



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:26 AM EDT

PDB ID : 2RDA
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

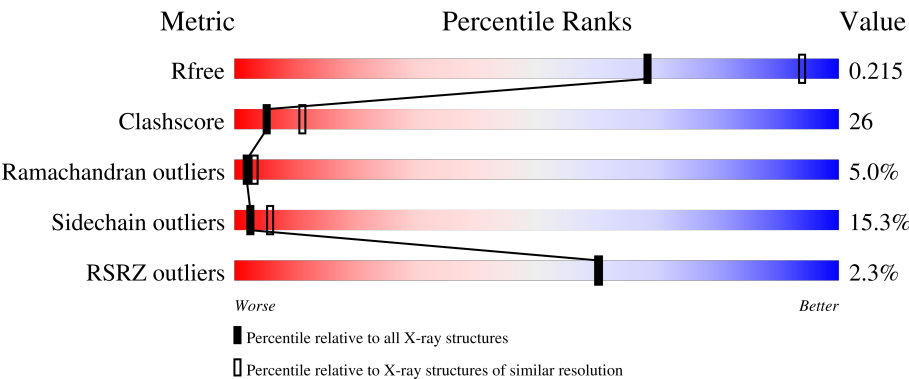
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.67 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (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	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>38%35%14%•10%</div></div>
1	B	313	<div><div></div><div></div><div></div><div></div><div></div></div> <div>42%39%7%•10%</div>
1	C	313	<div><div></div><div></div><div></div><div></div><div></div></div> <div>42%34%10%•10%</div>
1	D	313	<div><div>%</div><div></div><div></div><div></div><div></div></div> <div>40%35%14%•10%</div>
1	E	313	<div><div>4%</div><div></div><div></div><div></div><div></div></div> <div>29%41%19%•10%</div>

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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
1	A	282	Total	C	N	O	S	0	0	0
			2279	1457	399	412	11			
1	B	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	C	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	D	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	E	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	F	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			

There are 6 discrepancies between the modelled and reference sequences:

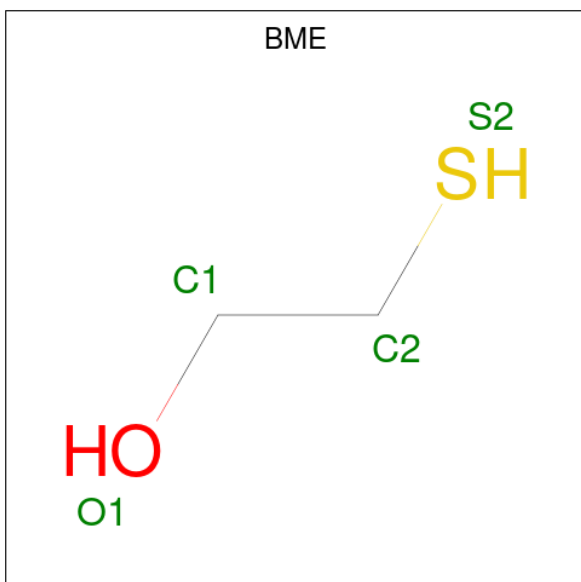
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LYS	ARG	engineered mutation	UNP P04818
B	163	LYS	ARG	engineered mutation	UNP P04818
C	163	LYS	ARG	engineered mutation	UNP P04818
D	163	LYS	ARG	engineered mutation	UNP P04818
E	163	LYS	ARG	engineered mutation	UNP P04818
F	163	LYS	ARG	engineered mutation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

- Molecule 2 is PHOSPHATE ION (three-letter code: 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 (three-letter code: BME) (formula: C_2H_6OS).



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		

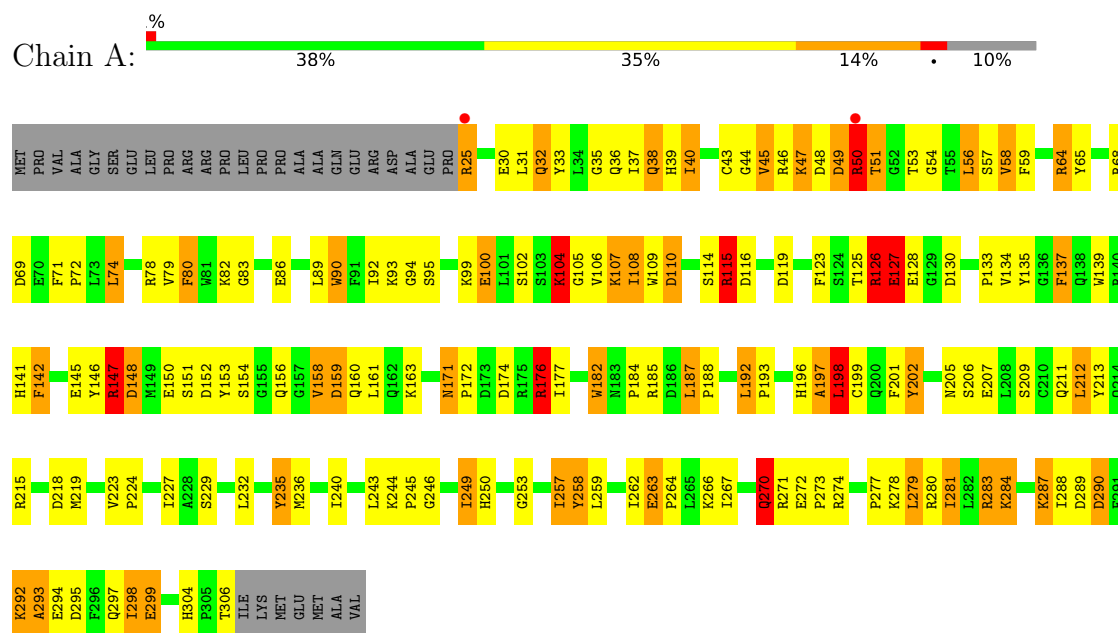
- Molecule 4 is water.

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		

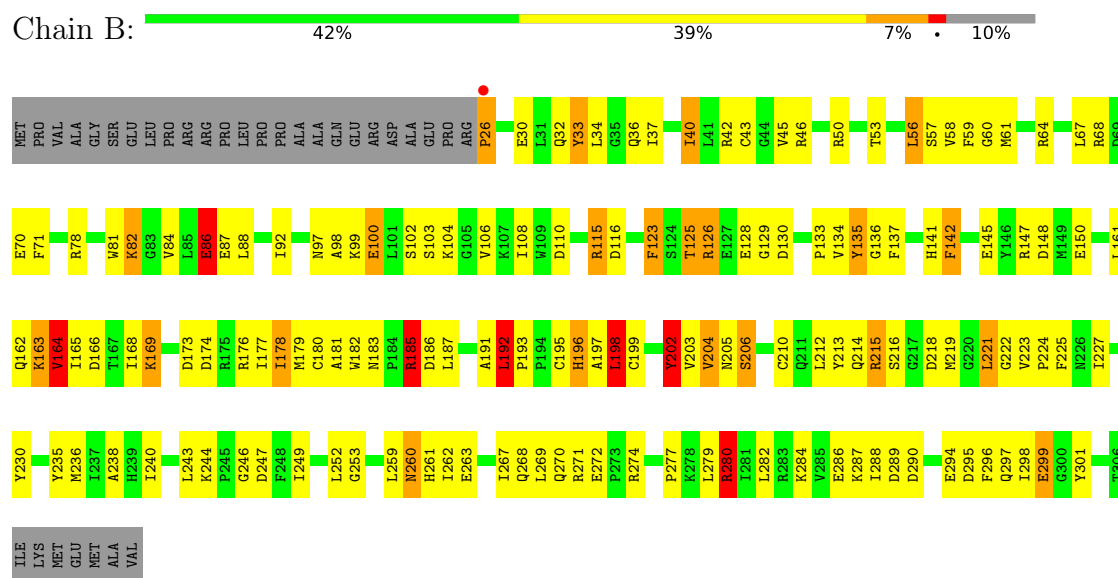
3 Residue-property plots

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

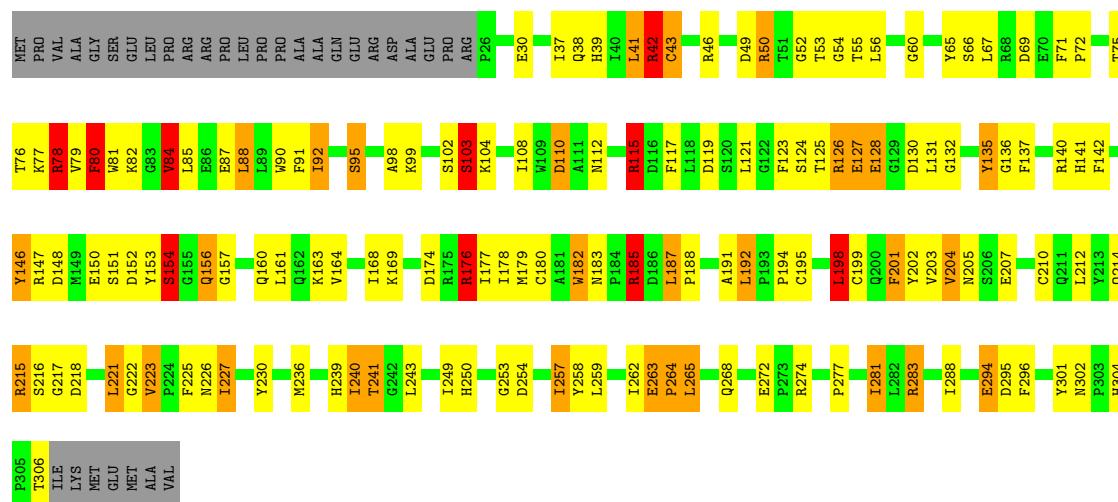


• Molecule 1: Thymidylate synthase




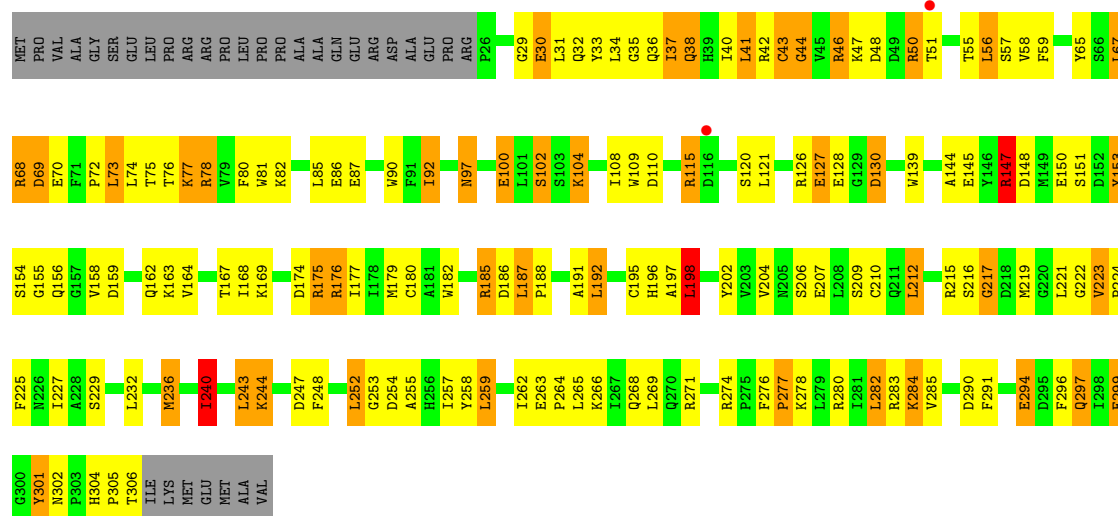
- Molecule 1: Thymidylate synthase

Chain C: 

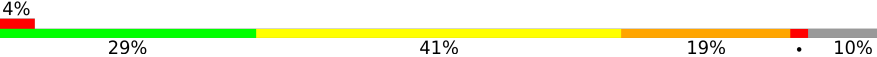


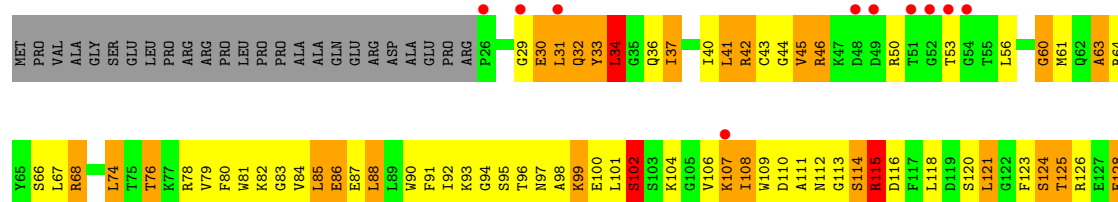
- Molecule 1: Thymidylate synthase

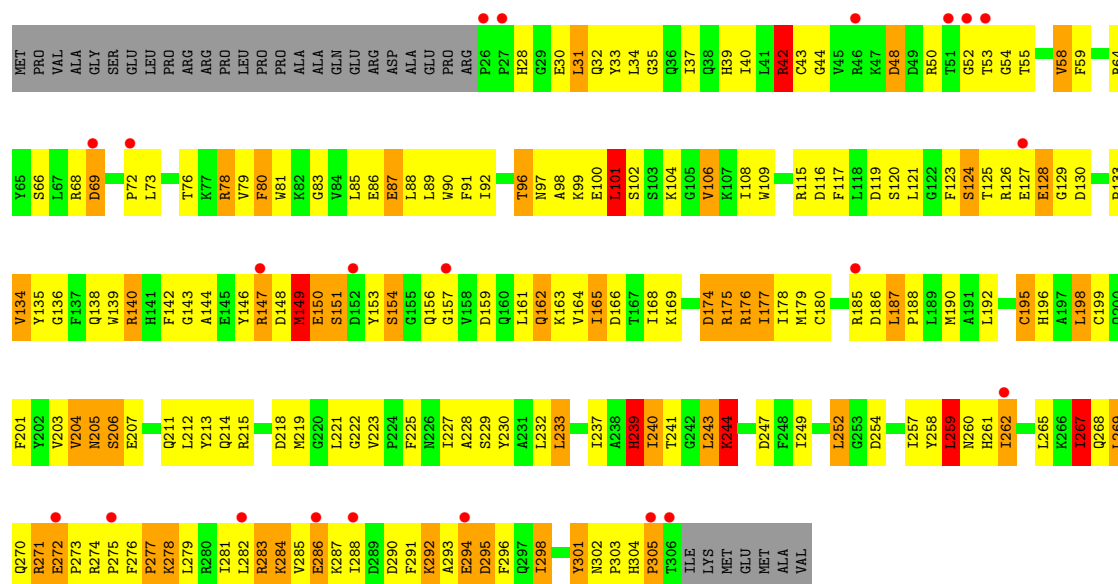
Chain D: 



- Molecule 1: Thymidylate synthase

Chain E: 





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 46.68 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.2 (107.21-2.67) 94.2 (46.68-2.64)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.279 0.210 , 0.215	Depositor DCC
R_{free} test set	7351 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	2.05	62/2339 (2.7%)	1.69	45/3165 (1.4%)
1	B	2.13	74/2328 (3.2%)	1.73	47/3150 (1.5%)
1	C	1.89	41/2328 (1.8%)	1.64	37/3150 (1.2%)
1	D	1.72	31/2328 (1.3%)	1.52	38/3150 (1.2%)
1	E	1.44	12/2328 (0.5%)	1.36	16/3150 (0.5%)
1	F	1.26	5/2328 (0.2%)	1.21	12/3150 (0.4%)
All	All	1.78	225/13979 (1.6%)	1.54	195/18915 (1.0%)

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 (225) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	GLU	CG-CD	13.31	1.72	1.51
1	C	199	CYS	CB-SG	-11.57	1.62	1.82
1	B	150	GLU	CB-CG	10.62	1.72	1.52
1	B	294	GLU	CD-OE1	10.57	1.37	1.25
1	B	195	CYS	CB-SG	-10.48	1.64	1.82
1	B	294	GLU	CG-CD	10.28	1.67	1.51
1	C	42	ARG	CG-CD	10.22	1.77	1.51
1	A	127	GLU	CG-CD	9.68	1.66	1.51
1	A	137	PHE	CE1-CZ	9.53	1.55	1.37
1	A	272	GLU	CG-CD	9.28	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	GLU	CD-OE1	9.01	1.35	1.25
1	A	213	TYR	CE1-CZ	-8.76	1.27	1.38
1	A	182	TRP	CE3-CZ3	8.60	1.53	1.38
1	C	84	VAL	CA-CB	-8.53	1.36	1.54
1	D	153	TYR	CD1-CE1	8.46	1.52	1.39
1	B	70	GLU	CG-CD	8.35	1.64	1.51
1	B	70	GLU	CD-OE2	8.25	1.34	1.25
1	A	272	GLU	CD-OE2	8.12	1.34	1.25
1	C	207	GLU	CG-CD	8.06	1.64	1.51
1	B	84	VAL	CB-CG2	8.03	1.69	1.52
1	B	272	GLU	CG-CD	7.93	1.63	1.51
1	F	267	ILE	CA-CB	7.91	1.73	1.54
1	C	201	PHE	CD1-CE1	-7.88	1.23	1.39
1	E	180	CYS	CB-SG	-7.85	1.68	1.82
1	B	64	ARG	CZ-NH2	7.83	1.43	1.33
1	B	294	GLU	CD-OE2	7.77	1.34	1.25
1	D	65	TYR	CE1-CZ	-7.72	1.28	1.38
1	A	142	PHE	CD1-CE1	-7.70	1.23	1.39
1	A	30	GLU	CD-OE1	7.61	1.34	1.25
1	B	173	ASP	CB-CG	7.60	1.67	1.51
1	B	199	CYS	CB-SG	-7.55	1.69	1.82
1	B	180	CYS	CB-SG	7.52	1.95	1.82
1	A	201	PHE	CE2-CZ	7.50	1.51	1.37
1	A	104	LYS	CE-NZ	7.49	1.67	1.49
1	B	240	ILE	CA-CB	-7.48	1.37	1.54
1	A	207	GLU	CG-CD	7.48	1.63	1.51
1	A	297	GLN	CG-CD	7.46	1.68	1.51
1	D	182	TRP	CB-CG	-7.44	1.36	1.50
1	A	163	LYS	CD-CE	7.43	1.69	1.51
1	D	297	GLN	CG-CD	7.41	1.68	1.51
1	A	45	VAL	CB-CG2	-7.39	1.37	1.52
1	D	30	GLU	CD-OE1	7.37	1.33	1.25
1	B	286	GLU	CD-OE1	7.32	1.33	1.25
1	A	80	PHE	CE1-CZ	7.27	1.51	1.37
1	A	134	VAL	CB-CG2	-7.26	1.37	1.52
1	D	301	TYR	CD1-CE1	7.26	1.50	1.39
1	B	98	ALA	CA-CB	-7.24	1.37	1.52
1	C	78	ARG	CG-CD	7.22	1.70	1.51
1	B	64	ARG	CB-CG	7.21	1.72	1.52
1	B	59	PHE	CB-CG	-7.19	1.39	1.51
1	B	290	ASP	CB-CG	7.14	1.66	1.51
1	B	230	TYR	CE1-CZ	7.11	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	65	TYR	CE1-CZ	-7.10	1.29	1.38
1	D	30	GLU	CD-OE2	7.01	1.33	1.25
1	B	100	GLU	CD-OE2	6.93	1.33	1.25
1	D	195	CYS	CB-SG	-6.92	1.70	1.82
1	C	150	GLU	CG-CD	6.92	1.62	1.51
1	C	146	TYR	CD2-CE2	6.85	1.49	1.39
1	B	33	TYR	CD2-CE2	-6.83	1.29	1.39
1	C	182	TRP	CB-CG	-6.81	1.38	1.50
1	B	299	GLU	CG-CD	6.79	1.62	1.51
1	B	137	PHE	CE1-CZ	6.79	1.50	1.37
1	D	207	GLU	CB-CG	-6.78	1.39	1.52
1	C	127	GLU	CG-CD	6.76	1.62	1.51
1	A	287	LYS	CD-CE	6.75	1.68	1.51
1	C	258	TYR	CD2-CE2	6.68	1.49	1.39
1	C	264	PRO	CA-C	6.67	1.66	1.52
1	B	286	GLU	CG-CD	6.65	1.61	1.51
1	B	185	ARG	CG-CD	6.65	1.68	1.51
1	A	142	PHE	CE2-CZ	-6.64	1.24	1.37
1	B	30	GLU	CD-OE2	6.63	1.32	1.25
1	A	235	TYR	CE2-CZ	6.53	1.47	1.38
1	E	199	CYS	CB-SG	-6.49	1.71	1.82
1	B	147	ARG	CZ-NH2	6.48	1.41	1.33
1	B	71	PHE	CB-CG	-6.43	1.40	1.51
1	C	80	PHE	CE1-CZ	6.43	1.49	1.37
1	A	229	SER	CA-CB	-6.42	1.43	1.52
1	E	294	GLU	CG-CD	6.39	1.61	1.51
1	E	207	GLU	CG-CD	6.35	1.61	1.51
1	B	299	GLU	CD-OE2	6.30	1.32	1.25
1	C	180	CYS	CB-SG	-6.30	1.71	1.82
1	B	195	CYS	N-CA	-6.28	1.33	1.46
1	A	39	HIS	CA-CB	-6.27	1.40	1.53
1	A	135	TYR	CD1-CE1	-6.23	1.30	1.39
1	D	87	GLU	CD-OE1	6.23	1.32	1.25
1	B	100	GLU	CD-OE1	6.21	1.32	1.25
1	D	90	TRP	CE3-CZ3	6.15	1.49	1.38
1	C	71	PHE	CB-CG	-6.15	1.41	1.51
1	B	210	CYS	CB-SG	6.14	1.92	1.82
1	B	182	TRP	CB-CG	-6.13	1.39	1.50
1	C	294	GLU	CB-CG	6.12	1.63	1.52
1	D	147	ARG	CZ-NH1	6.11	1.41	1.33
1	A	58	VAL	CB-CG2	-6.11	1.40	1.52
1	E	100	GLU	CG-CD	6.10	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	TRP	CB-CG	-6.10	1.39	1.50
1	E	86	GLU	CG-CD	6.09	1.61	1.51
1	A	32	GLN	CG-CD	-6.08	1.37	1.51
1	A	59	PHE	CD2-CE2	6.08	1.51	1.39
1	B	86	GLU	CG-CD	6.08	1.61	1.51
1	B	178	ILE	N-CA	-6.08	1.34	1.46
1	B	150	GLU	CD-OE2	6.08	1.32	1.25
1	C	207	GLU	CD-OE1	6.07	1.32	1.25
1	A	258	TYR	CE1-CZ	6.05	1.46	1.38
1	B	181	ALA	C-O	-6.02	1.11	1.23
1	A	292	LYS	CD-CE	6.00	1.66	1.51
1	B	26	PRO	CB-CG	5.94	1.79	1.50
1	C	50	ARG	CG-CD	5.94	1.66	1.51
1	B	87	GLU	CD-OE2	5.91	1.32	1.25
1	C	204	VAL	CB-CG1	5.91	1.65	1.52
1	D	164	VAL	CB-CG1	-5.86	1.40	1.52
1	C	42	ARG	CD-NE	5.86	1.56	1.46
1	E	115	ARG	CG-CD	5.85	1.66	1.51
1	C	43	CYS	CB-SG	5.85	1.92	1.82
1	D	197	ALA	CA-CB	-5.83	1.40	1.52
1	A	139	TRP	CB-CG	-5.83	1.39	1.50
1	A	209	SER	CA-CB	-5.83	1.44	1.52
1	F	58	VAL	CB-CG2	5.83	1.65	1.52
1	B	116	ASP	CB-CG	5.83	1.64	1.51
1	A	30	GLU	CG-CD	5.82	1.60	1.51
1	B	225	PHE	CD1-CE1	5.80	1.50	1.39
1	B	26	PRO	N-CA	5.80	1.57	1.47
1	A	83	GLY	N-CA	5.79	1.54	1.46
1	A	246	GLY	C-O	5.79	1.32	1.23
1	B	296	PHE	CE2-CZ	5.78	1.48	1.37
1	D	158	VAL	CB-CG1	5.78	1.65	1.52
1	A	65	TYR	N-CA	5.77	1.57	1.46
1	C	80	PHE	CE2-CZ	5.74	1.48	1.37
1	B	26	PRO	CA-C	5.71	1.64	1.52
1	C	202	TYR	CD2-CE2	-5.67	1.30	1.39
1	D	128	GLU	CG-CD	5.67	1.60	1.51
1	C	215	ARG	N-CA	-5.67	1.35	1.46
1	B	230	TYR	CD1-CE1	-5.67	1.30	1.39
1	D	145	GLU	CG-CD	5.67	1.60	1.51
1	D	225	PHE	CE2-CZ	5.67	1.48	1.37
1	C	225	PHE	CD1-CE1	5.65	1.50	1.39
1	B	86	GLU	CD-OE2	5.65	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ILE	CA-CB	-5.64	1.41	1.54
1	A	128	GLU	CG-CD	5.64	1.60	1.51
1	A	235	TYR	CD2-CE2	5.63	1.47	1.39
1	D	210	CYS	CB-SG	5.61	1.91	1.82
1	B	147	ARG	CZ-NH1	5.60	1.40	1.33
1	E	211	GLN	CG-CD	5.56	1.63	1.51
1	C	60	GLY	C-O	-5.55	1.14	1.23
1	C	263	GLU	CG-CD	5.55	1.60	1.51
1	C	294	GLU	CG-CD	5.50	1.60	1.51
1	B	253	GLY	CA-C	5.49	1.60	1.51
1	C	302	ASN	N-CA	-5.48	1.35	1.46
1	A	150	GLU	CG-CD	5.47	1.60	1.51
1	D	164	VAL	CB-CG2	-5.47	1.41	1.52
1	A	272	GLU	CB-CG	5.46	1.62	1.52
1	E	128	GLU	CG-CD	5.46	1.60	1.51
1	D	225	PHE	CD1-CE1	5.45	1.50	1.39
1	F	195	CYS	CB-SG	-5.44	1.73	1.81
1	A	290	ASP	CB-CG	5.42	1.63	1.51
1	C	223	VAL	CA-CB	-5.41	1.43	1.54
1	D	180	CYS	N-CA	-5.41	1.35	1.46
1	C	185	ARG	CB-CG	5.38	1.67	1.52
1	B	164	VAL	CB-CG1	-5.37	1.41	1.52
1	B	244	LYS	CE-NZ	5.36	1.62	1.49
1	A	158	VAL	C-O	5.35	1.33	1.23
1	C	241	THR	CA-CB	5.35	1.67	1.53
1	A	50	ARG	CB-CG	5.34	1.67	1.52
1	A	299	GLU	CD-OE1	5.34	1.31	1.25
1	B	123	PHE	CE2-CZ	5.34	1.47	1.37
1	A	147	ARG	CZ-NH1	5.34	1.40	1.33
1	A	299	GLU	CD-OE2	5.34	1.31	1.25
1	B	163	LYS	CE-NZ	5.33	1.62	1.49
1	A	80	PHE	C-O	5.33	1.33	1.23
1	A	289	ASP	CB-CG	5.32	1.62	1.51
1	B	58	VAL	CB-CG2	5.31	1.64	1.52
1	D	65	TYR	CD2-CE2	-5.31	1.31	1.39
1	A	90	TRP	CA-CB	-5.30	1.42	1.53
1	A	65	TYR	CD2-CE2	5.30	1.47	1.39
1	B	301	TYR	C-O	-5.29	1.13	1.23
1	B	225	PHE	CB-CG	-5.29	1.42	1.51
1	E	115	ARG	CB-CG	5.28	1.66	1.52
1	E	244	LYS	CD-CE	5.28	1.64	1.51
1	D	109	TRP	CE3-CZ3	5.27	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	GLU	CD-OE2	5.27	1.31	1.25
1	B	213	TYR	CD2-CE2	-5.27	1.31	1.39
1	B	192	LEU	CG-CD2	5.26	1.71	1.51
1	A	127	GLU	CD-OE2	5.26	1.31	1.25
1	B	165	ILE	N-CA	-5.25	1.35	1.46
1	C	223	VAL	CB-CG2	5.25	1.63	1.52
1	A	215	ARG	CG-CD	-5.23	1.38	1.51
1	B	297	GLN	CG-CD	5.23	1.63	1.51
1	C	210	CYS	CB-SG	-5.22	1.73	1.81
1	B	301	TYR	CB-CG	5.22	1.59	1.51
1	C	92	ILE	CA-CB	-5.22	1.42	1.54
1	A	135	TYR	CG-CD1	-5.21	1.32	1.39
1	C	195	CYS	CB-SG	-5.20	1.73	1.81
1	D	253	GLY	C-O	-5.20	1.15	1.23
1	B	135	TYR	CG-CD2	5.18	1.45	1.39
1	F	294	GLU	CG-CD	5.18	1.59	1.51
1	A	32	GLN	CA-CB	-5.16	1.42	1.53
1	A	135	TYR	CD2-CE2	5.16	1.47	1.39
1	B	42	ARG	CG-CD	5.15	1.64	1.51
1	A	213	TYR	CG-CD2	-5.15	1.32	1.39
1	B	238	ALA	CA-CB	-5.15	1.41	1.52
1	A	146	TYR	CD2-CE2	5.14	1.47	1.39
1	C	98	ALA	CA-CB	-5.14	1.41	1.52
1	B	145	GLU	CD-OE1	5.13	1.31	1.25
1	C	301	TYR	CD2-CE2	5.13	1.47	1.39
1	B	45	VAL	CB-CG1	5.12	1.63	1.52
1	A	65	TYR	CG-CD1	-5.12	1.32	1.39
1	A	197	ALA	CA-CB	-5.12	1.41	1.52
1	A	107	LYS	CD-CE	5.11	1.64	1.51
1	A	145	GLU	CG-CD	5.11	1.59	1.51
1	B	240	ILE	CB-CG2	-5.11	1.37	1.52
1	D	59	PHE	CE2-CZ	5.10	1.47	1.37
1	D	229	SER	CA-CB	-5.10	1.45	1.52
1	E	63	ALA	CA-CB	-5.10	1.41	1.52
1	B	280	ARG	CG-CD	5.09	1.64	1.51
1	B	284	LYS	CD-CE	5.09	1.64	1.51
1	D	162	GLN	CG-CD	5.08	1.62	1.51
1	B	137	PHE	CB-CG	-5.08	1.42	1.51
1	B	142	PHE	CG-CD2	-5.07	1.31	1.38
1	F	230	TYR	CE2-CZ	5.05	1.45	1.38
1	D	92	ILE	CA-CB	-5.05	1.43	1.54
1	A	100	GLU	CD-OE1	5.04	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	VAL	CB-CG1	5.04	1.63	1.52
1	A	82	LYS	CD-CE	5.02	1.63	1.51
1	C	91	PHE	CE1-CZ	5.02	1.46	1.37
1	B	287	LYS	N-CA	-5.01	1.36	1.46
1	C	207	GLU	CD-OE2	5.01	1.31	1.25

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ARG	NE-CZ-NH2	-11.27	114.67	120.30
1	E	34	LEU	CA-CB-CG	10.96	140.51	115.30
1	B	126	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	B	274	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	C	140	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	C	140	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	C	148	ASP	CB-CG-OD2	9.95	127.26	118.30
1	C	176	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	D	148	ASP	CB-CG-OD2	-9.51	109.74	118.30
1	B	247	ASP	CB-CG-OD1	8.96	126.36	118.30
1	B	274	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	49	ASP	CB-CG-OD1	8.76	126.19	118.30
1	C	78	ARG	NE-CZ-NH2	8.73	124.66	120.30
1	B	104	LYS	CD-CE-NZ	-8.70	91.70	111.70
1	C	88	LEU	CB-CG-CD2	-8.45	96.63	111.00
1	A	152	ASP	CB-CG-OD2	8.44	125.90	118.30
1	A	159	ASP	CB-CG-OD1	8.44	125.90	118.30
1	D	121	LEU	CA-CB-CG	8.39	134.60	115.30
1	D	115	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	E	85	LEU	CB-CG-CD2	-8.16	97.13	111.00
1	B	195	CYS	CA-CB-SG	-8.09	99.44	114.00
1	C	49	ASP	CB-CG-OD2	-8.02	111.09	118.30
1	D	148	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	215	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	E	180	CYS	CA-CB-SG	-7.92	99.75	114.00
1	C	249	ILE	CG1-CB-CG2	-7.79	94.27	111.40
1	E	115	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	198	LEU	CB-CG-CD2	-7.63	98.02	111.00
1	A	274	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	A	218	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	A	232	LEU	CB-CG-CD1	-7.59	98.10	111.00
1	B	56	LEU	CB-CG-CD2	-7.54	98.18	111.00
1	C	187	LEU	C-N-CD	7.53	144.22	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ILE	CG1-CB-CG2	-7.52	94.86	111.40
1	D	147	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	F	175	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	240	ILE	CB-CA-C	-7.45	96.70	111.60
1	E	236	MET	CG-SD-CE	-7.45	88.28	100.20
1	D	247	ASP	CB-CG-OD1	7.44	124.99	118.30
1	C	198	LEU	CA-CB-CG	7.32	132.14	115.30
1	D	115	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	56	LEU	CA-CB-CG	7.24	131.96	115.30
1	C	115	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	B	78	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	271	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	D	175	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	C	56	LEU	CB-CG-CD1	7.14	123.13	111.00
1	D	68	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	230	TYR	CZ-CE2-CD2	-7.11	113.40	119.80
1	B	176	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	64	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	C	176	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	240	ILE	CB-CG1-CD1	-7.04	94.19	113.90
1	C	110	ASP	CB-CG-OD1	7.04	124.63	118.30
1	C	119	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	243	LEU	CB-CG-CD2	7.03	122.95	111.00
1	A	185	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	F	175	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	161	LEU	CB-CG-CD2	-6.85	99.36	111.00
1	A	187	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	C	161	LEU	CB-CG-CD2	-6.79	99.47	111.00
1	E	85	LEU	CB-CG-CD1	6.78	122.53	111.00
1	A	126	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	E	37	ILE	CB-CA-C	-6.74	98.13	111.60
1	A	218	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	212	LEU	CB-CG-CD1	-6.73	99.56	111.00
1	E	232	LEU	CB-CG-CD1	6.72	122.43	111.00
1	B	247	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	B	163	LYS	CD-CE-NZ	6.69	127.09	111.70
1	D	43	CYS	CA-CB-SG	-6.69	101.96	114.00
1	A	278	LYS	CB-CG-CD	-6.68	94.23	111.60
1	D	195	CYS	CA-CB-SG	-6.66	102.02	114.00
1	A	58	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	A	270	GLN	CB-CA-C	-6.62	97.16	110.40
1	C	295	ASP	CB-CG-OD1	6.60	124.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	161	LEU	CB-CG-CD1	6.50	122.04	111.00
1	D	44	GLY	N-CA-C	-6.48	96.91	113.10
1	D	97	ASN	CB-CA-C	-6.47	97.46	110.40
1	D	247	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	E	74	LEU	CA-CB-CG	-6.43	100.50	115.30
1	A	148	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	236	MET	CG-SD-CE	-6.40	89.96	100.20
1	D	259	LEU	CA-CB-CG	-6.38	100.62	115.30
1	A	295	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	67	LEU	CB-CG-CD1	-6.36	100.18	111.00
1	B	236	MET	CG-SD-CE	6.29	110.26	100.20
1	F	101	LEU	CA-CB-CG	6.26	129.71	115.30
1	B	43	CYS	CB-CA-C	-6.21	97.97	110.40
1	A	25	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	259	LEU	CA-CB-CG	6.09	129.31	115.30
1	D	185	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	B	130	ASP	CB-CG-OD1	6.05	123.75	118.30
1	D	128	GLU	N-CA-CB	6.04	121.48	110.60
1	A	253	GLY	N-CA-C	-6.04	98.00	113.10
1	C	203	VAL	CB-CA-C	-5.94	100.11	111.40
1	D	187	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	A	257	ILE	CB-CA-C	-5.90	99.80	111.60
1	C	115	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	C	221	LEU	CA-CB-CG	5.88	128.81	115.30
1	A	45	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	C	148	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	D	159	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	243	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	D	282	LEU	CA-CB-CG	-5.82	101.92	115.30
1	D	243	LEU	CB-CG-CD1	-5.81	101.13	111.00
1	B	284	LYS	CD-CE-NZ	5.79	125.03	111.70
1	C	253	GLY	N-CA-C	-5.79	98.63	113.10
1	C	131	LEU	CB-CG-CD1	-5.77	101.20	111.00
1	C	265	LEU	CB-CG-CD2	5.74	120.75	111.00
1	B	61	MET	CG-SD-CE	-5.73	91.04	100.20
1	A	115	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	210	CYS	CB-CA-C	-5.68	99.03	110.40
1	F	42	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	198	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	C	41	LEU	CA-CB-CG	-5.67	102.27	115.30
1	D	104	LYS	CD-CE-NZ	-5.65	98.70	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	LEU	N-CA-C	5.64	126.24	111.00
1	A	187	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	C	199	CYS	CA-CB-SG	-5.61	103.90	114.00
1	A	119	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	180	CYS	CA-CB-SG	-5.60	103.92	114.00
1	B	195	CYS	CB-CA-C	5.59	121.58	110.40
1	A	280	ARG	CG-CD-NE	-5.57	100.11	111.80
1	B	215	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	218	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	73	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	B	249	ILE	CG1-CB-CG2	-5.55	99.18	111.40
1	E	134	VAL	CB-CA-C	-5.55	100.86	111.40
1	A	284	LYS	CB-CA-C	5.54	121.47	110.40
1	B	218	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	57	SER	CB-CA-C	-5.52	99.61	110.10
1	B	221	LEU	CB-CG-CD1	5.50	120.34	111.00
1	D	212	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	A	94	GLY	C-N-CA	-5.48	108.00	121.70
1	E	102	SER	N-CA-C	5.47	125.78	111.00
1	B	130	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	79	VAL	CG1-CB-CG2	5.46	119.64	110.90
1	F	252	LEU	CA-CB-CG	-5.45	102.76	115.30
1	B	148	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	176	ARG	CB-CA-C	-5.42	99.56	110.40
1	A	74	LEU	CB-CG-CD2	5.42	120.21	111.00
1	B	53	THR	C-N-CA	-5.40	110.96	122.30
1	A	89	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	159	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	304	HIS	C-N-CD	5.37	139.68	128.40
1	B	203	VAL	CB-CA-C	-5.36	101.21	111.40
1	D	297	GLN	CB-CA-C	5.36	121.12	110.40
1	F	265	LEU	CB-CG-CD2	5.35	120.10	111.00
1	A	229	SER	CA-CB-OG	-5.35	96.76	111.20
1	A	25	ARG	C-N-CD	5.34	139.60	128.40
1	F	186	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	78	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	E	243	LEU	CA-CB-CG	-5.30	103.10	115.30
1	C	207	GLU	CB-CA-C	5.30	121.00	110.40
1	B	161	LEU	CB-CG-CD1	5.30	120.00	111.00
1	C	154	SER	CB-CA-C	-5.30	100.04	110.10
1	E	249	ILE	CB-CA-C	-5.29	101.03	111.60
1	A	110	ASP	CB-CG-OD1	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ILE	CG1-CB-CG2	-5.28	99.79	111.40
1	A	290	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	171	ASN	C-N-CD	5.27	139.47	128.40
1	A	280	ARG	O-C-N	5.27	131.13	122.70
1	C	126	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	D	110	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	185	ARG	CG-CD-NE	5.25	122.84	111.80
1	C	137	PHE	CG-CD2-CE2	5.24	126.56	120.80
1	B	126	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	202	TYR	N-CA-CB	-5.20	101.24	110.60
1	A	135	TYR	CB-CG-CD2	5.20	124.12	121.00
1	B	169	LYS	CD-CE-NZ	-5.18	99.78	111.70
1	D	69	ASP	N-CA-C	5.18	124.98	111.00
1	C	161	LEU	CB-CG-CD1	5.17	119.80	111.00
1	D	147	ARG	CB-CA-C	5.17	120.74	110.40
1	F	212	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	D	68	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	E	247	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	B	238	ALA	N-CA-CB	5.15	117.31	110.10
1	B	204	VAL	CA-CB-CG2	-5.15	103.17	110.90
1	D	130	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	196	HIS	CB-CA-C	-5.14	100.12	110.40
1	E	134	VAL	CG1-CB-CG2	5.14	119.12	110.90
1	D	180	CYS	CA-CB-SG	-5.13	104.77	114.00
1	A	119	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	F	203	VAL	CB-CA-C	-5.12	101.67	111.40
1	D	198	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	254	ASP	CB-CG-OD1	5.08	122.88	118.30
1	D	186	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	227	ILE	CG1-CB-CG2	-5.07	100.25	111.40
1	C	42	ARG	CA-CB-CG	5.07	124.55	113.40
1	D	78	ARG	CB-CG-CD	5.03	124.69	111.60
1	B	295	ASP	CB-CG-OD1	5.03	122.83	118.30
1	F	244	LYS	CA-CB-CG	5.03	124.46	113.40
1	B	213	TYR	N-CA-C	-5.01	97.48	111.00
1	B	271	ARG	CD-NE-CZ	5.01	130.61	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	LYS	Peptide

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Mol	Chain	Res	Type	Group
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	115	0
1	B	2268	0	2235	70	0
1	C	2268	0	2235	96	0
1	D	2268	0	2235	93	0
1	E	2268	0	2235	190	0
1	F	2268	0	2235	162	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
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	715	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 26.

All (715) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:198:LEU:C	1:A:198:LEU:HD12	1.97	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:306:THR:O	1:D:306:THR:HG23	1.81	0.80
1:E:111:ALA:HA	1:E:115:ARG:HH22	1.46	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:C:92:ILE:HD11	1:C:236:MET:HE2	1.64	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: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
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:C:198:LEU:C	1:C:198:LEU:HD12	2.06	0.75
1:F:97:ASN:HA	1:F:129:GLY:O	1.86	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:C	1:A:51:THR:H	1.92	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: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: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:C:191:ALA:C	1:C:192:LEU:HD12	2.12	0.70
1:D:168:ILE:HD11	1:D:177:ILE:HG21	1.73	0.70
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: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: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:D:198:LEU:HD12	1:D:198:LEU:C	2.12	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:126:ARG:HD3	1:C:130:ASP:CG	2.13	0.68
1:D:297:GLN:NE2	1:D:299:GLU:HB3	2.06	0.68
1:D:126:ARG:HD3	1:D:130:ASP:CG	2.14	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: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: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:E:98:ALA:HB2	1:E:131:LEU:HD11	1.76	0.66
1:F:206:SER:HA	1:F:243:LEU:HD22	1.77	0.66
1:D:198:LEU:C	1:D:198:LEU:CD1	2.64	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:58:VAL:HG12	1:D:58:VAL:O	1.98	0.64
1:A:50:ARG:HA	4:A:675:HOH:O	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:233:LEU:HD12	1:F:233:LEU:C	2.19	0.62
1:F:294:GLU:C	1:F:296:PHE:H	2.01	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: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
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:E:114:SER:OG	1:E:115:ARG:N	2.30	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:C:78:ARG:HH11	1:C:78:ARG:CG	2.14	0.61
1:E:271:ARG:HH11	1:E:304:HIS:CB	2.13	0.61
1:D:139:TRP:CD2	1:D:179:MET:HE1	2.35	0.60
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:D:294:GLU:CD	1:D:294:GLU:H	2.05	0.60
1:E:219:MET:HB2	1:E:257:ILE:HG13	1.83	0.60
1:E:192:LEU:HD13	1:E:192:LEU:C	2.21	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:198:LEU:C	1:C:198:LEU:CD1	2.70	0.60
1:D:240:ILE:HG22	1:D:240:ILE:O	2.01	0.60
1:F:88:LEU:HD23	1:F:88:LEU:C	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:211:GLN:HG3	1:E:249:ILE:HB	1.85	0.59
1:A:198:LEU:C	1:A:198:LEU:CD1	2.68	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
1:E:115:ARG:CD	1:E:116:ASP:H	2.17	0.58
1:F:198:LEU:C	1:F:198:LEU:HD23	2.24	0.58
1:C:66:SER:O	1:C:67:LEU:HD23	2.04	0.58
1:F:88:LEU:O	1:F:92:ILE:HG13	2.04	0.58
1:A:292:LYS:O	1:A:293:ALA:C	2.41	0.58
1:E:84:VAL:O	1:E:85:LEU:C	2.40	0.57
1:A:92:ILE:CD1	1:A:236:MET:HE1	2.34	0.57
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:A:46:ARG:C	1:A:48:ASP:H	2.08	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:259:LEU:C	1:E:261:HIS:H	2.08	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:F:81:TRP:CE2	1:F:85:LEU:HD11	2.40	0.56
1:F:143:GLY:O	1:F:144:ALA:C	2.39	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: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: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:F:69:ASP:O	1:F:278:LYS:HG3	2.06	0.55
1:F:301:TYR:C	1:F:303:PRO:HD3	2.26	0.55
1:B:164:VAL:HG22	1:B:177:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:618:PO4:O2	3:E:628:BME:H21	2.05	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:C:87:GLU:O	1:C:88:LEU:C	2.41	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
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:A:92:ILE:HD11	1:A:236:MET:HE1	1.88	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:C:135:TYR:O	1:C:136:GLY:C	2.42	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:F:39:HIS:O	1:F:40:ILE:C	2.43	0.54
1:A:197:ALA:O	1:A:198:LEU:HB3	2.08	0.54
1:C:79:VAL:O	1:C:81:TRP:N	2.38	0.54
1:C:102:SER:C	1:C:104:LYS:H	2.11	0.54
1:E:271:ARG:NH1	1:E:304:HIS:HB3	2.22	0.54
1:E:198:LEU:C	1:E:198:LEU:HD12	2.28	0.54
1:F:134:VAL:HG12	1:F:190:MET:HE3	1.89	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:C:72:PRO:O	1:C:72:PRO:HG2	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:130:ASP:CG	1:E:149:MET:HB3	2.29	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
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: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: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:C:263:GLU:O	1:C:264:PRO:C	2.47	0.53
1:D:47:LYS:HG2	1:D:48:ASP:N	2.18	0.53
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:D:198:LEU:HD12	1:D:198:LEU:O	2.09	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:F:80:PHE:CD2	1:F:83:GLY:HA3	2.45	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:E:31:LEU:C	1:E:32:GLN:HG2	2.23	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:F:109:TRP:CZ3	1:F:192:LEU:HD21	2.44	0.51
1:C:257:ILE:CD1	1:C:265:LEU:CD1	2.86	0.51
1:F:292:LYS:O	1:F:295:ASP:OD1	2.29	0.51
1:E:124:SER:C	1:E:126:ARG:H	2.14	0.51
1:F:267:ILE:C	1:F:269:LEU:H	2.14	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:D:139:TRP:CE2	1:D:179:MET:HE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:GLU:HG2	1:E:244:LYS:HG3	1.92	0.51
1:F:239:HIS:C	1:F:241:THR:H	2.14	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:E:135:TYR:O	1:E:136:GLY:C	2.49	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:127:GLU:CD	1:A:127:GLU:H	2.13	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:33:TYR:O	1:E:34:LEU:C	2.49	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: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:90:TRP:NE1	1:E:95:SER:OG	2.43	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:E:289:ASP:C	4:E:629:HOH:O	2.49	0.50
1:F:285:VAL:HG12	1:F:286:GLU:N	2.27	0.50
1:E:274:ARG:O	1:E:275:PRO:C	2.48	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
1:B:235:TYR:CD1	1:B:279:LEU:HD23	2.47	0.50
1:E:66:SER:HA	1:E:247:ASP:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:ASP:C	1:A:51:THR:N	2.64	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:E:292:LYS:C	1:E:294:GLU:H	2.16	0.49
1:A:263:GLU:HB2	1:A:264:PRO:HD3	1.94	0.49
1:E:32:GLN:HG3	1:E:64:ARG:N	2.27	0.49
1:A:171:ASN:O	1:A:172:PRO:C	2.48	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: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:C:127:GLU:CD	1:C:127:GLU:H	2.16	0.49
1:A:133:PRO:HB3	1:A:137:PHE:CD2	2.47	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: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: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:B:99:LYS:HZ1	1:B:128:GLU:HG3	1.77	0.48
1:E:88:LEU:O	1:E:92:ILE:HG13	2.14	0.48
1:E:131:LEU:C	1:E:132:GLY:O	2.51	0.48
1:E:133:PRO:HG2	1:E:186:ASP:HB3	1.95	0.48
1:E:237:ILE:O	1:E:241:THR:OG1	2.26	0.48
1:E:298:ILE:HG22	1:E:301:TYR:HB2	1.95	0.48
1:E:32:GLN:HB3	1:E:63:ALA:HB1	1.96	0.48
1:F:228:ALA:O	1:F:229:SER:C	2.51	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:294:GLU:C	1:F:296:PHE:N	2.66	0.47
1:B:100:GLU:HG3	1:B:100:GLU:O	2.13	0.47
1:B:183:ASN:C	1:B:183:ASN:OD1	2.52	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
1:E:192:LEU:C	1:E:192:LEU:CD1	2.82	0.47
1:E:289:ASP:OD1	1:E:289:ASP:N	2.41	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:257:ILE:O	1:C:257:ILE:CG2	2.63	0.47
1:E:303:PRO:O	1:E:304:HIS:C	2.51	0.47
1:F:99:LYS:C	1:F:101:LEU:H	2.17	0.47
1:F:124:SER:C	1:F:126:ARG:H	2.17	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:43:CYS:O	1:A:44:GLY:C	2.49	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:C:262:ILE:O	1:C:263:GLU:C	2.52	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: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:127:GLU:O	1:C:128:GLU:C	2.53	0.47
1:D:32:GLN:O	1:D:36:GLN:HG3	2.14	0.47
1:E:292:LYS:C	1:E:294:GLU:N	2.68	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:A:115:ARG:O	1:A:116:ASP:C	2.50	0.46
1:C:121:LEU:HD12	1:C:123:PHE:CE2	2.51	0.46
1:C:141:HIS:O	1:C:142:PHE:C	2.54	0.46
1:E:240:ILE:HD11	1:E:288:ILE:HD12	1.97	0.46
1:F:267:ILE:C	1:F:269:LEU:N	2.68	0.46
1:A:153:TYR:O	1:A:154:SER:C	2.54	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:E:94:GLY:C	1:E:95:SER:O	2.52	0.46
1:A:40:ILE:HD12	1:A:219:MET:HG3	1.97	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:F:232:LEU:O	1:F:233:LEU:C	2.53	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: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:B:141:HIS:O	1:B:142:PHE:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:82:LYS:O	1:B:86:GLU:HB2	2.16	0.46
1:A:43:CYS:C	1:A:44:GLY:O	2.51	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: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:D:276:PHE:HA	1:D:277:PRO:HD2	1.42	0.45
1:E:261:HIS:CA	1:E:264:PRO:HG2	2.34	0.45
1:A:141:HIS:O	1:A:142:PHE:C	2.55	0.45
1:A:267:ILE:O	1:A:270:GLN:HG3	2.17	0.45
1:C:53:THR:HG22	1:C:54:GLY:N	2.31	0.45
1:F:30:GLU:C	1:F:32:GLN:N	2.68	0.45
1:C:46:ARG:HA	1:C:55:THR:O	2.17	0.45
1:C:66:SER:C	1:C:67:LEU:HD23	2.37	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: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
1:E:239:HIS:HE2	1:E:284:LYS:HA	1.82	0.44
1:F:282:LEU:O	1:F:283:ARG:HB2	2.16	0.44
1:D:268:GLN:O	1:D:271:ARG:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:202:TYR:C	1:A:202:TYR:CD2	2.90	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:139:TRP:CD2	1:D:179:MET:CE	3.00	0.44
1:D:223:VAL:O	1:D:227:ILE:HG12	2.18	0.44
1:E:195:CYS:O	1:E:214:GLN:HA	2.18	0.44
1:D:57:SER:O	1:D:58:VAL:HG23	2.17	0.44
1:D:222:GLY:C	1:D:224:PRO:HD2	2.38	0.44
1:A:46:ARG:C	1:A:48:ASP:N	2.70	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: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:E:239:HIS:ND1	1:E:281:ILE:HG13	2.33	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:B:223:VAL:O	1:B:224:PRO:C	2.57	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: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
1:C:80:PHE:O	1:C:81:TRP:C	2.56	0.43
1:E:114:SER:O	1:E:118:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:60:GLY:C	1:E:61:MET:CG	2.86	0.43
1:F:97:ASN:ND2	1:F:100:GLU:H	2.14	0.43
1:F:139:TRP:CD2	1:F:179:MET:HE1	2.53	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:A:236:MET:HE3	1:A:236:MET:HB3	1.81	0.43
1:E:87:GLU:O	1:E:88:LEU:C	2.52	0.43
1:E:262:ILE:HG12	1:E:262:ILE:H	1.65	0.43
1:E:294:GLU:C	1:E:296:PHE:H	2.19	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:271:ARG:HD3	1:A:304:HIS:CG	2.54	0.42
1:C:168:ILE:HG22	1:C:168:ILE:O	2.18	0.42
1:E:274:ARG:O	1:E:275:PRO:O	2.36	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:O	1:D:168:ILE:C	2.57	0.42
1:C:77:LYS:O	1:C:78:ARG:C	2.58	0.42
1:C:214:GLN:OE1	1:C:250:HIS:CE1	2.70	0.42
1:E:236:MET:HE2	1:E:288:ILE:HD11	2.01	0.42
1:F:30:GLU:C	1:F:32:GLN:H	2.23	0.42
1:F:135:TYR:HH	1:F:196:HIS:HD1	1.66	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:B:198:LEU:HD12	1:B:198:LEU:C	2.40	0.42
1:C:81:TRP:O	1:C:82:LYS:C	2.54	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:C:81:TRP:O	1:C:84:VAL:HB	2.20	0.42
1:E:187:LEU:N	1:E:188:PRO:HD2	2.34	0.42
1:E:259:LEU:C	1:E:261:HIS:N	2.73	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:B:134:VAL:O	1:B:135:TYR:C	2.57	0.41
1:C:177:ILE:CG2	1:C:201:PHE:HB2	2.50	0.41
1:B:202:TYR:CD2	1:B:202:TYR:C	2.93	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
1:B:206:SER:HA	1:B:243:LEU:HD22	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:O	1:D:35:GLY:N	2.35	0.41
1:D:139:TRP:CE3	1:D:179:MET:HE1	2.56	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: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:90:TRP:HE1	1:A:95:SER:HG	1.68	0.41
1:A:283:ARG:HH11	1:A:283:ARG:HB2	1.85	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:CE1	2.94	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:A:108:ILE:HG21	1:A:108:ILE:HD12	1.79	0.41
1:B:222:GLY:O	1:B:223:VAL:C	2.60	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:183:ASN:OD1	1:C:183:ASN:C	2.58	0.41
1:C:185:ARG:O	1:C:188:PRO:HD2	2.20	0.41
1:D:139:TRP:CE2	1:D:179:MET:HE1	2.55	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
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:D:168:ILE:HD13	1:D:177:ILE:HG21	1.99	0.41
1:E:121:LEU:HB2	1:E:123:PHE:CE1	2.57	0.40
1:E:196:HIS:HB3	1:E:212:LEU:HD11	2.03	0.40
1:F:54:GLY:C	1:F:55:THR:CG2	2.90	0.40
1:F:139:TRP:CD2	1:F:179:MET:CE	3.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:283:ARG:C	1:F:284:LYS:HG2	2.42	0.40
1:B:259:LEU:C	1:B:261:HIS:N	2.74	0.40
1:C:39:HIS:CE1	1:C:43:CYS:SG	3.14	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:C:254:ASP:C	1:C:254:ASP:OD1	2.60	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/313 (90%)	251 (90%)	21 (8%)	8 (3%)	4	9
1	B	279/313 (89%)	254 (91%)	20 (7%)	5 (2%)	8	19
1	C	279/313 (89%)	239 (86%)	32 (12%)	8 (3%)	4	9
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%)	2	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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	217 (88%)	29 (12%)	5	11
1	B	245/271 (90%)	221 (90%)	24 (10%)	8	17
1	C	245/271 (90%)	216 (88%)	29 (12%)	5	11
1	D	245/271 (90%)	208 (85%)	37 (15%)	3	6
1	E	245/271 (90%)	193 (79%)	52 (21%)	1	2
1	F	245/271 (90%)	191 (78%)	54 (22%)	1	2
All	All	1471/1626 (90%)	1246 (85%)	225 (15%)	2	6

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	31	LEU
1	A	38	GLN
1	A	50	ARG
1	A	51	THR
1	A	56	LEU
1	A	72	PRO
1	A	93	LYS
1	A	104	LYS
1	A	108	ILE
1	A	114	SER
1	A	115	ARG
1	A	125	THR
1	A	126	ARG
1	A	127	GLU
1	A	147	ARG
1	A	148	ASP
1	A	151	SER
1	A	176	ARG
1	A	192	LEU
1	A	198	LEU
1	A	202	TYR

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Mol	Chain	Res	Type
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	298	ILE
1	B	40	ILE
1	B	50	ARG
1	B	56	LEU
1	B	57	SER
1	B	82	LYS
1	B	86	GLU
1	B	103	SER
1	B	108	ILE
1	B	115	ARG
1	B	125	THR
1	B	164	VAL
1	B	174	ASP
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	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	69	ASP
1	C	78	ARG
1	C	95	SER
1	C	103	SER
1	C	108	ILE
1	C	115	ARG
1	C	147	ARG
1	C	151	SER
1	C	154	SER

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Mol	Chain	Res	Type
1	C	156	GLN
1	C	163	LYS
1	C	176	ARG
1	C	178	ILE
1	C	179	MET
1	C	185	ARG
1	C	192	LEU
1	C	198	LEU
1	C	216	SER
1	C	221	LEU
1	C	227	ILE
1	C	240	ILE
1	C	257	ILE
1	C	272	GLU
1	C	281	ILE
1	C	283	ARG
1	C	294	GLU
1	C	306	THR
1	D	37	ILE
1	D	38	GLN
1	D	41	LEU
1	D	46	ARG
1	D	50	ARG
1	D	51	THR
1	D	56	LEU
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	115	ARG
1	D	120	SER
1	D	127	GLU
1	D	147	ARG
1	D	150	GLU
1	D	163	LYS
1	D	169	LYS
1	D	175	ARG
1	D	176	ARG
1	D	185	ARG

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Mol	Chain	Res	Type
1	D	192	LEU
1	D	198	LEU
1	D	204	VAL
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	299	GLU
1	D	302	ASN
1	E	30	GLU
1	E	34	LEU
1	E	40	ILE
1	E	41	LEU
1	E	42	ARG
1	E	45	VAL
1	E	46	ARG
1	E	50	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	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	165	ILE

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Mol	Chain	Res	Type
1	E	168	ILE
1	E	176	ARG
1	E	187	LEU
1	E	192	LEU
1	E	198	LEU
1	E	221	LEU
1	E	237	ILE
1	E	241	THR
1	E	257	ILE
1	E	262	ILE
1	E	265	LEU
1	E	267	ILE
1	E	278	LYS
1	E	280	ARG
1	E	281	ILE
1	E	283	ARG
1	E	284	LYS
1	E	286	GLU
1	E	289	ASP
1	E	294	GLU
1	E	299	GLU
1	E	302	ASN
1	E	306	THR
1	F	31	LEU
1	F	42	ARG
1	F	48	ASP
1	F	53	THR
1	F	69	ASP
1	F	76	THR
1	F	78	ARG
1	F	87	GLU
1	F	96	THR
1	F	101	LEU
1	F	102	SER
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

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Mol	Chain	Res	Type
1	F	147	ARG
1	F	149	MET
1	F	151	SER
1	F	154	SER
1	F	162	GLN
1	F	165	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	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
1	F	286	GLU
1	F	287	LYS
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 (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	141	HIS
1	A	160	GLN

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Mol	Chain	Res	Type
1	A	171	ASN
1	A	302	ASN
1	B	196	HIS
1	B	250	HIS
1	B	297	GLN
1	B	302	ASN
1	C	36	GLN
1	C	39	HIS
1	C	226	ASN
1	C	250	HIS
1	C	268	GLN
1	D	38	GLN
1	D	156	GLN
1	D	162	GLN
1	D	270	GLN
1	D	297	GLN
1	D	302	ASN
1	E	156	GLN
1	E	160	GLN
1	E	196	HIS
1	E	200	GLN
1	E	226	ASN
1	E	250	HIS
1	E	261	HIS
1	E	302	ASN
1	F	97	ASN
1	F	112	ASN
1	F	156	GLN
1	F	171	ASN
1	F	214	GLN
1	F	261	HIS
1	F	270	GLN
1	F	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
3	BME	C	626	-	3,3,3	0.64	0	1,2,2	1.37	0
2	PO4	C	616	-	4,4,4	1.38	1 (25%)	6,6,6	2.69	4 (66%)
2	PO4	E	619	-	4,4,4	0.78	0	6,6,6	1.18	0
2	PO4	E	618	-	4,4,4	0.61	0	6,6,6	1.26	1 (16%)
2	PO4	A	615	-	4,4,4	0.79	0	6,6,6	1.62	2 (33%)
2	PO4	D	617	-	4,4,4	1.26	0	6,6,6	0.98	0
3	BME	E	628	-	3,3,3	0.19	0	1,2,2	1.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-2.15	1.48	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	616	PO4	O4-P-O3	4.34	121.90	107.97
2	C	616	PO4	O3-P-O1	-3.81	96.97	110.89
2	A	615	PO4	O2-P-O1	-3.30	98.82	110.89
2	C	616	PO4	O4-P-O1	-2.32	102.42	110.89
2	E	618	PO4	O2-P-O1	-2.25	102.65	110.89
2	C	616	PO4	O4-P-O2	2.10	114.72	107.97
2	A	615	PO4	O4-P-O1	2.05	118.41	110.89

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	C	626	BME	3	0
2	E	619	PO4	3	0
2	E	618	PO4	2	0
3	E	628	BME	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.57	2 (0%) 87 88	5, 26, 51, 82	0
1	B	281/313 (89%)	-0.69	1 (0%) 92 93	3, 21, 48, 58	0
1	C	281/313 (89%)	-0.56	0 100 100	9, 33, 56, 65	0
1	D	281/313 (89%)	-0.39	2 (0%) 87 88	13, 40, 70, 93	0
1	E	281/313 (89%)	0.20	11 (3%) 39 37	29, 60, 99, 108	0
1	F	281/313 (89%)	0.44	22 (7%) 13 11	30, 76, 102, 114	0
All	All	1687/1878 (89%)	-0.26	38 (2%) 60 60	3, 39, 91, 114	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	31	LEU	5.0
1	F	147	ARG	4.0
1	E	51	THR	3.9
1	E	53	THR	3.9
1	E	26	PRO	3.6
1	E	29	GLY	3.6
1	F	306	THR	3.5
1	E	107	LYS	3.3
1	E	52	GLY	3.2
1	F	27	PRO	3.2
1	F	51	THR	3.0
1	A	50	ARG	2.9
1	F	305	PRO	2.9
1	E	269	LEU	2.8
1	F	52	GLY	2.8
1	E	54	GLY	2.6
1	F	152	ASP	2.6
1	F	157	GLY	2.6
1	F	275	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	69	ASP	2.4
1	F	46	ARG	2.4
1	F	288	ILE	2.4
1	E	48	ASP	2.3
1	F	262	ILE	2.2
1	F	185	ARG	2.2
1	F	127	GLU	2.1
1	F	272	GLU	2.1
1	F	282	LEU	2.1
1	F	286	GLU	2.1
1	D	51	THR	2.1
1	F	72	PRO	2.1
1	A	25	ARG	2.1
1	F	294	GLU	2.0
1	E	49	ASP	2.0
1	F	53	THR	2.0
1	F	26	PRO	2.0
1	D	116	ASP	2.0
1	B	26	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
3	BME	E	628	4/4	0.76	0.23	71,78,82,89	0
3	BME	C	626	4/4	0.84	0.22	45,47,50,58	0
2	PO4	E	618	5/5	0.95	0.11	98,99,100,102	0
2	PO4	D	617	5/5	0.97	0.14	70,72,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	E	619	5/5	0.98	0.10	75,77,79,80	0
2	PO4	C	616	5/5	0.99	0.13	31,33,40,43	0
2	PO4	A	615	5/5	0.99	0.10	36,38,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.