



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 AM GMT

PDB ID : 2NZ9
Title : Crystal structure of botulinum neurotoxin type A complexed with monoclonal antibody AR2
Authors : Stevens, R.C.; Arndt, J.W.
Deposited on : 2006-11-22
Resolution : 3.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

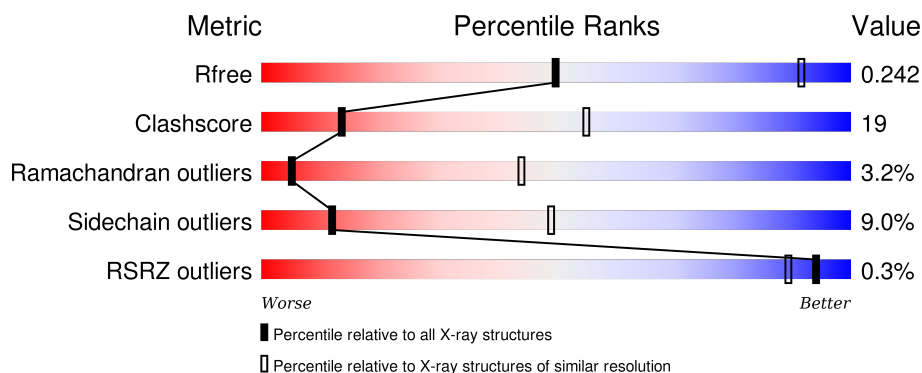
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1295	<div> <div></div> <div>61% 31% 5% ..</div> </div>
1	B	1295	<div> <div>%</div> <div>63% 30% 5% ..</div> </div>
2	C	218	<div> <div></div> <div>60% 33% 6% .</div> </div>
2	E	218	<div> <div></div> <div>62% 30% 6% ..</div> </div>
3	D	224	<div> <div></div> <div>63% 27% 5% ..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	224	<div><div></div><div>63%</div><div>29%</div><div></div><div>.</div><div>.</div><div>.</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26985 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1267	Total	C	N	O	S	0	0	0
			10200	6541	1691	1937	31			
1	B	1267	Total	C	N	O	S	0	0	0
			10203	6543	1691	1938	31			

- Molecule 2 is a protein called AR2 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	216	Total	C	N	O	S	0	0	0
			1657	1039	279	334	5			
2	E	216	Total	C	N	O	S	0	0	0
			1657	1039	279	334	5			

- Molecule 3 is a protein called AR2 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1632	1025	271	329	7			
3	F	217	Total	C	N	O	S	0	0	0
			1632	1025	271	329	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		

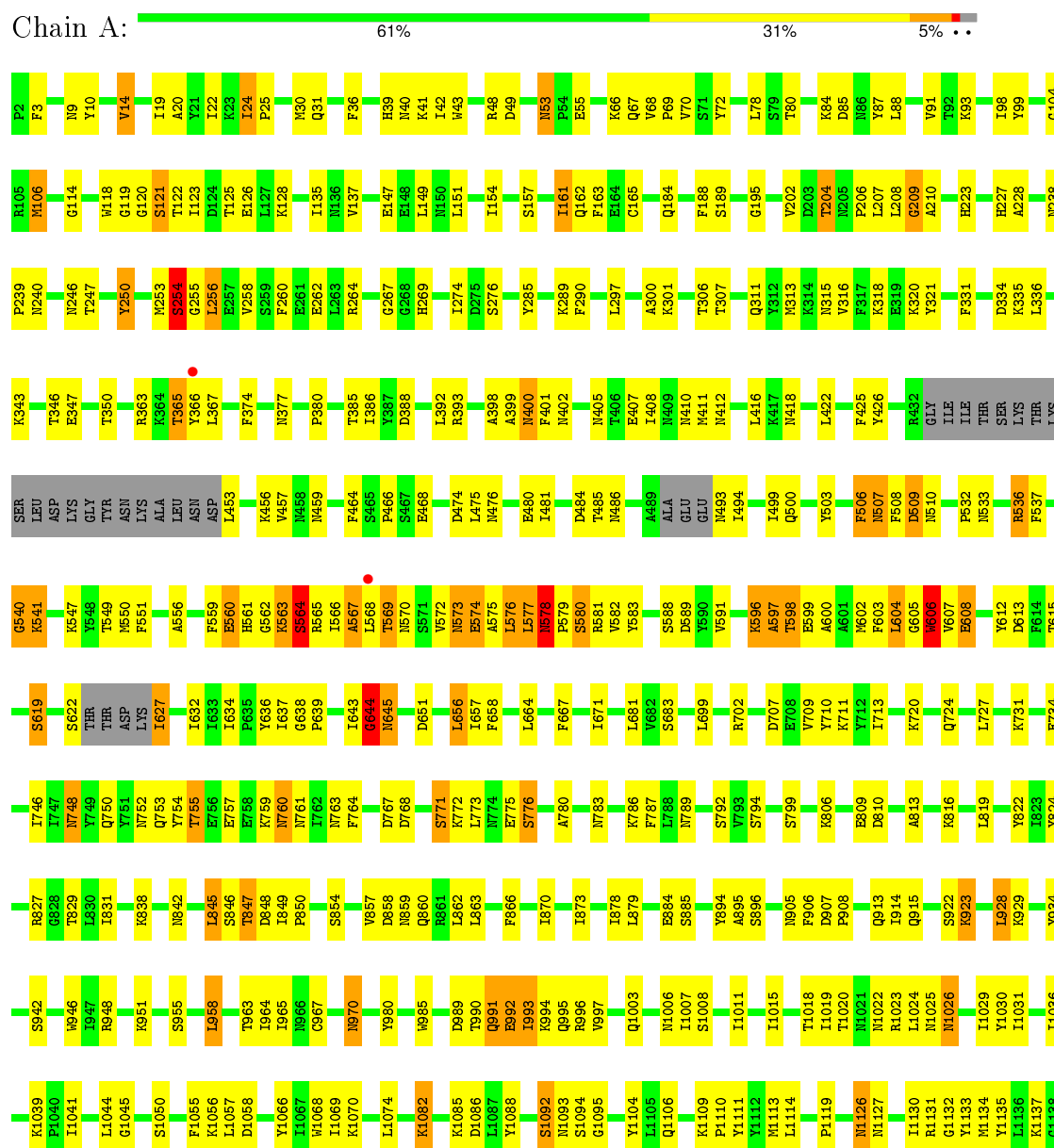
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

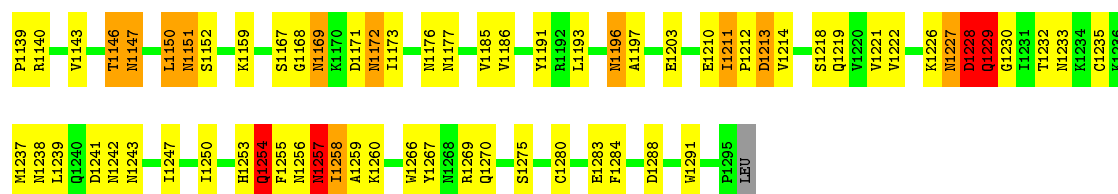
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Ca 1	0	0
5	A	1	Total 1	Ca 1	0	0

3 Residue-property plots

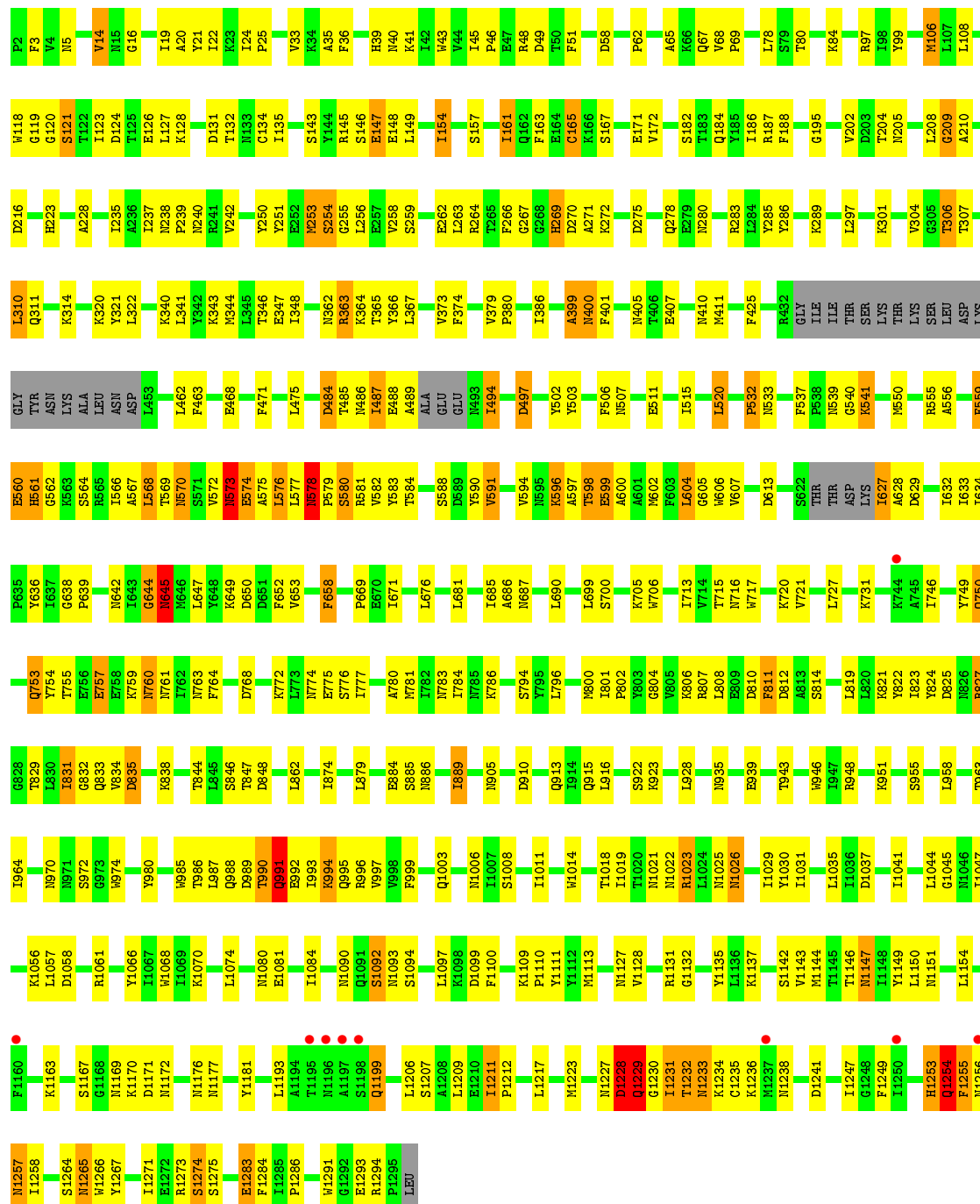
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Botulinum neurotoxin type A

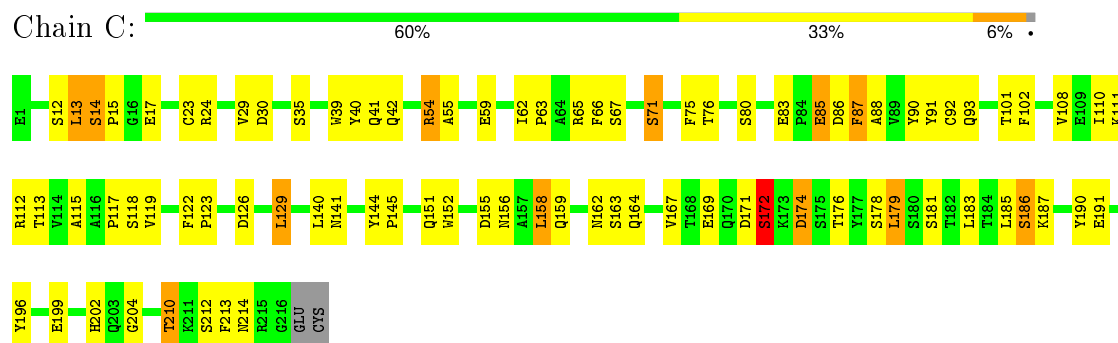




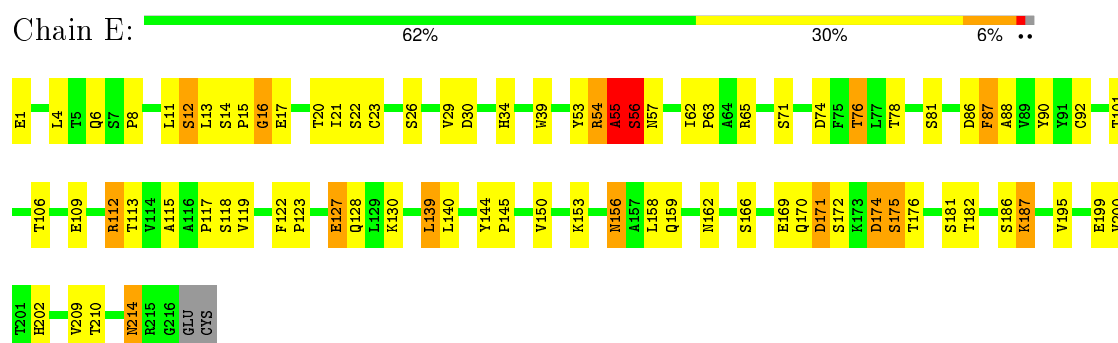
• Molecule 1: Botulinum neurotoxin type A



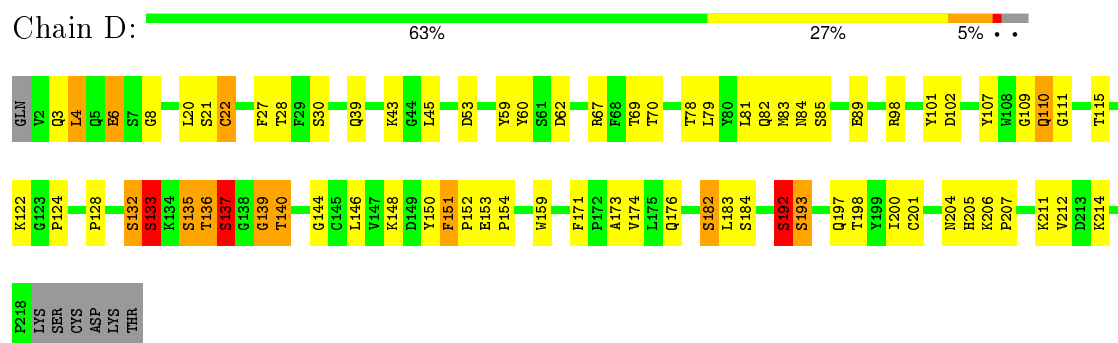
- Molecule 2: AR2 monoclonal antibody



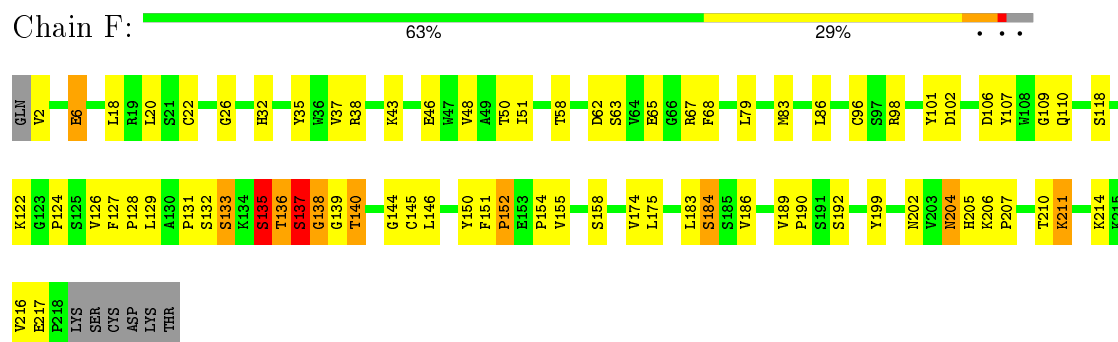
- Molecule 2: AR2 monoclonal antibody



- Molecule 3: AR2 monoclonal antibody



- Molecule 3: AR2 monoclonal antibody



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.97Å 197.60Å 146.10Å 90.00° 91.18° 90.00°	Depositor
Resolution (Å)	40.00 – 3.79 48.97 – 3.79	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.00-3.79) 95.5 (48.97-3.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.278 0.203 , 0.242	Depositor DCC
R_{free} test set	2686 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 112.2	EDS
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 52593 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26985	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.64	0/10416	0.67	0/14098
1	B	0.64	0/10420	0.66	0/14104
2	C	0.64	0/1695	0.60	0/2303
2	E	0.65	1/1695 (0.1%)	0.62	0/2303
3	D	0.56	0/1673	0.66	1/2281 (0.0%)
3	F	0.52	0/1673	0.64	0/2281
All	All	0.63	1/27572 (0.0%)	0.65	1/37370 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	26
1	B	0	27
2	C	0	3
2	E	0	3
3	D	0	6
3	F	0	5
All	All	0	70

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	127	GLU	CD-OE1	5.77	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	153	GLU	C-N-CD	-8.33	102.27	120.60

There are no chirality outliers.

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1139	PRO	Peptide
1	A	1167	SER	Peptide
1	A	118	TRP	Peptide
1	A	119	GLY	Peptide
1	A	1226	LYS	Peptide
1	A	1227	ASN	Peptide
1	A	1228	ASP	Peptide
1	A	1232	THR	Peptide
1	A	1254	GLN	Peptide
1	A	1257	ASN	Peptide
1	A	484	ASP	Peptide
1	A	507	ASN	Peptide
1	A	547	LYS	Peptide
1	A	564	SER	Peptide
1	A	573	ASN	Peptide
1	A	574	GLU	Peptide
1	A	578	ASN	Peptide
1	A	596	LYS	Peptide
1	A	598	THR	Peptide
1	A	604	LEU	Peptide
1	A	644	GLY	Peptide
1	A	645	ASN	Peptide
1	A	753	GLN	Peptide
1	A	847	THR	Peptide
1	A	989	ASP	Peptide
1	A	992	GLU	Peptide
1	B	118	TRP	Peptide
1	B	119	GLY	Peptide
1	B	120	GLY	Peptide
1	B	1228	ASP	Peptide
1	B	1229	GLN	Peptide
1	B	1232	THR	Peptide
1	B	1254	GLN	Peptide
1	B	148	GLU	Peptide
1	B	487	ILE	Peptide
1	B	532	PRO	Peptide
1	B	559	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	564	SER	Peptide
1	B	573	ASN	Peptide
1	B	574	GLU	Peptide
1	B	578	ASN	Peptide
1	B	596	LYS	Peptide
1	B	604	LEU	Peptide
1	B	644	GLY	Peptide
1	B	645	ASN	Peptide
1	B	649	LYS	Peptide
1	B	650	ASP	Peptide
1	B	753	GLN	Peptide
1	B	847	THR	Peptide
1	B	989	ASP	Peptide
1	B	990	THR	Peptide
1	B	991	GLN	Peptide
1	B	994	LYS	Peptide
2	C	117	PRO	Peptide
2	C	171	ASP	Peptide
2	C	172	SER	Peptide
3	D	133	SER	Peptide
3	D	135	SER	Peptide
3	D	136	THR	Peptide
3	D	137	SER	Peptide
3	D	139	GLY	Peptide
3	D	8	GLY	Peptide
2	E	171	ASP	Peptide
2	E	172	SER	Peptide
2	E	55	ALA	Peptide
3	F	133	SER	Peptide
3	F	135	SER	Peptide
3	F	136	THR	Peptide
3	F	137	SER	Peptide
3	F	152	PRO	Peptide

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	10200	0	10003	357	0
1	B	10203	0	9999	372	0
2	C	1657	0	1595	64	0
2	E	1657	0	1595	70	0
3	D	1632	0	1552	64	0
3	F	1632	0	1552	73	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	26985	0	26296	992	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (992) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:HIS:CD2	1:B:365:THR:HG21	1.40	1.56
1:A:596:LYS:CB	1:A:597:ALA:HB3	1.39	1.47
3:F:132:SER:HA	3:F:133:SER:CB	1.42	1.46
1:B:540:GLY:CA	1:B:541:LYS:HB2	1.40	1.43
1:B:578:ASN:HB3	1:B:579:PRO:CA	1.41	1.43
1:B:540:GLY:HA2	1:B:541:LYS:CB	1.44	1.40
3:D:139:GLY:N	3:D:140:THR:HB	1.34	1.38
1:A:578:ASN:HB3	1:A:579:PRO:C	1.43	1.37
3:D:132:SER:HA	3:D:133:SER:CB	1.44	1.34
3:D:132:SER:CA	3:D:133:SER:HB3	1.59	1.33
3:F:132:SER:CA	3:F:133:SER:HB3	1.62	1.29
1:B:578:ASN:HB3	1:B:579:PRO:C	1.53	1.28
1:A:596:LYS:HB2	1:A:597:ALA:CB	1.64	1.27
1:A:992:GLU:CA	1:A:993:ILE:HG13	1.63	1.26
1:A:1044:LEU:HB3	1:A:1045:GLY:CA	1.65	1.24
1:A:578:ASN:HB3	1:A:579:PRO:CA	1.62	1.23
1:B:488:GLU:HA	1:B:489:ALA:CB	1.60	1.23
3:F:139:GLY:CA	3:F:140:THR:HB	1.69	1.22
1:B:573:ASN:HA	1:B:575:ALA:H	1.06	1.21
1:A:1044:LEU:CB	1:A:1045:GLY:HA2	1.69	1.21
3:F:139:GLY:HA3	3:F:140:THR:CB	1.72	1.20
3:D:139:GLY:CA	3:D:140:THR:HB	1.70	1.18
3:D:136:THR:HB	3:D:137:SER:CA	1.73	1.17
1:B:532:PRO:HA	1:B:533:ASN:CB	1.74	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:PRO:HA	1:A:581:ARG:H	1.09	1.14
2:C:14:SER:O	2:C:17:GLU:HG3	1.42	1.13
1:B:488:GLU:CA	1:B:489:ALA:HB3	1.77	1.13
1:B:269:HIS:CD2	1:B:365:THR:CG2	2.31	1.12
1:B:532:PRO:HA	1:B:533:ASN:HB2	1.15	1.12
1:B:578:ASN:HB3	1:B:579:PRO:HA	1.17	1.12
3:F:136:THR:HB	3:F:137:SER:CA	1.81	1.10
2:E:12:SER:O	2:E:13:LEU:HD12	1.52	1.09
1:A:67:GLN:HA	1:A:425:PHE:CE1	1.88	1.09
1:A:540:GLY:HA2	1:A:541:LYS:HB2	1.13	1.09
2:E:144:TYR:CG	2:E:145:PRO:HA	1.88	1.08
1:B:68:VAL:CG2	1:B:69:PRO:HD2	1.84	1.08
1:B:135:ILE:HG23	1:B:149:LEU:HD22	1.36	1.08
1:B:573:ASN:HA	1:B:575:ALA:N	1.66	1.08
1:A:992:GLU:CA	1:A:993:ILE:CG1	2.29	1.08
1:B:578:ASN:CB	1:B:579:PRO:CA	2.30	1.06
1:B:578:ASN:CB	1:B:579:PRO:HA	1.85	1.06
1:B:627:ILE:HD12	1:B:628:ALA:H	1.11	1.06
1:B:1228:ASP:HB3	1:B:1229:GLN:CB	1.85	1.05
1:B:1228:ASP:HB3	1:B:1229:GLN:HB3	1.37	1.05
1:B:579:PRO:HA	1:B:581:ARG:H	1.18	1.03
1:A:540:GLY:HA2	1:A:541:LYS:CB	1.89	1.03
1:B:1211:ILE:CG1	1:B:1212:PRO:HD3	1.90	1.02
1:A:540:GLY:CA	1:A:541:LYS:HB2	1.90	1.01
1:A:532:PRO:HA	1:A:533:ASN:CB	1.88	1.01
3:D:139:GLY:CA	3:D:140:THR:CB	2.37	1.00
1:A:209:GLY:HA3	1:A:405:ASN:ND2	1.75	1.00
1:A:596:LYS:CA	1:A:597:ALA:HB3	1.93	0.99
1:A:14:VAL:HG12	1:A:20:ALA:HA	1.42	0.99
1:A:1044:LEU:HB3	1:A:1045:GLY:HA2	1.00	0.97
3:D:136:THR:CB	3:D:137:SER:CA	2.41	0.97
1:B:209:GLY:HA3	1:B:405:ASN:HD21	1.24	0.97
1:B:1044:LEU:HB3	1:B:1045:GLY:HA2	1.47	0.97
1:B:135:ILE:HG23	1:B:149:LEU:CD2	1.94	0.96
1:A:596:LYS:CA	1:A:597:ALA:CB	2.44	0.96
2:E:174:ASP:HB2	2:E:176:THR:HG22	1.44	0.95
1:B:269:HIS:HD2	1:B:365:THR:CG2	1.74	0.95
3:F:204:ASN:ND2	3:F:211:LYS:HG3	1.82	0.95
1:A:578:ASN:CB	1:A:579:PRO:C	2.34	0.94
1:B:364:LYS:O	1:B:365:THR:HG23	1.65	0.94
3:F:136:THR:CB	3:F:137:SER:CA	2.45	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:HIS:NE2	1:B:365:THR:HG21	1.84	0.92
1:A:604:LEU:N	1:A:605:GLY:HA3	1.83	0.92
1:A:578:ASN:CB	1:A:579:PRO:CA	2.48	0.91
1:B:68:VAL:HG23	1:B:69:PRO:HD2	1.49	0.91
1:B:67:GLN:HA	1:B:425:PHE:CE1	2.06	0.91
1:A:579:PRO:HA	1:A:581:ARG:N	1.84	0.91
3:D:139:GLY:HA3	3:D:140:THR:CB	1.99	0.90
1:A:532:PRO:HA	1:A:533:ASN:HB2	1.49	0.90
1:B:578:ASN:CB	1:B:579:PRO:C	2.39	0.90
1:A:561:HIS:N	1:A:562:GLY:HA3	1.84	0.90
2:E:144:TYR:CD1	2:E:145:PRO:HA	2.06	0.90
1:B:1211:ILE:HG13	1:B:1212:PRO:HD3	1.50	0.90
1:B:264:ARG:HD2	1:B:346:THR:HB	1.54	0.89
1:B:270:ASP:OD1	1:B:365:THR:HB	1.71	0.89
1:B:627:ILE:HD12	1:B:628:ALA:N	1.88	0.89
1:A:993:ILE:CG2	1:A:1044:LEU:HD11	2.02	0.88
1:B:532:PRO:CA	1:B:533:ASN:CB	2.49	0.88
3:D:132:SER:HA	3:D:133:SER:HB2	1.53	0.88
1:B:209:GLY:HA3	1:B:405:ASN:ND2	1.88	0.88
3:D:139:GLY:H	3:D:140:THR:CB	1.84	0.88
1:B:269:HIS:HD2	1:B:365:THR:HG21	1.11	0.87
3:F:132:SER:CA	3:F:133:SER:CB	2.32	0.87
3:D:132:SER:CA	3:D:133:SER:CB	2.31	0.87
1:B:1044:LEU:HB3	1:B:1045:GLY:CA	2.04	0.87
1:B:68:VAL:HG22	1:B:69:PRO:HD2	1.54	0.86
3:F:204:ASN:HD21	3:F:211:LYS:HG3	1.37	0.86
1:B:594:VAL:HA	1:B:606:TRP:HZ2	1.41	0.86
3:F:139:GLY:HA3	3:F:140:THR:HB	0.88	0.86
1:B:569:THR:HA	1:B:582:VAL:HG13	1.58	0.85
1:B:1273:ARG:O	1:B:1274:SER:HB2	1.75	0.85
1:B:579:PRO:HA	1:B:581:ARG:N	1.91	0.84
1:A:596:LYS:HA	1:A:597:ALA:CB	2.07	0.84
3:D:132:SER:HA	3:D:133:SER:HB3	0.85	0.84
1:B:364:LYS:O	1:B:365:THR:CG2	2.26	0.84
2:E:119:VAL:HG21	2:E:209:VAL:HG21	1.59	0.84
1:A:578:ASN:HB3	1:A:579:PRO:HA	1.58	0.84
1:B:135:ILE:CG2	1:B:149:LEU:HD22	2.08	0.83
1:A:264:ARG:HD2	1:A:346:THR:HB	1.60	0.83
1:B:596:LYS:HB2	1:B:597:ALA:HB3	1.58	0.83
1:B:561:HIS:N	1:B:562:GLY:HA2	1.92	0.83
1:B:604:LEU:N	1:B:605:GLY:HA3	1.93	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ARG:HG3	2:E:54:ARG:HH11	1.42	0.82
3:F:98:ARG:NH1	3:F:107:TYR:HD1	1.78	0.82
1:B:488:GLU:HA	1:B:489:ALA:HB3	0.83	0.81
2:C:144:TYR:CD1	2:C:145:PRO:HA	2.15	0.81
2:C:13:LEU:HG	2:C:17:GLU:OE1	1.80	0.81
3:D:135:SER:OG	3:D:136:THR:HA	1.80	0.81
3:F:204:ASN:HD21	3:F:211:LYS:CG	1.94	0.80
1:B:573:ASN:CA	1:B:575:ALA:H	1.90	0.80
1:B:1044:LEU:CB	1:B:1045:GLY:HA2	2.09	0.80
1:B:1228:ASP:CB	1:B:1229:GLN:HB3	2.12	0.80
1:A:561:HIS:H	1:A:562:GLY:CA	1.95	0.80
1:B:596:LYS:CA	1:B:597:ALA:HB3	2.12	0.80
1:A:596:LYS:CB	1:A:597:ALA:CB	2.34	0.80
1:A:532:PRO:CA	1:A:533:ASN:CB	2.59	0.80
1:B:596:LYS:CB	1:B:597:ALA:HB3	2.11	0.80
1:A:532:PRO:HA	1:A:533:ASN:HB3	1.64	0.80
1:B:238:ASN:HD22	1:B:239:PRO:HD2	1.46	0.80
1:A:385:THR:HG23	1:A:392:LEU:HD21	1.64	0.79
3:D:139:GLY:H	3:D:140:THR:HB	0.99	0.79
1:B:1228:ASP:C	1:B:1230:GLY:H	1.86	0.79
1:A:561:HIS:N	1:A:562:GLY:CA	2.46	0.78
1:B:1253:HIS:O	1:B:1254:GLN:HB2	1.82	0.78
3:D:139:GLY:HA3	3:D:140:THR:OG1	1.82	0.78
1:B:379:VAL:HB	1:B:380:PRO:HD3	1.63	0.78
1:A:857:VAL:HG12	1:A:859:ASN:H	1.49	0.78
1:A:125:THR:O	1:A:300:ALA:HA	1.84	0.77
1:A:596:LYS:HA	1:A:597:ALA:HB2	1.65	0.77
1:B:1193:LEU:HD11	1:B:1206:LEU:HD13	1.65	0.77
1:B:532:PRO:CA	1:B:533:ASN:HB2	2.07	0.76
1:A:569:THR:HA	1:A:582:VAL:HG13	1.66	0.76
1:A:532:PRO:CA	1:A:533:ASN:HB3	2.15	0.76
1:A:121:SER:OG	1:A:126:GLU:CG	2.33	0.76
1:B:24:ILE:HG23	1:B:25:PRO:HD2	1.67	0.76
1:B:561:HIS:H	1:B:562:GLY:HA2	1.48	0.76
1:A:992:GLU:CA	1:A:993:ILE:CB	2.63	0.76
1:A:573:ASN:HA	1:A:575:ALA:N	2.00	0.75
3:D:132:SER:CB	3:D:133:SER:HB3	2.16	0.75
1:A:209:GLY:HA3	1:A:405:ASN:HD22	1.49	0.75
1:B:1211:ILE:CD1	1:B:1212:PRO:HD3	2.17	0.75
1:A:964:ILE:HG22	1:A:1057:LEU:HD23	1.69	0.75
1:A:407:GLU:O	1:A:410:ASN:HB3	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:ASN:OD1	1:A:1127:ASN:N	2.19	0.75
1:B:67:GLN:HE22	1:B:537:PHE:H	1.31	0.74
1:B:45:ILE:HB	1:B:154:ILE:HG23	1.68	0.74
1:B:488:GLU:CA	1:B:489:ALA:CB	2.49	0.74
1:B:1211:ILE:HG13	1:B:1212:PRO:CD	2.17	0.74
2:E:54:ARG:O	2:E:55:ALA:HB3	1.87	0.74
3:D:135:SER:HA	3:D:136:THR:O	1.88	0.74
1:A:106:MET:HG2	1:A:506:PHE:CE1	2.23	0.73
1:B:596:LYS:HA	1:B:597:ALA:HB3	1.69	0.73
1:A:121:SER:OG	1:A:126:GLU:HG3	1.87	0.73
1:A:759:LYS:O	1:A:761:ASN:N	2.20	0.73
1:B:774:ASN:HA	1:B:777:ILE:HD12	1.71	0.73
1:B:596:LYS:HA	1:B:597:ALA:CB	2.17	0.73
1:A:607:VAL:HG12	1:A:608:GLU:N	2.03	0.73
1:A:767:ASP:O	1:A:771:SER:HB2	1.87	0.73
1:B:40:ASN:HD22	1:B:511:GLU:HG2	1.54	0.73
1:B:559:PHE:HB2	1:B:560:GLU:CA	2.18	0.73
1:A:238:ASN:HD22	1:A:239:PRO:CD	2.02	0.73
1:A:604:LEU:H	1:A:605:GLY:HA3	1.54	0.72
3:D:139:GLY:HA3	3:D:140:THR:HB	1.64	0.72
1:A:135:ILE:HG12	1:A:149:LEU:HD22	1.71	0.72
1:A:1113:MET:HE2	1:A:1284:PHE:HA	1.69	0.72
1:B:1254:GLN:O	1:B:1255:PHE:CD2	2.43	0.72
1:A:568:LEU:N	1:A:580:SER:OG	2.23	0.71
3:F:20:LEU:HD11	3:F:83:MET:HE1	1.72	0.71
1:A:238:ASN:HD22	1:A:239:PRO:HD2	1.54	0.71
1:A:1227:ASN:O	1:A:1230:GLY:N	2.23	0.71
1:A:1221:VAL:HG11	1:A:1237:MET:HB3	1.72	0.71
1:B:1273:ARG:O	1:B:1274:SER:CB	2.39	0.71
3:F:98:ARG:NH1	3:F:107:TYR:CD1	2.58	0.71
2:E:144:TYR:CG	2:E:145:PRO:CA	2.71	0.71
1:B:238:ASN:ND2	1:B:239:PRO:HD2	2.05	0.71
1:A:573:ASN:HA	1:A:574:GLU:C	2.12	0.71
1:A:757:GLU:O	1:A:760:ASN:N	2.23	0.71
1:A:3:PHE:O	1:A:39:HIS:HD2	1.73	0.70
2:E:16:GLY:HA2	2:E:81:SER:HB2	1.72	0.70
3:F:132:SER:HA	3:F:133:SER:HB3	0.74	0.70
1:A:576:LEU:O	1:A:581:ARG:HB3	1.92	0.70
1:A:1239:LEU:HG	1:A:1247:ILE:HD12	1.72	0.69
1:B:561:HIS:N	1:B:562:GLY:CA	2.56	0.69
1:A:68:VAL:CG2	1:A:69:PRO:HD2	2.21	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:TYR:HA	2:E:145:PRO:O	1.92	0.69
1:B:716:ASN:OD1	1:B:720:LYS:HE3	1.92	0.69
3:F:132:SER:HA	3:F:133:SER:HB2	1.63	0.69
2:E:54:ARG:O	2:E:55:ALA:CB	2.41	0.69
1:B:988:GLN:HG3	1:B:994:LYS:HG3	1.75	0.68
2:E:139:LEU:HD22	3:F:186:VAL:HG21	1.74	0.68
2:C:29:VAL:HG12	2:C:29:VAL:O	1.93	0.68
1:A:573:ASN:CB	1:A:575:ALA:H	2.07	0.68
1:B:532:PRO:HA	1:B:533:ASN:HB3	1.73	0.68
2:E:153:LYS:HB3	2:E:156:ASN:HA	1.75	0.68
1:B:568:LEU:N	1:B:580:SER:OG	2.23	0.68
1:A:634:ILE:HB	1:A:637:ILE:HD12	1.74	0.68
3:D:20:LEU:HG	3:D:83:MET:HE3	1.74	0.68
1:A:1211:ILE:CG1	1:A:1212:PRO:HD3	2.24	0.68
1:B:285:TYR:CZ	1:B:289:LYS:HE3	2.29	0.67
1:B:1228:ASP:C	1:B:1230:GLY:N	2.45	0.67
1:B:344:MET:HA	1:B:348:ILE:HD12	1.77	0.67
1:A:40:ASN:O	1:A:41:LYS:HB2	1.93	0.67
1:A:503:TYR:O	1:A:506:PHE:HB2	1.95	0.67
1:B:627:ILE:CD1	1:B:628:ALA:H	1.97	0.67
2:E:12:SER:C	2:E:13:LEU:HD12	2.15	0.67
3:D:139:GLY:N	3:D:140:THR:CB	2.31	0.66
2:E:8:PRO:O	2:E:106:THR:HG23	1.96	0.66
1:B:1199:GLN:O	1:B:1199:GLN:HG2	1.95	0.66
1:A:67:GLN:HA	1:A:425:PHE:CZ	2.30	0.66
1:B:604:LEU:O	1:B:607:VAL:HB	1.95	0.66
1:A:568:LEU:H	1:A:580:SER:CB	2.09	0.66
1:A:1211:ILE:N	1:A:1212:PRO:HD2	2.11	0.66
1:A:70:VAL:HA	1:A:418:ASN:ND2	2.11	0.66
1:B:1023:ARG:HH12	1:B:1047:ILE:H	1.43	0.65
3:D:98:ARG:NH1	3:D:107:TYR:HD1	1.94	0.65
3:F:98:ARG:NH1	3:F:106:ASP:OD1	2.28	0.65
1:B:121:SER:H	1:B:128:LYS:HE2	1.62	0.65
1:B:1211:ILE:HD12	1:B:1212:PRO:HD3	1.78	0.65
2:E:54:ARG:NH1	2:E:54:ARG:HG3	2.11	0.65
1:B:40:ASN:ND2	1:B:511:GLU:HG2	2.11	0.65
1:A:1113:MET:HE1	1:A:1284:PHE:CD2	2.30	0.65
1:B:1233:ASN:ND2	1:B:1235:CYS:H	1.94	0.65
1:A:849:ILE:HG23	1:A:850:PRO:HD2	1.77	0.65
1:A:575:ALA:O	1:A:576:LEU:C	2.34	0.65
1:A:596:LYS:HB2	1:A:597:ALA:HB3	0.70	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ILE:HG13	1:B:264:ARG:NH2	2.11	0.65
2:E:214:ASN:N	2:E:214:ASN:OD1	2.30	0.65
1:A:163:PHE:CD1	1:A:188:PHE:HA	2.31	0.65
1:B:347:GLU:HB3	1:B:494:ILE:HD11	1.77	0.65
2:E:174:ASP:HB2	2:E:176:THR:CG2	2.24	0.65
1:B:68:VAL:CG2	1:B:69:PRO:CD	2.69	0.64
3:F:51:ILE:HG13	3:F:58:THR:HG22	1.79	0.64
1:B:1227:ASN:O	1:B:1230:GLY:N	2.30	0.64
2:C:144:TYR:CG	2:C:145:PRO:HA	2.31	0.64
1:B:40:ASN:O	1:B:41:LYS:HB2	1.98	0.64
1:B:806:LYS:NZ	1:B:810:ASP:OD2	2.24	0.64
1:B:573:ASN:HA	1:B:574:GLU:C	2.17	0.64
1:A:578:ASN:CB	1:A:579:PRO:HA	2.22	0.64
1:A:1203:GLU:OE1	1:A:1253:HIS:HB2	1.97	0.64
1:A:993:ILE:HG22	1:A:1044:LEU:HD21	1.79	0.64
1:B:182:SER:O	1:B:184:GLN:NE2	2.30	0.64
2:E:159:GLN:HG2	2:E:162:ASN:HD21	1.62	0.64
1:A:1150:LEU:HG	1:A:1150:LEU:O	1.97	0.64
1:B:1227:ASN:O	1:B:1229:GLN:C	2.36	0.64
2:C:112:ARG:HH12	2:C:115:ALA:HB2	1.62	0.64
1:B:14:VAL:HG12	1:B:20:ALA:HA	1.78	0.64
2:C:30:ASP:OD1	2:C:35:SER:HA	1.98	0.64
1:A:964:ILE:HA	1:A:1056:LYS:O	1.98	0.64
1:B:365:THR:O	1:B:367:LEU:N	2.31	0.64
1:B:575:ALA:O	1:B:577:LEU:N	2.31	0.64
1:A:209:GLY:CA	1:A:405:ASN:ND2	2.57	0.63
1:A:1026:ASN:HB3	1:A:1039:LYS:O	1.98	0.63
1:B:1113:MET:HE2	1:B:1284:PHE:HA	1.80	0.63
1:A:10:TYR:N	1:A:85:ASP:OD1	2.27	0.63
1:B:596:LYS:CA	1:B:597:ALA:CB	2.75	0.63
3:F:6:GLU:HA	3:F:22:CYS:HA	1.79	0.63
1:A:866:PHE:CZ	1:A:870:ILE:HD11	2.33	0.63
1:B:681:LEU:HD11	1:B:819:LEU:HD23	1.81	0.63
1:B:67:GLN:HE22	1:B:537:PHE:N	1.96	0.63
1:A:754:TYR:O	1:A:755:THR:C	2.37	0.63
3:D:6:GLU:OE1	3:D:111:GLY:N	2.32	0.63
1:B:579:PRO:CA	1:B:581:ARG:H	2.02	0.63
1:A:24:ILE:HG23	1:A:25:PRO:HD2	1.81	0.62
3:D:140:THR:O	3:D:140:THR:HG22	1.98	0.62
1:A:532:PRO:CB	1:A:533:ASN:HB3	2.29	0.62
2:E:112:ARG:NH1	2:E:115:ALA:HB2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1228:ASP:O	1:B:1230:GLY:N	2.30	0.62
1:A:1113:MET:CE	1:A:1284:PHE:HA	2.29	0.62
1:A:68:VAL:HG22	1:A:69:PRO:HD2	1.81	0.62
1:A:1176:ASN:O	1:A:1177:ASN:HB2	1.99	0.62
1:B:1113:MET:HE1	1:B:1284:PHE:CD2	2.35	0.62
1:B:280:ASN:OD1	1:B:283:ARG:NH2	2.33	0.62
1:A:388:ASP:OD2	1:A:393:ARG:HG2	1.99	0.62
3:F:124:PRO:HD2	3:F:210:THR:HG21	1.80	0.62
1:B:68:VAL:HG22	1:B:69:PRO:CD	2.29	0.62
1:B:24:ILE:HG22	1:B:25:PRO:O	2.00	0.62
1:A:494:ILE:O	1:A:494:ILE:HG22	2.00	0.62
1:A:578:ASN:HB3	1:A:580:SER:N	2.10	0.61
1:B:993:ILE:CB	1:B:1044:LEU:HD11	2.30	0.61
1:B:343:LYS:HG3	1:B:347:GLU:OE1	1.99	0.61
2:E:12:SER:HB2	2:E:109:GLU:HB3	1.80	0.61
1:A:1211:ILE:HD12	1:A:1212:PRO:HD3	1.83	0.61
1:B:634:ILE:HD11	1:B:783:ASN:HB3	1.81	0.61
3:F:124:PRO:HB3	3:F:150:TYR:HB3	1.82	0.61
1:B:272:LYS:O	1:B:715:THR:HG23	1.99	0.61
1:B:1100:PHE:HD1	1:B:1283:GLU:HG2	1.66	0.61
1:A:599:GLU:HB2	1:A:600:ALA:HB2	1.82	0.61
1:A:567:ALA:HA	1:A:580:SER:OG	2.00	0.61
2:C:87:PHE:HB3	2:C:110:ILE:HG12	1.82	0.61
1:A:204:THR:O	1:A:206:PRO:HD3	2.00	0.61
1:B:270:ASP:CG	1:B:365:THR:HB	2.21	0.61
1:B:575:ALA:O	1:B:576:LEU:C	2.37	0.61
2:C:112:ARG:NH1	2:C:115:ALA:HB2	2.16	0.61
1:B:578:ASN:HB3	1:B:580:SER:N	2.13	0.61
1:A:1211:ILE:HG13	1:A:1212:PRO:HD3	1.81	0.61
3:D:204:ASN:ND2	3:D:211:LYS:HG3	2.16	0.61
1:B:699:LEU:HD22	1:B:844:THR:HG21	1.83	0.61
1:A:993:ILE:HG23	1:A:1044:LEU:HD11	1.83	0.61
1:A:1258:ILE:O	1:A:1260:LYS:N	2.34	0.61
1:B:1008:SER:OG	1:B:1011:ILE:HG13	2.00	0.61
1:A:1211:ILE:N	1:A:1212:PRO:CD	2.63	0.60
3:F:150:TYR:OH	3:F:155:VAL:HG22	2.01	0.60
2:C:202:HIS:CD2	2:C:204:GLY:H	2.19	0.60
1:A:615:THR:O	1:A:619:SER:HB2	2.01	0.60
2:E:20:THR:HG23	2:E:78:THR:HG22	1.84	0.60
3:F:101:TYR:CE2	3:F:102:ASP:HB2	2.36	0.60
1:A:70:VAL:HA	1:A:418:ASN:HD21	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:140:LEU:HD21	2:E:200:VAL:HG11	1.84	0.60
1:A:985:TRP:HB3	1:A:997:VAL:HG23	1.83	0.60
2:E:150:VAL:HG11	2:E:181:SER:HB2	1.83	0.60
1:B:757:GLU:O	1:B:760:ASN:N	2.35	0.60
1:B:1241:ASP:HB3	1:B:1247:ILE:HD11	1.83	0.60
3:F:204:ASN:CG	3:F:211:LYS:HG3	2.22	0.59
1:A:806:LYS:HG3	1:A:934:TYR:HB3	1.83	0.59
1:B:1230:GLY:O	1:B:1231:ILE:C	2.40	0.59
1:A:246:ASN:C	1:A:247:THR:HG23	2.22	0.59
1:B:823:ILE:CG2	1:B:834:VAL:HG13	2.31	0.59
1:A:1127:ASN:O	1:A:1132:GLY:HA3	2.01	0.59
1:A:993:ILE:HG22	1:A:1044:LEU:HD11	1.81	0.59
1:A:1169:ASN:O	1:A:1171:ASP:N	2.35	0.59
1:A:238:ASN:ND2	1:A:239:PRO:HD2	2.18	0.59
1:B:1066:TYR:C	1:B:1066:TYR:CD1	2.76	0.59
1:B:567:ALA:HB1	1:B:746:ILE:CG1	2.33	0.59
1:B:579:PRO:HB3	1:B:580:SER:HA	1.85	0.59
1:A:627:ILE:HG12	1:A:657:ILE:HG23	1.85	0.58
1:B:750:GLN:HE21	1:B:750:GLN:HA	1.68	0.58
1:B:301:LYS:O	1:B:310:LEU:HD12	2.03	0.58
1:B:532:PRO:CA	1:B:533:ASN:HB3	2.29	0.58
1:A:859:ASN:OD1	1:A:862:LEU:HD12	2.04	0.58
1:A:253:MET:O	1:A:254:SER:C	2.41	0.58
1:A:604:LEU:N	1:A:605:GLY:CA	2.63	0.58
1:B:559:PHE:CB	1:B:560:GLU:CA	2.81	0.58
1:A:1253:HIS:O	1:A:1254:GLN:HB2	2.03	0.58
1:A:114:GLY:HA2	1:A:320:LYS:HG3	1.85	0.58
1:B:579:PRO:CB	1:B:580:SER:HA	2.34	0.58
3:F:205:HIS:CD2	3:F:207:PRO:HD2	2.38	0.58
1:A:1019:ILE:HD13	1:A:1029:ILE:HG13	1.85	0.58
1:B:1022:ASN:H	1:B:1041:ILE:HD11	1.67	0.58
1:A:634:ILE:HB	1:A:637:ILE:CD1	2.33	0.58
1:A:816:LYS:HB2	1:A:845:LEU:HD23	1.86	0.58
1:A:1119:PRO:O	1:A:1140:ARG:HD2	2.04	0.58
1:B:972:SER:HA	1:B:988:GLN:O	2.02	0.58
1:A:121:SER:OG	1:A:126:GLU:HG2	2.03	0.58
1:A:1211:ILE:CD1	1:A:1212:PRO:HD3	2.34	0.58
1:B:1254:GLN:O	1:B:1255:PHE:HD2	1.87	0.58
2:C:159:GLN:HG2	2:C:162:ASN:HD21	1.69	0.58
3:F:128:PRO:HB2	3:F:216:VAL:HG13	1.85	0.57
3:F:132:SER:CB	3:F:133:SER:HB3	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:THR:O	1:A:1147:ASN:HB2	2.05	0.57
2:C:119:VAL:HG22	2:C:140:LEU:HG	1.85	0.57
1:A:1104:TYR:HB3	1:A:1173:ILE:HG23	1.85	0.57
1:A:643:ILE:HG21	1:A:664:LEU:HD23	1.87	0.57
1:A:253:MET:CE	1:A:256:LEU:HD22	2.35	0.57
2:E:171:ASP:O	2:E:174:ASP:O	2.23	0.57
1:A:575:ALA:O	1:A:577:LEU:N	2.38	0.57
3:F:135:SER:HA	3:F:136:THR:O	2.05	0.57
1:A:1019:ILE:CD1	1:A:1029:ILE:HG13	2.34	0.57
1:B:964:ILE:HG22	1:B:1057:LEU:HD23	1.87	0.57
1:B:946:TRP:HB2	1:B:1070:LYS:HG2	1.87	0.57
1:B:127:LEU:O	1:B:304:VAL:HG22	2.06	0.56
1:A:120:GLY:O	1:A:121:SER:C	2.43	0.56
1:A:709:VAL:O	1:A:713:ILE:HG13	2.05	0.56
1:A:195:GLY:HA3	1:A:374:PHE:HE1	1.70	0.56
1:A:993:ILE:CG2	1:A:1044:LEU:CD1	2.81	0.56
1:A:67:GLN:HE22	1:A:537:PHE:N	2.03	0.56
1:A:67:GLN:HE22	1:A:537:PHE:H	1.53	0.56
2:E:119:VAL:HG21	2:E:209:VAL:CG2	2.33	0.56
1:B:45:ILE:HB	1:B:154:ILE:CG2	2.35	0.56
3:D:204:ASN:HD21	3:D:211:LYS:HG3	1.70	0.56
2:E:150:VAL:HG23	2:E:200:VAL:HG22	1.87	0.56
1:A:1169:ASN:C	1:A:1171:ASP:H	2.08	0.56
1:A:567:ALA:CA	1:A:580:SER:OG	2.53	0.56
1:B:717:TRP:HH2	1:B:862:LEU:HD13	1.71	0.56
1:B:238:ASN:OD1	1:B:240:ASN:HB2	2.05	0.56
1:A:1113:MET:HA	1:A:1113:MET:HE2	1.86	0.56
1:B:310:LEU:HD22	1:B:314:LYS:HG3	1.88	0.56
1:B:205:ASN:HB3	1:B:400:ASN:HB3	1.86	0.56
1:A:951:LYS:HE2	1:A:1151:ASN:OD1	2.05	0.56
1:B:1227:ASN:ND2	1:B:1231:ILE:O	2.39	0.56
1:A:702:ARG:HD2	1:A:845:LEU:HD11	1.88	0.56
2:C:12:SER:O	2:C:13:LEU:HD13	2.06	0.56
2:C:196:TYR:HB2	2:C:213:PHE:CE1	2.41	0.56
1:A:599:GLU:HB2	1:A:600:ALA:CA	2.36	0.56
3:D:206:LYS:N	3:D:207:PRO:CD	2.69	0.56
1:A:992:GLU:CA	1:A:993:ILE:HB	2.35	0.55
1:B:21:TYR:HA	1:B:33:VAL:O	2.05	0.55
1:B:974:TRP:HB3	1:B:987:LEU:CD2	2.36	0.55
1:B:821:LYS:NZ	1:B:825:ASP:OD2	2.34	0.55
1:B:713:ILE:HD11	1:B:804:GLY:HA3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:948:ARG:HG3	1:B:1014:TRP:HA	1.88	0.55
1:A:573:ASN:HA	1:A:575:ALA:H	1.70	0.55
1:B:167:SER:OG	1:B:184:GLN:NE2	2.38	0.55
1:B:1154:LEU:HD12	1:B:1291:TRP:CE2	2.41	0.55
3:F:150:TYR:CZ	3:F:155:VAL:HG22	2.41	0.55
1:A:209:GLY:HA3	1:A:405:ASN:HD21	1.67	0.55
2:E:65:ARG:HH21	2:E:86:ASP:CG	2.10	0.55
2:C:54:ARG:O	2:C:55:ALA:HB3	2.07	0.55
1:A:1211:ILE:O	1:A:1214:VAL:HG23	2.07	0.55
1:B:757:GLU:O	1:B:759:LYS:CA	2.55	0.55
1:A:579:PRO:HB3	1:A:580:SER:HA	1.89	0.54
1:A:992:GLU:CA	1:A:993:ILE:CD1	2.84	0.54
1:B:24:ILE:HG23	1:B:25:PRO:CD	2.34	0.54
2:C:152:TRP:HE1	2:C:181:SER:HG	1.54	0.54
1:B:184:GLN:HG3	1:B:228:ALA:HA	1.88	0.54
3:F:154:PRO:O	3:F:205:HIS:HD2	1.89	0.54
2:C:199:GLU:HG3	2:C:210:THR:HG22	1.88	0.54
1:B:1234:LYS:O	1:B:1236:LYS:HG2	2.07	0.54
1:B:347:GLU:HB3	1:B:494:ILE:CD1	2.37	0.54
1:A:1150:LEU:C	1:A:1150:LEU:HD12	2.28	0.54
1:B:195:GLY:HA3	1:B:374:PHE:HE1	1.71	0.54
1:B:14:VAL:HA	1:B:19:ILE:O	2.07	0.54
1:A:699:LEU:O	1:A:702:ARG:HB3	2.06	0.54
1:A:824:TYR:O	1:A:827:ARG:HB3	2.08	0.54
1:B:97:ARG:HA	1:B:386:ILE:HG23	1.89	0.54
1:B:570:ASN:O	1:B:583:TYR:HA	2.08	0.54
1:B:135:ILE:CG2	1:B:149:LEU:CD2	2.76	0.54
1:A:560:GLU:N	1:A:561:HIS:CA	2.71	0.54
1:B:1135:TYR:HE1	1:B:1137:LYS:HB3	1.73	0.54
2:C:39:TRP:CZ3	2:C:92:CYS:HB3	2.42	0.54
1:B:364:LYS:C	1:B:365:THR:HG23	2.28	0.54
1:A:573:ASN:CA	1:A:575:ALA:H	2.21	0.54
1:B:322:LEU:HD12	1:B:341:LEU:HB2	1.88	0.54
2:C:83:GLU:HB2	2:C:85:GLU:HG2	1.88	0.54
3:F:35:TYR:CE1	3:F:50:THR:HG23	2.43	0.54
3:F:37:VAL:HG13	3:F:46:GLU:O	2.08	0.54
2:C:202:HIS:HD2	2:C:204:GLY:H	1.56	0.54
1:A:905:ASN:HB3	1:A:915:GLN:HB3	1.89	0.54
3:F:101:TYR:CD2	3:F:102:ASP:HB2	2.43	0.53
2:C:140:LEU:HD12	2:C:140:LEU:N	2.23	0.53
2:E:139:LEU:CD2	3:F:186:VAL:HG21	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:GLU:HA	3:D:22:CYS:HA	1.91	0.53
1:A:809:GLU:HB3	1:A:934:TYR:CD1	2.44	0.53
2:C:159:GLN:CG	2:C:162:ASN:HD21	2.21	0.53
1:B:146:SER:CB	1:B:520:LEU:HD22	2.38	0.53
1:B:638:GLY:HA3	1:B:652:PHE:HB2	1.91	0.53
1:A:946:TRP:HB2	1:A:1070:LYS:HG2	1.89	0.53
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.72	0.53
1:A:965:ILE:HG12	1:A:1055:PHE:CD2	2.44	0.53
3:D:200:ILE:HG22	3:D:201:CYS:H	1.74	0.53
1:A:573:ASN:HB3	1:A:575:ALA:H	1.72	0.53
1:B:596:LYS:O	1:B:598:THR:HG22	2.09	0.53
2:E:34:HIS:CD2	2:E:54:ARG:HE	2.27	0.53
2:E:140:LEU:HD21	2:E:200:VAL:CG1	2.39	0.53
1:B:1018:THR:HG21	1:B:1084:ILE:HG12	1.91	0.53
1:B:463:PHE:CD2	1:B:727:LEU:HD23	2.44	0.53
1:A:599:GLU:HB2	1:A:600:ALA:CB	2.38	0.53
1:A:1257:ASN:C	1:A:1258:ILE:HG12	2.29	0.53
3:F:2:VAL:HG13	3:F:26:GLY:O	2.09	0.53
3:F:131:PRO:O	3:F:133:SER:HB2	2.08	0.53
3:F:189:VAL:HB	3:F:190:PRO:CD	2.39	0.53
2:E:144:TYR:CD2	2:E:145:PRO:CA	2.92	0.53
2:E:54:ARG:HB2	2:E:57:ASN:OD1	2.09	0.53
1:B:485:THR:HG22	1:B:486:ASN:N	2.24	0.53
1:A:636:TYR:C	1:A:639:PRO:HD2	2.29	0.53
3:F:129:LEU:HD21	3:F:146:LEU:HB2	1.91	0.53
1:A:1113:MET:HA	1:A:1113:MET:CE	2.38	0.52
1:A:894:TYR:O	1:A:929:LYS:HG3	2.09	0.52
1:B:658:PHE:C	1:B:658:PHE:CD2	2.80	0.52
3:F:98:ARG:NH1	3:F:106:ASP:CG	2.62	0.52
1:B:1008:SER:CB	1:B:1011:ILE:HG13	2.39	0.52
1:B:567:ALA:HB1	1:B:746:ILE:HG12	1.91	0.52
3:F:189:VAL:HB	3:F:190:PRO:HD2	1.92	0.52
1:B:1211:ILE:N	1:B:1212:PRO:CD	2.71	0.52
1:A:1211:ILE:HG13	1:A:1212:PRO:CD	2.39	0.52
1:A:1133:TYR:CD1	1:A:1260:LYS:HG2	2.45	0.52
1:B:885:SER:O	1:B:886:ASN:HB2	2.09	0.52
1:A:632:ILE:O	1:A:787:PHE:HD1	1.93	0.52
1:A:576:LEU:O	1:A:578:ASN:N	2.42	0.52
3:F:189:VAL:HG11	3:F:199:TYR:CE2	2.44	0.52
1:A:80:THR:O	1:A:84:LYS:HG3	2.08	0.52
1:A:72:TYR:CE1	1:A:416:LEU:HD13	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:MET:CE	1:B:1113:MET:HA	2.39	0.52
1:B:658:PHE:C	1:B:658:PHE:HD2	2.13	0.52
1:A:267:GLY:HA3	1:A:350:THR:HB	1.92	0.52
3:F:126:VAL:HG12	3:F:214:LYS:HG2	1.92	0.52
1:B:574:GLU:N	1:B:574:GLU:OE1	2.42	0.52
1:B:1113:MET:HE2	1:B:1113:MET:HA	1.92	0.52
1:A:985:TRP:HB3	1:A:997:VAL:CG2	2.39	0.52
1:A:838:LYS:O	1:A:842:ASN:HB2	2.09	0.52
1:A:658:PHE:CD2	1:A:658:PHE:C	2.83	0.52
1:A:579:PRO:CB	1:A:580:SER:HA	2.40	0.51
2:E:55:ALA:HB3	2:E:56:SER:HB3	1.91	0.51
2:E:65:ARG:NH2	2:E:86:ASP:OD1	2.38	0.51
1:B:146:SER:OG	1:B:520:LEU:HD22	2.10	0.51
1:A:426:TYR:CE1	1:A:456:LYS:HG2	2.46	0.51
1:A:48:ARG:HG2	1:A:78:LEU:HD23	1.92	0.51
1:A:963:THR:HB	1:A:1058:ASP:HB3	1.92	0.51
2:E:144:TYR:HA	2:E:145:PRO:C	2.29	0.51
1:A:1266:TRP:CH2	1:A:1270:GLN:HG3	2.44	0.51
1:A:683:SER:HG	1:A:822:TYR:HE1	1.57	0.51
3:F:98:ARG:HH11	3:F:107:TYR:HD1	1.56	0.51
1:A:859:ASN:O	1:A:863:LEU:HG	2.11	0.51
1:B:46:PRO:O	1:B:84:LYS:HD3	2.10	0.51
3:F:6:GLU:OE2	3:F:96:CYS:N	2.38	0.51
1:A:990:THR:O	1:A:991:GLN:CB	2.59	0.51
1:A:377:ASN:OD1	1:A:380:PRO:HD3	2.11	0.51
1:B:379:VAL:CB	1:B:380:PRO:HD3	2.35	0.51
1:A:854:SER:HA	1:A:863:LEU:HD22	1.92	0.51
1:A:3:PHE:HB2	1:A:99:TYR:CD2	2.45	0.51
1:A:934:TYR:CD2	1:A:934:TYR:N	2.78	0.51
1:B:1061:ARG:HG2	1:B:1061:ARG:NH1	2.25	0.51
2:E:199:GLU:HB2	2:E:210:THR:HG22	1.93	0.51
1:B:1254:GLN:NE2	1:B:1255:PHE:HA	2.25	0.51
1:B:49:ASP:C	1:B:49:ASP:OD1	2.48	0.51
1:B:99:TYR:HB2	1:B:108:LEU:CD1	2.40	0.51
1:B:990:THR:O	1:B:991:GLN:CB	2.59	0.51
1:A:993:ILE:HG22	1:A:993:ILE:O	2.11	0.51
1:A:188:PHE:CG	1:A:189:SER:N	2.79	0.51
1:B:963:THR:HB	1:B:1058:ASP:HB3	1.93	0.51
1:A:464:PHE:CD2	1:A:466:PRO:HD3	2.46	0.51
2:C:183:LEU:HD21	2:C:185:LEU:HD11	1.92	0.51
1:B:306:THR:OG1	1:B:307:THR:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:144:TYR:CD2	2:E:145:PRO:HA	2.40	0.51
1:A:599:GLU:HB2	1:A:600:ALA:HA	1.92	0.51
1:B:242:VAL:HG12	1:B:259:SER:HA	1.93	0.51
1:A:578:ASN:C	1:A:581:ARG:HG2	2.31	0.51
1:B:1211:ILE:CB	1:B:1212:PRO:HD3	2.37	0.51
1:A:68:VAL:HG13	1:A:68:VAL:O	2.11	0.51
1:A:125:THR:O	1:A:301:LYS:N	2.37	0.50
1:A:636:TYR:O	1:A:639:PRO:HD2	2.12	0.50
2:C:155:ASP:O	2:C:156:ASN:ND2	2.44	0.50
1:A:634:ILE:HD11	1:A:783:ASN:HB3	1.93	0.50
1:A:1254:GLN:HG2	1:A:1256:ASN:H	1.76	0.50
1:B:1127:ASN:O	1:B:1132:GLY:HA3	2.11	0.50
3:D:146:LEU:HD21	3:D:148:LYS:HD3	1.93	0.50
1:B:67:GLN:HA	1:B:425:PHE:CZ	2.47	0.50
1:A:238:ASN:ND2	1:A:240:ASN:H	2.09	0.50
1:A:72:TYR:CZ	1:A:416:LEU:HD13	2.46	0.50
3:F:135:SER:CB	3:F:136:THR:HA	2.41	0.50
1:B:1233:ASN:ND2	1:B:1235:CYS:N	2.60	0.50
1:A:1257:ASN:O	1:A:1258:ILE:HG12	2.12	0.50
2:E:62:ILE:HG23	2:E:63:PRO:HD2	1.94	0.50
1:A:464:PHE:CE2	1:A:466:PRO:HD3	2.46	0.50
1:B:1273:ARG:HG3	1:B:1273:ARG:O	2.10	0.50
1:B:80:THR:O	1:B:84:LYS:HG3	2.11	0.50
1:B:780:ALA:O	1:B:783:ASN:HB2	2.12	0.50
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	1.94	0.50
1:B:487:ILE:HD12	1:B:700:SER:HB2	1.94	0.50
1:B:997:VAL:HB	1:B:1037:ASP:HB3	1.93	0.50
1:A:923:LYS:HG3	1:A:923:LYS:O	2.12	0.50
1:A:1044:LEU:CG	1:A:1045:GLY:HA2	2.40	0.50
1:B:267:GLY:HA2	1:B:271:ALA:HB2	1.93	0.50
3:D:98:ARG:NH1	3:D:107:TYR:CD1	2.79	0.50
1:B:49:ASP:OD2	1:B:187:ARG:NE	2.35	0.50
1:A:313:MET:O	1:A:316:VAL:HB	2.11	0.50
1:B:594:VAL:HA	1:B:606:TRP:CZ2	2.32	0.50
1:A:120:GLY:O	1:A:121:SER:O	2.30	0.50
1:B:995:GLN:HB3	1:B:1041:ILE:HG22	1.94	0.50
1:B:16:GLY:O	1:B:145:ARG:NH2	2.45	0.50
1:A:42:ILE:HG12	1:A:151:LEU:HB3	1.94	0.49
3:D:151:PHE:CD2	3:D:151:PHE:C	2.86	0.49
1:B:831:ILE:HG23	1:B:832:GLY:N	2.26	0.49
1:B:22:ILE:HG12	1:B:35:ALA:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:CG1	1:A:149:LEU:HD22	2.41	0.49
1:A:955:SER:HA	1:A:958:LEU:HD12	1.94	0.49
2:E:39:TRP:CZ3	2:E:92:CYS:HB3	2.47	0.49
1:B:1169:ASN:O	1:B:1171:ASP:N	2.39	0.49
1:B:1229:GLN:HG2	1:B:1229:GLN:O	2.12	0.49
1:A:559:PHE:HB2	1:A:560:GLU:CA	2.42	0.49
2:C:29:VAL:CG1	2:C:29:VAL:O	2.60	0.49
1:B:1111:TYR:CD2	1:B:1284:PHE:HB3	2.47	0.49
1:B:463:PHE:CE2	1:B:727:LEU:HD23	2.47	0.49
1:A:1026:ASN:CB	1:A:1039:LYS:O	2.60	0.49
1:B:681:LEU:CD1	1:B:819:LEU:HD23	2.42	0.49
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.46	0.49
2:C:83:GLU:CB	2:C:85:GLU:HG2	2.42	0.49
1:B:399:ALA:O	1:B:401:PHE:N	2.46	0.49
1:B:939:GLU:HB3	1:B:1023:ARG:HB2	1.94	0.49
1:B:485:THR:CG2	1:B:486:ASN:N	2.76	0.49
1:A:819:LEU:O	1:A:822:TYR:HB3	2.13	0.49
1:B:669:PRO:HG3	1:B:721:VAL:CG2	2.42	0.49
1:B:555:ARG:HD3	1:B:581:ARG:HH12	1.76	0.49
3:F:68:PHE:CZ	3:F:83:MET:HG2	2.47	0.49
3:F:101:TYR:HA	3:F:102:ASP:HA	1.50	0.49
1:B:1238:ASN:HB2	1:B:1249:PHE:CE2	2.48	0.49
1:B:1249:PHE:HB2	1:B:1267:TYR:HB2	1.95	0.49
1:B:590:TYR:O	1:B:594:VAL:HG22	2.13	0.49
3:F:206:LYS:N	3:F:207:PRO:CD	2.76	0.49
2:E:150:VAL:HG13	2:E:150:VAL:O	2.12	0.49
1:B:717:TRP:CD1	1:B:796:LEU:HB2	2.48	0.49
2:C:39:TRP:CH2	2:C:92:CYS:HB3	2.47	0.49
1:A:878:ILE:HD11	1:A:1074:LEU:HG	1.95	0.49
1:B:539:ASN:O	1:B:540:GLY:C	2.51	0.48
1:B:596:LYS:NZ	1:B:598:THR:HB	2.28	0.48
2:C:71:SER:HA	2:C:75:PHE:CE2	2.48	0.48
1:A:561:HIS:H	1:A:562:GLY:HA2	1.75	0.48
1:A:68:VAL:HG23	1:A:69:PRO:HD2	1.92	0.48
1:A:1150:LEU:CG	1:A:1150:LEU:O	2.61	0.48
3:D:205:HIS:CD2	3:D:207:PRO:HD2	2.48	0.48
1:B:905:ASN:HB3	1:B:915:GLN:HB3	1.96	0.48
2:E:12:SER:HB2	2:E:109:GLU:OE1	2.12	0.48
3:F:150:TYR:CZ	3:F:155:VAL:CG2	2.96	0.48
3:F:205:HIS:HB3	3:F:210:THR:HB	1.95	0.48
1:B:1169:ASN:C	1:B:1171:ASP:H	2.16	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:MET:HA	1:B:784:ILE:HD12	1.95	0.48
1:B:568:LEU:H	1:B:580:SER:CB	2.22	0.48
1:A:607:VAL:HG12	1:A:608:GLU:H	1.76	0.48
2:C:88:ALA:HB3	2:C:90:TYR:CE1	2.48	0.48
1:A:786:LYS:O	1:A:789:ASN:HB2	2.13	0.48
2:E:21:ILE:HG22	2:E:22:SER:N	2.27	0.48
1:B:910:ASP:O	1:B:913:GLN:HG3	2.13	0.48
1:A:599:GLU:N	1:A:599:GLU:OE2	2.46	0.48
2:E:4:LEU:HD13	2:E:23:CYS:SG	2.53	0.48
1:B:379:VAL:N	1:B:380:PRO:CD	2.76	0.48
1:A:494:ILE:CG2	1:A:494:ILE:O	2.61	0.48
2:C:54:ARG:HG3	2:C:54:ARG:HH11	1.78	0.48
1:A:1022:ASN:H	1:A:1041:ILE:HD11	1.78	0.48
1:A:556:ALA:HB1	1:A:583:TYR:HB3	1.95	0.48
1:B:811:PHE:C	1:B:811:PHE:CD2	2.87	0.48
1:A:53:ASN:ND2	1:A:55:GLU:H	2.12	0.48
2:E:29:VAL:O	2:E:29:VAL:CG1	2.61	0.48
1:A:3:PHE:O	1:A:39:HIS:CD2	2.62	0.47
2:C:129:LEU:HD21	2:C:190:TYR:CD2	2.49	0.47
1:A:906:PHE:CE2	1:A:914:ILE:HG12	2.48	0.47
1:A:588:SER:HA	1:A:591:VAL:HG13	1.96	0.47
2:C:179:LEU:HA	3:D:171:PHE:HE2	1.79	0.47
1:B:955:SER:O	1:B:958:LEU:HD12	2.14	0.47
3:F:139:GLY:N	3:F:140:THR:HB	2.24	0.47
1:A:1257:ASN:N	1:A:1257:ASN:OD1	2.48	0.47
1:B:1022:ASN:ND2	1:B:1025:ASN:OD1	2.47	0.47
1:A:563:LYS:O	1:A:565:ARG:N	2.47	0.47
1:B:1228:ASP:HB3	1:B:1229:GLN:HB2	1.90	0.47
1:A:605:GLY:O	1:A:606:TRP:C	2.53	0.47
1:A:1006:ASN:ND2	1:A:1006:ASN:H	2.10	0.47
2:C:172:SER:OG	2:C:172:SER:O	2.30	0.47
1:A:315:ASN:ND2	1:A:318:LYS:HD3	2.28	0.47
1:B:1233:ASN:HD21	1:B:1235:CYS:HB2	1.79	0.47
1:A:163:PHE:HD1	1:A:188:PHE:HA	1.77	0.47
1:A:1135:TYR:CE1	1:A:1137:LYS:HB3	2.49	0.47
1:B:556:ALA:HB2	1:B:576:LEU:CD1	2.45	0.47
1:A:385:THR:HG23	1:A:392:LEU:CD2	2.42	0.47
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.49	0.47
1:B:362:ASN:ND2	1:B:363:ARG:O	2.46	0.47
2:E:128:GLN:HA	3:F:127:PHE:CE2	2.50	0.47
1:B:62:PRO:HG2	1:B:65:ALA:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ILE:HD13	1:A:1114:LEU:HD21	1.95	0.47
1:B:588:SER:HA	1:B:591:VAL:HG22	1.97	0.47
1:B:772:LYS:O	1:B:775:GLU:HB2	2.15	0.47
1:B:578:ASN:HB2	1:B:581:ARG:N	2.29	0.47
3:D:6:GLU:O	3:D:6:GLU:HG2	2.14	0.47
1:B:195:GLY:CA	1:B:374:PHE:HE1	2.28	0.47
2:E:186:SER:O	2:E:187:LYS:C	2.52	0.47
3:D:101:TYR:CE2	3:D:102:ASP:HB2	2.49	0.47
3:D:53:ASP:OD1	3:D:53:ASP:N	2.48	0.47
1:B:43:TRP:CD1	1:B:149:LEU:HD13	2.50	0.47
1:A:238:ASN:ND2	1:A:239:PRO:CD	2.73	0.47
1:B:471:PHE:CE1	1:B:720:LYS:HE2	2.49	0.47
1:A:1022:ASN:HB3	1:A:1025:ASN:HB2	1.96	0.47
2:C:167:VAL:HG22	2:C:179:LEU:HD12	1.96	0.47
1:A:22:ILE:HG22	1:A:137:VAL:HA	1.96	0.47
1:A:223:HIS:CE1	1:A:262:GLU:OE2	2.66	0.47
2:C:59:GLU:HB3	2:C:62:ILE:HG13	1.95	0.47
1:B:1003:GLN:HA	1:B:1011:ILE:HD11	1.96	0.47
1:B:995:GLN:OE1	1:B:996:ARG:N	2.46	0.47
1:B:131:ASP:OD1	1:B:132:THR:HG23	2.14	0.47
1:B:208:LEU:O	1:B:209:GLY:O	2.32	0.47
1:A:759:LYS:C	1:A:761:ASN:N	2.68	0.47
1:A:1093:ASN:O	1:A:1095:GLY:N	2.48	0.47
1:B:165:CYS:SG	1:B:186:ILE:HG12	2.54	0.47
1:B:644:GLY:H	1:B:645:ASN:CA	2.28	0.47
1:A:536:ARG:HB3	1:A:536:ARG:HE	1.54	0.47
1:A:1082:LYS:HE3	1:A:1086:ASP:OD2	2.16	0.47
1:A:43:TRP:CD1	1:A:149:LEU:HD13	2.50	0.46
2:E:150:VAL:HG11	2:E:181:SER:CB	2.44	0.46
3:D:200:ILE:HG22	3:D:201:CYS:N	2.30	0.46
1:A:1228:ASP:O	1:A:1229:GLN:C	2.52	0.46
1:B:520:LEU:HD22	1:B:520:LEU:H	1.80	0.46
1:A:318:LYS:HB2	1:A:331:PHE:CE1	2.50	0.46
1:B:676:LEU:HD22	1:B:705:LYS:HE3	1.97	0.46
1:A:710:TYR:O	1:A:711:LYS:C	2.54	0.46
1:B:1227:ASN:CG	1:B:1227:ASN:O	2.53	0.46
1:B:596:LYS:HZ3	1:B:598:THR:HB	1.80	0.46
1:A:1031:ILE:HG12	1:A:1036:ILE:HG13	1.98	0.46
1:B:1080:ASN:O	1:B:1081:GLU:C	2.53	0.46
1:A:573:ASN:CA	1:A:575:ALA:N	2.74	0.46
2:E:23:CYS:HB2	2:E:39:TRP:CH2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:ASN:HD22	1:A:1197:ALA:N	2.14	0.46
1:B:598:THR:O	1:B:754:TYR:OH	2.33	0.46
2:C:87:PHE:HB3	2:C:110:ILE:CG1	2.46	0.46
2:C:62:ILE:CG2	2:C:63:PRO:HD2	2.45	0.46
1:B:636:TYR:C	1:B:639:PRO:HD2	2.36	0.46
1:B:1099:ASP:OD1	1:B:1099:ASP:C	2.53	0.46
1:A:567:ALA:HB1	1:A:746:ILE:HG12	1.97	0.46
1:A:816:LYS:CB	1:A:845:LEU:HD23	2.46	0.46
1:B:131:ASP:OD1	1:B:132:THR:N	2.49	0.46
2:E:6:GLN:NE2	2:E:90:TYR:O	2.40	0.46
1:B:687:ASN:ND2	1:B:690:LEU:HD13	2.30	0.46
1:B:468:GLU:OE1	1:B:720:LYS:NZ	2.49	0.46
2:C:163:SER:HB3	2:C:183:LEU:HA	1.97	0.46
3:D:4:LEU:HD21	3:D:27:PHE:CZ	2.51	0.46
1:B:216:ASP:C	1:B:216:ASP:OD1	2.55	0.46
1:B:573:ASN:HB2	1:B:576:LEU:HD13	1.97	0.46
1:B:1254:GLN:HG2	1:B:1256:ASN:H	1.81	0.46
1:B:22:ILE:HD11	1:B:45:ILE:HD11	1.98	0.46
3:D:144:GLY:HA2	3:D:159:TRP:HH2	1.82	0.46
1:A:93:LYS:HG3	1:A:386:ILE:HG13	1.98	0.46
1:A:1241:ASP:C	1:A:1243:ASN:H	2.19	0.45
1:A:948:ARG:NH2	1:A:1288:ASP:OD2	2.49	0.45
1:A:98:ILE:O	1:A:104:GLY:HA3	2.16	0.45
1:A:879:LEU:HD12	1:A:879:LEU:HA	1.80	0.45
1:B:488:GLU:HG2	1:B:489:ALA:HB3	1.98	0.45
2:E:144:TYR:CD2	2:E:145:PRO:N	2.84	0.45
1:A:24:ILE:HG23	1:A:25:PRO:CD	2.45	0.45
1:B:915:GLN:HB2	1:B:1068:TRP:CZ3	2.51	0.45
2:C:140:LEU:CD1	2:C:140:LEU:N	2.79	0.45
1:B:974:TRP:HB3	1:B:987:LEU:HD23	1.98	0.45
2:C:23:CYS:HB2	2:C:39:TRP:CH2	2.52	0.45
2:C:93:GLN:HB2	2:C:102:PHE:CD2	2.52	0.45
1:A:468:GLU:OE1	1:A:720:LYS:NZ	2.33	0.45
2:E:87:PHE:C	2:E:87:PHE:CD1	2.90	0.45
1:B:532:PRO:CB	1:B:533:ASN:HB3	2.46	0.45
1:A:607:VAL:O	1:A:608:GLU:C	2.54	0.45
1:A:1211:ILE:H	1:A:1211:ILE:HG13	1.53	0.45
1:A:227:HIS:CE1	1:A:262:GLU:OE1	2.69	0.45
1:A:1092:SER:O	1:A:1093:ASN:HB2	2.15	0.45
1:B:407:GLU:O	1:B:410:ASN:HB3	2.16	0.45
3:D:84:ASN:O	3:D:85:SER:C	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:HG2	1:B:78:LEU:HD23	1.99	0.45
1:A:1210:GLU:C	1:A:1212:PRO:HD2	2.36	0.45
1:A:246:ASN:C	1:A:247:THR:CG2	2.85	0.45
2:C:42:GLN:HE22	3:D:39:GLN:HE22	1.65	0.45
1:A:907:ASP:HB2	1:A:1068:TRP:CZ3	2.51	0.45
1:A:772:LYS:O	1:A:775:GLU:HB2	2.17	0.45
3:D:78:THR:HG22	3:D:79:LEU:N	2.31	0.45
1:B:3:PHE:O	1:B:39:HIS:HD2	1.99	0.45
3:D:197:GLN:NE2	3:D:198:THR:O	2.48	0.45
1:B:638:GLY:O	1:B:642:ASN:N	2.49	0.45
2:C:62:ILE:HG22	2:C:66:PHE:HD1	1.82	0.45
1:B:993:ILE:CB	1:B:1044:LEU:CD1	2.94	0.45
1:A:9:ASN:HA	1:A:85:ASP:OD1	2.17	0.45
1:A:599:GLU:CB	1:A:600:ALA:CA	2.93	0.45
1:A:1029:ILE:HG23	1:A:1029:ILE:O	2.17	0.45
1:A:253:MET:HE3	1:A:256:LEU:HD22	1.98	0.45
1:A:780:ALA:O	1:A:783:ASN:HB2	2.16	0.45
1:A:1253:HIS:O	1:A:1254:GLN:CB	2.64	0.45
1:B:645:ASN:O	1:B:647:LEU:N	2.49	0.45
1:B:134:CYS:HB3	1:B:147:GLU:O	2.17	0.45
3:D:176:GLN:CD	3:D:182:SER:HB3	2.38	0.45
3:D:192:SER:HB3	3:D:193:SER:H	1.64	0.45
1:A:1222:VAL:N	1:A:1238:ASN:O	2.46	0.45
2:E:174:ASP:C	2:E:176:THR:H	2.20	0.45
1:A:942:SER:OG	1:A:1020:THR:HA	2.17	0.45
3:F:204:ASN:HD21	3:F:211:LYS:HG2	1.79	0.44
1:B:255:GLY:HA3	1:B:537:PHE:CG	2.52	0.44
2:C:54:ARG:NH1	2:C:54:ARG:HG3	2.32	0.44
1:B:1146:THR:O	1:B:1147:ASN:HB2	2.16	0.44
2:C:91:TYR:CD1	3:D:45:LEU:HD12	2.52	0.44
1:A:457:VAL:HG21	1:A:551:PHE:HB3	1.99	0.44
2:E:21:ILE:HG22	2:E:22:SER:H	1.81	0.44
2:E:87:PHE:O	2:E:88:ALA:HB2	2.18	0.44
1:A:334:ASP:O	1:A:335:LYS:C	2.55	0.44
1:B:1142:SER:HB3	1:B:1150:LEU:HD11	2.00	0.44
1:B:1209:LEU:CD2	1:B:1217:LEU:HD13	2.46	0.44
2:C:62:ILE:HG22	2:C:63:PRO:HD2	1.98	0.44
1:A:285:TYR:CZ	1:A:289:LYS:HE2	2.53	0.44
1:B:43:TRP:CD1	1:B:149:LEU:CD1	3.00	0.44
3:F:35:TYR:CE1	3:F:50:THR:CG2	3.00	0.44
1:A:1267:TYR:O	1:A:1270:GLN:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASP:O	1:A:476:ASN:N	2.50	0.44
1:B:1018:THR:HB	1:B:1030:TYR:HB2	1.99	0.44
2:E:117:PRO:HD3	2:E:202:HIS:CD2	2.52	0.44
1:B:161:ILE:HG12	1:B:161:ILE:H	1.62	0.44
1:A:207:LEU:HA	1:A:207:LEU:HD12	1.88	0.44
1:B:686:ALA:HA	1:B:829:THR:HG23	1.99	0.44
3:F:137:SER:C	3:F:138:GLY:O	2.55	0.44
1:B:1284:PHE:O	1:B:1286:PRO:HD3	2.18	0.44
1:B:1144:MET:HB3	1:B:1150:LEU:HD13	1.98	0.44
1:B:502:TYR:O	1:B:503:TYR:C	2.56	0.44
3:F:144:GLY:O	3:F:216:VAL:HG21	2.18	0.44
1:B:1026:ASN:HA	1:B:1041:ILE:HG12	2.00	0.44
2:C:122:PHE:HA	2:C:123:PRO:HD2	1.68	0.44
3:F:38:ARG:HG2	3:F:48:VAL:CG2	2.48	0.44
1:B:1113:MET:CE	1:B:1284:PHE:HA	2.45	0.44
1:B:948:ARG:HG3	1:B:1014:TRP:CA	2.48	0.44
2:E:127:GLU:HA	2:E:130:LYS:HE3	2.00	0.44
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	2.00	0.44
1:A:393:ARG:HA	1:A:398:ALA:HB2	2.00	0.43
1:B:1022:ASN:HB3	1:B:1025:ASN:HB2	2.00	0.43
1:B:146:SER:HB3	1:B:520:LEU:CD2	2.48	0.43
2:C:118:SER:O	2:C:141:ASN:N	2.45	0.43
1:B:1257:ASN:CG	1:B:1258:ILE:H	2.21	0.43
2:E:122:PHE:HA	2:E:123:PRO:HD3	1.78	0.43
2:C:174:ASP:O	2:C:176:THR:N	2.43	0.43
1:B:1019:ILE:CD1	1:B:1029:ILE:HG13	2.48	0.43
2:E:170:GLN:NE2	2:E:175:SER:HB3	2.33	0.43
1:B:599:GLU:HA	1:B:600:ALA:HA	1.72	0.43
1:A:14:VAL:HA	1:A:19:ILE:O	2.18	0.43
1:A:857:VAL:HG12	1:A:858:ASP:N	2.33	0.43
1:A:320:LYS:HD3	1:A:321:TYR:CE1	2.53	0.43
1:B:1176:ASN:O	1:B:1177:ASN:HB2	2.18	0.43
2:C:14:SER:O	2:C:17:GLU:CG	2.36	0.43
1:B:1233:ASN:HD21	1:B:1235:CYS:H	1.64	0.43
1:B:636:TYR:O	1:B:639:PRO:HD2	2.18	0.43
1:B:251:TYR:O	1:B:462:LEU:HB3	2.18	0.43
1:A:727:LEU:O	1:A:731:LYS:HG3	2.18	0.43
1:B:550:MET:HE3	1:B:731:LYS:HD2	1.99	0.43
1:A:87:TYR:O	1:A:91:VAL:HG23	2.19	0.43
2:E:54:ARG:NH1	2:E:54:ARG:CG	2.77	0.43
3:F:128:PRO:HA	3:F:216:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:GLN:HB2	2:C:90:TYR:CE2	2.54	0.43
1:A:260:PHE:HE2	1:A:274:ILE:HG23	1.83	0.43
1:A:1085:LYS:O	1:A:1088:TYR:HB3	2.18	0.43
3:D:124:PRO:HB3	3:D:150:TYR:HB3	1.99	0.43
1:A:66:LYS:HE3	1:A:162:GLN:NE2	2.34	0.43
2:E:15:PRO:C	2:E:17:GLU:H	2.21	0.43
1:A:250:TYR:CD1	1:A:250:TYR:C	2.91	0.43
1:A:254:SER:HB2	1:A:459:ASN:CG	2.39	0.43
1:B:49:ASP:CG	1:B:49:ASP:O	2.57	0.43
1:B:1264:SER:C	1:B:1266:TRP:H	2.20	0.43
3:F:158:SER:OG	3:F:202:ASN:HB2	2.19	0.43
1:A:485:THR:CG2	1:A:486:ASN:N	2.82	0.43
1:A:1134:MET:HB3	1:A:1134:MET:HE2	1.87	0.43
3:F:136:THR:OG1	3:F:137:SER:CA	2.66	0.43
1:A:1168:GLY:O	1:A:1169:ASN:O	2.37	0.43
1:B:974:TRP:HB3	1:B:987:LEU:HD21	2.01	0.43
1:A:884:GLU:O	1:A:885:SER:C	2.56	0.43
1:A:1109:LYS:HA	1:A:1110:PRO:HD3	1.78	0.43
1:B:568:LEU:O	1:B:580:SER:HB3	2.19	0.43
1:A:560:GLU:H	1:A:561:HIS:CA	2.32	0.43
1:B:1264:SER:C	1:B:1266:TRP:N	2.72	0.43
1:B:223:HIS:CE1	1:B:262:GLU:OE2	2.71	0.43
1:A:36:PHE:N	1:A:36:PHE:CD1	2.87	0.43
1:B:573:ASN:CB	1:B:576:LEU:HD13	2.49	0.43
1:B:575:ALA:O	1:B:581:ARG:HB3	2.19	0.43
1:B:916:LEU:O	1:B:1066:TYR:HB2	2.18	0.43
1:A:365:THR:OG1	1:A:367:LEU:HB2	2.18	0.43
1:A:773:LEU:HA	1:A:776:SER:HB2	2.01	0.43
1:B:365:THR:C	1:B:367:LEU:N	2.70	0.43
1:B:1228:ASP:HB3	1:B:1229:GLN:CA	2.32	0.43
3:F:98:ARG:NH1	3:F:106:ASP:OD2	2.51	0.43
2:E:8:PRO:HG3	2:E:11:LEU:HD13	2.01	0.43
2:C:111:LYS:O	2:C:112:ARG:HB3	2.18	0.43
1:B:634:ILE:CD1	1:B:783:ASN:HB3	2.49	0.43
1:A:1228:ASP:HB3	1:A:1229:GLN:H	1.65	0.43
1:B:253:MET:O	1:B:254:SER:C	2.56	0.43
1:B:632:ILE:HG13	1:B:786:LYS:HD3	2.01	0.43
2:E:76:THR:O	2:E:76:THR:CG2	2.66	0.43
1:A:106:MET:SD	1:A:503:TYR:HA	2.59	0.43
3:D:151:PHE:HA	3:D:152:PRO:HA	1.83	0.43
1:A:895:ALA:HA	1:A:928:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:HG13	1:B:515:ILE:O	2.18	0.43
3:D:6:GLU:OE1	3:D:110:GLN:N	2.52	0.42
1:B:195:GLY:HA3	1:B:374:PHE:CE1	2.53	0.42
1:A:638:GLY:N	1:A:639:PRO:CD	2.82	0.42
1:A:550:MET:HE3	1:A:731:LYS:HD2	2.01	0.42
1:A:754:TYR:HB3	1:A:755:THR:H	1.59	0.42
1:A:643:ILE:HA	1:A:644:GLY:HA3	1.76	0.42
1:A:563:LYS:O	1:A:564:SER:C	2.58	0.42
1:B:629:ASP:N	1:B:629:ASP:OD1	2.51	0.42
1:B:999:PHE:CD1	1:B:1031:ILE:HG13	2.54	0.42
3:F:140:THR:HA	3:F:189:VAL:O	2.19	0.42
3:F:98:ARG:HH12	3:F:106:ASP:CG	2.21	0.42
2:E:170:GLN:HG2	2:E:175:SER:O	2.19	0.42
1:A:1106:GLN:HA	1:A:1172:ASN:O	2.19	0.42
1:B:1163:LYS:HB2	1:B:1181:TYR:HB2	2.01	0.42
1:A:1057:LEU:HD11	1:A:1066:TYR:HA	2.02	0.42
1:A:253:MET:HE1	1:A:256:LEU:HD22	2.01	0.42
3:D:128:PRO:HD3	3:D:214:LYS:HE2	1.99	0.42
2:E:112:ARG:HH11	2:E:115:ALA:HB2	1.84	0.42
2:C:86:ASP:O	2:C:108:VAL:HG11	2.19	0.42
1:B:824:TYR:O	1:B:827:ARG:HB3	2.19	0.42
1:A:1018:THR:HB	1:A:1030:TYR:HB2	2.02	0.42
3:D:183:LEU:HD12	3:D:183:LEU:C	2.40	0.42
3:F:155:VAL:HG23	3:F:183:LEU:HD21	2.02	0.42
1:B:951:LYS:HD3	1:B:1149:TYR:CG	2.54	0.42
1:B:1265:ASN:HD22	1:B:1265:ASN:HA	1.66	0.42
3:F:18:LEU:O	3:F:83:MET:HB2	2.19	0.42
1:B:1030:TYR:CE2	1:B:1035:LEU:HD13	2.55	0.42
1:A:366:TYR:OH	1:A:464:PHE:CE1	2.72	0.42
1:B:1238:ASN:HA	1:B:1249:PHE:HA	2.01	0.42
1:A:1193:LEU:HD21	1:A:1250:ILE:HD13	2.01	0.42
1:A:603:PHE:O	1:A:603:PHE:CD2	2.72	0.42
3:D:139:GLY:HA3	3:D:140:THR:HG1	1.84	0.42
1:B:627:ILE:CD1	1:B:628:ALA:N	2.69	0.42
1:B:819:LEU:O	1:B:822:TYR:HB3	2.20	0.42
1:B:884:GLU:CG	1:B:889:ILE:HD11	2.49	0.42
1:B:879:LEU:HA	1:B:879:LEU:HD12	1.83	0.42
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.77	0.42
3:F:20:LEU:CD1	3:F:83:MET:HE1	2.46	0.42
1:A:255:GLY:O	1:A:256:LEU:HB2	2.19	0.42
1:A:1146:THR:O	1:A:1147:ASN:CB	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:GLN:CG	1:A:996:ARG:H	2.33	0.42
3:F:145:CYS:O	3:F:184:SER:HA	2.19	0.42
1:B:800:MET:N	1:B:802:PRO:HD2	2.34	0.42
1:A:967:CYS:SG	1:A:1050:SER:HB3	2.59	0.42
1:A:1066:TYR:C	1:A:1066:TYR:CD1	2.93	0.42
2:C:87:PHE:CD1	2:C:87:PHE:C	2.92	0.42
3:D:204:ASN:HD21	3:D:211:LYS:CG	2.33	0.42
1:A:809:GLU:CB	1:A:934:TYR:CD1	3.03	0.42
2:C:213:PHE:CD1	2:C:213:PHE:C	2.94	0.42
3:D:101:TYR:CD2	3:D:102:ASP:HB2	2.55	0.42
2:C:164:GLN:HE22	3:D:176:GLN:HA	1.85	0.42
1:A:1008:SER:CB	1:A:1011:ILE:HG13	2.50	0.42
1:A:995:GLN:HG3	1:A:996:ARG:H	1.84	0.42
1:B:106:MET:HG2	1:B:506:PHE:CE1	2.54	0.42
1:A:1186:VAL:HB	1:A:1191:TYR:CE1	2.55	0.42
1:B:1109:LYS:HA	1:B:1110:PRO:HD3	1.90	0.42
1:A:184:GLN:HG3	1:A:228:ALA:HA	2.02	0.42
2:E:53:TYR:CE1	2:E:57:ASN:HB2	2.54	0.41
2:C:42:GLN:HE22	3:D:39:GLN:NE2	2.18	0.41
1:A:907:ASP:HA	1:A:908:PRO:HD3	1.81	0.41
2:C:40:TYR:N	2:C:91:TYR:O	2.43	0.41
3:D:59:TYR:N	3:D:59:TYR:CD1	2.88	0.41
1:A:10:TYR:CZ	1:A:84:LYS:HD2	2.55	0.41
1:B:1291:TRP:CD1	1:B:1293:GLU:HB3	2.55	0.41
1:B:633:ILE:HG21	1:B:653:VAL:HG22	2.01	0.41
1:A:499:ILE:O	1:A:500:GLN:C	2.57	0.41
1:A:343:LYS:HG3	1:A:347:GLU:OE1	2.21	0.41
2:E:30:ASP:HA	2:E:34:HIS:O	2.20	0.41
2:E:65:ARG:HD2	2:E:81:SER:O	2.21	0.41
3:F:6:GLU:OE1	3:F:109:GLY:HA3	2.21	0.41
3:D:6:GLU:OE1	3:D:109:GLY:C	2.58	0.41
2:E:144:TYR:C	2:E:144:TYR:CD2	2.93	0.41
1:B:754:TYR:O	1:B:755:THR:C	2.59	0.41
3:F:83:MET:HB3	3:F:86:LEU:HD21	2.03	0.41
2:C:112:ARG:HG3	2:C:113:THR:O	2.21	0.41
1:B:320:LYS:HE2	1:B:321:TYR:CZ	2.55	0.41
1:B:270:ASP:OD1	1:B:365:THR:CB	2.55	0.41
1:B:135:ILE:HG12	1:B:149:LEU:HD22	2.01	0.41
2:E:62:ILE:CG2	2:E:63:PRO:HD2	2.50	0.41
1:B:171:GLU:HG2	1:B:172:VAL:H	1.85	0.41
1:A:161:ILE:H	1:A:161:ILE:HG12	1.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASN:C	1:A:402:ASN:N	2.74	0.41
1:B:269:HIS:HD2	1:B:365:THR:HG22	1.73	0.41
1:A:567:ALA:HB1	1:A:746:ILE:CG1	2.50	0.41
1:A:1169:ASN:C	1:A:1171:ASP:N	2.70	0.41
1:B:1209:LEU:HD21	1:B:1217:LEU:HD13	2.03	0.41
3:D:150:TYR:OH	3:D:173:ALA:HB2	2.21	0.41
3:D:60:TYR:CE2	3:D:70:THR:HG22	2.56	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.88	0.41
3:F:151:PHE:HA	3:F:152:PRO:HA	1.87	0.41
3:D:81:LEU:HG	3:D:83:MET:HE2	2.02	0.41
1:A:1210:GLU:HB2	1:A:1213:ASP:HB2	2.03	0.41
1:A:951:LYS:HE3	1:A:1291:TRP:CZ3	2.56	0.41
2:C:151:GLN:HB3	2:C:158:LEU:HD21	2.03	0.41
1:A:748:ASN:O	1:A:752:ASN:ND2	2.51	0.41
1:A:481:ILE:N	1:A:481:ILE:HD13	2.36	0.41
3:D:82:GLN:NE2	3:D:83:MET:H	2.18	0.41
3:F:22:CYS:HB3	3:F:79:LEU:HB3	2.01	0.41
1:A:809:GLU:HG3	1:A:934:TYR:CE1	2.56	0.41
1:A:1233:ASN:HD21	1:A:1235:CYS:HB2	1.86	0.41
1:A:1235:CYS:HA	1:A:1280:CYS:O	2.21	0.41
1:B:964:ILE:HA	1:B:1056:LYS:O	2.21	0.41
1:B:915:GLN:HB2	1:B:1068:TRP:CH2	2.56	0.41
1:B:1264:SER:O	1:B:1266:TRP:N	2.54	0.41
1:A:509:ASP:HB3	1:A:510:ASN:H	1.57	0.41
1:A:810:ASP:O	1:A:813:ALA:HB3	2.21	0.41
1:B:163:PHE:CD1	1:B:188:PHE:HA	2.56	0.41
1:B:835:ASP:O	1:B:838:LYS:N	2.54	0.41
2:C:186:SER:O	2:C:187:LYS:C	2.59	0.41
2:C:187:LYS:O	2:C:191:GLU:HG2	2.20	0.41
1:A:1269:ARG:HD3	1:A:1269:ARG:HA	1.54	0.41
1:B:266:PHE:C	1:B:266:PHE:CD2	2.93	0.41
1:B:235:ILE:HA	1:B:286:TYR:CE2	2.55	0.41
1:B:749:TYR:O	1:B:753:GLN:HG2	2.21	0.41
1:B:365:THR:C	1:B:367:LEU:H	2.24	0.41
3:F:150:TYR:CE1	3:F:155:VAL:HG13	2.56	0.41
1:B:1135:TYR:CE1	1:B:1137:LYS:HB3	2.56	0.41
1:B:484:ASP:O	1:B:485:THR:O	2.37	0.41
1:A:306:THR:OG1	1:A:307:THR:N	2.54	0.41
1:A:656:LEU:HG	1:A:656:LEU:O	2.19	0.41
1:B:1233:ASN:HD21	1:B:1235:CYS:CB	2.35	0.40
3:D:144:GLY:HA2	3:D:159:TRP:CH2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:71:SER:HA	2:C:75:PHE:HE2	1.85	0.40
1:B:475:LEU:HB3	1:B:676:LEU:HD23	2.02	0.40
1:A:365:THR:C	1:A:367:LEU:N	2.74	0.40
1:A:667:PHE:CE1	1:A:724:GLN:NE2	2.90	0.40
1:B:497:ASP:N	1:B:497:ASP:OD1	2.54	0.40
1:A:405:ASN:HB3	1:A:408:ILE:HB	2.03	0.40
1:A:1126:ASN:CG	1:A:1127:ASN:N	2.75	0.40
1:B:567:ALA:HB1	1:B:746:ILE:HG13	2.02	0.40
1:A:290:PHE:CE2	1:A:321:TYR:HD2	2.39	0.40
1:B:1097:LEU:HD21	1:B:1223:MET:HB3	2.02	0.40
2:C:65:ARG:HA	2:C:80:SER:OG	2.21	0.40
1:B:1233:ASN:OD1	1:B:1271:ILE:HG23	2.22	0.40
1:B:801:ILE:N	1:B:802:PRO:CD	2.84	0.40
1:B:171:GLU:HG2	1:B:172:VAL:N	2.37	0.40
1:B:275:ASP:OD1	1:B:278:GLN:NE2	2.53	0.40
1:B:1092:SER:O	1:B:1093:ASN:HB2	2.21	0.40
1:B:36:PHE:CD1	1:B:36:PHE:N	2.89	0.40
1:A:121:SER:H	1:A:128:LYS:HB3	1.87	0.40
1:B:45:ILE:HA	1:B:46:PRO:HD3	1.88	0.40
1:B:559:PHE:CD1	1:B:560:GLU:CA	3.04	0.40
1:B:520:LEU:HD13	1:B:520:LEU:N	2.36	0.40
3:D:159:TRP:CE3	3:D:200:ILE:O	2.74	0.40
1:B:985:TRP:CE2	1:B:1019:ILE:HG21	2.56	0.40
1:B:706:TRP:CG	1:B:808:LEU:HD22	2.57	0.40
1:B:1074:LEU:HD12	1:B:1074:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1259/1295 (97%)	1084 (86%)	130 (10%)	45 (4%)	4	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1259/1295 (97%)	1081 (86%)	139 (11%)	39 (3%)	5	45
2	C	214/218 (98%)	182 (85%)	30 (14%)	2 (1%)	21	68
2	E	214/218 (98%)	193 (90%)	14 (6%)	7 (3%)	5	43
3	D	215/224 (96%)	182 (85%)	24 (11%)	9 (4%)	3	36
3	F	215/224 (96%)	192 (89%)	17 (8%)	6 (3%)	6	47
All	All	3376/3474 (97%)	2914 (86%)	354 (10%)	108 (3%)	5	44

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	400	ASN
1	A	560	GLU
1	A	564	SER
1	A	566	ILE
1	A	576	LEU
1	A	606	TRP
1	A	755	THR
1	A	760	ASN
1	A	831	ILE
1	A	991	GLN
1	A	993	ILE
1	A	1169	ASN
1	A	1229	GLN
1	A	1257	ASN
1	B	209	GLY
1	B	256	LEU
1	B	560	GLU
1	B	566	ILE
1	B	576	LEU
1	B	578	ASN
1	B	645	ASN
1	B	760	ASN
1	B	833	GLN
1	B	848	ASP
1	B	991	GLN
1	B	992	GLU
1	B	1167	SER
1	B	1170	LYS
1	B	1229	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1274	SER
3	D	137	SER
3	D	192	SER
3	F	137	SER
3	F	138	GLY
1	A	209	GLY
1	A	210	ALA
1	A	256	LEU
1	A	399	ALA
1	A	401	PHE
1	A	540	GLY
1	A	578	ASN
1	A	645	ASN
1	A	848	ASP
1	A	1254	GLN
1	A	1258	ILE
1	A	1259	ALA
1	B	121	SER
1	B	399	ALA
1	B	980	TYR
1	B	1231	ILE
1	B	1254	GLN
3	D	30	SER
3	D	140	THR
3	D	193	SER
2	E	55	ALA
2	E	156	ASN
1	A	49	ASP
1	A	254	SER
1	A	541	LYS
1	A	577	LEU
1	A	597	ALA
1	A	608	GLU
1	A	980	TYR
1	B	210	ALA
1	B	366	TYR
1	B	541	LYS
1	B	835	ASP
1	B	1094	SER
2	C	71	SER
3	D	28	THR
2	E	56	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	71	SER
3	F	140	THR
3	F	175	LEU
3	F	192	SER
1	A	563	LYS
1	A	567	ALA
1	A	589	ASP
1	A	970	ASN
1	A	1094	SER
1	A	1146	THR
1	B	124	ASP
1	B	400	ASN
1	B	561	HIS
1	B	757	GLU
1	B	761	ASN
1	B	1257	ASN
3	D	154	PRO
3	F	135	SER
1	A	475	LEU
1	A	644	GLY
1	A	1147	ASN
1	B	763	ASN
1	B	970	ASN
3	D	133	SER
2	E	16	GLY
2	E	175	SER
2	E	187	LYS
1	A	1242	ASN
1	B	572	VAL
1	B	831	ILE
1	B	1147	ASN
2	C	15	PRO
1	B	494	ILE
1	A	572	VAL
1	B	685	ILE
3	D	151	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1124/1178 (95%)	1020 (91%)	104 (9%)	11	47
1	B	1124/1178 (95%)	1037 (92%)	87 (8%)	16	56
2	C	186/190 (98%)	165 (89%)	21 (11%)	7	38
2	E	186/190 (98%)	165 (89%)	21 (11%)	7	38
3	D	181/190 (95%)	162 (90%)	19 (10%)	8	41
3	F	181/190 (95%)	165 (91%)	16 (9%)	12	50
All	All	2982/3116 (96%)	2714 (91%)	268 (9%)	12	49

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	24	ILE
1	A	30	MET
1	A	31	GLN
1	A	53	ASN
1	A	106	MET
1	A	122	THR
1	A	123	ILE
1	A	147	GLU
1	A	154	ILE
1	A	157	SER
1	A	161	ILE
1	A	165	CYS
1	A	202	VAL
1	A	204	THR
1	A	208	LEU
1	A	250	TYR
1	A	254	SER
1	A	258	VAL
1	A	269	HIS
1	A	276	SER
1	A	297	LEU
1	A	311	GLN
1	A	336	LEU
1	A	363	ARG
1	A	365	THR
1	A	411	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	412	ASN
1	A	422	LEU
1	A	453	LEU
1	A	480	GLU
1	A	493	ASN
1	A	506	PHE
1	A	507	ASN
1	A	508	PHE
1	A	509	ASP
1	A	536	ARG
1	A	549	THR
1	A	569	THR
1	A	570	ASN
1	A	580	SER
1	A	598	THR
1	A	602	MET
1	A	606	TRP
1	A	612	TYR
1	A	613	ASP
1	A	619	SER
1	A	622	SER
1	A	627	ILE
1	A	651	ASP
1	A	656	LEU
1	A	671	ILE
1	A	681	LEU
1	A	707	ASP
1	A	734	GLU
1	A	748	ASN
1	A	750	GLN
1	A	763	ASN
1	A	764	PHE
1	A	768	ASP
1	A	771	SER
1	A	776	SER
1	A	792	SER
1	A	794	SER
1	A	799	SER
1	A	829	THR
1	A	845	LEU
1	A	846	SER
1	A	847	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	860	GLN
1	A	873	ILE
1	A	896	SER
1	A	913	GLN
1	A	922	SER
1	A	923	LYS
1	A	928	LEU
1	A	958	LEU
1	A	970	ASN
1	A	994	LYS
1	A	1015	ILE
1	A	1023	ARG
1	A	1024	LEU
1	A	1026	ASN
1	A	1069	ILE
1	A	1082	LYS
1	A	1092	SER
1	A	1126	ASN
1	A	1130	ILE
1	A	1131	ARG
1	A	1143	VAL
1	A	1150	LEU
1	A	1151	ASN
1	A	1152	SER
1	A	1172	ASN
1	A	1196	ASN
1	A	1211	ILE
1	A	1213	ASP
1	A	1218	SER
1	A	1219	GLN
1	A	1228	ASP
1	A	1229	GLN
1	A	1255	PHE
1	A	1275	SER
1	A	1283	GLU
1	B	5	ASN
1	B	14	VAL
1	B	51	PHE
1	B	58	ASP
1	B	106	MET
1	B	123	ILE
1	B	126	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	143	SER
1	B	147	GLU
1	B	154	ILE
1	B	157	SER
1	B	161	ILE
1	B	165	CYS
1	B	202	VAL
1	B	204	THR
1	B	250	TYR
1	B	253	MET
1	B	254	SER
1	B	258	VAL
1	B	269	HIS
1	B	297	LEU
1	B	306	THR
1	B	310	LEU
1	B	311	GLN
1	B	340	LYS
1	B	363	ARG
1	B	373	VAL
1	B	411	MET
1	B	484	ASP
1	B	497	ASP
1	B	507	ASN
1	B	520	LEU
1	B	568	LEU
1	B	570	ASN
1	B	573	ASN
1	B	580	SER
1	B	584	THR
1	B	591	VAL
1	B	598	THR
1	B	599	GLU
1	B	602	MET
1	B	613	ASP
1	B	627	ILE
1	B	658	PHE
1	B	671	ILE
1	B	750	GLN
1	B	764	PHE
1	B	768	ASP
1	B	776	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	794	SER
1	B	807	ARG
1	B	811	PHE
1	B	812	ASP
1	B	814	SER
1	B	827	ARG
1	B	846	SER
1	B	874	ILE
1	B	889	ILE
1	B	922	SER
1	B	923	LYS
1	B	928	LEU
1	B	935	ASN
1	B	943	THR
1	B	986	THR
1	B	1006	ASN
1	B	1021	ASN
1	B	1023	ARG
1	B	1026	ASN
1	B	1090	ASN
1	B	1092	SER
1	B	1128	VAL
1	B	1131	ARG
1	B	1143	VAL
1	B	1151	ASN
1	B	1172	ASN
1	B	1199	GLN
1	B	1207	SER
1	B	1211	ILE
1	B	1228	ASP
1	B	1232	THR
1	B	1233	ASN
1	B	1253	HIS
1	B	1255	PHE
1	B	1265	ASN
1	B	1275	SER
1	B	1283	GLU
1	B	1294	ARG
2	C	13	LEU
2	C	14	SER
2	C	24	ARG
2	C	54	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	67	SER
2	C	76	THR
2	C	85	GLU
2	C	87	PHE
2	C	101	THR
2	C	126	ASP
2	C	129	LEU
2	C	158	LEU
2	C	169	GLU
2	C	172	SER
2	C	174	ASP
2	C	178	SER
2	C	179	LEU
2	C	186	SER
2	C	210	THR
2	C	212	SER
2	C	214	ASN
3	D	3	GLN
3	D	4	LEU
3	D	6	GLU
3	D	21	SER
3	D	22	CYS
3	D	43	LYS
3	D	62	ASP
3	D	67	ARG
3	D	69	THR
3	D	89	GLU
3	D	110	GLN
3	D	115	THR
3	D	122	LYS
3	D	132	SER
3	D	174	VAL
3	D	182	SER
3	D	184	SER
3	D	192	SER
3	D	212	VAL
2	E	1	GLU
2	E	12	SER
2	E	14	SER
2	E	26	SER
2	E	54	ARG
2	E	56	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	74	ASP
2	E	76	THR
2	E	87	PHE
2	E	101	THR
2	E	112	ARG
2	E	113	THR
2	E	118	SER
2	E	139	LEU
2	E	158	LEU
2	E	166	SER
2	E	169	GLU
2	E	174	ASP
2	E	182	THR
2	E	195	VAL
2	E	214	ASN
3	F	6	GLU
3	F	32	HIS
3	F	43	LYS
3	F	62	ASP
3	F	63	SER
3	F	65	GLU
3	F	67	ARG
3	F	110	GLN
3	F	118	SER
3	F	122	LYS
3	F	135	SER
3	F	174	VAL
3	F	184	SER
3	F	204	ASN
3	F	211	LYS
3	F	217	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	53	ASN
1	A	67	GLN
1	A	162	GLN
1	A	170	HIS
1	A	238	ASN
1	A	315	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	353	ASN
1	A	383	ASN
1	A	609	GLN
1	A	642	ASN
1	A	774	ASN
1	A	960	ASN
1	A	1006	ASN
1	A	1196	ASN
1	A	1233	ASN
1	A	1253	HIS
1	A	1256	ASN
1	A	1265	ASN
1	B	39	HIS
1	B	40	ASN
1	B	53	ASN
1	B	67	GLN
1	B	139	GLN
1	B	205	ASN
1	B	238	ASN
1	B	246	ASN
1	B	269	HIS
1	B	383	ASN
1	B	833	GLN
1	B	960	ASN
1	B	1090	ASN
1	B	1172	ASN
1	B	1196	ASN
1	B	1227	ASN
1	B	1233	ASN
1	B	1254	GLN
1	B	1256	ASN
1	B	1265	ASN
2	C	156	ASN
2	C	164	GLN
2	C	202	HIS
2	C	214	ASN
3	D	39	GLN
3	D	82	GLN
2	E	34	HIS
2	E	128	GLN
2	E	202	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1267/1295 (97%)	-0.14	2 (0%) 95 91	29, 84, 98, 110	0
1	B	1267/1295 (97%)	-0.12	9 (0%) 89 80	33, 85, 97, 111	0
2	C	216/218 (99%)	-0.12	0 100 100	62, 84, 92, 95	0
2	E	216/218 (99%)	-0.23	0 100 100	67, 85, 92, 95	0
3	D	217/224 (96%)	-0.13	0 100 100	75, 85, 95, 103	0
3	F	217/224 (96%)	-0.15	0 100 100	72, 84, 92, 99	0
All	All	3400/3474 (97%)	-0.14	11 (0%) 94 89	29, 84, 97, 111	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	TYR	3.2
1	B	1198	SER	2.9
1	B	1237	MET	2.4
1	B	1160	PHE	2.3
1	B	1256	ASN	2.3
1	B	1197	ALA	2.1
1	B	1196	ASN	2.1
1	B	744	LYS	2.1
1	B	1195	THR	2.0
1	A	568	LEU	2.0
1	B	1250	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	B	1298	1/1	0.91	0.14	-	110,110,110,110	0
4	ZN	B	1297	1/1	0.99	0.13	-	72,72,72,72	0
4	ZN	A	1	1/1	0.96	0.15	-	81,81,81,81	0
5	CA	A	1297	1/1	0.85	0.23	-	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.