



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:33 am BST

PDB ID : 2NYY  
Title : Crystal structure of botulinum neurotoxin type A complexed with monoclonal antibody CR1  
Authors : Stevens, R.C.; Arndt, J.W.  
Deposited on : 2006-11-21  
Resolution : 2.61 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](mailto: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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

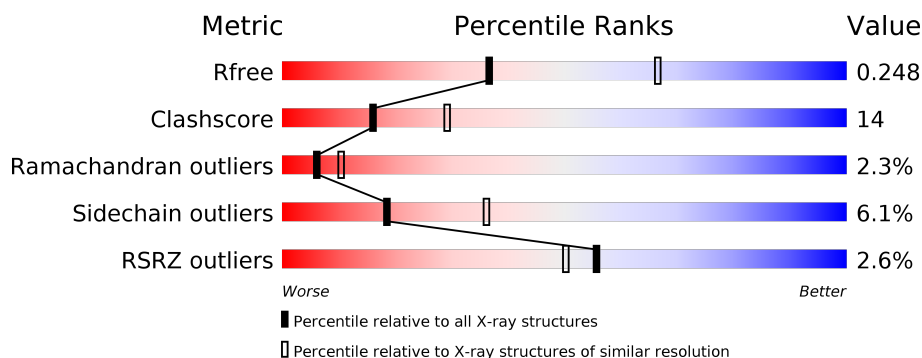
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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>3%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• • •</div> </div> </div>
2	C	218	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
3	D	223	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13507 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
			10211	6549	1691	1940	31			

- Molecule 2 is a protein called CR1 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			

- Molecule 3 is a protein called CR1 monoclonal antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1637	1031	270	329	7			

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

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

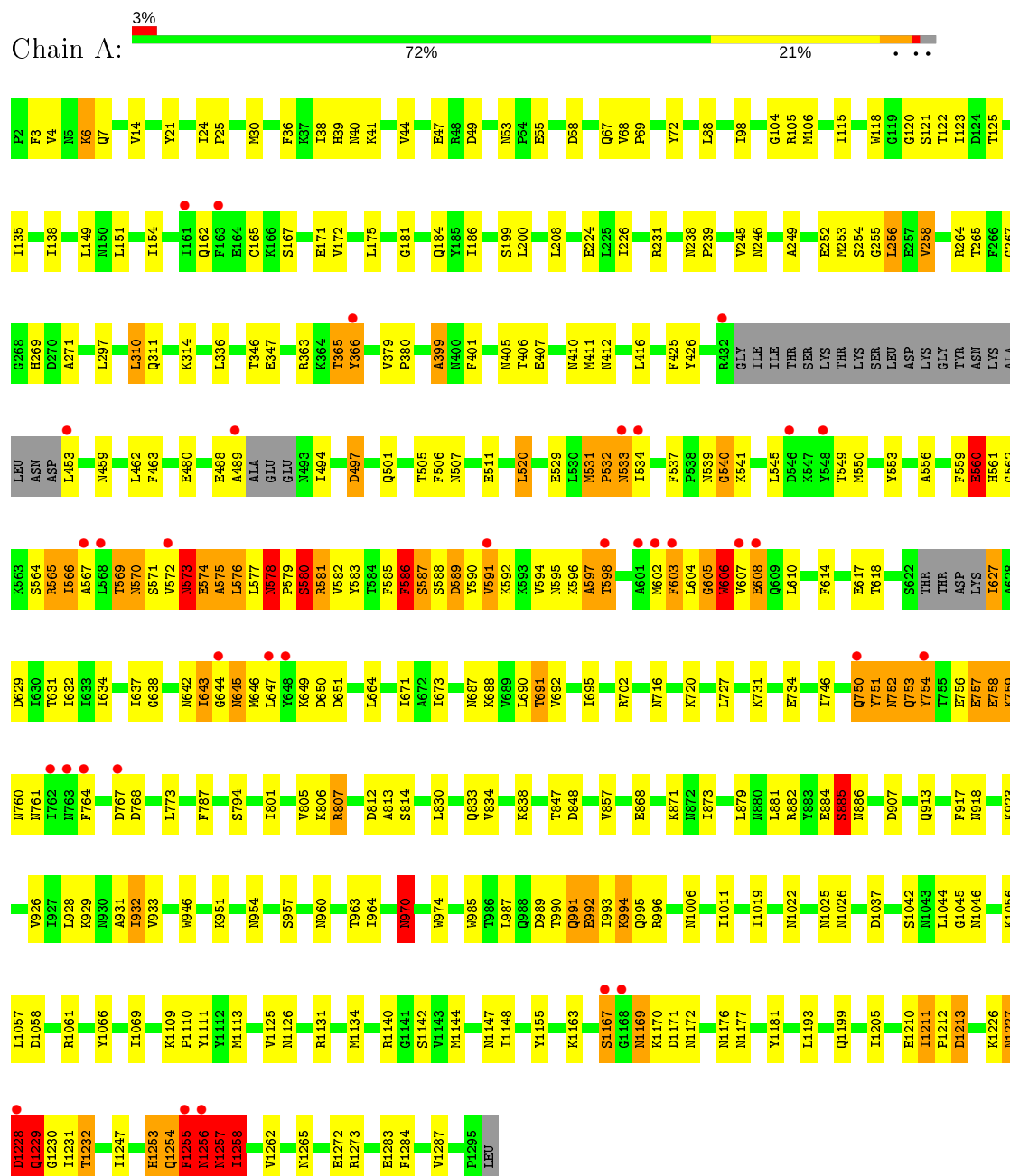
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

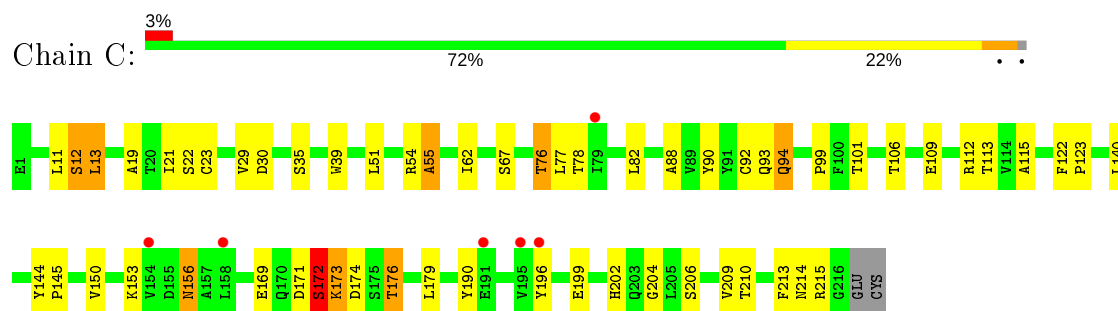
### 3 Residue-property plots

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 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.

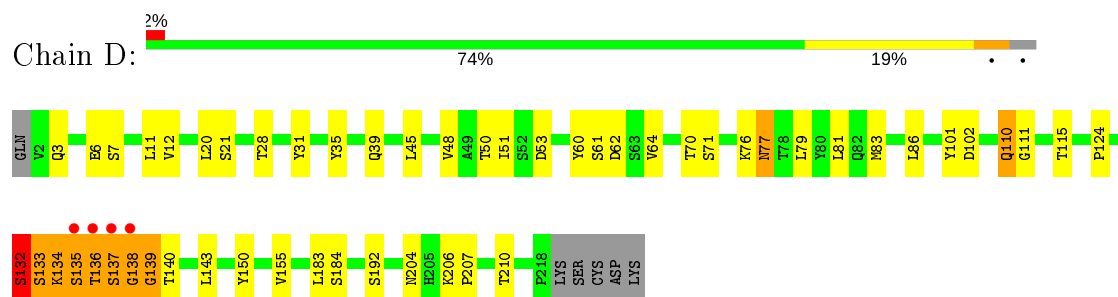
#### • Molecule 1: Botulinum neurotoxin type A



- Molecule 2: CR1 monoclonal antibody



- Molecule 3: CR1 monoclonal antibody



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.05Å 148.25Å 196.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 43.05 – 2.61	Depositor EDS
% Data completeness (in resolution range)	89.4 (50.00-2.61) 89.4 (43.05-2.61)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.246 0.211 , 0.248	Depositor DCC
$R_{free}$ test set	3912 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0/10428	0.70	3/14115 (0.0%)
2	C	0.58	0/1695	0.67	0/2303
3	D	0.56	0/1678	0.65	0/2287
All	All	0.62	0/13801	0.69	3/18705 (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	46
2	C	0	2
3	D	0	5
All	All	0	53

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1140	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	1037	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	154	ILE	CB-CA-C	-5.03	101.55	111.60

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	1167	SER	Peptide
1	A	118	TRP	Peptide
1	A	1228	ASP	Peptide
1	A	1229	GLN	Peptide
1	A	1232	THR	Peptide
1	A	1253	HIS	Peptide
1	A	1254	GLN	Peptide
1	A	1255	PHE	Peptide
1	A	1256	ASN	Peptide
1	A	1257	ASN	Peptide
1	A	1258	ILE	Peptide
1	A	532	PRO	Peptide
1	A	534	ILE	Peptide
1	A	539	ASN	Peptide
1	A	540	GLY	Peptide
1	A	559	PHE	Peptide
1	A	560	GLU	Peptide
1	A	561	HIS	Peptide
1	A	564	SER	Peptide
1	A	565	ARG	Peptide
1	A	573	ASN	Peptide
1	A	574	GLU	Peptide
1	A	575	ALA	Peptide
1	A	578	ASN	Peptide
1	A	580	SER	Peptide
1	A	585	PHE	Peptide
1	A	586	PHE	Peptide
1	A	587	SER	Peptide
1	A	6	LYS	Peptide
1	A	603	PHE	Peptide
1	A	605	GLY	Peptide
1	A	644	GLY	Peptide
1	A	645	ASN	Peptide
1	A	647	LEU	Peptide
1	A	649	LYS	Peptide
1	A	650	ASP	Peptide
1	A	753	GLN	Peptide
1	A	754	TYR	Peptide
1	A	757	GLU	Peptide
1	A	758	GLU	Peptide
1	A	847	THR	Peptide
1	A	885	SER	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	989	ASP	Peptide
1	A	992	GLU	Peptide
1	A	994	LYS	Peptide
2	C	172	SER	Peptide
2	C	173	LYS	Peptide
3	D	132	SER	Peptide
3	D	135	SER	Peptide
3	D	136	THR	Peptide
3	D	138	GLY	Peptide
3	D	139	GLY	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	10211	0	10013	292	0
2	C	1657	0	1595	36	0
3	D	1637	0	1562	58	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
All	All	13507	0	13170	386	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 14.

All (386) 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:578:ASN:HB3	1:A:579:PRO:C	1.38	1.43
1:A:1228:ASP:HB3	1:A:1229:GLN:CB	1.51	1.38
1:A:578:ASN:HB3	1:A:579:PRO:CA	1.48	1.33
3:D:139:GLY:N	3:D:140:THR:HB	1.40	1.32
1:A:604:LEU:N	1:A:605:GLY:HA3	1.55	1.15
3:D:139:GLY:H	3:D:140:THR:CB	1.60	1.14
1:A:588:SER:HA	1:A:591:VAL:HG13	1.13	1.11
1:A:453:LEU:HD12	1:A:576:LEU:HD23	1.32	1.11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:THR:HA	1:A:582:VAL:CG1	1.81	1.10
1:A:569:THR:HA	1:A:582:VAL:HG13	1.12	1.10
2:C:174:ASP:HB2	2:C:176:THR:HG22	1.31	1.09
1:A:1228:ASP:HB3	1:A:1229:GLN:HB3	1.26	1.09
3:D:139:GLY:CA	3:D:140:THR:HB	1.82	1.08
1:A:1228:ASP:HB3	1:A:1229:GLN:HB2	1.33	1.06
1:A:578:ASN:CB	1:A:579:PRO:CA	2.34	1.05
1:A:578:ASN:CB	1:A:579:PRO:C	2.27	1.02
1:A:631:THR:HG22	1:A:632:ILE:HD13	1.40	1.01
3:D:136:THR:HB	3:D:137:SER:CA	1.90	1.00
1:A:578:ASN:HB2	1:A:581:ARG:H	1.27	0.99
1:A:598:THR:HG21	1:A:606:TRP:CE2	1.97	0.99
3:D:136:THR:CB	3:D:137:SER:CA	2.40	0.98
3:D:139:GLY:H	3:D:140:THR:HB	0.86	0.98
1:A:578:ASN:HB3	1:A:579:PRO:HA	1.43	0.97
1:A:540:GLY:HA2	1:A:541:LYS:HB2	1.44	0.96
1:A:604:LEU:N	1:A:605:GLY:CA	2.30	0.95
1:A:567:ALA:HA	1:A:580:SER:OG	1.67	0.94
1:A:24:ILE:HG22	1:A:25:PRO:O	1.65	0.94
1:A:1228:ASP:CB	1:A:1229:GLN:HB3	1.97	0.93
1:A:1228:ASP:CB	1:A:1229:GLN:CB	2.46	0.92
3:D:132:SER:HA	3:D:133:SER:HB2	1.50	0.92
1:A:578:ASN:HB2	1:A:581:ARG:N	1.85	0.91
1:A:603:PHE:O	1:A:606:TRP:HB3	1.74	0.87
1:A:993:ILE:HG22	1:A:994:LYS:H	1.37	0.87
3:D:20:LEU:HG	3:D:83:MET:HE3	1.57	0.86
1:A:578:ASN:CB	1:A:579:PRO:HA	2.03	0.86
1:A:560:GLU:O	1:A:562:GLY:HA3	1.74	0.86
1:A:532:PRO:HA	1:A:533:ASN:HB2	1.57	0.85
3:D:140:THR:O	3:D:140:THR:HG22	1.76	0.84
1:A:588:SER:CA	1:A:591:VAL:HG13	2.05	0.82
1:A:567:ALA:CA	1:A:580:SER:OG	2.28	0.82
1:A:579:PRO:HA	1:A:581:ARG:H	1.45	0.81
1:A:604:LEU:H	1:A:605:GLY:HA3	1.41	0.81
1:A:579:PRO:HA	1:A:581:ARG:N	1.96	0.81
1:A:596:LYS:HB2	1:A:597:ALA:HB3	1.63	0.80
1:A:631:THR:HG22	1:A:632:ILE:CD1	2.12	0.80
1:A:588:SER:HA	1:A:591:VAL:CG1	2.05	0.80
1:A:578:ASN:CB	1:A:581:ARG:H	1.95	0.79
2:C:174:ASP:CB	2:C:176:THR:HG22	2.12	0.78
1:A:596:LYS:HA	1:A:597:ALA:HB3	1.65	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:GLU:HG3	1:A:993:ILE:HG12	1.65	0.76
1:A:596:LYS:HA	1:A:597:ALA:CB	2.15	0.76
1:A:604:LEU:H	1:A:605:GLY:CA	1.95	0.76
2:C:174:ASP:HB2	2:C:176:THR:CG2	2.14	0.76
1:A:1227:ASN:HD21	1:A:1231:ILE:HB	1.51	0.75
1:A:993:ILE:HG22	1:A:994:LYS:N	2.01	0.74
1:A:135:ILE:HG12	1:A:149:LEU:HD22	1.70	0.74
1:A:453:LEU:CD1	1:A:576:LEU:HD23	2.15	0.74
1:A:238:ASN:HD22	1:A:239:PRO:HD2	1.53	0.73
1:A:1227:ASN:O	1:A:1230:GLY:N	2.22	0.72
3:D:136:THR:OG1	3:D:137:SER:CA	2.37	0.72
1:A:596:LYS:CA	1:A:597:ALA:HB3	2.19	0.72
1:A:691:THR:CG2	1:A:830:LEU:HD21	2.21	0.71
1:A:135:ILE:HG23	1:A:149:LEU:CD2	2.20	0.70
2:C:150:VAL:HG13	2:C:150:VAL:O	1.91	0.69
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.27	0.69
1:A:691:THR:HG22	1:A:830:LEU:HD21	1.72	0.69
1:A:575:ALA:O	1:A:581:ARG:HB3	1.93	0.69
1:A:614:PHE:O	1:A:618:THR:HG23	1.93	0.69
1:A:586:PHE:CD1	1:A:586:PHE:N	2.58	0.69
1:A:750:GLN:HE21	1:A:750:GLN:HA	1.57	0.69
3:D:139:GLY:H	3:D:140:THR:CG2	2.06	0.68
1:A:596:LYS:CB	1:A:597:ALA:HB3	2.23	0.68
3:D:135:SER:HA	3:D:136:THR:O	1.94	0.68
1:A:1211:ILE:HD12	1:A:1212:PRO:HD3	1.75	0.68
1:A:995:GLN:HG3	1:A:996:ARG:H	1.59	0.68
1:A:488:GLU:HA	1:A:489:ALA:HB3	1.75	0.67
1:A:570:ASN:O	1:A:583:TYR:HA	1.94	0.67
1:A:603:PHE:CZ	1:A:751:TYR:HB2	2.30	0.67
1:A:603:PHE:C	1:A:605:GLY:HA3	2.16	0.66
3:D:139:GLY:CA	3:D:140:THR:CB	2.66	0.66
1:A:638:GLY:O	1:A:642:ASN:N	2.29	0.66
3:D:132:SER:O	3:D:135:SER:HB3	1.96	0.65
1:A:605:GLY:O	1:A:608:GLU:HB3	1.97	0.65
3:D:150:TYR:CE1	3:D:155:VAL:HG13	2.32	0.65
1:A:1113:MET:HE1	1:A:1284:PHE:HA	1.79	0.64
1:A:532:PRO:CA	1:A:533:ASN:HB2	2.26	0.64
1:A:587:SER:O	1:A:589:ASP:N	2.30	0.64
1:A:801:ILE:O	1:A:805:VAL:HG23	1.98	0.64
2:C:94:GLN:HG3	2:C:94:GLN:O	1.98	0.64
1:A:1228:ASP:O	1:A:1230:GLY:N	2.31	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LYS:HE2	1:A:115:ILE:HD12	1.78	0.64
1:A:1148:ILE:N	1:A:1148:ILE:HD12	2.12	0.63
1:A:1257:ASN:CG	1:A:1258:ILE:N	2.51	0.63
1:A:531:MET:HB3	1:A:532:PRO:HD2	1.79	0.63
1:A:566:ILE:O	1:A:567:ALA:HB3	1.99	0.63
1:A:1113:MET:HE3	1:A:1284:PHE:CD2	2.34	0.63
1:A:993:ILE:CG2	1:A:994:LYS:H	2.09	0.63
2:C:171:ASP:O	2:C:173:LYS:N	2.31	0.63
1:A:1228:ASP:CB	1:A:1229:GLN:HB2	2.21	0.63
1:A:627:ILE:HD12	1:A:629:ASP:OD1	1.99	0.62
1:A:1227:ASN:ND2	1:A:1231:ILE:HB	2.13	0.62
1:A:607:VAL:HG12	1:A:608:GLU:N	2.13	0.62
2:C:51:LEU:HD23	2:C:62:ILE:HD12	1.81	0.61
3:D:132:SER:O	3:D:135:SER:CB	2.48	0.61
1:A:1228:ASP:C	1:A:1230:GLY:N	2.51	0.61
3:D:140:THR:O	3:D:140:THR:CG2	2.48	0.61
3:D:35:TYR:CD1	3:D:50:THR:HG23	2.36	0.61
1:A:245:VAL:HG12	1:A:246:ASN:O	2.00	0.61
1:A:596:LYS:CA	1:A:597:ALA:CB	2.78	0.61
1:A:946:TRP:O	1:A:1069:ILE:HD12	2.01	0.61
1:A:1044:LEU:HB3	1:A:1045:GLY:HA2	1.83	0.61
1:A:267:GLY:HA2	1:A:271:ALA:HB2	1.83	0.61
1:A:756:GLU:N	1:A:757:GLU:CA	2.63	0.61
3:D:133:SER:O	3:D:135:SER:N	2.34	0.61
1:A:1199:GLN:HE22	1:A:1205:ILE:H	1.48	0.61
1:A:929:LYS:O	1:A:932:ILE:HG22	2.01	0.60
1:A:1254:GLN:HG2	1:A:1256:ASN:H	1.64	0.60
3:D:139:GLY:HA3	3:D:140:THR:HB	1.80	0.60
1:A:1254:GLN:HG2	1:A:1256:ASN:N	2.16	0.60
1:A:960:ASN:HD21	1:A:1061:ARG:H	1.49	0.59
1:A:1255:PHE:CD1	1:A:1255:PHE:N	2.70	0.59
1:A:995:GLN:HG3	1:A:996:ARG:N	2.17	0.59
1:A:1227:ASN:ND2	1:A:1231:ILE:O	2.36	0.59
1:A:1227:ASN:O	1:A:1227:ASN:ND2	2.36	0.59
1:A:573:ASN:OD1	1:A:583:TYR:CD1	2.56	0.59
3:D:139:GLY:N	3:D:140:THR:CB	2.31	0.59
1:A:72:TYR:CZ	1:A:416:LEU:HD13	2.37	0.59
1:A:806:LYS:HE2	1:A:933:VAL:O	2.03	0.59
1:A:1147:ASN:C	1:A:1148:ILE:HD12	2.23	0.58
2:C:99:PRO:O	2:C:101:THR:HG23	2.02	0.58
1:A:687:ASN:ND2	1:A:690:LEU:HD13	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:20:LEU:CD1	3:D:83:MET:HE1	2.34	0.58
1:A:1228:ASP:C	1:A:1230:GLY:H	2.05	0.58
1:A:264:ARG:HD2	1:A:346:THR:HB	1.84	0.58
1:A:588:SER:O	1:A:590:TYR:N	2.37	0.58
3:D:81:LEU:HG	3:D:83:MET:HE2	1.86	0.58
1:A:24:ILE:CG2	1:A:25:PRO:N	2.67	0.58
3:D:20:LEU:CG	3:D:83:MET:HE3	2.32	0.58
3:D:28:THR:HG21	3:D:31:TYR:CD2	2.39	0.57
1:A:453:LEU:HD12	1:A:576:LEU:CD2	2.22	0.57
1:A:569:THR:CA	1:A:582:VAL:CG1	2.71	0.57
1:A:459:ASN:HA	1:A:462:LEU:HD12	1.85	0.57
1:A:1254:GLN:HE21	1:A:1257:ASN:H	1.51	0.57
1:A:587:SER:O	1:A:589:ASP:HB2	2.04	0.57
1:A:598:THR:O	1:A:754:TYR:OH	2.23	0.57
1:A:208:LEU:HD23	1:A:208:LEU:O	2.05	0.56
1:A:692:VAL:HA	1:A:695:ILE:HD12	1.86	0.56
3:D:20:LEU:CD1	3:D:83:MET:CE	2.84	0.56
1:A:578:ASN:HB3	1:A:580:SER:N	2.15	0.56
1:A:579:PRO:HB3	1:A:580:SER:HA	1.87	0.56
1:A:1247:ILE:O	1:A:1265:ASN:ND2	2.38	0.56
1:A:24:ILE:HG23	1:A:25:PRO:HD2	1.86	0.56
3:D:124:PRO:HB3	3:D:150:TYR:HB3	1.87	0.55
1:A:587:SER:O	1:A:590:TYR:N	2.38	0.55
1:A:24:ILE:CG2	1:A:25:PRO:O	2.46	0.55
1:A:573:ASN:HA	1:A:575:ALA:N	2.21	0.55
1:A:497:ASP:OD1	1:A:497:ASP:N	2.38	0.55
1:A:556:ALA:HB2	1:A:576:LEU:CD1	2.37	0.55
1:A:580:SER:HB3	1:A:582:VAL:HG12	1.88	0.55
1:A:990:THR:O	1:A:991:GLN:CB	2.54	0.55
1:A:951:LYS:HG3	1:A:1011:ILE:HG21	1.89	0.54
1:A:463:PHE:CE2	1:A:727:LEU:HD23	2.42	0.54
1:A:575:ALA:C	1:A:581:ARG:HA	2.27	0.54
1:A:531:MET:HB3	1:A:532:PRO:CD	2.37	0.54
1:A:990:THR:HB	1:A:1046:ASN:O	2.08	0.54
1:A:575:ALA:O	1:A:577:LEU:N	2.41	0.54
1:A:594:VAL:CG1	1:A:610:LEU:HD21	2.38	0.53
1:A:598:THR:HG21	1:A:606:TRP:NE1	2.23	0.53
1:A:604:LEU:O	1:A:604:LEU:HD12	2.08	0.53
1:A:1210:GLU:HB2	1:A:1213:ASP:HB2	1.90	0.53
1:A:588:SER:O	1:A:592:LYS:N	2.32	0.53
1:A:540:GLY:HA2	1:A:541:LYS:CB	2.30	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MET:O	1:A:255:GLY:N	2.41	0.53
1:A:258:VAL:HG21	1:A:366:TYR:OH	2.09	0.53
3:D:83:MET:HG2	3:D:86:LEU:HD21	1.89	0.53
3:D:35:TYR:CE1	3:D:50:THR:HG23	2.45	0.52
1:A:532:PRO:CA	1:A:533:ASN:CB	2.88	0.52
1:A:565:ARG:C	1:A:566:ILE:O	2.46	0.52
3:D:48:VAL:HG13	3:D:64:VAL:HG21	1.92	0.52
1:A:586:PHE:HB3	1:A:617:GLU:CD	2.30	0.52
1:A:104:GLY:C	1:A:106:MET:H	2.12	0.52
1:A:553:TYR:CE2	1:A:642:ASN:HB2	2.44	0.52
1:A:960:ASN:ND2	1:A:1061:ARG:H	2.08	0.52
1:A:1057:LEU:HD11	1:A:1066:TYR:HA	1.92	0.52
3:D:206:LYS:N	3:D:207:PRO:CD	2.72	0.52
1:A:963:THR:HB	1:A:1058:ASP:HB3	1.91	0.51
1:A:310:LEU:HD22	1:A:314:LYS:HD2	1.92	0.51
1:A:884:GLU:O	1:A:885:SER:C	2.46	0.51
1:A:579:PRO:CB	1:A:580:SER:HA	2.40	0.51
1:A:463:PHE:CD2	1:A:727:LEU:HD23	2.45	0.51
1:A:588:SER:C	1:A:590:TYR:N	2.63	0.51
1:A:885:SER:O	1:A:886:ASN:HB2	2.11	0.51
2:C:150:VAL:O	2:C:150:VAL:CG1	2.57	0.51
2:C:172:SER:HA	2:C:174:ASP:O	2.11	0.51
1:A:167:SER:OG	1:A:184:GLN:NE2	2.44	0.51
1:A:716:ASN:OD1	1:A:720:LYS:HE3	2.10	0.50
1:A:550:MET:HE3	1:A:731:LYS:CD	2.40	0.50
1:A:226:ILE:CG2	1:A:265:THR:HG23	2.41	0.50
1:A:68:VAL:CG2	1:A:69:PRO:HD2	2.41	0.50
1:A:347:GLU:HB3	1:A:494:ILE:HD11	1.94	0.50
2:C:112:ARG:HG3	2:C:113:THR:O	2.11	0.50
3:D:132:SER:CA	3:D:133:SER:HB2	2.32	0.50
1:A:985:TRP:CG	1:A:1019:ILE:HG21	2.46	0.50
1:A:643:ILE:HG21	1:A:664:LEU:HD23	1.92	0.50
2:C:29:VAL:CG1	2:C:29:VAL:O	2.58	0.50
1:A:1044:LEU:HB3	1:A:1045:GLY:CA	2.42	0.50
1:A:1211:ILE:CD1	1:A:1212:PRO:HD3	2.40	0.50
1:A:1226:LYS:HA	1:A:1232:THR:HA	1.94	0.50
1:A:565:ARG:O	1:A:566:ILE:O	2.30	0.49
1:A:917:PHE:C	1:A:1057:LEU:HD12	2.32	0.49
1:A:256:LEU:HD21	1:A:366:TYR:OH	2.13	0.49
2:C:30:ASP:OD1	2:C:35:SER:OG	2.26	0.49
3:D:11:LEU:O	3:D:12:VAL:HG23	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:O	1:A:589:ASP:C	2.50	0.49
3:D:133:SER:O	3:D:135:SER:O	2.30	0.49
1:A:1148:ILE:CD1	1:A:1148:ILE:N	2.76	0.49
1:A:1163:LYS:HB2	1:A:1181:TYR:HB2	1.95	0.49
1:A:594:VAL:HG12	1:A:610:LEU:HD11	1.93	0.49
1:A:974:TRP:HB3	1:A:987:LEU:HD23	1.94	0.49
1:A:587:SER:O	1:A:588:SER:C	2.50	0.49
1:A:586:PHE:HB3	1:A:617:GLU:OE2	2.12	0.49
2:C:199:GLU:HG3	2:C:210:THR:HG22	1.95	0.48
1:A:1254:GLN:CG	1:A:1255:PHE:HA	2.43	0.48
1:A:1229:GLN:OE1	1:A:1272:GLU:OE1	2.31	0.48
1:A:637:ILE:HD13	1:A:787:PHE:CE2	2.49	0.48
1:A:750:GLN:O	1:A:752:ASN:N	2.46	0.48
3:D:110:GLN:NE2	3:D:111:GLY:O	2.46	0.48
1:A:569:THR:HA	1:A:582:VAL:HG11	1.86	0.48
1:A:642:ASN:ND2	1:A:646:MET:O	2.47	0.48
3:D:35:TYR:CE1	3:D:50:THR:CG2	2.97	0.48
1:A:399:ALA:O	1:A:401:PHE:N	2.46	0.48
3:D:143:LEU:C	3:D:143:LEU:HD12	2.34	0.48
1:A:575:ALA:HB1	1:A:581:ARG:HA	1.96	0.48
2:C:76:THR:O	2:C:76:THR:CG2	2.61	0.48
3:D:28:THR:CG2	3:D:31:TYR:CD2	2.97	0.48
2:C:23:CYS:HB2	2:C:39:TRP:CH2	2.49	0.48
1:A:634:ILE:HB	1:A:637:ILE:HD12	1.95	0.47
1:A:575:ALA:O	1:A:576:LEU:C	2.51	0.47
1:A:687:ASN:CG	1:A:690:LEU:HD13	2.34	0.47
3:D:133:SER:O	3:D:134:LYS:C	2.53	0.47
1:A:1254:GLN:HG2	1:A:1255:PHE:CA	2.44	0.47
1:A:550:MET:HE3	1:A:731:LYS:HD2	1.95	0.47
2:C:140:LEU:HD22	2:C:179:LEU:HD22	1.95	0.47
3:D:20:LEU:HD11	3:D:83:MET:HE1	1.96	0.47
1:A:1022:ASN:ND2	1:A:1025:ASN:OD1	2.48	0.47
3:D:133:SER:C	3:D:135:SER:N	2.68	0.47
1:A:545:LEU:HD12	1:A:549:THR:CG2	2.44	0.47
1:A:673:ILE:O	1:A:807:ARG:HD2	2.15	0.47
1:A:1254:GLN:HG2	1:A:1255:PHE:HA	1.97	0.47
1:A:995:GLN:CG	1:A:996:ARG:H	2.27	0.47
3:D:137:SER:N	3:D:138:GLY:HA2	2.30	0.47
1:A:14:VAL:HG11	1:A:21:TYR:CD1	2.51	0.46
1:A:24:ILE:HG23	1:A:25:PRO:CD	2.45	0.46
1:A:574:GLU:N	1:A:574:GLU:OE1	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:VAL:O	1:A:608:GLU:C	2.53	0.46
1:A:598:THR:HG21	1:A:606:TRP:CZ2	2.48	0.46
1:A:605:GLY:C	1:A:607:VAL:N	2.68	0.46
2:C:144:TYR:CG	2:C:145:PRO:HA	2.50	0.46
1:A:1227:ASN:HD21	1:A:1231:ILE:CB	2.24	0.46
1:A:985:TRP:CE2	1:A:1019:ILE:HG21	2.50	0.46
2:C:93:GLN:NE2	2:C:94:GLN:O	2.49	0.46
3:D:132:SER:HA	3:D:133:SER:CB	2.35	0.46
1:A:106:MET:HG3	1:A:506:PHE:CE1	2.51	0.46
1:A:573:ASN:HA	1:A:574:GLU:C	2.36	0.46
1:A:582:VAL:O	1:A:582:VAL:HG13	2.16	0.46
1:A:569:THR:HG23	1:A:595:ASN:OD1	2.16	0.46
1:A:964:ILE:HA	1:A:1056:LYS:O	2.16	0.46
1:A:501:GLN:O	1:A:505:THR:HG23	2.15	0.46
2:C:196:TYR:HB2	2:C:213:PHE:CE1	2.51	0.46
1:A:806:LYS:HD3	1:A:931:ALA:O	2.16	0.45
1:A:1113:MET:CE	1:A:1284:PHE:CD2	2.99	0.45
1:A:758:GLU:O	1:A:761:ASN:CA	2.64	0.45
3:D:60:TYR:CE2	3:D:70:THR:HG22	2.51	0.45
1:A:1066:TYR:C	1:A:1066:TYR:CD1	2.90	0.45
1:A:590:TYR:O	1:A:594:VAL:HG22	2.16	0.45
2:C:54:ARG:O	2:C:55:ALA:HB3	2.15	0.45
1:A:1006:ASN:H	1:A:1006:ASN:ND2	2.15	0.45
1:A:1155:TYR:CE2	1:A:1287:VAL:HG22	2.51	0.45
2:C:11:LEU:HG	2:C:13:LEU:HD22	1.98	0.45
1:A:1125:VAL:HG22	1:A:1134:MET:CE	2.47	0.45
3:D:132:SER:O	3:D:135:SER:HB2	2.16	0.45
2:C:140:LEU:N	2:C:140:LEU:HD12	2.31	0.45
1:A:970:ASN:N	1:A:970:ASN:HD22	2.16	0.44
1:A:688:LYS:O	1:A:692:VAL:HG13	2.16	0.44
1:A:53:ASN:HD21	1:A:55:GLU:HG2	1.81	0.44
1:A:992:GLU:HG3	1:A:993:ILE:CG1	2.43	0.44
1:A:181:GLY:HA2	1:A:231:ARG:O	2.17	0.44
1:A:4:VAL:HG12	1:A:6:LYS:O	2.18	0.44
1:A:138:ILE:N	1:A:138:ILE:HD12	2.32	0.44
1:A:560:GLU:O	1:A:562:GLY:CA	2.55	0.44
3:D:12:VAL:HG11	3:D:86:LEU:HD12	2.00	0.44
1:A:123:ILE:HG22	1:A:125:THR:H	1.82	0.44
1:A:881:LEU:O	1:A:882:ARG:HD3	2.18	0.44
3:D:133:SER:HB3	3:D:134:LYS:H	1.51	0.44
1:A:594:VAL:HG13	1:A:610:LEU:HD21	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:PHE:O	1:A:606:TRP:CB	2.54	0.44
1:A:576:LEU:C	1:A:581:ARG:HB3	2.38	0.44
1:A:868:GLU:OE1	1:A:871:LYS:HE2	2.17	0.44
2:C:35:SER:O	2:C:54:ARG:HA	2.17	0.44
2:C:39:TRP:CZ3	2:C:92:CYS:HB3	2.53	0.44
1:A:1257:ASN:CG	1:A:1258:ILE:H	2.20	0.43
1:A:598:THR:CG2	1:A:606:TRP:CE2	2.86	0.43
2:C:112:ARG:NH1	2:C:115:ALA:HB2	2.33	0.43
1:A:199:SER:O	1:A:200:LEU:HD22	2.18	0.43
1:A:3:PHE:O	1:A:39:HIS:HD2	2.00	0.43
1:A:594:VAL:CG1	1:A:610:LEU:CD2	2.95	0.43
1:A:578:ASN:CB	1:A:581:ARG:N	2.64	0.43
1:A:426:TYR:O	1:A:540:GLY:HA3	2.17	0.43
1:A:49:ASP:OD1	1:A:49:ASP:C	2.55	0.43
1:A:520:LEU:H	1:A:520:LEU:HD22	1.83	0.43
2:C:88:ALA:HB3	2:C:90:TYR:CE1	2.54	0.43
1:A:310:LEU:HD22	1:A:314:LYS:CD	2.49	0.43
1:A:36:PHE:N	1:A:36:PHE:CD1	2.87	0.43
1:A:379:VAL:HB	1:A:380:PRO:HD3	2.01	0.43
1:A:569:THR:HG22	1:A:746:ILE:CD1	2.49	0.43
3:D:101:TYR:HA	3:D:102:ASP:HA	1.80	0.43
1:A:1134:MET:SD	1:A:1193:LEU:HD13	2.60	0.42
1:A:1256:ASN:HB2	1:A:1257:ASN:OD1	2.18	0.42
1:A:879:LEU:HA	1:A:879:LEU:HD12	1.81	0.42
2:C:13:LEU:HB3	2:C:82:LEU:CD1	2.48	0.42
3:D:51:ILE:HG21	3:D:79:LEU:HD11	2.00	0.42
3:D:20:LEU:HD12	3:D:83:MET:HE1	2.02	0.42
1:A:40:ASN:HD22	1:A:511:GLU:HG2	1.85	0.42
1:A:918:ASN:N	1:A:1057:LEU:HD12	2.34	0.42
2:C:190:TYR:CE2	2:C:215:ARG:HD3	2.54	0.42
1:A:38:ILE:HD13	1:A:44:VAL:HG23	2.01	0.42
1:A:575:ALA:O	1:A:581:ARG:CB	2.64	0.42
1:A:567:ALA:N	1:A:580:SER:OG	2.52	0.42
1:A:614:PHE:CD2	1:A:773:LEU:HD22	2.54	0.42
3:D:183:LEU:HD12	3:D:184:SER:N	2.34	0.42
3:D:20:LEU:CD1	3:D:83:MET:HE3	2.49	0.42
3:D:61:SER:OG	3:D:64:VAL:HG22	2.18	0.42
1:A:135:ILE:HG23	1:A:149:LEU:HD23	1.98	0.42
1:A:135:ILE:CG2	1:A:149:LEU:CD2	2.96	0.42
1:A:405:ASN:OD1	1:A:407:GLU:HB2	2.20	0.42
1:A:67:GLN:HA	1:A:425:PHE:CZ	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:SER:HA	2:C:109:GLU:O	2.20	0.42
2:C:67:SER:O	2:C:77:LEU:HD12	2.20	0.42
1:A:550:MET:CE	1:A:731:LYS:HD2	2.49	0.42
1:A:954:ASN:O	1:A:957:SER:HB2	2.20	0.42
3:D:39:GLN:HB2	3:D:45:LEU:HD23	2.02	0.42
1:A:365:THR:O	1:A:365:THR:HG23	2.20	0.42
3:D:155:VAL:CG2	3:D:183:LEU:HD21	2.49	0.42
1:A:578:ASN:CB	1:A:580:SER:N	2.81	0.42
1:A:907:ASP:OD2	1:A:913:GLN:NE2	2.53	0.42
1:A:1254:GLN:O	1:A:1255:PHE:CG	2.73	0.42
1:A:255:GLY:HA3	1:A:537:PHE:CD1	2.55	0.42
1:A:651:ASP:OD1	1:A:651:ASP:O	2.38	0.42
1:A:98:ILE:O	1:A:104:GLY:HA3	2.20	0.42
1:A:759:LYS:C	1:A:761:ASN:H	2.24	0.41
1:A:578:ASN:CG	1:A:579:PRO:C	2.77	0.41
1:A:750:GLN:HE21	1:A:750:GLN:CA	2.29	0.41
2:C:122:PHE:HA	2:C:123:PRO:HD3	1.92	0.41
2:C:202:HIS:CD2	2:C:204:GLY:H	2.38	0.41
1:A:175:LEU:O	1:A:181:GLY:N	2.45	0.41
1:A:834:VAL:HG12	1:A:838:LYS:NZ	2.35	0.41
1:A:1109:LYS:HA	1:A:1110:PRO:HD3	1.94	0.41
1:A:151:LEU:HD11	1:A:186:ILE:HG13	2.02	0.41
1:A:186:ILE:HD13	1:A:224:GLU:HB3	2.02	0.41
1:A:410:ASN:C	1:A:412:ASN:H	2.24	0.41
1:A:567:ALA:HA	1:A:580:SER:HG	1.77	0.41
1:A:751:TYR:O	1:A:754:TYR:HB2	2.21	0.41
1:A:812:ASP:O	1:A:813:ALA:C	2.59	0.41
3:D:124:PRO:HD2	3:D:210:THR:HG21	2.02	0.41
1:A:1111:TYR:CD2	1:A:1284:PHE:HB3	2.56	0.41
1:A:1176:ASN:O	1:A:1177:ASN:HB2	2.21	0.41
1:A:171:GLU:HG2	1:A:172:VAL:HG23	2.03	0.41
1:A:556:ALA:HB2	1:A:576:LEU:HD13	2.03	0.41
1:A:879:LEU:HD21	1:A:926:VAL:HG11	2.02	0.41
3:D:76:LYS:O	3:D:77:ASN:C	2.59	0.41
1:A:1253:HIS:HB2	1:A:1262:VAL:HG11	2.02	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD12	1.72	0.41
2:C:19:ALA:O	2:C:78:THR:HA	2.21	0.41
1:A:995:GLN:CG	1:A:996:ARG:N	2.83	0.40
1:A:1257:ASN:ND2	1:A:1258:ILE:HB	2.36	0.40
1:A:578:ASN:HD22	1:A:580:SER:N	2.20	0.40
1:A:575:ALA:C	1:A:581:ARG:HB3	2.42	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:53:ASP:OD1	3:D:53:ASP:N	2.55	0.40
1:A:1254:GLN:HE21	1:A:1256:ASN:H	1.70	0.40
1:A:627:ILE:HA	1:A:627:ILE:HD13	1.95	0.40
1:A:6:LYS:HB3	1:A:7:GLN:O	2.21	0.40
2:C:21:ILE:HG12	2:C:106:THR:HG21	2.02	0.40
1:A:1169:ASN:C	1:A:1171:ASP:N	2.74	0.40
1:A:249:ALA:HB3	1:A:252:GLU:HG3	2.03	0.40
1:A:24:ILE:HG23	1:A:25:PRO:N	2.36	0.40
2:C:153:LYS:HB3	2:C:156:ASN:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1259/1295 (97%)	1112 (88%)	117 (9%)	30 (2%)	6	9
2	C	214/218 (98%)	198 (92%)	13 (6%)	3 (1%)	11	21
3	D	215/223 (96%)	193 (90%)	17 (8%)	5 (2%)	6	10
All	All	1688/1736 (97%)	1503 (89%)	147 (9%)	38 (2%)	6	10

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	560	GLU
1	A	566	ILE
1	A	576	LEU
1	A	578	ASN
1	A	581	ARG
1	A	589	ASP
1	A	606	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	759	LYS
1	A	848	ASP
1	A	1229	GLN
1	A	1257	ASN
3	D	137	SER
3	D	192	SER
1	A	254	SER
1	A	399	ALA
1	A	597	ALA
1	A	645	ASN
1	A	751	TYR
1	A	970	ASN
1	A	991	GLN
2	C	156	ASN
2	C	172	SER
3	D	134	LYS
1	A	256	LEU
1	A	608	GLU
1	A	760	ASN
1	A	1169	ASN
1	A	1258	ILE
3	D	77	ASN
3	D	132	SER
1	A	885	SER
1	A	1167	SER
1	A	120	GLY
1	A	533	ASN
1	A	572	VAL
1	A	1170	LYS
2	C	55	ALA

### 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	1126/1178 (96%)	1055 (94%)	71 (6%)	18	35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	186/190 (98%)	176 (95%)	10 (5%)	22	42
3	D	181/189 (96%)	171 (94%)	10 (6%)	21	41
All	All	1493/1557 (96%)	1402 (94%)	91 (6%)	18	36

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	47	GLU
1	A	58	ASP
1	A	122	THR
1	A	162	GLN
1	A	165	CYS
1	A	258	VAL
1	A	269	HIS
1	A	297	LEU
1	A	310	LEU
1	A	311	GLN
1	A	336	LEU
1	A	363	ARG
1	A	365	THR
1	A	366	TYR
1	A	406	THR
1	A	411	MET
1	A	480	GLU
1	A	497	ASP
1	A	507	ASN
1	A	520	LEU
1	A	529	GLU
1	A	531	MET
1	A	569	THR
1	A	570	ASN
1	A	571	SER
1	A	573	ASN
1	A	580	SER
1	A	586	PHE
1	A	591	VAL
1	A	598	THR
1	A	602	MET
1	A	606	TRP
1	A	627	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	643	ILE
1	A	671	ILE
1	A	691	THR
1	A	702	ARG
1	A	734	GLU
1	A	750	GLN
1	A	752	ASN
1	A	753	GLN
1	A	764	PHE
1	A	767	ASP
1	A	768	ASP
1	A	794	SER
1	A	807	ARG
1	A	814	SER
1	A	833	GLN
1	A	857	VAL
1	A	873	ILE
1	A	885	SER
1	A	923	LYS
1	A	928	LEU
1	A	932	ILE
1	A	970	ASN
1	A	1026	ASN
1	A	1042	SER
1	A	1126	ASN
1	A	1131	ARG
1	A	1142	SER
1	A	1144	MET
1	A	1172	ASN
1	A	1211	ILE
1	A	1213	ASP
1	A	1227	ASN
1	A	1228	ASP
1	A	1255	PHE
1	A	1256	ASN
1	A	1273	ARG
1	A	1283	GLU
2	C	12	SER
2	C	13	LEU
2	C	22	SER
2	C	76	THR
2	C	94	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	169	GLU
2	C	176	THR
2	C	206	SER
2	C	209	VAL
2	C	214	ASN
3	D	3	GLN
3	D	6	GLU
3	D	7	SER
3	D	21	SER
3	D	62	ASP
3	D	71	SER
3	D	110	GLN
3	D	115	THR
3	D	133	SER
3	D	204	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	39	HIS
1	A	40	ASN
1	A	53	ASN
1	A	238	ASN
1	A	383	ASN
1	A	400	ASN
1	A	514	ASN
1	A	527	GLN
1	A	573	ASN
1	A	609	GLN
1	A	750	GLN
1	A	752	ASN
1	A	960	ASN
1	A	970	ASN
1	A	988	GLN
1	A	1006	ASN
1	A	1093	ASN
1	A	1196	ASN
1	A	1199	GLN
1	A	1227	ASN
1	A	1254	GLN
1	A	1256	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	202	HIS
3	D	13	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1267/1295 (97%)	-0.05	34 (2%) 54 49	2, 10, 33, 45	0
2	C	216/218 (99%)	0.05	6 (2%) 53 47	2, 14, 31, 38	0
3	D	217/223 (97%)	-0.16	4 (1%) 68 64	2, 17, 29, 30	0
All	All	1700/1736 (97%)	-0.05	44 (2%) 56 50	2, 11, 32, 45	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	TYR	5.4
1	A	489	ALA	4.9
1	A	603	PHE	4.7
3	D	136	THR	4.3
1	A	644	GLY	4.3
1	A	763	ASN	4.1
1	A	1255	PHE	4.0
1	A	762	ILE	3.9
1	A	648	TYR	3.9
3	D	137	SER	3.5
1	A	1167	SER	3.4
1	A	568	LEU	3.3
1	A	764	PHE	3.3
1	A	601	ALA	3.2
1	A	602	MET	3.1
1	A	598	THR	3.1
1	A	607	VAL	3.1
2	C	154	VAL	3.0
1	A	767	ASP	3.0
1	A	534	ILE	3.0
3	D	135	SER	2.9
1	A	432	ARG	2.8
1	A	1256	ASN	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	750	GLN	2.7
3	D	138	GLY	2.5
1	A	533	ASN	2.5
1	A	163	PHE	2.5
1	A	548	TYR	2.5
2	C	191	GLU	2.4
1	A	1168	GLY	2.4
1	A	591	VAL	2.4
2	C	158	LEU	2.3
2	C	196	TYR	2.3
2	C	79	ILE	2.2
1	A	572	VAL	2.1
1	A	567	ALA	2.1
1	A	546	ASP	2.1
1	A	1228	ASP	2.1
1	A	647	LEU	2.1
1	A	366	TYR	2.1
1	A	453	LEU	2.0
2	C	195	VAL	2.0
1	A	161	ILE	2.0
1	A	608	GLU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	A	1297	1/1	0.58	0.13	63,63,63,63	0
4	ZN	A	1	1/1	0.99	0.04	3,3,3,3	0

## 6.5 Other polymers

There are no such residues in this entry.