



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:07 pm BST

PDB ID : 1MCW
Title : THREE-DIMENSIONAL STRUCTURE OF A HYBRID LIGHT CHAIN DIMER. PROTEIN ENGINEERING OF A BINDING CAVITY
Authors : Ely, K.R.; Herron, J.N.; Edmundson, A.B.
Deposited on : 1989-05-09
Resolution : 3.50 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 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) : 2.11

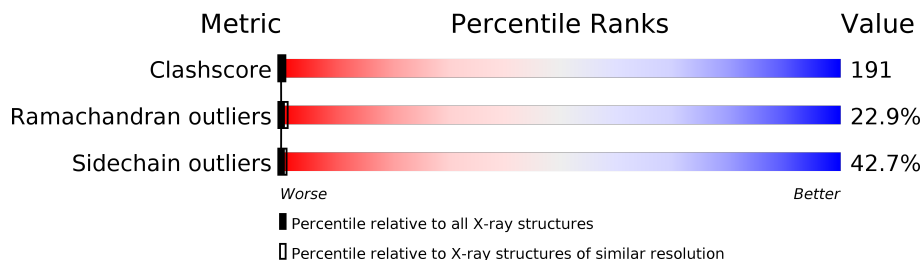
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 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	W	216	
2	M	216	

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
1	PCA	W	1	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3217 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 IMMUNOGLOBULIN WEIR (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	W	216	1611	1010	266	329	6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	20	VAL	ILE	conflict	PIR S25758
W	23	ALA	THR	conflict	PIR S25758
W	25	HIS	SER	conflict	PIR S25758
W	26	THR	SER	conflict	PIR S25758
W	30	ALA	GLY	conflict	PIR S25758
W	31	ASP	GLY	conflict	PIR S25758
W	32	SER	TYR	conflict	PIR S25758
W	34	SER	TYR	conflict	PIR S25758
W	35	ILE	VAL	conflict	PIR S25758
W	38	PHE	TYR	conflict	PIR S25758
W	43	ASP	GLY	conflict	PIR S25758
W	49	LEU	MET	conflict	PIR S25758
W	52	ALA	ASP	conflict	PIR S25758
W	55	PHE	ASN	conflict	PIR S25758
W	60	ILE	VAL	conflict	PIR S25758
W	61	PRO	SER	conflict	PIR S25758
W	62	LEU	ASN	conflict	PIR S25758
W	81	LEU	GLN	conflict	PIR S25758
W	83	ASP	GLU	conflict	PIR S25758
W	89	PHE	TYR	conflict	PIR S25758
W	91	MET	THR	conflict	PIR S25758
W	93	TYR	LYS	conflict	PIR S25758
W	94	LEU	THR	conflict	PIR S25758
W	96	ASP	-	insertion	PIR S25758
W	97	ALA	SER	conflict	PIR S25758
W	?	-	TYR	deletion	PIR S25758
W	103	SER	THR	conflict	PIR S25758

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Chain	Residue	Modelled	Actual	Comment	Reference
W	108	THR	SER	conflict	PIR S25758
W	111	ARG	GLY	conflict	PIR S25758
W	160	GLU	LYS	conflict	PIR S25758

- Molecule 2 is a protein called IMMUNOGLOBULIN MCG (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	216	1606	1000	266	335	5	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

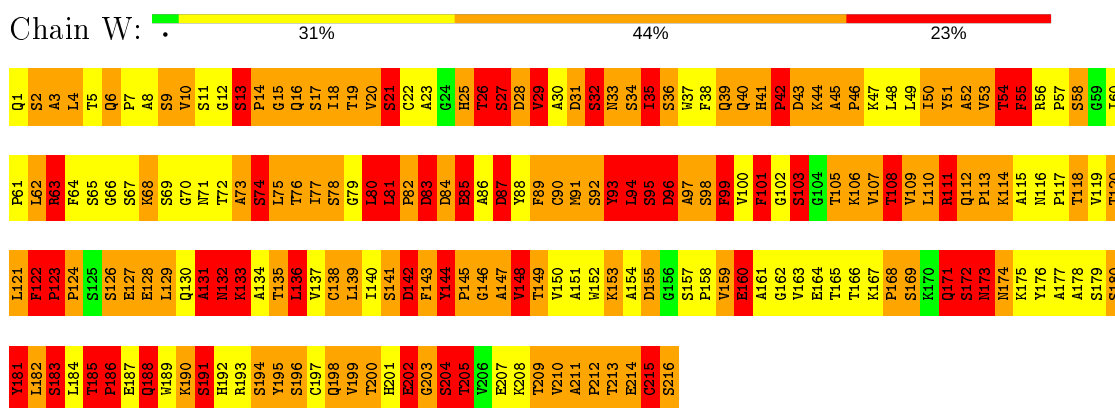
Chain	Residue	Modelled	Actual	Comment	Reference
M	20	ILE	PHE	conflict	PIR S14675
M	23	THR	SER	conflict	PIR S14675
M	29	VAL	ILE	conflict	PIR S14675
M	31	GLY	ASN	conflict	PIR S14675
M	39	GLN	ARG	conflict	PIR S14675
M	42	ALA	PRO	conflict	PIR S14675
M	48	VAL	LEU	conflict	PIR S14675
M	49	ILE	MET	conflict	PIR S14675
M	54	ASN	THR	conflict	PIR S14675
M	62	ASP	ASN	conflict	PIR S14675
M	94	GLU	ALA	conflict	PIR S14675
M	97	ASP	ASN	conflict	PIR S14675
M	98	ASN	SER	conflict	PIR S14675
M	99	PHE	LEU	conflict	PIR S14675
M	100	VAL	ILE	conflict	PIR S14675
M	103	THR	GLY	conflict	PIR S14675
M	106	LYS	ARG	conflict	PIR S14675
M	107	VAL	LEU	conflict	PIR S14675
M	116	ASN	ALA	conflict	PIR S14675
M	118	THR	SER	conflict	PIR S14675
M	156	GLY	SER	conflict	PIR S14675
M	167	LYS	THR	conflict	PIR S14675

3 Residue-property plots

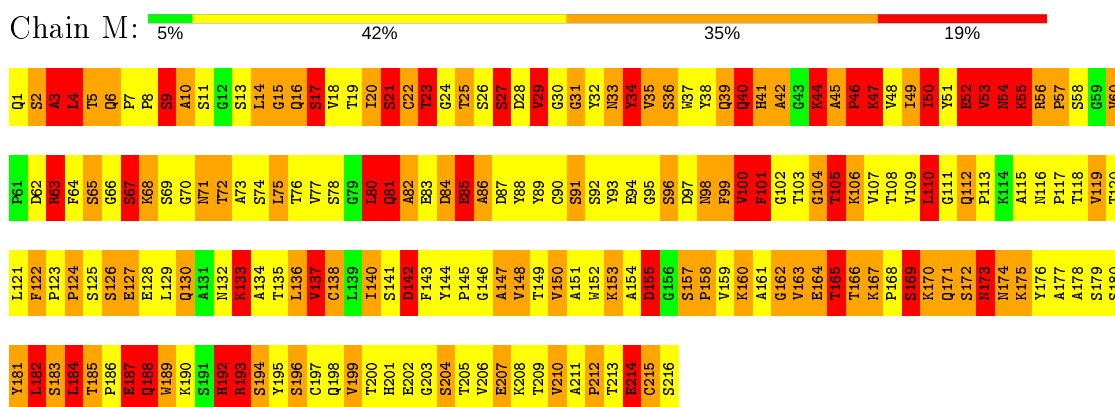
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



- Molecule 2: IMMUNOGLOBULIN MCG (LIGHT CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.30Å 72.30Å 185.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: PCA

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	W	1.31	6/1644 (0.4%)	2.41	108/2245 (4.8%)
2	M	1.24	2/1637 (0.1%)	2.36	89/2233 (4.0%)
All	All	1.28	8/3281 (0.2%)	2.38	197/4478 (4.4%)

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	W	0	1
2	M	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	164	GLU	CG-CD	-6.44	1.42	1.51
1	W	98	SER	CA-CB	-6.38	1.43	1.52
2	M	85	GLU	CD-OE1	-6.21	1.18	1.25
2	M	105	THR	CA-CB	6.00	1.69	1.53
1	W	164	GLU	CD-OE2	5.72	1.31	1.25
1	W	169	SER	CA-CB	-5.70	1.44	1.52
1	W	42	PRO	N-CD	5.19	1.55	1.47
1	W	103	SER	CB-OG	-5.04	1.35	1.42

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	63	ARG	NE-CZ-NH1	23.08	131.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	136	LEU	CA-CB-CG	16.80	153.95	115.30
2	M	63	ARG	NE-CZ-NH2	-15.45	112.58	120.30
1	W	164	GLU	CB-CG-CD	11.08	144.11	114.20
2	M	81	GLN	CA-CB-CG	11.01	137.62	113.40
1	W	111	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	W	136	LEU	CB-CA-C	10.68	130.50	110.20
1	W	101	PHE	CA-CB-CG	10.25	138.50	113.90
2	M	192	HIS	CA-CB-CG	-9.96	96.66	113.60
2	M	116	ASN	CA-CB-CG	9.88	135.13	113.40
2	M	155	ASP	CB-CG-OD1	9.83	127.15	118.30
2	M	104	GLY	C-N-CA	9.81	146.22	121.70
2	M	192	HIS	N-CA-C	9.14	135.67	111.00
2	M	193	ARG	CD-NE-CZ	-9.01	110.98	123.60
1	W	21	SER	N-CA-CB	8.93	123.89	110.50
2	M	34	TYR	CB-CG-CD1	8.88	126.33	121.00
1	W	93	TYR	CA-CB-CG	8.82	130.16	113.40
2	M	105	THR	N-CA-C	8.75	134.62	111.00
2	M	187	GLU	CB-CG-CD	8.70	137.69	114.20
1	W	142	ASP	CA-CB-CG	8.62	132.38	113.40
1	W	108	THR	CB-CA-C	-8.58	88.43	111.60
2	M	187	GLU	CA-CB-CG	8.49	132.07	113.40
1	W	132	ASN	CA-CB-CG	8.37	131.80	113.40
1	W	25	HIS	CB-CA-C	-8.27	93.86	110.40
1	W	111	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	W	33	ASN	CB-CA-C	8.17	126.74	110.40
2	M	33	ASN	CA-CB-CG	7.91	130.81	113.40
1	W	146	GLY	C-N-CA	7.89	141.42	121.70
1	W	148	VAL	CA-C-O	-7.88	103.54	120.10
1	W	174	ASN	CA-CB-CG	7.79	130.55	113.40
1	W	164	GLU	CG-CD-OE1	7.71	133.72	118.30
2	M	54	ASN	CB-CA-C	7.70	125.80	110.40
1	W	13	SER	N-CA-CB	7.62	121.94	110.50
1	W	180	SER	N-CA-CB	7.59	121.89	110.50
1	W	107	VAL	CB-CA-C	7.50	125.65	111.40
1	W	169	SER	N-CA-CB	7.46	121.69	110.50
1	W	63	ARG	CA-CB-CG	7.41	129.70	113.40
1	W	147	ALA	N-CA-CB	7.20	120.18	110.10
2	M	120	THR	N-CA-CB	7.17	123.93	110.30
1	W	80	LEU	CB-CA-C	7.16	123.80	110.20
2	M	137	VAL	CB-CA-C	7.12	124.93	111.40
1	W	29	VAL	CB-CA-C	7.11	124.91	111.40
1	W	191	SER	N-CA-CB	7.10	121.15	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	16	GLN	CA-CB-CG	7.04	128.88	113.40
1	W	87	ASP	CB-CG-OD1	6.98	124.58	118.30
1	W	204	SER	CA-CB-OG	6.96	130.00	111.20
2	M	21	SER	CB-CA-C	-6.95	96.90	110.10
2	M	23	THR	N-CA-CB	6.92	123.45	110.30
2	M	27	SER	N-CA-CB	6.92	120.87	110.50
1	W	20	VAL	C-N-CA	6.89	138.92	121.70
1	W	41	HIS	CA-CB-CG	6.86	125.26	113.60
1	W	42	PRO	N-CD-CG	-6.85	92.92	103.20
2	M	34	TYR	CB-CG-CD2	-6.83	116.90	121.00
2	M	110	LEU	CA-CB-CG	6.83	131.01	115.30
1	W	103	SER	N-CA-C	6.83	129.44	111.00
1	W	44	LYS	N-CA-CB	6.81	122.86	110.60
2	M	67	SER	N-CA-CB	6.78	120.67	110.50
2	M	188	GLN	CB-CG-CD	6.71	129.06	111.60
1	W	146	GLY	CA-C-O	6.62	132.52	120.60
1	W	101	PHE	N-CA-CB	6.58	122.45	110.60
1	W	95	SER	N-CA-CB	6.54	120.31	110.50
1	W	188	GLN	CA-CB-CG	6.52	127.75	113.40
2	M	133	LYS	N-CA-CB	6.46	122.23	110.60
2	M	184	LEU	CA-C-O	6.46	133.67	120.10
1	W	41	HIS	N-CA-CB	6.44	122.19	110.60
2	M	52	GLU	CG-CD-OE1	6.41	131.13	118.30
2	M	17	SER	N-CA-CB	6.35	120.03	110.50
1	W	90	CYS	N-CA-CB	-6.34	99.19	110.60
1	W	159	VAL	CA-CB-CG1	6.30	120.35	110.90
1	W	96	ASP	CB-CA-C	6.28	122.96	110.40
2	M	81	GLN	CB-CG-CD	6.23	127.81	111.60
2	M	104	GLY	CA-C-O	6.20	131.76	120.60
2	M	55	LYS	N-CA-CB	6.20	121.75	110.60
2	M	85	GLU	CG-CD-OE2	-6.20	105.91	118.30
2	M	150	VAL	CA-CB-CG1	6.19	120.18	110.90
2	M	4	LEU	N-CA-CB	6.18	122.77	110.40
2	M	87	ASP	CB-CG-OD2	6.17	123.85	118.30
1	W	31	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	W	202	GLU	CA-CB-CG	6.12	126.86	113.40
1	W	160	GLU	N-CA-CB	6.09	121.57	110.60
2	M	69	SER	CB-CA-C	6.09	121.68	110.10
2	M	39	GLN	CB-CA-C	-6.07	98.26	110.40
2	M	39	GLN	CA-CB-CG	-6.05	100.09	113.40
1	W	204	SER	N-CA-C	-6.04	94.68	111.00
2	M	164	GLU	CG-CD-OE2	-6.04	106.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	160	GLU	OE1-CD-OE2	6.04	130.54	123.30
2	M	194	SER	CA-CB-OG	6.03	127.48	111.20
2	M	101	PHE	CA-CB-CG	6.03	128.37	113.90
1	W	98	SER	N-CA-CB	6.01	119.51	110.50
2	M	138	CYS	CA-CB-SG	5.95	124.71	114.00
1	W	63	ARG	CD-NE-CZ	5.93	131.91	123.60
1	W	155	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	M	55	LYS	CA-CB-CG	5.91	126.39	113.40
2	M	193	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	M	63	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
2	M	54	ASN	N-CA-C	-5.90	95.08	111.00
1	W	81	LEU	CB-CA-C	5.90	121.40	110.20
1	W	90	CYS	CA-CB-SG	-5.89	103.41	114.00
2	M	104	GLY	O-C-N	-5.87	113.31	122.70
2	M	173	ASN	C-N-CA	5.86	136.36	121.70
2	M	132	ASN	CA-CB-CG	-5.86	100.51	113.40
2	M	132	ASN	N-CA-CB	-5.80	100.15	110.60
1	W	205	THR	N-CA-CB	5.79	121.29	110.30
1	W	111	ARG	N-CA-CB	5.75	120.95	110.60
1	W	129	LEU	C-N-CA	5.75	136.07	121.70
1	W	123	PRO	N-CA-C	-5.75	97.16	112.10
2	M	71	ASN	CA-C-N	-5.74	104.58	117.20
1	W	15	GLY	N-CA-C	-5.73	98.78	113.10
1	W	74	SER	O-C-N	5.73	131.87	122.70
1	W	171	GLN	N-CA-CB	5.71	120.87	110.60
1	W	186	PRO	CA-N-CD	-5.69	103.53	111.50
1	W	26	THR	N-CA-CB	-5.68	99.51	110.30
1	W	169	SER	CA-CB-OG	5.66	126.49	111.20
2	M	100	VAL	N-CA-CB	-5.66	99.05	111.50
1	W	50	ILE	CB-CA-C	5.66	122.92	111.60
1	W	84	ASP	CB-CG-OD1	5.66	123.39	118.30
2	M	40	GLN	O-C-N	5.65	131.74	122.70
2	M	105	THR	CB-CA-C	-5.65	96.35	111.60
2	M	207	GLU	CB-CA-C	-5.65	99.11	110.40
1	W	185	THR	N-CA-CB	5.64	121.01	110.30
1	W	96	ASP	CB-CG-OD1	5.62	123.36	118.30
1	W	148	VAL	O-C-N	5.60	131.66	122.70
1	W	128	GLU	CG-CD-OE1	5.60	129.49	118.30
1	W	128	GLU	CB-CG-CD	5.59	129.31	114.20
2	M	182	LEU	CA-CB-CG	5.59	128.15	115.30
1	W	147	ALA	N-CA-C	-5.58	95.94	111.00
2	M	33	ASN	O-C-N	5.53	131.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	ALA	C-N-CA	5.52	135.50	121.70
1	W	186	PRO	N-CA-CB	-5.51	96.54	102.60
1	W	54	THR	CA-CB-CG2	5.49	120.08	112.40
2	M	40	GLN	N-CA-CB	5.48	120.46	110.60
1	W	144	TYR	O-C-N	5.46	131.48	121.10
1	W	55	PHE	CB-CA-C	5.45	121.31	110.40
1	W	89	PHE	O-C-N	5.45	131.41	122.70
2	M	137	VAL	CA-CB-CG1	5.45	119.07	110.90
1	W	94	LEU	CB-CA-C	5.44	120.53	110.20
2	M	71	ASN	CA-C-O	5.43	131.51	120.10
1	W	45	ALA	CB-CA-C	5.43	118.24	110.10
2	M	87	ASP	CA-CB-CG	5.43	125.34	113.40
1	W	131	ALA	CB-CA-C	5.41	118.22	110.10
1	W	205	THR	CA-CB-CG2	5.40	119.95	112.40
2	M	63	ARG	CG-CD-NE	5.39	123.13	111.80
1	W	40	GLN	N-CA-CB	5.39	120.30	110.60
2	M	40	GLN	N-CA-C	-5.38	96.47	111.00
1	W	83	ASP	CB-CG-OD2	5.38	123.14	118.30
1	W	204	SER	N-CA-CB	5.37	118.56	110.50
2	M	142	ASP	CB-CG-OD1	5.37	123.13	118.30
1	W	172	SER	N-CA-CB	-5.36	102.46	110.50
1	W	96	ASP	CB-CG-OD2	5.34	123.10	118.30
1	W	89	PHE	C-N-CA	-5.34	108.36	121.70
2	M	87	ASP	OD1-CG-OD2	-5.34	113.16	123.30
2	M	203	GLY	N-CA-C	-5.34	99.76	113.10
2	M	39	GLN	O-C-N	5.31	131.20	122.70
2	M	164	GLU	CG-CD-OE1	5.31	128.92	118.30
1	W	98	SER	CA-C-O	-5.30	108.98	120.10
2	M	52	GLU	C-N-CA	5.28	134.90	121.70
2	M	60	VAL	O-C-N	5.28	131.13	121.10
2	M	67	SER	CA-CB-OG	5.27	125.44	111.20
2	M	54	ASN	CA-CB-CG	5.27	125.00	113.40
1	W	183	SER	CA-C-O	5.26	131.15	120.10
1	W	173	ASN	N-CA-CB	5.25	120.05	110.60
1	W	99	PHE	N-CA-CB	5.25	120.04	110.60
1	W	122	PHE	CA-CB-CG	5.24	126.47	113.90
2	M	71	ASN	CA-CB-CG	5.23	124.91	113.40
1	W	85	GLU	CA-CB-CG	5.23	124.90	113.40
1	W	164	GLU	CG-CD-OE2	-5.23	107.84	118.30
2	M	80	LEU	CB-CA-C	5.22	120.11	110.20
2	M	104	GLY	N-CA-C	5.20	126.11	113.10
1	W	73	ALA	CA-C-O	5.20	131.01	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	215	CYS	O-C-N	5.19	131.01	122.70
1	W	149	THR	N-CA-CB	5.19	120.16	110.30
2	M	10	ALA	N-CA-CB	5.19	117.36	110.10
2	M	87	ASP	CB-CG-OD1	5.19	122.97	118.30
2	M	53	VAL	N-CA-CB	5.16	122.84	111.50
1	W	148	VAL	CB-CA-C	-5.15	101.62	111.40
1	W	181	TYR	CA-CB-CG	5.15	123.18	113.40
1	W	96	ASP	OD1-CG-OD2	-5.14	113.52	123.30
1	W	98	SER	CB-CA-C	5.14	119.86	110.10
2	M	27	SER	CA-CB-OG	5.14	125.08	111.20
1	W	173	ASN	CA-CB-CG	5.13	124.70	113.40
1	W	174	ASN	CB-CG-OD1	5.13	131.87	121.60
2	M	194	SER	CA-C-O	-5.12	109.34	120.10
1	W	195	TYR	CB-CG-CD1	5.12	124.07	121.00
1	W	148	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	W	98	SER	N-CA-C	-5.10	97.24	111.00
2	M	181	TYR	CB-CA-C	5.07	120.54	110.40
1	W	63	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	W	144	TYR	N-CA-CB	5.06	119.71	110.60
1	W	141	SER	N-CA-CB	5.06	118.09	110.50
2	M	86	ALA	N-CA-CB	5.05	117.17	110.10
1	W	99	PHE	CB-CA-C	-5.04	100.32	110.40
2	M	86	ALA	CB-CA-C	5.03	117.64	110.10
2	M	149	THR	CA-CB-CG2	5.03	119.43	112.40
2	M	207	GLU	O-C-N	5.03	130.74	122.70
2	M	50	ILE	N-CA-CB	5.02	122.36	110.80
2	M	44	LYS	CB-CG-CD	5.02	124.66	111.60
2	M	194	SER	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	56	ARG	Sidechain
2	M	63	ARG	Sidechain
1	W	111	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	W	1611	0	1559	666	7
2	M	1606	0	1536	578	4
All	All	3217	0	3095	1205	10

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 191.

All (1205) 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:W:13:SER:HB2	1:W:16:GLN:NE2	1.22	1.44
2:M:51:TYR:O	2:M:55:LYS:HB2	1.24	1.28
1:W:185:THR:CB	1:W:186:PRO:HD3	1.66	1.26
1:W:81:LEU:HD21	1:W:83:ASP:OD2	1.35	1.25
1:W:19:THR:HA	1:W:75:LEU:O	1.25	1.25
1:W:13:SER:CB	1:W:14:PRO:HD3	1.60	1.22
2:M:20:ILE:CG2	2:M:105:THR:HB	1.71	1.20
1:W:21:SER:HA	1:W:73:ALA:O	1.36	1.20
1:W:18:ILE:O	1:W:76:THR:HA	1.39	1.19
1:W:13:SER:HB3	1:W:14:PRO:CD	1.72	1.19
2:M:20:ILE:HG23	2:M:105:THR:CB	1.72	1.18
2:M:56:ARG:HE	2:M:62:ASP:HA	1.09	1.16
1:W:185:THR:OG1	1:W:186:PRO:HD3	1.42	1.16
2:M:84:ASP:HB3	2:M:106:LYS:HZ2	1.07	1.15
2:M:155:ASP:HA	2:M:194:SER:HB3	1.26	1.14
1:W:133:LYS:HD3	1:W:134:ALA:H	1.09	1.13
1:W:93:TYR:HA	1:W:99:PHE:CD1	1.83	1.13
1:W:81:LEU:HG	1:W:82:PRO:HD2	1.14	1.13
2:M:63:ARG:HH22	2:M:81:GLN:HG2	1.13	1.12
1:W:41:HIS:HB2	1:W:42:PRO:HD2	1.23	1.12
1:W:186:PRO:HD2	1:W:187:GLU:H	0.96	1.11
2:M:53:VAL:HG13	2:M:54:ASN:H	1.11	1.11
2:M:117:PRO:HB3	2:M:143:PHE:HD1	1.04	1.10
1:W:168:PRO:HA	1:W:177:ALA:O	1.51	1.10
2:M:52:GLU:HB2	2:M:55:LYS:HG2	1.21	1.10
1:W:53:VAL:CG1	1:W:54:THR:H	1.64	1.10
2:M:20:ILE:HA	2:M:105:THR:HG21	1.28	1.09
1:W:13:SER:CB	1:W:16:GLN:NE2	2.15	1.09
2:M:63:ARG:HH22	2:M:81:GLN:CG	1.64	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:48:LEU:HG	1:W:57:PRO:CG	1.83	1.09
1:W:31:ASP:O	1:W:32:SER:HB3	1.48	1.09
2:M:88:TYR:CE1	2:M:106:LYS:HG3	1.88	1.09
2:M:84:ASP:HB3	2:M:106:LYS:NZ	1.66	1.09
1:W:167:LYS:CG	1:W:168:PRO:HD2	1.81	1.08
2:M:85:GLU:HB3	2:M:109:VAL:HG13	1.25	1.08
2:M:117:PRO:HB3	2:M:143:PHE:CD1	1.88	1.08
2:M:51:TYR:CD2	2:M:55:LYS:HB3	1.89	1.08
1:W:210:VAL:HG22	1:W:211:ALA:H	1.08	1.08
2:M:23:THR:HG23	2:M:72:THR:HG23	1.32	1.07
2:M:93:TYR:HA	2:M:99:PHE:HB3	1.27	1.07
2:M:169:SER:HA	2:M:176:TYR:CD2	1.89	1.07
1:W:215:CYS:SG	2:M:214:GLU:O	2.12	1.07
2:M:7:PRO:HD2	2:M:21:SER:OG	1.56	1.06
1:W:133:LYS:HD3	1:W:134:ALA:N	1.71	1.06
1:W:48:LEU:HG	1:W:57:PRO:HG3	1.12	1.06
1:W:94:LEU:HB3	1:W:98:SER:HB3	1.10	1.06
2:M:39:GLN:HB2	2:M:49:ILE:HG21	1.32	1.06
2:M:151:ALA:HB3	2:M:198:GLN:HG3	1.33	1.06
1:W:108:THR:O	1:W:109:VAL:HG23	1.53	1.05
1:W:169:SER:HB2	2:M:166:THR:CG2	1.86	1.05
1:W:153:LYS:HG2	1:W:158:PRO:HA	1.37	1.05
1:W:94:LEU:CB	1:W:98:SER:HB3	1.87	1.05
1:W:68:LYS:HA	1:W:72:THR:O	1.55	1.05
1:W:167:LYS:HG3	1:W:168:PRO:HD2	1.07	1.04
1:W:173:ASN:HD21	1:W:175:LYS:HB2	1.14	1.04
1:W:40:GLN:O	1:W:86:ALA:HB1	1.57	1.03
1:W:121:LEU:HB2	1:W:208:LYS:HD3	1.34	1.03
1:W:187:GLU:O	1:W:191:SER:HB2	1.58	1.03
1:W:53:VAL:HG13	1:W:54:THR:H	0.87	1.03
2:M:68:LYS:HB2	2:M:73:ALA:CB	1.88	1.02
2:M:171:GLN:OE1	2:M:177:ALA:HB2	1.59	1.02
1:W:138:CYS:HB3	1:W:152:TRP:CZ2	1.94	1.01
1:W:56:ARG:NH2	1:W:62:LEU:HD13	1.75	1.01
1:W:53:VAL:HG13	1:W:54:THR:N	1.70	1.01
2:M:4:LEU:HG	2:M:5:THR:H	0.89	1.01
2:M:56:ARG:HH21	2:M:62:ASP:N	1.59	1.00
1:W:133:LYS:HE3	1:W:183:SER:OG	1.59	1.00
2:M:143:PHE:O	2:M:175:LYS:HB2	1.61	1.00
1:W:186:PRO:CD	1:W:187:GLU:H	1.75	1.00
1:W:182:LEU:HD21	1:W:184:LEU:HD21	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:123:PRO:HB2	1:W:124:PRO:HD3	1.40	1.00
1:W:124:PRO:HG2	1:W:129:LEU:HD21	1.41	1.00
2:M:81:GLN:HG3	2:M:84:ASP:OD1	1.60	0.99
1:W:124:PRO:CG	1:W:129:LEU:HD21	1.93	0.99
1:W:51:TYR:O	1:W:51:TYR:CD1	2.15	0.99
2:M:4:LEU:HG	2:M:5:THR:N	1.68	0.98
2:M:50:ILE:HG12	2:M:53:VAL:O	1.64	0.98
2:M:14:LEU:HD22	2:M:111:GLY:O	1.63	0.98
1:W:7:PRO:HD2	1:W:20:VAL:HG23	1.46	0.98
1:W:21:SER:CA	1:W:73:ALA:O	2.11	0.97
1:W:154:ALA:HB2	1:W:195:TYR:CD2	1.99	0.97
1:W:64:PHE:CD1	1:W:77:ILE:HG22	1.99	0.97
2:M:124:PRO:HD3	2:M:136:LEU:CD1	1.94	0.97
2:M:165:THR:OG1	2:M:180:SER:HA	1.63	0.97
1:W:123:PRO:HB2	1:W:124:PRO:CD	1.94	0.97
2:M:14:LEU:HA	2:M:80:LEU:HD11	1.45	0.96
2:M:4:LEU:HD21	2:M:22:CYS:SG	2.05	0.96
2:M:75:LEU:O	2:M:75:LEU:HD23	1.65	0.96
1:W:63:ARG:HB2	1:W:78:SER:H	1.30	0.96
2:M:37:TRP:CG	2:M:75:LEU:HD13	1.99	0.96
1:W:142:ASP:HB2	1:W:175:LYS:HE2	1.47	0.96
2:M:56:ARG:NE	2:M:62:ASP:HA	1.79	0.96
1:W:38:PHE:CE2	1:W:91:MET:SD	2.58	0.96
2:M:186:PRO:HA	2:M:189:TRP:CD1	2.01	0.96
2:M:169:SER:HA	2:M:176:TYR:HD2	1.24	0.95
1:W:143:PHE:CE1	1:W:148:VAL:HG21	2.02	0.95
1:W:143:PHE:HE1	1:W:148:VAL:CG2	1.80	0.95
2:M:56:ARG:HH11	2:M:56:ARG:HB2	1.31	0.94
2:M:39:GLN:HE21	2:M:47:LYS:NZ	1.65	0.94
1:W:185:THR:HB	1:W:186:PRO:HD3	1.46	0.94
1:W:185:THR:CB	1:W:186:PRO:CD	2.44	0.94
2:M:189:TRP:NE1	2:M:190:LYS:HG2	1.82	0.94
1:W:186:PRO:HD2	1:W:187:GLU:N	1.81	0.94
1:W:35:ILE:HA	1:W:91:MET:O	1.67	0.94
2:M:30:GLY:HA2	2:M:71:ASN:HA	1.49	0.93
1:W:130:GLN:HE21	1:W:131:ALA:N	1.66	0.93
1:W:20:VAL:HG21	1:W:37:TRP:HH2	1.29	0.93
1:W:143:PHE:HE1	1:W:148:VAL:HG21	1.33	0.93
1:W:168:PRO:CA	1:W:178:ALA:HB2	1.98	0.93
2:M:117:PRO:HA	2:M:141:SER:O	1.67	0.93
1:W:13:SER:HB2	1:W:16:GLN:HE22	1.21	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:26:THR:HA	1:W:30:ALA:HB3	1.50	0.93
1:W:94:LEU:HB3	1:W:98:SER:CB	1.99	0.93
2:M:160:LYS:NZ	2:M:160:LYS:HB2	1.84	0.93
1:W:12:GLY:HA3	1:W:108:THR:O	1.67	0.92
1:W:20:VAL:HG11	1:W:37:TRP:CZ2	2.05	0.92
2:M:53:VAL:HG13	2:M:54:ASN:N	1.84	0.92
2:M:18:VAL:CG2	2:M:77:VAL:HB	2.00	0.92
2:M:185:THR:HG22	2:M:187:GLU:HB2	1.48	0.92
2:M:51:TYR:O	2:M:55:LYS:CB	2.17	0.92
1:W:196:SER:OG	1:W:209:THR:HA	1.67	0.92
1:W:148:VAL:HG12	1:W:199:VAL:HG23	1.52	0.92
2:M:65:SER:O	2:M:75:LEU:HA	1.70	0.92
1:W:216:SER:H	2:M:215:CYS:HB3	1.33	0.92
2:M:145:PRO:HB2	2:M:201:HIS:NE2	1.86	0.91
1:W:169:SER:HB2	2:M:166:THR:HG23	1.52	0.91
1:W:13:SER:CB	1:W:14:PRO:CD	2.41	0.91
2:M:62:ASP:O	2:M:64:PHE:N	2.03	0.91
1:W:169:SER:HB2	2:M:166:THR:CB	2.00	0.91
2:M:124:PRO:HD3	2:M:136:LEU:HD12	1.53	0.91
2:M:51:TYR:HE1	2:M:57:PRO:N	1.69	0.91
2:M:51:TYR:CE2	2:M:55:LYS:HB3	2.06	0.91
1:W:133:LYS:HZ3	1:W:185:THR:HG23	1.36	0.90
2:M:117:PRO:HB2	2:M:140:ILE:HG22	1.51	0.90
2:M:154:ALA:HB2	2:M:159:VAL:CG2	2.01	0.90
1:W:198:GLN:HG3	1:W:207:GLU:HG3	1.53	0.90
1:W:19:THR:CA	1:W:75:LEU:O	2.18	0.90
2:M:151:ALA:CB	2:M:198:GLN:HE21	1.84	0.90
2:M:196:SER:HB3	2:M:209:THR:OG1	1.72	0.90
2:M:39:GLN:HE21	2:M:47:LYS:HZ2	1.16	0.90
2:M:94:GLU:HB2	2:M:98:ASN:HD22	1.37	0.90
1:W:48:LEU:CG	1:W:57:PRO:HG3	2.00	0.90
2:M:94:GLU:HG3	2:M:99:PHE:HA	1.53	0.90
1:W:7:PRO:HD2	1:W:20:VAL:CG2	2.02	0.89
1:W:48:LEU:O	1:W:57:PRO:HG2	1.72	0.89
2:M:20:ILE:HG22	2:M:37:TRP:CZ3	2.07	0.89
2:M:68:LYS:HB2	2:M:73:ALA:CA	2.01	0.89
1:W:118:THR:CG2	1:W:141:SER:HB3	2.01	0.89
1:W:169:SER:OG	2:M:167:LYS:HD3	1.72	0.89
2:M:51:TYR:CE1	2:M:57:PRO:N	2.41	0.89
2:M:14:LEU:HA	2:M:80:LEU:CD1	2.02	0.89
1:W:18:ILE:CG2	1:W:80:LEU:HD11	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:41:HIS:HB2	1:W:42:PRO:CD	2.02	0.89
1:W:169:SER:CB	2:M:166:THR:OG1	2.21	0.89
1:W:143:PHE:CE1	1:W:148:VAL:CG2	2.56	0.89
1:W:4:LEU:HD23	1:W:22:CYS:HB3	1.52	0.89
2:M:17:SER:OG	2:M:78:SER:HA	1.73	0.88
1:W:13:SER:HB2	1:W:16:GLN:HE21	1.06	0.88
1:W:173:ASN:ND2	1:W:175:LYS:HB2	1.88	0.88
2:M:123:PRO:HA	2:M:136:LEU:HG	1.55	0.88
1:W:13:SER:HB3	1:W:14:PRO:HD3	0.90	0.88
1:W:20:VAL:HG21	1:W:37:TRP:CH2	2.07	0.88
2:M:82:ALA:HA	2:M:109:VAL:HG21	1.55	0.88
2:M:39:GLN:NE2	2:M:47:LYS:NZ	2.21	0.88
1:W:143:PHE:CD2	1:W:176:TYR:HB3	2.10	0.87
2:M:39:GLN:NE2	2:M:47:LYS:HZ2	1.71	0.87
1:W:167:LYS:HG3	1:W:168:PRO:CD	1.99	0.87
1:W:39:GLN:HB3	1:W:47:LYS:HB2	1.57	0.87
1:W:18:ILE:HG23	1:W:80:LEU:HD21	1.53	0.87
1:W:133:LYS:HD2	1:W:134:ALA:O	1.75	0.87
1:W:204:SER:O	1:W:205:THR:HG22	1.75	0.87
1:W:210:VAL:HG22	1:W:211:ALA:N	1.90	0.87
1:W:196:SER:OG	1:W:208:LYS:O	1.93	0.86
1:W:56:ARG:HB3	1:W:60:ILE:HG23	1.57	0.86
2:M:140:ILE:HG13	2:M:178:ALA:HB3	1.55	0.86
1:W:90:CYS:O	1:W:101:PHE:HA	1.76	0.86
1:W:89:PHE:C	1:W:90:CYS:SG	2.53	0.86
2:M:34:TYR:CB	2:M:93:TYR:HB3	2.05	0.86
2:M:39:GLN:CB	2:M:49:ILE:HG21	2.03	0.86
2:M:28:ASP:HB2	2:M:92:SER:HB3	1.55	0.86
1:W:171:GLN:HE22	1:W:176:TYR:N	1.72	0.86
1:W:194:SER:HB2	1:W:210:VAL:O	1.75	0.86
1:W:94:LEU:O	1:W:96:ASP:N	2.09	0.85
1:W:110:LEU:HD23	1:W:111:ARG:H	1.39	0.85
2:M:153:LYS:HZ2	2:M:153:LYS:HA	1.40	0.85
1:W:64:PHE:HD1	1:W:77:ILE:HG22	1.38	0.85
2:M:77:VAL:HG11	2:M:106:LYS:HZ3	1.42	0.85
1:W:159:VAL:O	1:W:160:GLU:HG3	1.75	0.85
2:M:153:LYS:NZ	2:M:153:LYS:HA	1.89	0.85
1:W:81:LEU:HG	1:W:82:PRO:CD	2.03	0.85
1:W:13:SER:C	1:W:109:VAL:HG22	1.97	0.85
1:W:144:TYR:HB3	1:W:145:PRO:HD3	1.57	0.85
1:W:182:LEU:HD23	1:W:182:LEU:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:56:ARG:HB3	1:W:60:ILE:CG2	2.07	0.85
1:W:40:GLN:HE22	2:M:40:GLN:HE22	1.23	0.84
2:M:50:ILE:CG1	2:M:53:VAL:O	2.25	0.84
1:W:140:ILE:HG21	1:W:148:VAL:HG11	1.60	0.84
1:W:212:PRO:O	1:W:213:THR:OG1	1.95	0.84
2:M:56:ARG:CB	2:M:56:ARG:HH11	1.89	0.84
1:W:35:ILE:HA	1:W:91:MET:C	1.97	0.84
2:M:151:ALA:HB2	2:M:198:GLN:HE21	1.43	0.84
2:M:186:PRO:HA	2:M:189:TRP:HD1	1.41	0.83
1:W:20:VAL:O	1:W:74:SER:HA	1.78	0.83
2:M:20:ILE:HG23	2:M:105:THR:HB	0.86	0.83
1:W:80:LEU:HB3	1:W:109:VAL:HG21	1.60	0.83
1:W:151:ALA:O	1:W:197:CYS:HA	1.76	0.83
2:M:68:LYS:HD3	2:M:73:ALA:HB2	1.58	0.83
1:W:185:THR:OG1	1:W:186:PRO:CD	2.26	0.83
1:W:55:PHE:HD2	1:W:55:PHE:N	1.75	0.83
2:M:68:LYS:CD	2:M:73:ALA:HB2	2.08	0.83
1:W:31:ASP:O	1:W:32:SER:CB	2.26	0.83
1:W:38:PHE:HE2	1:W:91:MET:SD	2.01	0.83
2:M:81:GLN:HG3	2:M:84:ASP:CG	1.99	0.83
1:W:201:HIS:O	1:W:202:GLU:C	2.17	0.83
1:W:118:THR:HG22	1:W:141:SER:HB3	1.58	0.83
2:M:171:GLN:HG3	2:M:175:LYS:O	1.79	0.83
1:W:64:PHE:HA	1:W:76:THR:O	1.79	0.83
1:W:35:ILE:CA	1:W:91:MET:O	2.26	0.83
2:M:108:THR:HG22	2:M:110:LEU:HD22	1.61	0.82
2:M:6:GLN:NE2	2:M:90:CYS:HB3	1.93	0.82
1:W:112:GLN:CB	1:W:144:TYR:OH	2.27	0.82
1:W:81:LEU:CG	1:W:82:PRO:HD2	2.03	0.82
1:W:13:SER:O	1:W:109:VAL:HA	1.79	0.82
2:M:68:LYS:HB2	2:M:73:ALA:HA	1.61	0.82
1:W:21:SER:OG	1:W:22:CYS:N	2.08	0.82
2:M:138:CYS:O	2:M:179:SER:HA	1.80	0.82
2:M:122:PHE:HD2	2:M:137:VAL:HG12	1.44	0.82
2:M:148:VAL:HG23	2:M:199:VAL:HG12	1.60	0.82
1:W:184:LEU:O	1:W:185:THR:OG1	1.97	0.82
2:M:185:THR:HB	2:M:188:GLN:HG3	1.60	0.82
2:M:143:PHE:HE2	2:M:176:TYR:HB2	1.43	0.81
2:M:51:TYR:C	2:M:55:LYS:HB2	1.98	0.81
1:W:169:SER:HB2	2:M:166:THR:OG1	1.80	0.81
2:M:105:THR:O	2:M:106:LYS:HB3	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:68:LYS:HG3	2:M:72:THR:O	1.78	0.81
2:M:51:TYR:HE1	2:M:57:PRO:CA	1.93	0.81
2:M:148:VAL:HG23	2:M:199:VAL:CG1	2.11	0.81
2:M:20:ILE:HD13	2:M:105:THR:O	1.80	0.81
1:W:101:PHE:CZ	2:M:46:PRO:HB2	2.14	0.81
1:W:113:PRO:HG2	1:W:144:TYR:CD2	2.16	0.81
2:M:84:ASP:CB	2:M:106:LYS:NZ	2.43	0.81
1:W:20:VAL:HG11	1:W:37:TRP:CH2	2.15	0.81
1:W:68:LYS:CA	1:W:72:THR:O	2.28	0.81
1:W:155:ASP:OD2	1:W:192:HIS:HB3	1.81	0.81
2:M:54:ASN:HB3	2:M:66:GLY:H	1.46	0.81
2:M:144:TYR:HB2	2:M:175:LYS:HZ2	1.47	0.80
2:M:93:TYR:HA	2:M:99:PHE:CB	2.08	0.80
2:M:34:TYR:HB2	2:M:93:TYR:HB3	1.62	0.80
1:W:34:SER:O	1:W:35:ILE:HG13	1.82	0.80
2:M:136:LEU:O	2:M:181:TYR:HA	1.82	0.80
2:M:143:PHE:CE2	2:M:176:TYR:HB2	2.17	0.80
2:M:6:GLN:OE1	2:M:89:TYR:HA	1.82	0.80
1:W:14:PRO:HD2	1:W:15:GLY:O	1.82	0.80
1:W:213:THR:HG22	1:W:214:GLU:H	1.45	0.80
2:M:51:TYR:CD1	2:M:55:LYS:O	2.35	0.79
1:W:120:THR:OG1	1:W:139:LEU:HD23	1.82	0.79
1:W:84:ASP:O	1:W:107:VAL:HG13	1.81	0.79
1:W:55:PHE:CD2	1:W:55:PHE:N	2.46	0.79
1:W:117:PRO:HG3	1:W:143:PHE:CB	2.11	0.79
1:W:19:THR:OG1	1:W:76:THR:HG22	1.82	0.79
1:W:56:ARG:NE	1:W:62:LEU:HB2	1.98	0.79
1:W:198:GLN:CG	1:W:207:GLU:HG3	2.13	0.79
1:W:20:VAL:HG22	1:W:21:SER:H	1.47	0.79
1:W:171:GLN:NE2	1:W:176:TYR:N	2.31	0.78
1:W:62:LEU:O	1:W:62:LEU:HD12	1.83	0.78
2:M:7:PRO:O	2:M:104:GLY:HA3	1.83	0.78
1:W:210:VAL:CG2	1:W:211:ALA:H	1.90	0.78
2:M:23:THR:CG2	2:M:72:THR:HG23	2.13	0.78
1:W:166:THR:HG22	1:W:179:SER:N	1.98	0.78
1:W:185:THR:HB	1:W:186:PRO:CD	2.09	0.78
2:M:25:THR:HG23	2:M:28:ASP:OD2	1.83	0.78
2:M:30:GLY:CA	2:M:71:ASN:HA	2.14	0.78
2:M:63:ARG:NH2	2:M:81:GLN:HG2	1.97	0.78
2:M:81:GLN:NE2	2:M:83:GLU:OE1	2.15	0.78
1:W:122:PHE:HD2	2:M:123:PRO:O	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:154:ALA:HB2	1:W:195:TYR:CG	2.18	0.78
1:W:159:VAL:HG22	1:W:161:ALA:H	1.48	0.78
1:W:133:LYS:HZ3	1:W:185:THR:CG2	1.97	0.78
1:W:1:PCA:O	1:W:2:SER:HB2	1.82	0.78
2:M:144:TYR:HB2	2:M:175:LYS:NZ	1.99	0.78
1:W:117:PRO:HG3	1:W:143:PHE:HA	1.66	0.78
1:W:41:HIS:HB3	1:W:86:ALA:HA	1.65	0.78
1:W:201:HIS:O	1:W:204:SER:HB2	1.85	0.77
2:M:85:GLU:HB2	2:M:107:VAL:O	1.83	0.77
1:W:198:GLN:HB2	1:W:207:GLU:CG	2.15	0.77
2:M:144:TYR:CD1	2:M:145:PRO:HD3	2.20	0.77
1:W:37:TRP:HZ3	1:W:88:TYR:HB2	1.49	0.77
2:M:20:ILE:HG23	2:M:105:THR:CG2	2.14	0.77
2:M:81:GLN:CG	2:M:84:ASP:OD1	2.31	0.77
2:M:163:VAL:HG12	2:M:182:LEU:HB2	1.66	0.77
2:M:163:VAL:HG13	2:M:182:LEU:HD23	1.65	0.77
2:M:85:GLU:HB3	2:M:109:VAL:CG1	2.12	0.77
2:M:213:THR:O	2:M:214:GLU:HB3	1.84	0.77
2:M:46:PRO:O	2:M:47:LYS:HB3	1.84	0.77
2:M:20:ILE:CA	2:M:105:THR:HG21	2.12	0.77
2:M:155:ASP:OD2	2:M:192:HIS:O	2.02	0.77
1:W:9:SER:OG	1:W:202:GLU:OE1	2.01	0.77
1:W:91:MET:HA	1:W:100:VAL:O	1.85	0.76
1:W:130:GLN:HE21	1:W:131:ALA:H	1.33	0.76
2:M:126:SER:O	2:M:129:LEU:HB2	1.86	0.76
2:M:154:ALA:HB2	2:M:159:VAL:HG23	1.65	0.76
1:W:13:SER:CB	1:W:16:GLN:HE22	1.86	0.76
1:W:200:THR:HA	1:W:205:THR:HA	1.67	0.76
2:M:14:LEU:HD12	2:M:109:VAL:HG23	1.66	0.76
1:W:168:PRO:HA	1:W:178:ALA:HB2	1.65	0.76
2:M:38:TYR:CE1	2:M:48:VAL:HB	2.20	0.76
1:W:144:TYR:CB	1:W:145:PRO:HD3	2.15	0.76
1:W:74:SER:OG	1:W:75:LEU:N	2.15	0.76
2:M:63:ARG:NH2	2:M:81:GLN:CG	2.46	0.76
1:W:134:ALA:HB3	1:W:185:THR:H	1.47	0.76
2:M:23:THR:HG23	2:M:72:THR:CG2	2.16	0.76
2:M:117:PRO:CB	2:M:143:PHE:HD1	1.93	0.76
2:M:56:ARG:CB	2:M:56:ARG:NH1	2.48	0.76
1:W:166:THR:HG22	1:W:179:SER:H	1.49	0.76
2:M:63:ARG:O	2:M:77:VAL:HA	1.86	0.75
1:W:133:LYS:NZ	1:W:185:THR:HG23	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:52:ALA:HB3	1:W:55:PHE:CE2	2.21	0.75
2:M:165:THR:OG1	2:M:180:SER:CA	2.34	0.75
1:W:48:LEU:HD11	1:W:50:ILE:O	1.87	0.75
1:W:80:LEU:O	1:W:81:LEU:CB	2.34	0.75
2:M:110:LEU:HD23	2:M:110:LEU:H	1.51	0.75
2:M:214:GLU:HG3	2:M:215:CYS:N	2.00	0.75
1:W:112:GLN:HB3	1:W:144:TYR:OH	1.86	0.75
1:W:112:GLN:HB2	1:W:144:TYR:OH	1.87	0.75
1:W:115:ALA:H	1:W:144:TYR:HB3	1.52	0.75
2:M:13:SER:O	2:M:16:GLN:HB2	1.87	0.75
2:M:25:THR:O	2:M:28:ASP:OD1	2.05	0.75
1:W:200:THR:HA	1:W:205:THR:HB	1.69	0.75
1:W:77:ILE:HD13	1:W:84:ASP:OD2	1.86	0.75
2:M:93:TYR:CD1	2:M:94:GLU:N	2.55	0.75
1:W:75:LEU:HG	1:W:76:THR:N	2.02	0.74
2:M:52:GLU:CB	2:M:55:LYS:HG2	2.09	0.74
2:M:82:ALA:CA	2:M:109:VAL:HG21	2.16	0.74
1:W:143:PHE:CD2	1:W:176:TYR:CB	2.71	0.74
2:M:160:LYS:HZ2	2:M:160:LYS:HB2	1.50	0.74
1:W:153:LYS:HB3	1:W:157:SER:O	1.87	0.74
1:W:23:ALA:CB	1:W:72:THR:HG22	2.18	0.74
2:M:6:GLN:HB2	2:M:21:SER:O	1.86	0.74
2:M:33:ASN:O	2:M:34:TYR:CG	2.41	0.74
1:W:42:PRO:O	1:W:43:ASP:OD2	2.04	0.74
2:M:117:PRO:CB	2:M:140:ILE:HG22	2.17	0.74
1:W:169:SER:HB3	2:M:166:THR:OG1	1.86	0.74
2:M:186:PRO:CA	2:M:189:TRP:HD1	2.00	0.74
2:M:95:GLY:O	2:M:96:SER:HB3	1.88	0.73
1:W:133:LYS:CD	1:W:134:ALA:N	2.49	0.73
2:M:51:TYR:CE1	2:M:57:PRO:CD	2.71	0.73
2:M:195:TYR:O	2:M:209:THR:HA	1.88	0.73
2:M:151:ALA:HB3	2:M:198:GLN:CG	2.16	0.73
1:W:95:SER:O	1:W:95:SER:OG	2.05	0.73
1:W:88:TYR:HE2	1:W:107:VAL:HG12	1.54	0.73
1:W:41:HIS:CB	1:W:86:ALA:HA	2.18	0.73
2:M:25:THR:O	2:M:30:GLY:N	2.21	0.73
2:M:33:ASN:O	2:M:34:TYR:CD1	2.40	0.73
2:M:25:THR:OG1	2:M:26:SER:N	2.17	0.73
2:M:75:LEU:HD23	2:M:75:LEU:C	2.08	0.73
1:W:64:PHE:CD1	1:W:77:ILE:CG2	2.70	0.73
1:W:133:LYS:CD	1:W:134:ALA:H	1.95	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:56:ARG:HH21	2:M:62:ASP:CA	2.02	0.72
1:W:2:SER:CA	1:W:100:VAL:HG21	2.19	0.72
2:M:8:PRO:O	2:M:9:SER:HB2	1.88	0.72
1:W:119:VAL:HB	1:W:199:VAL:HG11	1.69	0.72
1:W:142:ASP:HA	1:W:176:TYR:O	1.89	0.72
2:M:50:ILE:CG2	2:M:75:LEU:HD12	2.20	0.72
1:W:152:TRP:HE1	1:W:180:SER:HB3	1.53	0.72
1:W:171:GLN:HE22	1:W:176:TYR:CA	2.03	0.72
1:W:5:THR:O	1:W:22:CYS:HA	1.90	0.72
2:M:68:LYS:HB2	2:M:73:ALA:HB2	1.70	0.72
1:W:122:PHE:CD2	2:M:123:PRO:O	2.41	0.72
1:W:155:ASP:OD1	1:W:193:ARG:HB2	1.89	0.72
2:M:196:SER:HA	2:M:208:LYS:O	1.89	0.71
2:M:93:TYR:HD1	2:M:98:ASN:O	1.73	0.71
1:W:150:VAL:HG21	1:W:180:SER:HB2	1.71	0.71
1:W:57:PRO:O	1:W:60:ILE:HG22	1.89	0.71
2:M:144:TYR:HB3	2:M:145:PRO:CD	2.20	0.71
2:M:16:GLN:H	2:M:80:LEU:H	1.36	0.71
1:W:23:ALA:HB2	1:W:72:THR:HG22	1.72	0.71
1:W:56:ARG:CB	1:W:60:ILE:HG23	2.21	0.71
2:M:51:TYR:CD1	2:M:57:PRO:HD3	2.26	0.71
1:W:110:LEU:CD2	1:W:111:ARG:H	2.04	0.71
1:W:65:SER:O	1:W:75:LEU:HA	1.91	0.71
2:M:37:TRP:CD1	2:M:75:LEU:HD13	2.26	0.71
2:M:96:SER:O	2:M:97:ASP:HB2	1.89	0.71
1:W:168:PRO:N	1:W:178:ALA:HB2	2.05	0.71
1:W:68:LYS:CB	1:W:72:THR:O	2.39	0.71
2:M:155:ASP:CA	2:M:194:SER:HB3	2.14	0.71
1:W:171:GLN:O	1:W:173:ASN:N	2.24	0.71
1:W:18:ILE:HG21	1:W:80:LEU:HD11	1.70	0.70
1:W:216:SER:N	2:M:215:CYS:HB3	2.05	0.70
2:M:11:SER:HA	2:M:108:THR:HB	1.72	0.70
2:M:37:TRP:HB2	2:M:49:ILE:O	1.92	0.70
2:M:4:LEU:CG	2:M:5:THR:H	1.83	0.70
2:M:84:ASP:CB	2:M:106:LYS:HZ2	1.96	0.70
1:W:26:THR:O	1:W:27:SER:C	2.30	0.70
2:M:14:LEU:HD12	2:M:109:VAL:CG2	2.21	0.70
2:M:172:SER:O	2:M:173:ASN:ND2	2.25	0.70
2:M:18:VAL:HG11	2:M:106:LYS:HB2	1.72	0.70
2:M:68:LYS:CB	2:M:73:ALA:CB	2.70	0.70
2:M:53:VAL:HG22	2:M:54:ASN:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:81:GLN:NE2	2:M:83:GLU:CD	2.44	0.70
1:W:88:TYR:CE2	1:W:107:VAL:HG12	2.26	0.70
1:W:4:LEU:HD11	1:W:92:SER:OG	1.92	0.70
2:M:82:ALA:CB	2:M:109:VAL:HG21	2.21	0.70
1:W:25:HIS:O	1:W:26:THR:O	2.09	0.70
2:M:81:GLN:HE21	2:M:83:GLU:CD	1.95	0.70
1:W:168:PRO:CA	1:W:177:ALA:O	2.34	0.70
1:W:86:ALA:O	1:W:87:ASP:HB2	1.89	0.70
1:W:8:ALA:O	1:W:9:SER:HB2	1.92	0.70
2:M:126:SER:O	2:M:129:LEU:N	2.25	0.69
2:M:184:LEU:HD22	2:M:185:THR:O	1.91	0.69
2:M:80:LEU:HD12	2:M:81:GLN:N	2.06	0.69
1:W:152:TRP:HA	1:W:196:SER:O	1.92	0.69
1:W:171:GLN:HB2	2:M:164:GLU:OE1	1.92	0.69
1:W:135:THR:HA	1:W:183:SER:HA	1.73	0.69
1:W:2:SER:CA	1:W:100:VAL:HG11	2.23	0.69
2:M:89:TYR:CE2	2:M:103:THR:OG1	2.44	0.69
1:W:117:PRO:HG3	1:W:143:PHE:HB3	1.74	0.69
2:M:185:THR:CG2	2:M:187:GLU:HB2	2.21	0.69
2:M:34:TYR:HB3	2:M:93:TYR:HB3	1.73	0.69
2:M:37:TRP:HD1	2:M:50:ILE:HD12	1.57	0.69
1:W:77:ILE:HD11	1:W:80:LEU:CD2	2.22	0.69
1:W:13:SER:O	1:W:109:VAL:HG22	1.93	0.69
2:M:20:ILE:CG2	2:M:37:TRP:CZ3	2.76	0.69
1:W:10:VAL:HG13	1:W:105:THR:OG1	1.92	0.69
2:M:50:ILE:HG21	2:M:75:LEU:HD12	1.74	0.69
1:W:40:GLN:O	1:W:86:ALA:CB	2.38	0.69
1:W:56:ARG:CZ	1:W:62:LEU:HD13	2.22	0.69
2:M:51:TYR:CD2	2:M:55:LYS:CB	2.73	0.69
1:W:1:PCA:N	1:W:94:LEU:HD13	2.07	0.69
2:M:25:THR:CA	2:M:28:ASP:OD1	2.41	0.69
2:M:94:GLU:HB2	2:M:98:ASN:ND2	2.05	0.69
1:W:36:SER:OG	1:W:91:MET:CE	2.41	0.69
2:M:124:PRO:HD3	2:M:136:LEU:HD11	1.72	0.68
2:M:154:ALA:O	2:M:157:SER:OG	2.08	0.68
2:M:51:TYR:CE1	2:M:57:PRO:HD3	2.28	0.68
1:W:149:THR:O	1:W:199:VAL:HA	1.93	0.68
2:M:56:ARG:HH21	2:M:62:ASP:H	1.38	0.68
2:M:25:THR:C	2:M:28:ASP:OD1	2.32	0.68
1:W:134:ALA:O	1:W:135:THR:HB	1.92	0.68
1:W:36:SER:OG	1:W:91:MET:HE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:92:SER:O	1:W:99:PHE:HD1	1.77	0.68
2:M:51:TYR:HE1	2:M:57:PRO:CD	2.06	0.68
1:W:198:GLN:HB2	1:W:207:GLU:HG3	1.75	0.68
1:W:117:PRO:HG3	1:W:143:PHE:CA	2.23	0.68
1:W:41:HIS:CB	1:W:42:PRO:HD2	2.08	0.68
2:M:168:PRO:O	2:M:169:SER:HB2	1.94	0.68
1:W:101:PHE:CE2	2:M:46:PRO:HB2	2.30	0.68
1:W:132:ASN:ND2	1:W:132:ASN:O	2.22	0.67
2:M:56:ARG:NH2	2:M:62:ASP:N	2.40	0.67
1:W:30:ALA:HA	1:W:70:GLY:O	1.94	0.67
1:W:81:LEU:CD2	1:W:83:ASP:OD2	2.29	0.67
1:W:80:LEU:O	1:W:81:LEU:HB2	1.94	0.67
1:W:135:THR:HG23	1:W:136:LEU:N	2.10	0.67
2:M:66:GLY:O	2:M:67:SER:HB3	1.94	0.67
1:W:209:THR:CG2	1:W:210:VAL:H	2.07	0.67
1:W:20:VAL:CG1	1:W:75:LEU:HB3	2.25	0.67
1:W:171:GLN:NE2	1:W:175:LYS:C	2.47	0.67
2:M:127:GLU:HA	2:M:127:GLU:OE2	1.95	0.67
1:W:17:SER:HA	1:W:77:ILE:O	1.95	0.67
2:M:121:LEU:HD21	2:M:210:VAL:HG22	1.76	0.67
1:W:112:GLN:O	1:W:113:PRO:O	2.13	0.66
1:W:52:ALA:HB3	1:W:55:PHE:CZ	2.30	0.66
2:M:112:GLN:OE1	2:M:144:TYR:CG	2.48	0.66
2:M:85:GLU:O	2:M:85:GLU:HG3	1.94	0.66
1:W:133:LYS:HA	1:W:185:THR:HA	1.75	0.66
1:W:198:GLN:HB2	1:W:207:GLU:HG2	1.76	0.66
2:M:150:VAL:CG2	2:M:197:CYS:SG	2.83	0.66
2:M:198:GLN:HB3	2:M:207:GLU:HG2	1.77	0.66
1:W:94:LEU:HB2	1:W:99:PHE:N	2.11	0.66
2:M:88:TYR:CD1	2:M:106:LYS:HG3	2.29	0.66
2:M:17:SER:HA	2:M:77:VAL:O	1.96	0.66
2:M:93:TYR:HD1	2:M:94:GLU:H	1.41	0.66
1:W:6:GLN:HB2	1:W:21:SER:O	1.94	0.66
2:M:160:LYS:HZ3	2:M:160:LYS:HB2	1.58	0.66
1:W:6:GLN:NE2	1:W:102:GLY:O	2.28	0.66
1:W:123:PRO:CB	1:W:124:PRO:CD	2.67	0.66
1:W:12:GLY:HA2	1:W:80:LEU:CD1	2.26	0.66
2:M:18:VAL:CB	2:M:77:VAL:HB	2.26	0.66
2:M:60:VAL:HG12	2:M:60:VAL:O	1.96	0.66
2:M:94:GLU:OE1	2:M:100:VAL:HG13	1.96	0.66
1:W:110:LEU:HD23	1:W:111:ARG:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:118:THR:HG22	1:W:141:SER:CB	2.26	0.66
2:M:91:SER:HA	2:M:100:VAL:O	1.96	0.66
1:W:188:GLN:N	1:W:188:GLN:HE21	1.94	0.66
2:M:39:GLN:CB	2:M:49:ILE:CG2	2.74	0.66
1:W:13:SER:CB	1:W:16:GLN:HE21	1.97	0.66
1:W:213:THR:HG22	1:W:214:GLU:N	2.09	0.66
1:W:216:SER:OXT	2:M:215:CYS:HA	1.97	0.65
1:W:20:VAL:HG22	1:W:21:SER:O	1.95	0.65
2:M:40:GLN:O	2:M:86:ALA:HB1	1.96	0.65
1:W:166:THR:O	1:W:178:ALA:HB1	1.96	0.65
1:W:12:GLY:CA	1:W:108:THR:O	2.41	0.65
1:W:144:TYR:CD2	1:W:144:TYR:O	2.49	0.65
1:W:82:PRO:O	1:W:84:ASP:N	2.26	0.65
2:M:51:TYR:HE1	2:M:57:PRO:CB	2.10	0.65
1:W:166:THR:HG22	1:W:179:SER:HB2	1.78	0.65
1:W:1:PCA:O	1:W:2:SER:CB	2.45	0.65
2:M:10:ALA:HB2	2:M:105:THR:HG23	1.78	0.65
2:M:14:LEU:HD11	2:M:82:ALA:HB2	1.79	0.65
1:W:20:VAL:HG22	1:W:21:SER:N	2.11	0.65
2:M:80:LEU:CD1	2:M:109:VAL:HB	2.27	0.65
2:M:117:PRO:HG2	2:M:117:PRO:O	1.97	0.65
2:M:25:THR:HG23	2:M:28:ASP:CG	2.17	0.65
2:M:68:LYS:CB	2:M:73:ALA:HB2	2.26	0.65
1:W:201:HIS:HB3	1:W:204:SER:HB2	1.79	0.65
1:W:41:HIS:HA	1:W:86:ALA:HA	1.79	0.65
2:M:56:ARG:HB3	2:M:56:ARG:NH1	2.11	0.65
1:W:173:ASN:HD22	1:W:175:LYS:H	1.45	0.65
1:W:212:PRO:O	1:W:213:THR:CB	2.45	0.65
1:W:110:LEU:HD23	1:W:111:ARG:N	2.11	0.65
1:W:182:LEU:CD2	1:W:184:LEU:HD21	2.23	0.65
1:W:189:TRP:CH2	1:W:212:PRO:HA	2.32	0.65
2:M:112:GLN:NE2	2:M:113:PRO:HD2	2.12	0.64
2:M:186:PRO:HG2	2:M:187:GLU:H	1.62	0.64
1:W:108:THR:O	1:W:109:VAL:CG2	2.38	0.64
1:W:186:PRO:CD	1:W:187:GLU:N	2.48	0.64
1:W:181:TYR:HE2	2:M:171:GLN:OE1	1.80	0.64
2:M:41:HIS:O	2:M:42:ALA:CB	2.45	0.64
2:M:151:ALA:HB3	2:M:198:GLN:HE21	1.61	0.64
2:M:80:LEU:C	2:M:80:LEU:HD12	2.17	0.64
1:W:44:LYS:O	1:W:46:PRO:HD3	1.97	0.64
1:W:148:VAL:HG12	1:W:199:VAL:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:20:VAL:CG1	1:W:37:TRP:CZ2	2.79	0.64
1:W:48:LEU:CD1	1:W:50:ILE:O	2.45	0.64
2:M:64:PHE:CD2	2:M:77:VAL:HG13	2.32	0.64
1:W:213:THR:CG2	1:W:214:GLU:H	2.11	0.64
1:W:51:TYR:O	1:W:52:ALA:CB	2.46	0.64
2:M:29:VAL:HG12	2:M:68:LYS:HD3	1.80	0.64
2:M:53:VAL:HG12	2:M:55:LYS:NZ	2.12	0.64
2:M:80:LEU:CD2	2:M:109:VAL:HB	2.28	0.64
2:M:81:GLN:O	2:M:82:ALA:HB3	1.97	0.64
1:W:205:THR:O	1:W:205:THR:OG1	2.16	0.64
2:M:152:TRP:HE1	2:M:180:SER:HG	0.64	0.64
2:M:50:ILE:CG2	2:M:75:LEU:CD1	2.76	0.64
1:W:126:SER:O	1:W:127:GLU:C	2.36	0.64
1:W:20:VAL:HG12	1:W:75:LEU:HB3	1.80	0.63
2:M:14:LEU:CD1	2:M:109:VAL:HG23	2.27	0.63
2:M:84:ASP:HB3	2:M:106:LYS:CE	2.28	0.63
1:W:85:GLU:HG3	1:W:107:VAL:O	1.98	0.63
2:M:109:VAL:CG2	2:M:109:VAL:O	2.47	0.63
2:M:25:THR:N	2:M:28:ASP:OD1	2.31	0.63
2:M:53:VAL:CG1	2:M:54:ASN:H	1.80	0.63
2:M:144:TYR:CB	2:M:145:PRO:CD	2.76	0.63
2:M:170:LYS:HB3	2:M:173:ASN:O	1.98	0.63
1:W:2:SER:HA	1:W:100:VAL:CB	2.29	0.63
1:W:97:ALA:HB2	2:M:51:TYR:OH	1.99	0.63
2:M:105:THR:O	2:M:106:LYS:CB	2.47	0.63
2:M:18:VAL:HB	2:M:77:VAL:HG23	1.81	0.63
2:M:82:ALA:HB2	2:M:109:VAL:HG21	1.81	0.63
1:W:153:LYS:HA	1:W:157:SER:O	1.98	0.63
2:M:10:ALA:CB	2:M:105:THR:HG23	2.29	0.63
1:W:13:SER:HB2	1:W:14:PRO:HD3	1.71	0.63
2:M:44:LYS:O	2:M:45:ALA:CB	2.45	0.62
1:W:123:PRO:HB2	1:W:189:TRP:CH2	2.33	0.62
1:W:9:SER:CB	1:W:202:GLU:OE1	2.47	0.62
2:M:18:VAL:CG1	2:M:106:LYS:HB2	2.30	0.62
2:M:122:PHE:CD2	2:M:137:VAL:HG12	2.32	0.62
2:M:18:VAL:HB	2:M:77:VAL:HB	1.81	0.62
2:M:5:THR:O	2:M:22:CYS:HA	1.99	0.62
1:W:38:PHE:HB2	1:W:89:PHE:HB2	1.80	0.62
1:W:37:TRP:CE3	1:W:88:TYR:HB3	2.34	0.62
2:M:118:THR:O	2:M:119:VAL:O	2.15	0.62
1:W:37:TRP:CD2	1:W:90:CYS:SG	2.89	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:126:SER:O	2:M:127:GLU:C	2.36	0.62
2:M:51:TYR:CE1	2:M:57:PRO:CA	2.79	0.62
1:W:152:TRP:HE1	1:W:180:SER:CB	2.12	0.62
2:M:168:PRO:CB	2:M:177:ALA:O	2.48	0.62
2:M:18:VAL:HG21	2:M:77:VAL:HB	1.82	0.62
1:W:62:LEU:O	1:W:62:LEU:CG	2.48	0.62
1:W:96:ASP:N	1:W:96:ASP:OD2	2.31	0.62
2:M:108:THR:CG2	2:M:110:LEU:HD22	2.29	0.62
2:M:150:VAL:HG23	2:M:197:CYS:SG	2.40	0.62
1:W:56:ARG:CZ	1:W:62:LEU:HB2	2.30	0.62
1:W:64:PHE:CE1	1:W:77:ILE:CG2	2.82	0.62
2:M:141:SER:OG	2:M:171:GLN:NE2	2.33	0.61
1:W:209:THR:HG22	1:W:210:VAL:N	2.15	0.61
1:W:62:LEU:O	1:W:62:LEU:CD1	2.47	0.61
1:W:65:SER:OG	1:W:76:THR:HG23	2.01	0.61
2:M:50:ILE:HG23	2:M:75:LEU:CD1	2.31	0.61
2:M:186:PRO:HG2	2:M:187:GLU:N	2.15	0.61
2:M:50:ILE:HD13	2:M:50:ILE:C	2.21	0.61
2:M:83:GLU:HG3	2:M:173:ASN:CG	2.21	0.61
1:W:8:ALA:O	1:W:9:SER:CB	2.47	0.61
2:M:109:VAL:HG22	2:M:109:VAL:O	2.01	0.61
2:M:140:ILE:HG13	2:M:178:ALA:CB	2.29	0.61
2:M:6:GLN:NE2	2:M:37:TRP:CH2	2.68	0.61
2:M:214:GLU:OE1	2:M:216:SER:OG	2.18	0.61
1:W:107:VAL:CG2	1:W:108:THR:H	2.13	0.61
1:W:133:LYS:C	1:W:185:THR:O	2.39	0.61
2:M:118:THR:C	2:M:119:VAL:O	2.39	0.61
1:W:20:VAL:O	1:W:74:SER:CA	2.49	0.61
1:W:105:THR:O	1:W:106:LYS:CB	2.49	0.61
1:W:119:VAL:HB	1:W:199:VAL:CG1	2.31	0.61
1:W:20:VAL:CG2	1:W:21:SER:H	2.13	0.61
1:W:39:GLN:HB2	1:W:49:LEU:HD13	1.83	0.61
1:W:6:GLN:OE1	1:W:88:TYR:O	2.19	0.61
2:M:165:THR:OG1	2:M:180:SER:CB	2.49	0.60
1:W:2:SER:HA	1:W:100:VAL:HG11	1.82	0.60
1:W:131:ALA:O	1:W:132:ASN:HB3	2.01	0.60
1:W:171:GLN:HB2	2:M:164:GLU:CD	2.22	0.60
1:W:209:THR:CG2	1:W:210:VAL:N	2.64	0.60
1:W:216:SER:H	2:M:215:CYS:CB	2.10	0.60
1:W:92:SER:O	1:W:99:PHE:CD1	2.54	0.60
1:W:10:VAL:HG22	1:W:106:LYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:15:GLY:O	1:W:16:GLN:HB2	2.00	0.60
1:W:198:GLN:CB	1:W:207:GLU:HG3	2.31	0.60
2:M:152:TRP:O	2:M:153:LYS:NZ	2.35	0.60
1:W:173:ASN:C	1:W:173:ASN:HD22	2.05	0.60
1:W:2:SER:HA	1:W:100:VAL:HG21	1.82	0.60
2:M:189:TRP:CD1	2:M:190:LYS:HG2	2.36	0.60
2:M:7:PRO:HD2	2:M:21:SER:HG	1.65	0.60
1:W:52:ALA:O	1:W:53:VAL:HG12	2.02	0.60
2:M:18:VAL:HB	2:M:77:VAL:CG2	2.32	0.60
2:M:65:SER:O	2:M:75:LEU:CA	2.48	0.60
1:W:77:ILE:HD11	1:W:80:LEU:HD22	1.83	0.59
1:W:132:ASN:O	1:W:133:LYS:HB2	2.00	0.59
2:M:88:TYR:CZ	2:M:106:LYS:HG3	2.37	0.59
2:M:6:GLN:NE2	2:M:37:TRP:CZ3	2.70	0.59
2:M:83:GLU:HG3	2:M:173:ASN:ND2	2.17	0.59
1:W:119:VAL:O	1:W:120:THR:HG23	2.01	0.59
1:W:60:ILE:HG12	1:W:61:PRO:O	2.03	0.59
1:W:18:ILE:HG23	1:W:80:LEU:HD11	1.84	0.59
2:M:144:TYR:HB3	2:M:145:PRO:HD2	1.85	0.59
2:M:39:GLN:NE2	2:M:47:LYS:HZ1	2.01	0.59
1:W:51:TYR:CG	1:W:51:TYR:O	2.56	0.59
2:M:63:ARG:N	2:M:63:ARG:HD3	2.16	0.59
2:M:89:TYR:HB3	2:M:102:GLY:O	2.03	0.59
1:W:39:GLN:O	1:W:46:PRO:HA	2.02	0.59
1:W:41:HIS:HB3	1:W:86:ALA:CA	2.33	0.59
2:M:122:PHE:HD2	2:M:137:VAL:CG1	2.14	0.59
1:W:135:THR:O	1:W:136:LEU:CB	2.48	0.59
2:M:110:LEU:CD2	2:M:110:LEU:H	2.15	0.59
2:M:153:LYS:HZ1	2:M:158:PRO:HA	1.67	0.59
2:M:82:ALA:HA	2:M:109:VAL:CG2	2.30	0.59
1:W:166:THR:CG2	1:W:179:SER:HB2	2.33	0.59
1:W:38:PHE:CZ	1:W:91:MET:CE	2.86	0.59
2:M:125:SER:C	2:M:129:LEU:HD12	2.23	0.58
2:M:193:ARG:HA	2:M:212:PRO:HD2	1.84	0.58
1:W:118:THR:HG22	1:W:141:SER:CA	2.32	0.58
1:W:49:LEU:O	1:W:57:PRO:HD2	2.03	0.58
1:W:64:PHE:CE1	1:W:77:ILE:HG21	2.38	0.58
2:M:18:VAL:O	2:M:76:THR:HA	2.02	0.58
1:W:2:SER:O	1:W:3:ALA:CB	2.50	0.58
2:M:176:TYR:N	2:M:176:TYR:CD1	2.71	0.58
1:W:154:ALA:CB	1:W:195:TYR:CD2	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:63:ARG:HH22	2:M:81:GLN:HG3	1.65	0.58
1:W:171:GLN:HE22	1:W:176:TYR:C	2.07	0.58
1:W:62:LEU:O	1:W:62:LEU:HG	2.04	0.58
2:M:84:ASP:CA	2:M:106:LYS:HE3	2.33	0.58
2:M:141:SER:OG	2:M:142:ASP:N	2.36	0.58
1:W:136:LEU:HD12	1:W:182:LEU:HD22	1.84	0.58
1:W:56:ARG:HB3	1:W:60:ILE:HG21	1.85	0.58
2:M:93:TYR:CD1	2:M:98:ASN:O	2.55	0.58
2:M:146:GLY:O	2:M:147:ALA:HB2	2.02	0.58
2:M:160:LYS:NZ	2:M:160:LYS:CB	2.59	0.58
1:W:209:THR:HG22	1:W:210:VAL:H	1.67	0.58
1:W:154:ALA:HB1	1:W:194:SER:O	2.03	0.58
1:W:48:LEU:C	1:W:57:PRO:HG2	2.24	0.58
2:M:18:VAL:HG11	2:M:106:LYS:HD3	1.86	0.57
1:W:216:SER:OXT	2:M:215:CYS:HB3	2.04	0.57
1:W:113:PRO:O	1:W:114:LYS:HB2	2.04	0.57
1:W:189:TRP:CZ2	1:W:212:PRO:HA	2.38	0.57
1:W:19:THR:OG1	1:W:76:THR:CG2	2.51	0.57
2:M:14:LEU:HD12	2:M:80:LEU:HD11	1.86	0.57
2:M:150:VAL:HA	2:M:198:GLN:O	2.05	0.57
1:W:171:GLN:HE21	1:W:175:LYS:C	2.07	0.57
1:W:201:HIS:O	1:W:204:SER:CB	2.52	0.57
1:W:77:ILE:HD11	1:W:80:LEU:HD23	1.85	0.57
2:M:147:ALA:H	2:M:148:VAL:HG12	1.68	0.57
1:W:152:TRP:O	1:W:159:VAL:HG12	2.04	0.57
1:W:2:SER:N	1:W:100:VAL:HG21	2.19	0.57
2:M:185:THR:HB	2:M:188:GLN:CG	2.32	0.57
1:W:77:ILE:O	1:W:77:ILE:HG13	2.02	0.57
1:W:37:TRP:CZ3	1:W:88:TYR:HB2	2.35	0.57
2:M:68:LYS:CG	2:M:73:ALA:HB2	2.34	0.57
2:M:68:LYS:HD2	2:M:70:GLY:O	2.04	0.57
2:M:18:VAL:HB	2:M:77:VAL:CB	2.34	0.57
2:M:89:TYR:CD2	2:M:103:THR:HB	2.39	0.57
2:M:89:TYR:CD2	2:M:103:THR:CB	2.88	0.56
1:W:109:VAL:O	1:W:109:VAL:HG12	2.05	0.56
1:W:48:LEU:CG	1:W:57:PRO:CG	2.71	0.56
1:W:63:ARG:HB2	1:W:78:SER:N	2.10	0.56
1:W:82:PRO:C	1:W:84:ASP:H	2.07	0.56
2:M:84:ASP:O	2:M:106:LYS:O	2.23	0.56
1:W:209:THR:O	1:W:210:VAL:HB	2.05	0.56
1:W:35:ILE:N	1:W:92:SER:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:81:GLN:O	2:M:82:ALA:CB	2.53	0.56
1:W:6:GLN:HA	1:W:21:SER:O	2.05	0.56
2:M:14:LEU:HB2	2:M:111:GLY:HA3	1.88	0.56
2:M:151:ALA:CB	2:M:198:GLN:NE2	2.62	0.56
2:M:110:LEU:N	2:M:110:LEU:CD2	2.69	0.56
1:W:114:LYS:HA	1:W:144:TYR:CD1	2.41	0.56
1:W:105:THR:O	1:W:106:LYS:HB2	2.06	0.56
1:W:166:THR:HG22	1:W:179:SER:CA	2.36	0.56
1:W:37:TRP:CZ3	1:W:88:TYR:CB	2.89	0.56
1:W:34:SER:C	1:W:92:SER:HA	2.27	0.56
2:M:4:LEU:CD2	2:M:22:CYS:SG	2.87	0.56
2:M:2:SER:O	2:M:3:ALA:HB2	2.05	0.56
1:W:141:SER:O	1:W:142:ASP:C	2.45	0.56
1:W:201:HIS:O	1:W:202:GLU:O	2.24	0.56
1:W:60:ILE:HD11	1:W:64:PHE:CD2	2.41	0.56
2:M:163:VAL:CG1	2:M:182:LEU:HB2	2.35	0.55
1:W:121:LEU:HB2	1:W:208:LYS:CD	2.24	0.55
2:M:155:ASP:CG	2:M:192:HIS:O	2.44	0.55
1:W:106:LYS:O	1:W:107:VAL:HB	2.06	0.55
1:W:153:LYS:CA	1:W:157:SER:O	2.54	0.55
2:M:20:ILE:HG13	2:M:75:LEU:O	2.06	0.55
2:M:25:THR:O	2:M:30:GLY:CA	2.54	0.55
2:M:40:GLN:CG	2:M:42:ALA:H	2.19	0.55
2:M:80:LEU:CD1	2:M:81:GLN:N	2.70	0.55
2:M:81:GLN:NE2	2:M:83:GLU:HB2	2.22	0.55
1:W:81:LEU:C	1:W:81:LEU:HD23	2.26	0.55
1:W:166:THR:CG2	1:W:179:SER:H	2.18	0.55
1:W:7:PRO:HD2	1:W:20:VAL:HG22	1.87	0.55
2:M:128:GLU:HB3	2:M:133:LYS:O	2.06	0.55
2:M:84:ASP:O	2:M:106:LYS:HE3	2.05	0.55
2:M:144:TYR:HA	2:M:175:LYS:HB3	1.88	0.55
2:M:153:LYS:HB3	2:M:196:SER:OG	2.07	0.55
1:W:29:VAL:CG2	1:W:71:ASN:O	2.54	0.55
2:M:51:TYR:CG	2:M:55:LYS:O	2.60	0.55
1:W:120:THR:O	1:W:138:CYS:HA	2.07	0.55
1:W:135:THR:O	1:W:136:LEU:CG	2.55	0.55
2:M:108:THR:HG22	2:M:110:LEU:CD2	2.35	0.55
2:M:163:VAL:HG12	2:M:182:LEU:CB	2.37	0.55
1:W:143:PHE:CE1	1:W:148:VAL:HG22	2.40	0.55
1:W:40:GLN:O	1:W:86:ALA:C	2.45	0.55
2:M:115:ALA:O	2:M:201:HIS:CE1	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:214:GLU:OE2	2:M:215:CYS:SG	2.65	0.55
1:W:91:MET:HG3	1:W:99:PHE:CE1	2.42	0.55
2:M:84:ASP:HA	2:M:106:LYS:HE3	1.89	0.54
2:M:171:GLN:OE1	2:M:177:ALA:CB	2.47	0.54
1:W:97:ALA:CB	2:M:51:TYR:OH	2.55	0.54
1:W:120:THR:OG1	1:W:139:LEU:CD2	2.54	0.54
1:W:77:ILE:HD11	1:W:80:LEU:HA	1.90	0.54
1:W:37:TRP:HE3	1:W:88:TYR:HB3	1.71	0.54
2:M:20:ILE:HG13	2:M:75:LEU:HD23	1.90	0.54
1:W:36:SER:CB	1:W:91:MET:HE2	2.37	0.54
1:W:120:THR:HA	1:W:208:LYS:HD2	1.90	0.54
1:W:210:VAL:HG13	1:W:211:ALA:N	2.23	0.54
2:M:14:LEU:CD1	2:M:82:ALA:HB2	2.37	0.54
2:M:173:ASN:CG	2:M:174:ASN:N	2.61	0.54
2:M:82:ALA:HA	2:M:109:VAL:HG11	1.90	0.54
1:W:12:GLY:HA3	1:W:108:THR:CB	2.38	0.54
1:W:80:LEU:HB3	1:W:109:VAL:CG2	2.36	0.54
2:M:13:SER:HB2	2:M:16:GLN:HG3	1.90	0.54
1:W:64:PHE:CA	1:W:76:THR:O	2.54	0.54
1:W:56:ARG:CB	1:W:60:ILE:CG2	2.82	0.54
2:M:84:ASP:OD2	2:M:106:LYS:NZ	2.41	0.54
1:W:13:SER:H	1:W:80:LEU:HD12	1.72	0.54
2:M:173:ASN:CG	2:M:174:ASN:H	2.10	0.53
2:M:35:VAL:HA	2:M:91:SER:O	2.08	0.53
1:W:2:SER:HA	1:W:100:VAL:CG1	2.38	0.53
1:W:150:VAL:HG11	1:W:165:THR:OG1	2.07	0.53
1:W:143:PHE:HE2	1:W:177:ALA:N	2.06	0.53
1:W:66:GLY:C	1:W:67:SER:OG	2.46	0.53
1:W:38:PHE:CE2	1:W:91:MET:CE	2.91	0.53
2:M:196:SER:CA	2:M:208:LYS:O	2.56	0.53
2:M:37:TRP:CD1	2:M:75:LEU:CD1	2.91	0.53
2:M:93:TYR:OH	2:M:96:SER:HA	2.08	0.53
2:M:144:TYR:HB3	2:M:145:PRO:HD3	1.90	0.53
1:W:40:GLN:CD	1:W:89:PHE:HE1	2.11	0.53
2:M:171:GLN:CG	2:M:175:LYS:O	2.54	0.53
2:M:38:TYR:CD1	2:M:48:VAL:HB	2.43	0.53
2:M:174:ASN:N	2:M:174:ASN:OD1	2.41	0.53
2:M:150:VAL:HG23	2:M:198:GLN:O	2.09	0.53
2:M:213:THR:O	2:M:214:GLU:CB	2.55	0.53
2:M:27:SER:O	2:M:32:TYR:CD1	2.62	0.53
1:W:130:GLN:O	1:W:131:ALA:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:18:VAL:HG23	2:M:77:VAL:HB	1.86	0.53
1:W:153:LYS:CB	1:W:157:SER:O	2.57	0.53
1:W:19:THR:HG1	1:W:76:THR:HG22	1.71	0.53
1:W:38:PHE:O	1:W:88:TYR:HA	2.09	0.53
2:M:183:SER:O	2:M:184:LEU:HB3	2.08	0.53
1:W:90:CYS:O	1:W:101:PHE:CA	2.54	0.53
2:M:34:TYR:HB3	2:M:93:TYR:CB	2.38	0.53
2:M:84:ASP:N	2:M:84:ASP:OD1	2.41	0.53
1:W:26:THR:O	1:W:27:SER:O	2.26	0.53
2:M:39:GLN:CD	2:M:41:HIS:HD2	2.13	0.53
1:W:135:THR:HA	1:W:183:SER:CA	2.39	0.53
1:W:136:LEU:HD12	1:W:152:TRP:CZ3	2.44	0.53
2:M:186:PRO:CG	2:M:187:GLU:H	2.22	0.52
2:M:148:VAL:CG2	2:M:199:VAL:CG1	2.85	0.52
1:W:40:GLN:NE2	2:M:40:GLN:HE22	1.99	0.52
2:M:41:HIS:O	2:M:42:ALA:HB2	2.09	0.52
1:W:130:GLN:C	1:W:130:GLN:HE21	2.12	0.52
1:W:136:LEU:CD1	1:W:182:LEU:HD22	2.39	0.52
1:W:51:TYR:O	1:W:52:ALA:HB3	2.08	0.52
2:M:185:THR:O	2:M:189:TRP:HB3	2.09	0.52
2:M:35:VAL:HG23	2:M:36:SER:N	2.22	0.52
1:W:106:LYS:HG3	1:W:107:VAL:N	2.24	0.52
1:W:144:TYR:CB	1:W:145:PRO:CD	2.87	0.52
1:W:93:TYR:HA	1:W:99:PHE:CE1	2.43	0.52
1:W:121:LEU:HD12	1:W:208:LYS:HB2	1.91	0.52
1:W:4:LEU:HB3	1:W:102:GLY:HA3	1.92	0.52
1:W:169:SER:CB	2:M:166:THR:CG2	2.74	0.52
2:M:32:TYR:CE2	2:M:94:GLU:O	2.63	0.52
1:W:146:GLY:H	1:W:201:HIS:CE1	2.28	0.52
1:W:4:LEU:HD21	1:W:35:ILE:HG21	1.91	0.52
1:W:29:VAL:HG22	1:W:71:ASN:O	2.09	0.52
2:M:81:GLN:CB	2:M:84:ASP:OD1	2.58	0.52
1:W:2:SER:HA	1:W:100:VAL:CG2	2.39	0.52
1:W:109:VAL:CG1	1:W:109:VAL:O	2.57	0.52
1:W:196:SER:OG	1:W:209:THR:CA	2.49	0.52
1:W:199:VAL:O	1:W:205:THR:HA	2.10	0.52
1:W:68:LYS:HD2	1:W:70:GLY:HA2	1.91	0.52
1:W:23:ALA:HB1	1:W:72:THR:HG22	1.89	0.52
1:W:93:TYR:C	1:W:99:PHE:HA	2.30	0.52
2:M:150:VAL:HG21	2:M:197:CYS:SG	2.50	0.52
2:M:82:ALA:C	2:M:84:ASP:H	2.05	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:89:TYR:HD2	2:M:103:THR:HB	1.74	0.52
2:M:186:PRO:CG	2:M:187:GLU:N	2.72	0.52
2:M:88:TYR:CE1	2:M:106:LYS:O	2.63	0.52
1:W:80:LEU:O	1:W:81:LEU:HB3	2.10	0.52
2:M:151:ALA:HB3	2:M:198:GLN:NE2	2.23	0.52
2:M:57:PRO:HG2	2:M:60:VAL:CG2	2.39	0.52
1:W:121:LEU:H	1:W:208:LYS:CD	2.23	0.52
2:M:18:VAL:HG23	2:M:77:VAL:O	2.10	0.51
1:W:57:PRO:C	1:W:60:ILE:HG22	2.30	0.51
1:W:6:GLN:HE22	1:W:90:CYS:HB2	1.75	0.51
1:W:77:ILE:CD1	1:W:80:LEU:HD23	2.40	0.51
2:M:44:LYS:O	2:M:45:ALA:HB2	2.10	0.51
1:W:107:VAL:HG22	1:W:108:THR:H	1.75	0.51
1:W:145:PRO:O	1:W:176:TYR:CE1	2.64	0.51
1:W:143:PHE:HE2	1:W:177:ALA:CA	2.23	0.51
2:M:51:TYR:CE1	2:M:55:LYS:O	2.62	0.51
1:W:81:LEU:CA	1:W:109:VAL:HG11	2.41	0.51
2:M:6:GLN:HG2	2:M:103:THR:N	2.25	0.51
1:W:133:LYS:HE3	1:W:183:SER:HG	1.69	0.51
1:W:4:LEU:HD11	1:W:92:SER:HG	1.74	0.51
1:W:93:TYR:CA	1:W:99:PHE:CD1	2.75	0.51
2:M:1:PCA:O	2:M:2:SER:HB2	2.11	0.51
2:M:15:GLY:N	2:M:80:LEU:HG	2.25	0.51
2:M:37:TRP:HA	2:M:89:TYR:O	2.11	0.51
1:W:145:PRO:O	1:W:176:TYR:CD1	2.63	0.51
2:M:24:GLY:HA3	2:M:29:VAL:HG21	1.92	0.51
2:M:20:ILE:HG13	2:M:75:LEU:CD2	2.41	0.51
1:W:153:LYS:HB3	1:W:157:SER:C	2.31	0.51
2:M:134:ALA:HB3	2:M:184:LEU:O	2.11	0.51
1:W:106:LYS:HG3	1:W:107:VAL:H	1.76	0.51
1:W:12:GLY:N	1:W:108:THR:OG1	2.43	0.51
1:W:144:TYR:CD1	1:W:145:PRO:HD3	2.46	0.51
1:W:159:VAL:HG22	1:W:160:GLU:N	2.26	0.51
2:M:144:TYR:HA	2:M:175:LYS:CB	2.41	0.51
1:W:123:PRO:CB	1:W:124:PRO:HD3	2.21	0.51
1:W:60:ILE:HD11	1:W:64:PHE:HD2	1.76	0.51
2:M:117:PRO:HB2	2:M:140:ILE:CG2	2.32	0.50
2:M:20:ILE:HG22	2:M:37:TRP:CH2	2.46	0.50
2:M:40:GLN:HG2	2:M:42:ALA:C	2.31	0.50
1:W:143:PHE:HE1	1:W:148:VAL:CG1	2.24	0.50
1:W:6:GLN:NE2	1:W:90:CYS:SG	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:154:ALA:CB	1:W:195:TYR:CG	2.93	0.50
1:W:204:SER:O	1:W:205:THR:CG2	2.56	0.50
1:W:11:SER:OG	1:W:202:GLU:OE2	2.24	0.50
1:W:79:GLY:O	1:W:80:LEU:O	2.30	0.50
1:W:37:TRP:CE3	1:W:90:CYS:SG	3.04	0.50
2:M:123:PRO:CB	2:M:124:PRO:HD2	2.42	0.50
2:M:29:VAL:HB	2:M:71:ASN:O	2.12	0.50
2:M:37:TRP:CD1	2:M:50:ILE:HD12	2.44	0.50
2:M:82:ALA:C	2:M:84:ASP:N	2.63	0.50
1:W:166:THR:HG22	1:W:179:SER:CB	2.42	0.50
1:W:9:SER:HB3	1:W:202:GLU:OE1	2.11	0.50
1:W:91:MET:HB2	1:W:92:SER:O	2.12	0.50
2:M:60:VAL:CG1	2:M:60:VAL:O	2.59	0.50
2:M:81:GLN:HG3	2:M:84:ASP:OD2	2.10	0.50
2:M:26:SER:O	2:M:31:GLY:HA3	2.11	0.50
1:W:143:PHE:CD1	1:W:146:GLY:HA2	2.46	0.50
1:W:144:TYR:C	1:W:144:TYR:CD2	2.83	0.50
2:M:39:GLN:O	2:M:39:GLN:HG2	1.98	0.50
2:M:6:GLN:HE22	2:M:90:CYS:HB3	1.76	0.50
1:W:110:LEU:CG	1:W:111:ARG:H	2.23	0.50
1:W:18:ILE:O	1:W:76:THR:CA	2.34	0.50
1:W:4:LEU:HD21	1:W:35:ILE:CG2	2.42	0.50
2:M:150:VAL:HB	2:M:199:VAL:HG13	1.93	0.49
1:W:187:GLU:O	1:W:191:SER:CB	2.47	0.49
1:W:121:LEU:CB	1:W:208:LYS:HD3	2.25	0.49
1:W:51:TYR:CZ	1:W:55:PHE:CD1	3.00	0.49
2:M:163:VAL:HG12	2:M:182:LEU:HA	1.94	0.49
1:W:119:VAL:HA	1:W:139:LEU:O	2.12	0.49
1:W:143:PHE:HD2	1:W:176:TYR:CB	2.22	0.49
2:M:153:LYS:NZ	2:M:158:PRO:HA	2.26	0.49
1:W:135:THR:HA	1:W:183:SER:CB	2.42	0.49
1:W:64:PHE:HE1	1:W:77:ILE:HG21	1.77	0.49
2:M:152:TRP:CG	2:M:163:VAL:HG11	2.46	0.49
2:M:28:ASP:O	2:M:31:GLY:N	2.32	0.49
1:W:216:SER:OXT	2:M:215:CYS:CA	2.60	0.49
2:M:4:LEU:CG	2:M:5:THR:N	2.53	0.49
1:W:135:THR:O	1:W:136:LEU:HG	2.12	0.49
1:W:194:SER:CB	1:W:210:VAL:O	2.54	0.49
2:M:186:PRO:O	2:M:187:GLU:C	2.49	0.49
1:W:48:LEU:HG	1:W:57:PRO:HG2	1.85	0.49
1:W:137:VAL:HG11	2:M:122:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:193:ARG:O	2:M:193:ARG:HG2	2.13	0.49
1:W:11:SER:HA	1:W:202:GLU:OE2	2.13	0.49
1:W:141:SER:O	1:W:142:ASP:O	2.31	0.49
1:W:37:TRP:HZ3	1:W:88:TYR:CB	2.20	0.49
1:W:68:LYS:NZ	1:W:70:GLY:HA2	2.28	0.49
2:M:20:ILE:O	2:M:74:SER:HA	2.12	0.49
2:M:39:GLN:O	2:M:39:GLN:CG	2.56	0.49
2:M:13:SER:O	2:M:14:LEU:C	2.52	0.49
1:W:166:THR:O	1:W:166:THR:CG2	2.61	0.49
1:W:136:LEU:HG	1:W:182:LEU:CD2	2.43	0.49
1:W:7:PRO:HD3	1:W:21:SER:O	2.13	0.49
1:W:39:GLN:HG2	1:W:47:LYS:HD2	1.94	0.49
2:M:211:ALA:O	2:M:213:THR:N	2.45	0.49
2:M:37:TRP:CG	2:M:75:LEU:CD1	2.86	0.49
1:W:10:VAL:CG2	1:W:106:LYS:O	2.61	0.49
1:W:173:ASN:ND2	1:W:175:LYS:H	2.08	0.49
1:W:188:GLN:HB2	1:W:195:TYR:OH	2.13	0.49
2:M:140:ILE:CG1	2:M:178:ALA:HB3	2.36	0.48
2:M:205:THR:HG23	2:M:205:THR:O	2.12	0.48
1:W:88:TYR:CE2	1:W:107:VAL:CG1	2.95	0.48
1:W:166:THR:O	1:W:166:THR:HG23	2.13	0.48
2:M:16:GLN:N	2:M:80:LEU:H	2.09	0.48
1:W:130:GLN:O	1:W:130:GLN:HG3	2.07	0.48
2:M:51:TYR:CE1	2:M:57:PRO:CB	2.95	0.48
1:W:162:GLY:C	1:W:163:VAL:HG12	2.32	0.48
1:W:37:TRP:H	1:W:50:ILE:HG12	1.77	0.48
1:W:53:VAL:O	1:W:55:PHE:N	2.47	0.48
1:W:95:SER:C	1:W:97:ALA:N	2.67	0.48
2:M:28:ASP:O	2:M:29:VAL:C	2.52	0.48
2:M:80:LEU:HD13	2:M:109:VAL:HB	1.95	0.48
1:W:17:SER:O	1:W:18:ILE:HG22	2.13	0.48
1:W:35:ILE:HG23	1:W:92:SER:OG	2.13	0.48
2:M:118:THR:O	2:M:119:VAL:C	2.52	0.48
1:W:47:LYS:HB3	1:W:48:LEU:H	1.43	0.48
1:W:86:ALA:O	1:W:87:ASP:CB	2.60	0.48
2:M:67:SER:O	2:M:74:SER:O	2.31	0.48
1:W:2:SER:N	1:W:100:VAL:HG11	2.28	0.48
1:W:12:GLY:HA2	1:W:80:LEU:HD12	1.94	0.48
1:W:95:SER:C	1:W:97:ALA:H	2.17	0.48
2:M:53:VAL:CG1	2:M:55:LYS:NZ	2.76	0.48
1:W:137:VAL:HG21	2:M:137:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:117:PRO:HA	1:W:142:ASP:O	2.14	0.48
1:W:159:VAL:HG22	1:W:160:GLU:H	1.79	0.48
1:W:77:ILE:CD1	1:W:80:LEU:CD2	2.90	0.48
2:M:37:TRP:CZ2	2:M:90:CYS:HB2	2.49	0.47
1:W:142:ASP:CA	1:W:176:TYR:O	2.61	0.47
2:M:108:THR:O	2:M:108:THR:HG22	2.14	0.47
2:M:63:ARG:H	2:M:63:ARG:CD	2.26	0.47
1:W:77:ILE:CG1	1:W:80:LEU:CD2	2.91	0.47
1:W:95:SER:HA	1:W:96:ASP:OD2	2.14	0.47
2:M:40:GLN:OE1	2:M:46:PRO:HD3	2.14	0.47
2:M:53:VAL:CG1	2:M:54:ASN:N	2.50	0.47
1:W:144:TYR:CD1	1:W:145:PRO:HG3	2.49	0.47
1:W:146:GLY:H	1:W:201:HIS:HE1	1.62	0.47
1:W:169:SER:CA	2:M:166:THR:HG21	2.45	0.47
1:W:169:SER:H	2:M:166:THR:HG21	1.78	0.47
1:W:28:ASP:O	1:W:29:VAL:C	2.53	0.47
2:M:6:GLN:HG2	2:M:102:GLY:C	2.35	0.47
2:M:94:GLU:HG3	2:M:99:PHE:CA	2.36	0.47
1:W:42:PRO:O	1:W:43:ASP:CG	2.52	0.47
1:W:54:THR:C	1:W:55:PHE:HD2	2.18	0.47
1:W:82:PRO:C	1:W:84:ASP:N	2.68	0.47
1:W:6:GLN:HE22	1:W:90:CYS:CB	2.28	0.47
1:W:97:ALA:HB1	2:M:57:PRO:HA	1.97	0.47
2:M:77:VAL:CG1	2:M:106:LYS:HZ3	2.21	0.47
2:M:151:ALA:HB2	2:M:198:GLN:NE2	2.19	0.47
1:W:200:THR:HA	1:W:205:THR:CB	2.43	0.47
1:W:200:THR:OG1	1:W:205:THR:HB	2.14	0.47
1:W:121:LEU:N	1:W:208:LYS:HD3	2.29	0.47
1:W:91:MET:CA	1:W:100:VAL:O	2.58	0.47
1:W:118:THR:O	1:W:118:THR:HG23	2.15	0.47
2:M:154:ALA:CB	2:M:159:VAL:HG23	2.42	0.47
2:M:53:VAL:HG22	2:M:54:ASN:OD1	2.14	0.47
1:W:121:LEU:HD21	1:W:152:TRP:CZ3	2.50	0.47
1:W:181:TYR:CE2	2:M:171:GLN:OE1	2.64	0.47
1:W:216:SER:OXT	2:M:215:CYS:CB	2.63	0.47
2:M:77:VAL:HG11	2:M:106:LYS:NZ	2.23	0.47
1:W:16:GLN:H	1:W:80:LEU:H	1.63	0.47
1:W:40:GLN:HB2	1:W:46:PRO:HG3	1.97	0.47
2:M:53:VAL:CG1	2:M:55:LYS:HZ3	2.27	0.47
1:W:110:LEU:CD2	1:W:111:ARG:HG3	2.41	0.47
2:M:144:TYR:HD1	2:M:145:PRO:HD3	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:112:GLN:HA	1:W:113:PRO:HD2	1.73	0.47
2:M:115:ALA:O	2:M:201:HIS:HE1	1.96	0.46
2:M:49:ILE:HG13	2:M:49:ILE:O	2.12	0.46
1:W:195:TYR:O	1:W:196:SER:HB2	2.15	0.46
1:W:1:PCA:CD	1:W:2:SER:H	2.26	0.46
1:W:48:LEU:HD21	1:W:51:TYR:HB2	1.96	0.46
2:M:50:ILE:HG23	2:M:75:LEU:HD12	1.90	0.46
2:M:40:GLN:HG2	2:M:42:ALA:CA	2.45	0.46
2:M:51:TYR:CE1	2:M:57:PRO:HB3	2.50	0.46
1:W:173:ASN:ND2	1:W:175:LYS:CB	2.70	0.46
1:W:11:SER:CA	1:W:202:GLU:OE2	2.64	0.46
2:M:89:TYR:CE2	2:M:103:THR:CB	2.98	0.46
2:M:144:TYR:CB	2:M:145:PRO:HD3	2.45	0.46
1:W:136:LEU:CD2	1:W:189:TRP:CE3	2.98	0.46
2:M:124:PRO:HB3	2:M:135:THR:H	1.80	0.46
2:M:153:LYS:HE3	2:M:157:SER:C	2.35	0.46
2:M:39:GLN:OE1	2:M:41:HIS:CD2	2.68	0.46
1:W:107:VAL:CG2	1:W:108:THR:N	2.79	0.46
2:M:37:TRP:O	2:M:49:ILE:O	2.34	0.46
1:W:135:THR:HA	1:W:183:SER:OG	2.15	0.46
1:W:166:THR:CG2	1:W:179:SER:N	2.75	0.46
1:W:36:SER:O	1:W:91:MET:CE	2.63	0.46
1:W:45:ALA:O	1:W:46:PRO:O	2.33	0.46
2:M:39:GLN:HG2	2:M:40:GLN:O	2.14	0.46
2:M:50:ILE:HG21	2:M:75:LEU:CD1	2.40	0.46
2:M:53:VAL:CG2	2:M:54:ASN:N	2.67	0.46
2:M:186:PRO:O	2:M:187:GLU:O	2.33	0.46
2:M:196:SER:HB3	2:M:209:THR:HG1	1.76	0.46
1:W:60:ILE:HD11	1:W:64:PHE:HB2	1.98	0.46
2:M:122:PHE:CD2	2:M:137:VAL:CG1	2.98	0.46
2:M:49:ILE:CG1	2:M:49:ILE:O	2.64	0.46
1:W:144:TYR:H	1:W:145:PRO:CD	2.28	0.46
1:W:18:ILE:HG23	1:W:80:LEU:CD2	2.37	0.46
2:M:155:ASP:HB2	2:M:192:HIS:CD2	2.51	0.45
1:W:143:PHE:CE2	1:W:176:TYR:HB3	2.50	0.45
2:M:144:TYR:CG	2:M:145:PRO:HD3	2.52	0.45
2:M:84:ASP:CB	2:M:106:LYS:HZ1	2.28	0.45
1:W:81:LEU:HA	1:W:109:VAL:HG11	1.99	0.45
2:M:90:CYS:O	2:M:101:PHE:HA	2.16	0.45
1:W:123:PRO:HB2	1:W:124:PRO:HD2	1.91	0.45
2:M:20:ILE:HG23	2:M:105:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:15:GLY:H	2:M:80:LEU:HG	1.81	0.45
1:W:41:HIS:CB	1:W:42:PRO:CD	2.79	0.45
2:M:157:SER:HA	2:M:158:PRO:HD2	1.76	0.45
2:M:39:GLN:N	2:M:49:ILE:HG23	2.32	0.45
1:W:110:LEU:CG	1:W:111:ARG:N	2.79	0.45
1:W:11:SER:OG	1:W:202:GLU:HG2	2.17	0.45
1:W:171:GLN:O	1:W:172:SER:C	2.54	0.45
2:M:160:LYS:CB	2:M:160:LYS:HZ3	2.25	0.45
2:M:16:GLN:HB3	2:M:17:SER:H	1.46	0.45
2:M:1:PCA:CD	2:M:2:SER:H	2.29	0.45
2:M:6:GLN:OE1	2:M:88:TYR:O	2.34	0.45
1:W:121:LEU:HD12	1:W:208:LYS:CB	2.46	0.45
1:W:117:PRO:CG	1:W:143:PHE:CD1	3.00	0.45
2:M:14:LEU:CB	2:M:111:GLY:HA3	2.47	0.45
2:M:214:GLU:HG3	2:M:215:CYS:O	2.17	0.45
1:W:79:GLY:C	1:W:80:LEU:O	2.54	0.45
2:M:62:ASP:C	2:M:62:ASP:OD2	2.54	0.45
1:W:136:LEU:HD21	1:W:189:TRP:CE3	2.51	0.45
1:W:135:THR:CG2	1:W:136:LEU:N	2.76	0.45
1:W:188:GLN:N	1:W:188:GLN:NE2	2.64	0.45
2:M:14:LEU:CD1	2:M:109:VAL:CG2	2.92	0.45
1:W:169:SER:CB	2:M:166:THR:HG23	2.36	0.45
1:W:138:CYS:HB3	1:W:152:TRP:HZ2	1.65	0.45
1:W:34:SER:O	1:W:35:ILE:CG1	2.60	0.45
1:W:67:SER:HB2	1:W:74:SER:HB3	1.98	0.45
1:W:95:SER:C	1:W:96:ASP:CG	2.75	0.45
2:M:88:TYR:CD1	2:M:106:LYS:CG	2.98	0.44
1:W:38:PHE:HD1	1:W:47:LYS:O	1.99	0.44
1:W:77:ILE:HG13	1:W:80:LEU:CD2	2.47	0.44
1:W:93:TYR:O	1:W:94:LEU:CG	2.65	0.44
2:M:83:GLU:CG	2:M:173:ASN:ND2	2.80	0.44
2:M:195:TYR:H	2:M:209:THR:HG22	1.81	0.44
1:W:154:ALA:CB	1:W:195:TYR:HA	2.46	0.44
2:M:123:PRO:HB2	2:M:124:PRO:HD2	1.99	0.44
2:M:39:GLN:N	2:M:49:ILE:CG2	2.80	0.44
1:W:81:LEU:HD22	1:W:84:ASP:CG	2.38	0.44
2:M:89:TYR:HE2	2:M:103:THR:OG1	1.99	0.44
2:M:186:PRO:O	2:M:190:LYS:HB2	2.18	0.44
2:M:195:TYR:C	2:M:209:THR:HG23	2.38	0.44
1:W:81:LEU:CG	1:W:82:PRO:CD	2.81	0.44
2:M:186:PRO:HA	2:M:189:TRP:CG	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:134:ALA:HB3	1:W:184:LEU:HB2	1.98	0.44
1:W:41:HIS:HB3	1:W:86:ALA:CB	2.48	0.44
1:W:169:SER:N	2:M:166:THR:HG21	2.32	0.44
1:W:6:GLN:HG2	1:W:103:SER:HB2	2.00	0.44
2:M:57:PRO:O	2:M:58:SER:C	2.55	0.44
2:M:37:TRP:CE2	2:M:90:CYS:HB2	2.53	0.44
1:W:14:PRO:HD2	1:W:16:GLN:HB2	2.00	0.44
1:W:185:THR:HB	1:W:186:PRO:CG	2.48	0.44
1:W:22:CYS:SG	1:W:90:CYS:CB	3.05	0.44
2:M:14:LEU:CD2	2:M:111:GLY:O	2.51	0.44
2:M:126:SER:N	2:M:129:LEU:HD12	2.33	0.44
2:M:152:TRP:NE1	2:M:180:SER:OG	2.01	0.44
2:M:51:TYR:O	2:M:53:VAL:N	2.51	0.44
1:W:143:PHE:CE2	1:W:177:ALA:N	2.86	0.43
1:W:135:THR:CA	1:W:183:SER:OG	2.66	0.43
2:M:18:VAL:O	2:M:76:THR:CA	2.66	0.43
2:M:52:GLU:HB2	2:M:55:LYS:CG	2.15	0.43
2:M:49:ILE:HD12	2:M:64:PHE:CD2	2.53	0.43
1:W:51:TYR:CE1	2:M:97:ASP:HB3	2.53	0.43
1:W:143:PHE:CE1	1:W:148:VAL:CG1	3.01	0.43
1:W:41:HIS:HA	1:W:86:ALA:O	2.17	0.43
1:W:95:SER:C	1:W:96:ASP:OD2	2.57	0.43
1:W:168:PRO:O	1:W:168:PRO:HG2	2.18	0.43
1:W:50:ILE:HG21	1:W:50:ILE:HD13	1.71	0.43
1:W:5:THR:O	1:W:22:CYS:CA	2.64	0.43
2:M:56:ARG:NH2	2:M:62:ASP:CA	2.75	0.43
1:W:200:THR:HA	1:W:205:THR:CA	2.43	0.43
2:M:26:SER:HA	2:M:30:GLY:C	2.39	0.43
1:W:122:PHE:N	1:W:122:PHE:CD1	2.87	0.43
1:W:119:VAL:CG2	1:W:197:CYS:SG	3.07	0.43
1:W:1:PCA:CD	1:W:2:SER:N	2.81	0.43
1:W:93:TYR:HA	1:W:99:PHE:HA	2.01	0.43
2:M:88:TYR:CD1	2:M:106:LYS:HB3	2.54	0.43
2:M:63:ARG:HD3	2:M:63:ARG:H	1.80	0.43
2:M:6:GLN:HG3	2:M:103:THR:C	2.39	0.43
2:M:63:ARG:HG2	2:M:78:SER:O	2.18	0.43
1:W:117:PRO:HG2	1:W:143:PHE:CD1	2.54	0.43
1:W:16:GLN:O	1:W:80:LEU:N	2.50	0.43
1:W:17:SER:HB3	1:W:78:SER:HA	2.01	0.43
1:W:81:LEU:HD22	1:W:84:ASP:OD1	2.19	0.43
2:M:153:LYS:HA	2:M:153:LYS:HZ3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:163:VAL:HG12	2:M:182:LEU:CA	2.48	0.43
2:M:24:GLY:HA3	2:M:29:VAL:CG2	2.48	0.43
2:M:57:PRO:HD2	2:M:60:VAL:HG11	2.01	0.43
2:M:56:ARG:CZ	2:M:60:VAL:O	2.67	0.43
1:W:144:TYR:CG	1:W:145:PRO:HD3	2.54	0.43
1:W:168:PRO:CB	1:W:178:ALA:HB2	2.48	0.43
1:W:136:LEU:HD21	1:W:189:TRP:HE3	1.83	0.43
1:W:56:ARG:CD	1:W:62:LEU:HB2	2.48	0.43
2:M:63:ARG:NH2	2:M:81:GLN:HG3	2.29	0.43
1:W:130:GLN:O	1:W:131:ALA:HB3	2.19	0.43
1:W:213:THR:CG2	1:W:214:GLU:N	2.74	0.43
2:M:38:TYR:HA	2:M:48:VAL:HA	2.01	0.42
2:M:85:GLU:O	2:M:85:GLU:CG	2.64	0.42
2:M:95:GLY:O	2:M:96:SER:CB	2.61	0.42
2:M:56:ARG:CZ	2:M:56:ARG:HB3	2.49	0.42
2:M:25:THR:O	2:M:30:GLY:HA3	2.18	0.42
2:M:7:PRO:HD2	2:M:21:SER:CB	2.46	0.42
1:W:118:THR:HG21	1:W:141:SER:HB3	1.96	0.42
2:M:62:ASP:C	2:M:64:PHE:H	2.07	0.42
1:W:2:SER:O	1:W:3:ALA:HB2	2.19	0.42
1:W:93:TYR:O	1:W:94:LEU:HG	2.18	0.42
2:M:37:TRP:CH2	2:M:90:CYS:HB2	2.53	0.42
2:M:89:TYR:HD2	2:M:103:THR:CB	2.30	0.42
2:M:8:PRO:O	2:M:9:SER:CB	2.63	0.42
1:W:2:SER:HA	1:W:100:VAL:HB	1.98	0.42
2:M:168:PRO:HA	2:M:177:ALA:O	2.19	0.42
2:M:50:ILE:CD1	2:M:50:ILE:C	2.88	0.42
1:W:130:GLN:CA	1:W:130:GLN:HE21	2.32	0.42
1:W:35:ILE:HA	1:W:92:SER:N	2.32	0.42
1:W:63:ARG:NH2	1:W:81:LEU:HD13	2.34	0.42
2:M:41:HIS:CE1	2:M:173:ASN:HB2	2.55	0.42
2:M:68:LYS:CG	2:M:70:GLY:H	2.32	0.42
1:W:130:GLN:CA	1:W:130:GLN:NE2	2.83	0.42
1:W:141:SER:OG	1:W:142:ASP:N	2.52	0.42
1:W:154:ALA:HB2	1:W:195:TYR:HA	2.02	0.42
1:W:38:PHE:CD1	1:W:47:LYS:O	2.72	0.42
1:W:60:ILE:HA	1:W:61:PRO:HD2	1.73	0.42
2:M:2:SER:O	2:M:3:ALA:CB	2.66	0.42
1:W:110:LEU:HD23	1:W:111:ARG:CG	2.48	0.42
1:W:20:VAL:C	1:W:74:SER:HA	2.37	0.42
2:M:153:LYS:NZ	2:M:153:LYS:CA	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:36:SER:OG	2:M:48:VAL:HG23	2.20	0.42
2:M:53:VAL:HG12	2:M:55:LYS:HZ3	1.83	0.42
1:W:134:ALA:H	1:W:185:THR:HA	1.84	0.42
1:W:188:GLN:H	1:W:188:GLN:NE2	2.18	0.42
1:W:155:ASP:CG	1:W:193:ARG:H	2.20	0.42
1:W:160:GLU:HA	1:W:163:VAL:HG13	2.02	0.42
2:M:14:LEU:HA	2:M:80:LEU:CG	2.48	0.41
2:M:151:ALA:O	2:M:197:CYS:HA	2.20	0.41
2:M:189:TRP:CE2	2:M:190:LYS:HG2	2.52	0.41
2:M:214:GLU:HG3	2:M:215:CYS:H	1.80	0.41
1:W:25:HIS:O	1:W:26:THR:C	2.58	0.41
1:W:37:TRP:CZ3	1:W:88:TYR:HB3	2.55	0.41
1:W:48:LEU:HD21	1:W:51:TYR:CB	2.50	0.41
2:M:168:PRO:HB3	2:M:178:ALA:HB2	2.02	0.41
2:M:37:TRP:CB	2:M:49:ILE:O	2.64	0.41
1:W:2:SER:H	1:W:100:VAL:HG21	1.82	0.41
1:W:23:ALA:HB2	1:W:72:THR:CG2	2.46	0.41
2:M:13:SER:O	2:M:16:GLN:CB	2.61	0.41
1:W:169:SER:CA	2:M:166:THR:CG2	2.98	0.41
1:W:101:PHE:HZ	2:M:46:PRO:HB2	1.78	0.41
1:W:134:ALA:N	1:W:185:THR:O	2.54	0.41
1:W:136:LEU:HG	1:W:184:LEU:HD11	2.02	0.41
1:W:20:VAL:HG12	1:W:75:LEU:CB	2.48	0.41
1:W:56:ARG:NH1	1:W:64:PHE:O	2.53	0.41
1:W:7:PRO:CD	1:W:21:SER:O	2.68	0.41
2:M:154:ALA:HB2	2:M:159:VAL:HG22	1.93	0.41
2:M:88:TYR:CE1	2:M:106:LYS:CG	2.80	0.41
2:M:14:LEU:HB2	2:M:111:GLY:CA	2.49	0.41
2:M:39:GLN:NE2	2:M:41:HIS:CD2	2.89	0.41
2:M:68:LYS:HG3	2:M:70:GLY:H	1.86	0.41
1:W:45:ALA:HA	1:W:46:PRO:HD2	1.93	0.41
1:W:63:ARG:HH22	1:W:81:LEU:HD13	1.86	0.41
1:W:202:GLU:O	1:W:203:GLY:C	2.59	0.41
1:W:57:PRO:O	1:W:58:SER:O	2.39	0.41
1:W:40:GLN:O	1:W:86:ALA:CA	2.69	0.41
1:W:116:ASN:HA	1:W:117:PRO:HD3	1.75	0.41
1:W:134:ALA:O	1:W:135:THR:CB	2.66	0.41
1:W:167:LYS:O	1:W:169:SER:N	2.54	0.41
1:W:6:GLN:CB	1:W:21:SER:O	2.68	0.41
1:W:37:TRP:CE2	1:W:90:CYS:SG	3.01	0.41
2:M:7:PRO:HA	2:M:8:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:124:PRO:HG3	1:W:129:LEU:HD21	1.96	0.41
1:W:190:LYS:HE3	1:W:190:LYS:HB2	1.66	0.41
1:W:19:THR:HG23	1:W:20:VAL:N	2.36	0.41
2:M:168:PRO:CA	2:M:177:ALA:O	2.69	0.41
1:W:117:PRO:HG3	1:W:143:PHE:CG	2.56	0.41
1:W:215:CYS:SG	2:M:214:GLU:C	2.96	0.41
1:W:33:ASN:OD1	1:W:68:LYS:HE2	2.21	0.41
2:M:51:TYR:C	2:M:53:VAL:H	2.24	0.40
1:W:135:THR:C	1:W:182:LEU:O	2.60	0.40
1:W:171:GLN:NE2	1:W:176:TYR:O	2.51	0.40
1:W:98:SER:O	1:W:99:PHE:HB2	2.21	0.40
2:M:173:ASN:OD1	2:M:174:ASN:N	2.55	0.40
2:M:82:ALA:O	2:M:85:GLU:HG2	2.21	0.40
2:M:20:ILE:CD1	2:M:106:LYS:HB2	2.51	0.40
1:W:12:GLY:HA3	1:W:108:THR:HB	2.03	0.40
1:W:144:TYR:CD1	1:W:145:PRO:CD	3.05	0.40
1:W:93:TYR:O	1:W:94:LEU:CB	2.69	0.40
2:M:80:LEU:HD21	2:M:109:VAL:HB	2.02	0.40
2:M:80:LEU:HD22	2:M:109:VAL:HB	2.01	0.40
2:M:140:ILE:O	2:M:177:ALA:HA	2.22	0.40
2:M:51:TYR:O	2:M:55:LYS:CA	2.69	0.40
2:M:93:TYR:CE1	2:M:94:GLU:O	2.74	0.40
1:W:171:GLN:HG2	1:W:171:GLN:O	2.21	0.40
1:W:57:PRO:O	1:W:58:SER:C	2.59	0.40
2:M:162:GLY:H	2:M:163:VAL:HG22	1.86	0.40
2:M:1:PCA:O	2:M:2:SER:CB	2.69	0.40
1:W:51:TYR:CE1	1:W:55:PHE:CE1	3.10	0.40
1:W:93:TYR:HA	1:W:99:PHE:HD1	1.66	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:78:SER:OG	1:W:78:SER:OG[4_646]	1.27	0.93
1:W:61:PRO:CA	1:W:216:SER:OG[3_654]	1.64	0.56
1:W:61:PRO:N	1:W:216:SER:OG[3_654]	1.64	0.56
1:W:61:PRO:CD	1:W:216:SER:OG[3_654]	1.91	0.29
1:W:78:SER:O	1:W:78:SER:O[4_646]	1.95	0.25
1:W:61:PRO:N	1:W:216:SER:CB[3_654]	2.07	0.13
1:W:31:ASP:CG	2:M:19:THR:OG1[4_546]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:95:GLY:O	2:M:202:GLU:OE1[4_546]	2.09	0.11
2:M:97:ASP:OD2	2:M:130:GLN:NE2[3_654]	2.12	0.08
2:M:32:TYR:OH	2:M:202:GLU:CA[4_546]	2.15	0.05

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	W	214/216 (99%)	118 (55%)	40 (19%)	56 (26%)	0	0
2	M	214/216 (99%)	141 (66%)	31 (14%)	42 (20%)	0	2
All	All	428/432 (99%)	259 (60%)	71 (17%)	98 (23%)	0	1

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	2	SER
1	W	3	ALA
1	W	9	SER
1	W	13	SER
1	W	14	PRO
1	W	26	THR
1	W	28	ASP
1	W	32	SER
1	W	35	ILE
1	W	42	PRO
1	W	46	PRO
1	W	52	ALA
1	W	53	VAL
1	W	54	THR
1	W	83	ASP
1	W	87	ASP
1	W	95	SER

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Mol	Chain	Res	Type
1	W	97	ALA
1	W	99	PHE
1	W	109	VAL
1	W	113	PRO
1	W	114	LYS
1	W	131	ALA
1	W	132	ASN
1	W	133	LYS
1	W	135	THR
1	W	145	PRO
1	W	172	SER
1	W	173	ASN
1	W	185	THR
1	W	186	PRO
1	W	205	THR
1	W	210	VAL
1	W	212	PRO
1	W	213	THR
2	M	3	ALA
2	M	9	SER
2	M	42	ALA
2	M	44	LYS
2	M	45	ALA
2	M	46	PRO
2	M	52	GLU
2	M	53	VAL
2	M	67	SER
2	M	106	LYS
2	M	119	VAL
2	M	147	ALA
2	M	170	LYS
2	M	174	ASN
2	M	204	SER
2	M	214	GLU
2	M	215	CYS
1	W	27	SER
1	W	58	SER
1	W	80	LEU
1	W	106	LYS
1	W	123	PRO
1	W	136	LEU
1	W	142	ASP

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Mol	Chain	Res	Type
1	W	202	GLU
1	W	203	GLY
1	W	204	SER
2	M	4	LEU
2	M	50	ILE
2	M	63	ARG
2	M	82	ALA
2	M	96	SER
2	M	127	GLU
2	M	173	ASN
1	W	103	SER
1	W	147	ALA
1	W	160	GLU
2	M	34	TYR
2	M	126	SER
2	M	161	ALA
2	M	165	THR
2	M	193	ARG
1	W	124	PRO
1	W	144	TYR
2	M	2	SER
2	M	31	GLY
2	M	105	THR
2	M	187	GLU
1	W	10	VAL
1	W	82	PRO
1	W	215	CYS
2	M	47	LYS
2	M	169	SER
2	M	171	GLN
1	W	168	PRO
2	M	212	PRO
1	W	81	LEU
2	M	29	VAL
2	M	162	GLY
1	W	211	ALA
2	M	158	PRO
2	M	57	PRO
2	M	15	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	183/183 (100%)	103 (56%)	80 (44%)	0	0
2	M	180/180 (100%)	105 (58%)	75 (42%)	0	0
All	All	363/363 (100%)	208 (57%)	155 (43%)	0	0

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	4	LEU
1	W	6	GLN
1	W	13	SER
1	W	17	SER
1	W	18	ILE
1	W	19	THR
1	W	21	SER
1	W	27	SER
1	W	29	VAL
1	W	32	SER
1	W	34	SER
1	W	35	ILE
1	W	36	SER
1	W	39	GLN
1	W	43	ASP
1	W	51	TYR
1	W	55	PHE
1	W	62	LEU
1	W	63	ARG
1	W	68	LYS
1	W	69	SER
1	W	74	SER
1	W	75	LEU
1	W	76	THR
1	W	77	ILE
1	W	78	SER
1	W	80	LEU

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Mol	Chain	Res	Type
1	W	81	LEU
1	W	85	GLU
1	W	87	ASP
1	W	91	MET
1	W	92	SER
1	W	93	TYR
1	W	94	LEU
1	W	95	SER
1	W	96	ASP
1	W	99	PHE
1	W	101	PHE
1	W	105	THR
1	W	108	THR
1	W	110	LEU
1	W	112	GLN
1	W	118	THR
1	W	120	THR
1	W	121	LEU
1	W	122	PHE
1	W	126	SER
1	W	127	GLU
1	W	128	GLU
1	W	132	ASN
1	W	133	LYS
1	W	136	LEU
1	W	138	CYS
1	W	139	LEU
1	W	142	ASP
1	W	143	PHE
1	W	144	TYR
1	W	148	VAL
1	W	153	LYS
1	W	171	GLN
1	W	172	SER
1	W	173	ASN
1	W	174	ASN
1	W	181	TYR
1	W	182	LEU
1	W	183	SER
1	W	185	THR
1	W	188	GLN
1	W	190	LYS

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Mol	Chain	Res	Type
1	W	191	SER
1	W	194	SER
1	W	196	SER
1	W	198	GLN
1	W	199	VAL
1	W	200	THR
1	W	202	GLU
1	W	205	THR
1	W	209	THR
1	W	214	GLU
1	W	216	SER
2	M	5	THR
2	M	6	GLN
2	M	9	SER
2	M	14	LEU
2	M	16	GLN
2	M	17	SER
2	M	20	ILE
2	M	21	SER
2	M	22	CYS
2	M	23	THR
2	M	25	THR
2	M	27	SER
2	M	29	VAL
2	M	35	VAL
2	M	36	SER
2	M	40	GLN
2	M	41	HIS
2	M	46	PRO
2	M	47	LYS
2	M	49	ILE
2	M	50	ILE
2	M	54	ASN
2	M	55	LYS
2	M	63	ARG
2	M	65	SER
2	M	67	SER
2	M	68	LYS
2	M	72	THR
2	M	75	LEU
2	M	80	LEU
2	M	81	GLN

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Mol	Chain	Res	Type
2	M	84	ASP
2	M	85	GLU
2	M	91	SER
2	M	98	ASN
2	M	99	PHE
2	M	100	VAL
2	M	101	PHE
2	M	110	LEU
2	M	112	GLN
2	M	122	PHE
2	M	124	PRO
2	M	130	GLN
2	M	133	LYS
2	M	136	LEU
2	M	137	VAL
2	M	140	ILE
2	M	142	ASP
2	M	148	VAL
2	M	153	LYS
2	M	155	ASP
2	M	157	SER
2	M	160	LYS
2	M	163	VAL
2	M	165	THR
2	M	166	THR
2	M	167	LYS
2	M	169	SER
2	M	172	SER
2	M	175	LYS
2	M	182	LEU
2	M	183	SER
2	M	184	LEU
2	M	185	THR
2	M	187	GLU
2	M	188	GLN
2	M	189	TRP
2	M	192	HIS
2	M	196	SER
2	M	199	VAL
2	M	200	THR
2	M	204	SER
2	M	206	VAL

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Mol	Chain	Res	Type
2	M	210	VAL
2	M	214	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	W	6	GLN
1	W	16	GLN
1	W	40	GLN
1	W	41	HIS
1	W	112	GLN
1	W	130	GLN
1	W	171	GLN
1	W	173	ASN
1	W	188	GLN
1	W	192	HIS
1	W	201	HIS
2	M	39	GLN
2	M	98	ASN
2	M	171	GLN
2	M	192	HIS
2	M	198	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	W	1	1	7,8,9	2.68	1 (14%)	9,10,12	4.20	3 (33%)
2	PCA	M	1	2	7,8,9	2.83	1 (14%)	9,10,12	2.30	4 (44%)

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
1	PCA	W	1	1	-	0/0/11/13	0/1/1/1
2	PCA	M	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	PCA	CD-N	7.07	1.53	1.34
1	W	1	PCA	CD-N	6.88	1.53	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	1	PCA	OE-CD-N	-11.54	97.95	124.86
2	M	1	PCA	CB-CA-C	-3.88	107.36	112.70
2	M	1	PCA	OE-CD-CG	-3.73	120.26	126.76
1	W	1	PCA	OE-CD-CG	-3.11	121.33	126.76
1	W	1	PCA	CA-N-CD	-2.72	104.27	113.58
2	M	1	PCA	OE-CD-N	-2.26	119.60	124.86
2	M	1	PCA	CA-N-CD	-2.01	106.70	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	W	1	PCA	5	0
2	M	1	PCA	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.