



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:01 PM EDT

PDB ID : 4CPA
Title : REFINED CRYSTAL STRUCTURE OF THE POTATO INHIBITOR COMPLEX OF CARBOXYPEPTIDASE A AT 2.5 ANGSTROMS RESOLUTION
Authors : Lipscomb, W.N.; Rees, D.C.
Deposited on : 1982-03-24
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

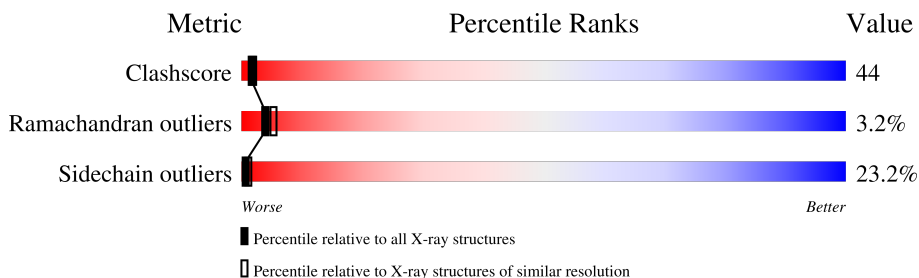
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	31% 40% 21% 9%
1	B	307	31% 39% 21% 9%
2	I	38	18% 32% 34% 13% .
2	J	38	18% 32% 34% 13% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	A	308	-	X	-	-
3	GLY	B	308	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5456 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2437	1561	406	465	5	0	0	0
1	B	307	2437	1561	406	465	5	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLN	GLU	conflict	UNP P00730
A	31	GLU	GLN	conflict	UNP P00730
A	89	ASN	ASP	conflict	UNP P00730
A	93	ASN	ASP	conflict	UNP P00730
A	114	ASN	ASP	conflict	UNP P00730
A	122	GLU	GLN	conflict	UNP P00730
A	185	ASN	ASP	conflict	UNP P00730
A	228	ALA	GLU	conflict	UNP P00730
A	305	VAL	LEU	conflict	UNP P00730
B	28	GLN	GLU	conflict	UNP P00730
B	31	GLU	GLN	conflict	UNP P00730
B	89	ASN	ASP	conflict	UNP P00730
B	93	ASN	ASP	conflict	UNP P00730
B	114	ASN	ASP	conflict	UNP P00730
B	122	GLU	GLN	conflict	UNP P00730
B	185	ASN	ASP	conflict	UNP P00730
B	228	ALA	GLU	conflict	UNP P00730
B	305	VAL	LEU	conflict	UNP P00730

- Molecule 2 is a protein called METALLOCARBOXYPEPTIDASE INHIBITOR.

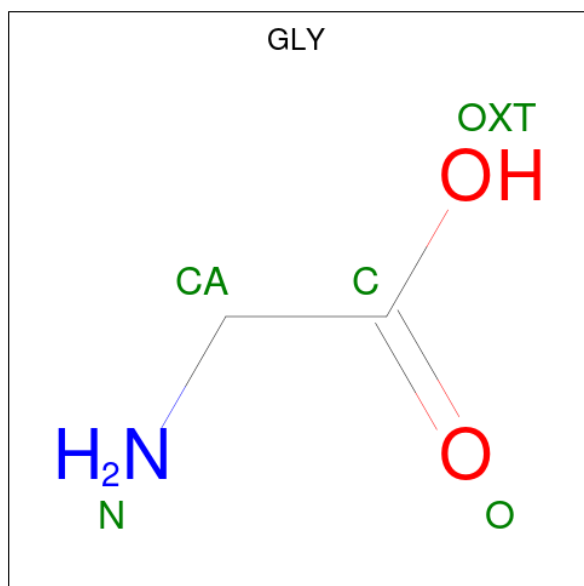
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	X			
2	I	37	285	174	51	52	6	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				X
2	J	37	285	174	51	52	6	2	0	0	0

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	5	2	1	2	0	0
3	B	1	5	2	1	2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

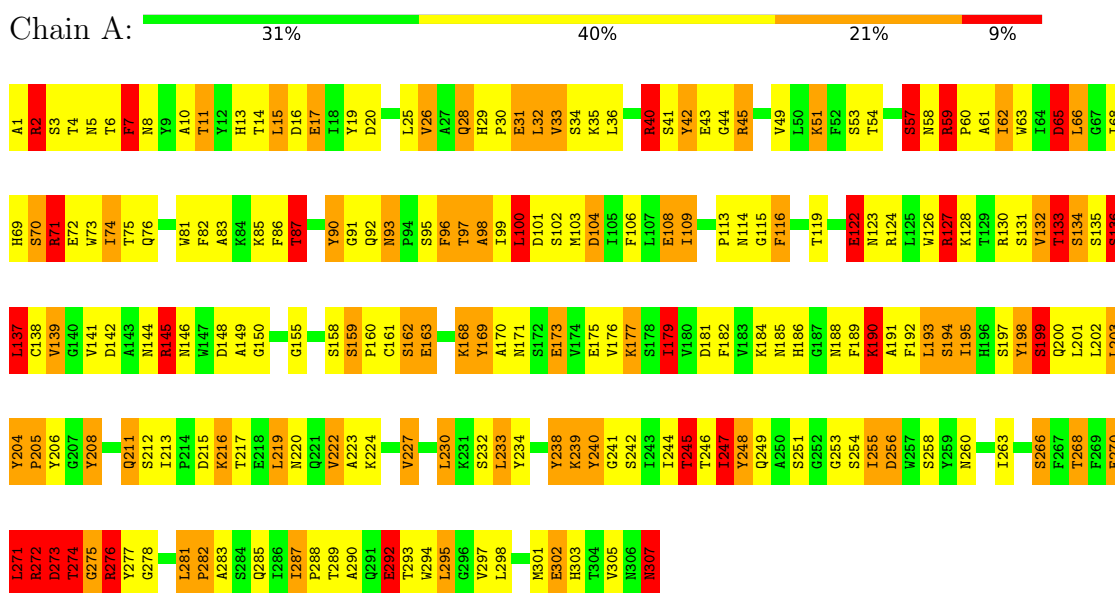
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	I	1	1	1	0	0
4	J	1	1	1	0	0

3 Residue-property plots

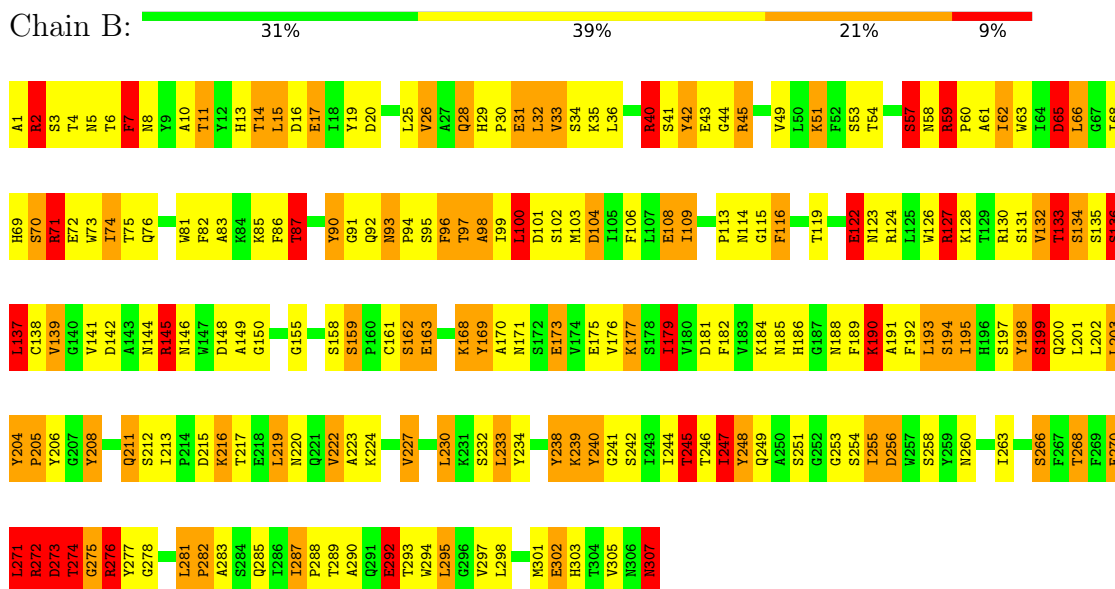
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

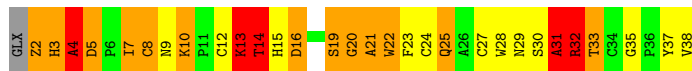
- Molecule 1: CARBOXYPEPTIDASE A



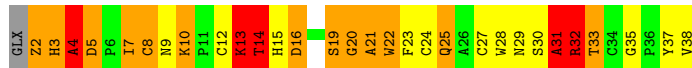
- Molecule 1: CARBOXYPEPTIDASE A



• Molecule 2: METALLOCARBOXYPEPTIDASE INHIBITOR

Chain I:  18% 32% 34% 13%

• Molecule 2: METALLOCARBOXYPEPTIDASE INHIBITOR

Chain J:  18% 32% 34% 13%

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	53.45Å 53.45Å 218.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5456	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.31	3/2503 (0.1%)	2.61	166/3402 (4.9%)
1	B	1.31	3/2503 (0.1%)	2.61	165/3402 (4.9%)
2	I	1.36	0/287	2.87	27/392 (6.9%)
2	J	1.36	0/287	2.87	27/392 (6.9%)
All	All	1.31	6/5580 (0.1%)	2.64	385/7588 (5.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	12
2	I	0	3
2	J	0	3
All	All	0	30

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	302	GLU	CD-OE2	9.00	1.35	1.25
1	A	302	GLU	CD-OE2	8.96	1.35	1.25
1	A	292	GLU	CD-OE1	-5.94	1.19	1.25
1	B	292	GLU	CD-OE1	-5.94	1.19	1.25
1	A	57	SER	CB-OG	5.21	1.49	1.42
1	B	57	SER	CB-OG	5.19	1.49	1.42

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH2	25.23	132.91	120.30
1	A	127	ARG	NE-CZ-NH2	25.06	132.83	120.30
1	A	2	ARG	CA-CB-CG	23.71	165.56	113.40
1	B	2	ARG	CA-CB-CG	23.70	165.53	113.40
1	B	40	ARG	NE-CZ-NH1	22.37	131.49	120.30
1	A	40	ARG	NE-CZ-NH1	22.27	131.44	120.30
1	B	273	ASP	CB-CG-OD1	21.57	137.72	118.30
1	A	273	ASP	CB-CG-OD1	21.53	137.68	118.30
1	A	136	SER	C-N-CA	19.21	169.72	121.70
1	B	136	SER	C-N-CA	19.19	169.67	121.70
1	A	273	ASP	CB-CG-OD2	-18.48	101.67	118.30
1	B	273	ASP	CB-CG-OD2	-18.48	101.67	118.30
2	J	5	ASP	CB-CG-OD1	16.41	133.07	118.30
2	I	5	ASP	CB-CG-OD1	16.40	133.06	118.30
1	B	71	ARG	NE-CZ-NH2	15.48	128.04	120.30
1	A	71	ARG	NE-CZ-NH2	15.38	127.99	120.30
1	B	71	ARG	NE-CZ-NH1	-15.22	112.69	120.30
1	B	127	ARG	NH1-CZ-NH2	-15.16	102.73	119.40
1	A	71	ARG	NE-CZ-NH1	-15.15	112.72	120.30
1	A	127	ARG	NH1-CZ-NH2	-15.14	102.74	119.40
1	A	208	TYR	CB-CG-CD1	14.33	129.60	121.00
1	B	208	TYR	CB-CG-CD1	14.31	129.59	121.00
1	A	40	ARG	NE-CZ-NH2	-13.99	113.30	120.30
1	B	40	ARG	NE-CZ-NH2	-13.94	113.33	120.30
2	I	32	ARG	NE-CZ-NH1	13.63	127.11	120.30
2	J	32	ARG	NE-CZ-NH1	13.62	127.11	120.30
2	J	5	ASP	CB-CG-OD2	-13.30	106.33	118.30
2	I	5	ASP	CB-CG-OD2	-13.29	106.34	118.30
1	A	45	ARG	NE-CZ-NH1	-12.86	113.87	120.30
1	B	45	ARG	NE-CZ-NH1	-12.82	113.89	120.30
1	B	101	ASP	CB-CG-OD1	12.27	129.34	118.30
1	A	101	ASP	CB-CG-OD1	12.24	129.32	118.30
1	A	272	ARG	C-N-CA	11.47	150.38	121.70
1	B	272	ARG	C-N-CA	11.46	150.34	121.70
1	A	276	ARG	NE-CZ-NH1	-10.77	114.91	120.30
1	B	276	ARG	NE-CZ-NH1	-10.75	114.92	120.30
1	A	130	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	B	130	ARG	NE-CZ-NH2	10.48	125.54	120.30
2	J	32	ARG	CA-CB-CG	10.30	136.05	113.40
2	I	32	ARG	CA-CB-CG	10.29	136.03	113.40
1	B	130	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	130	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	240	TYR	CB-CG-CD1	-9.97	115.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	TYR	CB-CG-CD1	-9.92	115.05	121.00
1	B	248	TYR	CB-CG-CD1	9.86	126.92	121.00
1	B	20	ASP	CB-CG-OD1	9.83	127.15	118.30
1	A	248	TYR	CB-CG-CD1	9.79	126.88	121.00
1	A	20	ASP	CB-CG-OD1	9.77	127.10	118.30
1	B	208	TYR	CB-CG-CD2	-9.76	115.15	121.00
2	I	21	ALA	N-CA-CB	-9.71	96.50	110.10
2	J	21	ALA	N-CA-CB	-9.68	96.54	110.10
1	A	208	TYR	CB-CG-CD2	-9.68	115.19	121.00
1	B	130	ARG	NH1-CZ-NH2	-9.42	109.03	119.40
1	A	130	ARG	NH1-CZ-NH2	-9.40	109.06	119.40
1	B	145	ARG	NE-CZ-NH2	9.39	124.99	120.30
1	A	206	TYR	CB-CG-CD1	-9.32	115.41	121.00
1	A	145	ARG	NE-CZ-NH2	9.29	124.95	120.30
1	B	206	TYR	CB-CG-CD1	-9.26	115.44	121.00
2	I	32	ARG	NH1-CZ-NH2	-8.89	109.62	119.40
2	J	32	ARG	NH1-CZ-NH2	-8.83	109.68	119.40
1	A	104	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	B	145	ARG	CD-NE-CZ	8.78	135.88	123.60
1	B	104	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	B	177	LYS	CA-CB-CG	8.74	132.63	113.40
1	A	177	LYS	CA-CB-CG	8.73	132.62	113.40
1	A	145	ARG	CD-NE-CZ	8.73	135.82	123.60
2	I	20	GLY	O-C-N	8.73	136.66	122.70
2	J	20	GLY	O-C-N	8.70	136.63	122.70
1	A	305	VAL	CA-CB-CG1	8.58	123.77	110.90
1	A	276	ARG	CA-CB-CG	8.54	132.19	113.40
1	B	276	ARG	CA-CB-CG	8.53	132.16	113.40
1	B	305	VAL	CA-CB-CG1	8.52	123.69	110.90
1	B	270	GLU	OE1-CD-OE2	8.46	133.45	123.30
1	B	211	GLN	CG-CD-OE1	-8.45	104.71	121.60
1	B	124	ARG	CD-NE-CZ	8.43	135.41	123.60
1	A	270	GLU	OE1-CD-OE2	8.41	133.39	123.30
1	A	211	GLN	CG-CD-OE1	-8.40	104.80	121.60
1	A	124	ARG	CD-NE-CZ	8.39	135.34	123.60
1	B	19	TYR	CB-CG-CD1	8.38	126.03	121.00
1	A	127	ARG	CB-CG-CD	8.36	133.33	111.60
1	A	19	TYR	CB-CG-CD1	8.35	126.01	121.00
1	A	59	ARG	NE-CZ-NH1	-8.35	116.12	120.30
1	B	127	ARG	CB-CG-CD	8.35	133.30	111.60
1	B	137	LEU	C-N-CA	8.30	142.46	121.70
1	A	137	LEU	C-N-CA	8.30	142.45	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	A	59	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	59	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	17	GLU	CG-CD-OE1	8.01	134.33	118.30
1	B	17	GLU	CG-CD-OE1	7.99	134.28	118.30
1	B	124	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	A	124	ARG	NE-CZ-NH1	-7.93	116.34	120.30
1	B	247	ILE	CA-CB-CG1	7.92	126.05	111.00
1	A	305	VAL	CB-CA-C	7.91	126.42	111.40
1	B	305	VAL	CB-CA-C	7.91	126.43	111.40
1	A	247	ILE	CA-CB-CG1	7.90	126.00	111.00
1	A	17	GLU	CG-CD-OE2	-7.75	102.81	118.30
1	B	247	ILE	N-CA-CB	7.74	128.61	110.80
1	A	247	ILE	N-CA-CB	7.72	128.56	110.80
1	A	161	CYS	CA-CB-SG	-7.72	100.11	114.00
1	B	17	GLU	CG-CD-OE2	-7.71	102.88	118.30
1	B	161	CYS	CA-CB-SG	-7.68	100.17	114.00
1	A	302	GLU	CB-CG-CD	7.65	134.86	114.20
1	B	227	VAL	CA-CB-CG1	7.64	122.36	110.90
1	B	302	GLU	CB-CG-CD	7.64	134.82	114.20
1	A	227	VAL	CA-CB-CG1	7.62	122.33	110.90
1	A	282	PRO	O-C-N	-7.59	110.55	122.70
1	B	90	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	B	282	PRO	O-C-N	-7.50	110.70	122.70
1	A	116	PHE	CB-CG-CD1	-7.50	115.55	120.80
1	B	116	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	A	127	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	199	SER	N-CA-CB	7.46	121.68	110.50
1	B	2	ARG	N-CA-CB	7.44	123.99	110.60
1	B	271	LEU	CA-CB-CG	7.43	132.39	115.30
1	A	199	SER	N-CA-CB	7.43	121.64	110.50
1	A	271	LEU	CA-CB-CG	7.43	132.38	115.30
1	B	161	CYS	O-C-N	7.43	134.58	122.70
1	B	211	GLN	OE1-CD-NE2	7.42	138.96	121.90
1	A	2	ARG	N-CA-CB	7.41	123.93	110.60
1	A	161	CYS	O-C-N	7.39	134.52	122.70
1	A	90	TYR	CB-CG-CD1	-7.38	116.57	121.00
1	A	211	GLN	OE1-CD-NE2	7.36	138.83	121.90
1	A	248	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	B	127	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	248	TYR	CB-CG-CD2	-7.31	116.62	121.00
1	A	133	THR	CB-CA-C	-7.30	91.90	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	THR	CB-CA-C	-7.30	91.90	111.60
1	B	133	THR	N-CA-CB	7.23	124.04	110.30
1	A	133	THR	N-CA-CB	7.22	124.01	110.30
1	A	302	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	B	302	GLU	OE1-CD-OE2	-7.18	114.68	123.30
1	B	65	ASP	CB-CG-OD1	7.17	124.75	118.30
1	B	260	ASN	CA-CB-CG	7.17	129.16	113.40
1	A	260	ASN	CA-CB-CG	7.16	129.15	113.40
2	J	5	ASP	CA-CB-CG	-7.11	97.75	113.40
1	B	179	ILE	O-C-N	7.10	134.06	122.70
2	I	5	ASP	CA-CB-CG	-7.10	97.79	113.40
1	A	11	THR	CA-CB-CG2	-7.09	102.47	112.40
1	A	179	ILE	O-C-N	7.08	134.03	122.70
1	B	11	THR	CA-CB-CG2	-7.07	102.51	112.40
1	A	65	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	136	SER	O-C-N	-7.03	111.46	122.70
1	B	136	SER	O-C-N	-7.01	111.48	122.70
1	A	45	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	272	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	96	PHE	N-CA-CB	6.93	123.07	110.60
1	B	96	PHE	N-CA-CB	6.93	123.07	110.60
1	B	45	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	B	136	SER	CA-C-O	6.83	134.45	120.10
1	B	272	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	136	SER	CA-C-O	6.82	134.41	120.10
1	B	2	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	A	2	ARG	NE-CZ-NH2	6.77	123.68	120.30
2	I	28	TRP	CA-C-O	-6.75	105.93	120.10
1	A	268	THR	N-CA-CB	6.74	123.10	110.30
2	J	28	TRP	CA-C-O	-6.72	106.00	120.10
1	B	268	THR	N-CA-CB	6.71	123.05	110.30
1	B	276	ARG	CD-NE-CZ	-6.70	114.22	123.60
1	A	302	GLU	CA-CB-CG	6.69	128.12	113.40
1	A	59	ARG	NH1-CZ-NH2	6.66	126.73	119.40
1	A	276	ARG	CD-NE-CZ	-6.66	114.28	123.60
1	B	42	TYR	CA-CB-CG	-6.66	100.75	113.40
1	B	59	ARG	NH1-CZ-NH2	6.65	126.71	119.40
1	B	302	GLU	CA-CB-CG	6.65	128.02	113.40
1	A	42	TYR	CA-CB-CG	-6.64	100.78	113.40
1	B	198	TYR	CZ-CE2-CD2	-6.64	113.83	119.80
1	A	198	TYR	CZ-CE2-CD2	-6.63	113.83	119.80
1	A	185	ASN	O-C-N	6.62	133.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	O-C-N	6.60	133.26	122.70
1	A	198	TYR	CG-CD2-CE2	6.59	126.57	121.30
2	J	13	LYS	C-N-CA	6.57	138.13	121.70
1	B	90	TYR	CB-CG-CD2	6.57	124.94	121.00
1	B	275	GLY	CA-C-O	-6.57	108.78	120.60
2	I	13	LYS	C-N-CA	6.55	138.09	121.70
1	A	275	GLY	CA-C-O	-6.55	108.81	120.60
1	A	148	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	B	11	THR	CA-CB-OG1	6.53	122.71	109.00
1	A	11	THR	CA-CB-OG1	6.53	122.70	109.00
1	B	198	TYR	CG-CD2-CE2	6.52	126.52	121.30
1	B	175	GLU	O-C-N	6.51	133.12	122.70
1	B	148	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	245	THR	CA-CB-CG2	6.50	121.50	112.40
1	A	206	TYR	CB-CG-CD2	6.48	124.89	121.00
1	A	245	THR	CA-CB-CG2	6.47	121.45	112.40
1	B	206	TYR	CB-CG-CD2	6.46	124.88	121.00
1	A	175	GLU	O-C-N	6.45	133.02	122.70
1	A	137	LEU	CA-C-O	6.44	133.63	120.10
1	B	276	ARG	CB-CA-C	-6.42	97.55	110.40
1	B	137	LEU	CA-C-O	6.42	133.58	120.10
1	A	276	ARG	CB-CA-C	-6.41	97.57	110.40
1	A	90	TYR	CB-CG-CD2	6.41	124.85	121.00
1	A	248	TYR	CA-CB-CG	6.41	125.58	113.40
1	B	248	TYR	CA-CB-CG	6.39	125.54	113.40
1	B	194	SER	N-CA-CB	6.34	120.02	110.50
1	A	194	SER	N-CA-CB	6.33	119.99	110.50
1	A	122	GLU	OE1-CD-OE2	-6.29	115.76	123.30
2	I	14	THR	CA-CB-CG2	6.29	121.20	112.40
1	A	182	PHE	CG-CD1-CE1	-6.28	113.89	120.80
1	B	122	GLU	OE1-CD-OE2	-6.26	115.78	123.30
2	J	14	THR	CA-CB-CG2	6.26	121.16	112.40
2	J	15	HIS	CA-C-O	6.25	133.22	120.10
1	B	182	PHE	CG-CD1-CE1	-6.25	113.93	120.80
2	I	15	HIS	CA-C-O	6.24	133.21	120.10
1	A	28	GLN	O-C-N	-6.24	112.71	122.70
1	A	137	LEU	N-CA-CB	-6.24	97.92	110.40
1	B	205	PRO	O-C-N	-6.24	112.72	122.70
1	B	137	LEU	N-CA-CB	-6.24	97.93	110.40
1	A	271	LEU	CB-CG-CD1	6.23	121.59	111.00
1	B	28	GLN	O-C-N	-6.23	112.73	122.70
1	A	205	PRO	O-C-N	-6.20	112.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	LEU	CB-CG-CD1	6.20	121.54	111.00
2	I	33	THR	CA-CB-CG2	6.19	121.07	112.40
1	B	163	GLU	OE1-CD-OE2	6.14	130.67	123.30
2	J	33	THR	CA-CB-CG2	6.14	121.00	112.40
1	A	163	GLU	OE1-CD-OE2	6.10	130.62	123.30
1	A	133	THR	O-C-N	6.09	132.45	122.70
2	I	20	GLY	CA-C-N	-6.09	103.81	117.20
1	B	133	THR	O-C-N	6.08	132.43	122.70
2	J	20	GLY	CA-C-N	-6.07	103.84	117.20
1	B	16	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	234	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	16	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	16	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	65	ASP	CA-CB-CG	5.89	126.37	113.40
1	A	132	VAL	O-C-N	-5.89	113.27	122.70
1	A	234	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	A	65	ASP	CA-CB-CG	5.88	126.33	113.40
1	B	132	VAL	O-C-N	-5.88	113.29	122.70
1	A	7	PHE	CB-CG-CD1	-5.87	116.69	120.80
1	B	273	ASP	C-N-CA	5.86	136.36	121.70
2	J	16	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	273	ASP	C-N-CA	5.86	136.35	121.70
1	B	16	ASP	CB-CG-OD1	-5.85	113.04	118.30
2	I	16	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	7	PHE	CB-CG-CD1	-5.83	116.72	120.80
1	B	137	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	137	LEU	CA-CB-CG	5.82	128.69	115.30
2	I	35	GLY	N-CA-C	-5.82	98.55	113.10
2	J	35	GLY	N-CA-C	-5.81	98.58	113.10
1	A	190	LYS	N-CA-CB	5.80	121.05	110.60
2	I	32	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	B	190	LYS	N-CA-CB	5.79	121.02	110.60
1	B	33	VAL	CA-CB-CG2	5.79	119.58	110.90
1	A	33	VAL	CA-CB-CG2	5.78	119.56	110.90
1	B	276	ARG	CG-CD-NE	-5.78	99.67	111.80
1	A	31	GLU	OE1-CD-OE2	-5.77	116.37	123.30
2	J	16	ASP	N-CA-CB	-5.77	100.21	110.60
1	A	276	ARG	CG-CD-NE	-5.76	99.70	111.80
1	A	185	ASN	CB-CA-C	-5.76	98.88	110.40
2	I	16	ASP	N-CA-CB	-5.76	100.23	110.60
1	B	100	LEU	CB-CG-CD1	-5.76	101.21	111.00
1	B	185	ASN	CB-CA-C	-5.76	98.88	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	LEU	CB-CG-CD1	-5.75	101.22	111.00
1	B	31	GLU	OE1-CD-OE2	-5.75	116.39	123.30
1	A	7	PHE	CB-CG-CD2	5.75	124.82	120.80
1	B	33	VAL	C-N-CA	5.71	135.97	121.70
1	A	33	VAL	C-N-CA	5.70	135.96	121.70
1	B	254	SER	C-N-CA	5.70	135.95	121.70
1	B	5	ASN	OD1-CG-ND2	5.69	134.98	121.90
1	A	254	SER	C-N-CA	5.67	135.88	121.70
1	B	7	PHE	CB-CG-CD2	5.67	124.77	120.80
2	J	32	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	A	5	ASN	OD1-CG-ND2	5.65	134.89	121.90
2	J	8	CYS	CA-C-O	-5.62	108.29	120.10
1	A	28	GLN	CB-CA-C	5.61	121.63	110.40
2	I	8	CYS	CA-C-O	-5.61	108.32	120.10
1	A	270	GLU	CG-CD-OE2	-5.61	107.09	118.30
1	B	270	GLU	CG-CD-OE2	-5.60	107.10	118.30
1	B	44	GLY	N-CA-C	5.60	127.10	113.10
1	B	28	GLN	CB-CA-C	5.60	121.59	110.40
1	A	44	GLY	N-CA-C	5.60	127.09	113.10
1	A	31	GLU	CG-CD-OE1	5.59	129.49	118.30
1	A	96	PHE	CA-C-O	-5.59	108.35	120.10
1	B	31	GLU	CG-CD-OE1	5.59	129.49	118.30
1	B	96	PHE	CA-C-O	-5.59	108.37	120.10
1	B	240	TYR	CB-CG-CD2	5.57	124.34	121.00
1	A	240	TYR	CB-CG-CD2	5.54	124.32	121.00
2	J	33	THR	CA-C-N	5.52	129.35	117.20
1	A	93	ASN	CA-CB-CG	5.52	125.55	113.40
1	B	93	ASN	CA-CB-CG	5.52	125.54	113.40
2	I	33	THR	CA-C-N	5.50	129.29	117.20
1	A	93	ASN	CB-CG-OD1	5.50	132.59	121.60
1	B	93	ASN	CB-CG-OD1	5.50	132.59	121.60
2	I	31	ALA	N-CA-CB	5.48	117.77	110.10
1	A	274	THR	N-CA-CB	5.47	120.69	110.30
2	J	31	ALA	N-CA-CB	5.47	117.75	110.10
1	B	274	THR	N-CA-CB	5.46	120.68	110.30
1	B	275	GLY	CA-C-N	5.46	129.21	117.20
1	A	16	ASP	OD1-CG-OD2	5.45	133.66	123.30
1	B	16	ASP	OD1-CG-OD2	5.45	133.65	123.30
1	A	275	GLY	CA-C-N	5.44	129.18	117.20
2	I	4	ALA	O-C-N	5.44	131.40	122.70
2	I	16	ASP	CB-CA-C	5.42	121.24	110.40
1	A	169	TYR	CB-CA-C	5.42	121.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	TYR	CB-CA-C	5.42	121.23	110.40
2	J	4	ALA	O-C-N	5.41	131.36	122.70
2	J	16	ASP	CB-CA-C	5.39	121.17	110.40
1	A	177	LYS	CG-CD-CE	5.38	128.03	111.90
1	B	177	LYS	CG-CD-CE	5.37	128.02	111.90
1	B	230	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	A	230	LEU	CB-CG-CD1	-5.37	101.88	111.00
1	B	66	LEU	CB-CA-C	5.35	120.36	110.20
1	A	104	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	104	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	98	ALA	C-N-CA	5.34	135.06	121.70
1	A	10	ALA	C-N-CA	5.34	135.04	121.70
1	A	98	ALA	C-N-CA	5.33	135.03	121.70
1	B	57	SER	C-N-CA	5.33	135.04	121.70
1	A	66	LEU	CB-CA-C	5.33	120.32	110.20
1	B	10	ALA	C-N-CA	5.32	135.00	121.70
1	B	133	THR	CA-C-N	-5.32	105.49	117.20
1	A	133	THR	CA-C-N	-5.32	105.50	117.20
1	A	181	ASP	C-N-CA	5.32	135.00	121.70
2	I	35	GLY	O-C-N	5.32	131.21	121.10
1	B	181	ASP	C-N-CA	5.32	134.99	121.70
1	A	57	SER	C-N-CA	5.31	134.98	121.70
1	A	113	PRO	C-N-CA	5.31	134.98	121.70
1	B	113	PRO	C-N-CA	5.31	134.97	121.70
2	J	35	GLY	O-C-N	5.31	131.18	121.10
1	A	256	ASP	CA-CB-CG	-5.30	101.74	113.40
1	B	256	ASP	CA-CB-CG	-5.29	101.77	113.40
1	B	108	GLU	C-N-CA	5.28	134.90	121.70
1	A	116	PHE	CB-CG-CD2	5.26	124.48	120.80
1	A	108	GLU	C-N-CA	5.25	134.83	121.70
2	I	3	HIS	N-CA-CB	5.25	120.06	110.60
1	A	217	THR	CA-CB-CG2	5.23	119.72	112.40
1	A	59	ARG	CD-NE-CZ	5.21	130.90	123.60
1	B	266	SER	O-C-N	5.21	131.04	122.70
2	J	3	HIS	N-CA-CB	5.21	119.97	110.60
1	B	270	GLU	CA-C-O	-5.20	109.18	120.10
1	A	65	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	217	THR	CA-CB-CG2	5.20	119.68	112.40
1	A	204	TYR	CB-CG-CD2	5.20	124.12	121.00
1	B	116	PHE	CB-CG-CD2	5.20	124.44	120.80
1	A	266	SER	O-C-N	5.20	131.01	122.70
1	A	270	GLU	CA-C-O	-5.19	109.19	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	179	ILE	CB-CA-C	-5.18	101.24	111.60
1	B	59	ARG	CD-NE-CZ	5.18	130.85	123.60
1	A	87	THR	O-C-N	-5.18	114.42	122.70
1	A	185	ASN	N-CA-CB	5.18	119.92	110.60
1	B	185	ASN	N-CA-CB	5.17	119.91	110.60
1	A	233	LEU	N-CA-CB	-5.16	100.07	110.40
1	B	87	THR	O-C-N	-5.16	114.44	122.70
1	B	204	TYR	CB-CG-CD2	5.16	124.10	121.00
1	B	292	GLU	CA-CB-CG	5.15	124.74	113.40
1	A	179	ILE	CB-CA-C	-5.15	101.30	111.60
1	A	73	TRP	CA-C-O	-5.15	109.29	120.10
1	B	73	TRP	CA-C-O	-5.15	109.29	120.10
1	B	233	LEU	N-CA-CB	-5.15	100.11	110.40
1	B	34	SER	CB-CA-C	-5.14	100.33	110.10
1	A	34	SER	CB-CA-C	-5.13	100.35	110.10
1	B	2	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	292	GLU	CA-CB-CG	5.12	124.66	113.40
1	A	179	ILE	N-CA-CB	5.12	122.57	110.80
1	B	179	ILE	N-CA-CB	5.12	122.57	110.80
1	A	137	LEU	O-C-N	-5.11	114.52	122.70
1	B	247	ILE	CB-CA-C	-5.09	101.41	111.60
1	A	247	ILE	CB-CA-C	-5.08	101.43	111.60
1	B	193	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	219	LEU	CB-CA-C	5.08	119.85	110.20
1	A	159	SER	CA-CB-OG	-5.08	97.49	111.20
1	A	193	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	159	SER	CA-CB-OG	-5.08	97.49	111.20
1	B	137	LEU	O-C-N	-5.07	114.58	122.70
2	I	12	CYS	N-CA-CB	-5.07	101.47	110.60
1	B	219	LEU	CB-CA-C	5.06	119.81	110.20
2	J	12	CYS	N-CA-CB	-5.05	101.51	110.60
1	A	282	PRO	C-N-CA	5.05	134.33	121.70
1	B	282	PRO	C-N-CA	5.05	134.32	121.70
1	A	307	ASN	CA-C-O	-5.05	109.50	120.10
1	A	2	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	43	GLU	C-N-CA	5.04	132.89	122.30
1	B	51	LYS	C-N-CA	5.04	134.30	121.70
1	B	307	ASN	CA-C-O	-5.04	109.52	120.10
1	B	62	ILE	CA-C-O	-5.03	109.54	120.10
1	A	253	GLY	C-N-CA	5.03	134.26	121.70
1	B	253	GLY	C-N-CA	5.03	134.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ILE	CA-C-O	-5.02	109.56	120.10
1	B	43	GLU	C-N-CA	5.02	132.84	122.30
1	A	51	LYS	C-N-CA	5.01	134.23	121.70
1	A	148	ASP	CB-CG-OD1	5.01	122.81	118.30
2	I	27	CYS	O-C-N	5.00	130.71	122.70
2	J	27	CYS	O-C-N	5.00	130.71	122.70

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	135	SER	Mainchain
1	A	145	ARG	Sidechain
1	A	2	ARG	Sidechain
1	A	238	TYR	Mainchain
1	A	247	ILE	Mainchain
1	A	272	ARG	Sidechain,Peptide
1	A	276	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	59	ARG	Sidechain
1	A	71	ARG	Sidechain
1	B	127	ARG	Sidechain
1	B	135	SER	Mainchain
1	B	145	ARG	Sidechain
1	B	2	ARG	Sidechain
1	B	238	TYR	Mainchain
1	B	247	ILE	Mainchain
1	B	272	ARG	Sidechain,Peptide
1	B	276	ARG	Sidechain
1	B	40	ARG	Sidechain
1	B	59	ARG	Sidechain
1	B	71	ARG	Sidechain
2	I	2	GLX	Mainchain
2	I	31	ALA	Mainchain
2	I	32	ARG	Sidechain
2	J	2	GLX	Mainchain
2	J	31	ALA	Mainchain
2	J	32	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2350	201	0
1	B	2437	0	2350	197	0
2	I	285	0	243	44	0
2	J	285	0	243	43	0
3	A	5	0	2	1	0
3	B	5	0	2	1	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	5456	0	5190	468	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 44.

All (468) 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:134:SER:HB3	1:B:136:SER:HB2	1.25	1.18
1:A:134:SER:HB3	1:A:136:SER:HB2	1.25	1.17
1:B:136:SER:HA	1:B:137:LEU:HD22	1.32	1.10
1:B:60:PRO:HB3	1:B:190:LYS:HD2	1.33	1.09
1:A:136:SER:HA	1:A:137:LEU:HD22	1.32	1.08
1:B:208:TYR:HB3	1:B:251:SER:HA	1.31	1.08
1:A:60:PRO:HB3	1:A:190:LYS:HD2	1.33	1.04
1:A:208:TYR:HB3	1:A:251:SER:HA	1.31	1.04
1:B:74:ILE:HD13	1:B:281:LEU:HD12	1.45	0.98
2:J:21:ALA:O	2:J:23:PHE:N	1.97	0.97
1:A:74:ILE:HD13	1:A:281:LEU:HD12	1.44	0.96
2:I:21:ALA:O	2:I:23:PHE:N	1.97	0.96
1:B:74:ILE:HD13	1:B:281:LEU:CD1	1.96	0.95
2:I:5:ASP:CG	2:I:21:ALA:HB1	1.86	0.95
2:J:5:ASP:CG	2:J:21:ALA:HB1	1.86	0.94
1:A:74:ILE:HD13	1:A:281:LEU:CD1	1.96	0.94
1:B:134:SER:CB	1:B:136:SER:HB2	1.98	0.93
2:I:9:ASN:HA	2:I:33:THR:HG23	1.51	0.93
2:J:9:ASN:HA	2:J:33:THR:HG23	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:CB	1:A:136:SER:HB2	1.98	0.92
1:A:186:HIS:HD2	1:A:188:ASN:H	1.11	0.92
1:B:186:HIS:HD2	1:B:188:ASN:H	1.11	0.92
1:A:289:THR:O	1:A:293:THR:HG22	1.70	0.92
1:B:289:THR:O	1:B:293:THR:HG22	1.70	0.91
1:A:283:ALA:HB3	1:B:122:GLU:HG3	1.52	0.89
1:A:122:GLU:HG3	1:B:283:ALA:HB3	1.53	0.89
1:B:132:VAL:O	1:B:133:THR:OG1	1.90	0.89
1:A:132:VAL:O	1:A:133:THR:OG1	1.90	0.88
2:J:5:ASP:OD2	2:J:21:ALA:O	1.92	0.88
2:J:5:ASP:OD1	2:J:21:ALA:HB1	1.73	0.87
2:I:5:ASP:OD2	2:I:21:ALA:O	1.92	0.86
1:B:171:ASN:O	1:B:177:LYS:HE2	1.75	0.86
1:A:92:GLN:HA	1:A:92:GLN:NE2	1.90	0.86
1:B:92:GLN:HA	1:B:92:GLN:NE2	1.90	0.86
1:A:136:SER:HA	1:A:137:LEU:CD2	2.05	0.86
1:B:136:SER:HA	1:B:137:LEU:CD2	2.05	0.86
2:I:5:ASP:OD1	2:I:21:ALA:HB1	1.74	0.85
1:A:283:ALA:HB2	1:B:122:GLU:HA	1.58	0.85
1:A:171:ASN:O	1:A:177:LYS:HE2	1.75	0.85
1:A:245:THR:HG22	1:A:246:THR:CG2	2.08	0.84
1:A:122:GLU:HA	1:B:283:ALA:HB2	1.60	0.84
1:A:245:THR:HG22	1:A:246:THR:HG23	1.59	0.83
1:B:245:THR:HG22	1:B:246:THR:CG2	2.08	0.83
1:B:245:THR:HG22	1:B:246:THR:HG23	1.59	0.82
2:J:31:ALA:HA	2:J:32:ARG:NH1	1.95	0.81
1:B:134:SER:HB3	1:B:136:SER:CB	2.09	0.81
2:J:5:ASP:OD2	2:J:21:ALA:HB1	1.80	0.81
2:I:31:ALA:HA	2:I:32:ARG:NH1	1.95	0.80
1:A:93:ASN:O	1:A:97:THR:HG23	1.82	0.80
1:A:134:SER:HB3	1:A:136:SER:CB	2.09	0.80
1:A:186:HIS:CD2	1:A:188:ASN:H	1.99	0.79
2:I:5:ASP:OD2	2:I:21:ALA:HB1	1.80	0.79
1:A:208:TYR:CB	1:A:251:SER:HA	2.13	0.78
1:B:93:ASN:O	1:B:97:THR:HG23	1.82	0.78
1:B:208:TYR:CB	1:B:251:SER:HA	2.13	0.78
1:A:91:GLY:H	1:A:97:THR:HG22	1.48	0.78
1:B:186:HIS:CD2	1:B:188:ASN:H	1.99	0.78
1:A:131:SER:O	1:A:139:VAL:HG23	1.83	0.77
1:B:131:SER:O	1:B:139:VAL:HG23	1.83	0.77
2:J:5:ASP:HB3	2:J:8:CYS:SG	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:ASP:HB3	2:I:8:CYS:SG	2.24	0.77
2:I:7:ILE:HD12	2:I:20:GLY:H	1.50	0.77
1:B:91:GLY:H	1:B:97:THR:HG22	1.48	0.77
2:J:7:ILE:HD12	2:J:20:GLY:H	1.50	0.76
1:B:26:VAL:HG13	1:B:33:VAL:HG23	1.68	0.75
1:A:26:VAL:HG13	1:A:33:VAL:HG23	1.68	0.75
1:A:91:GLY:H	1:A:97:THR:CG2	2.00	0.75
1:B:91:GLY:H	1:B:97:THR:CG2	2.00	0.74
1:A:159:SER:O	1:A:162:SER:HB2	1.88	0.74
2:I:31:ALA:CA	2:I:32:ARG:NH1	2.51	0.74
1:B:159:SER:O	1:B:162:SER:HB2	1.88	0.73
1:B:224:LYS:HD2	1:B:240:TYR:OH	1.88	0.73
1:A:224:LYS:HD2	1:A:240:TYR:OH	1.88	0.73
2:J:31:ALA:CA	2:J:32:ARG:NH1	2.51	0.73
1:B:26:VAL:HA	1:B:33:VAL:HG22	1.72	0.72
1:B:297:VAL:HG12	1:B:301:MET:CE	2.19	0.72
1:A:297:VAL:HG12	1:A:301:MET:CE	2.19	0.72
1:B:136:SER:CA	1:B:137:LEU:HD22	2.16	0.72
1:A:297:VAL:O	1:A:301:MET:HG3	1.90	0.72
1:B:303:HIS:O	1:B:307:ASN:ND2	2.23	0.72
1:B:297:VAL:O	1:B:301:MET:HG3	1.90	0.71
1:A:303:HIS:O	1:A:307:ASN:ND2	2.23	0.71
2:J:32:ARG:HH11	2:J:32:ARG:H	1.40	0.70
1:A:26:VAL:HA	1:A:33:VAL:HG22	1.72	0.70
2:I:31:ALA:CA	2:I:32:ARG:HH11	2.05	0.70
1:B:83:ALA:O	1:B:87:THR:HG23	1.92	0.70
1:A:136:SER:CA	1:A:137:LEU:HD22	2.16	0.69
2:J:5:ASP:OD1	2:J:21:ALA:CB	2.40	0.69
1:A:273:ASP:OD2	1:A:274:THR:N	2.22	0.69
2:I:32:ARG:HH11	2:I:32:ARG:H	1.40	0.69
1:A:83:ALA:O	1:A:87:THR:HG23	1.92	0.69
2:J:31:ALA:CA	2:J:32:ARG:HH11	2.05	0.69
1:B:273:ASP:OD2	1:B:274:THR:N	2.22	0.69
2:I:5:ASP:OD1	2:I:21:ALA:CB	2.40	0.68
2:I:32:ARG:HH11	2:I:32:ARG:N	1.92	0.68
1:A:119:THR:HA	1:A:123:ASN:O	1.94	0.68
1:B:213:ILE:O	1:B:216:LYS:HB2	1.94	0.68
1:B:91:GLY:N	1:B:97:THR:HG22	2.09	0.68
1:A:213:ILE:O	1:A:216:LYS:HB2	1.94	0.68
1:B:3:SER:HA	1:B:28:GLN:HE22	1.59	0.67
1:A:3:SER:HA	1:A:28:GLN:HE22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:N	1:A:97:THR:HG22	2.09	0.67
1:B:119:THR:HA	1:B:123:ASN:O	1.94	0.67
1:A:273:ASP:OD2	1:A:275:GLY:N	2.27	0.67
2:J:32:ARG:HH11	2:J:32:ARG:N	1.92	0.67
2:I:9:ASN:HD21	2:J:3:HIS:H	1.42	0.67
2:J:7:ILE:O	2:J:10:LYS:HB3	1.94	0.67
2:J:31:ALA:HA	2:J:32:ARG:HH12	1.59	0.67
2:I:7:ILE:O	2:I:10:LYS:HB3	1.94	0.67
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.60	0.67
1:A:297:VAL:HG12	1:A:301:MET:HE3	1.76	0.67
2:I:31:ALA:O	2:I:33:THR:HB	1.95	0.67
1:A:179:ILE:N	1:A:179:ILE:HD12	2.10	0.66
1:B:26:VAL:HG13	1:B:33:VAL:CG2	2.25	0.66
2:I:3:HIS:H	2:J:9:ASN:HD21	1.44	0.66
1:B:273:ASP:OD2	1:B:275:GLY:N	2.27	0.66
1:B:192:PHE:O	1:B:266:SER:HA	1.95	0.66
2:J:31:ALA:O	2:J:33:THR:HB	1.95	0.66
1:A:26:VAL:HG13	1:A:33:VAL:CG2	2.25	0.66
1:A:192:PHE:O	1:A:266:SER:HA	1.95	0.66
1:B:179:ILE:HD12	1:B:179:ILE:N	2.10	0.65
1:A:70:SER:HB3	1:A:116:PHE:N	2.11	0.65
1:A:186:HIS:HD2	1:A:188:ASN:N	1.92	0.65
1:B:58:ASN:HD21	1:B:188:ASN:HB2	1.60	0.65
2:I:31:ALA:HA	2:I:32:ARG:HH12	1.60	0.65
1:B:70:SER:HB3	1:B:116:PHE:N	2.11	0.65
1:A:201:LEU:HA	1:A:239:LYS:O	1.97	0.65
1:B:201:LEU:HA	1:B:239:LYS:O	1.97	0.65
1:B:81:TRP:CH2	1:B:85:LYS:HD3	2.32	0.64
1:A:81:TRP:CH2	1:A:85:LYS:HD3	2.32	0.64
1:A:149:ALA:HB1	1:A:256:ASP:HB3	1.80	0.64
1:A:283:ALA:CB	1:B:122:GLU:HA	2.28	0.63
1:B:149:ALA:HB1	1:B:256:ASP:HB3	1.80	0.63
1:A:179:ILE:H	1:A:179:ILE:CD1	2.12	0.63
2:I:21:ALA:O	2:I:22:TRP:CD1	2.52	0.63
1:B:91:GLY:HA2	1:B:97:THR:HG21	1.81	0.63
1:B:297:VAL:HG12	1:B:301:MET:HE3	1.81	0.63
1:B:69:HIS:NE2	1:B:127:ARG:NH2	2.46	0.63
1:A:122:GLU:HA	1:B:283:ALA:CB	2.29	0.62
1:A:91:GLY:HA2	1:A:97:THR:HG21	1.81	0.62
2:J:21:ALA:O	2:J:22:TRP:CD1	2.52	0.62
1:A:51:LYS:HG3	1:A:106:PHE:CZ	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:HIS:CE1	1:B:127:ARG:NH2	2.68	0.61
1:B:179:ILE:H	1:B:179:ILE:CD1	2.12	0.61
2:I:7:ILE:HB	2:I:21:ALA:HB2	1.82	0.61
1:A:69:HIS:CE1	1:A:127:ARG:NH2	2.68	0.61
1:B:186:HIS:HD2	1:B:188:ASN:N	1.92	0.61
1:B:51:LYS:HG3	1:B:106:PHE:CZ	2.35	0.61
1:A:213:ILE:CD1	1:A:219:LEU:HD22	2.31	0.61
1:A:146:ASN:O	1:A:170:ALA:HA	2.01	0.61
1:A:91:GLY:N	1:A:97:THR:CG2	2.64	0.60
1:B:213:ILE:CD1	1:B:219:LEU:HD22	2.31	0.60
2:J:3:HIS:O	2:J:4:ALA:HB2	2.01	0.60
2:J:7:ILE:HB	2:J:21:ALA:HB2	1.82	0.60
2:I:3:HIS:O	2:I:4:ALA:HB2	2.01	0.60
1:A:69:HIS:NE2	1:A:127:ARG:NH2	2.46	0.60
1:A:91:GLY:CA	1:A:97:THR:HG21	2.31	0.60
1:B:91:GLY:CA	1:B:97:THR:HG21	2.31	0.60
1:B:146:ASN:O	1:B:170:ALA:HA	2.01	0.60
1:B:171:ASN:O	1:B:177:LYS:CE	2.49	0.60
1:A:42:TYR:C	1:A:42:TYR:CD2	2.75	0.59
1:B:233:LEU:CD1	1:B:295:LEU:HD22	2.33	0.59
1:A:233:LEU:CD1	1:A:295:LEU:HD22	2.33	0.59
1:A:63:TRP:HB2	1:A:189:PHE:CE2	2.38	0.59
1:B:42:TYR:C	1:B:42:TYR:CD2	2.75	0.59
1:B:63:TRP:HB2	1:B:189:PHE:CE2	2.38	0.59
1:B:242:SER:OG	1:B:245:THR:HB	2.03	0.59
1:B:289:THR:O	1:B:293:THR:CG2	2.49	0.59
1:B:297:VAL:HG12	1:B:301:MET:HE2	1.83	0.59
1:A:70:SER:HB2	1:A:119:THR:HG21	1.85	0.59
1:B:58:ASN:ND2	1:B:188:ASN:HB2	2.18	0.59
1:B:150:GLY:O	1:B:251:SER:HB2	2.03	0.59
1:B:211:GLN:HG2	1:B:212:SER:N	2.17	0.59
1:A:127:ARG:NH2	1:A:142:ASP:OD2	2.36	0.58
1:B:66:LEU:N	1:B:108:GLU:O	2.36	0.58
1:B:70:SER:HB2	1:B:119:THR:HG21	1.85	0.58
1:B:198:TYR:HA	1:B:271:LEU:O	2.03	0.58
1:A:150:GLY:O	1:A:251:SER:HB2	2.03	0.58
1:A:242:SER:OG	1:A:245:THR:HB	2.03	0.58
1:B:127:ARG:NH2	1:B:142:ASP:OD2	2.36	0.58
1:A:171:ASN:HD22	1:A:176:VAL:HG12	1.68	0.58
1:A:192:PHE:HB2	1:A:263:ILE:HG21	1.86	0.58
1:A:211:GLN:HG2	1:A:212:SER:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:TYR:HA	1:A:271:LEU:O	2.03	0.58
1:B:192:PHE:HB2	1:B:263:ILE:HG21	1.86	0.58
1:A:58:ASN:ND2	1:A:188:ASN:HB2	2.18	0.58
1:A:136:SER:CA	1:A:137:LEU:HD13	2.34	0.58
1:B:91:GLY:N	1:B:97:THR:CG2	2.64	0.58
1:A:171:ASN:O	1:A:177:LYS:CE	2.49	0.57
1:B:136:SER:CA	1:B:137:LEU:HD13	2.34	0.57
1:B:195:ILE:CG2	1:B:271:LEU:HD21	2.35	0.57
1:A:41:SER:N	1:A:45:ARG:O	2.30	0.57
1:B:233:LEU:HD12	1:B:295:LEU:HD22	1.87	0.57
1:B:245:THR:HG22	1:B:246:THR:HG22	1.85	0.57
1:A:86:PHE:HE1	1:A:294:TRP:HE1	1.53	0.57
1:B:171:ASN:HD22	1:B:176:VAL:HG12	1.68	0.57
3:B:308:GLY:HA2	2:J:38:VAL:OXT	2.04	0.57
1:A:179:ILE:HD12	1:A:179:ILE:H	1.68	0.57
1:A:233:LEU:HD12	1:A:295:LEU:HD22	1.87	0.57
1:A:74:ILE:CD1	1:A:281:LEU:HD12	2.29	0.57
1:B:61:ALA:HA	1:B:104:ASP:O	2.05	0.57
1:A:215:ASP:O	1:A:219:LEU:HD13	2.05	0.57
1:A:25:LEU:HD11	1:A:87:THR:HG21	1.87	0.56
3:A:308:GLY:HA2	2:I:38:VAL:OXT	2.05	0.56
1:B:74:ILE:HG13	1:B:74:ILE:O	2.05	0.56
1:A:66:LEU:N	1:A:108:GLU:O	2.36	0.56
1:A:195:ILE:CG2	1:A:271:LEU:HD21	2.35	0.56
1:A:245:THR:HG22	1:A:246:THR:HG22	1.85	0.56
1:B:72:GLU:HB3	1:B:197:SER:HB3	1.87	0.56
1:B:86:PHE:HE1	1:B:294:TRP:HE1	1.53	0.56
2:J:21:ALA:O	2:J:22:TRP:CG	2.59	0.56
1:A:289:THR:O	1:A:293:THR:CG2	2.49	0.56
1:B:25:LEU:HD11	1:B:87:THR:HG21	1.87	0.56
1:B:179:ILE:HD12	1:B:179:ILE:H	1.68	0.56
2:I:21:ALA:O	2:I:22:TRP:CG	2.59	0.56
1:A:61:ALA:HA	1:A:104:ASP:O	2.05	0.56
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.71	0.56
1:A:69:HIS:CE1	1:A:127:ARG:HH21	2.24	0.56
1:B:276:ARG:HG2	1:B:276:ARG:HH11	1.71	0.56
1:A:115:GLY:O	1:A:119:THR:HG23	2.06	0.56
1:A:212:SER:OG	1:A:216:LYS:HG3	2.06	0.55
1:A:281:LEU:HD21	1:A:285:GLN:NE2	2.22	0.55
1:B:215:ASP:O	1:B:219:LEU:HD13	2.05	0.55
1:B:258:SER:HB2	1:B:263:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:TYR:HD1	1:A:256:ASP:OD2	1.89	0.55
1:A:72:GLU:HB3	1:A:197:SER:HB3	1.87	0.55
1:A:74:ILE:HG13	1:A:74:ILE:O	2.05	0.55
1:B:95:SER:OG	1:B:302:GLU:OE2	2.25	0.55
1:A:66:LEU:HD22	1:A:75:THR:O	2.07	0.55
2:I:29:ASN:N	2:I:29:ASN:HD22	2.04	0.55
1:B:115:GLY:O	1:B:119:THR:HG23	2.06	0.55
1:A:131:SER:C	1:A:139:VAL:HG23	2.28	0.54
1:A:297:VAL:HG12	1:A:301:MET:HE2	1.87	0.54
1:B:127:ARG:HH11	2:J:37:TYR:CB	2.20	0.54
1:B:63:TRP:HE1	1:B:65:ASP:HB3	1.72	0.54
1:B:281:LEU:HD21	1:B:285:GLN:NE2	2.22	0.54
1:B:66:LEU:HD22	1:B:75:THR:O	2.07	0.54
1:B:179:ILE:N	1:B:179:ILE:CD1	2.70	0.54
1:B:208:TYR:HD1	1:B:256:ASP:OD2	1.89	0.54
1:B:212:SER:OG	1:B:216:LYS:HG3	2.06	0.54
1:A:95:SER:OG	1:A:302:GLU:OE2	2.25	0.54
1:A:1:ALA:N	1:A:7:PHE:HB2	2.23	0.54
1:A:63:TRP:HE1	1:A:65:ASP:HB3	1.73	0.54
1:B:45:ARG:HH11	1:B:114:ASN:ND2	2.06	0.54
1:B:131:SER:C	1:B:139:VAL:HG23	2.27	0.54
1:A:7:PHE:CD1	1:A:7:PHE:C	2.82	0.54
1:A:70:SER:HB2	1:A:119:THR:CG2	2.38	0.54
1:B:70:SER:HB2	1:B:119:THR:CG2	2.38	0.54
2:J:7:ILE:CD1	2:J:20:GLY:H	2.20	0.54
1:A:127:ARG:HH11	2:I:37:TYR:CB	2.21	0.53
1:A:136:SER:HA	1:A:137:LEU:HD13	1.90	0.53
2:I:31:ALA:C	2:I:32:ARG:HH11	2.11	0.53
1:B:136:SER:HA	1:B:137:LEU:HD13	1.91	0.53
1:A:258:SER:HB2	1:A:263:ILE:HD12	1.89	0.53
1:B:195:ILE:HG22	1:B:271:LEU:CD2	2.38	0.53
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.06	0.53
1:A:195:ILE:HG22	1:A:271:LEU:CD2	2.39	0.53
1:B:93:ASN:O	1:B:97:THR:CG2	2.56	0.53
1:B:199:SER:N	1:B:271:LEU:O	2.42	0.53
2:J:31:ALA:C	2:J:32:ARG:HH11	2.11	0.53
1:B:1:ALA:N	1:B:7:PHE:HB2	2.23	0.52
1:A:29:HIS:HB2	1:A:33:VAL:HG13	1.92	0.52
2:I:7:ILE:CD1	2:I:20:GLY:H	2.21	0.52
1:A:204:TYR:HB2	1:A:205:PRO:HD2	1.91	0.52
1:B:7:PHE:CD1	1:B:7:PHE:C	2.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:THR:O	1:A:134:SER:HB2	2.10	0.52
1:A:199:SER:N	1:A:271:LEU:O	2.42	0.52
1:B:204:TYR:HB2	1:B:205:PRO:HD2	1.91	0.52
1:A:60:PRO:HA	1:A:188:ASN:O	2.10	0.52
1:A:26:VAL:HG12	1:A:33:VAL:O	2.11	0.51
1:A:213:ILE:HD11	1:A:216:LYS:HA	1.91	0.51
1:B:204:TYR:O	1:B:242:SER:HA	2.10	0.51
1:B:213:ILE:HD11	1:B:216:LYS:HA	1.91	0.51
1:A:25:LEU:CD2	1:A:83:ALA:HB1	2.41	0.51
1:B:25:LEU:CD2	1:B:83:ALA:HB1	2.41	0.51
1:B:74:ILE:CD1	1:B:281:LEU:HD12	2.29	0.51
1:A:69:HIS:HE2	1:A:127:ARG:HH21	1.54	0.51
1:B:41:SER:N	1:B:45:ARG:O	2.30	0.51
1:B:95:SER:O	1:B:99:ILE:HD12	2.10	0.51
1:B:133:THR:O	1:B:134:SER:HB2	2.10	0.51
1:A:179:ILE:N	1:A:179:ILE:CD1	2.70	0.51
1:A:136:SER:HA	1:A:137:LEU:CD1	2.41	0.51
1:B:26:VAL:HG12	1:B:33:VAL:O	2.11	0.51
1:B:136:SER:HA	1:B:137:LEU:CD1	2.41	0.51
1:B:213:ILE:O	1:B:213:ILE:HG13	2.10	0.51
1:B:60:PRO:HA	1:B:188:ASN:O	2.10	0.50
1:A:95:SER:O	1:A:99:ILE:HD12	2.10	0.50
1:A:213:ILE:O	1:A:213:ILE:HG13	2.10	0.50
1:A:204:TYR:O	1:A:242:SER:HA	2.10	0.50
1:B:293:THR:O	1:B:297:VAL:HG23	2.12	0.50
1:B:29:His:HB2	1:B:33:VAL:HG13	1.92	0.50
1:A:93:ASN:ND2	1:A:96:PHE:HB2	2.27	0.49
1:A:293:THR:O	1:A:297:VAL:HG23	2.12	0.49
1:B:69:HIS:CE1	1:B:127:ARG:HH21	2.24	0.49
1:B:54:THR:HG21	1:B:90:TYR:CZ	2.47	0.49
1:A:54:THR:HG21	1:A:90:TYR:CZ	2.47	0.49
2:J:29:ASN:N	2:J:29:ASN:HD22	2.04	0.49
1:A:93:ASN:O	1:A:97:THR:CG2	2.56	0.49
1:A:133:THR:O	1:A:134:SER:CB	2.61	0.49
1:A:195:ILE:HG22	1:A:271:LEU:HD22	1.95	0.49
2:I:2:GLX:O	2:I:2:GLX:HG2	2.12	0.49
1:A:93:ASN:HD22	1:A:96:PHE:CB	2.26	0.49
1:A:203:LEU:HD11	1:A:246:THR:OG1	2.13	0.49
1:B:93:ASN:ND2	1:B:96:PHE:HB2	2.27	0.49
1:B:144:ASN:O	1:B:145:ARG:HD2	2.12	0.49
1:A:93:ASN:HD22	1:A:96:PHE:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:O	1:A:145:ARG:HD2	2.13	0.48
1:B:93:ASN:HD22	1:B:96:PHE:CB	2.26	0.48
2:J:2:GLX:O	2:J:2:GLX:HG2	2.12	0.48
2:I:9:ASN:HA	2:I:33:THR:CG2	2.34	0.48
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.44	0.48
1:B:93:ASN:HD22	1:B:96:PHE:HB2	1.78	0.48
1:B:195:ILE:HG21	1:B:271:LEU:HD21	1.96	0.48
1:B:133:THR:O	1:B:134:SER:CB	2.61	0.48
1:B:203:LEU:HD11	1:B:246:THR:OG1	2.13	0.48
1:A:195:ILE:HG21	1:A:271:LEU:HD21	1.96	0.48
2:I:31:ALA:O	2:I:33:THR:N	2.47	0.48
1:B:297:VAL:CG1	1:B:301:MET:HE2	2.43	0.48
1:B:203:LEU:HD12	1:B:241:GLY:O	2.14	0.48
2:J:14:THR:HB	2:J:16:ASP:HB3	1.95	0.48
1:A:203:LEU:HD12	1:A:241:GLY:O	2.14	0.47
2:J:9:ASN:HA	2:J:33:THR:CG2	2.34	0.47
1:A:8:ASN:O	1:A:11:THR:CG2	2.62	0.47
2:I:14:THR:HB	2:I:16:ASP:HB3	1.95	0.47
1:B:272:ARG:HD3	1:B:285:GLN:HE21	1.79	0.47
1:A:127:ARG:HH11	2:I:37:TYR:HB2	1.79	0.47
1:A:272:ARG:HD3	1:A:285:GLN:HE21	1.79	0.47
1:B:186:HIS:CD2	1:B:188:ASN:N	2.76	0.47
1:B:136:SER:OG	1:B:138:CYS:HB2	2.15	0.47
1:B:8:ASN:O	1:B:11:THR:CG2	2.62	0.47
1:B:69:HIS:HE2	1:B:127:ARG:HH21	1.54	0.47
1:B:127:ARG:HH11	2:J:37:TYR:HB2	1.78	0.47
1:B:195:ILE:HG22	1:B:271:LEU:HD22	1.95	0.47
1:B:205:PRO:HB2	1:B:213:ILE:HG21	1.97	0.47
1:A:144:ASN:C	1:A:145:ARG:HD2	2.35	0.47
2:J:31:ALA:O	2:J:33:THR:N	2.47	0.47
1:A:82:PHE:CE1	1:A:294:TRP:HB2	2.49	0.47
1:A:276:ARG:HG2	1:A:276:ARG:NH1	2.30	0.47
1:B:62:ILE:HD12	1:B:191:ALA:HB3	1.97	0.47
1:B:132:VAL:O	1:B:133:THR:CB	2.60	0.47
1:A:136:SER:OG	1:A:138:CYS:HB2	2.15	0.47
1:B:144:ASN:C	1:B:145:ARG:HD2	2.35	0.47
1:A:62:ILE:HD12	1:A:191:ALA:HB3	1.97	0.47
1:A:36:LEU:HB2	1:A:49:VAL:O	2.15	0.47
1:B:36:LEU:HB2	1:B:49:VAL:O	2.15	0.47
1:A:200:GLN:HB3	1:A:238:TYR:CD1	2.50	0.46
1:A:205:PRO:HB2	1:A:213:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:CG2	1:B:271:LEU:CD2	2.93	0.46
1:B:204:TYR:HB2	1:B:205:PRO:CD	2.44	0.46
1:A:277:TYR:CG	1:A:282:PRO:HD3	2.51	0.46
2:I:3:HIS:O	2:I:4:ALA:CB	2.61	0.46
2:I:5:ASP:OD2	2:I:21:ALA:CB	2.59	0.46
1:B:82:PHE:CE1	1:B:294:TRP:HB2	2.49	0.46
1:B:200:GLN:HB3	1:B:238:TYR:CD1	2.50	0.46
1:A:54:THR:HG21	1:A:90:TYR:CE1	2.51	0.46
1:A:4:THR:HG23	1:A:28:GLN:OE1	2.15	0.46
1:A:132:VAL:O	1:A:133:THR:CB	2.60	0.46
1:B:93:ASN:HA	1:B:94:PRO:HD2	1.64	0.46
1:B:136:SER:C	1:B:137:LEU:HD13	2.36	0.46
1:A:136:SER:C	1:A:137:LEU:HD13	2.36	0.46
1:B:95:SER:O	1:B:98:ALA:HB3	2.15	0.46
1:B:4:THR:HG23	1:B:28:GLN:OE1	2.15	0.46
1:B:54:THR:HG21	1:B:90:TYR:CE1	2.51	0.46
1:B:126:TRP:NE1	1:B:128:LYS:O	2.50	0.46
1:A:95:SER:O	1:A:98:ALA:HB3	2.15	0.45
2:I:31:ALA:O	2:I:33:THR:CB	2.63	0.45
1:A:287:ILE:HD13	1:A:287:ILE:N	2.32	0.45
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.79	0.45
1:B:271:LEU:HB3	1:B:272:ARG:H	1.63	0.45
1:A:36:LEU:O	1:A:49:VAL:N	2.40	0.45
2:I:29:ASN:N	2:I:29:ASN:ND2	2.63	0.45
1:B:287:ILE:HD13	1:B:287:ILE:N	2.31	0.45
1:A:126:TRP:NE1	1:A:128:LYS:O	2.50	0.45
1:A:168:LYS:HG3	1:A:169:TYR:CD2	2.51	0.45
2:I:21:ALA:C	2:I:23:PHE:N	2.70	0.45
1:B:220:ASN:O	1:B:223:ALA:HB3	2.16	0.45
1:B:171:ASN:HB3	1:B:177:LYS:HD3	1.99	0.45
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.75	0.45
1:A:13:HIS:HA	1:A:17:GLU:OE1	2.17	0.45
1:B:13:HIS:HA	1:B:17:GLU:OE1	2.17	0.45
1:B:277:TYR:CG	1:B:282:PRO:HD3	2.51	0.45
1:A:1:ALA:H1	1:A:7:PHE:HB2	1.81	0.45
1:A:198:TYR:O	1:A:199:SER:CB	2.65	0.45
1:A:220:ASN:O	1:A:223:ALA:HB3	2.16	0.45
1:A:297:VAL:CG1	1:A:301:MET:HE2	2.47	0.45
1:B:276:ARG:HG2	1:B:276:ARG:NH1	2.30	0.45
1:B:168:LYS:HG3	1:B:169:TYR:CD2	2.51	0.44
1:B:205:PRO:HG3	1:B:255:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:CG2	1:A:271:LEU:CD2	2.93	0.44
2:J:31:ALA:O	2:J:33:THR:CB	2.63	0.44
2:J:29:ASN:N	2:J:29:ASN:ND2	2.63	0.44
1:A:134:SER:C	1:A:136:SER:N	2.71	0.44
1:A:287:ILE:N	1:A:288:PRO:CD	2.81	0.44
1:B:290:ALA:HA	1:B:293:THR:CG2	2.48	0.44
1:A:76:GLN:HG3	1:A:109:ILE:O	2.18	0.44
1:A:290:ALA:HA	1:A:293:THR:CG2	2.48	0.44
1:B:186:HIS:NE2	1:B:188:ASN:HB3	2.33	0.44
2:J:5:ASP:OD2	2:J:21:ALA:CB	2.59	0.44
1:A:45:ARG:HH11	1:A:45:ARG:HD2	1.50	0.44
1:A:208:TYR:CD1	1:A:256:ASP:OD2	2.69	0.44
1:B:29:HIS:N	1:B:30:PRO:HD3	2.33	0.44
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.86	0.44
1:A:127:ARG:NH1	2:I:37:TYR:HB3	2.33	0.44
2:J:3:HIS:O	2:J:4:ALA:CB	2.61	0.44
1:A:186:HIS:NE2	1:A:188:ASN:HB3	2.33	0.43
1:B:127:ARG:NH1	2:J:37:TYR:HB3	2.33	0.43
1:A:171:ASN:HB3	1:A:177:LYS:HD3	1.99	0.43
1:B:76:GLN:HG3	1:B:109:ILE:O	2.18	0.43
1:B:134:SER:C	1:B:136:SER:N	2.71	0.43
1:B:198:TYR:O	1:B:199:SER:CB	2.65	0.43
1:A:194:SER:O	1:A:268:THR:HG23	2.19	0.43
1:A:205:PRO:HG3	1:A:255:ILE:HG23	2.00	0.43
1:B:287:ILE:HB	1:B:288:PRO:HD3	2.01	0.43
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.86	0.43
2:J:7:ILE:HG13	2:J:21:ALA:HB2	2.01	0.43
2:J:21:ALA:C	2:J:23:PHE:N	2.69	0.43
1:A:29:HIS:N	1:A:30:PRO:HD3	2.33	0.43
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.75	0.42
1:A:233:LEU:HD12	1:A:292:GLU:HA	2.01	0.42
1:B:57:SER:HB3	1:B:58:ASN:H	1.66	0.42
1:B:287:ILE:N	1:B:288:PRO:CD	2.81	0.42
1:B:220:ASN:O	1:B:224:LYS:N	2.52	0.42
1:B:247:ILE:HD13	1:B:247:ILE:HG21	1.85	0.42
1:A:142:ASP:HB2	1:A:163:GLU:O	2.20	0.42
1:A:159:SER:HA	1:A:160:PRO:HD3	1.75	0.42
1:B:142:ASP:HB2	1:B:163:GLU:O	2.19	0.42
1:A:287:ILE:HB	1:A:288:PRO:HD3	2.01	0.42
1:B:208:TYR:CD1	1:B:256:ASP:OD2	2.69	0.42
1:A:54:THR:H	1:A:59:ARG:HH22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:HB3	1:A:138:CYS:O	2.19	0.42
1:B:222:VAL:HG21	1:B:303:HIS:CG	2.55	0.42
2:I:7:ILE:HG13	2:I:21:ALA:HB2	2.01	0.42
1:B:233:LEU:HD12	1:B:292:GLU:HA	2.01	0.42
1:A:186:HIS:CD2	1:A:188:ASN:N	2.76	0.42
1:B:54:THR:H	1:B:59:ARG:HH22	1.68	0.42
1:A:276:ARG:O	2:J:22:TRP:CZ2	2.73	0.42
1:B:91:GLY:CA	1:B:97:THR:CG2	2.98	0.42
1:B:194:SER:O	1:B:268:THR:HG23	2.19	0.42
1:A:127:ARG:NH1	2:I:37:TYR:CB	2.83	0.42
1:A:247:ILE:HD13	1:A:247:ILE:HG21	1.85	0.42
1:B:136:SER:HB3	1:B:138:CYS:O	2.19	0.42
1:A:71:ARG:HH11	1:A:71:ARG:HD2	1.48	0.42
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.79	0.41
2:I:22:TRP:CZ2	1:B:276:ARG:O	2.73	0.41
1:A:287:ILE:N	1:A:287:ILE:CD1	2.84	0.41
1:B:155:GLY:HA3	1:B:251:SER:H	1.86	0.41
1:B:168:LYS:H	1:B:168:LYS:HG2	1.48	0.41
2:J:8:CYS:HA	2:J:24:CYS:CB	2.50	0.41
1:B:59:ARG:HA	1:B:60:PRO:HD3	1.76	0.41
1:B:141:VAL:HG21	1:B:173:GLU:OE2	2.21	0.41
1:A:91:GLY:CA	1:A:97:THR:CG2	2.98	0.41
1:A:290:ALA:HA	1:A:293:THR:HG22	2.03	0.41
1:B:277:TYR:O	1:B:278:GLY:C	2.59	0.41
2:I:8:CYS:HA	2:I:24:CYS:CB	2.50	0.41
1:A:222:VAL:HG21	1:A:303:HIS:CG	2.55	0.41
1:B:14:THR:O	1:B:15:LEU:C	2.59	0.41
1:A:155:GLY:HA3	1:A:251:SER:H	1.86	0.41
1:A:58:ASN:ND2	1:A:188:ASN:CB	2.84	0.41
1:A:141:VAL:HG21	1:A:173:GLU:OE2	2.21	0.41
1:A:220:ASN:O	1:A:224:LYS:N	2.52	0.40
1:A:239:LYS:HZ3	1:A:239:LYS:HG2	1.82	0.40
1:A:277:TYR:O	1:A:278:GLY:C	2.59	0.40
2:I:23:PHE:O	2:I:25:GLN:HG3	2.21	0.40
1:B:32:LEU:HD11	1:B:54:THR:HG22	2.02	0.40
1:B:287:ILE:N	1:B:287:ILE:CD1	2.83	0.40
1:A:198:TYR:CA	1:A:271:LEU:O	2.70	0.40
2:J:23:PHE:O	2:J:25:GLN:HG3	2.21	0.40
1:A:32:LEU:HD11	1:A:54:THR:HG22	2.02	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	305/307 (99%)	274 (90%)	27 (9%)	4 (1%)	12	21
1	B	305/307 (99%)	274 (90%)	27 (9%)	4 (1%)	12	21
2	I	35/38 (92%)	22 (63%)	6 (17%)	7 (20%)	0	0
2	J	35/38 (92%)	22 (63%)	6 (17%)	7 (20%)	0	0
All	All	680/690 (99%)	592 (87%)	66 (10%)	22 (3%)	4	5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	134	SER
1	A	199	SER
1	A	273	ASP
2	I	4	ALA
2	I	32	ARG
1	B	57	SER
1	B	134	SER
1	B	199	SER
1	B	273	ASP
2	J	4	ALA
2	J	32	ARG
2	I	19	SER
2	I	22	TRP
2	I	31	ALA
2	J	19	SER
2	J	22	TRP
2	J	31	ALA
2	I	30	SER
2	J	30	SER
2	I	13	LYS
2	J	13	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/263 (100%)	202 (77%)	61 (23%)	1	1
1	B	263/263 (100%)	202 (77%)	61 (23%)	1	1
2	I	30/30 (100%)	23 (77%)	7 (23%)	1	1
2	J	30/30 (100%)	23 (77%)	7 (23%)	1	1
All	All	586/586 (100%)	450 (77%)	136 (23%)	1	1

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	THR
1	A	7	PHE
1	A	14	THR
1	A	15	LEU
1	A	26	VAL
1	A	31	GLU
1	A	32	LEU
1	A	35	LYS
1	A	40	ARG
1	A	53	SER
1	A	57	SER
1	A	65	ASP
1	A	68	ILE
1	A	70	SER
1	A	71	ARG
1	A	74	ILE
1	A	87	THR
1	A	97	THR
1	A	100	LEU
1	A	102	SER
1	A	103	MET
1	A	109	ILE
1	A	122	GLU

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Mol	Chain	Res	Type
1	A	127	ARG
1	A	133	THR
1	A	136	SER
1	A	137	LEU
1	A	139	VAL
1	A	158	SER
1	A	162	SER
1	A	168	LYS
1	A	173	GLU
1	A	179	ILE
1	A	184	LYS
1	A	190	LYS
1	A	193	LEU
1	A	195	ILE
1	A	202	LEU
1	A	203	LEU
1	A	216	LYS
1	A	222	VAL
1	A	227	VAL
1	A	230	LEU
1	A	232	SER
1	A	239	LYS
1	A	244	ILE
1	A	245	THR
1	A	248	TYR
1	A	249	GLN
1	A	255	ILE
1	A	270	GLU
1	A	271	LEU
1	A	272	ARG
1	A	274	THR
1	A	281	LEU
1	A	287	ILE
1	A	292	GLU
1	A	295	LEU
1	A	298	LEU
1	A	307	ASN
2	I	7	ILE
2	I	10	LYS
2	I	13	LYS
2	I	14	THR
2	I	19	SER

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Mol	Chain	Res	Type
2	I	25	GLN
2	I	32	ARG
1	B	2	ARG
1	B	6	THR
1	B	7	PHE
1	B	14	THR
1	B	15	LEU
1	B	26	VAL
1	B	31	GLU
1	B	32	LEU
1	B	35	LYS
1	B	40	ARG
1	B	53	SER
1	B	57	SER
1	B	65	ASP
1	B	68	ILE
1	B	70	SER
1	B	71	ARG
1	B	74	ILE
1	B	87	THR
1	B	97	THR
1	B	100	LEU
1	B	102	SER
1	B	103	MET
1	B	109	ILE
1	B	122	GLU
1	B	127	ARG
1	B	133	THR
1	B	136	SER
1	B	137	LEU
1	B	139	VAL
1	B	158	SER
1	B	162	SER
1	B	168	LYS
1	B	173	GLU
1	B	179	ILE
1	B	184	LYS
1	B	190	LYS
1	B	193	LEU
1	B	195	ILE
1	B	202	LEU
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	216	LYS
1	B	222	VAL
1	B	227	VAL
1	B	230	LEU
1	B	232	SER
1	B	239	LYS
1	B	244	ILE
1	B	245	THR
1	B	248	TYR
1	B	249	GLN
1	B	255	ILE
1	B	270	GLU
1	B	271	LEU
1	B	272	ARG
1	B	274	THR
1	B	281	LEU
1	B	287	ILE
1	B	292	GLU
1	B	295	LEU
1	B	298	LEU
1	B	307	ASN
2	J	7	ILE
2	J	10	LYS
2	J	13	LYS
2	J	14	THR
2	J	19	SER
2	J	25	GLN
2	J	32	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	58	ASN
1	A	92	GLN
1	A	93	ASN
1	A	112	ASN
1	A	114	ASN
1	A	171	ASN
1	A	186	HIS
1	A	221	GLN
1	A	285	GLN

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Mol	Chain	Res	Type
2	I	9	ASN
2	I	25	GLN
2	I	29	ASN
1	B	29	HIS
1	B	58	ASN
1	B	92	GLN
1	B	93	ASN
1	B	112	ASN
1	B	114	ASN
1	B	171	ASN
1	B	186	HIS
1	B	221	GLN
1	B	285	GLN
2	J	9	ASN
2	J	25	GLN
2	J	29	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	GLY	B	308	-	4,4,4	1.26	1 (25%)	3,4,4	1.93	1 (33%)
3	GLY	A	308	-	4,4,4	1.27	1 (25%)	3,4,4	1.93	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	B	308	-	-	2/2/2/2	-
3	GLY	A	308	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	308	GLY	O-C	2.03	1.28	1.22
3	A	308	GLY	O-C	2.03	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	308	GLY	OXT-C-O	-3.30	115.06	123.30
3	A	308	GLY	OXT-C-O	-3.30	115.07	123.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	308	GLY	O-C-CA-N
3	B	308	GLY	O-C-CA-N
3	A	308	GLY	OXT-C-CA-N
3	B	308	GLY	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	308	GLY	1	0
3	A	308	GLY	1	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.