



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:34 PM GMT

PDB ID : 4CPA
Title : REFINED CRYSTAL STRUCTURE OF THE POTATO INHIBITOR COM-
PLEX 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

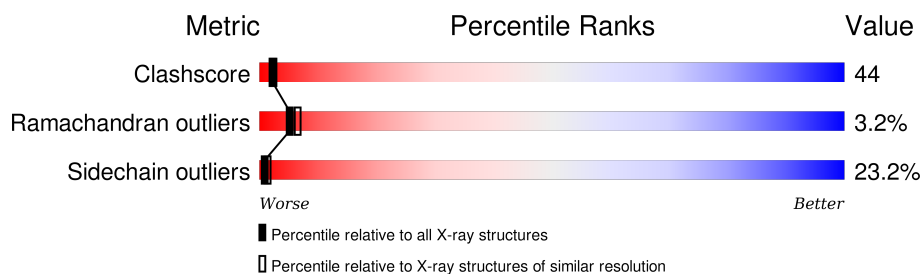
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	 31% 39% 21% 8%
1	B	307	 30% 40% 21% 9%
2	I	38	 21% 29% 34% 13% •
2	J	38	 21% 29% 34% 13% •

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
1	A	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			
1	B	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			

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
2	I	37	Total	C	N	O	S	X	0	0	0
			285	174	51	52	6	2			

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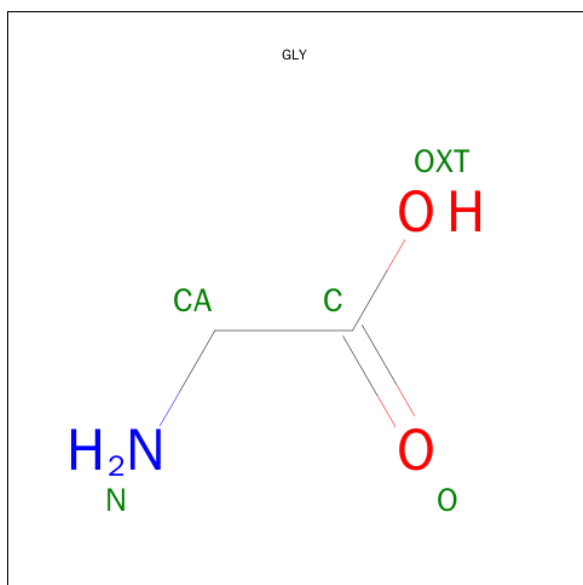
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	J	37	Total	C	N	O	S	X	0	0	0
			285	174	51	52	6	2			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



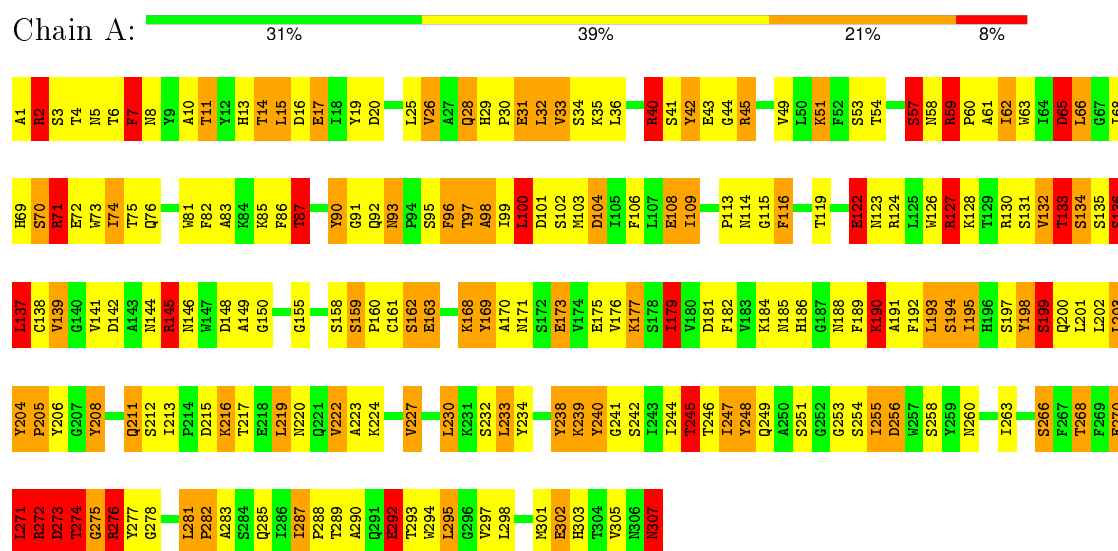
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	2	1	2		
4	B	1	Total	C	N	O	0	0
			5	2	1	2		

3 Residue-property plots

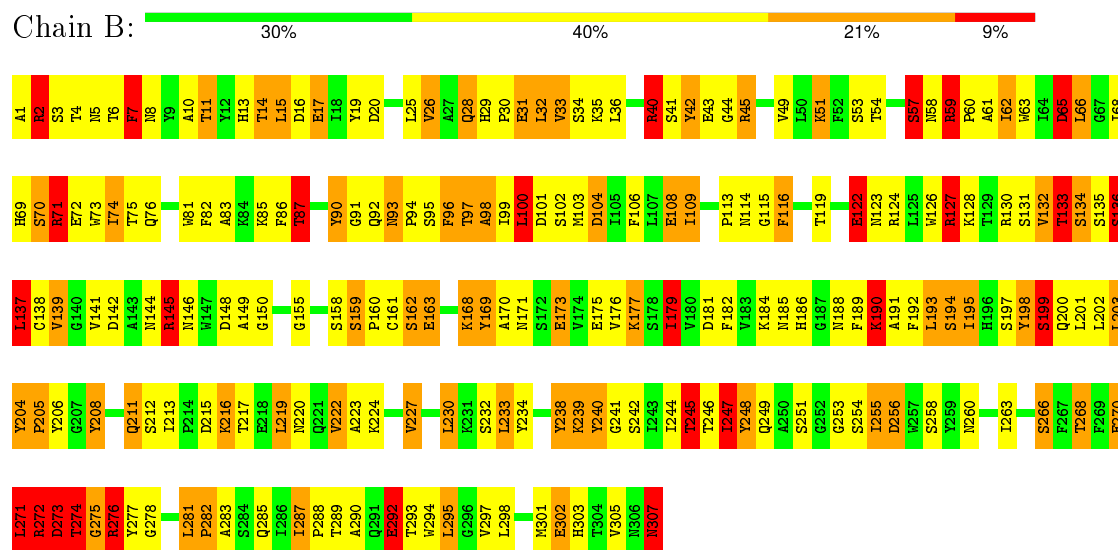
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

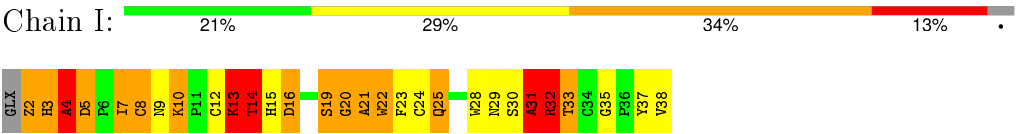
• Molecule 1: CARBOXYPEPTIDASE A



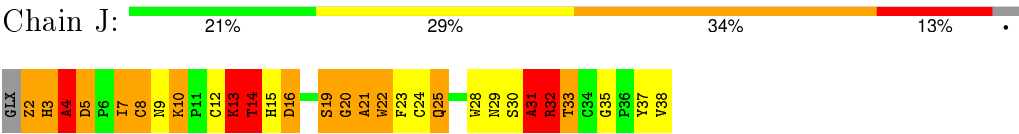
• Molecule 1: CARBOXYPEPTIDASE A



● Molecule 2: METALLOCARBOXYPEPTIDASE INHIBITOR



● Molecule 2: METALLOCARBOXYPEPTIDASE INHIBITOR



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtriage
Total number of atoms	5456	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	165/3402 (4.9%)
1	B	1.31	3/2503 (0.1%)	2.61	165/3402 (4.9%)
2	I	1.36	0/287	2.87	26/392 (6.6%)
2	J	1.35	0/287	2.87	26/392 (6.6%)
All	All	1.31	6/5580 (0.1%)	2.64	382/7588 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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	8.98	1.35	1.25
1	A	302	GLU	CD-OE2	8.95	1.35	1.25
1	B	292	GLU	CD-OE1	-5.92	1.19	1.25
1	A	292	GLU	CD-OE1	-5.92	1.19	1.25
1	A	57	SER	CB-OG	5.22	1.49	1.42
1	B	57	SER	CB-OG	5.19	1.49	1.42

All (382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH2	25.09	132.85	120.30
1	A	127	ARG	NE-CZ-NH2	25.07	132.84	120.30
1	B	2	ARG	CA-CB-CG	23.71	165.56	113.40
1	A	2	ARG	CA-CB-CG	23.70	165.53	113.40
1	B	40	ARG	NE-CZ-NH1	22.30	131.45	120.30
1	A	40	ARG	NE-CZ-NH1	22.23	131.41	120.30
1	A	273	ASP	CB-CG-OD1	21.57	137.72	118.30
1	B	273	ASP	CB-CG-OD1	21.55	137.70	118.30
1	A	136	SER	C-N-CA	19.22	169.74	121.70
1	B	136	SER	C-N-CA	19.20	169.70	121.70
1	A	273	ASP	CB-CG-OD2	-18.48	101.67	118.30
1	B	273	ASP	CB-CG-OD2	-18.46	101.68	118.30
2	J	5	ASP	CB-CG-OD1	16.43	133.09	118.30
2	I	5	ASP	CB-CG-OD1	16.39	133.05	118.30
1	B	71	ARG	NE-CZ-NH2	15.42	128.01	120.30
1	A	71	ARG	NE-CZ-NH2	15.42	128.01	120.30
1	A	71	ARG	NE-CZ-NH1	-15.22	112.69	120.30
1	B	71	ARG	NE-CZ-NH1	-15.19	112.70	120.30
1	A	127	ARG	NH1-CZ-NH2	-15.15	102.74	119.40
1	B	127	ARG	NH1-CZ-NH2	-15.13	102.75	119.40
1	A	208	TYR	CB-CG-CD1	14.34	129.61	121.00
1	B	208	TYR	CB-CG-CD1	14.29	129.57	121.00
1	A	40	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	B	40	ARG	NE-CZ-NH2	-13.96	113.32	120.30
2	I	32	ARG	NE-CZ-NH1	13.64	127.12	120.30
2	J	32	ARG	NE-CZ-NH1	13.63	127.11	120.30
2	J	5	ASP	CB-CG-OD2	-13.30	106.33	118.30
2	I	5	ASP	CB-CG-OD2	-13.26	106.37	118.30
1	A	45	ARG	NE-CZ-NH1	-12.83	113.89	120.30
1	B	45	ARG	NE-CZ-NH1	-12.81	113.89	120.30
1	B	101	ASP	CB-CG-OD1	12.27	129.34	118.30
1	A	101	ASP	CB-CG-OD1	12.20	129.28	118.30
1	A	272	ARG	C-N-CA	11.49	150.42	121.70
1	B	272	ARG	C-N-CA	11.46	150.36	121.70
1	A	276	ARG	NE-CZ-NH1	-10.77	114.92	120.30
1	B	276	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	A	130	ARG	NE-CZ-NH2	10.53	125.56	120.30
1	B	130	ARG	NE-CZ-NH2	10.47	125.54	120.30
2	I	32	ARG	CA-CB-CG	10.29	136.04	113.40
2	J	32	ARG	CA-CB-CG	10.29	136.04	113.40
1	B	130	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	A	130	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	A	240	TYR	CB-CG-CD1	-9.92	115.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	TYR	CB-CG-CD1	-9.87	115.08	121.00
1	B	20	ASP	CB-CG-OD1	9.85	127.17	118.30
1	A	20	ASP	CB-CG-OD1	9.84	127.15	118.30
1	B	248	TYR	CB-CG-CD1	9.82	126.89	121.00
1	A	248	TYR	CB-CG-CD1	9.81	126.89	121.00
1	B	208	TYR	CB-CG-CD2	-9.75	115.15	121.00
2	I	21	ALA	N-CA-CB	-9.70	96.52	110.10
1	A	208	TYR	CB-CG-CD2	-9.70	115.18	121.00
2	J	21	ALA	N-CA-CB	-9.69	96.54	110.10
1	B	145	ARG	NE-CZ-NH2	9.41	125.00	120.30
1	B	130	ARG	NH1-CZ-NH2	-9.40	109.06	119.40
1	A	130	ARG	NH1-CZ-NH2	-9.39	109.07	119.40
1	A	145	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	B	206	TYR	CB-CG-CD1	-9.29	115.43	121.00
1	A	206	TYR	CB-CG-CD1	-9.28	115.43	121.00
2	I	32	ARG	NH1-CZ-NH2	-8.88	109.63	119.40
2	J	32	ARG	NH1-CZ-NH2	-8.84	109.68	119.40
1	A	104	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	B	104	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	B	145	ARG	CD-NE-CZ	8.76	135.87	123.60
1	A	145	ARG	CD-NE-CZ	8.74	135.84	123.60
1	B	177	LYS	CA-CB-CG	8.73	132.60	113.40
1	A	177	LYS	CA-CB-CG	8.72	132.58	113.40
2	I	20	GLY	O-C-N	8.72	136.65	122.70
2	J	20	GLY	O-C-N	8.71	136.64	122.70
1	A	305	VAL	CA-CB-CG1	8.57	123.76	110.90
1	A	276	ARG	CA-CB-CG	8.55	132.22	113.40
1	B	276	ARG	CA-CB-CG	8.53	132.17	113.40
1	B	305	VAL	CA-CB-CG1	8.52	123.67	110.90
1	A	270	GLU	OE1-CD-OE2	8.44	133.43	123.30
1	B	270	GLU	OE1-CD-OE2	8.44	133.43	123.30
1	B	211	GLN	CG-CD-OE1	-8.43	104.73	121.60
1	B	124	ARG	CD-NE-CZ	8.42	135.39	123.60
1	A	211	GLN	CG-CD-OE1	-8.42	104.76	121.60
1	A	124	ARG	CD-NE-CZ	8.38	135.34	123.60
1	B	19	TYR	CB-CG-CD1	8.37	126.02	121.00
1	A	19	TYR	CB-CG-CD1	8.36	126.02	121.00
1	A	127	ARG	CB-CG-CD	8.36	133.34	111.60
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	59	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	B	137	LEU	C-N-CA	8.31	142.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	LEU	C-N-CA	8.29	142.43	121.70
1	B	59	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	17	GLU	CG-CD-OE1	8.01	134.32	118.30
1	B	17	GLU	CG-CD-OE1	8.00	134.30	118.30
1	A	59	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	124	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	B	305	VAL	CB-CA-C	7.93	126.47	111.40
1	A	247	ILE	CA-CB-CG1	7.91	126.02	111.00
1	B	247	ILE	CA-CB-CG1	7.91	126.03	111.00
1	A	305	VAL	CB-CA-C	7.90	126.42	111.40
1	A	124	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	B	247	ILE	N-CA-CB	7.75	128.63	110.80
1	A	247	ILE	N-CA-CB	7.74	128.59	110.80
1	A	17	GLU	CG-CD-OE2	-7.73	102.83	118.30
1	B	17	GLU	CG-CD-OE2	-7.72	102.86	118.30
1	A	161	CYS	CA-CB-SG	-7.71	100.11	114.00
1	B	161	CYS	CA-CB-SG	-7.69	100.16	114.00
1	A	302	GLU	CB-CG-CD	7.67	134.90	114.20
1	B	302	GLU	CB-CG-CD	7.64	134.84	114.20
1	B	227	VAL	CA-CB-CG1	7.63	122.35	110.90
1	A	227	VAL	CA-CB-CG1	7.63	122.35	110.90
1	A	282	PRO	O-C-N	-7.54	110.64	122.70
1	B	282	PRO	O-C-N	-7.53	110.66	122.70
1	A	116	PHE	CB-CG-CD1	-7.50	115.55	120.80
1	B	90	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	127	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	199	SER	N-CA-CB	7.45	121.68	110.50
1	B	2	ARG	N-CA-CB	7.43	123.98	110.60
1	B	271	LEU	CA-CB-CG	7.43	132.40	115.30
1	A	199	SER	N-CA-CB	7.43	121.64	110.50
1	B	116	PHE	CB-CG-CD1	-7.42	115.60	120.80
1	A	90	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	A	271	LEU	CA-CB-CG	7.42	132.36	115.30
1	B	127	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	2	ARG	N-CA-CB	7.40	123.93	110.60
1	A	161	CYS	O-C-N	7.39	134.53	122.70
1	B	211	GLN	OE1-CD-NE2	7.39	138.91	121.90
1	B	161	CYS	O-C-N	7.39	134.53	122.70
1	A	211	GLN	OE1-CD-NE2	7.38	138.88	121.90
1	A	248	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	A	133	THR	CB-CA-C	-7.31	91.87	111.60
1	B	248	TYR	CB-CG-CD2	-7.30	116.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	THR	CB-CA-C	-7.30	91.89	111.60
1	A	133	THR	N-CA-CB	7.22	124.01	110.30
1	B	133	THR	N-CA-CB	7.21	124.01	110.30
1	A	302	GLU	OE1-CD-OE2	-7.20	114.66	123.30
1	B	302	GLU	OE1-CD-OE2	-7.19	114.67	123.30
1	B	65	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	260	ASN	CA-CB-CG	7.14	129.12	113.40
1	B	260	ASN	CA-CB-CG	7.13	129.10	113.40
2	J	5	ASP	CA-CB-CG	-7.11	97.75	113.40
2	I	5	ASP	CA-CB-CG	-7.09	97.80	113.40
1	A	179	ILE	O-C-N	7.09	134.04	122.70
1	A	11	THR	CA-CB-CG2	-7.08	102.49	112.40
1	B	179	ILE	O-C-N	7.08	134.03	122.70
1	A	65	ASP	CB-CG-OD1	7.06	124.66	118.30
1	B	11	THR	CA-CB-CG2	-7.06	102.52	112.40
1	A	136	SER	O-C-N	-7.03	111.45	122.70
1	B	136	SER	O-C-N	-7.02	111.47	122.70
1	A	45	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	A	272	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	96	PHE	N-CA-CB	6.93	123.07	110.60
1	B	96	PHE	N-CA-CB	6.92	123.06	110.60
1	B	45	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	B	136	SER	CA-C-O	6.83	134.44	120.10
1	A	136	SER	CA-C-O	6.83	134.44	120.10
1	B	272	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	2	ARG	NE-CZ-NH2	6.75	123.67	120.30
2	I	28	TRP	CA-C-O	-6.74	105.94	120.10
1	B	2	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	268	THR	N-CA-CB	6.73	123.08	110.30
2	J	28	TRP	CA-C-O	-6.72	105.98	120.10
1	B	268	THR	N-CA-CB	6.71	123.05	110.30
1	B	276	ARG	CD-NE-CZ	-6.69	114.24	123.60
1	A	276	ARG	CD-NE-CZ	-6.69	114.24	123.60
1	A	302	GLU	CA-CB-CG	6.68	128.09	113.40
1	B	198	TYR	CZ-CE2-CD2	-6.67	113.80	119.80
1	B	302	GLU	CA-CB-CG	6.66	128.06	113.40
1	A	198	TYR	CZ-CE2-CD2	-6.66	113.81	119.80
1	A	42	TYR	CA-CB-CG	-6.66	100.75	113.40
1	B	42	TYR	CA-CB-CG	-6.65	100.76	113.40
1	B	59	ARG	NH1-CZ-NH2	6.65	126.72	119.40
1	A	59	ARG	NH1-CZ-NH2	6.65	126.71	119.40
1	A	185	ASN	O-C-N	6.63	133.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	O-C-N	6.62	133.30	122.70
1	A	198	TYR	CG-CD2-CE2	6.58	126.56	121.30
2	J	13	LYS	C-N-CA	6.57	138.12	121.70
2	I	13	LYS	C-N-CA	6.55	138.09	121.70
1	B	275	GLY	CA-C-O	-6.55	108.81	120.60
1	A	11	THR	CA-CB-OG1	6.55	122.76	109.00
1	B	198	TYR	CG-CD2-CE2	6.55	126.54	121.30
1	B	11	THR	CA-CB-OG1	6.54	122.74	109.00
1	A	275	GLY	CA-C-O	-6.54	108.82	120.60
1	B	90	TYR	CB-CG-CD2	6.53	124.92	121.00
1	A	148	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	148	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	175	GLU	O-C-N	6.50	133.09	122.70
1	B	245	THR	CA-CB-CG2	6.49	121.49	112.40
1	A	245	THR	CA-CB-CG2	6.46	121.45	112.40
1	A	175	GLU	O-C-N	6.46	133.04	122.70
1	A	206	TYR	CB-CG-CD2	6.45	124.87	121.00
1	B	206	TYR	CB-CG-CD2	6.45	124.87	121.00
1	B	137	LEU	CA-C-O	6.44	133.63	120.10
1	A	90	TYR	CB-CG-CD2	6.44	124.86	121.00
1	A	137	LEU	CA-C-O	6.44	133.62	120.10
1	A	248	TYR	CA-CB-CG	6.41	125.58	113.40
1	B	276	ARG	CB-CA-C	-6.41	97.59	110.40
1	A	276	ARG	CB-CA-C	-6.40	97.60	110.40
1	B	248	TYR	CA-CB-CG	6.39	125.55	113.40
1	B	194	SER	N-CA-CB	6.35	120.02	110.50
1	A	194	SER	N-CA-CB	6.33	119.99	110.50
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
2	J	14	THR	CA-CB-CG2	6.27	121.17	112.40
1	A	28	GLN	O-C-N	-6.26	112.69	122.70
1	A	122	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	B	182	PHE	CG-CD1-CE1	-6.25	113.93	120.80
1	B	122	GLU	OE1-CD-OE2	-6.24	115.81	123.30
2	J	15	HIS	CA-C-O	6.24	133.21	120.10
1	B	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	A	271	LEU	CB-CG-CD1	6.24	121.61	111.00
1	B	137	LEU	N-CA-CB	-6.24	97.92	110.40
2	I	15	HIS	CA-C-O	6.23	133.19	120.10
1	B	205	PRO	O-C-N	-6.23	112.73	122.70
1	A	205	PRO	O-C-N	-6.21	112.76	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	LEU	CB-CG-CD1	6.21	121.56	111.00
2	I	33	THR	CA-CB-CG2	6.20	121.07	112.40
2	J	33	THR	CA-CB-CG2	6.16	121.02	112.40
1	B	163	GLU	OE1-CD-OE2	6.13	130.65	123.30
1	A	163	GLU	OE1-CD-OE2	6.11	130.63	123.30
2	I	20	GLY	CA-C-N	-6.09	103.80	117.20
2	J	20	GLY	CA-C-N	-6.08	103.82	117.20
1	A	133	THR	O-C-N	6.08	132.43	122.70
1	B	133	THR	O-C-N	6.08	132.42	122.70
1	B	16	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	B	234	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	16	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	16	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	132	VAL	O-C-N	-5.91	113.24	122.70
1	A	16	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	A	7	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	234	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	65	ASP	CA-CB-CG	5.89	126.36	113.40
1	A	65	ASP	CA-CB-CG	5.88	126.34	113.40
1	B	132	VAL	O-C-N	-5.88	113.29	122.70
2	J	16	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	273	ASP	C-N-CA	5.86	136.34	121.70
1	B	273	ASP	C-N-CA	5.86	136.34	121.70
1	B	7	PHE	CB-CG-CD1	-5.84	116.71	120.80
2	I	16	ASP	CB-CG-OD2	-5.84	113.05	118.30
2	I	35	GLY	N-CA-C	-5.83	98.54	113.10
1	A	137	LEU	CA-CB-CG	5.82	128.68	115.30
2	J	35	GLY	N-CA-C	-5.82	98.56	113.10
1	B	137	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	190	LYS	N-CA-CB	5.80	121.04	110.60
1	B	33	VAL	CA-CB-CG2	5.79	119.59	110.90
1	B	190	LYS	N-CA-CB	5.78	121.01	110.60
1	A	33	VAL	CA-CB-CG2	5.78	119.57	110.90
1	B	276	ARG	CG-CD-NE	-5.78	99.66	111.80
2	I	32	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	A	7	PHE	CB-CG-CD2	5.77	124.84	120.80
1	B	31	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	B	185	ASN	CB-CA-C	-5.76	98.87	110.40
1	A	185	ASN	CB-CA-C	-5.76	98.87	110.40
1	A	276	ARG	CG-CD-NE	-5.76	99.70	111.80
2	J	16	ASP	N-CA-CB	-5.76	100.23	110.60
2	I	16	ASP	N-CA-CB	-5.76	100.24	110.60

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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	100	LEU	CB-CG-CD1	-5.74	101.23	111.00
1	A	31	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	B	33	VAL	C-N-CA	5.72	136.00	121.70
1	A	33	VAL	C-N-CA	5.71	135.98	121.70
1	B	7	PHE	CB-CG-CD2	5.71	124.80	120.80
1	A	254	SER	C-N-CA	5.69	135.91	121.70
1	B	254	SER	C-N-CA	5.68	135.91	121.70
2	J	32	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	5	ASN	OD1-CG-ND2	5.67	134.95	121.90
1	A	5	ASN	OD1-CG-ND2	5.65	134.90	121.90
2	J	8	CYS	CA-C-O	-5.62	108.29	120.10
1	B	44	GLY	N-CA-C	5.61	127.14	113.10
1	A	44	GLY	N-CA-C	5.61	127.11	113.10
1	A	28	GLN	CB-CA-C	5.60	121.61	110.40
1	A	270	GLU	CG-CD-OE2	-5.60	107.10	118.30
2	I	8	CYS	CA-C-O	-5.60	108.33	120.10
1	B	31	GLU	CG-CD-OE1	5.60	129.50	118.30
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	28	GLN	CB-CA-C	5.59	121.58	110.40
1	B	270	GLU	CG-CD-OE2	-5.59	107.12	118.30
1	B	96	PHE	CA-C-O	-5.58	108.38	120.10
1	B	240	TYR	CB-CG-CD2	5.58	124.35	121.00
1	A	240	TYR	CB-CG-CD2	5.55	124.33	121.00
1	A	93	ASN	CA-CB-CG	5.53	125.56	113.40
1	B	93	ASN	CA-CB-CG	5.52	125.55	113.40
2	J	33	THR	CA-C-N	5.51	129.33	117.20
2	I	33	THR	CA-C-N	5.50	129.31	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	J	31	ALA	N-CA-CB	5.48	117.78	110.10
2	I	31	ALA	N-CA-CB	5.47	117.76	110.10
1	B	16	ASP	OD1-CG-OD2	5.47	133.69	123.30
1	B	274	THR	N-CA-CB	5.47	120.69	110.30
1	A	274	THR	N-CA-CB	5.46	120.68	110.30
1	A	16	ASP	OD1-CG-OD2	5.46	133.67	123.30
2	I	4	ALA	O-C-N	5.45	131.42	122.70
1	B	275	GLY	CA-C-N	5.45	129.19	117.20
1	A	275	GLY	CA-C-N	5.45	129.18	117.20
2	J	4	ALA	O-C-N	5.43	131.38	122.70
1	B	169	TYR	CB-CA-C	5.42	121.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	TYR	CB-CA-C	5.42	121.23	110.40
2	I	16	ASP	CB-CA-C	5.41	121.21	110.40
1	A	177	LYS	CG-CD-CE	5.39	128.06	111.90
1	B	177	LYS	CG-CD-CE	5.38	128.05	111.90
2	J	16	ASP	CB-CA-C	5.38	121.16	110.40
1	A	230	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	B	230	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	B	104	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	104	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	98	ALA	C-N-CA	5.34	135.06	121.70
1	B	66	LEU	CB-CA-C	5.34	120.35	110.20
1	A	98	ALA	C-N-CA	5.34	135.05	121.70
1	B	10	ALA	C-N-CA	5.33	135.04	121.70
1	A	10	ALA	C-N-CA	5.33	135.03	121.70
1	A	66	LEU	CB-CA-C	5.33	120.32	110.20
1	A	181	ASP	C-N-CA	5.32	135.01	121.70
1	A	57	SER	C-N-CA	5.32	135.00	121.70
1	A	133	THR	CA-C-N	-5.32	105.50	117.20
1	B	57	SER	C-N-CA	5.32	135.00	121.70
1	B	133	THR	CA-C-N	-5.32	105.50	117.20
1	B	181	ASP	C-N-CA	5.32	135.00	121.70
1	A	113	PRO	C-N-CA	5.31	134.97	121.70
2	I	35	GLY	O-C-N	5.30	131.18	121.10
1	B	113	PRO	C-N-CA	5.30	134.96	121.70
1	A	256	ASP	CA-CB-CG	-5.30	101.74	113.40
2	J	35	GLY	O-C-N	5.30	131.17	121.10
1	B	256	ASP	CA-CB-CG	-5.29	101.77	113.40
1	B	108	GLU	C-N-CA	5.28	134.89	121.70
1	A	116	PHE	CB-CG-CD2	5.27	124.49	120.80
2	I	3	HIS	N-CA-CB	5.27	120.08	110.60
1	A	108	GLU	C-N-CA	5.26	134.86	121.70
2	J	3	HIS	N-CA-CB	5.23	120.02	110.60
1	A	217	THR	CA-CB-CG2	5.22	119.71	112.40
1	A	59	ARG	CD-NE-CZ	5.20	130.89	123.60
1	B	266	SER	O-C-N	5.20	131.03	122.70
1	A	204	TYR	CB-CG-CD2	5.20	124.12	121.00
1	B	217	THR	CA-CB-CG2	5.20	119.68	112.40
1	A	266	SER	O-C-N	5.20	131.01	122.70
1	B	65	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	185	ASN	N-CA-CB	5.19	119.94	110.60
1	B	270	GLU	CA-C-O	-5.19	109.21	120.10
1	A	270	GLU	CA-C-O	-5.18	109.22	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	87	THR	O-C-N	-5.18	114.41	122.70
1	B	204	TYR	CB-CG-CD2	5.18	124.11	121.00
1	B	59	ARG	CD-NE-CZ	5.18	130.85	123.60
1	B	185	ASN	N-CA-CB	5.18	119.92	110.60
1	B	87	THR	O-C-N	-5.17	114.42	122.70
1	B	116	PHE	CB-CG-CD2	5.17	124.42	120.80
1	A	233	LEU	N-CA-CB	-5.17	100.07	110.40
1	B	179	ILE	CB-CA-C	-5.16	101.28	111.60
1	A	179	ILE	CB-CA-C	-5.15	101.29	111.60
1	B	34	SER	CB-CA-C	-5.15	100.32	110.10
1	B	233	LEU	N-CA-CB	-5.14	100.11	110.40
1	B	292	GLU	CA-CB-CG	5.14	124.72	113.40
1	A	34	SER	CB-CA-C	-5.14	100.33	110.10
1	B	73	TRP	CA-C-O	-5.14	109.31	120.10
1	A	73	TRP	CA-C-O	-5.14	109.31	120.10
1	B	179	ILE	N-CA-CB	5.12	122.59	110.80
1	A	292	GLU	CA-CB-CG	5.12	124.67	113.40
1	A	179	ILE	N-CA-CB	5.11	122.55	110.80
1	B	137	LEU	O-C-N	-5.10	114.53	122.70
1	A	2	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	2	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	247	ILE	CB-CA-C	-5.09	101.41	111.60
1	A	137	LEU	O-C-N	-5.09	114.55	122.70
1	B	159	SER	CA-CB-OG	-5.09	97.46	111.20
1	A	247	ILE	CB-CA-C	-5.09	101.42	111.60
1	A	159	SER	CA-CB-OG	-5.09	97.47	111.20
1	A	219	LEU	CB-CA-C	5.08	119.86	110.20
1	A	193	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	193	LEU	CA-CB-CG	5.07	126.97	115.30
1	B	219	LEU	CB-CA-C	5.07	119.84	110.20
2	J	12	CYS	N-CA-CB	-5.07	101.48	110.60
1	A	307	ASN	CA-C-O	-5.06	109.48	120.10
1	B	282	PRO	C-N-CA	5.05	134.34	121.70
2	I	12	CYS	N-CA-CB	-5.05	101.50	110.60
1	B	307	ASN	CA-C-O	-5.05	109.50	120.10
1	A	43	GLU	C-N-CA	5.04	132.88	122.30
1	B	51	LYS	C-N-CA	5.04	134.29	121.70
1	B	43	GLU	C-N-CA	5.04	132.87	122.30
1	B	62	ILE	CA-C-O	-5.03	109.53	120.10
1	A	282	PRO	C-N-CA	5.03	134.27	121.70
1	B	253	GLY	C-N-CA	5.03	134.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ILE	CA-C-O	-5.03	109.55	120.10
1	A	51	LYS	C-N-CA	5.02	134.25	121.70
1	A	253	GLY	C-N-CA	5.02	134.25	121.70

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	198	0
1	B	2437	0	2350	199	0
2	I	285	0	243	45	0
2	J	285	0	243	45	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	5	0	2	1	0
4	B	5	0	2	1	0
All	All	5456	0	5190	469	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 (469) 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	1.19
1:A:134:SER:HB3	1:A:136:SER:HB2	1.25	1.16
1:B:136:SER:HA	1:B:137:LEU:HD22	1.32	1.10
1:B:208:TYR:HB3	1:B:251:SER:HA	1.31	1.08
1:B:60:PRO:HB3	1:B:190:LYS:HD2	1.33	1.08
1:A:208:TYR:HB3	1:A:251:SER:HA	1.31	1.06
1:A:136:SER:HA	1:A:137:LEU:HD22	1.32	1.06
1:A:60:PRO:HB3	1:A:190:LYS:HD2	1.33	1.05
2:J:21:ALA:O	2:J:23:PHE:N	1.97	0.98
2:I:21:ALA:O	2:I:23:PHE:N	1.97	0.98
1:A:74:ILE:HD13	1:A:281:LEU:HD12	1.44	0.97
1:B:74:ILE:HD13	1:B:281:LEU:HD12	1.45	0.96
2:I:5:ASP:CG	2:I:21:ALA:HB1	1.86	0.96
2:J:5:ASP:CG	2:J:21:ALA:HB1	1.86	0.96
1:A:74:ILE:HD13	1:A:281:LEU:CD1	1.96	0.94
1:B:74:ILE:HD13	1:B:281:LEU:CD1	1.96	0.94
2:J:9:ASN:HA	2:J:33:THR:HG23	1.51	0.93
2:I:9:ASN:HA	2:I:33:THR:HG23	1.51	0.93
1:B:134:SER:CB	1:B:136:SER:HB2	1.98	0.92
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	0.91
1:B:289:THR:O	1:B:293:THR:HG22	1.70	0.91
1:A:289:THR:O	1:A:293:THR:HG22	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:HIS:HD2	1:B:188:ASN:H	1.11	0.90
1:A:283:ALA:HB3	1:B:122:GLU:HG3	1.51	0.90
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:I:5:ASP:OD2	2:I:21:ALA:O	1.92	0.87
1:B:171:ASN:O	1:B:177:LYS:HE2	1.75	0.87
2:J:5:ASP:OD1	2:J:21:ALA:HB1	1.73	0.86
1:A:171:ASN:O	1:A:177:LYS:HE2	1.75	0.86
1:A:92:GLN:NE2	1:A:92:GLN:HA	1.90	0.86
1:A:136:SER:HA	1:A:137:LEU:CD2	2.05	0.86
2:I:5:ASP:OD1	2:I:21:ALA:HB1	1.73	0.86
1:A:283:ALA:HB2	1:B:122:GLU:HA	1.58	0.86
1:B:136:SER:HA	1:B:137:LEU:CD2	2.05	0.85
1:B:92:GLN:NE2	1:B:92:GLN:HA	1.90	0.85
1:A:245:THR:HG22	1:A:246:THR:CG2	2.08	0.84
1:A:245:THR:HG22	1:A:246:THR:HG23	1.60	0.83
1:B:245:THR:HG22	1:B:246:THR:CG2	2.08	0.83
1:A:122:GLU:HA	1:B:283:ALA:HB2	1.60	0.82
2:J:5:ASP:OD2	2:J:21:ALA:HB1	1.80	0.82
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:I:5:ASP:OD2	2:I:21:ALA:HB1	1.80	0.80
2:I:31:ALA:HA	2:I:32:ARG:NH1	1.95	0.80
1:B:93:ASN:O	1:B:97:THR:HG23	1.82	0.80
1:A:93:ASN:O	1:A:97:THR:HG23	1.82	0.80
1:A:208:TYR:CB	1:A:251:SER:HA	2.13	0.79
1:A:131:SER:O	1:A:139:VAL:HG23	1.83	0.79
1:A:134:SER:HB3	1:A:136:SER:CB	2.09	0.78
1:B:131:SER:O	1:B:139:VAL:HG23	1.83	0.78
1:B:186:HIS:CD2	1:B:188:ASN:H	1.99	0.77
2:J:5:ASP:HB3	2:J:8:CYS:SG	2.24	0.77
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
1:A:91:GLY:H	1:A:97:THR:HG22	1.48	0.77
1:B:208:TYR:CB	1:B:251:SER:HA	2.13	0.76
1:A:186:HIS:CD2	1:A:188:ASN:H	1.99	0.75
2:J:7:ILE:HD12	2:J:20:GLY:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:HG13	1:B: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:26:VAL:HG13	1:A:33:VAL:HG23	1.68	0.74
2:I:31:ALA:CA	2:I:32:ARG:NH1	2.51	0.74
1:A:224:LYS:HD2	1:A:240:TYR:OH	1.88	0.74
1:A:159:SER:O	1:A:162:SER:HB2	1.88	0.73
1:B:224:LYS:HD2	1:B:240:TYR:OH	1.88	0.73
1:B:136:SER:CA	1:B:137:LEU:HD22	2.16	0.73
1:B:297:VAL:HG12	1:B:301:MET:HE3	1.71	0.73
1:B:159:SER:O	1:B:162:SER:HB2	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:A:297:VAL:HG12	1:A:301:MET:CE	2.19	0.72
1:B:297:VAL:O	1:B:301:MET:HG3	1.90	0.71
1:B:297:VAL:HG12	1:B:301:MET:CE	2.19	0.71
1:A:303:HIS:O	1:A:307:ASN:ND2	2.23	0.71
1:A:297:VAL:HG12	1:A:301:MET:HE3	1.72	0.71
1:A:297:VAL:O	1:A:301:MET:HG3	1.90	0.71
1:B:303:HIS:O	1:B:307:ASN:ND2	2.23	0.71
1:A:26:VAL:HA	1:A:33:VAL:HG22	1.72	0.71
2:J:32:ARG:H	2:J:32:ARG:HH11	1.40	0.70
2:I:32:ARG:H	2:I:32:ARG:HH11	1.40	0.70
1:A:83:ALA:O	1:A:87:THR:HG23	1.92	0.70
2:J:5:ASP:OD1	2:J:21:ALA:CB	2.40	0.70
2:I:31:ALA:CA	2:I:32:ARG:HH11	2.05	0.70
1:A:273:ASP:OD2	1:A:274:THR:N	2.22	0.70
2:I:5:ASP:OD1	2:I:21:ALA:CB	2.40	0.69
2:J:31:ALA:CA	2:J:32:ARG:HH11	2.05	0.69
1:B:83:ALA:O	1:B:87:THR:HG23	1.92	0.69
1:A:136:SER:CA	1:A:137:LEU:HD22	2.16	0.69
1:A:119:THR:HA	1:A:123:ASN:O	1.94	0.68
2:J:7:ILE:O	2:J:10:LYS:HB3	1.94	0.68
1:B:213:ILE:O	1:B:216:LYS:HB2	1.94	0.68
2:I:32:ARG:N	2:I:32:ARG:HH11	1.92	0.68
1:B:119:THR:HA	1:B:123:ASN:O	1.94	0.68
1:B:273:ASP:OD2	1:B:274:THR:N	2.22	0.68
1:A:3:SER:HA	1:A:28:GLN:HE22	1.59	0.68
1:B:91:GLY:N	1:B:97:THR:HG22	2.09	0.67
1:A:91:GLY:N	1:A:97:THR:HG22	2.09	0.67
1:B:3:SER:HA	1:B:28:GLN:HE22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:ALA:HA	2:J:32:ARG:HH12	1.59	0.67
2:J:32:ARG:N	2:J:32:ARG:HH11	1.92	0.67
2:I:31:ALA:O	2:I:33:THR:HB	1.95	0.67
1:A:213:ILE:O	1:A:216:LYS:HB2	1.94	0.67
2:I:9:ASN:HD21	2:J:3:HIS:H	1.42	0.67
2:I:31:ALA:HA	2:I:32:ARG:HH12	1.59	0.67
2:J:31:ALA:O	2:J:33:THR:HB	1.95	0.67
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.60	0.66
2:I:7:ILE:O	2:I:10:LYS:HB3	1.94	0.66
1:B:26:VAL:HG13	1:B:33:VAL:CG2	2.25	0.66
1:A:192:PHE:O	1:A:266:SER:HA	1.95	0.66
2:I:3:HIS:H	2:J:9:ASN:HD21	1.44	0.66
1:A:70:SER:HB3	1:A:116:PHE:N	2.11	0.66
1:B:273:ASP:OD2	1:B:275:GLY:N	2.27	0.66
1:A:26:VAL:HG13	1:A:33:VAL:CG2	2.25	0.66
1:B:58:ASN:HD21	1:B:188:ASN:HB2	1.60	0.65
1:A:179:ILE:N	1:A:179:ILE:HD12	2.10	0.65
1:B:192:PHE:O	1:B:266:SER:HA	1.95	0.65
1:B:70:SER:HB3	1:B:116:PHE:N	2.11	0.65
1:B:179:ILE:HD12	1:B:179:ILE:N	2.10	0.65
1:A:283:ALA:CB	1:B:122:GLU:HA	2.28	0.64
1:B:201:LEU:HA	1:B:239:LYS:O	1.97	0.64
1:A:201:LEU:HA	1:A:239:LYS:O	1.97	0.64
1:A:81:TRP:CH2	1:A:85:LYS:HD3	2.32	0.64
1:B:81:TRP:CH2	1:B:85:LYS:HD3	2.32	0.64
1:A:91:GLY:HA2	1:A:97:THR:HG21	1.81	0.63
1:B:149:ALA:HB1	1:B:256:ASP:HB3	1.80	0.63
1:A:149:ALA:HB1	1:A:256:ASP:HB3	1.80	0.63
1:A:273:ASP:OD2	1:A:275:GLY:N	2.27	0.63
1:A:179:ILE:H	1:A:179:ILE:CD1	2.12	0.63
1:B:69:HIS:NE2	1:B:127:ARG:NH2	2.46	0.62
2:J:21:ALA:O	2:J:22:TRP:CD1	2.52	0.62
2:I:21:ALA:O	2:I:22:TRP:CD1	2.52	0.62
1:B:91:GLY:HA2	1:B:97:THR:HG21	1.81	0.62
1:B:179:ILE:CD1	1:B:179:ILE:H	2.12	0.62
1:B:69:HIS:CE1	1:B:127:ARG:NH2	2.68	0.62
1:B:51:LYS:HG3	1:B:106:PHE:CZ	2.35	0.62
1:A:122:GLU:HA	1:B:283:ALA:CB	2.29	0.61
1:A:69:HIS:CE1	1:A:127:ARG:NH2	2.68	0.61
2:I:7:ILE:HB	2:I:21:ALA:HB2	1.82	0.61
1:A:69:HIS:NE2	1:A:127:ARG:NH2	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:CD1	1:B:219:LEU:HD22	2.31	0.61
1:A:213:ILE:CD1	1:A:219:LEU:HD22	2.31	0.60
1:A:51:LYS:HG3	1:A:106:PHE:CZ	2.35	0.60
1:A:91:GLY:N	1:A:97:THR:CG2	2.64	0.60
1:A:42:TYR:C	1:A:42:TYR:CD2	2.75	0.60
1:A:146:ASN:O	1:A:170:ALA:HA	2.01	0.60
1:B:42:TYR:CD2	1:B:42:TYR:C	2.75	0.60
1:B:146:ASN:O	1:B:170:ALA:HA	2.01	0.60
2:I:3:HIS:O	2:I:4:ALA:HB2	2.01	0.60
2:J:3:HIS:O	2:J:4:ALA:HB2	2.01	0.60
1:B:91:GLY:CA	1:B:97:THR:HG21	2.31	0.59
1:B:171:ASN:O	1:B:177:LYS:CE	2.49	0.59
1:A:186:HIS:HD2	1:A:188:ASN:N	1.92	0.59
2:J:7:ILE:HB	2:J:21:ALA:HB2	1.82	0.59
1:B:211:GLN:HG2	1:B:212:SER:N	2.18	0.59
1:A:63:TRP:HB2	1:A:189:PHE:CE2	2.38	0.59
1:A:91:GLY:CA	1:A:97:THR:HG21	2.31	0.59
1:A:233:LEU:CD1	1:A:295:LEU:HD22	2.33	0.59
1:A:211:GLN:HG2	1:A:212:SER:N	2.18	0.59
1:A:242:SER:OG	1:A:245:THR:HB	2.03	0.59
1:B:63:TRP:HB2	1:B:189:PHE:CE2	2.38	0.59
1:B:66:LEU:N	1:B:108:GLU:O	2.36	0.59
1:B:242:SER:OG	1:B:245:THR:HB	2.03	0.59
1:A:70:SER:HB2	1:A:119:THR:HG21	1.85	0.59
1:B:70:SER:HB2	1:B:119:THR:HG21	1.85	0.59
1:B:127:ARG:NH2	1:B:142:ASP:OD2	2.36	0.59
1:B:233:LEU:CD1	1:B:295:LEU:HD22	2.33	0.59
1:A:127:ARG:NH2	1:A:142:ASP:OD2	2.36	0.58
1:A:192:PHE:HB2	1:A:263:ILE:HG21	1.86	0.58
1:B:192:PHE:HB2	1:B:263:ILE:HG21	1.86	0.58
1:A:198:TYR:HA	1:A:271:LEU:O	2.03	0.58
1:A:150:GLY:O	1:A:251:SER:HB2	2.03	0.58
1:A:171:ASN:O	1:A:177:LYS:CE	2.49	0.58
1:B:91:GLY:N	1:B:97:THR:CG2	2.64	0.58
1:B:186:HIS:HD2	1:B:188:ASN:N	1.91	0.58
1:B:289:THR:O	1:B:293:THR:CG2	2.49	0.58
1:B:58:ASN:ND2	1:B:188:ASN:HB2	2.18	0.58
1:B:245:THR:HG22	1:B:246:THR:HG22	1.85	0.58
1:A:171:ASN:HD22	1:A:176:VAL:HG12	1.68	0.58
1:B:136:SER:CA	1:B:137:LEU:HD13	2.34	0.58
1:B:198:TYR:HA	1:B:271:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLY:O	1:B:251:SER:HB2	2.03	0.57
1:A:66:LEU:N	1:A:108:GLU:O	2.36	0.57
1:A:58:ASN:ND2	1:A:188:ASN:HB2	2.18	0.57
1:B:233:LEU:HD12	1:B:295:LEU:HD22	1.87	0.57
1:A:41:SER:N	1:A:45:ARG:O	2.30	0.57
1:B:171:ASN:HD22	1:B:176:VAL:HG12	1.68	0.57
1:B:195:ILE:CG2	1:B:271:LEU:HD21	2.35	0.57
1:A:86:PHE:HE1	1:A:294:TRP:HE1	1.53	0.57
1:A:136:SER:CA	1:A:137:LEU:HD13	2.34	0.57
1:B:61:ALA:HA	1:B:104:ASP:O	2.05	0.57
4:B:308:GLY:HA2	2:J:38:VAL:OXT	2.04	0.57
1:B:86:PHE:HE1	1:B:294:TRP:HE1	1.53	0.57
1:A:195:ILE:CG2	1:A:271:LEU:HD21	2.35	0.57
1:B:25:LEU:HD11	1:B:87:THR:HG21	1.87	0.56
1:B:72:GLU:HB3	1:B:197:SER:HB3	1.87	0.56
2:I:21:ALA:O	2:I:22:TRP:CG	2.59	0.56
1:B:74:ILE:CD1	1:B:281:LEU:HD12	2.30	0.56
1:A:289:THR:O	1:A:293:THR:CG2	2.49	0.56
1:B:215:ASP:O	1:B:219:LEU:HD13	2.05	0.56
1:B:74:ILE:HG13	1:B:74:ILE:O	2.05	0.56
1:A:25:LEU:HD11	1:A:87:THR:HG21	1.87	0.56
1:A:179:ILE:H	1:A:179:ILE:HD12	1.68	0.56
1:A:233:LEU:HD12	1:A:295:LEU:HD22	1.87	0.56
1:A:72:GLU:HB3	1:A:197:SER:HB3	1.87	0.56
1:A:61:ALA:HA	1:A:104:ASP:O	2.05	0.56
2:J:21:ALA:O	2:J:22:TRP:CG	2.59	0.56
1:A:115:GLY:O	1:A:119:THR:HG23	2.06	0.56
4:A:308:GLY:HA2	2:I:38:VAL:OXT	2.05	0.56
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.71	0.55
1:B:276:ARG:HH11	1:B:276:ARG:HG2	1.71	0.55
1:A:215:ASP:O	1:A:219:LEU:HD13	2.05	0.55
1:B:258:SER:HB2	1:B:263:ILE:HD12	1.89	0.55
1:A:69:HIS:HE2	1:A:127:ARG:HH21	1.54	0.55
1:B:212:SER:OG	1:B:216:LYS:HG3	2.06	0.55
1:A:281:LEU:HD21	1:A:285:GLN:NE2	2.22	0.55
1:A:212:SER:OG	1:A:216:LYS:HG3	2.06	0.55
1:A:245:THR:HG22	1:A:246:THR:HG22	1.85	0.55
1:A:74:ILE:HG13	1:A:74:ILE:O	2.05	0.55
1:A:208:TYR:HD1	1:A:256:ASP:OD2	1.89	0.55
1:A:131:SER:C	1:A:139:VAL:HG23	2.28	0.55
1:B:115:GLY:O	1:B:119:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:HH11	2:J:37:TYR:CB	2.20	0.54
1:A:66:LEU:HD22	1:A:75:THR:O	2.07	0.54
1:B:208:TYR:HD1	1:B:256:ASP:OD2	1.89	0.54
1:B:131:SER:C	1:B:139:VAL:HG23	2.27	0.54
1:B:70:SER:HB2	1:B:119:THR:CG2	2.38	0.54
1:B:95:SER:OG	1:B:302:GLU:OE2	2.25	0.54
1:B:45:ARG:HH11	1:B:114:ASN:ND2	2.06	0.54
1:B:41:SER:N	1:B:45:ARG:O	2.30	0.54
1:B:281:LEU:HD21	1:B:285:GLN:NE2	2.22	0.54
1:B:179:ILE:CD1	1:B:179:ILE:N	2.70	0.54
1:B:7:PHE:CD1	1:B:7:PHE:C	2.81	0.54
2:J:7:ILE:CD1	2:J:20:GLY:H	2.21	0.54
1:A:258:SER:HB2	1:A:263:ILE:HD12	1.89	0.54
1:B:69:HIS:HE2	1:B:127:ARG:HH21	1.54	0.54
1:A:127:ARG:HH11	2:I:37:TYR:CB	2.21	0.54
1:B:136:SER:HA	1:B:137:LEU:HD13	1.91	0.53
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.06	0.53
1:B:1:ALA:N	1:B:7:PHE:HB2	2.23	0.53
1:A:7:PHE:C	1:A:7:PHE:CD1	2.82	0.53
1:B:179:ILE:HD12	1:B:179:ILE:H	1.68	0.53
1:B:66:LEU:HD22	1:B:75:THR:O	2.07	0.53
1:A:1:ALA:N	1:A:7:PHE:HB2	2.23	0.53
1:A:136:SER:HA	1:A:137:LEU:HD13	1.90	0.53
1:A:70:SER:HB2	1:A:119:THR:CG2	2.38	0.53
1:A:179:ILE:N	1:A:179:ILE:CD1	2.70	0.53
1:A:195:ILE:HG22	1:A:271:LEU:CD2	2.39	0.53
2:I:31:ALA:C	2:I:32:ARG:HH11	2.11	0.53
1:B:63:TRP:HE1	1:B:65:ASP:HB3	1.72	0.53
1:B:199:SER:N	1:B:271:LEU:O	2.42	0.53
1:A:95:SER:OG	1:A:302:GLU:OE2	2.25	0.53
1:B:195:ILE:HG22	1:B:271:LEU:CD2	2.38	0.53
2:I:7:ILE:CD1	2:I:20:GLY:H	2.21	0.53
2:J:31:ALA:C	2:J:32:ARG:HH11	2.11	0.53
1:A:204:TYR:HB2	1:A:205:PRO:HD2	1.91	0.53
1:B:204:TYR:HB2	1:B:205:PRO:HD2	1.91	0.52
1:A:213:ILE:HD11	1:A:216:LYS:HA	1.92	0.52
1:A:29:HIS:HB2	1:A:33:VAL:HG13	1.92	0.52
1:A:63:TRP:HE1	1:A:65:ASP:HB3	1.73	0.52
1:A:93:ASN:O	1:A:97:THR:CG2	2.56	0.52
1:A:199:SER:N	1:A:271:LEU:O	2.42	0.52
1:B:213:ILE:HG13	1:B:213:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:O	1:B:134:SER:HB2	2.10	0.52
1:A:213:ILE:O	1:A:213:ILE:HG13	2.10	0.51
1:B:95:SER:O	1:B:99:ILE:HD12	2.10	0.51
1:B:204:TYR:O	1:B:242:SER:HA	2.10	0.51
1:A:69:HIS:CE1	1:A:127:ARG:HH21	2.24	0.51
1:A:60:PRO:HA	1:A:188:ASN:O	2.10	0.51
1:B:25:LEU:CD2	1:B:83:ALA:HB1	2.41	0.51
1:A:95:SER:O	1:A:99:ILE:HD12	2.10	0.51
1:B:60:PRO:HA	1:B:188:ASN:O	2.10	0.51
1:A:26:VAL:HG12	1:A:33:VAL:O	2.11	0.51
1:B:29:HIS:HB2	1:B:33:VAL:HG13	1.92	0.51
1:A:25:LEU:CD2	1:A:83:ALA:HB1	2.41	0.51
1:A:133:THR:O	1:A:134:SER:HB2	2.10	0.51
1:A:204:TYR:O	1:A:242:SER:HA	2.10	0.51
1:B:136:SER:HA	1:B:137:LEU:CD1	2.41	0.50
2:J:9:ASN:HA	2:J:33:THR:CG2	2.34	0.50
1:B:69:HIS:CE1	1:B:127:ARG:HH21	2.24	0.50
1:B:54:THR:HG21	1:B:90:TYR:CZ	2.47	0.50
1:A:136:SER:HA	1:A:137:LEU:CD1	2.41	0.50
1:B:293:THR:O	1:B:297:VAL:HG23	2.12	0.50
1:A:297:VAL:HG12	1:A:301:MET:HE2	1.92	0.50
1:B:213:ILE:HD11	1:B:216:LYS:HA	1.91	0.50
1:B:26:VAL:HG12	1:B:33:VAL:O	2.11	0.50
1:A:54:THR:HG21	1:A:90:TYR:CZ	2.47	0.50
1:A:293:THR:O	1:A:297:VAL:HG23	2.12	0.49
1:B:93:ASN:ND2	1:B:96:PHE:HB2	2.27	0.49
2:I:2:GLX:O	2:I:2:GLX:HG2	2.12	0.49
1:A:93:ASN:ND2	1:A:96:PHE:HB2	2.27	0.49
1:A:195:ILE:HG22	1:A:271:LEU:HD22	1.95	0.49
1:A:203:LEU:HD11	1:A:246:THR:OG1	2.13	0.49
1:B:127:ARG:HH11	2:J:37:TYR:HB2	1.78	0.48
1:A:93:ASN:HD22	1:A:96:PHE:HB2	1.78	0.48
2:J:2:GLX:HG2	2:J:2:GLX:O	2.12	0.48
1:B:133:THR:O	1:B:134:SER:CB	2.61	0.48
1:A:133:THR:O	1:A:134:SER:CB	2.61	0.48
1:B:93:ASN:HD22	1:B:96:PHE:HB2	1.78	0.48
1:B:297:VAL:HG12	1:B:301:MET:HE2	1.93	0.48
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.44	0.48
1:B:195:ILE:HG21	1:B:271:LEU:HD21	1.96	0.48
1:B:144:ASN:O	1:B:145:ARG:HD2	2.12	0.48
1:A:127:ARG:HH11	2:I:37:TYR:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:ASN:HD22	2:I:29:ASN:N	2.04	0.48
1:A:144:ASN:O	1:A:145:ARG:HD2	2.13	0.48
1:A:195:ILE:HG21	1:A:271:LEU:HD21	1.96	0.48
1:B:272:ARG:HD3	1:B:285:GLN:HE21	1.79	0.48
1:B:195:ILE:HG22	1:B:271:LEU:HD22	1.95	0.48
1:B:203:LEU:HD11	1:B:246:THR:OG1	2.13	0.48
1:B:82:PHE:CE1	1:B:294:TRP:HB2	2.49	0.48
2:I:31:ALA:O	2:I:33:THR:N	2.47	0.47
1:B:136:SER:OG	1:B:138:CYS:HB2	2.14	0.47
1:A:93:ASN:HD22	1:A:96:PHE:CB	2.26	0.47
2:J:14:THR:HB	2:J:16:ASP:HB3	1.95	0.47
1:B:132:VAL:O	1:B:133:THR:CB	2.60	0.47
2:J:31:ALA:O	2:J:33:THR:N	2.47	0.47
1:B:204:TYR:HB2	1:B:205:PRO:CD	2.44	0.47
1:B:93:ASN:HD22	1:B:96:PHE:CB	2.26	0.47
1:B:93:ASN:O	1:B:97:THR:CG2	2.56	0.47
1:A:74:ILE:CD1	1:A:281:LEU:HD12	2.29	0.47
1:A:203:LEU:HD12	1:A:241:GLY:O	2.14	0.47
1:B:205:PRO:HB2	1:B:213:ILE:HG21	1.97	0.47
1:B:203:LEU:HD12	1:B:241:GLY:O	2.14	0.47
2:I:14:THR:HB	2:I:16:ASP:HB3	1.95	0.47
1:A:8:ASN:O	1:A:11:THR:CG2	2.62	0.47
1:A:136:SER:OG	1:A:138:CYS:HB2	2.15	0.47
1:A:272:ARG:HD3	1:A:285:GLN:HE21	1.79	0.47
1:A:82:PHE:CE1	1:A:294:TRP:HB2	2.49	0.47
2:J:29:ASN:HD22	2:J:29:ASN:N	2.04	0.47
2:J:31:ALA:O	2:J:33:THR:CB	2.63	0.47
1:A:205:PRO:HB2	1:A:213:ILE:HG21	1.97	0.47
1:B:8:ASN:O	1:B:11:THR:CG2	2.62	0.47
1:A:132:VAL:O	1:A:133:THR:CB	2.60	0.47
1:A:200:GLN:HB3	1:A:238:TYR:CD1	2.50	0.47
1:A:144:ASN:C	1:A:145:ARG:HD2	2.35	0.47
1:B:195:ILE:CG2	1:B:271:LEU:CD2	2.93	0.47
1:B:62:ILE:HD12	1:B:191:ALA:HB3	1.97	0.47
1:A:95:SER:O	1:A:98:ALA:HB3	2.15	0.46
1:B:71:ARG:HH11	1:B:71:ARG:HD2	1.48	0.46
1:A:62:ILE:HD12	1:A:191:ALA:HB3	1.97	0.46
1:B:36:LEU:HB2	1:B:49:VAL:O	2.15	0.46
2:I:31:ALA:O	2:I:33:THR:CB	2.63	0.46
1:B:144:ASN:C	1:B:145:ARG:HD2	2.35	0.46
1:A:36:LEU:HB2	1:A:49:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:THR:HG21	1:B:90:TYR:CE1	2.51	0.46
2:J:3:HIS:O	2:J:4:ALA:CB	2.61	0.46
1:A:4:THR:HG23	1:A:28:GLN:OE1	2.15	0.46
1:A:1:ALA:H1	1:A:7:PHE:HB2	1.80	0.46
1:A:45:ARG:HH11	1:A:45:ARG:HD2	1.50	0.46
1:A:54:THR:HG21	1:A:90:TYR:CE1	2.51	0.46
1:A:36:LEU:O	1:A:49:VAL:N	2.40	0.46
1:A:277:TYR:CG	1:A:282:PRO:HD3	2.51	0.46
1:B:136:SER:C	1:B:137:LEU:HD13	2.36	0.46
1:A:276:ARG:HG2	1:A:276:ARG:NH1	2.30	0.46
1:B:4:THR:HG23	1:B:28:GLN:OE1	2.15	0.46
1:B:277:TYR:CG	1:B:282:PRO:HD3	2.51	0.46
1:B:95:SER:O	1:B:98:ALA:HB3	2.16	0.46
1:A:136:SER:C	1:A:137:LEU:HD13	2.36	0.45
2:I:9:ASN:HA	2:I:33:THR:CG2	2.34	0.45
1:A:220:ASN:O	1:A:223:ALA:HB3	2.16	0.45
1:B:159:SER:HA	1:B:160:PRO:HD3	1.75	0.45
1:B:200:GLN:HB3	1:B:238:TYR:CD1	2.50	0.45
1:A:168:LYS:HG3	1:A:169:TYR:CD2	2.51	0.45
1:A:287:ILE:N	1:A:287:ILE:HD13	2.32	0.45
1:A:159:SER:HA	1:A:160:PRO:HD3	1.75	0.45
1:B:220:ASN:O	1:B:223:ALA:HB3	2.16	0.45
1:A:195:ILE:CG2	1:A:271:LEU:CD2	2.93	0.45
1:B:126:TRP:NE1	1:B:128:LYS:O	2.50	0.45
1:A:13:HIS:HA	1:A:17:GLU:OE1	2.17	0.45
1:A:126:TRP:NE1	1:A:128:LYS:O	2.50	0.45
1:B:168:LYS:HG3	1:B:169:TYR:CD2	2.51	0.45
1:B:186:HIS:CD2	1:B:188:ASN:N	2.76	0.45
2:I:21:ALA:C	2:I:23:PHE:N	2.69	0.45
2:I:3:HIS:O	2:I:4:ALA:CB	2.61	0.45
1:B:171:ASN:HB3	1:B:177:LYS:HD3	1.99	0.45
1:A:198:TYR:O	1:A:199:SER:CB	2.65	0.44
1:B:205:PRO:HG3	1:B:255:ILE:HG23	2.00	0.44
1:A:168:LYS:HG2	1:A:168:LYS:H	1.48	0.44
1:A:208:TYR:CD1	1:A:256:ASP:OD2	2.69	0.44
1:B:287:ILE:N	1:B:287:ILE:HD13	2.32	0.44
1:B:127:ARG:NH1	2:J:37:TYR:HB3	2.33	0.44
1:B:13:HIS:HA	1:B:17:GLU:OE1	2.17	0.44
1:B:168:LYS:HG2	1:B:168:LYS:H	1.48	0.44
1:B:186:HIS:NE2	1:B:188:ASN:HB3	2.33	0.44
1:A:127:ARG:NH1	2:I:37:TYR:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:N	1:A:288:PRO:CD	2.81	0.44
1:B:134:SER:C	1:B:136:SER:N	2.71	0.44
1:A:134:SER:C	1:A:136:SER:N	2.71	0.44
1:A:29:HIS:N	1:A:30:PRO:HD3	2.33	0.44
1:A:76:GLN:HG3	1:A:109:ILE:O	2.18	0.44
1:B:198:TYR:O	1:B:199:SER:CB	2.65	0.44
1:B:76:GLN:HG3	1:B:109:ILE:O	2.18	0.44
1:A:171:ASN:HB3	1:A:177:LYS:HD3	1.99	0.43
1:A:205:PRO:HG3	1:A:255:ILE:HG23	2.00	0.43
2:I:7:ILE:HG13	2:I:21:ALA:HB2	2.01	0.43
1:B:29:HIS:N	1:B:30:PRO:HD3	2.33	0.43
1:B:290:ALA:HA	1:B:293:THR:CG2	2.48	0.43
1:A:290:ALA:HA	1:A:293:THR:CG2	2.48	0.43
1:B:208:TYR:CD1	1:B:256:ASP:OD2	2.69	0.43
2:J:21:ALA:C	2:J:23:PHE:N	2.69	0.43
1:B:287:ILE:N	1:B:288:PRO:CD	2.81	0.43
1:A:57:SER:HB3	1:A:58:ASN:H	1.66	0.43
1:B:45:ARG:HD2	1:B:45:ARG:HH11	1.50	0.43
1:B:287:ILE:HB	1:B:288:PRO:HD3	2.01	0.43
1:A:186:HIS:NE2	1:A:188:ASN:HB3	2.33	0.43
2:I:29:ASN:ND2	2:I:29:ASN:N	2.63	0.43
1:B:136:SER:HB3	1:B:138:CYS:O	2.19	0.43
1:B:276:ARG:HG2	1:B:276:ARG:NH1	2.30	0.43
1:B:142:ASP:HB2	1:B:163:GLU:O	2.19	0.43
2:I:38:VAL:H	2:I:38:VAL:HG22	1.59	0.43
1:B:233:LEU:HD12	1:B:292:GLU:HA	2.01	0.42
1:B:54:THR:H	1:B:59:ARG:HH22	1.67	0.42
1:B:203:LEU:HA	1:B:203:LEU:HD12	1.75	0.42
1:A:233:LEU:HD12	1:A:292:GLU:HA	2.01	0.42
1:A:71:ARG:HH11	1:A:71:ARG:HD2	1.48	0.42
1:A:194:SER:O	1:A:268:THR:HG23	2.19	0.42
1:B:93:ASN:HA	1:B:94:PRO:HD2	1.64	0.42
1:A:287:ILE:HB	1:A:288:PRO:HD3	2.01	0.42
1:B:194:SER:O	1:B:268:THR:HG23	2.19	0.42
1:A:136:SER:HB3	1:A:138:CYS:O	2.19	0.42
1:A:276:ARG:O	2:J:22:TRP:CZ2	2.73	0.42
2:J:7:ILE:HG13	2:J:21:ALA:HB2	2.01	0.42
2:J:5:ASP:OD2	2:J:21:ALA:CB	2.59	0.42
2:I:22:TRP:CZ2	1:B:276:ARG:O	2.73	0.42
1:B:1:ALA:H1	1:B:7:PHE:HB2	1.85	0.42
1:B:100:LEU:HA	1:B:100:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:H	1:A:59:ARG:HH22	1.68	0.42
1:B:247:ILE:HG21	1:B:247:ILE:HD13	1.85	0.42
2:J:8:CYS:HA	2:J:24:CYS:CB	2.50	0.42
1:B:91:GLY:CA	1:B:97:THR:CG2	2.98	0.42
1:A:127:ARG:NH1	2:I:37:TYR:CB	2.83	0.42
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.86	0.42
2:J:5:ASP:CB	2:J:8:CYS:SG	3.04	0.42
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.79	0.42
2:I:5:ASP:CB	2:I:8:CYS:SG	3.04	0.41
1:B:222:VAL:HG21	1:B:303:HIS:CG	2.55	0.41
1:A:142:ASP:HB2	1:A:163:GLU:O	2.20	0.41
1:B:277:TYR:O	1:B:278:GLY:C	2.59	0.41
1:A:287:ILE:N	1:A:287:ILE:CD1	2.83	0.41
1:A:91:GLY:CA	1:A:97:THR:CG2	2.98	0.41
1:A:155:GLY:HA3	1:A:251:SER:H	1.86	0.41
1:A:222:VAL:HG21	1:A:303:HIS:CG	2.55	0.41
1:B:127:ARG:NH1	2:J:37:TYR:CB	2.83	0.41
1:B:14:THR:O	1:B:15:LEU:C	2.59	0.41
1:B:155:GLY:HA3	1:B:251:SER:H	1.86	0.41
1:A:58:ASN:ND2	1:A:188:ASN:CB	2.84	0.41
2:I:8:CYS:HA	2:I:24:CYS:CB	2.50	0.41
1:A:290:ALA:HA	1:A:293:THR:HG22	2.03	0.41
1:B:32:LEU:HD11	1:B:54:THR:HG22	2.02	0.41
1:B:287:ILE:N	1:B:287:ILE:CD1	2.83	0.41
1:A:32:LEU:HD11	1:A:54:THR:HG22	2.02	0.41
1:B:141:VAL:HG21	1:B:173:GLU:OE2	2.21	0.41
2:I:23:PHE:O	2:I:25:GLN:HG3	2.21	0.40
1:A:277:TYR:O	1:A:278:GLY:C	2.59	0.40
1:A:141:VAL:HG21	1:A:173:GLU:OE2	2.21	0.40
1:A:14:THR:O	1:A:15:LEU:C	2.60	0.40
1:B:220:ASN:O	1:B:224:LYS:N	2.52	0.40
2:J:23:PHE:O	2:J:25:GLN:HG3	2.21	0.40
1:A:220:ASN:O	1:A:224:LYS:N	2.52	0.40
1:B:11:THR:HG23	1:B:13:HIS:NE2	2.37	0.40
1:B:14:THR:HG23	1:B:17:GLU:OE1	2.22	0.40
2:J:29:ASN:ND2	2:J:29:ASN:N	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/307 (99%)	274 (90%)	27 (9%)	4 (1%)	15	26
1	B	305/307 (99%)	274 (90%)	27 (9%)	4 (1%)	15	26
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%)	5	6

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 ⓘ

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

Some 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 carbohydrates 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
4	GLY	A	308	-	1,4,4	0.60	0	0,4,4	0.00	-
4	GLY	B	308	-	1,4,4	0.60	0	0,4,4	0.00	-

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
4	GLY	A	308	-	-	0/0/2/2	0/0/0/0
4	GLY	B	308	-	-	0/0/2/2	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	308	GLY	1	0
4	B	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.