB	1:E:106:VAL:O	2.61	0.49
1:D:263:GLU:N	1:D:264:PRO:HD2	2.28	0.49
1:A:263:GLU:HB2	1:A:264:PRO:HD3	1.94	0.49
1:C:66:SER:C	1:C:67:LEU:HD23	2.37	0.49
1:E:32:GLN:HG3	1:E:64:ARG:N	2.27	0.49
1:D:215:ARG:HG3	1:D:216:SER:N	2.28	0.49
1:E:175:ARG:HG2	1:F:254:ASP:OD2	2.13	0.49
1:A:202:TYR:C	1:A:202:TYR:CD2	2.90	0.49
1:B:81:TRP:CE2	1:B:298:ILE:HG13	2.48	0.49
1:B:33:TYR:OH	1:B:219:MET:O	2.21	0.49
1:A:133:PRO:HB3	1:A:137:PHE:CD2	2.47	0.49
1:A:153:TYR:O	1:A:154:SER:C	2.54	0.49
1:C:112:ASN:HA	1:C:117:PHE:CD2	2.48	0.49
1:C:240:ILE:HG22	1:C:240:ILE:O	2.13	0.49
1:D:222:GLY:C	1:D:224:PRO:HD2	2.38	0.49
1:B:164:VAL:HG22	1:B:177:ILE:CG2	2.43	0.48
1:E:272:GLU:HA	1:E:273:PRO:HD2	1.51	0.48
1:F:28:HIS:HB3	1:F:31:LEU:HD11	1.94	0.48
1:B:141:HIS:O	1:B:142:PHE:C	2.48	0.48
1:D:126:ARG:HG2	1:D:130:ASP:HB3	1.94	0.48
1:D:126:ARG:CG	1:D:130:ASP:HB3	2.43	0.48
1:E:114:SER:OG	1:E:115:ARG:N	2.30	0.48
1:E:88:LEU:O	1:E:92:ILE:HG13	2.14	0.48
1:E:133:PRO:HG2	1:E:186:ASP:HB3	1.95	0.48
1:E:298:ILE:HG22	1:E:301:TYR:HB2	1.95	0.48
1:A:46:ARG:C	1:A:48:ASP:N	2.70	0.48
1:E:32:GLN:HB3	1:E:63:ALA:HB1	1.96	0.48
1:C:80:PHE:O	1:C:81:TRP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:PRO:O	1:E:304:HIS:O	2.31	0.48
1:F:44:GLY:HA2	1:F:58:VAL:HG23	1.95	0.48
1:A:174:ASP:OD1	1:A:176:ARG:HB2	2.14	0.48
1:C:169:LYS:HG3	1:C:241:THR:HG22	1.95	0.48
1:E:160:GLN:O	1:E:164:VAL:HG23	2.14	0.48
1:E:233:LEU:O	1:E:237:ILE:CG1	2.60	0.48
1:A:102:SER:HA	1:A:106:VAL:O	2.14	0.48
1:E:200:GLN:N	1:E:211:GLN:O	2.40	0.48
1:E:214:GLN:HB3	1:E:252:LEU:HD23	1.96	0.48
1:F:98:ALA:N	1:F:129:GLY:O	2.47	0.48
1:F:199:CYS:HA	1:F:211:GLN:O	2.13	0.48
1:E:60:GLY:C	1:E:61:MET:CG	2.86	0.48
1:F:164:VAL:O	1:F:168:ILE:HG13	2.13	0.48
1:B:214:GLN:HB3	1:B:252:LEU:HD23	1.95	0.48
1:C:90:TRP:NE1	1:C:95:SER:OG	2.46	0.48
1:B:185:ARG:HH21	1:B:185:ARG:CG	2.25	0.47
1:C:182:TRP:CZ2	1:C:187:LEU:HD11	2.49	0.47
1:E:202:TYR:CD1	1:F:59:PHE:CD2	3.02	0.47
1:F:192:LEU:H	1:F:192:LEU:HD23	1.79	0.47
1:C:30:GLU:OE1	1:C:76:THR:HG23	2.14	0.47
1:D:151:SER:HB2	1:D:153:TYR:CZ	2.49	0.47
1:E:294:GLU:C	1:E:296:PHE:H	2.19	0.47
1:F:96:THR:CG2	1:F:146:TYR:OH	2.62	0.47
1:F:257:ILE:HG22	1:F:258:TYR:O	2.14	0.47
1:B:100:GLU:HG3	1:B:100:GLU:O	2.13	0.47
1:C:240:ILE:O	1:C:240:ILE:CG2	2.62	0.47
1:D:217:GLY:HA3	1:D:252:LEU:HD21	1.95	0.47
2:E:618:PO4:O2	3:E:628:BME:C2	2.63	0.47
1:B:68:ARG:HG3	1:B:68:ARG:NH1	2.28	0.47
1:C:262:ILE:O	1:C:263:GLU:C	2.52	0.47
1:E:87:GLU:O	1:E:88:LEU:C	2.52	0.47
1:A:262:ILE:O	1:A:266:LYS:HB2	2.15	0.47
1:E:126:ARG:HD3	1:E:130:ASP:OD1	2.15	0.47
1:E:265:LEU:HD12	1:E:268:GLN:HB2	1.96	0.47
1:F:80:PHE:CE2	1:F:106:VAL:HG13	2.48	0.47
1:A:56:LEU:HD13	1:A:259:LEU:HD21	1.96	0.47
1:A:99:LYS:HA	4:A:635:HOH:O	2.15	0.47
1:B:267:ILE:O	1:B:270:GLN:HB2	2.13	0.47
1:D:167:THR:O	1:D:168:ILE:C	2.57	0.47
1:F:133:PRO:HD2	1:F:190:MET:HG2	1.95	0.47
1:F:285:VAL:HG12	1:F:286:GLU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HG22	1:A:298:ILE:O	2.15	0.47
1:B:198:LEU:HD12	1:B:198:LEU:C	2.40	0.47
1:C:77:LYS:O	1:C:78:ARG:C	2.58	0.47
1:D:187:LEU:N	1:D:188:PRO:CD	2.77	0.47
1:F:86:GLU:HB3	1:F:101:LEU:HD23	1.96	0.47
1:C:81:TRP:O	1:C:82:LYS:C	2.54	0.47
1:D:32:GLN:O	1:D:36:GLN:HG3	2.14	0.47
1:F:169:LYS:HE3	1:F:241:THR:HA	1.97	0.47
1:E:132:GLY:HA3	1:E:190:MET:HA	1.96	0.47
1:E:211:GLN:HG3	1:E:249:ILE:O	2.14	0.47
1:E:301:TYR:CE1	1:E:303:PRO:HG3	2.49	0.47
1:F:30:GLU:C	1:F:32:GLN:H	2.23	0.47
1:E:259:LEU:C	1:E:261:HIS:N	2.73	0.46
1:C:121:LEU:HD12	1:C:123:PHE:CE2	2.51	0.46
1:E:240:ILE:HD11	1:E:288:ILE:HD12	1.97	0.46
1:A:257:ILE:HG22	1:A:258:TYR:O	2.16	0.46
1:E:45:VAL:HG23	1:F:204:VAL:HG21	1.94	0.46
1:A:40:ILE:HD12	1:A:219:MET:HG3	1.97	0.46
1:B:202:TYR:CD2	1:B:202:TYR:C	2.93	0.46
1:E:286:GLU:H	1:E:286:GLU:HG3	1.66	0.46
1:F:204:VAL:O	1:F:207:GLU:CB	2.52	0.46
1:F:240:ILE:HD13	1:F:288:ILE:HB	1.97	0.46
1:A:107:LYS:HD2	1:A:110:ASP:OD2	2.15	0.46
1:C:204:VAL:CG2	1:C:205:ASN:H	2.29	0.46
1:D:126:ARG:HD2	1:D:130:ASP:HB3	1.93	0.46
1:D:196:HIS:HB3	1:D:212:LEU:HD11	1.98	0.46
1:D:206:SER:HA	1:D:243:LEU:HD22	1.98	0.46
1:E:60:GLY:O	1:E:61:MET:CG	2.62	0.46
1:F:96:THR:HG21	1:F:146:TYR:OH	2.15	0.46
1:A:182:TRP:CZ2	1:A:187:LEU:HD11	2.51	0.46
1:A:199:CYS:HA	1:A:211:GLN:O	2.16	0.46
1:B:134:VAL:O	1:B:135:TYR:C	2.57	0.46
1:F:177:ILE:CG2	1:F:201:PHE:HB2	2.46	0.46
1:F:282:LEU:O	1:F:283:ARG:CB	2.63	0.46
1:A:158:VAL:HG12	1:A:159:ASP:N	2.29	0.46
1:D:277:PRO:HG3	1:D:301:TYR:CD1	2.51	0.46
1:F:144:ALA:H	1:F:157:GLY:HA3	1.80	0.46
1:A:279:LEU:HD13	1:A:298:ILE:CD1	2.46	0.46
1:C:217:GLY:HA2	3:C:626:BME:H22	1.98	0.46
1:E:171:ASN:ND2	1:E:174:ASP:HB2	2.30	0.46
1:E:107:LYS:O	1:E:108:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:PRO:C	1:F:276:PHE:CE1	2.94	0.46
1:F:139:TRP:CD2	1:F:179:MET:HE1	2.51	0.46
1:B:82:LYS:O	1:B:86:GLU:HB2	2.16	0.46
1:C:92:ILE:HD11	1:C:236:MET:HE2	1.97	0.45
1:C:183:ASN:OD1	1:C:183:ASN:C	2.58	0.45
1:F:215:ARG:HG3	1:F:215:ARG:HH11	1.81	0.45
1:A:279:LEU:HB2	1:A:298:ILE:CD1	2.47	0.45
1:B:97:ASN:HA	1:B:129:GLY:O	2.17	0.45
1:B:222:GLY:O	1:B:223:VAL:C	2.60	0.45
1:D:223:VAL:N	1:D:224:PRO:HD3	2.27	0.45
1:E:33:TYR:HA	1:E:36:GLN:HB2	1.98	0.45
1:A:74:LEU:HD12	1:A:224:PRO:HB3	1.98	0.45
1:C:102:SER:HB2	1:C:110:ASP:OD1	2.15	0.45
1:E:271:ARG:NH1	1:E:304:HIS:CB	2.78	0.45
1:F:161:LEU:HG	1:F:165:ILE:HD11	1.99	0.45
1:A:287:LYS:O	1:A:290:ASP:HB3	2.16	0.45
1:E:178:ILE:HG22	1:E:179:MET:N	2.31	0.45
1:E:279:LEU:CD1	1:E:298:ILE:HD13	2.45	0.45
1:F:54:GLY:C	1:F:55:THR:CG2	2.90	0.45
1:D:276:PHE:HA	1:D:277:PRO:HD2	1.42	0.45
1:F:283:ARG:C	1:F:284:LYS:HG2	2.42	0.45
1:E:261:HIS:CA	1:E:264:PRO:HG2	2.34	0.45
1:A:267:ILE:O	1:A:270:GLN:HG3	2.17	0.45
1:B:165:ILE:O	1:B:166:ASP:C	2.57	0.45
1:C:254:ASP:OD1	1:C:254:ASP:C	2.60	0.45
1:C:46:ARG:HA	1:C:55:THR:O	2.17	0.45
1:C:121:LEU:CD1	1:C:123:PHE:CE2	3.00	0.45
1:D:81:TRP:O	1:D:81:TRP:CG	2.66	0.45
1:F:119:ASP:OD1	1:F:124:SER:HB3	2.16	0.45
1:F:233:LEU:CD1	1:F:237:ILE:HG12	2.47	0.45
1:A:68:ARG:O	1:A:69:ASP:HB2	2.16	0.45
1:C:50:ARG:NH1	1:C:50:ARG:HG2	2.32	0.45
1:E:192:LEU:O	1:E:192:LEU:CD1	2.60	0.45
1:A:86:GLU:HG2	1:A:104:LYS:CB	2.47	0.44
1:C:53:THR:HG22	1:C:54:GLY:N	2.31	0.44
1:C:212:LEU:HD22	1:C:230:TYR:CD2	2.52	0.44
1:D:38:GLN:O	1:D:42:ARG:HB2	2.17	0.44
1:E:78:ARG:CG	1:E:79:VAL:N	2.80	0.44
1:E:260:ASN:N	1:E:260:ASN:OD1	2.50	0.44
1:F:301:TYR:CZ	1:F:303:PRO:HG3	2.52	0.44
1:D:33:TYR:O	1:D:37:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:LEU:O	1:F:283:ARG:HB2	2.16	0.44
1:B:254:ASP:C	1:B:254:ASP:OD1	2.59	0.44
1:D:139:TRP:CD2	1:D:179:MET:CE	3.00	0.44
1:D:268:GLN:O	1:D:271:ARG:HB2	2.16	0.44
1:D:283:ARG:HB2	1:D:284:LYS:H	1.44	0.44
1:E:271:ARG:O	1:E:273:PRO:HD2	2.17	0.44
1:F:272:GLU:HA	1:F:273:PRO:HD3	1.69	0.44
1:D:168:ILE:CD1	1:D:177:ILE:HD13	2.46	0.44
1:F:34:LEU:O	1:F:37:ILE:N	2.50	0.44
1:F:187:LEU:HB3	1:F:188:PRO:HD3	1.99	0.44
1:D:223:VAL:O	1:D:227:ILE:HG12	2.18	0.44
1:D:274:ARG:O	1:D:275:PRO:C	2.59	0.44
1:E:195:CYS:O	1:E:214:GLN:HA	2.18	0.44
1:F:232:LEU:C	1:F:234:THR:N	2.73	0.44
1:D:57:SER:O	1:D:58:VAL:HG23	2.17	0.44
1:D:126:ARG:CD	1:D:130:ASP:CB	2.93	0.44
1:F:43:CYS:O	1:F:44:GLY:O	2.35	0.44
1:A:78:ARG:NH2	4:A:618:HOH:O	2.47	0.44
1:A:259:LEU:HD23	1:A:262:ILE:HD11	1.99	0.44
1:B:162:GLN:NE2	1:B:166:ASP:OD2	2.46	0.44
1:C:102:SER:C	1:C:104:LYS:N	2.76	0.44
1:E:259:LEU:O	1:E:261:HIS:N	2.51	0.44
1:F:30:GLU:O	1:F:30:GLU:HG2	2.18	0.44
1:C:30:GLU:OE2	1:C:75:THR:N	2.36	0.43
1:D:67:LEU:HD21	1:D:248:PHE:HB3	2.00	0.43
1:D:236:MET:CE	1:D:291:PHE:CD2	3.01	0.43
1:F:162:GLN:O	1:F:165:ILE:HG12	2.18	0.43
1:F:187:LEU:HA	1:F:187:LEU:HD12	1.66	0.43
1:F:206:SER:HA	1:F:243:LEU:HD23	2.00	0.43
1:A:223:VAL:HG13	1:A:250:HIS:CE1	2.53	0.43
1:D:86:GLU:HG2	1:D:104:LYS:HB2	2.00	0.43
1:D:126:ARG:HD3	1:D:130:ASP:CB	2.48	0.43
1:F:100:GLU:O	1:F:100:GLU:CG	2.65	0.43
1:F:279:LEU:CD1	1:F:298:ILE:CD1	2.95	0.43
1:B:34:LEU:O	1:B:37:ILE:N	2.50	0.43
1:D:277:PRO:HG3	1:D:301:TYR:HD1	1.83	0.43
1:F:270:GLN:O	1:F:271:ARG:C	2.60	0.43
1:F:288:ILE:HD12	1:F:291:PHE:CE2	2.53	0.43
1:A:126:ARG:HG2	1:A:130:ASP:CB	2.42	0.43
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.87	0.43
1:B:102:SER:HA	1:B:106:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:SER:O	1:E:118:LEU:HG	2.17	0.43
1:F:161:LEU:HD12	1:F:161:LEU:HA	1.73	0.43
1:F:215:ARG:HG3	1:F:215:ARG:NH1	2.34	0.43
1:B:68:ARG:HG3	1:B:68:ARG:HH11	1.83	0.43
1:B:125:THR:HG23	1:B:125:THR:O	2.17	0.43
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.54	0.43
1:B:280:ARG:HH11	1:B:280:ARG:HG2	1.77	0.43
1:C:218:ASP:H	3:C:626:BME:C2	2.31	0.43
1:E:46:ARG:HH11	1:E:259:LEU:HD11	1.84	0.43
1:A:78:ARG:NH1	4:A:618:HOH:O	2.24	0.43
1:A:270:GLN:H	1:A:270:GLN:HG2	1.12	0.43
1:B:259:LEU:C	1:B:261:HIS:H	2.25	0.43
1:F:97:ASN:ND2	1:F:100:GLU:H	2.14	0.43
1:A:105:GLY:HA2	1:A:107:LYS:HZ3	1.84	0.43
1:D:278:LYS:HD3	1:D:299:GLU:OE2	2.18	0.43
1:A:48:ASP:O	1:A:54:GLY:HA2	2.18	0.43
1:A:211:GLN:HA	1:A:249:ILE:O	2.19	0.43
1:E:100:GLU:O	1:E:101:LEU:C	2.61	0.43
1:E:262:ILE:HG12	1:E:262:ILE:H	1.65	0.43
1:A:110:ASP:O	1:A:111:ALA:C	2.61	0.43
1:A:134:VAL:O	1:A:135:TYR:C	2.60	0.43
1:B:236:MET:HE2	1:B:291:PHE:CD2	2.53	0.43
1:C:124:SER:OG	1:C:125:THR:N	2.52	0.43
1:A:212:LEU:HA	1:A:212:LEU:HD12	1.77	0.42
1:A:213:TYR:CD1	1:A:213:TYR:C	2.97	0.42
1:A:271:ARG:HD3	1:A:304:HIS:CG	2.54	0.42
1:C:168:ILE:O	1:C:168:ILE:HG22	2.18	0.42
1:C:222:GLY:O	1:C:223:VAL:C	2.62	0.42
1:A:196:HIS:CD2	1:A:212:LEU:HD21	2.54	0.42
1:E:92:ILE:O	1:E:140:ARG:NH1	2.51	0.42
1:E:184:PRO:HD2	1:F:142:PHE:CE2	2.54	0.42
1:E:271:ARG:HD3	1:E:304:HIS:CG	2.54	0.42
1:F:68:ARG:C	1:F:69:ASP:CG	2.87	0.42
1:F:239:HIS:C	1:F:241:THR:N	2.76	0.42
1:A:64:ARG:NH1	1:B:60:GLY:O	2.52	0.42
1:A:133:PRO:HB3	1:A:137:PHE:CE2	2.53	0.42
1:B:192:LEU:HD13	1:B:192:LEU:H	1.84	0.42
1:B:223:VAL:O	1:B:224:PRO:C	2.57	0.42
1:E:99:LYS:HA	1:E:99:LYS:HD3	1.72	0.42
1:E:102:SER:HA	1:E:106:VAL:O	2.19	0.42
1:A:240:ILE:HD13	1:A:240:ILE:HG21	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLU:CB	1:A:264:PRO:CD	2.98	0.42
1:C:37:ILE:HG22	1:C:41:LEU:HD12	2.02	0.42
1:C:112:ASN:O	1:C:117:PHE:HD2	2.01	0.42
1:C:257:ILE:O	1:C:257:ILE:CG2	2.63	0.42
1:E:274:ARG:O	1:E:275:PRO:O	2.36	0.42
1:F:163:LYS:HA	1:F:166:ASP:OD1	2.20	0.42
1:B:37:ILE:HD12	1:B:37:ILE:HG23	1.68	0.42
1:B:123:PHE:C	1:B:125:THR:N	2.76	0.42
1:C:186:ASP:O	1:C:187:LEU:C	2.61	0.42
1:C:214:GLN:OE1	1:C:250:HIS:CE1	2.70	0.42
1:D:222:GLY:C	1:D:224:PRO:CD	2.93	0.42
1:A:115:ARG:NH1	1:A:115:ARG:CG	2.64	0.42
1:A:184:PRO:HD2	1:B:142:PHE:CE2	2.55	0.42
1:C:142:PHE:C	1:C:142:PHE:CD2	2.97	0.42
1:E:236:MET:HE3	1:E:236:MET:HB3	1.78	0.42
1:F:119:ASP:O	1:F:120:SER:C	2.62	0.42
1:A:187:LEU:N	1:A:188:PRO:CD	2.83	0.42
1:A:205:ASN:O	1:A:206:SER:HB2	2.19	0.42
1:B:178:ILE:CG2	1:B:179:MET:N	2.82	0.42
1:B:259:LEU:C	1:B:261:HIS:N	2.74	0.42
1:C:81:TRP:O	1:C:84:VAL:HB	2.20	0.42
1:D:46:ARG:C	1:D:46:ARG:HD3	2.44	0.42
1:E:187:LEU:N	1:E:188:PRO:HD2	2.34	0.42
2:E:619:PO4:O4	1:F:215:ARG:NH1	2.52	0.42
1:B:46:ARG:HB3	1:B:46:ARG:NH2	2.34	0.42
1:B:133:PRO:HG2	1:B:186:ASP:HB3	2.01	0.42
1:C:152:ASP:OD1	1:C:154:SER:HB2	2.20	0.42
1:E:187:LEU:HD22	1:E:187:LEU:HA	1.78	0.42
1:E:203:VAL:HA	1:E:207:GLU:O	2.20	0.42
1:B:196:HIS:HB3	1:B:212:LEU:HD11	2.01	0.42
1:D:41:LEU:HA	1:D:56:LEU:HD22	2.02	0.42
1:F:31:LEU:O	1:F:35:GLY:N	2.37	0.42
1:F:135:TYR:O	1:F:136:GLY:C	2.62	0.42
1:B:123:PHE:C	1:B:125:THR:H	2.28	0.41
1:C:97:ASN:O	1:C:98:ALA:C	2.62	0.41
1:C:177:ILE:CG2	1:C:201:PHE:HB2	2.50	0.41
1:A:292:LYS:C	1:A:294:GLU:N	2.78	0.41
1:D:37:ILE:HG12	1:D:37:ILE:H	1.60	0.41
1:D:147:ARG:HH12	1:D:156:GLN:NE2	2.11	0.41
1:E:200:GLN:NE2	1:F:213:TYR:OH	2.51	0.41
1:E:252:LEU:HD13	1:E:255:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:SER:HA	1:B:243:LEU:HD22	2.01	0.41
1:C:205:ASN:O	1:C:206:SER:C	2.62	0.41
1:D:265:LEU:HD23	1:D:265:LEU:HA	1.91	0.41
1:E:82:LYS:O	1:E:86:GLU:CB	2.65	0.41
1:E:97:ASN:C	1:E:99:LYS:N	2.78	0.41
1:E:199:CYS:HA	1:E:211:GLN:O	2.20	0.41
1:E:210:CYS:O	1:E:248:PHE:HA	2.20	0.41
1:C:222:GLY:HA3	3:C:626:BME:H21	2.02	0.41
1:C:274:ARG:H	1:C:274:ARG:HG3	1.64	0.41
1:D:30:GLU:OE1	1:D:76:THR:HG23	2.20	0.41
1:E:206:SER:HA	1:E:243:LEU:CD2	2.50	0.41
1:D:31:LEU:O	1:D:35:GLY:N	2.35	0.41
1:E:159:ASP:OD1	1:E:159:ASP:C	2.63	0.41
1:A:279:LEU:HB2	1:A:298:ILE:HD13	2.01	0.41
1:C:72:PRO:O	1:C:72:PRO:CG	2.65	0.41
1:C:115:ARG:HH11	1:C:115:ARG:HD2	1.61	0.41
1:D:252:LEU:HD12	4:D:635:HOH:O	2.20	0.41
1:D:263:GLU:CD	1:D:263:GLU:H	2.28	0.41
1:E:124:SER:C	1:E:126:ARG:N	2.78	0.41
1:E:199:CYS:HB3	1:E:212:LEU:HD12	2.02	0.41
1:F:91:PHE:CD1	1:F:135:TYR:HB2	2.52	0.41
1:A:283:ARG:HH11	1:A:283:ARG:HB2	1.85	0.41
1:D:141:HIS:O	1:D:142:PHE:C	2.59	0.41
1:E:258:TYR:HB2	1:E:261:HIS:CD2	2.55	0.41
1:F:72:PRO:C	1:F:276:PHE:HE1	2.29	0.41
1:A:103:SER:C	1:A:105:GLY:H	2.28	0.41
1:A:105:GLY:HA2	1:A:107:LYS:NZ	2.36	0.41
1:A:177:ILE:HD13	1:A:177:ILE:HG21	1.71	0.41
1:B:185:ARG:HG2	1:B:185:ARG:NH2	2.30	0.41
1:C:77:LYS:HB2	1:C:268:GLN:NE2	2.35	0.41
1:C:194:PRO:O	1:C:215:ARG:NE	2.45	0.41
1:F:233:LEU:C	1:F:233:LEU:CD1	2.86	0.41
1:A:108:ILE:HG21	1:A:108:ILE:HD12	1.79	0.41
1:B:135:TYR:O	1:B:136:GLY:C	2.64	0.41
1:B:260:ASN:OD1	1:B:260:ASN:N	2.48	0.41
1:C:85:LEU:CD1	1:C:296:PHE:CD1	3.03	0.41
1:C:142:PHE:HB2	1:C:160:GLN:HE21	1.86	0.41
1:C:185:ARG:O	1:C:188:PRO:HD2	2.20	0.41
1:D:80:PHE:CD1	1:D:80:PHE:C	2.97	0.41
1:E:169:LYS:HG3	1:E:241:THR:HG22	2.03	0.41
1:E:266:LYS:HE3	1:E:266:LYS:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:619:PO4:O4	1:F:215:ARG:NH2	2.54	0.41
1:F:37:ILE:O	1:F:37:ILE:CG2	2.68	0.41
1:F:50:ARG:HE	1:F:50:ARG:HB3	1.58	0.41
1:F:66:SER:OG	1:F:68:ARG:HB2	2.21	0.41
1:F:108:ILE:HG13	1:F:109:TRP:CD1	2.55	0.41
1:F:195:CYS:O	1:F:214:GLN:HA	2.21	0.41
1:F:304:HIS:HA	1:F:305:PRO:HD3	1.79	0.41
1:A:288:ILE:C	1:A:290:ASP:H	2.29	0.41
1:D:168:ILE:HD13	1:D:177:ILE:HG21	1.99	0.41
1:D:236:MET:HE2	1:D:236:MET:HB3	1.62	0.41
1:E:60:GLY:C	1:E:61:MET:HG3	2.46	0.41
1:C:130:ASP:CG	1:C:149:MET:HB3	2.46	0.40
1:D:28:HIS:HD1	1:D:30:GLU:HB3	1.86	0.40
1:D:202:TYR:CD2	1:D:202:TYR:C	2.99	0.40
1:E:121:LEU:HB2	1:E:123:PHE:CE1	2.57	0.40
1:E:140:ARG:C	1:E:141:HIS:CG	2.98	0.40
1:E:196:HIS:HB3	1:E:212:LEU:HD11	2.03	0.40
1:F:139:TRP:CD2	1:F:179:MET:CE	3.05	0.40
1:B:52:GLY:O	1:B:53:THR:C	2.63	0.40
1:B:197:ALA:O	1:B:198:LEU:HB3	2.21	0.40
1:C:257:ILE:HD13	1:C:257:ILE:HG21	1.76	0.40
1:E:254:ASP:OD2	1:F:175:ARG:CD	2.67	0.40
1:F:121:LEU:HD13	1:F:123:PHE:HE2	1.86	0.40
1:F:159:ASP:CG	1:F:162:GLN:HB2	2.45	0.40
1:F:169:LYS:HG3	1:F:241:THR:HG22	2.02	0.40
1:F:277:PRO:HG3	1:F:301:TYR:HA	2.02	0.40
1:C:39:HIS:CE1	1:C:43:CYS:SG	3.14	0.40
1:D:71:PHE:CD1	1:D:71:PHE:C	2.98	0.40
1:E:30:GLU:O	1:E:30:GLU:CD	2.62	0.40
1:B:169:LYS:HE2	1:B:169:LYS:HB3	1.80	0.40
1:B:223:VAL:O	1:B:227:ILE:HG12	2.21	0.40
1:D:92:ILE:O	1:D:92:ILE:HG22	2.21	0.40
1:F:301:TYR:CE1	1:F:303:PRO:HG3	2.56	0.40
1:A:71:PHE:HD2	1:A:235:TYR:CE2	2.40	0.40
1:B:192:LEU:N	1:B:192:LEU:CD1	2.84	0.40
1:D:50:ARG:H	1:D:50:ARG:HG3	1.71	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	280/313 (90%)	251 (90%)	21 (8%)	8 (3%)	3	8
1	B	279/313 (89%)	254 (91%)	20 (7%)	5 (2%)	6	15
1	C	279/313 (89%)	239 (86%)	32 (12%)	8 (3%)	3	8
1	D	279/313 (89%)	235 (84%)	32 (12%)	12 (4%)	2	4
1	E	279/313 (89%)	210 (75%)	41 (15%)	28 (10%)	0	0
1	F	279/313 (89%)	208 (75%)	49 (18%)	22 (8%)	1	1
All	All	1675/1878 (89%)	1397 (83%)	195 (12%)	83 (5%)	1	3

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	50	ARG
1	A	53	THR
1	C	103	SER
1	D	69	ASP
1	D	155	GLY
1	E	31	LEU
1	E	32	GLN
1	E	34	LEU
1	E	41	LEU
1	E	80	PHE
1	E	101	LEU
1	E	102	SER
1	E	114	SER
1	E	132	GLY
1	E	134	VAL
1	E	144	ALA
1	E	295	ASP
1	F	127	GLU
1	F	134	VAL

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Mol	Chain	Res	Type
1	F	154	SER
1	F	240	ILE
1	F	271	ARG
1	F	277	PRO
1	F	283	ARG
1	A	80	PHE
1	A	293	ALA
1	C	80	PHE
1	C	154	SER
1	D	191	ALA
1	E	29	GLY
1	E	33	TYR
1	E	154	SER
1	E	260	ASN
1	E	277	PRO
1	F	80	PHE
1	F	149	MET
1	F	150	GLU
1	F	260	ASN
1	F	301	TYR
1	F	305	PRO
1	B	136	GLY
1	C	135	TYR
1	C	277	PRO
1	D	277	PRO
1	D	294	GLU
1	E	189	LEU
1	E	220	GLY
1	E	273	PRO
1	E	275	PRO
1	E	304	HIS
1	F	174	ASP
1	F	261	HIS
1	B	191	ALA
1	B	268	GLN
1	C	128	GLU
1	D	29	GLY
1	D	144	ALA
1	D	154	SER
1	D	202	TYR
1	E	128	GLU
1	F	177	ILE

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Mol	Chain	Res	Type
1	F	222	GLY
1	F	239	HIS
1	F	268	GLN
1	F	275	PRO
1	D	72	PRO
1	D	102	SER
1	D	305	PRO
1	E	147	ARG
1	F	205	ASN
1	A	47	LYS
1	A	273	PRO
1	B	110	ASP
1	E	125	THR
1	F	293	ALA
1	B	277	PRO
1	E	108	ILE
1	C	84	VAL
1	E	83	GLY
1	A	277	PRO
1	C	157	GLY
1	E	60	GLY

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	246/271 (91%)	215 (87%)	31 (13%)	4 10
1	B	245/271 (90%)	215 (88%)	30 (12%)	5 10
1	C	245/271 (90%)	210 (86%)	35 (14%)	3 7
1	D	245/271 (90%)	203 (83%)	42 (17%)	2 5
1	E	245/271 (90%)	187 (76%)	58 (24%)	1 2
1	F	245/271 (90%)	184 (75%)	61 (25%)	0 2
All	All	1471/1626 (90%)	1214 (82%)	257 (18%)	2 4

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	31	LEU
1	A	37	ILE
1	A	38	GLN
1	A	51	THR
1	A	56	LEU
1	A	72	PRO
1	A	82	LYS
1	A	93	LYS
1	A	99	LYS
1	A	108	ILE
1	A	114	SER
1	A	115	ARG
1	A	125	THR
1	A	127	GLU
1	A	148	ASP
1	A	151	SER
1	A	164	VAL
1	A	176	ARG
1	A	192	LEU
1	A	198	LEU
1	A	202	TYR
1	A	263	GLU
1	A	270	GLN
1	A	279	LEU
1	A	281	ILE
1	A	283	ARG
1	A	284	LYS
1	A	292	LYS
1	A	295	ASP
1	A	298	ILE
1	B	40	ILE
1	B	45	VAL
1	B	50	ARG
1	B	56	LEU
1	B	57	SER
1	B	58	VAL
1	B	82	LYS
1	B	86	GLU
1	B	103	SER
1	B	108	ILE
1	B	115	ARG

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Mol	Chain	Res	Type
1	B	125	THR
1	B	127	GLU
1	B	147	ARG
1	B	164	VAL
1	B	184	PRO
1	B	185	ARG
1	B	192	LEU
1	B	198	LEU
1	B	202	TYR
1	B	206	SER
1	B	216	SER
1	B	221	LEU
1	B	240	ILE
1	B	260	ASN
1	B	263	GLU
1	B	280	ARG
1	B	282	LEU
1	B	288	ILE
1	B	289	ASP
1	C	38	GLN
1	C	42	ARG
1	C	56	LEU
1	C	69	ASP
1	C	78	ARG
1	C	95	SER
1	C	103	SER
1	C	108	ILE
1	C	115	ARG
1	C	126	ARG
1	C	127	GLU
1	C	128	GLU
1	C	147	ARG
1	C	151	SER
1	C	154	SER
1	C	156	GLN
1	C	163	LYS
1	C	164	VAL
1	C	168	ILE
1	C	176	ARG
1	C	178	ILE
1	C	179	MET
1	C	185	ARG

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Mol	Chain	Res	Type
1	C	192	LEU
1	C	198	LEU
1	C	216	SER
1	C	221	LEU
1	C	227	ILE
1	C	236	MET
1	C	240	ILE
1	C	257	ILE
1	C	281	ILE
1	C	283	ARG
1	C	294	GLU
1	C	306	THR
1	D	32	GLN
1	D	37	ILE
1	D	38	GLN
1	D	41	LEU
1	D	50	ARG
1	D	51	THR
1	D	56	LEU
1	D	58	VAL
1	D	68	ARG
1	D	70	GLU
1	D	75	THR
1	D	77	LYS
1	D	100	GLU
1	D	102	SER
1	D	108	ILE
1	D	120	SER
1	D	127	GLU
1	D	147	ARG
1	D	149	MET
1	D	150	GLU
1	D	163	LYS
1	D	164	VAL
1	D	168	ILE
1	D	169	LYS
1	D	176	ARG
1	D	185	ARG
1	D	187	LEU
1	D	192	LEU
1	D	198	LEU
1	D	204	VAL

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Mol	Chain	Res	Type
1	D	209	SER
1	D	232	LEU
1	D	240	ILE
1	D	244	LYS
1	D	252	LEU
1	D	266	LYS
1	D	280	ARG
1	D	284	LYS
1	D	285	VAL
1	D	294	GLU
1	D	299	GLU
1	D	302	ASN
1	E	30	GLU
1	E	34	LEU
1	E	37	ILE
1	E	40	ILE
1	E	41	LEU
1	E	42	ARG
1	E	45	VAL
1	E	46	ARG
1	E	53	THR
1	E	68	ARG
1	E	74	LEU
1	E	76	THR
1	E	88	LEU
1	E	93	LYS
1	E	96	THR
1	E	99	LYS
1	E	104	LYS
1	E	107	LYS
1	E	108	ILE
1	E	112	ASN
1	E	115	ARG
1	E	121	LEU
1	E	124	SER
1	E	125	THR
1	E	145	GLU
1	E	147	ARG
1	E	148	ASP
1	E	151	SER
1	E	156	GLN
1	E	163	LYS

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Mol	Chain	Res	Type
1	E	165	ILE
1	E	168	ILE
1	E	170	THR
1	E	176	ARG
1	E	187	LEU
1	E	192	LEU
1	E	198	LEU
1	E	221	LEU
1	E	232	LEU
1	E	237	ILE
1	E	241	THR
1	E	249	ILE
1	E	257	ILE
1	E	262	ILE
1	E	265	LEU
1	E	267	ILE
1	E	272	GLU
1	E	278	LYS
1	E	279	LEU
1	E	280	ARG
1	E	281	ILE
1	E	283	ARG
1	E	286	GLU
1	E	288	ILE
1	E	289	ASP
1	E	294	GLU
1	E	299	GLU
1	E	306	THR
1	F	31	LEU
1	F	42	ARG
1	F	50	ARG
1	F	53	THR
1	F	58	VAL
1	F	69	ASP
1	F	73	LEU
1	F	74	LEU
1	F	76	THR
1	F	87	GLU
1	F	92	ILE
1	F	96	THR
1	F	101	LEU
1	F	102	SER

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Mol	Chain	Res	Type
1	F	106	VAL
1	F	116	ASP
1	F	117	PHE
1	F	120	SER
1	F	124	SER
1	F	125	THR
1	F	128	GLU
1	F	140	ARG
1	F	147	ARG
1	F	149	MET
1	F	151	SER
1	F	154	SER
1	F	162	GLN
1	F	164	VAL
1	F	165	ILE
1	F	166	ASP
1	F	168	ILE
1	F	176	ARG
1	F	178	ILE
1	F	180	CYS
1	F	185	ARG
1	F	187	LEU
1	F	198	LEU
1	F	204	VAL
1	F	205	ASN
1	F	206	SER
1	F	221	LEU
1	F	233	LEU
1	F	237	ILE
1	F	239	HIS
1	F	243	LEU
1	F	244	LYS
1	F	247	ASP
1	F	252	LEU
1	F	259	LEU
1	F	262	ILE
1	F	267	ILE
1	F	269	LEU
1	F	272	GLU
1	F	278	LYS
1	F	281	ILE
1	F	284	LYS

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Mol	Chain	Res	Type
1	F	285	VAL
1	F	286	GLU
1	F	292	LYS
1	F	295	ASP
1	F	298	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	38	GLN
1	A	62	GLN
1	A	97	ASN
1	A	112	ASN
1	A	141	HIS
1	A	160	GLN
1	A	171	ASN
1	A	211	GLN
1	A	297	GLN
1	A	302	ASN
1	B	196	HIS
1	B	250	HIS
1	C	39	HIS
1	C	141	HIS
1	C	156	GLN
1	C	226	ASN
1	C	250	HIS
1	C	268	GLN
1	D	38	GLN
1	D	112	ASN
1	D	156	GLN
1	D	268	GLN
1	D	270	GLN
1	D	297	GLN
1	D	302	ASN
1	E	112	ASN
1	E	160	GLN
1	E	196	HIS
1	E	200	GLN
1	E	205	ASN
1	E	226	ASN
1	E	250	HIS

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Mol	Chain	Res	Type
1	E	261	HIS
1	E	302	ASN
1	F	97	ASN
1	F	112	ASN
1	F	156	GLN
1	F	160	GLN
1	F	211	GLN
1	F	260	ASN
1	F	261	HIS
1	F	302	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	PO4	A	615	-	4,4,4	0.83	0	6,6,6	1.68	2 (33%)
2	PO4	C	616	-	4,4,4	1.42	1 (25%)	6,6,6	2.79	4 (66%)
3	BME	E	628	-	3,3,3	0.19	0	2,2,2	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	E	618	-	4,4,4	0.65	0	6,6,6	1.31	1 (16%)
2	PO4	D	617	-	4,4,4	1.30	0	6,6,6	1.02	0
3	BME	C	626	-	3,3,3	0.62	0	2,2,2	0.99	0
2	PO4	E	619	-	4,4,4	0.83	0	6,6,6	1.23	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	E	628	-	-	0/1/1/1	-
3	BME	C	626	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	616	PO4	P-O4	-2.23	1.48	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	616	PO4	O4-P-O3	4.50	121.90	107.91
2	C	616	PO4	O3-P-O1	-3.96	96.97	110.95
2	A	615	PO4	O2-P-O1	-3.43	98.82	110.95
2	C	616	PO4	O4-P-O1	-2.41	102.42	110.95
2	E	618	PO4	O2-P-O1	-2.35	102.65	110.95
2	C	616	PO4	O4-P-O2	2.19	114.72	107.91
2	A	615	PO4	O4-P-O1	2.11	118.41	110.95
2	E	619	PO4	O4-P-O1	-2.02	103.81	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	628	BME	2	0
2	E	618	PO4	2	0
3	C	626	BME	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	619	PO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	282/313 (90%)	-0.47	4 (1%) 73 71	5, 26, 51, 82	0
1	B	281/313 (89%)	-0.68	0 100 100	3, 21, 48, 58	0
1	C	281/313 (89%)	-0.28	0 100 100	9, 33, 56, 65	0
1	D	281/313 (89%)	0.00	5 (1%) 67 65	13, 40, 70, 93	0
1	E	281/313 (89%)	0.90	34 (12%) 8 7	29, 60, 99, 108	0
1	F	281/313 (89%)	1.21	55 (19%) 3 2	30, 76, 102, 114	0
All	All	1687/1878 (89%)	0.11	98 (5%) 29 25	3, 39, 91, 114	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	265	LEU	5.8
1	E	29	GLY	5.7
1	E	31	LEU	5.4
1	E	306	THR	5.0
1	F	306	THR	4.3
1	E	45	VAL	4.1
1	E	269	LEU	3.8
1	F	147	ARG	3.8
1	F	117	PHE	3.7
1	F	282	LEU	3.6
1	E	192	LEU	3.6
1	E	259	LEU	3.6
1	F	127	GLU	3.5
1	D	53	THR	3.4
1	F	72	PRO	3.4
1	F	148	ASP	3.4
1	F	146	TYR	3.4
1	F	26	PRO	3.4
1	E	34	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	74	LEU	3.2
1	F	267	ILE	3.2
1	F	192	LEU	3.2
1	E	26	PRO	3.2
1	E	107	LYS	3.1
1	E	53	THR	3.0
1	F	296	PHE	3.0
1	E	109	TRP	3.0
1	F	153	TYR	2.9
1	E	49	ASP	2.9
1	E	96	THR	2.9
1	F	149	MET	2.8
1	F	99	LYS	2.8
1	F	50	ARG	2.8
1	E	267	ILE	2.8
1	E	52	GLY	2.8
1	F	108	ILE	2.7
1	F	106	VAL	2.7
1	F	281	ILE	2.7
1	F	152	ASP	2.7
1	E	46	ARG	2.7
1	F	244	LYS	2.6
1	F	293	ALA	2.6
1	E	27	PRO	2.6
1	E	51	THR	2.6
1	F	275	PRO	2.6
1	F	101	LEU	2.6
1	E	294	GLU	2.6
1	E	264	PRO	2.6
1	F	191	ALA	2.6
1	E	102	SER	2.6
1	F	125	THR	2.6
1	F	186	ASP	2.5
1	F	243	LEU	2.5
1	F	105	GLY	2.5
1	F	154	SER	2.5
1	E	305	PRO	2.5
1	F	118	LEU	2.4
1	F	121	LEU	2.4
1	A	49	ASP	2.4
1	E	300	GLY	2.4
1	E	115	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	109	TRP	2.4
1	F	204	VAL	2.3
1	E	56	LEU	2.3
1	F	185	ARG	2.3
1	F	285	VAL	2.3
1	E	298	ILE	2.3
1	F	145	GLU	2.3
1	F	69	ASP	2.3
1	F	157	GLY	2.3
1	F	52	GLY	2.2
1	E	77	LYS	2.2
1	A	26	PRO	2.2
1	D	273	PRO	2.2
1	E	275	PRO	2.2
1	F	131	LEU	2.2
1	F	288	ILE	2.2
1	F	291	PHE	2.2
1	F	112	ASN	2.2
1	D	51	THR	2.1
1	E	155	GLY	2.1
1	E	111	ALA	2.1
1	F	51	THR	2.1
1	F	305	PRO	2.1
1	F	221	LEU	2.1
1	F	155	GLY	2.1
1	A	50	ARG	2.1
1	E	55	THR	2.1
1	F	172	PRO	2.1
1	E	262	ILE	2.1
1	F	30	GLU	2.0
1	A	51	THR	2.0
1	D	26	PRO	2.0
1	F	298	ILE	2.0
1	D	128	GLU	2.0
1	F	104	LYS	2.0
1	F	144	ALA	2.0
1	F	156	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BME	E	628	4/4	0.77	0.22	71,78,82,89	0
2	PO4	E	618	5/5	0.88	0.12	98,99,100,102	0
3	BME	C	626	4/4	0.90	0.15	45,47,50,58	0
2	PO4	E	619	5/5	0.91	0.13	75,77,79,80	0
2	PO4	D	617	5/5	0.92	0.14	70,72,74,76	0
2	PO4	A	615	5/5	0.97	0.07	36,38,40,42	0
2	PO4	C	616	5/5	0.98	0.05	31,33,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.