



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:12 PM UTC

PDB ID : 3GNT / pdb_00003gnt
Title : Crystal Structure of the Staphylococcus aureus Enoyl-Acyl Carrier Protein Reductase (FabI) in apo form (two molecules in AU)
Authors : Priyadarshi, A.; Hwang, K.Y.
Deposited on : 2009-03-18
Resolution : 2.75 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
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

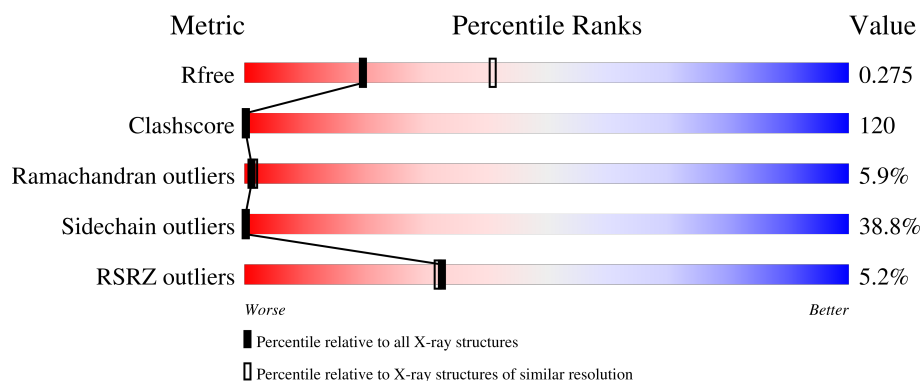
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	256	5% 21% 34% 22% 19%
1	B	256	3% 21% 37% 17% 22%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3157 atoms, of which 0 are hydrogens and 0 are deuteriums.

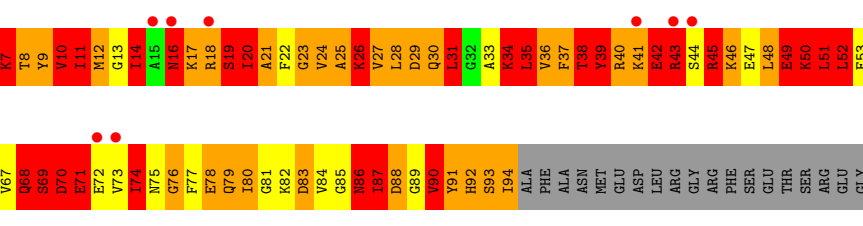
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1608	1017	276	312	3			
1	B	200	Total	C	N	O	S	0	0	0
			1549	978	267	301	3			

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.

- Chain A: 



- Chain B:
-
- | Amino Acid | Frequency (%) |
|------------|---------------|
| H1 | 3% |
| L2 | |
| N3 | |
| L4 | |
| E5 | |
| N6 | |
| K7 | |
| T8 | |
| V9 | |
| V10 | |
| I11 | |
| M12 | |
| G13 | |
| A14 | |
| A15 | |
| M16 | |
| K17 | |
| R18 | |
| S19 | |
| L20 | |
| F21 | |
| F22 | |
| G23 | |
| V24 | |
| A25 | |
| K26 | |
| V27 | |
| L28 | |
| D29 | |
| Q30 | |
| L31 | |
| G32 | |
| A33 | |
| K34 | |
| L35 | |
| V36 | |
| F37 | |
| T38 | |
| Y39 | |
| R40 | |
| K41 | |
| E42 | |
| R43 | |
| S44 | |
| R45 | |
| K46 | |
| E47 | |
| L48 | |
| E49 | |
| K50 | |
| L51 | |
| L52 | |
| E53 | |
| D54 | |
| L55 | |
| N56 | |
| D57 | |
| P58 | |
| E59 | |
| L60 | |

T242	G243	E244	N245	I246	H247	V248	D249	S250	G251	F252	H253	A254	I255	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.10Å 74.46Å 70.61Å 90.00° 119.35° 90.00°	Depositor
Resolution (Å)	34.96 – 2.75 34.96 – 2.75	Depositor EDS
% Data completeness (in resolution range)	84.0 (34.96-2.75) 83.9 (34.96-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.278 0.252 , 0.275	Depositor DCC
R_{free} test set	564 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for -1/2*h+1/2*k+1,1/2*h-1/2*k+1,1/2*h+1/2*k 0.030 for -1/2*h-1/2*k+1,-1/2*h-1/2*k-1,1/2*h-1/2*k	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3157	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% 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

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	2.58	103/1627 (6.3%)	2.64	148/2190 (6.8%)
1	B	2.59	106/1567 (6.8%)	2.60	120/2110 (5.7%)
All	All	2.59	209/3194 (6.5%)	2.62	268/4300 (6.2%)

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	19
1	B	0	24
All	All	0	43

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ILE	CA-CB	-15.79	1.34	1.54
1	A	86	ASN	CA-C	11.26	1.66	1.52
1	A	170	ASN	CA-C	-11.20	1.37	1.52
1	B	241	VAL	CA-CB	-11.02	1.40	1.54
1	B	64	GLN	CA-C	-10.29	1.40	1.52
1	A	28	LEU	CA-C	-9.99	1.41	1.52
1	B	35	LEU	N-CA	-9.91	1.34	1.46
1	B	230	ALA	CA-CB	-9.81	1.38	1.53
1	B	37	PHE	CA-C	-9.70	1.40	1.52
1	B	38	THR	CA-CB	-9.62	1.39	1.53
1	B	145	THR	C-O	-9.50	1.13	1.24
1	B	19	SER	C-O	9.41	1.35	1.23
1	A	170	ASN	C-O	-9.25	1.12	1.24
1	B	180	PRO	N-CA	-9.12	1.35	1.47
1	A	194	ARG	N-CA	8.84	1.57	1.46
1	A	19	SER	N-CA	-8.77	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	ILE	CA-CB	-8.62	1.42	1.54
1	B	143	VAL	C-O	8.61	1.32	1.24
1	A	25	ALA	N-CA	8.47	1.56	1.46
1	B	146	THR	CA-C	-8.47	1.41	1.53
1	B	232	TYR	N-CA	8.39	1.56	1.46
1	A	171	VAL	CA-CB	-8.32	1.43	1.54
1	B	63	TYR	CA-C	-8.25	1.42	1.52
1	A	26	LYS	N-CA	-8.23	1.36	1.46
1	A	230	ALA	CA-CB	-8.23	1.40	1.53
1	B	222	ASP	CB-CG	-8.20	1.31	1.52
1	A	16	ASN	C-O	8.11	1.32	1.24
1	B	40	ARG	CA-C	-8.05	1.42	1.53
1	A	235	SER	N-CA	7.94	1.56	1.46
1	A	245	ASN	C-O	-7.93	1.14	1.24
1	A	80	ILE	C-O	7.88	1.32	1.24
1	A	52	LEU	C-N	7.87	1.45	1.33
1	B	173	TYR	CA-C	-7.82	1.42	1.52
1	A	188	ILE	CA-C	-7.81	1.43	1.52
1	A	10	VAL	CA-CB	7.78	1.63	1.54
1	A	8	THR	CA-C	-7.78	1.43	1.52
1	A	146	THR	CA-C	-7.75	1.43	1.52
1	B	143	VAL	N-CA	-7.70	1.37	1.46
1	B	188	ILE	CA-CB	-7.69	1.45	1.54
1	B	38	THR	N-CA	-7.66	1.34	1.46
1	B	183	ILE	C-O	7.62	1.31	1.24
1	B	247	HIS	CA-CB	-7.60	1.43	1.53
1	A	186	ASN	CA-C	-7.60	1.43	1.52
1	A	185	VAL	CA-CB	-7.54	1.43	1.54
1	A	39	TYR	N-CA	7.48	1.55	1.46
1	B	220	ASN	CA-C	7.48	1.62	1.52
1	B	220	ASN	C-O	7.48	1.33	1.24
1	B	175	ALA	CA-C	7.46	1.62	1.52
1	B	132	ALA	CA-CB	-7.40	1.41	1.53
1	B	14	ILE	C-O	-7.38	1.16	1.23
1	A	86	ASN	C-O	7.28	1.33	1.23
1	B	7	LYS	N-CA	-7.24	1.36	1.45
1	A	16	ASN	CA-C	7.23	1.61	1.53
1	A	1	MET	CG-SD	7.19	1.98	1.80
1	B	248	VAL	CA-C	-7.10	1.43	1.52
1	B	12	MET	N-CA	-7.08	1.36	1.46
1	A	83	ASP	CA-C	7.08	1.62	1.52
1	B	45	ARG	CA-C	-7.04	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	GLU	C-O	7.04	1.32	1.23
1	A	22	PHE	N-CA	-7.04	1.37	1.46
1	B	246	ILE	CA-CB	-7.00	1.45	1.54
1	A	87	ILE	C-O	6.99	1.32	1.23
1	B	190	ALA	CA-CB	6.98	1.64	1.53
1	A	141	SER	N-CA	-6.94	1.37	1.46
1	A	14	ILE	N-CA	-6.88	1.37	1.46
1	A	26	LYS	CA-C	-6.86	1.44	1.52
1	A	45	ARG	CA-C	-6.85	1.44	1.53
1	B	65	ILE	CA-CB	6.82	1.63	1.54
1	A	224	VAL	CA-CB	-6.82	1.45	1.54
1	B	226	VAL	C-O	-6.78	1.15	1.24
1	B	241	VAL	N-CA	-6.73	1.38	1.46
1	A	33	ALA	CA-CB	-6.71	1.42	1.53
1	B	36	VAL	CA-C	6.71	1.60	1.52
1	B	22	PHE	N-CA	-6.70	1.37	1.46
1	B	140	GLY	C-O	6.69	1.33	1.24
1	A	190	ALA	CA-C	-6.64	1.44	1.52
1	A	87	ILE	CA-C	6.61	1.62	1.53
1	A	194	ARG	CA-C	6.56	1.61	1.52
1	B	135	LEU	N-CA	6.54	1.55	1.46
1	B	15	ALA	CA-C	6.53	1.61	1.52
1	A	130	HIS	CA-C	6.53	1.61	1.52
1	B	11	ILE	CA-C	-6.52	1.44	1.52
1	B	237	LEU	C-O	6.50	1.32	1.24
1	B	227	GLY	C-O	-6.49	1.15	1.23
1	A	190	ALA	C-O	6.48	1.31	1.24
1	A	76	GLY	N-CA	6.44	1.54	1.45
1	A	93	SER	N-CA	6.43	1.53	1.46
1	B	146	THR	N-CA	-6.39	1.37	1.45
1	B	28	LEU	C-O	6.33	1.32	1.24
1	B	185	VAL	CA-C	-6.30	1.44	1.52
1	A	236	ASP	N-CA	6.28	1.54	1.46
1	B	238	SER	C-O	6.26	1.33	1.23
1	A	136	MET	C-N	-6.24	1.27	1.34
1	B	61	HIS	CA-C	-6.23	1.44	1.53
1	A	36	VAL	C-O	-6.23	1.17	1.24
1	A	231	ALA	CA-CB	-6.20	1.43	1.53
1	B	192	PRO	N-CA	-6.13	1.40	1.47
1	B	46	LYS	N-CA	-6.13	1.38	1.46
1	A	144	ALA	N-CA	-6.13	1.38	1.46
1	A	40	ARG	CA-C	-6.11	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	ILE	CA-C	6.08	1.60	1.52
1	B	184	ARG	C-O	6.06	1.31	1.24
1	A	91	TYR	N-CA	-6.05	1.38	1.46
1	A	20	ILE	CB-CG2	-6.05	1.32	1.52
1	B	70	ASP	N-CA	-6.05	1.39	1.46
1	A	34	LYS	C-O	6.01	1.31	1.24
1	A	92	HIS	CA-CB	-6.00	1.45	1.52
1	B	231	ALA	CA-CB	-5.99	1.43	1.53
1	A	37	PHE	N-CA	5.96	1.53	1.46
1	B	30	GLN	N-CA	-5.94	1.39	1.46
1	B	42	GLU	CA-CB	5.93	1.64	1.53
1	B	74	ILE	CA-CB	-5.92	1.47	1.54
1	B	215	ALA	CA-C	-5.89	1.46	1.53
1	A	241	VAL	CA-CB	-5.87	1.46	1.54
1	A	55	LEU	CA-C	-5.87	1.44	1.52
1	B	222	ASP	CG-OD2	-5.87	1.14	1.25
1	A	56	ASN	CA-C	-5.86	1.45	1.52
1	A	178	LEU	N-CA	5.84	1.53	1.46
1	B	80	ILE	CA-C	-5.84	1.45	1.52
1	A	226	VAL	CA-CB	5.81	1.63	1.54
1	A	176	LEU	N-CA	5.80	1.53	1.46
1	B	39	TYR	N-CA	5.80	1.52	1.46
1	B	14	ILE	CA-C	-5.79	1.46	1.53
1	B	21	ALA	CA-C	5.79	1.60	1.52
1	A	30	GLN	CA-CB	-5.79	1.44	1.53
1	A	10	VAL	C-O	-5.76	1.18	1.24
1	A	139	GLY	N-CA	5.75	1.53	1.45
1	B	225	GLU	CA-C	-5.74	1.45	1.52
1	B	248	VAL	C-O	-5.74	1.17	1.24
1	A	249	ASP	N-CA	5.74	1.52	1.46
1	B	224	VAL	N-CA	-5.73	1.40	1.46
1	A	14	ILE	CA-CB	5.71	1.60	1.54
1	B	87	ILE	CA-CB	-5.69	1.46	1.55
1	B	33	ALA	CA-C	-5.67	1.45	1.52
1	A	74	ILE	CA-C	5.67	1.59	1.52
1	B	20	ILE	CG1-CD1	-5.67	1.29	1.51
1	B	34	LYS	N-CA	-5.66	1.39	1.45
1	A	228	LYS	CA-C	5.65	1.59	1.52
1	B	75	ASN	C-O	5.63	1.31	1.24
1	A	243	GLY	C-O	-5.61	1.16	1.24
1	B	186	ASN	N-CA	5.61	1.52	1.45
1	B	20	ILE	N-CA	5.60	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	HIS	N-CA	5.60	1.53	1.46
1	B	229	THR	C-O	5.60	1.30	1.24
1	B	236	ASP	N-CA	5.59	1.53	1.46
1	A	222	ASP	C-O	-5.59	1.17	1.24
1	A	208	LEU	N-CA	-5.59	1.39	1.46
1	B	144	ALA	CA-CB	-5.59	1.44	1.53
1	B	30	GLN	CD-OE1	5.59	1.34	1.23
1	A	170	ASN	CA-CB	-5.58	1.45	1.53
1	B	176	LEU	N-CA	5.57	1.53	1.46
1	B	222	ASP	CG-OD1	-5.57	1.14	1.25
1	B	231	ALA	N-CA	-5.56	1.38	1.46
1	A	73	VAL	N-CA	-5.56	1.39	1.46
1	B	129	ALA	C-O	-5.55	1.16	1.23
1	B	175	ALA	C-O	5.55	1.30	1.24
1	A	65	ILE	N-CA	5.55	1.54	1.46
1	A	12	MET	C-O	5.52	1.31	1.23
1	B	211	ILE	CA-C	-5.52	1.46	1.52
1	A	142	ILE	C-O	5.51	1.29	1.24
1	A	79	GLN	N-CA	-5.51	1.39	1.46
1	B	164	LYS	CE-NZ	5.50	1.65	1.49
1	B	126	THR	CA-C	-5.49	1.46	1.52
1	B	189	SER	CA-CB	5.48	1.61	1.53
1	A	132	ALA	CA-CB	-5.47	1.43	1.53
1	A	230	ALA	N-CA	-5.47	1.39	1.46
1	A	29	ASP	N-CA	-5.45	1.39	1.46
1	A	64	GLN	CA-C	-5.45	1.45	1.52
1	A	228	LYS	CA-CB	5.44	1.61	1.53
1	A	88	ASP	CA-C	5.42	1.59	1.52
1	A	23	GLY	C-O	5.38	1.30	1.23
1	A	76	GLY	C-O	5.37	1.31	1.23
1	A	145	THR	CA-CB	-5.36	1.44	1.53
1	B	247	HIS	CA-C	-5.34	1.46	1.52
1	A	184	ARG	NE-CZ	5.33	1.39	1.33
1	B	215	ALA	CA-CB	-5.29	1.42	1.53
1	B	44	SER	N-CA	-5.28	1.39	1.46
1	A	93	SER	CA-C	-5.26	1.46	1.52
1	B	8	THR	CA-CB	-5.26	1.44	1.53
1	A	183	ILE	C-O	-5.25	1.18	1.24
1	A	227	GLY	C-O	-5.24	1.17	1.23
1	A	90	VAL	CA-C	5.23	1.59	1.52
1	B	145	THR	N-CA	5.23	1.52	1.46
1	A	73	VAL	CA-CB	5.23	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	SER	CA-C	5.23	1.58	1.53
1	A	226	VAL	CA-C	5.22	1.59	1.52
1	B	236	ASP	CA-C	5.21	1.59	1.52
1	B	45	ARG	C-O	-5.21	1.17	1.24
1	A	236	ASP	C-O	-5.20	1.17	1.24
1	B	16	ASN	C-O	5.18	1.28	1.24
1	A	82	LYS	CA-CB	5.14	1.61	1.53
1	B	192	PRO	CG-CD	-5.13	1.33	1.50
1	A	235	SER	CA-CB	5.13	1.62	1.53
1	B	171	VAL	CA-CB	-5.11	1.47	1.54
1	B	126	THR	C-O	-5.11	1.18	1.24
1	A	235	SER	CA-C	5.10	1.59	1.52
1	A	181	ASP	CA-CB	5.09	1.60	1.53
1	A	122	SER	C-O	5.08	1.30	1.24
1	A	170	ASN	N-CA	-5.08	1.39	1.46
1	B	244	GLU	CA-C	5.08	1.58	1.52
1	B	249	ASP	N-CA	5.08	1.52	1.46
1	A	184	ARG	CG-CD	-5.07	1.37	1.52
1	B	216	PRO	N-CA	-5.07	1.41	1.47
1	B	33	ALA	CA-CB	-5.06	1.45	1.53
1	A	169	ALA	CA-CB	-5.05	1.45	1.53
1	B	67	VAL	C-N	-5.05	1.24	1.34
1	A	139	GLY	C-O	5.04	1.29	1.23
1	B	129	ALA	CA-CB	-5.02	1.45	1.53
1	B	34	LYS	CA-C	-5.01	1.46	1.52

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLN	CA-C-N	-18.37	102.57	120.21
1	A	57	GLN	C-N-CA	-18.37	102.57	120.21
1	A	49	GLU	CB-CA-C	-17.53	84.34	111.17
1	B	80	ILE	CB-CA-C	-15.18	92.16	112.04
1	B	146	THR	N-CA-C	-14.37	92.00	110.53
1	B	4	LEU	N-CA-C	14.09	140.81	110.80
1	B	56	ASN	N-CA-C	-13.63	87.41	109.76
1	B	78	GLU	N-CA-C	-12.55	97.68	111.36
1	A	11	ILE	CB-CA-C	-12.16	92.32	110.81
1	B	125	LEU	N-CA-C	-12.15	98.24	113.55
1	B	44	SER	N-CA-C	-11.81	98.83	113.01
1	A	73	VAL	N-CA-C	-11.55	100.23	110.74
1	A	86	ASN	N-CA-C	11.34	127.42	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ILE	N-CA-C	11.19	124.84	108.96
1	B	223	GLN	O-C-N	-11.15	110.50	122.09
1	B	27	VAL	N-CA-C	-11.02	101.20	111.67
1	B	63	TYR	N-CA-C	-10.97	92.39	109.07
1	B	122	SER	N-CA-C	10.83	127.54	110.32
1	A	65	ILE	N-CA-C	10.73	125.71	106.61
1	B	225	GLU	N-CA-C	-10.62	100.44	113.50
1	B	221	VAL	CA-C-N	-10.41	108.42	122.16
1	B	221	VAL	C-N-CA	-10.41	108.42	122.16
1	B	29	ASP	N-CA-C	-10.36	99.99	111.07
1	A	43	ARG	N-CA-C	-10.31	100.64	113.01
1	B	70	ASP	N-CA-C	-10.27	98.78	111.11
1	B	12	MET	CB-CG-SD	-10.20	82.10	112.70
1	A	169	ALA	CA-C-N	-10.05	104.53	121.92
1	A	169	ALA	C-N-CA	-10.05	104.53	121.92
1	A	220	ASN	N-CA-C	9.98	124.58	109.41
1	B	74	ILE	N-CA-C	9.80	120.65	110.36
1	B	43	ARG	N-CA-C	-9.62	103.66	114.62
1	B	209	LYS	N-CA-C	-9.61	98.03	112.54
1	B	45	ARG	N-CA-C	-9.59	100.34	112.90
1	A	19	SER	N-CA-C	-9.55	94.09	109.76
1	A	123	TYR	N-CA-C	-9.51	100.48	111.03
1	A	132	ALA	N-CA-C	-9.35	101.13	112.54
1	B	4	LEU	CB-CA-C	-9.27	91.97	110.42
1	B	124	SER	N-CA-C	-9.19	98.66	112.54
1	A	185	VAL	N-CA-C	9.14	121.98	108.45
1	B	127	ILE	CB-CA-C	-9.10	100.44	111.81
1	A	70	ASP	N-CA-C	-8.88	101.60	111.28
1	B	126	THR	N-CA-C	-8.84	101.34	110.97
1	A	38	THR	CA-CB-OG1	8.79	122.79	109.60
1	B	180	PRO	N-CA-C	-8.78	102.08	113.57
1	B	66	ASP	N-CA-C	8.73	124.06	113.23
1	B	169	ALA	CA-C-N	-8.46	109.11	122.65
1	B	169	ALA	C-N-CA	-8.46	109.11	122.65
1	B	143	VAL	N-CA-C	-8.43	95.86	108.17
1	B	188	ILE	CA-C-N	-8.33	111.26	123.00
1	B	188	ILE	C-N-CA	-8.33	111.26	123.00
1	A	168	GLU	N-CA-C	-8.26	102.96	112.87
1	A	62	LEU	N-CA-C	-8.06	98.55	110.48
1	A	51	LEU	N-CA-C	-8.00	93.77	110.80
1	A	16	ASN	N-CA-C	7.96	119.05	108.07
1	A	191	GLY	N-CA-C	-7.90	102.52	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ILE	CA-C-N	-7.88	108.31	121.39
1	A	183	ILE	C-N-CA	-7.88	108.31	121.39
1	B	241	VAL	N-CA-C	7.70	119.57	108.48
1	B	184	ARG	N-CA-C	7.69	121.06	108.52
1	A	52	LEU	CA-C-N	-7.68	111.11	122.86
1	A	52	LEU	C-N-CA	-7.68	111.11	122.86
1	A	238	SER	N-CA-C	-7.65	103.51	112.92
1	A	143	VAL	CB-CA-C	-7.61	99.22	110.33
1	B	182	ASN	N-CA-C	-7.59	101.04	111.28
1	B	67	VAL	O-C-N	-7.58	113.09	122.57
1	B	1	MET	CB-CA-C	7.58	124.50	110.10
1	B	64	GLN	N-CA-C	-7.56	96.58	108.90
1	B	129	ALA	N-CA-C	-7.56	103.67	113.12
1	A	188	ILE	CB-CA-C	-7.55	99.07	110.55
1	B	75	ASN	O-C-N	7.53	132.01	122.37
1	A	1	MET	CA-CB-CG	-7.49	99.11	114.10
1	B	166	SER	N-CA-C	7.48	120.53	110.35
1	B	211	ILE	N-CA-C	-7.39	103.13	110.30
1	A	55	LEU	N-CA-C	-7.32	104.87	114.31
1	A	45	ARG	N-CA-C	-7.32	101.50	112.04
1	B	82	LYS	N-CA-C	7.21	121.17	112.38
1	B	66	ASP	CB-CA-C	-7.18	94.97	109.55
1	A	244	GLU	CA-C-N	7.12	133.03	122.99
1	A	244	GLU	C-N-CA	7.12	133.03	122.99
1	A	38	THR	CB-CA-C	-7.05	94.95	110.67
1	A	73	VAL	CB-CA-C	7.05	121.25	111.94
1	B	140	GLY	O-C-N	7.05	129.65	123.80
1	B	45	ARG	CA-C-N	-6.96	110.38	120.82
1	B	45	ARG	C-N-CA	-6.96	110.38	120.82
1	A	182	ASN	CA-C-N	-6.94	114.09	123.12
1	A	182	ASN	C-N-CA	-6.94	114.09	123.12
1	A	14	ILE	N-CA-C	-6.91	97.90	107.99
1	B	222	ASP	N-CA-C	6.91	121.44	108.65
1	B	164	LYS	O-C-N	-6.90	111.97	123.00
1	A	207	ILE	CA-C-N	-6.88	111.08	120.44
1	A	207	ILE	C-N-CA	-6.88	111.08	120.44
1	A	21	ALA	N-CA-C	-6.88	104.15	112.54
1	A	24	VAL	N-CA-C	-6.87	103.82	110.42
1	B	57	GLN	N-CA-C	6.84	124.92	109.81
1	B	31	LEU	N-CA-C	6.81	121.30	113.19
1	B	46	LYS	N-CA-C	-6.81	100.13	111.37
1	A	190	ALA	N-CA-C	-6.78	98.20	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	MET	CB-CG-SD	-6.77	92.39	112.70
1	A	58	PRO	N-CA-C	-6.77	101.74	111.22
1	B	250	SER	N-CA-C	6.76	120.86	112.47
1	A	9	TYR	N-CA-C	6.76	120.55	109.06
1	B	11	ILE	CB-CA-C	-6.74	100.24	111.29
1	A	50	LYS	N-CA-C	6.74	121.03	110.32
1	A	48	LEU	CA-C-N	-6.72	111.71	122.66
1	A	48	LEU	C-N-CA	-6.72	111.71	122.66
1	A	28	LEU	CA-CB-CG	-6.72	92.80	116.30
1	A	69	SER	N-CA-C	6.71	119.88	109.07
1	B	246	ILE	CA-C-N	-6.67	113.56	122.42
1	B	246	ILE	C-N-CA	-6.67	113.56	122.42
1	B	8	THR	CB-CA-C	6.64	121.34	109.38
1	B	215	ALA	N-CA-C	-6.63	101.70	109.93
1	B	64	GLN	CB-CA-C	-6.61	97.61	109.71
1	A	189	SER	CB-CA-C	6.54	120.51	111.23
1	A	223	GLN	CA-C-N	-6.54	109.92	120.64
1	A	223	GLN	C-N-CA	-6.54	109.92	120.64
1	B	237	LEU	N-CA-C	-6.53	105.18	113.01
1	B	22	PHE	CA-C-N	-6.51	112.74	120.03
1	B	22	PHE	C-N-CA	-6.51	112.74	120.03
1	B	146	THR	CB-CA-C	-6.49	96.96	110.40
1	A	206	THR	N-CA-C	-6.46	102.91	111.24
1	B	7	LYS	CB-CA-C	6.43	120.51	109.51
1	A	24	VAL	CB-CA-C	6.42	120.18	111.97
1	B	211	ILE	CB-CA-C	-6.41	103.80	111.81
1	B	76	GLY	N-CA-C	-6.30	98.25	113.18
1	A	180	PRO	CA-C-N	-6.30	112.65	122.67
1	A	180	PRO	C-N-CA	-6.30	112.65	122.67
1	B	132	ALA	N-CA-C	6.28	121.74	111.37
1	A	60	ALA	N-CA-C	-6.27	106.17	113.88
1	A	211	ILE	CA-C-N	-6.26	112.09	120.54
1	A	211	ILE	C-N-CA	-6.26	112.09	120.54
1	A	136	MET	CG-SD-CE	-6.25	87.14	100.90
1	A	238	SER	O-C-N	6.24	129.83	122.34
1	A	172	LYS	CA-C-N	-6.23	111.45	120.29
1	A	172	LYS	C-N-CA	-6.23	111.45	120.29
1	A	79	GLN	N-CA-C	-6.22	103.80	111.33
1	A	204	PHE	CA-C-N	-6.20	110.11	121.52
1	A	204	PHE	C-N-CA	-6.20	110.11	121.52
1	B	194	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	B	61	HIS	N-CA-CB	-6.18	102.78	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	GLU	CA-C-N	-6.16	113.37	120.88
1	A	72	GLU	C-N-CA	-6.16	113.37	120.88
1	A	71	GLU	CA-C-N	-6.14	112.82	122.65
1	A	71	GLU	C-N-CA	-6.14	112.82	122.65
1	A	127	ILE	CB-CA-C	-6.14	104.49	111.55
1	A	78	GLU	N-CA-C	-6.09	103.98	112.45
1	A	6	ASN	CA-C-N	-6.09	111.28	123.09
1	A	6	ASN	C-N-CA	-6.09	111.28	123.09
1	A	6	ASN	CB-CA-C	-6.08	98.33	110.42
1	A	31	LEU	N-CA-C	6.07	121.75	113.37
1	A	229	THR	N-CA-C	6.03	123.65	110.80
1	A	208	LEU	N-CA-C	-6.03	104.63	111.14
1	A	188	ILE	CA-C-N	-6.01	113.46	122.47
1	A	188	ILE	C-N-CA	-6.01	113.46	122.47
1	A	26	LYS	N-CA-C	-6.00	104.43	110.97
1	A	183	ILE	O-C-N	-5.99	116.09	123.10
1	A	83	ASP	N-CA-C	5.98	123.54	110.80
1	A	1	MET	CG-SD-CE	5.97	114.03	100.90
1	B	240	GLY	N-CA-C	-5.95	105.44	115.80
1	A	7	LYS	N-CA-C	-5.94	100.38	109.65
1	B	34	LYS	CA-C-N	5.94	132.22	121.89
1	B	34	LYS	C-N-CA	5.94	132.22	121.89
1	A	2	LEU	CA-CB-CG	-5.92	95.57	116.30
1	B	135	LEU	N-CA-CB	5.90	118.85	111.00
1	A	12	MET	CB-CA-C	-5.90	103.40	111.95
1	B	7	LYS	CA-C-N	-5.90	114.38	122.93
1	B	7	LYS	C-N-CA	-5.90	114.38	122.93
1	A	29	ASP	N-CA-C	-5.89	101.71	111.37
1	A	23	GLY	N-CA-C	-5.84	105.55	113.37
1	A	28	LEU	CB-CA-C	-5.83	100.50	110.24
1	A	136	MET	N-CA-C	5.83	122.69	109.81
1	B	138	GLU	N-CA-C	-5.76	106.38	113.41
1	A	90	VAL	CA-C-N	-5.75	115.36	122.84
1	A	90	VAL	C-N-CA	-5.75	115.36	122.84
1	A	138	GLU	N-CA-C	-5.75	106.25	113.72
1	A	193	ILE	CA-C-O	-5.74	113.61	120.78
1	B	174	LEU	N-CA-C	-5.73	105.17	111.82
1	B	140	GLY	N-CA-C	-5.71	102.80	111.42
1	A	61	HIS	N-CA-C	5.69	122.92	110.80
1	A	1	MET	N-CA-C	5.69	126.92	111.00
1	A	45	ARG	NE-CZ-NH2	-5.68	114.08	119.20
1	B	184	ARG	NE-CZ-NH1	-5.64	115.86	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ASP	N-CA-CB	5.60	118.35	110.24
1	B	28	LEU	CB-CA-C	-5.59	100.28	110.63
1	A	136	MET	CA-C-N	5.59	125.30	119.82
1	A	136	MET	C-N-CA	5.59	125.30	119.82
1	A	90	VAL	O-C-N	-5.58	116.61	123.03
1	B	59	GLU	CA-CB-CG	5.58	125.25	114.10
1	A	252	PHE	N-CA-C	5.57	119.17	112.38
1	A	28	LEU	N-CA-C	-5.56	105.29	112.68
1	B	6	ASN	N-CA-CB	-5.56	107.83	114.17
1	B	75	ASN	N-CA-C	-5.55	106.71	112.93
1	B	176	LEU	CA-CB-CG	-5.55	96.87	116.30
1	A	92	HIS	CA-C-O	-5.55	115.15	120.92
1	A	37	PHE	N-CA-C	5.54	118.52	109.59
1	A	2	LEU	CD1-CG-CD2	5.54	122.99	110.80
1	B	74	ILE	CA-C-N	-5.53	113.47	122.65
1	B	74	ILE	C-N-CA	-5.53	113.47	122.65
1	A	12	MET	CA-C-N	-5.52	110.59	121.41
1	A	12	MET	C-N-CA	-5.52	110.59	121.41
1	A	227	GLY	N-CA-C	-5.51	105.98	113.37
1	A	83	ASP	CA-C-N	5.51	129.67	120.64
1	A	83	ASP	C-N-CA	5.51	129.67	120.64
1	A	248	VAL	N-CA-C	-5.51	97.89	109.34
1	A	92	HIS	N-CA-C	5.50	117.67	107.99
1	A	30	GLN	N-CA-C	5.47	117.68	111.11
1	B	185	VAL	N-CA-C	5.47	115.73	107.75
1	A	223	GLN	N-CA-C	5.46	117.93	111.33
1	A	211	ILE	N-CA-C	5.45	116.23	110.72
1	B	8	THR	CA-CB-OG1	-5.45	101.42	109.60
1	B	226	VAL	N-CA-C	-5.45	105.06	111.00
1	A	133	LYS	CA-C-O	5.45	126.08	119.49
1	B	220	ASN	N-CA-C	5.44	116.53	108.86
1	A	24	VAL	CA-C-O	-5.44	115.40	121.17
1	B	177	ASP	N-CA-C	-5.43	105.45	112.68
1	A	186	ASN	N-CA-C	-5.43	99.83	109.06
1	A	68	GLN	CA-C-N	-5.38	115.57	123.00
1	A	68	GLN	C-N-CA	-5.38	115.57	123.00
1	A	65	ILE	CB-CA-C	-5.38	105.12	111.09
1	B	12	MET	N-CA-C	-5.38	100.92	109.96
1	B	23	GLY	N-CA-C	-5.37	106.28	112.83
1	B	136	MET	CA-C-N	5.37	126.55	119.84
1	B	136	MET	C-N-CA	5.37	126.55	119.84
1	B	30	GLN	N-CA-C	5.37	117.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	LYS	CA-C-N	-5.35	113.11	120.28
1	B	228	LYS	C-N-CA	-5.35	113.11	120.28
1	A	234	LEU	CB-CA-C	-5.34	100.10	110.46
1	B	87	ILE	N-CA-C	5.32	117.05	108.85
1	B	170	ASN	N-CA-CB	5.31	118.32	110.56
1	A	39	TYR	CA-C-N	-5.28	114.64	122.56
1	A	39	TYR	C-N-CA	-5.28	114.64	122.56
1	A	194	ARG	CG-CD-NE	-5.27	100.40	112.00
1	A	186	ASN	CA-C-O	-5.26	114.28	120.60
1	B	214	ARG	CG-CD-NE	5.24	123.53	112.00
1	A	65	ILE	CA-C-N	-5.23	113.69	122.17
1	A	65	ILE	C-N-CA	-5.23	113.69	122.17
1	A	64	GLN	CA-C-O	-5.23	114.69	120.70
1	A	35	LEU	N-CA-C	5.22	117.58	108.76
1	B	69	SER	CA-C-N	-5.20	113.52	120.54
1	B	69	SER	C-N-CA	-5.20	113.52	120.54
1	A	130	HIS	N-CA-C	5.19	116.62	111.07
1	A	27	VAL	N-CA-C	-5.18	104.43	111.89
1	B	189	SER	CB-CA-C	5.18	118.76	110.16
1	B	184	ARG	CA-C-N	-5.18	116.21	123.10
1	B	184	ARG	C-N-CA	-5.18	116.21	123.10
1	A	174	LEU	CA-CB-CG	5.17	134.40	116.30
1	B	11	ILE	CA-C-N	-5.15	114.47	122.09
1	B	11	ILE	C-N-CA	-5.15	114.47	122.09
1	A	233	LEU	CA-C-O	-5.15	115.48	120.89
1	A	18	ARG	CA-C-N	-5.13	115.01	122.65
1	A	18	ARG	C-N-CA	-5.13	115.01	122.65
1	B	180	PRO	CB-CG-CD	-5.13	89.69	106.10
1	A	253	HIS	N-CA-C	5.12	121.71	110.80
1	A	54	GLN	CA-CB-CG	-5.12	103.86	114.10
1	B	143	VAL	O-C-N	5.11	128.59	123.07
1	B	146	THR	N-CA-CB	-5.11	103.14	110.44
1	B	38	THR	OG1-CB-CG2	5.11	119.51	109.30
1	A	184	ARG	CG-CD-NE	5.10	123.23	112.00
1	B	39	TYR	CA-CB-CG	5.10	123.09	113.90
1	B	57	GLN	CA-C-N	-5.09	113.47	119.84
1	B	57	GLN	C-N-CA	-5.09	113.47	119.84
1	A	92	HIS	CB-CA-C	-5.09	102.65	111.30
1	B	141	SER	N-CA-CB	-5.09	103.16	111.66
1	A	218	LYS	N-CA-C	5.08	118.61	111.90
1	B	28	LEU	O-C-N	5.07	128.15	122.22
1	B	38	THR	N-CA-C	-5.04	102.43	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	N-CA-CB	5.04	118.98	110.92
1	B	185	VAL	N-CA-CB	5.03	118.18	111.64
1	B	7	LYS	N-CA-C	-5.00	102.36	110.32

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ILE	Peptide
1	A	127	ILE	Peptide
1	A	146	THR	Peptide
1	A	164	LYS	Peptide
1	A	165	ALA	Peptide
1	A	166	SER	Peptide
1	A	185	VAL	Peptide
1	A	2	LEU	Peptide
1	A	38	THR	Peptide
1	A	42	GLU	Peptide
1	A	49	GLU	Peptide
1	A	50	LYS	Peptide
1	A	51	LEU	Peptide
1	A	57	GLN	Peptide
1	A	59	GLU	Peptide
1	A	6	ASN	Peptide
1	A	60	ALA	Peptide
1	A	71	GLU	Mainchain
1	A	86	ASN	Peptide
1	B	1	MET	Peptide
1	B	121	SER	Peptide
1	B	122	SER	Peptide
1	B	165	ALA	Peptide
1	B	167	LEU	Peptide
1	B	169	ALA	Peptide
1	B	176	LEU	Peptide
1	B	193	ILE	Peptide
1	B	2	LEU	Peptide
1	B	208	LEU	Peptide
1	B	221	VAL	Peptide
1	B	224	VAL	Mainchain
1	B	24	VAL	Peptide
1	B	254	ALA	Peptide
1	B	3	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	34	LYS	Peptide
1	B	38	THR	Peptide
1	B	41	LYS	Peptide
1	B	42	GLU	Peptide
1	B	51	LEU	Peptide
1	B	52	LEU	Peptide
1	B	53	GLU	Peptide
1	B	54	GLN	Peptide
1	B	67	VAL	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	1608	0	1640	374	0
1	B	1549	0	1576	399	0
All	All	3157	0	3216	764	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 120.

All (764) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:CG2	1:B:73:VAL:HG12	1.39	1.49
1:B:59:GLU:HG3	1:B:61:HIS:N	1.39	1.36
1:B:8:THR:CG2	1:B:87:ILE:HD11	1.55	1.36
1:B:52:LEU:HA	1:B:54:GLN:CG	1.55	1.36
1:B:147:TYR:CD1	1:B:147:TYR:C	1.99	1.35
1:B:89:GLY:HA2	1:B:136:MET:CE	1.60	1.31
1:B:75:ASN:O	1:B:79:GLN:HB2	1.35	1.26
1:B:167:LEU:HD13	1:B:167:LEU:O	1.31	1.25
1:B:167:LEU:HA	1:B:168:GLU:CB	1.69	1.20
1:A:194:ARG:HB3	1:A:194:ARG:NH1	1.56	1.20
1:B:52:LEU:CA	1:B:54:GLN:HG2	1.70	1.20
1:B:135:LEU:O	1:B:137:PRO:HD3	1.41	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB3	1:B:2:LEU:HD23	1.26	1.16
1:B:65:ILE:HG22	1:B:73:VAL:CG1	1.76	1.16
1:A:166:SER:HB3	1:A:169:ALA:CB	1.76	1.15
1:B:1:MET:HB3	1:B:2:LEU:CD2	1.75	1.15
1:B:10:VAL:HG13	1:B:36:VAL:HG12	1.27	1.15
1:B:59:GLU:N	1:B:60:ALA:HA	1.55	1.14
1:A:39:TYR:CE1	1:A:64:GLN:HG2	1.83	1.13
1:B:59:GLU:CG	1:B:61:HIS:H	1.60	1.13
1:A:171:VAL:HG21	1:A:187:ALA:HB2	1.28	1.13
1:B:34:LYS:NZ	1:B:34:LYS:HB3	1.43	1.12
1:B:194:ARG:HG2	1:B:194:ARG:HH11	1.06	1.12
1:B:65:ILE:CG2	1:B:73:VAL:CG1	2.26	1.11
1:B:65:ILE:HG22	1:B:73:VAL:HG12	1.22	1.11
1:B:65:ILE:HG21	1:B:73:VAL:HG12	1.21	1.09
1:A:123:TYR:CG	1:A:127:ILE:HD11	1.87	1.09
1:A:93:SER:O	1:A:94:ILE:HB	1.44	1.08
1:B:194:ARG:HH11	1:B:194:ARG:CG	1.55	1.08
1:A:166:SER:HB3	1:A:169:ALA:HB3	1.17	1.08
1:B:8:THR:HB	1:B:87:ILE:CD1	1.84	1.07
1:B:123:TYR:HD2	1:B:123:TYR:C	1.61	1.07
1:A:39:TYR:CD1	1:A:39:TYR:C	2.33	1.07
1:A:123:TYR:O	1:A:127:ILE:HG13	1.55	1.06
1:B:194:ARG:NH1	1:B:194:ARG:HB3	1.68	1.06
1:B:43:ARG:O	1:B:46:LYS:HB2	1.54	1.05
1:B:194:ARG:NH1	1:B:194:ARG:CB	2.19	1.05
1:B:89:GLY:HA2	1:B:136:MET:HE2	1.37	1.04
1:A:4:LEU:HD12	1:A:236:ASP:CG	1.83	1.04
1:B:8:THR:CG2	1:B:87:ILE:CD1	2.37	1.03
1:B:123:TYR:C	1:B:123:TYR:CD2	2.30	1.03
1:B:167:LEU:CA	1:B:168:GLU:HB2	1.88	1.03
1:A:59:GLU:H	1:A:60:ALA:HA	1.20	1.02
1:B:177:ASP:HB3	1:B:178:LEU:HD13	1.39	1.02
1:B:182:ASN:O	1:B:183:ILE:HD12	1.59	1.02
1:B:123:TYR:CE2	1:B:127:ILE:CG1	2.42	1.02
1:B:124:SER:O	1:B:128:VAL:HG23	1.58	1.01
1:B:167:LEU:CA	1:B:168:GLU:CB	2.38	1.01
1:A:124:SER:O	1:A:128:VAL:HG23	1.58	1.00
1:B:8:THR:CB	1:B:87:ILE:HD11	1.90	1.00
1:B:139:GLY:HA2	1:B:183:ILE:HD11	1.38	1.00
1:B:8:THR:HB	1:B:87:ILE:HD12	1.41	1.00
1:A:49:GLU:O	1:A:49:GLU:HG2	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:TYR:HE2	1:B:127:ILE:CD1	1.73	1.00
1:B:123:TYR:HE2	1:B:127:ILE:HD11	1.26	1.00
1:B:5:GLU:O	1:B:6:ASN:HB2	1.58	1.00
1:A:39:TYR:C	1:A:39:TYR:HD1	1.67	0.99
1:A:170:ASN:N	1:A:170:ASN:HD22	1.54	0.99
1:B:147:TYR:C	1:B:147:TYR:HD1	1.47	0.98
1:B:8:THR:HG22	1:B:87:ILE:HD11	1.01	0.98
1:B:10:VAL:HG22	1:B:36:VAL:HB	1.43	0.98
1:A:51:LEU:HB3	1:A:52:LEU:C	1.87	0.97
1:B:2:LEU:C	1:B:3:ASN:CG	2.29	0.97
1:B:167:LEU:O	1:B:167:LEU:CD1	2.12	0.97
1:B:167:LEU:HD13	1:B:167:LEU:C	1.89	0.97
1:B:8:THR:CB	1:B:87:ILE:CD1	2.42	0.97
1:B:6:ASN:HA	1:B:34:LYS:HD2	1.47	0.96
1:B:34:LYS:HB3	1:B:34:LYS:HZ3	0.93	0.96
1:B:2:LEU:HB2	1:B:3:ASN:ND2	1.81	0.96
1:B:17:LYS:O	1:B:17:LYS:HG2	1.66	0.96
1:A:194:ARG:HH11	1:A:194:ARG:CB	1.78	0.96
1:A:89:GLY:HA2	1:A:136:MET:HE1	1.45	0.95
1:A:130:HIS:O	1:A:133:LYS:HB3	1.66	0.95
1:A:55:LEU:O	1:A:57:GLN:HG3	1.66	0.95
1:B:8:THR:HG22	1:B:87:ILE:CD1	1.92	0.95
1:B:54:GLN:O	1:B:54:GLN:HG3	1.63	0.95
1:A:4:LEU:CD1	1:A:236:ASP:CG	2.40	0.95
1:B:167:LEU:HA	1:B:168:GLU:HB2	0.97	0.95
1:A:29:ASP:HB2	1:A:54:GLN:NE2	1.81	0.94
1:A:237:LEU:HD12	1:B:228:LYS:HD2	1.48	0.94
1:B:8:THR:HA	1:B:34:LYS:O	1.67	0.94
1:A:38:THR:HG23	1:A:39:TYR:H	1.30	0.94
1:B:45:ARG:O	1:B:45:ARG:HG2	1.66	0.93
1:A:5:GLU:HG3	1:A:6:ASN:N	1.80	0.93
1:A:194:ARG:NH1	1:A:194:ARG:CB	2.31	0.92
1:A:207:ILE:HD12	1:A:207:ILE:C	1.95	0.92
1:B:194:ARG:CG	1:B:194:ARG:NH1	2.20	0.92
1:A:50:LYS:HG3	1:A:51:LEU:N	1.83	0.92
1:A:38:THR:CG2	1:A:39:TYR:N	2.33	0.91
1:B:39:TYR:CZ	1:B:64:GLN:HB2	2.06	0.91
1:B:39:TYR:CE1	1:B:64:GLN:HB2	2.06	0.91
1:B:167:LEU:HD22	1:B:168:GLU:HB3	1.51	0.91
1:A:60:ALA:O	1:A:61:HIS:CD2	2.23	0.90
1:B:123:TYR:HE2	1:B:127:ILE:CG1	1.81	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:C	1:A:45:ARG:H	1.78	0.89
1:A:60:ALA:O	1:A:61:HIS:CG	2.25	0.89
1:A:188:ILE:CG2	1:A:189:SER:N	2.35	0.89
1:A:39:TYR:HE1	1:A:64:GLN:HG2	1.32	0.89
1:B:169:ALA:O	1:B:173:TYR:CD2	2.25	0.89
1:A:1:MET:HE3	1:A:1:MET:HA	1.54	0.89
1:A:2:LEU:N	1:A:2:LEU:HD12	1.82	0.89
1:B:52:LEU:HA	1:B:54:GLN:HG2	0.90	0.89
1:B:139:GLY:HA2	1:B:183:ILE:CD1	2.02	0.88
1:A:23:GLY:O	1:A:27:VAL:HG23	1.73	0.88
1:B:44:SER:O	1:B:48:LEU:HD23	1.72	0.88
1:B:123:TYR:CE2	1:B:127:ILE:HD11	2.08	0.88
1:B:3:ASN:HB3	1:B:236:ASP:H	1.38	0.88
1:B:38:THR:HB	1:B:65:ILE:HG13	1.55	0.87
1:B:182:ASN:O	1:B:183:ILE:CD1	2.23	0.87
1:B:4:LEU:HD22	1:B:31:LEU:HB3	1.57	0.87
1:A:59:GLU:H	1:A:60:ALA:CA	1.86	0.87
1:A:4:LEU:CD1	1:A:236:ASP:OD2	2.22	0.87
1:A:39:TYR:OH	1:A:64:GLN:HG3	1.74	0.87
1:A:167:LEU:HD13	1:A:187:ALA:HB1	1.57	0.86
1:A:166:SER:CB	1:A:169:ALA:HB3	2.05	0.86
1:B:69:SER:O	1:B:70:ASP:C	2.15	0.86
1:A:57:GLN:OE1	1:A:58:PRO:HD2	1.75	0.86
1:B:193:ILE:HG12	1:B:222:ASP:HA	1.57	0.86
1:B:89:GLY:CA	1:B:136:MET:CE	2.51	0.86
1:B:34:LYS:NZ	1:B:34:LYS:CB	2.29	0.86
1:B:89:GLY:HA2	1:B:136:MET:HE3	1.54	0.86
1:A:57:GLN:OE1	1:A:57:GLN:N	2.09	0.85
1:B:139:GLY:CA	1:B:183:ILE:HD11	2.06	0.85
1:A:11:ILE:HG22	1:A:12:MET:N	1.92	0.85
1:B:194:ARG:CB	1:B:194:ARG:CZ	2.52	0.85
1:A:169:ALA:O	1:A:173:TYR:HD2	1.59	0.85
1:A:194:ARG:HD2	1:A:194:ARG:O	1.74	0.85
1:B:2:LEU:HB2	1:B:3:ASN:HD21	1.36	0.85
1:A:208:LEU:HB3	1:A:209:LYS:HD2	1.57	0.84
1:B:66:ASP:CG	1:B:66:ASP:O	2.17	0.84
1:A:86:ASN:C	1:A:86:ASN:HD22	1.85	0.84
1:B:123:TYR:CD2	1:B:123:TYR:O	2.29	0.84
1:B:123:TYR:CE2	1:B:127:ILE:HG13	2.11	0.84
1:B:76:GLY:O	1:B:80:ILE:HG13	1.77	0.84
1:A:5:GLU:O	1:A:6:ASN:HB2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HD13	1:A:234:LEU:H	1.41	0.83
1:B:35:LEU:HB2	1:B:56:ASN:HD21	1.42	0.83
1:A:236:ASP:O	1:A:239:SER:HB2	1.79	0.83
1:B:4:LEU:CD2	1:B:31:LEU:HB3	2.07	0.83
1:A:38:THR:CG2	1:A:39:TYR:H	1.91	0.83
1:A:47:GLU:O	1:A:50:LYS:HB3	1.79	0.83
1:A:51:LEU:HB3	1:A:52:LEU:O	1.78	0.83
1:A:86:ASN:C	1:A:86:ASN:ND2	2.36	0.83
1:A:147:TYR:CD1	1:A:147:TYR:O	2.32	0.83
1:B:10:VAL:CG1	1:B:36:VAL:HG12	2.07	0.83
1:A:146:THR:CG2	1:A:167:LEU:HD12	2.09	0.82
1:B:52:LEU:C	1:B:54:GLN:HB3	2.03	0.82
1:A:194:ARG:HB3	1:A:194:ARG:HH11	1.29	0.82
1:B:254:ALA:C	1:B:255:ILE:HG22	2.04	0.82
1:A:188:ILE:HG22	1:A:189:SER:N	1.95	0.82
1:B:254:ALA:C	1:B:255:ILE:CG2	2.52	0.82
1:B:59:GLU:HG3	1:B:61:HIS:CA	2.08	0.82
1:A:5:GLU:CG	1:A:6:ASN:N	2.42	0.81
1:B:125:LEU:O	1:B:129:ALA:HB2	1.78	0.81
1:A:1:MET:HA	1:A:1:MET:CE	2.10	0.81
1:A:39:TYR:CZ	1:A:42:GLU:HB3	2.14	0.81
1:A:204:PHE:HA	1:A:207:ILE:HG13	1.62	0.81
1:A:39:TYR:CD1	1:A:39:TYR:O	2.33	0.81
1:A:204:PHE:HA	1:A:207:ILE:CG1	2.09	0.81
1:B:184:ARG:HD2	1:B:241:VAL:O	1.81	0.81
1:A:24:VAL:HG21	1:A:91:TYR:CE1	2.16	0.80
1:B:2:LEU:HB2	1:B:3:ASN:CG	2.06	0.80
1:B:45:ARG:O	1:B:49:GLU:HG2	1.82	0.80
1:B:2:LEU:CB	1:B:3:ASN:OD1	2.30	0.80
1:B:58:PRO:C	1:B:60:ALA:HA	2.07	0.80
1:A:50:LYS:C	1:A:52:LEU:N	2.31	0.80
1:B:60:ALA:O	1:B:62:LEU:HD13	1.82	0.80
1:B:169:ALA:O	1:B:173:TYR:HD2	1.64	0.80
1:B:5:GLU:O	1:B:6:ASN:CB	2.30	0.79
1:A:59:GLU:N	1:A:60:ALA:HA	1.97	0.79
1:A:81:GLY:O	1:A:85:GLY:HA2	1.81	0.79
1:A:254:ALA:O	1:A:255:ILE:HG22	1.82	0.79
1:B:43:ARG:O	1:B:46:LYS:CB	2.30	0.79
1:A:124:SER:O	1:A:128:VAL:CG2	2.30	0.79
1:A:194:ARG:O	1:A:194:ARG:CD	2.30	0.79
1:B:48:LEU:HA	1:B:51:LEU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ALA:O	1:A:173:TYR:CD2	2.36	0.78
1:A:170:ASN:N	1:A:170:ASN:ND2	2.24	0.78
1:A:171:VAL:CG2	1:A:187:ALA:HB2	2.13	0.78
1:B:164:LYS:HB3	1:B:165:ALA:HB2	1.63	0.78
1:A:77:PHE:HA	1:A:80:ILE:HD12	1.65	0.78
1:B:6:ASN:HA	1:B:34:LYS:CD	2.15	0.77
1:B:59:GLU:N	1:B:60:ALA:CA	2.41	0.77
1:A:10:VAL:HG21	1:A:77:PHE:HE2	1.49	0.77
1:B:45:ARG:O	1:B:45:ARG:CG	2.30	0.77
1:B:167:LEU:CD2	1:B:168:GLU:HB3	2.14	0.77
1:B:254:ALA:O	1:B:255:ILE:HG22	1.85	0.77
1:B:10:VAL:HG13	1:B:36:VAL:CG1	2.11	0.77
1:B:120:ILE:HA	1:B:121:SER:HB2	1.67	0.77
1:A:48:LEU:HG	1:A:62:LEU:HD22	1.67	0.77
1:B:59:GLU:H	1:B:60:ALA:HA	1.49	0.77
1:B:75:ASN:O	1:B:79:GLN:CB	2.26	0.77
1:A:92:HIS:CE1	1:A:124:SER:HG	2.03	0.76
1:A:24:VAL:HG11	1:A:91:TYR:CG	2.21	0.76
1:B:67:VAL:HG22	1:B:67:VAL:O	1.85	0.76
1:A:50:LYS:C	1:A:52:LEU:H	1.92	0.76
1:A:234:LEU:H	1:A:234:LEU:CD1	1.99	0.76
1:B:67:VAL:CG2	1:B:124:SER:HB2	2.15	0.76
1:B:54:GLN:CG	1:B:54:GLN:O	2.34	0.76
1:B:86:ASN:CB	1:B:135:LEU:O	2.32	0.76
1:B:39:TYR:CE2	1:B:45:ARG:NH1	2.54	0.76
1:B:67:VAL:HG23	1:B:124:SER:HB2	1.67	0.76
1:B:39:TYR:HE2	1:B:45:ARG:HH12	1.31	0.75
1:A:4:LEU:HD11	1:A:236:ASP:OD2	1.86	0.75
1:A:193:ILE:CG2	1:A:221:VAL:O	2.35	0.75
1:A:29:ASP:CB	1:A:54:GLN:HE21	1.98	0.75
1:A:193:ILE:HG21	1:A:221:VAL:O	1.86	0.75
1:A:204:PHE:CA	1:A:207:ILE:HG13	2.15	0.75
1:B:39:TYR:HE2	1:B:45:ARG:NH1	1.82	0.75
1:A:211:ILE:HG23	1:A:215:ALA:HB2	1.68	0.74
1:A:7:LYS:HG2	1:A:88:ASP:CG	2.12	0.74
1:B:171:VAL:HG21	1:B:187:ALA:HB2	1.68	0.74
1:B:187:ALA:O	1:B:245:ASN:HA	1.88	0.74
1:B:45:ARG:O	1:B:46:LYS:C	2.22	0.74
1:A:94:ILE:CG2	1:A:94:ILE:O	2.35	0.73
1:B:125:LEU:O	1:B:129:ALA:CB	2.35	0.73
1:A:1:MET:C	1:A:2:LEU:HG	2.12	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:HB2	1:A:54:GLN:HE21	1.53	0.73
1:A:93:SER:O	1:A:94:ILE:CB	2.27	0.73
1:A:221:VAL:HA	1:A:225:GLU:OE1	1.88	0.73
1:A:1:MET:O	1:A:1:MET:HG3	1.89	0.72
1:A:129:ALA:CB	1:A:174:LEU:HD11	2.19	0.72
1:A:211:ILE:HD12	1:A:211:ILE:H	1.52	0.72
1:A:35:LEU:HB2	1:A:56:ASN:ND2	2.05	0.72
1:A:193:ILE:HG21	1:A:222:ASP:HA	1.72	0.72
1:A:42:GLU:O	1:A:45:ARG:CB	2.37	0.71
1:B:66:ASP:O	1:B:66:ASP:OD2	2.08	0.71
1:A:39:TYR:CE1	1:A:64:GLN:CG	2.68	0.71
1:A:178:LEU:N	1:A:178:LEU:HD13	2.05	0.71
1:B:48:LEU:O	1:B:51:LEU:HB2	1.90	0.71
1:B:146:THR:HG23	1:B:147:TYR:N	2.05	0.71
1:B:147:TYR:CD1	1:B:147:TYR:O	2.42	0.71
1:A:171:VAL:HG21	1:A:187:ALA:CB	2.16	0.71
1:A:211:ILE:HD12	1:A:211:ILE:N	2.06	0.71
1:B:12:MET:HE3	1:B:77:PHE:HZ	1.55	0.71
1:B:35:LEU:HB2	1:B:56:ASN:ND2	2.04	0.71
1:A:10:VAL:HG13	1:A:36:VAL:CG1	2.20	0.71
1:B:1:MET:CB	1:B:2:LEU:CD2	2.63	0.71
1:B:60:ALA:O	1:B:61:HIS:C	2.34	0.71
1:A:42:GLU:O	1:A:42:GLU:OE2	2.09	0.71
1:A:45:ARG:HD3	1:A:62:LEU:HD13	1.71	0.71
1:A:5:GLU:HB2	1:A:31:LEU:O	1.90	0.70
1:B:193:ILE:CG1	1:B:222:ASP:HA	2.20	0.70
1:B:24:VAL:O	1:B:28:LEU:HB2	1.92	0.70
1:B:86:ASN:HB2	1:B:135:LEU:O	1.91	0.70
1:B:167:LEU:CA	1:B:168:GLU:HB3	2.21	0.70
1:A:16:ASN:HB3	1:A:47:GLU:OE1	1.91	0.69
1:B:65:ILE:HG22	1:B:73:VAL:HG13	1.72	0.69
1:B:59:GLU:CG	1:B:61:HIS:N	2.35	0.69
1:A:40:ARG:HH12	1:A:68:GLN:HE21	1.40	0.69
1:A:24:VAL:HG11	1:A:91:TYR:CD1	2.27	0.69
1:A:41:LYS:O	1:A:44:SER:HB2	1.93	0.69
1:A:70:ASP:O	1:A:74:ILE:HG13	1.92	0.69
1:A:71:GLU:O	1:A:75:ASN:ND2	2.26	0.69
1:B:124:SER:O	1:B:128:VAL:CG2	2.37	0.69
1:B:43:ARG:C	1:B:46:LYS:H	2.01	0.68
1:A:70:ASP:OD1	1:A:70:ASP:N	2.25	0.68
1:B:20:ILE:CG2	1:B:226:VAL:HG11	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD13	1:A:187:ALA:CB	2.23	0.68
1:B:86:ASN:H	1:B:86:ASN:ND2	1.88	0.68
1:A:166:SER:HB3	1:A:169:ALA:HB2	1.71	0.68
1:A:207:ILE:C	1:A:207:ILE:CD1	2.67	0.68
1:A:43:ARG:HA	1:A:46:LYS:HB2	1.74	0.68
1:B:2:LEU:HB2	1:B:3:ASN:OD1	1.93	0.68
1:B:139:GLY:CA	1:B:183:ILE:CD1	2.69	0.68
1:B:67:VAL:CG2	1:B:124:SER:CB	2.71	0.68
1:B:122:SER:OG	1:B:123:TYR:C	2.37	0.68
1:B:166:SER:OG	1:B:167:LEU:N	2.23	0.68
1:B:143:VAL:CG2	1:B:234:LEU:HD13	2.24	0.68
1:A:83:ASP:OD1	1:A:83:ASP:N	2.22	0.67
1:B:140:GLY:H	1:B:183:ILE:HD12	1.59	0.67
1:B:231:ALA:O	1:B:235:SER:HB3	1.94	0.67
1:A:129:ALA:CB	1:A:174:LEU:CD1	2.72	0.67
1:A:178:LEU:N	1:A:178:LEU:CD1	2.57	0.67
1:B:123:TYR:CE2	1:B:127:ILE:HG12	2.29	0.67
1:B:211:ILE:O	1:B:213:GLU:N	2.27	0.67
1:B:46:LYS:O	1:B:49:GLU:CG	2.42	0.67
1:B:89:GLY:CA	1:B:136:MET:HE3	2.21	0.67
1:B:43:ARG:C	1:B:45:ARG:N	2.47	0.67
1:A:43:ARG:O	1:A:43:ARG:HG2	1.94	0.67
1:A:51:LEU:HD13	1:A:53:GLU:HB2	1.76	0.66
1:A:170:ASN:O	1:A:171:VAL:C	2.34	0.66
1:B:66:ASP:O	1:B:67:VAL:HG12	1.94	0.66
1:B:23:GLY:O	1:B:27:VAL:HG23	1.95	0.66
1:B:27:VAL:O	1:B:30:GLN:HB3	1.95	0.66
1:A:170:ASN:C	1:A:172:LYS:H	2.03	0.66
1:A:216:PRO:HG2	1:A:251:GLY:HA3	1.76	0.66
1:A:231:ALA:O	1:A:235:SER:HB3	1.96	0.66
1:B:61:HIS:CD2	1:B:84:VAL:HG12	2.30	0.66
1:B:135:LEU:C	1:B:137:PRO:HD3	2.17	0.66
1:A:123:TYR:CD1	1:A:127:ILE:HD11	2.30	0.66
1:A:170:ASN:C	1:A:172:LYS:N	2.45	0.66
1:B:39:TYR:CE1	1:B:64:GLN:CB	2.79	0.66
1:B:123:TYR:HD2	1:B:124:SER:N	1.94	0.66
1:A:10:VAL:HG13	1:A:36:VAL:HG12	1.78	0.66
1:A:89:GLY:CA	1:A:136:MET:HE1	2.25	0.66
1:B:146:THR:CG2	1:B:147:TYR:N	2.53	0.66
1:A:169:ALA:C	1:A:170:ASN:HD22	2.03	0.66
1:B:135:LEU:HD23	1:B:135:LEU:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:H	1:A:56:ASN:HD21	1.43	0.65
1:A:123:TYR:CD2	1:A:127:ILE:HD11	2.31	0.65
1:B:2:LEU:HB3	1:B:3:ASN:OD1	1.96	0.65
1:B:122:SER:OG	1:B:123:TYR:N	2.29	0.65
1:B:120:ILE:O	1:B:120:ILE:HG22	1.96	0.65
1:B:211:ILE:CG2	1:B:215:ALA:HB2	2.27	0.65
1:A:76:GLY:O	1:A:80:ILE:HG13	1.96	0.65
1:B:17:LYS:HE2	1:B:18:ARG:NH2	2.11	0.65
1:A:146:THR:OG1	1:A:147:TYR:N	2.23	0.65
1:B:57:GLN:OE1	1:B:58:PRO:HD3	1.97	0.65
1:B:17:LYS:O	1:B:17:LYS:CG	2.43	0.65
1:B:249:ASP:OD1	1:B:253:HIS:HD2	1.80	0.65
1:B:2:LEU:CB	1:B:3:ASN:CG	2.70	0.64
1:A:217:LEU:O	1:A:219:ARG:HG2	1.97	0.64
1:A:1:MET:O	1:A:1:MET:CG	2.45	0.64
1:A:29:ASP:OD1	1:A:54:GLN:HB3	1.98	0.64
1:B:43:ARG:O	1:B:46:LYS:N	2.31	0.64
1:B:64:GLN:C	1:B:65:ILE:HG12	2.21	0.64
1:B:120:ILE:HA	1:B:121:SER:CB	2.25	0.64
1:B:123:TYR:CE2	1:B:127:ILE:CD1	2.64	0.64
1:A:2:LEU:N	1:A:2:LEU:CD1	2.43	0.64
1:A:167:LEU:CD1	1:A:187:ALA:HB1	2.28	0.64
1:A:171:VAL:HG12	1:A:243:GLY:HA2	1.80	0.64
1:B:2:LEU:O	1:B:3:ASN:ND2	2.30	0.63
1:A:38:THR:HG23	1:A:39:TYR:N	2.00	0.63
1:B:1:MET:HB3	1:B:2:LEU:CG	2.28	0.63
1:B:22:PHE:O	1:B:23:GLY:C	2.37	0.63
1:B:52:LEU:HA	1:B:54:GLN:CB	2.28	0.63
1:B:70:ASP:O	1:B:74:ILE:HG13	1.99	0.63
1:B:86:ASN:HB3	1:B:135:LEU:O	1.96	0.63
1:A:39:TYR:CZ	1:A:64:GLN:CG	2.81	0.63
1:A:137:PRO:HG2	1:A:138:GLU:HG2	1.80	0.63
1:A:39:TYR:CE1	1:A:42:GLU:HB3	2.34	0.63
1:B:48:LEU:CA	1:B:51:LEU:HB2	2.28	0.63
1:B:52:LEU:HA	1:B:54:GLN:HG3	1.74	0.63
1:A:38:THR:HG22	1:A:39:TYR:N	2.08	0.63
1:A:193:ILE:HD12	1:A:222:ASP:HA	1.80	0.62
1:A:187:ALA:N	1:A:244:GLU:O	2.31	0.62
1:B:130:HIS:HE1	1:B:177:ASP:OD2	1.82	0.62
1:B:59:GLU:HG3	1:B:61:HIS:H	0.69	0.62
1:B:223:GLN:OE1	1:B:223:GLN:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:HD12	1:A:2:LEU:H	1.63	0.62
1:A:208:LEU:HD13	1:A:209:LYS:NZ	2.15	0.62
1:B:89:GLY:CA	1:B:136:MET:HE2	2.21	0.62
1:B:127:ILE:C	1:B:129:ALA:H	2.08	0.62
1:A:140:GLY:O	1:A:184:ARG:N	2.33	0.62
1:A:147:TYR:CZ	1:A:192:PRO:HA	2.34	0.62
1:A:228:LYS:O	1:A:231:ALA:HB3	2.00	0.61
1:A:78:GLU:O	1:A:79:GLN:C	2.41	0.61
1:A:120:ILE:HG23	1:A:121:SER:N	2.14	0.61
1:B:164:LYS:CB	1:B:165:ALA:HB2	2.28	0.61
1:A:147:TYR:CD1	1:A:147:TYR:C	2.71	0.61
1:B:7:LYS:HD3	1:B:88:ASP:OD1	2.00	0.61
1:B:43:ARG:C	1:B:45:ARG:H	2.08	0.61
1:B:52:LEU:N	1:B:54:GLN:HG2	2.13	0.61
1:A:130:HIS:O	1:A:133:LYS:CD	2.48	0.61
1:A:7:LYS:CG	1:A:88:ASP:CG	2.74	0.61
1:A:39:TYR:CZ	1:A:42:GLU:CB	2.83	0.61
1:A:188:ILE:HD11	1:A:229:THR:HG22	1.82	0.61
1:B:2:LEU:C	1:B:3:ASN:ND2	2.57	0.61
1:B:143:VAL:HG21	1:B:234:LEU:HD13	1.82	0.61
1:A:25:ALA:HB1	1:A:35:LEU:CD1	2.30	0.61
1:A:42:GLU:O	1:A:45:ARG:HB2	2.01	0.61
1:B:77:PHE:HA	1:B:80:ILE:HG13	1.83	0.61
1:B:146:THR:HG21	1:B:189:SER:HB2	1.82	0.61
1:A:5:GLU:HG3	1:A:6:ASN:H	1.64	0.61
1:A:234:LEU:CD1	1:A:234:LEU:N	2.62	0.60
1:B:170:ASN:HA	1:B:173:TYR:HD2	1.66	0.60
1:A:3:ASN:HD21	1:A:236:ASP:HB2	1.66	0.60
1:B:12:MET:HE3	1:B:77:PHE:CZ	2.36	0.60
1:B:74:ILE:C	1:B:76:GLY:H	2.05	0.60
1:B:235:SER:OG	1:B:237:LEU:HB2	2.02	0.60
1:A:49:GLU:O	1:A:49:GLU:CG	2.21	0.60
1:B:123:TYR:HD2	1:B:124:SER:CA	2.14	0.60
1:A:45:ARG:HD2	1:A:45:ARG:O	2.02	0.59
1:A:210:GLU:HB3	1:A:211:ILE:HD12	1.85	0.59
1:B:139:GLY:C	1:B:183:ILE:HD11	2.26	0.59
1:B:43:ARG:O	1:B:43:ARG:HG2	1.98	0.59
1:B:84:VAL:HG23	1:B:85:GLY:N	2.17	0.59
1:A:207:ILE:HD12	1:A:207:ILE:O	2.00	0.59
1:B:3:ASN:HD21	1:B:237:LEU:HD13	1.68	0.59
1:A:7:LYS:HB3	1:A:9:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:CA	1:B:164:LYS:HE2	2.32	0.59
1:B:194:ARG:HG2	1:B:194:ARG:NH1	1.90	0.59
1:A:94:ILE:O	1:A:94:ILE:HG22	2.03	0.59
1:B:143:VAL:HG23	1:B:234:LEU:CD1	2.33	0.59
1:A:5:GLU:O	1:A:6:ASN:CB	2.49	0.58
1:A:207:ILE:O	1:A:211:ILE:HD13	2.02	0.58
1:B:236:ASP:C	1:B:238:SER:H	2.09	0.58
1:B:48:LEU:C	1:B:51:LEU:HB2	2.28	0.58
1:B:211:ILE:HG22	1:B:215:ALA:HB2	1.85	0.58
1:A:42:GLU:C	1:A:44:SER:N	2.61	0.58
1:A:42:GLU:HB2	1:A:45:ARG:HB2	1.86	0.58
1:A:45:ARG:C	1:A:45:ARG:CD	2.74	0.58
1:B:35:LEU:HD13	1:B:37:PHE:CZ	2.38	0.58
1:B:141:SER:C	1:B:142:ILE:HG13	2.29	0.58
1:B:146:THR:HG23	1:B:147:TYR:CA	2.33	0.58
1:A:136:MET:O	1:A:139:GLY:N	2.30	0.58
1:A:58:PRO:HB2	1:A:59:GLU:HB2	1.86	0.58
1:B:2:LEU:O	1:B:3:ASN:CG	2.47	0.58
1:B:211:ILE:O	1:B:212:GLU:C	2.45	0.58
1:A:10:VAL:CG1	1:A:36:VAL:HG12	2.34	0.57
1:A:170:ASN:O	1:A:172:LYS:N	2.37	0.57
1:B:38:THR:HA	1:B:63:TYR:O	2.03	0.57
1:B:45:ARG:C	1:B:47:GLU:N	2.58	0.57
1:B:24:VAL:HG22	1:B:227:GLY:HA2	1.86	0.57
1:B:178:LEU:O	1:B:179:GLY:C	2.45	0.57
1:A:130:HIS:O	1:A:133:LYS:HD3	2.04	0.57
1:B:9:TYR:O	1:B:36:VAL:N	2.34	0.57
1:B:194:ARG:HB3	1:B:194:ARG:CZ	2.25	0.57
1:A:129:ALA:HB1	1:A:174:LEU:HD13	1.86	0.57
1:A:45:ARG:HD2	1:A:45:ARG:C	2.17	0.57
1:A:215:ALA:O	1:A:218:LYS:HD3	2.03	0.57
1:B:20:ILE:HA	1:B:223:GLN:HG3	1.86	0.57
1:A:188:ILE:HG23	1:A:189:SER:N	2.20	0.57
1:A:29:ASP:CB	1:A:54:GLN:NE2	2.55	0.57
1:A:94:ILE:O	1:A:94:ILE:HG23	2.04	0.57
1:A:41:LYS:O	1:A:44:SER:CB	2.52	0.56
1:B:14:ILE:HG21	1:B:48:LEU:HD11	1.86	0.56
1:A:2:LEU:O	1:A:3:ASN:O	2.22	0.56
1:A:16:ASN:CB	1:A:47:GLU:OE1	2.53	0.56
1:A:60:ALA:C	1:A:61:HIS:CG	2.75	0.56
1:B:45:ARG:O	1:B:49:GLU:CG	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLY:H	1:B:183:ILE:CD1	2.18	0.56
1:A:205:ASN:O	1:A:209:LYS:HD3	2.05	0.56
1:A:69:SER:O	1:A:70:ASP:C	2.48	0.56
1:A:40:ARG:HH12	1:A:68:GLN:NE2	2.04	0.56
1:A:184:ARG:HG2	1:B:217:LEU:HD21	1.86	0.56
1:B:11:ILE:N	1:B:36:VAL:O	2.38	0.56
1:A:24:VAL:HG21	1:A:91:TYR:CZ	2.40	0.56
1:A:8:THR:HA	1:A:34:LYS:O	2.05	0.56
1:A:29:ASP:HB2	1:A:54:GLN:HE22	1.66	0.56
1:A:136:MET:O	1:A:138:GLU:N	2.39	0.56
1:A:193:ILE:HD13	1:A:221:VAL:HG23	1.88	0.55
1:A:206:THR:O	1:A:209:LYS:N	2.35	0.55
1:B:127:ILE:C	1:B:129:ALA:N	2.62	0.55
1:B:244:GLU:OE1	1:B:245:ASN:N	2.37	0.55
1:A:146:THR:CG2	1:A:167:LEU:CD1	2.83	0.55
1:A:50:LYS:HG3	1:A:51:LEU:H	1.71	0.55
1:A:165:ALA:C	1:A:166:SER:HG	2.14	0.55
1:B:52:LEU:CA	1:B:54:GLN:CG	2.48	0.55
1:A:57:GLN:OE1	1:A:58:PRO:CD	2.52	0.55
1:A:90:VAL:HG23	1:A:142:ILE:HG12	1.89	0.55
1:A:19:SER:O	1:A:20:ILE:C	2.49	0.54
1:B:44:SER:O	1:B:48:LEU:CD2	2.52	0.54
1:A:42:GLU:O	1:A:42:GLU:CD	2.50	0.54
1:B:92:HIS:N	1:B:143:VAL:O	2.40	0.54
1:B:164:LYS:HE2	1:B:164:LYS:N	2.21	0.54
1:B:44:SER:C	1:B:47:GLU:H	2.15	0.54
1:A:11:ILE:CG2	1:A:12:MET:N	2.62	0.54
1:A:46:LYS:HD2	1:A:46:LYS:O	2.06	0.54
1:A:185:VAL:O	1:A:243:GLY:N	2.40	0.54
1:B:28:LEU:O	1:B:33:ALA:HB3	2.07	0.54
1:B:193:ILE:HD12	1:B:193:ILE:N	2.22	0.54
1:B:66:ASP:C	1:B:67:VAL:HG12	2.31	0.54
1:B:127:ILE:O	1:B:128:VAL:C	2.51	0.54
1:B:140:GLY:N	1:B:183:ILE:CD1	2.71	0.54
1:A:14:ILE:HD12	1:A:37:PHE:HD1	1.73	0.54
1:A:211:ILE:H	1:A:211:ILE:CD1	2.19	0.54
1:B:168:GLU:O	1:B:169:ALA:HB2	2.07	0.54
1:B:27:VAL:HG21	1:B:227:GLY:HA3	1.91	0.53
1:A:167:LEU:C	1:A:169:ALA:H	2.14	0.53
1:A:167:LEU:C	1:A:169:ALA:N	2.58	0.53
1:B:10:VAL:HA	1:B:36:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:O	1:A:127:ILE:CG1	2.43	0.53
1:A:217:LEU:HD23	1:A:250:SER:O	2.08	0.53
1:A:230:ALA:O	1:A:233:LEU:N	2.41	0.53
1:A:35:LEU:N	1:A:56:ASN:HD21	2.05	0.53
1:B:3:ASN:ND2	1:B:237:LEU:HD13	2.23	0.53
1:A:204:PHE:O	1:A:208:LEU:HB2	2.08	0.53
1:B:23:GLY:O	1:B:26:LYS:HB3	2.09	0.53
1:B:127:ILE:O	1:B:129:ALA:N	2.41	0.53
1:A:9:TYR:N	1:A:34:LYS:O	2.37	0.53
1:A:204:PHE:C	1:A:207:ILE:HG13	2.34	0.53
1:A:120:ILE:HG23	1:A:121:SER:H	1.74	0.53
1:A:91:TYR:CE2	1:A:93:SER:HB3	2.44	0.53
1:B:236:ASP:C	1:B:238:SER:N	2.66	0.53
1:A:61:HIS:HB3	1:A:63:TYR:HE2	1.73	0.53
1:B:76:GLY:O	1:B:80:ILE:CG1	2.55	0.53
1:B:86:ASN:HB3	1:B:135:LEU:HB2	1.90	0.53
1:A:28:LEU:O	1:A:29:ASP:C	2.49	0.53
1:A:60:ALA:O	1:A:61:HIS:CB	2.57	0.53
1:A:26:LYS:C	1:A:28:LEU:H	2.17	0.52
1:B:86:ASN:CB	1:B:135:LEU:HB2	2.39	0.52
1:B:5:GLU:HB3	1:B:32:GLY:HA3	1.92	0.52
1:B:172:LYS:O	1:B:175:ALA:HB3	2.10	0.52
1:A:27:VAL:HG21	1:A:227:GLY:HA3	1.91	0.52
1:A:125:LEU:O	1:A:129:ALA:N	2.35	0.52
1:A:207:ILE:HD12	1:A:208:LEU:N	2.25	0.52
1:B:169:ALA:O	1:B:173:TYR:CE2	2.63	0.52
1:B:194:ARG:CZ	1:B:194:ARG:HB2	2.39	0.52
1:A:253:HIS:HE1	1:B:243:GLY:O	1.93	0.52
1:A:244:GLU:OE2	1:B:247:HIS:ND1	2.41	0.52
1:A:39:TYR:CZ	1:A:64:GLN:HG3	2.42	0.52
1:A:147:TYR:O	1:A:147:TYR:HD1	1.86	0.52
1:A:176:LEU:O	1:A:180:PRO:HD3	2.09	0.52
1:A:224:VAL:O	1:A:228:LYS:HG3	2.10	0.52
1:B:178:LEU:O	1:B:181:ASP:N	2.43	0.52
1:A:145:THR:HG22	1:A:146:THR:N	2.25	0.51
1:B:146:THR:CG2	1:B:189:SER:HB2	2.39	0.51
1:A:3:ASN:OD1	1:A:4:LEU:N	2.43	0.51
1:B:167:LEU:CB	1:B:168:GLU:HB3	2.40	0.51
1:B:229:THR:HB	1:B:248:VAL:HG21	1.91	0.51
1:B:211:ILE:HG22	1:B:215:ALA:CB	2.40	0.51
1:A:45:ARG:O	1:A:48:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLY:HA3	1:A:141:SER:O	2.11	0.51
1:A:228:LYS:HE3	1:B:236:ASP:O	2.11	0.51
1:B:46:LYS:O	1:B:49:GLU:HG3	2.11	0.51
1:B:52:LEU:O	1:B:54:GLN:HB3	2.09	0.51
1:B:208:LEU:O	1:B:212:GLU:HG3	2.10	0.51
1:A:10:VAL:HG22	1:A:87:ILE:HD11	1.92	0.51
1:A:20:ILE:HA	1:A:223:GLN:HG2	1.93	0.51
1:B:19:SER:O	1:B:22:PHE:N	2.44	0.51
1:A:2:LEU:HD12	1:A:2:LEU:C	2.21	0.51
1:A:194:ARG:NH1	1:A:194:ARG:CG	2.68	0.51
1:B:2:LEU:O	1:B:3:ASN:CB	2.56	0.51
1:B:86:ASN:HA	1:B:135:LEU:HB2	1.91	0.51
1:B:92:HIS:O	1:B:144:ALA:HA	2.10	0.51
1:A:7:LYS:HG2	1:A:88:ASP:CB	2.41	0.51
1:B:46:LYS:O	1:B:49:GLU:HG2	2.11	0.51
1:A:188:ILE:HG23	1:A:189:SER:H	1.76	0.50
1:A:211:ILE:CG2	1:A:215:ALA:HB2	2.38	0.50
1:A:253:HIS:NE2	1:B:242:THR:O	2.43	0.50
1:B:69:SER:HB2	1:B:72:GLU:HB2	1.93	0.50
1:A:66:ASP:OD1	1:A:66:ASP:C	2.54	0.50
1:A:237:LEU:HG	1:B:228:LYS:HB3	1.92	0.50
1:B:211:ILE:HG23	1:B:215:ALA:HB2	1.92	0.50
1:A:37:PHE:N	1:A:37:PHE:CD2	2.79	0.50
1:B:78:GLU:OE2	1:B:82:LYS:HE2	2.11	0.50
1:A:34:LYS:NZ	1:A:58:PRO:HG2	2.26	0.50
1:B:69:SER:O	1:B:70:ASP:O	2.30	0.50
1:A:87:ILE:CG2	1:A:136:MET:HE3	2.42	0.50
1:A:237:LEU:CD1	1:B:228:LYS:HB3	2.42	0.50
1:B:39:TYR:CE1	1:B:64:GLN:CG	2.95	0.50
1:A:39:TYR:HD1	1:A:40:ARG:N	2.06	0.50
1:A:184:ARG:HB3	1:A:242:THR:HB	1.92	0.50
1:B:75:ASN:ND2	1:B:78:GLU:OE1	2.45	0.50
1:B:180:PRO:C	1:B:182:ASN:H	2.20	0.50
1:A:62:LEU:O	1:A:63:TYR:CD2	2.65	0.50
1:A:208:LEU:HB3	1:A:209:LYS:CD	2.36	0.50
1:B:143:VAL:HG23	1:B:234:LEU:HD13	1.92	0.50
1:A:70:ASP:O	1:A:74:ILE:CG1	2.60	0.49
1:B:141:SER:O	1:B:142:ILE:HG13	2.12	0.49
1:B:241:VAL:O	1:B:242:THR:HB	2.11	0.49
1:A:4:LEU:HD12	1:A:236:ASP:CB	2.42	0.49
1:A:11:ILE:O	1:A:37:PHE:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HB3	1:A:174:LEU:HD11	1.94	0.49
1:A:185:VAL:O	1:A:243:GLY:HA2	2.12	0.49
1:B:86:ASN:ND2	1:B:86:ASN:N	2.49	0.49
1:A:194:ARG:HH11	1:A:194:ARG:CA	2.25	0.49
1:A:219:ARG:NH2	1:A:225:GLU:OE2	2.46	0.49
1:B:20:ILE:O	1:B:23:GLY:N	2.45	0.49
1:B:211:ILE:C	1:B:213:GLU:N	2.71	0.49
1:A:167:LEU:O	1:A:168:GLU:C	2.51	0.49
1:B:36:VAL:HG22	1:B:61:HIS:CB	2.43	0.49
1:B:238:SER:O	1:B:241:VAL:HB	2.13	0.49
1:B:67:VAL:O	1:B:67:VAL:CG2	2.57	0.49
1:B:75:ASN:HA	1:B:78:GLU:HB3	1.95	0.49
1:A:25:ALA:CB	1:A:35:LEU:CD1	2.91	0.49
1:B:49:GLU:C	1:B:51:LEU:H	2.20	0.49
1:B:58:PRO:HD2	1:B:58:PRO:O	2.12	0.49
1:A:42:GLU:O	1:A:45:ARG:HB3	2.13	0.49
1:B:78:GLU:O	1:B:79:GLN:C	2.55	0.49
1:A:26:LYS:C	1:A:28:LEU:N	2.68	0.48
1:A:77:PHE:HB3	1:A:135:LEU:HD11	1.94	0.48
1:B:8:THR:O	1:B:88:ASP:N	2.46	0.48
1:B:9:TYR:O	1:B:35:LEU:HA	2.13	0.48
1:A:10:VAL:HG21	1:A:77:PHE:CE2	2.38	0.48
1:A:121:SER:O	1:A:121:SER:OG	2.28	0.48
1:A:70:ASP:C	1:A:74:ILE:HG13	2.38	0.48
1:A:208:LEU:HD13	1:A:209:LYS:HZ3	1.78	0.48
1:A:20:ILE:HA	1:A:223:GLN:CG	2.44	0.48
1:A:84:VAL:HG23	1:A:85:GLY:N	2.29	0.48
1:A:185:VAL:N	1:A:242:THR:OG1	2.45	0.48
1:B:164:LYS:CA	1:B:165:ALA:HB2	2.43	0.48
1:A:11:ILE:HG22	1:A:12:MET:H	1.74	0.48
1:A:146:THR:HG23	1:A:167:LEU:HD12	1.94	0.48
1:B:146:THR:CG2	1:B:147:TYR:HA	2.43	0.48
1:B:178:LEU:O	1:B:181:ASP:HB2	2.14	0.48
1:B:5:GLU:HB3	1:B:31:LEU:O	2.13	0.48
1:B:34:LYS:H	1:B:34:LYS:HG2	1.52	0.48
1:B:36:VAL:HG22	1:B:61:HIS:HB3	1.95	0.47
1:B:146:THR:CG2	1:B:147:TYR:CA	2.91	0.47
1:A:89:GLY:CA	1:A:141:SER:O	2.62	0.47
1:A:123:TYR:O	1:A:124:SER:C	2.57	0.47
1:B:43:ARG:C	1:B:46:LYS:N	2.69	0.47
1:B:80:ILE:O	1:B:84:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:TYR:CD2	1:B:124:SER:HA	2.49	0.47
1:B:125:LEU:HA	1:B:128:VAL:HB	1.96	0.47
1:B:193:ILE:HG12	1:B:222:ASP:CA	2.38	0.47
1:B:229:THR:O	1:B:232:TYR:HB3	2.15	0.47
1:A:165:ALA:O	1:A:166:SER:OG	2.30	0.47
1:A:171:VAL:HG13	1:A:185:VAL:O	2.13	0.47
1:B:182:ASN:O	1:B:183:ILE:HD13	2.12	0.47
1:A:25:ALA:O	1:A:29:ASP:N	2.34	0.47
1:A:57:GLN:OE1	1:A:57:GLN:CA	2.62	0.47
1:A:92:HIS:O	1:A:92:HIS:ND1	2.47	0.47
1:B:52:LEU:HD21	1:B:56:ASN:O	2.14	0.47
1:B:218:LYS:HA	1:B:218:LYS:HD3	1.44	0.47
1:A:16:ASN:C	1:A:18:ARG:H	2.22	0.47
1:A:78:GLU:C	1:A:80:ILE:N	2.68	0.47
1:A:173:TYR:CD2	1:A:173:TYR:N	2.79	0.47
1:B:18:ARG:HG2	1:B:194:ARG:NH2	2.30	0.47
1:A:57:GLN:N	1:A:58:PRO:O	2.48	0.47
1:A:204:PHE:HA	1:A:207:ILE:HG12	1.95	0.47
1:B:3:ASN:HB3	1:B:236:ASP:N	2.18	0.47
1:A:48:LEU:O	1:A:50:LYS:O	2.32	0.47
1:B:247:HIS:CD2	1:B:253:HIS:HB3	2.50	0.47
1:B:18:ARG:HG2	1:B:194:ARG:HH21	1.80	0.47
1:B:25:ALA:HA	1:B:35:LEU:HD11	1.96	0.47
1:A:57:GLN:C	1:A:58:PRO:O	2.56	0.46
1:A:45:ARG:O	1:A:45:ARG:CD	2.62	0.46
1:A:87:ILE:HG23	1:A:136:MET:HE3	1.98	0.46
1:B:45:ARG:O	1:B:49:GLU:CD	2.58	0.46
1:A:47:GLU:O	1:A:50:LYS:CB	2.56	0.46
1:B:134:LYS:C	1:B:135:LEU:HD23	2.40	0.46
1:B:254:ALA:C	1:B:255:ILE:HG23	2.39	0.46
1:A:39:TYR:CE1	1:A:64:GLN:HA	2.50	0.46
1:A:178:LEU:O	1:A:179:GLY:C	2.56	0.46
1:B:146:THR:HG22	1:B:147:TYR:HA	1.98	0.46
1:A:50:LYS:HA	1:A:51:LEU:C	2.41	0.46
1:B:8:THR:N	1:B:88:ASP:HB2	2.30	0.46
1:A:194:ARG:C	1:A:195:THR:HG22	2.41	0.46
1:A:254:ALA:C	1:A:255:ILE:CG2	2.89	0.46
1:B:17:LYS:HE2	1:B:18:ARG:HH21	1.81	0.46
1:A:50:LYS:CG	1:A:51:LEU:N	2.66	0.45
1:A:123:TYR:CG	1:A:127:ILE:CD1	2.79	0.45
1:B:11:ILE:HD13	1:B:37:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ASP:O	1:B:67:VAL:CG1	2.62	0.45
1:B:251:GLY:O	1:B:252:PHE:C	2.57	0.45
1:A:140:GLY:O	1:A:183:ILE:HA	2.17	0.45
1:A:166:SER:C	1:A:169:ALA:H	2.24	0.45
1:B:67:VAL:HG22	1:B:124:SER:CB	2.45	0.45
1:A:29:ASP:CG	1:A:54:GLN:HE21	2.24	0.45
1:A:42:GLU:C	1:A:44:SER:H	2.24	0.45
1:A:91:TYR:HE2	1:A:93:SER:HB3	1.81	0.45
1:A:123:TYR:CD2	1:A:127:ILE:CD1	2.98	0.45
1:A:175:ALA:HA	1:A:185:VAL:HG13	1.97	0.45
1:A:77:PHE:CD2	1:A:80:ILE:HD12	2.51	0.45
1:A:90:VAL:CG2	1:A:142:ILE:HG12	2.46	0.45
1:A:171:VAL:O	1:A:175:ALA:HB2	2.16	0.45
1:A:62:LEU:H	1:A:62:LEU:HG	1.67	0.45
1:B:208:LEU:HB3	1:B:209:LYS:HD2	1.99	0.45
1:B:121:SER:H	1:B:122:SER:HA	1.82	0.45
1:A:178:LEU:HD13	1:A:178:LEU:H	1.77	0.45
1:A:255:ILE:HD13	1:A:255:ILE:HG21	1.48	0.45
1:B:16:ASN:OD1	1:B:19:SER:OG	2.33	0.45
1:B:123:TYR:HD2	1:B:124:SER:HA	1.81	0.45
1:A:127:ILE:HG13	1:A:127:ILE:H	1.67	0.45
1:A:194:ARG:CD	1:A:194:ARG:C	2.89	0.45
1:B:143:VAL:HG22	1:B:233:LEU:HB3	1.97	0.45
1:A:189:SER:HB3	1:A:245:ASN:HD21	1.82	0.44
1:B:25:ALA:O	1:B:29:ASP:N	2.47	0.44
1:B:164:LYS:HE2	1:B:164:LYS:HA	1.99	0.44
1:B:49:GLU:C	1:B:51:LEU:N	2.75	0.44
1:B:52:LEU:CA	1:B:54:GLN:HB3	2.47	0.44
1:B:179:GLY:O	1:B:180:PRO:C	2.59	0.44
1:A:19:SER:C	1:A:21:ALA:N	2.74	0.44
1:B:143:VAL:CG2	1:B:234:LEU:CD1	2.91	0.44
1:A:146:THR:HG21	1:A:167:LEU:HD12	1.98	0.44
1:A:168:GLU:HG3	1:A:172:LYS:NZ	2.32	0.44
1:B:8:THR:C	1:B:9:TYR:CG	2.96	0.44
1:B:16:ASN:OD1	1:B:16:ASN:N	2.50	0.44
1:B:41:LYS:C	1:B:43:ARG:H	2.24	0.44
1:B:48:LEU:HA	1:B:51:LEU:CB	2.43	0.44
1:A:87:ILE:HG21	1:A:87:ILE:HD13	1.61	0.44
1:A:45:ARG:CZ	1:A:49:GLU:HB2	2.47	0.44
1:B:1:MET:HB3	1:B:2:LEU:HD21	1.86	0.44
1:B:8:THR:H	1:B:88:ASP:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:PRO:CB	1:B:59:GLU:HA	2.48	0.44
1:A:50:LYS:O	1:A:52:LEU:N	2.30	0.44
1:A:172:LYS:HZ3	1:A:172:LYS:HG3	1.76	0.44
1:A:215:ALA:HB1	1:A:250:SER:HB3	2.00	0.44
1:B:183:ILE:HG23	1:B:184:ARG:N	2.32	0.44
1:A:34:LYS:HZ3	1:A:58:PRO:HG2	1.81	0.44
1:A:129:ALA:CB	1:A:174:LEU:HD13	2.43	0.44
1:B:86:ASN:HB3	1:B:135:LEU:CB	2.48	0.44
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.62	0.43
1:B:28:LEU:HA	1:B:28:LEU:HD23	1.59	0.43
1:A:146:THR:O	1:A:189:SER:HA	2.17	0.43
1:A:40:ARG:NH1	1:A:68:GLN:HE21	2.10	0.43
1:B:20:ILE:HG23	1:B:226:VAL:HG11	1.98	0.43
1:B:179:GLY:N	1:B:180:PRO:HD3	2.33	0.43
1:A:178:LEU:HB3	1:A:183:ILE:HD12	2.00	0.43
1:B:167:LEU:CD1	1:B:167:LEU:C	2.65	0.43
1:B:234:LEU:HD13	1:B:234:LEU:N	2.32	0.43
1:B:41:LYS:O	1:B:43:ARG:N	2.50	0.43
1:A:185:VAL:O	1:A:243:GLY:CA	2.67	0.43
1:A:233:LEU:O	1:A:238:SER:OG	2.31	0.43
1:B:86:ASN:CA	1:B:135:LEU:HB2	2.48	0.43
1:B:249:ASP:OD1	1:B:253:HIS:CD2	2.66	0.43
1:A:39:TYR:OH	1:A:42:GLU:HB3	2.17	0.43
1:A:58:PRO:CB	1:A:59:GLU:HB2	2.48	0.43
1:B:4:LEU:HD22	1:B:31:LEU:O	2.19	0.43
1:B:39:TYR:CE1	1:B:64:GLN:HG3	2.54	0.43
1:B:49:GLU:HG2	1:B:49:GLU:H	1.61	0.43
1:B:208:LEU:HB3	1:B:209:LYS:CD	2.48	0.43
1:A:143:VAL:HG21	1:A:233:LEU:HB2	2.01	0.43
1:B:140:GLY:N	1:B:183:ILE:HD11	2.33	0.43
1:A:207:ILE:O	1:A:208:LEU:C	2.59	0.43
1:A:254:ALA:O	1:A:255:ILE:CG2	2.58	0.43
1:A:79:GLN:O	1:A:83:ASP:CG	2.62	0.43
1:B:210:GLU:O	1:B:210:GLU:HG2	2.11	0.43
1:A:123:TYR:CD1	1:A:127:ILE:CD1	3.02	0.42
1:B:1:MET:CB	1:B:2:LEU:HG	2.48	0.42
1:A:65:ILE:HD13	1:A:65:ILE:HG21	1.63	0.42
1:A:176:LEU:HA	1:B:216:PRO:HB3	2.01	0.42
1:B:2:LEU:CB	1:B:3:ASN:ND2	2.68	0.42
1:B:10:VAL:HG13	1:B:36:VAL:C	2.43	0.42
1:B:84:VAL:CG2	1:B:85:GLY:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:O	1:A:168:GLU:CG	2.67	0.42
1:A:208:LEU:HD13	1:A:209:LYS:HZ2	1.84	0.42
1:A:209:LYS:HD2	1:A:209:LYS:N	2.34	0.42
1:B:183:ILE:HD12	1:B:183:ILE:HA	1.86	0.42
1:B:1:MET:CB	1:B:2:LEU:CG	2.97	0.42
1:B:5:GLU:HB2	1:B:32:GLY:O	2.18	0.42
1:B:52:LEU:CA	1:B:54:GLN:CB	2.95	0.42
1:A:210:GLU:HG3	1:A:214:ARG:HD2	2.01	0.42
1:B:89:GLY:HA2	1:B:136:MET:HE1	1.80	0.42
1:B:176:LEU:HA	1:B:176:LEU:HD13	1.43	0.42
1:B:214:ARG:O	1:B:255:ILE:CD1	2.68	0.42
1:B:60:ALA:O	1:B:62:LEU:N	2.51	0.42
1:A:27:VAL:O	1:A:30:GLN:HB3	2.20	0.42
1:A:42:GLU:O	1:A:45:ARG:N	2.49	0.42
1:B:19:SER:C	1:B:21:ALA:N	2.78	0.42
1:A:130:HIS:ND1	1:A:133:LYS:CD	2.83	0.42
1:B:7:LYS:HD3	1:B:88:ASP:CG	2.44	0.42
1:A:31:LEU:N	1:A:31:LEU:HD13	2.33	0.42
1:A:143:VAL:CG2	1:A:233:LEU:HB2	2.50	0.42
1:A:146:THR:HG22	1:A:167:LEU:CD1	2.49	0.42
1:A:167:LEU:HD22	1:A:171:VAL:HG23	2.01	0.42
1:A:184:ARG:HB3	1:A:242:THR:CB	2.50	0.42
1:A:186:ASN:OD1	1:A:242:THR:HA	2.20	0.42
1:B:43:ARG:O	1:B:46:LYS:CA	2.67	0.42
1:B:219:ARG:NH2	1:B:225:GLU:OE2	2.53	0.42
1:B:252:PHE:C	1:B:254:ALA:H	2.28	0.42
1:B:34:LYS:CB	1:B:34:LYS:HZ2	2.27	0.42
1:B:80:ILE:HG22	1:B:84:VAL:HG22	2.02	0.42
1:B:179:GLY:O	1:B:182:ASN:N	2.48	0.42
1:B:237:LEU:HD12	1:B:237:LEU:HA	1.95	0.42
1:A:249:ASP:OD2	1:A:253:HIS:N	2.53	0.41
1:A:14:ILE:HD12	1:A:37:PHE:CD1	2.53	0.41
1:A:39:TYR:OH	1:A:64:GLN:CG	2.54	0.41
1:B:58:PRO:HB2	1:B:59:GLU:HA	2.02	0.41
1:A:45:ARG:O	1:A:45:ARG:NE	2.54	0.41
1:A:215:ALA:O	1:A:216:PRO:C	2.63	0.41
1:B:254:ALA:HB3	1:B:255:ILE:CG2	2.50	0.41
1:A:48:LEU:C	1:A:50:LYS:N	2.78	0.41
1:A:185:VAL:O	1:A:185:VAL:HG22	2.18	0.41
1:B:74:ILE:O	1:B:78:GLU:HB2	2.19	0.41
1:A:35:LEU:HB2	1:A:56:ASN:HD21	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:C	1:B:43:ARG:N	2.78	0.41
1:A:140:GLY:H	1:A:183:ILE:HA	1.85	0.41
1:A:232:TYR:O	1:A:238:SER:HB3	2.20	0.41
1:B:65:ILE:HG23	1:B:73:VAL:HA	2.02	0.41
1:B:77:PHE:O	1:B:81:GLY:N	2.54	0.41
1:B:221:VAL:H	1:B:221:VAL:HG22	1.48	0.41
1:B:241:VAL:HG12	1:B:242:THR:N	2.36	0.41
1:B:61:HIS:CD2	1:B:84:VAL:CG1	3.02	0.40
1:A:214:ARG:NH2	1:A:256:LYS:HE2	2.37	0.40
1:B:59:GLU:CG	1:B:61:HIS:CA	2.91	0.40
1:B:214:ARG:O	1:B:255:ILE:HD11	2.21	0.40
1:A:237:LEU:C	1:A:239:SER:H	2.28	0.40
1:B:9:TYR:HA	1:B:89:GLY:O	2.21	0.40
1:B:211:ILE:O	1:B:214:ARG:N	2.54	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	199/256 (78%)	147 (74%)	41 (21%)	11 (6%)	1	2
1	B	192/256 (75%)	150 (78%)	30 (16%)	12 (6%)	1	1
All	All	391/512 (76%)	297 (76%)	71 (18%)	23 (6%)	1	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	B	3	ASN
1	B	52	LEU
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	58	PRO
1	B	168	GLU
1	B	169	ALA
1	B	128	VAL
1	B	212	GLU
1	A	3	ASN
1	A	6	ASN
1	A	17	LYS
1	B	53	GLU
1	A	57	GLN
1	B	167	LEU
1	A	2	LEU
1	A	128	VAL
1	A	216	PRO
1	B	176	LEU
1	B	165	ALA
1	A	74	ILE
1	A	207	ILE
1	A	13	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	175/210 (83%)	105 (60%)	70 (40%)	0	0
1	B	168/210 (80%)	105 (62%)	63 (38%)	0	0
All	All	343/420 (82%)	210 (61%)	133 (39%)	0	0

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	5	GLU
1	A	7	LYS

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Mol	Chain	Res	Type
1	A	10	VAL
1	A	11	ILE
1	A	14	ILE
1	A	16	ASN
1	A	17	LYS
1	A	19	SER
1	A	20	ILE
1	A	26	LYS
1	A	31	LEU
1	A	34	LYS
1	A	35	LEU
1	A	39	TYR
1	A	41	LYS
1	A	42	GLU
1	A	43	ARG
1	A	45	ARG
1	A	46	LYS
1	A	51	LEU
1	A	52	LEU
1	A	55	LEU
1	A	57	GLN
1	A	62	LEU
1	A	64	GLN
1	A	67	VAL
1	A	68	GLN
1	A	69	SER
1	A	70	ASP
1	A	74	ILE
1	A	86	ASN
1	A	87	ILE
1	A	90	VAL
1	A	94	ILE
1	A	127	ILE
1	A	133	LYS
1	A	135	LEU
1	A	137	PRO
1	A	138	GLU
1	A	146	THR
1	A	164	LYS
1	A	167	LEU
1	A	170	ASN
1	A	171	VAL

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Mol	Chain	Res	Type
1	A	178	LEU
1	A	181	ASP
1	A	185	VAL
1	A	188	ILE
1	A	193	ILE
1	A	194	ARG
1	A	195	THR
1	A	204	PHE
1	A	206	THR
1	A	207	ILE
1	A	208	LEU
1	A	211	ILE
1	A	213	GLU
1	A	214	ARG
1	A	219	ARG
1	A	224	VAL
1	A	234	LEU
1	A	235	SER
1	A	237	LEU
1	A	246	ILE
1	A	249	ASP
1	A	250	SER
1	A	255	ILE
1	A	256	LYS
1	B	1	MET
1	B	2	LEU
1	B	3	ASN
1	B	7	LYS
1	B	18	ARG
1	B	31	LEU
1	B	34	LYS
1	B	35	LEU
1	B	39	TYR
1	B	40	ARG
1	B	42	GLU
1	B	43	ARG
1	B	45	ARG
1	B	46	LYS
1	B	47	GLU
1	B	50	LYS
1	B	51	LEU
1	B	52	LEU

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Mol	Chain	Res	Type
1	B	54	GLN
1	B	55	LEU
1	B	56	ASN
1	B	57	GLN
1	B	59	GLU
1	B	62	LEU
1	B	65	ILE
1	B	66	ASP
1	B	68	GLN
1	B	69	SER
1	B	71	GLU
1	B	79	GLN
1	B	80	ILE
1	B	86	ASN
1	B	87	ILE
1	B	93	SER
1	B	120	ILE
1	B	123	TYR
1	B	124	SER
1	B	125	LEU
1	B	127	ILE
1	B	133	LYS
1	B	135	LEU
1	B	141	SER
1	B	146	THR
1	B	147	TYR
1	B	167	LEU
1	B	170	ASN
1	B	171	VAL
1	B	176	LEU
1	B	178	LEU
1	B	183	ILE
1	B	185	VAL
1	B	194	ARG
1	B	213	GLU
1	B	217	LEU
1	B	218	LYS
1	B	219	ARG
1	B	226	VAL
1	B	229	THR
1	B	233	LEU
1	B	234	LEU

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Mol	Chain	Res	Type
1	B	235	SER
1	B	246	ILE
1	B	255	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	54	GLN
1	A	56	ASN
1	A	68	GLN
1	A	86	ASN
1	A	170	ASN
1	A	182	ASN
1	A	245	ASN
1	A	247	HIS
1	B	6	ASN
1	B	54	GLN
1	B	56	ASN
1	B	75	ASN
1	B	86	ASN
1	B	130	HIS
1	B	220	ASN
1	B	253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/256 (80%)	0.43	14 (6%) 23 23	12, 34, 63, 73	0
1	B	200/256 (78%)	0.29	7 (3%) 47 44	8, 33, 56, 63	0
All	All	407/512 (79%)	0.36	21 (5%) 33 32	8, 34, 59, 73	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	ALA	4.7
1	A	44	SER	4.5
1	A	15	ALA	3.5
1	A	18	ARG	3.4
1	B	10	VAL	3.4
1	A	195	THR	3.3
1	A	173	TYR	3.2
1	A	6	ASN	3.0
1	A	61	HIS	3.0
1	A	43	ARG	2.9
1	A	72	GLU	2.8
1	B	6	ASN	2.6
1	B	52	LEU	2.6
1	A	73	VAL	2.5
1	A	16	ASN	2.3
1	B	2	LEU	2.3
1	B	4	LEU	2.3
1	B	66	ASP	2.2
1	A	41	LYS	2.1
1	A	3	ASN	2.1
1	B	123	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.