



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:18 pm BST

PDB ID : 2CNA
Title : THE COVALENT AND THREE-DIMENSIONAL STRUCTURE OF
CONCANAVALIN A, IV.ATOMIC COORDINATES,HYDROGEN BOND-
ING,AND QUATERNARY STRUCTURE
Authors : Reekejunior, G.N.; Becker, J.W.; Edelman, G.M.
Deposited on : 1975-04-01
Resolution : 2.00 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
Xtriage (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

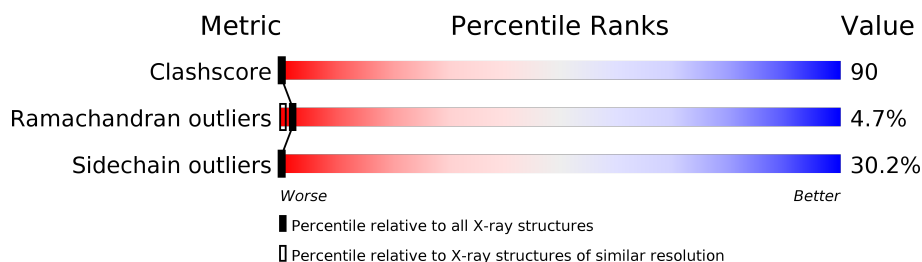
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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	A	237	<div> <div></div> <div>10%</div> <div>41%</div> <div>36%</div> <div>14%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1813 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 CONCANAVALIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1807	1139	300	366	2			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

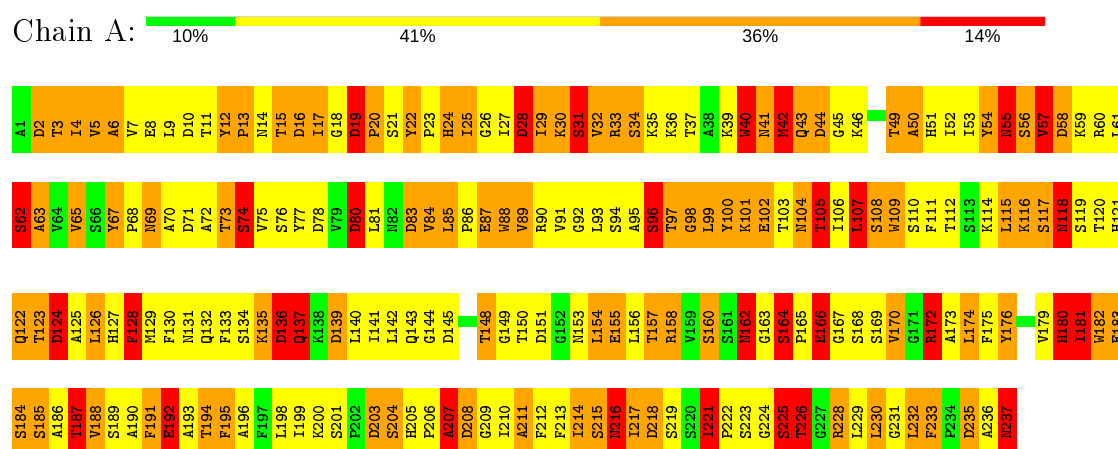
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		

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: CONCAVALIN A



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.91Å 87.23Å 63.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1813	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: CA, MN

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	1.22	22/1849 (1.2%)	2.32	151/2519 (6.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	TRP	NE1-CE2	-7.41	1.27	1.37
1	A	182	TRP	NE1-CE2	-7.37	1.27	1.37
1	A	40	TRP	NE1-CE2	-7.36	1.27	1.37
1	A	109	TRP	NE1-CE2	-7.35	1.27	1.37
1	A	118	ASN	CG-OD1	7.04	1.39	1.24
1	A	162	ASN	CG-OD1	7.03	1.39	1.24
1	A	41	ASN	CG-OD1	7.02	1.39	1.24
1	A	216	ASN	CG-OD1	7.02	1.39	1.24
1	A	153	ASN	CG-OD1	7.01	1.39	1.24
1	A	131	ASN	CG-OD1	7.00	1.39	1.24
1	A	69	ASN	CG-OD1	7.00	1.39	1.24
1	A	55	ASN	CG-OD1	7.00	1.39	1.24
1	A	14	ASN	CG-OD1	6.97	1.39	1.24
1	A	237	ASN	CG-OD1	6.96	1.39	1.24
1	A	104	ASN	CG-OD1	6.95	1.39	1.24
1	A	192	GLU	CD-OE1	-5.30	1.19	1.25
1	A	8	GLU	CD-OE1	-5.29	1.19	1.25
1	A	155	GLU	CD-OE1	-5.27	1.19	1.25
1	A	102	GLU	CD-OE1	-5.26	1.19	1.25
1	A	166	GLU	CD-OE1	-5.20	1.20	1.25
1	A	183	GLU	CD-OE1	-5.19	1.20	1.25
1	A	87	GLU	CD-OE1	-5.12	1.20	1.25

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	SER	N-CA-CB	-18.07	83.40	110.50
1	A	158	ARG	N-CA-CB	17.54	142.16	110.60
1	A	158	ARG	CB-CA-C	-16.56	77.27	110.40
1	A	95	ALA	CB-CA-C	-15.20	87.30	110.10
1	A	6	ALA	CB-CA-C	-12.33	91.60	110.10
1	A	182	TRP	CB-CA-C	-10.90	88.59	110.40
1	A	125	ALA	CB-CA-C	-10.64	94.14	110.10
1	A	99	LEU	N-CA-CB	-10.22	89.96	110.40
1	A	99	LEU	CB-CA-C	-9.93	91.34	110.20
1	A	180	HIS	N-CA-CB	9.27	127.29	110.60
1	A	121	HIS	CB-CA-C	-9.17	92.05	110.40
1	A	187	THR	N-CA-CB	-8.89	93.40	110.30
1	A	186	ALA	CB-CA-C	-8.55	97.28	110.10
1	A	182	TRP	N-CA-CB	-8.37	95.53	110.60
1	A	105	THR	N-CA-CB	-8.37	94.41	110.30
1	A	184	SER	N-CA-CB	8.31	122.97	110.50
1	A	193	ALA	N-CA-CB	8.29	121.71	110.10
1	A	63	ALA	CB-CA-C	-8.28	97.68	110.10
1	A	41	ASN	N-CA-CB	-8.25	95.75	110.60
1	A	54	TYR	N-CA-CB	-8.23	95.79	110.60
1	A	122	GLN	CB-CA-C	-8.12	94.16	110.40
1	A	101	LYS	N-CA-CB	-8.11	96.00	110.60
1	A	116	LYS	N-CA-CB	-8.10	96.03	110.60
1	A	122	GLN	N-CA-CB	8.07	125.13	110.60
1	A	181	ILE	CB-CA-C	7.91	127.42	111.60
1	A	223	SER	CB-CA-C	7.82	124.96	110.10
1	A	137	GLN	N-CA-CB	7.68	124.42	110.60
1	A	125	ALA	N-CA-C	7.64	131.63	111.00
1	A	213	PHE	N-CA-CB	-7.52	97.06	110.60
1	A	57	VAL	N-CA-CB	7.43	127.85	111.50
1	A	40	TRP	N-CA-CB	-7.42	97.25	110.60
1	A	28	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	31	SER	N-CA-CB	-7.40	99.40	110.50
1	A	193	ALA	CB-CA-C	-7.40	99.00	110.10
1	A	58	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	44	ASP	CB-CG-OD1	7.37	124.94	118.30
1	A	78	ASP	N-CA-CB	7.37	123.86	110.60
1	A	71	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	83	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	124	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	10	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	53	ILE	CB-CA-C	-7.32	96.95	111.60
1	A	80	ASP	CB-CG-OD1	7.32	124.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	203	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	16	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	128	PHE	CB-CA-C	7.29	124.99	110.40
1	A	235	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	136	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	145	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	195	PHE	N-CA-CB	7.27	123.69	110.60
1	A	139	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	78	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	218	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	172	ARG	CB-CA-C	-7.24	95.92	110.40
1	A	205	HIS	CB-CA-C	7.24	124.88	110.40
1	A	208	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	2	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	19	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	117	SER	N-CA-CB	-7.03	99.95	110.50
1	A	119	SER	N-CA-CB	-7.03	99.95	110.50
1	A	12	TYR	N-CA-CB	7.02	123.23	110.60
1	A	188	VAL	N-CA-CB	-7.02	96.06	111.50
1	A	125	ALA	N-CA-CB	-6.88	100.47	110.10
1	A	126	LEU	N-CA-C	6.88	129.57	111.00
1	A	72	ALA	CB-CA-C	-6.81	99.89	110.10
1	A	121	HIS	N-CA-CB	6.73	122.71	110.60
1	A	12	TYR	CB-CA-C	-6.64	97.13	110.40
1	A	78	ASP	CB-CA-C	-6.58	97.24	110.40
1	A	22	TYR	N-CA-CB	-6.57	98.78	110.60
1	A	7	VAL	N-CA-C	-6.56	93.29	111.00
1	A	228	ARG	N-CA-CB	-6.56	98.80	110.60
1	A	108	SER	N-CA-CB	-6.55	100.68	110.50
1	A	216	ASN	CB-CA-C	6.54	123.47	110.40
1	A	118	ASN	CB-CA-C	-6.50	97.40	110.40
1	A	107	LEU	CB-CA-C	6.49	122.54	110.20
1	A	126	LEU	N-CA-CB	-6.30	97.79	110.40
1	A	154	LEU	N-CA-CB	6.26	122.92	110.40
1	A	226	THR	N-CA-CB	6.26	122.19	110.30
1	A	81	LEU	CB-CA-C	6.24	122.05	110.20
1	A	194	THR	N-CA-CB	-6.22	98.48	110.30
1	A	136	ASP	CB-CA-C	6.22	122.83	110.40
1	A	144	GLY	N-CA-C	6.21	128.63	113.10
1	A	43	GLN	N-CA-CB	-6.21	99.42	110.60
1	A	164	SER	N-CA-CB	-6.18	101.22	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ILE	N-CA-CB	-6.15	96.66	110.80
1	A	95	ALA	N-CA-CB	6.10	118.64	110.10
1	A	221	ILE	CB-CA-C	-6.08	99.43	111.60
1	A	24	HIS	N-CA-CB	-5.99	99.82	110.60
1	A	37	THR	N-CA-CB	5.99	121.68	110.30
1	A	215	SER	N-CA-CB	-5.99	101.52	110.50
1	A	49	THR	CB-CA-C	-5.98	95.45	111.60
1	A	62	SER	CB-CA-C	-5.97	98.75	110.10
1	A	6	ALA	N-CA-CB	5.94	118.42	110.10
1	A	131	ASN	N-CA-CB	-5.91	99.96	110.60
1	A	163	GLY	N-CA-C	-5.88	98.40	113.10
1	A	213	PHE	N-CA-C	5.86	126.83	111.00
1	A	96	SER	N-CA-C	5.84	126.76	111.00
1	A	135	LYS	N-CA-C	-5.82	95.29	111.00
1	A	155	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	A	192	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	166	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	A	102	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	A	87	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	8	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	225	SER	CB-CA-C	5.75	121.02	110.10
1	A	25	ILE	CB-CA-C	-5.73	100.14	111.60
1	A	43	GLN	CB-CA-C	5.71	121.82	110.40
1	A	72	ALA	N-CA-C	5.70	126.38	111.00
1	A	183	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	A	115	LEU	N-CA-CB	-5.69	99.02	110.40
1	A	225	SER	N-CA-C	-5.62	95.82	111.00
1	A	99	LEU	N-CA-C	-5.61	95.86	111.00
1	A	124	ASP	N-CA-C	5.53	125.94	111.00
1	A	50	ALA	N-CA-CB	-5.51	102.38	110.10
1	A	74	SER	CB-CA-C	5.49	120.53	110.10
1	A	54	TYR	CB-CA-C	-5.47	99.46	110.40
1	A	74	SER	N-CA-CB	-5.45	102.33	110.50
1	A	235	ASP	N-CA-CB	-5.42	100.85	110.60
1	A	42	MET	N-CA-CB	-5.41	100.87	110.60
1	A	190	ALA	N-CA-CB	-5.37	102.58	110.10
1	A	19	ASP	N-CA-CB	5.25	120.05	110.60
1	A	84	VAL	CB-CA-C	-5.25	101.44	111.40
1	A	192	GLU	N-CA-CB	5.24	120.04	110.60
1	A	211	ALA	N-CA-CB	-5.24	102.76	110.10
1	A	154	LEU	N-CA-C	-5.23	96.88	111.00
1	A	207	ALA	N-CA-C	5.20	125.04	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	HIS	CB-CA-C	-5.20	100.00	110.40
1	A	204	SER	N-CA-CB	-5.19	102.72	110.50
1	A	192	GLU	CG-CD-OE2	-5.18	107.95	118.30
1	A	155	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	102	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	166	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	8	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	148	THR	N-CA-CB	5.14	120.06	110.30
1	A	214	ILE	CB-CA-C	-5.14	101.33	111.60
1	A	87	GLU	CG-CD-OE2	-5.13	108.05	118.30
1	A	183	GLU	CG-CD-OE2	-5.13	108.05	118.30
1	A	104	ASN	N-CA-CB	5.11	119.79	110.60
1	A	2	ASP	N-CA-CB	5.10	119.79	110.60
1	A	22	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	100	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	A	5	VAL	N-CA-C	-5.09	97.27	111.00
1	A	54	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	58	ASP	CB-CA-C	-5.08	100.24	110.40
1	A	29	ILE	CB-CA-C	-5.07	101.47	111.60
1	A	12	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	A	176	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	67	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	77	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	176	TYR	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

There are no planarity outliers.

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	1807	0	1746	320	4
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	0	1	0
All	All	1813	0	1746	320	4

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 90.

All (320) 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:A:11:THR:HB	1:A:42:MET:CE	1.61	1.31
1:A:174:LEU:N	1:A:174:LEU:HD23	1.44	1.25
1:A:85:LEU:HD11	1:A:214:ILE:HG21	1.20	1.19
1:A:116:LYS:HD3	1:A:188:VAL:HG12	1.27	1.16
1:A:110:SER:OG	1:A:194:THR:HG22	1.42	1.16
1:A:19:ASP:HB3	1:A:24:HIS:CE1	1.89	1.06
1:A:11:THR:HB	1:A:42:MET:HE1	1.07	1.06
1:A:97:THR:HG22	1:A:169:SER:H	1.17	1.06
1:A:116:LYS:HB2	1:A:188:VAL:O	1.54	1.05
1:A:216:ASN:OD1	1:A:216:ASN:N	1.87	1.05
1:A:54:TYR:CD2	1:A:55:ASN:N	2.25	1.05
1:A:174:LEU:CD2	1:A:174:LEU:N	2.14	1.02
1:A:210:ILE:HG23	1:A:211:ALA:H	1.25	1.02
1:A:11:THR:CB	1:A:42:MET:CE	2.37	1.01
1:A:36:LYS:HD3	1:A:75:VAL:HG23	1.43	1.00
1:A:90:ARG:HD2	1:A:217:ILE:HA	1.44	0.99
1:A:88:TRP:CE2	1:A:180:HIS:NE2	2.31	0.99
1:A:11:THR:CB	1:A:42:MET:HE1	1.92	0.99
1:A:191:PHE:HE1	1:A:214:ILE:HD11	1.27	0.98
1:A:143:GLN:OE1	1:A:172:ARG:HD2	1.64	0.98
1:A:56:SER:O	1:A:59:LYS:HG3	1.63	0.97
1:A:143:GLN:OE1	1:A:172:ARG:CD	2.14	0.96
1:A:137:GLN:HG3	1:A:140:LEU:HD12	1.48	0.95
1:A:142:LEU:HD23	1:A:173:ALA:HB2	1.46	0.94
1:A:210:ILE:CG2	1:A:211:ALA:N	2.30	0.94
1:A:133:PHE:CD2	1:A:154:LEU:HB2	2.03	0.92
1:A:4:ILE:HG12	1:A:5:VAL:N	1.84	0.92
1:A:19:ASP:HB3	1:A:24:HIS:NE2	1.85	0.92
1:A:173:ALA:C	1:A:174:LEU:HD23	1.89	0.91
1:A:174:LEU:H	1:A:174:LEU:HD23	1.29	0.91
1:A:128:PHE:CD1	1:A:175:PHE:CG	2.57	0.91
1:A:12:TYR:CE2	1:A:100:TYR:CE1	2.59	0.91
1:A:133:PHE:CE2	1:A:154:LEU:HB2	2.06	0.90
1:A:105:THR:HB	1:A:155:GLU:OE1	1.72	0.89
1:A:229:LEU:O	1:A:231:GLY:N	2.05	0.89
1:A:85:LEU:HD11	1:A:214:ILE:CG2	2.02	0.89
1:A:158:ARG:HB2	1:A:166:GLU:HG2	1.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:CE1	1:A:175:PHE:HB2	2.08	0.88
1:A:110:SER:OG	1:A:194:THR:CG2	2.22	0.88
1:A:103:THR:HG22	1:A:105:THR:HG22	1.56	0.86
1:A:19:ASP:CB	1:A:24:HIS:CE1	2.59	0.85
1:A:134:SER:OG	1:A:137:GLN:N	2.10	0.85
1:A:11:THR:HG22	1:A:42:MET:HE2	1.55	0.85
1:A:88:TRP:CD2	1:A:180:HIS:CD2	2.66	0.84
1:A:116:LYS:HD3	1:A:188:VAL:CG1	2.07	0.84
1:A:117:SER:HB2	1:A:123:THR:HG21	1.58	0.84
1:A:225:SER:HB3	1:A:231:GLY:HA2	1.58	0.83
1:A:93:LEU:HB3	1:A:156:LEU:HD11	1.59	0.82
1:A:162:ASN:H	1:A:162:ASN:ND2	1.77	0.82
1:A:143:GLN:N	1:A:172:ARG:O	2.12	0.81
1:A:88:TRP:CE2	1:A:180:HIS:CD2	2.69	0.81
1:A:173:ALA:C	1:A:174:LEU:CD2	2.46	0.81
1:A:210:ILE:HG23	1:A:211:ALA:N	1.93	0.80
1:A:25:ILE:HG21	1:A:65:VAL:HG21	1.62	0.80
1:A:54:TYR:CD2	1:A:54:TYR:C	2.55	0.80
1:A:133:PHE:HD2	1:A:154:LEU:N	1.79	0.79
1:A:85:LEU:CD1	1:A:214:ILE:HG21	2.09	0.79
1:A:133:PHE:CE2	1:A:154:LEU:CB	2.65	0.79
1:A:51:HIS:C	1:A:52:ILE:HG13	2.03	0.78
1:A:128:PHE:CD1	1:A:175:PHE:CD1	2.71	0.78
1:A:85:LEU:HD13	1:A:89:VAL:HG21	1.66	0.78
1:A:12:TYR:HB2	1:A:207:ALA:O	1.84	0.78
1:A:117:SER:CB	1:A:123:THR:HG21	2.14	0.78
1:A:11:THR:CG2	1:A:42:MET:HE2	2.13	0.78
1:A:89:VAL:HG22	1:A:215:SER:O	1.83	0.77
1:A:191:PHE:O	1:A:191:PHE:HD2	1.67	0.77
1:A:88:TRP:NE1	1:A:180:HIS:NE2	2.30	0.77
1:A:133:PHE:CD2	1:A:154:LEU:N	2.53	0.76
1:A:143:GLN:OE1	1:A:172:ARG:HD3	1.86	0.76
1:A:191:PHE:CE1	1:A:214:ILE:HD11	2.16	0.76
1:A:210:ILE:HG22	1:A:211:ALA:N	2.01	0.76
1:A:11:THR:CG2	1:A:42:MET:CE	2.64	0.75
1:A:65:VAL:O	1:A:73:THR:HG23	1.87	0.75
1:A:56:SER:O	1:A:59:LYS:CG	2.33	0.75
1:A:97:THR:CG2	1:A:167:GLY:HA2	2.16	0.75
1:A:105:THR:HG23	1:A:198:LEU:O	1.86	0.74
1:A:102:GLU:HG2	1:A:199:ILE:HG23	1.69	0.74
1:A:133:PHE:CD2	1:A:154:LEU:CB	2.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HG2	1:A:225:SER:OG	1.87	0.74
1:A:179:VAL:HG12	1:A:181:ILE:HD13	1.68	0.74
1:A:162:ASN:N	1:A:162:ASN:ND2	2.34	0.74
1:A:128:PHE:CE1	1:A:175:PHE:CB	2.71	0.74
1:A:187:THR:HG23	1:A:188:VAL:HG23	1.70	0.74
1:A:128:PHE:CE1	1:A:175:PHE:CG	2.77	0.73
1:A:162:ASN:HD22	1:A:162:ASN:N	1.87	0.72
1:A:55:ASN:O	1:A:59:LYS:N	2.21	0.72
1:A:141:ILE:O	1:A:173:ALA:HA	1.89	0.72
1:A:11:THR:O	1:A:13:PRO:HD3	1.90	0.71
1:A:36:LYS:HD2	1:A:76:SER:O	1.88	0.71
1:A:122:GLN:O	1:A:122:GLN:HG2	1.90	0.71
1:A:124:ASP:OD2	1:A:124:ASP:N	2.23	0.71
1:A:89:VAL:HG21	1:A:214:ILE:CG2	2.19	0.71
1:A:191:PHE:C	1:A:191:PHE:CD2	2.63	0.71
1:A:222:PRO:CD	1:A:225:SER:OG	2.39	0.71
1:A:105:THR:CG2	1:A:198:LEU:O	2.40	0.70
1:A:97:THR:HG22	1:A:169:SER:N	2.01	0.70
1:A:142:LEU:HD23	1:A:173:ALA:CB	2.20	0.70
1:A:157:THR:HG23	1:A:158:ARG:N	2.06	0.70
1:A:191:PHE:C	1:A:191:PHE:HD2	1.94	0.70
1:A:128:PHE:HD1	1:A:175:PHE:CD1	2.09	0.70
1:A:36:LYS:HD3	1:A:75:VAL:CG2	2.21	0.69
1:A:187:THR:CG2	1:A:188:VAL:HG23	2.23	0.69
1:A:179:VAL:HG12	1:A:181:ILE:CD1	2.22	0.69
1:A:89:VAL:HG12	1:A:179:VAL:HB	1.73	0.69
1:A:105:THR:HG23	1:A:198:LEU:HB3	1.75	0.68
1:A:107:LEU:HD23	1:A:107:LEU:N	2.09	0.68
1:A:222:PRO:HD2	1:A:225:SER:OG	1.93	0.68
1:A:89:VAL:CG2	1:A:215:SER:O	2.42	0.67
1:A:44:ASP:C	1:A:44:ASP:OD2	2.32	0.67
1:A:33:ARG:HE	1:A:237:ASN:HB2	1.60	0.67
1:A:116:LYS:CD	1:A:188:VAL:HG12	2.16	0.67
1:A:210:ILE:CG2	1:A:211:ALA:H	1.92	0.67
1:A:54:TYR:CD2	1:A:55:ASN:CA	2.78	0.67
1:A:55:ASN:HB2	1:A:189:SER:O	1.96	0.66
1:A:97:THR:HG21	1:A:167:GLY:HA2	1.78	0.66
1:A:222:PRO:HG2	1:A:225:SER:HG	1.60	0.65
1:A:173:ALA:CA	1:A:174:LEU:HD23	2.26	0.65
1:A:25:ILE:HD12	1:A:75:VAL:HG12	1.79	0.65
1:A:106:ILE:CD1	1:A:156:LEU:HG	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HA	1:A:59:LYS:HG2	1.80	0.64
1:A:103:THR:HG22	1:A:105:THR:CG2	2.25	0.64
1:A:148:THR:HG22	1:A:154:LEU:CD1	2.28	0.64
1:A:221:ILE:HG22	1:A:225:SER:CB	2.29	0.63
1:A:187:THR:C	1:A:188:VAL:HG23	2.18	0.63
1:A:222:PRO:CG	1:A:225:SER:OG	2.46	0.63
1:A:93:LEU:N	1:A:173:ALA:O	2.31	0.63
1:A:224:GLY:C	1:A:226:THR:H	2.02	0.62
1:A:25:ILE:HD13	1:A:65:VAL:HG23	1.79	0.62
1:A:224:GLY:C	1:A:226:THR:N	2.48	0.62
1:A:106:ILE:C	1:A:107:LEU:HD23	2.20	0.61
1:A:11:THR:CB	1:A:42:MET:HE2	2.24	0.61
1:A:96:SER:HB2	1:A:230:LEU:HA	1.82	0.61
1:A:85:LEU:HD22	1:A:86:PRO:HD2	1.82	0.61
1:A:215:SER:OG	1:A:219:SER:HB2	2.01	0.60
1:A:54:TYR:CG	1:A:55:ASN:N	2.68	0.60
1:A:28:ASP:HB3	1:A:31:SER:O	2.02	0.60
1:A:182:TRP:CG	1:A:183:GLU:N	2.70	0.60
1:A:17:ILE:O	1:A:33:ARG:NH1	2.35	0.60
1:A:157:THR:CG2	1:A:158:ARG:N	2.63	0.60
1:A:11:THR:CG2	1:A:42:MET:HE1	2.31	0.60
1:A:92:GLY:HA2	1:A:174:LEU:HA	1.83	0.60
1:A:183:GLU:HG2	1:A:184:SER:H	1.67	0.60
1:A:56:SER:O	1:A:57:VAL:C	2.39	0.60
1:A:9:LEU:O	1:A:209:GLY:HA3	2.02	0.59
1:A:134:SER:HG	1:A:137:GLN:H	1.50	0.59
1:A:148:THR:HG22	1:A:154:LEU:HD13	1.84	0.59
1:A:85:LEU:CD1	1:A:89:VAL:HG21	2.31	0.59
1:A:97:THR:HG23	1:A:167:GLY:HA2	1.84	0.59
1:A:100:TYR:CB	1:A:207:ALA:HA	2.32	0.59
1:A:44:ASP:OD2	1:A:45:GLY:N	2.36	0.58
1:A:12:TYR:CE2	1:A:100:TYR:CD1	2.91	0.58
1:A:133:PHE:CD2	1:A:154:LEU:CA	2.85	0.58
1:A:93:LEU:O	1:A:172:ARG:HB3	2.03	0.58
1:A:221:ILE:CG2	1:A:225:SER:CB	2.82	0.58
1:A:158:ARG:O	1:A:166:GLU:HB3	2.04	0.58
1:A:26:GLY:C	1:A:27:ILE:HD13	2.24	0.58
1:A:17:ILE:HG22	1:A:18:GLY:N	2.19	0.58
1:A:55:ASN:ND2	1:A:58:ASP:H	2.02	0.57
1:A:118:ASN:ND2	1:A:185:SER:O	2.38	0.57
1:A:123:THR:C	1:A:124:ASP:OD2	2.43	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:CG1	1:A:179:VAL:HB	2.35	0.57
1:A:85:LEU:HD13	1:A:89:VAL:CG2	2.34	0.57
1:A:128:PHE:CD1	1:A:175:PHE:CD2	2.92	0.57
1:A:137:GLN:OE1	1:A:137:GLN:HA	1.95	0.57
1:A:173:ALA:HA	1:A:174:LEU:HD23	1.86	0.56
1:A:33:ARG:HE	1:A:237:ASN:CB	2.18	0.56
1:A:141:ILE:O	1:A:174:LEU:HD23	2.06	0.56
1:A:27:ILE:HD13	1:A:27:ILE:N	2.21	0.56
1:A:102:GLU:CB	1:A:207:ALA:HB3	2.35	0.56
1:A:51:HIS:C	1:A:52:ILE:CG1	2.74	0.56
1:A:236:ALA:C	1:A:237:ASN:CG	2.63	0.56
1:A:112:THR:HB	1:A:192:GLU:HG2	1.86	0.56
1:A:173:ALA:C	1:A:174:LEU:HD22	2.24	0.56
1:A:19:ASP:O	1:A:20:PRO:O	2.23	0.55
1:A:211:ALA:HB2	1:A:230:LEU:HD23	1.87	0.55
1:A:4:ILE:HD11	1:A:6:ALA:HB2	1.87	0.55
1:A:12:TYR:CD2	1:A:100:TYR:CD1	2.94	0.55
1:A:198:LEU:HD23	1:A:198:LEU:C	2.26	0.55
1:A:98:GLY:HA2	1:A:168:SER:HA	1.88	0.55
1:A:12:TYR:HE2	1:A:100:TYR:CE1	2.21	0.55
1:A:11:THR:O	1:A:13:PRO:CD	2.54	0.55
1:A:211:ALA:HB1	1:A:232:LEU:HD21	1.90	0.53
1:A:27:ILE:CG2	1:A:61:LEU:HD23	2.38	0.53
1:A:27:ILE:HG23	1:A:61:LEU:HD23	1.91	0.53
1:A:54:TYR:C	1:A:54:TYR:HD2	2.08	0.53
1:A:80:ASP:O	1:A:84:VAL:HG23	2.09	0.53
1:A:28:ASP:N	1:A:28:ASP:OD2	2.42	0.52
1:A:12:TYR:CE2	1:A:100:TYR:HE1	2.21	0.52
1:A:162:ASN:HD22	1:A:162:ASN:H	1.47	0.52
1:A:102:GLU:HB3	1:A:207:ALA:HB3	1.91	0.52
1:A:54:TYR:HD2	1:A:55:ASN:N	2.02	0.52
1:A:133:PHE:CE2	1:A:154:LEU:HB3	2.44	0.52
1:A:49:THR:HA	1:A:196:ALA:HA	1.92	0.52
1:A:29:ILE:O	1:A:30:LYS:HB2	2.11	0.52
1:A:141:ILE:HD11	1:A:176:TYR:CE1	2.45	0.51
1:A:187:THR:C	1:A:188:VAL:CG2	2.78	0.51
1:A:225:SER:CB	1:A:231:GLY:HA2	2.33	0.51
1:A:211:ALA:HB1	1:A:232:LEU:CD2	2.41	0.50
1:A:117:SER:HB3	1:A:123:THR:HG21	1.93	0.50
1:A:86:PRO:HG3	1:A:216:ASN:HB3	1.94	0.50
1:A:12:TYR:C	1:A:12:TYR:CD1	2.84	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ILE:O	1:A:35:LYS:N	2.40	0.50
1:A:51:HIS:O	1:A:52:ILE:CG1	2.59	0.50
1:A:215:SER:OG	1:A:219:SER:CB	2.60	0.50
1:A:229:LEU:C	1:A:231:GLY:H	2.15	0.50
1:A:67:TYR:CB	1:A:70:ALA:HB3	2.42	0.50
1:A:68:PRO:C	1:A:70:ALA:H	2.15	0.50
1:A:97:THR:CG2	1:A:167:GLY:CA	2.88	0.50
1:A:55:ASN:HD21	1:A:58:ASP:H	1.59	0.49
1:A:88:TRP:CZ2	1:A:180:HIS:NE2	2.80	0.49
1:A:128:PHE:HB2	1:A:175:PHE:CZ	2.47	0.49
1:A:229:LEU:C	1:A:231:GLY:N	2.66	0.49
1:A:26:GLY:HA3	1:A:36:LYS:O	2.12	0.49
1:A:89:VAL:HG21	1:A:214:ILE:HG22	1.95	0.49
1:A:221:ILE:HG22	1:A:225:SER:HB2	1.92	0.49
1:A:128:PHE:HE1	1:A:175:PHE:HB2	1.75	0.49
1:A:149:GLY:O	1:A:150:THR:C	2.51	0.48
1:A:133:PHE:CG	1:A:154:LEU:HB2	2.48	0.48
1:A:212:PHE:CD1	1:A:212:PHE:C	2.85	0.48
1:A:106:ILE:HD12	1:A:156:LEU:HG	1.96	0.48
1:A:183:GLU:CG	1:A:184:SER:N	2.76	0.48
1:A:51:HIS:O	1:A:52:ILE:HG13	2.13	0.48
1:A:80:ASP:HB3	1:A:83:ASP:OD2	2.13	0.48
1:A:3:THR:H	1:A:216:ASN:HD21	1.61	0.48
1:A:28:ASP:HB2	1:A:233:PHE:CZ	2.48	0.48
1:A:63:ALA:O	1:A:74:SER:HB2	2.14	0.48
1:A:91:VAL:HG21	1:A:111:PHE:CZ	2.49	0.48
1:A:36:LYS:HB3	1:A:75:VAL:CG2	2.44	0.48
1:A:173:ALA:CA	1:A:174:LEU:CD2	2.91	0.47
1:A:32:VAL:O	1:A:34:SER:N	2.45	0.47
1:A:106:ILE:HD11	1:A:156:LEU:CD1	2.44	0.47
1:A:100:TYR:HB3	1:A:207:ALA:HA	1.96	0.47
1:A:225:SER:HB3	1:A:231:GLY:CA	2.38	0.47
1:A:54:TYR:CD2	1:A:55:ASN:HA	2.49	0.47
1:A:208:ASP:HB3	4:A:243:HOH:O	2.13	0.47
1:A:68:PRO:O	1:A:69:ASN:HB2	2.14	0.47
1:A:87:GLU:HG3	1:A:182:TRP:HE3	1.80	0.47
1:A:128:PHE:CB	1:A:175:PHE:CZ	2.98	0.46
1:A:104:ASN:OD1	1:A:199:ILE:HD13	2.15	0.46
1:A:97:THR:HG21	1:A:167:GLY:CA	2.45	0.46
1:A:141:ILE:HD11	1:A:176:TYR:CD1	2.51	0.46
1:A:22:TYR:HB2	1:A:23:PRO:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:O	1:A:137:GLN:C	2.53	0.46
1:A:232:LEU:HA	1:A:232:LEU:HD12	1.74	0.46
1:A:91:VAL:HG21	1:A:111:PHE:CE1	2.50	0.46
1:A:97:THR:CG2	1:A:168:SER:N	2.78	0.46
1:A:41:ASN:O	1:A:43:GLN:HG3	2.15	0.46
1:A:160:SER:HB2	1:A:164:SER:OG	2.17	0.45
1:A:108:SER:HA	1:A:130:PHE:O	2.16	0.45
1:A:221:ILE:CG2	1:A:225:SER:HB2	2.46	0.45
1:A:102:GLU:CG	1:A:199:ILE:HG23	2.43	0.45
1:A:50:ALA:O	1:A:194:THR:HA	2.17	0.45
1:A:181:ILE:N	1:A:181:ILE:HD13	2.32	0.45
1:A:92:GLY:CA	1:A:173:ALA:O	2.64	0.45
1:A:97:THR:HG22	1:A:168:SER:N	2.31	0.45
1:A:115:LEU:O	1:A:123:THR:HB	2.17	0.45
1:A:12:TYR:O	1:A:12:TYR:CD1	2.70	0.45
1:A:216:ASN:C	1:A:218:ASP:N	2.70	0.45
1:A:88:TRP:CZ2	1:A:180:HIS:CE1	3.05	0.45
1:A:111:PHE:CB	1:A:128:PHE:CE2	3.00	0.44
1:A:133:PHE:CZ	1:A:154:LEU:HB2	2.51	0.44
1:A:50:ALA:N	1:A:195:PHE:O	2.43	0.44
1:A:183:GLU:HG2	1:A:184:SER:N	2.32	0.44
1:A:11:THR:OG1	1:A:102:GLU:OE2	2.24	0.44
1:A:12:TYR:O	1:A:12:TYR:HD1	2.01	0.44
1:A:217:ILE:H	1:A:217:ILE:HG23	1.39	0.44
1:A:102:GLU:HB2	1:A:207:ALA:CB	2.47	0.44
1:A:103:THR:O	1:A:199:ILE:HA	2.17	0.44
1:A:51:HIS:CD2	1:A:194:THR:OG1	2.71	0.44
1:A:19:ASP:C	1:A:20:PRO:O	2.56	0.44
1:A:93:LEU:O	1:A:172:ARG:CB	2.66	0.44
1:A:103:THR:OG1	1:A:165:PRO:HB3	2.17	0.43
1:A:204:SER:C	1:A:206:PRO:HD3	2.38	0.43
1:A:212:PHE:CD1	1:A:212:PHE:O	2.71	0.43
1:A:89:VAL:CG2	1:A:214:ILE:CG2	2.94	0.43
1:A:67:TYR:HB3	1:A:70:ALA:HB3	1.99	0.43
1:A:228:ARG:C	1:A:230:LEU:H	2.20	0.43
1:A:228:ARG:HG3	1:A:229:LEU:N	2.33	0.43
1:A:136:ASP:O	1:A:137:GLN:O	2.36	0.43
1:A:148:THR:HG22	1:A:154:LEU:HD12	1.99	0.43
1:A:102:GLU:CB	1:A:207:ALA:CB	2.97	0.43
1:A:221:ILE:HG22	1:A:225:SER:OG	2.18	0.43
1:A:103:THR:HB	1:A:200:LYS:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:CD2	1:A:180:HIS:HD2	2.30	0.43
1:A:22:TYR:CD1	1:A:39:LYS:NZ	2.78	0.43
1:A:60:ARG:HE	1:A:76:SER:HB3	1.82	0.43
1:A:111:PHE:HB2	1:A:128:PHE:CE2	2.53	0.43
1:A:92:GLY:HA2	1:A:173:ALA:O	2.19	0.42
1:A:102:GLU:HB2	1:A:207:ALA:HB3	2.01	0.42
1:A:26:GLY:HA2	1:A:75:VAL:HG11	2.02	0.42
1:A:109:TRP:O	1:A:130:PHE:N	2.48	0.42
1:A:166:GLU:HG3	1:A:167:GLY:N	2.33	0.42
1:A:102:GLU:HB2	1:A:207:ALA:H	1.84	0.42
1:A:170:VAL:O	1:A:170:VAL:HG13	2.20	0.42
1:A:137:GLN:NE2	1:A:139:ASP:OD1	2.52	0.42
1:A:164:SER:HA	1:A:165:PRO:HD2	1.91	0.42
1:A:182:TRP:CE3	1:A:183:GLU:HA	2.55	0.42
1:A:43:GLN:OE1	1:A:70:ALA:HB2	2.19	0.42
1:A:142:LEU:HD11	1:A:148:THR:HG23	2.02	0.42
1:A:128:PHE:HB2	1:A:175:PHE:CE2	2.55	0.42
1:A:31:SER:OG	1:A:33:ARG:N	2.53	0.42
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.93	0.41
1:A:96:SER:CB	1:A:230:LEU:HA	2.49	0.41
1:A:222:PRO:CG	1:A:225:SER:HG	2.27	0.41
1:A:158:ARG:HB2	1:A:166:GLU:CG	2.37	0.41
1:A:229:LEU:O	1:A:230:LEU:C	2.57	0.41
1:A:80:ASP:CB	1:A:83:ASP:OD2	2.68	0.41
1:A:160:SER:CB	1:A:164:SER:OG	2.69	0.41
1:A:40:TRP:HE1	1:A:67:TYR:HE1	1.67	0.41
1:A:127:HIS:NE2	1:A:129:MET:HG3	2.36	0.41
1:A:101:LYS:NZ	1:A:203:ASP:OD1	2.54	0.41
1:A:204:SER:O	1:A:206:PRO:CD	2.69	0.41
1:A:102:GLU:HG2	1:A:199:ILE:CG2	2.46	0.41
1:A:36:LYS:CD	1:A:75:VAL:HG23	2.31	0.41
1:A:156:LEU:HD22	1:A:172:ARG:HA	2.03	0.41
1:A:102:GLU:CG	1:A:199:ILE:CG2	2.99	0.41
1:A:93:LEU:O	1:A:172:ARG:CA	2.69	0.40
1:A:228:ARG:HG3	1:A:229:LEU:HD23	2.03	0.40
1:A:97:THR:CG2	1:A:167:GLY:C	2.90	0.40
1:A:90:ARG:HB2	1:A:217:ILE:HA	2.04	0.40

All (4) 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:A:122:GLN:NE2	1:A:122:GLN:NE2[4_565]	1.49	0.71
1:A:57:VAL:CG1	1:A:62:SER:OG[3_655]	1.92	0.28
1:A:15:THR:OG1	1:A:184:SER:OG[8_555]	1.96	0.24
1:A:122:GLN:CD	1:A:122:GLN:NE2[4_565]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	235/237 (99%)	183 (78%)	41 (17%)	11 (5%)	2 0

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	123	THR
1	A	207	ALA
1	A	230	LEU
1	A	33	ARG
1	A	98	GLY
1	A	120	THR
1	A	137	GLN
1	A	13	PRO
1	A	57	VAL
1	A	170	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/202 (100%)	141 (70%)	61 (30%)	0 0

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	THR
1	A	4	ILE
1	A	15	THR
1	A	16	ASP
1	A	17	ILE
1	A	19	ASP
1	A	21	SER
1	A	28	ASP
1	A	30	LYS
1	A	31	SER
1	A	32	VAL
1	A	34	SER
1	A	40	TRP
1	A	42	MET
1	A	46	LYS
1	A	55	ASN
1	A	62	SER
1	A	65	VAL
1	A	73	THR
1	A	74	SER
1	A	80	ASP
1	A	85	LEU
1	A	89	VAL
1	A	94	SER
1	A	96	SER
1	A	97	THR
1	A	99	LEU
1	A	105	THR
1	A	107	LEU
1	A	114	LYS
1	A	118	ASN
1	A	124	ASP
1	A	126	LEU
1	A	128	PHE
1	A	132	GLN
1	A	135	LYS
1	A	136	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	137	GLN
1	A	157	THR
1	A	160	SER
1	A	162	ASN
1	A	164	SER
1	A	166	GLU
1	A	172	ARG
1	A	174	LEU
1	A	180	HIS
1	A	181	ILE
1	A	185	SER
1	A	187	THR
1	A	191	PHE
1	A	192	GLU
1	A	201	SER
1	A	216	ASN
1	A	221	ILE
1	A	225	SER
1	A	226	THR
1	A	232	LEU
1	A	233	PHE
1	A	235	ASP
1	A	237	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	55	ASN
1	A	82	ASN
1	A	118	ASN
1	A	131	ASN
1	A	162	ASN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.