



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 08:41 am GMT

PDB ID : 3V0B  
Title : 3.9 angstrom crystal structure of BoNT/Ai in complex with NTNHA  
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Deposited on : 2011-12-07  
Resolution : 3.90 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.

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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 : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

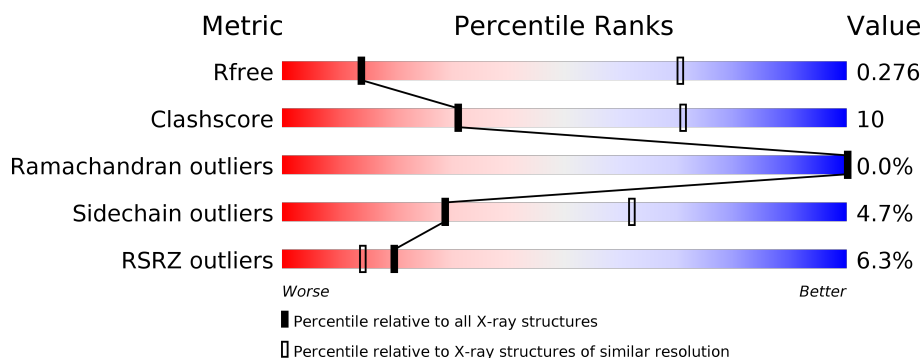
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	111664	1145 (4.20-3.60)
Clashscore	122126	1225 (4.20-3.60)
Ramachandran outliers	120053	1184 (4.20-3.60)
Sidechain outliers	120020	1175 (4.20-3.60)
RSRZ outliers	108989	1046 (4.20-3.60)

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. 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	1296	<div> <div>6%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
2	B	1196	<div> <div>6%</div> <div>71%</div> <div>22%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	1297	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19830 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 BoNT/A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1280	Total	C	N	O	S	36	0	0
			10418	6681	1721	1983	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLN	GLU	ENGINEERED MUTATION	UNP Q7B8V4
A	363	ALA	ARG	ENGINEERED MUTATION	UNP Q7B8V4
A	366	PHE	TYR	ENGINEERED MUTATION	UNP Q7B8V4
A	1158	ALA	THR	CONFLICT	UNP Q7B8V4

- Molecule 2 is a protein called NTN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	46	0	0
			9410	6022	1515	1841	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP Q45914
B	0	SER	-	EXPRESSION TAG	UNP Q45914
B	1194	PRO	-	EXPRESSION TAG	UNP Q45914

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

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

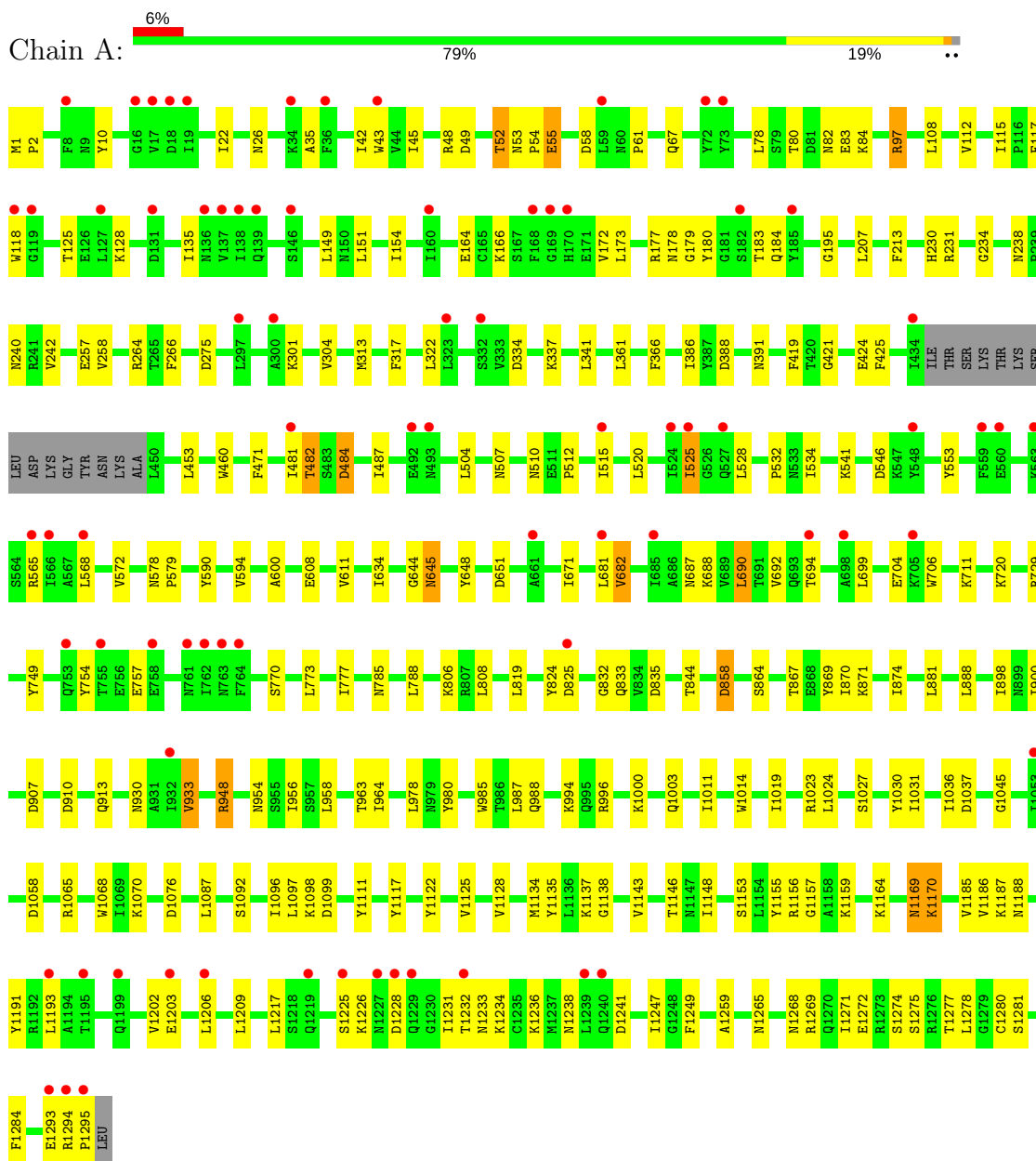
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

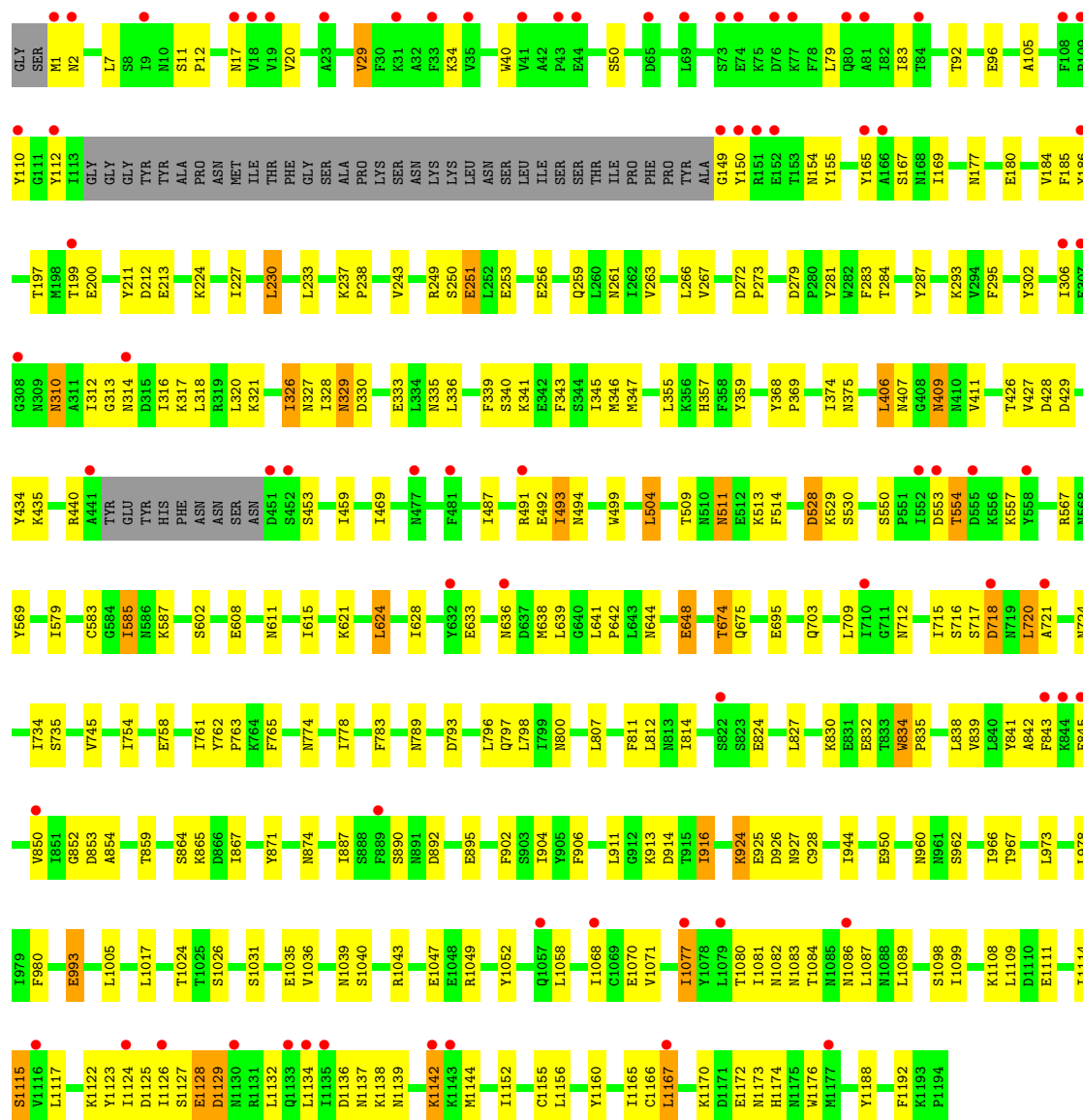
### 3 Residue-property plots [i](#)

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: BoNT/A



#### • Molecule 2: NTNH



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	282.23Å 282.23Å 374.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 3.90 48.88 – 3.90	Depositor EDS
% Data completeness (in resolution range)	92.1 (48.47-3.90) 92.1 (48.88-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.252 , 0.280 0.250 , 0.276	Depositor DCC
$R_{free}$ test set	3737 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	139.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 121.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	19830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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	0.31	0/10639	0.49	0/14405
2	B	0.32	0/9605	0.51	0/13015
All	All	0.31	0/20244	0.50	0/27420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10418	0	10297	190	30
2	B	9410	0	9202	214	31
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	19830	0	19499	382	32

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 10.

All (382) 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)
2:B:528:ASP:HB2	2:B:530:SER:H	1.07	1.09
2:B:426:THR:HB	2:B:427:VAL:HA	1.02	1.02
2:B:528:ASP:HB2	2:B:530:SER:N	1.76	1.00
2:B:426:THR:HB	2:B:427:VAL:CA	1.91	0.99
2:B:426:THR:CB	2:B:427:VAL:HA	1.93	0.98
1:A:421:GLY:H	1:A:424:GLU:HG3	1.33	0.92
2:B:528:ASP:CB	2:B:530:SER:H	1.88	0.87
1:A:1265:ASN:ND2	2:B:845:GLU:HG2	1.93	0.83
2:B:314:ASN:HB3	2:B:318:LEU:HD12	1.60	0.82
2:B:336:LEU:HB3	2:B:347:MET:HE1	1.60	0.82
2:B:1099:ILE:HD12	2:B:1099:ILE:H	1.44	0.81
1:A:10:TYR:CZ	1:A:84:LYS:HD3	2.16	0.81
1:A:80:THR:HG22	1:A:82:ASN:H	1.47	0.80
1:A:988:GLN:HG3	1:A:994:LYS:HB3	1.64	0.80
1:A:149:LEU:HD12	1:A:183:THR:CG2	2.12	0.80
2:B:715:ILE:HG22	2:B:720:LEU:HD22	1.61	0.80
2:B:426:THR:OG1	2:B:427:VAL:CG2	2.30	0.80
1:A:482:THR:HG22	1:A:484:ASP:H	1.46	0.79
1:A:525:ILE:HD12	1:A:525:ILE:H	1.47	0.78
1:A:52:THR:HG23	1:A:528:LEU:HD11	1.66	0.77
1:A:1265:ASN:HD22	2:B:845:GLU:HG2	1.48	0.77
1:A:487:ILE:HG23	1:A:704:GLU:OE2	1.85	0.76
2:B:602:SER:HB2	2:B:608:GLU:OE1	1.85	0.75
1:A:1271:ILE:HG13	2:B:854:ALA:HB1	1.67	0.75
2:B:426:THR:HG21	2:B:428:ASP:OD2	1.86	0.75
1:A:421:GLY:N	1:A:424:GLU:HG3	2.02	0.74
1:A:1271:ILE:HG13	2:B:854:ALA:CB	2.18	0.73
2:B:1031:SER:O	2:B:1035:GLU:HG2	1.89	0.73
2:B:1170:LYS:HE3	2:B:1173:ASN:HB3	1.69	0.73
1:A:1265:ASN:ND2	2:B:845:GLU:CG	2.51	0.73
1:A:1137:LYS:HG2	1:A:1138:GLY:H	1.53	0.73
2:B:336:LEU:HB3	2:B:347:MET:CE	2.18	0.72
2:B:426:THR:OG1	2:B:427:VAL:HG22	1.89	0.72
1:A:1275:SER:HA	2:B:827:LEU:HD21	1.70	0.72
2:B:251:GLU:HG2	2:B:357:HIS:HE1	1.54	0.71
2:B:243:VAL:HG13	2:B:259:GLN:HB2	1.72	0.71
1:A:149:LEU:HD12	1:A:183:THR:HG23	1.71	0.71
1:A:482:THR:HG22	1:A:484:ASP:N	2.07	0.70
1:A:1278:LEU:HD23	1:A:1281:SER:OG	1.92	0.70
1:A:1265:ASN:HD22	2:B:845:GLU:CG	2.03	0.69
2:B:834:TRP:HB2	2:B:835:PRO:HD2	1.74	0.69
2:B:96:GLU:HG2	2:B:459:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:VAL:CG1	2:B:259:GLN:HB2	2.22	0.68
2:B:1123:TYR:CE1	2:B:1138:LYS:HB2	2.28	0.68
1:A:870:ILE:O	1:A:874:ILE:HG13	1.93	0.67
1:A:1228:ASP:HB3	1:A:1232:THR:H	1.60	0.67
2:B:528:ASP:HB2	2:B:529:LYS:CA	2.25	0.67
2:B:715:ILE:CG2	2:B:720:LEU:HD22	2.24	0.67
2:B:426:THR:OG1	2:B:427:VAL:HG23	1.94	0.66
2:B:310:ASN:OD1	2:B:310:ASN:N	2.29	0.66
2:B:528:ASP:HB2	2:B:529:LYS:HA	1.76	0.66
1:A:1037:ASP:OD1	2:B:812:LEU:HD23	1.95	0.66
1:A:1170:LYS:H	1:A:1170:LYS:HD3	1.60	0.66
2:B:295:PHE:CD1	2:B:328:ILE:HD11	2.32	0.65
1:A:1269:ARG:HG2	2:B:841:TYR:CE1	2.32	0.65
2:B:340:SER:HB2	2:B:347:MET:CE	2.26	0.65
1:A:1236:LYS:NZ	1:A:1280:CYS:SG	2.70	0.65
2:B:302:TYR:OH	2:B:321:LYS:HB2	1.98	0.64
1:A:1170:LYS:N	1:A:1170:LYS:HD3	2.13	0.64
1:A:149:LEU:HD12	1:A:183:THR:HG21	1.79	0.64
1:A:80:THR:HG22	1:A:82:ASN:N	2.12	0.64
2:B:493:ILE:HD11	2:B:499:TRP:CZ2	2.33	0.64
1:A:453:LEU:HD23	1:A:453:LEU:H	1.62	0.63
1:A:1170:LYS:O	1:A:1170:LYS:HG2	1.99	0.63
2:B:251:GLU:HG2	2:B:357:HIS:CE1	2.34	0.63
2:B:409:ASN:OD1	2:B:409:ASN:N	2.31	0.63
1:A:149:LEU:CD1	1:A:183:THR:HG21	2.28	0.63
1:A:1:MET:N	1:A:2:PRO:HD3	2.14	0.62
2:B:1132:LEU:HD21	2:B:1165:ILE:HD13	1.79	0.62
1:A:135:ILE:HD13	1:A:149:LEU:CD2	2.30	0.62
2:B:340:SER:HB2	2:B:347:MET:HE2	1.82	0.62
1:A:117:PHE:HA	1:A:317:PHE:CE1	2.34	0.62
1:A:611:VAL:HG12	1:A:1024:LEU:HD11	1.81	0.62
1:A:1000:LYS:HE2	2:B:811:PHE:CE1	2.35	0.61
2:B:1142:LYS:HD3	2:B:1160:TYR:CE1	2.36	0.61
2:B:960:ASN:OD1	2:B:962:SER:HB3	2.00	0.61
1:A:681:LEU:HD23	1:A:694:THR:HG22	1.81	0.61
1:A:184:GLN:OE1	1:A:231:ARG:HD3	2.01	0.60
1:A:963:THR:HB	1:A:1058:ASP:HB3	1.84	0.60
2:B:715:ILE:HB	2:B:720:LEU:HD21	1.82	0.60
1:A:10:TYR:CZ	1:A:84:LYS:CD	2.84	0.60
1:A:482:THR:CG2	1:A:484:ASP:H	2.14	0.60
1:A:67:GLN:O	1:A:460:TRP:HZ2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1172:GLU:H	2:B:1174:HIS:H	1.50	0.59
1:A:52:THR:CG2	1:A:528:LEU:HD11	2.31	0.59
2:B:639:LEU:HD12	2:B:783:PHE:HE1	1.67	0.59
1:A:53:ASN:OD1	1:A:55:GLU:HB2	2.01	0.59
1:A:1092:SER:O	1:A:1098:LYS:NZ	2.34	0.59
2:B:639:LEU:HD12	2:B:783:PHE:CE1	2.37	0.59
2:B:1082:ASN:ND2	2:B:1084:THR:O	2.36	0.59
1:A:706:TRP:CD2	1:A:808:LEU:HD13	2.37	0.59
1:A:149:LEU:CD1	1:A:183:THR:CG2	2.81	0.58
2:B:169:ILE:CD1	2:B:199:THR:HB	2.33	0.58
2:B:924:LYS:HG3	2:B:928:CYS:O	2.03	0.58
1:A:1128:VAL:HG11	1:A:1191:TYR:CE2	2.38	0.58
2:B:79:LEU:O	2:B:83:ILE:HG13	2.03	0.58
1:A:388:ASP:HB3	1:A:391:ASN:O	2.03	0.58
2:B:1125:ASP:OD1	2:B:1126:ILE:N	2.36	0.58
2:B:110:TYR:O	2:B:150:TYR:HD1	1.87	0.58
1:A:687:ASN:ND2	1:A:690:LEU:HD22	2.19	0.58
1:A:568:LEU:HD12	1:A:594:VAL:HG11	1.85	0.57
2:B:313:GLY:H	2:B:317:LYS:HZ2	1.51	0.57
1:A:1271:ILE:HD11	2:B:839:VAL:HG21	1.86	0.57
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.40	0.57
1:A:1228:ASP:OD2	1:A:1231:ILE:HB	2.05	0.57
2:B:674:THR:HG22	2:B:675:GLN:HG3	1.85	0.57
2:B:281:TYR:OH	2:B:440:ARG:O	2.23	0.56
2:B:238:PRO:HG3	2:B:287:TYR:CZ	2.40	0.56
1:A:1277:THR:HG23	1:A:1277:THR:O	2.05	0.56
1:A:1122:TYR:CZ	1:A:1156:ARG:NE	2.74	0.56
1:A:35:ALA:HB2	1:A:45:ILE:HG12	1.88	0.55
2:B:283:PHE:HA	2:B:434:TYR:OH	2.06	0.55
1:A:1117:TYR:CD1	1:A:1277:THR:OG1	2.55	0.55
2:B:1137:ASN:OD1	2:B:1139:ASN:HB2	2.07	0.55
1:A:80:THR:HB	1:A:83:GLU:HG3	1.88	0.55
1:A:869:TYR:HD1	1:A:870:ILE:HD12	1.72	0.55
2:B:112:TYR:CE1	2:B:149:GLY:HA3	2.42	0.55
1:A:996:ARG:HE	2:B:807:LEU:HD11	1.72	0.55
1:A:1137:LYS:HG2	1:A:1138:GLY:N	2.21	0.55
1:A:67:GLN:HG2	1:A:425:PHE:CE1	2.41	0.55
1:A:648:TYR:O	1:A:651:ASP:HB2	2.07	0.54
1:A:49:ASP:OD1	1:A:52:THR:HB	2.06	0.54
1:A:1122:TYR:OH	1:A:1156:ARG:NE	2.40	0.54
2:B:169:ILE:HD13	2:B:199:THR:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TYR:CZ	1:A:572:VAL:HG21	2.43	0.54
1:A:1228:ASP:HB3	1:A:1232:THR:N	2.23	0.54
1:A:565:ARG:HB2	1:A:749:TYR:CZ	2.43	0.54
1:A:322:LEU:HD12	1:A:341:LEU:HB2	1.90	0.54
2:B:762:TYR:HB3	2:B:763:PRO:HD3	1.89	0.54
2:B:341:LYS:HA	2:B:824:GLU:HG2	1.90	0.54
1:A:61:PRO:HB3	1:A:419:PHE:CZ	2.43	0.53
1:A:1036:ILE:O	2:B:814:ILE:N	2.28	0.53
1:A:888:LEU:HB3	1:A:900:ILE:HD11	1.91	0.53
1:A:1271:ILE:HG22	1:A:1271:ILE:O	2.07	0.53
1:A:42:ILE:HD13	1:A:151:LEU:HB3	1.90	0.53
1:A:1228:ASP:OD1	1:A:1234:LYS:HD2	2.09	0.53
1:A:207:LEU:HD11	1:A:1076:ASP:HB3	1.91	0.53
2:B:513:LYS:HD2	2:B:514:PHE:H	1.74	0.53
1:A:67:GLN:O	1:A:460:TRP:CZ2	2.62	0.53
2:B:227:ILE:HD11	2:B:339:PHE:CE2	2.43	0.53
1:A:108:LEU:O	1:A:112:VAL:HG23	2.09	0.53
2:B:306:ILE:HG23	2:B:312:ILE:CD1	2.39	0.53
2:B:513:LYS:HD2	2:B:514:PHE:N	2.24	0.53
1:A:644:GLY:O	1:A:645:ASN:ND2	2.43	0.52
1:A:1241:ASP:HB3	1:A:1247:ILE:HD11	1.91	0.52
2:B:40:TRP:CD1	2:B:167:SER:HB2	2.45	0.52
2:B:887:ILE:HG23	2:B:1005:LEU:HB3	1.92	0.52
1:A:1122:TYR:OH	1:A:1137:LYS:HD2	2.09	0.52
2:B:329:ASN:O	2:B:333:GLU:HG2	2.10	0.52
2:B:112:TYR:HE1	2:B:149:GLY:HA3	1.75	0.52
2:B:227:ILE:HG22	2:B:267:VAL:HG22	1.92	0.52
2:B:266:LEU:O	2:B:335:ASN:HB3	2.10	0.52
2:B:1043:ARG:HB3	2:B:1047:GLU:HA	1.92	0.51
1:A:1031:ILE:HG12	1:A:1036:ILE:HG13	1.92	0.51
1:A:52:THR:HG22	1:A:53:ASN:N	2.25	0.51
2:B:336:LEU:O	2:B:347:MET:HE3	2.11	0.51
1:A:864:SER:HA	1:A:867:THR:HB	1.93	0.51
1:A:1209:LEU:CD1	1:A:1217:LEU:HD13	2.40	0.51
1:A:1037:ASP:HA	2:B:814:ILE:HD12	1.93	0.51
1:A:115:ILE:HD11	1:A:512:PRO:HB2	1.92	0.51
1:A:1278:LEU:HG	1:A:1280:CYS:SG	2.51	0.51
1:A:706:TRP:CE3	1:A:808:LEU:HD13	2.46	0.51
1:A:671:ILE:O	1:A:671:ILE:HG23	2.11	0.51
2:B:1058:LEU:HD23	2:B:1068:ILE:HG13	1.93	0.50
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:ASN:HB2	1:A:1249:PHE:CE1	2.46	0.50
1:A:729:ARG:HD2	1:A:785:ASN:OD1	2.11	0.50
1:A:699:LEU:HD22	1:A:844:THR:HG21	1.93	0.50
2:B:426:THR:CB	2:B:427:VAL:CA	2.69	0.50
1:A:504:LEU:O	2:B:1170:LYS:HB2	2.12	0.50
1:A:525:ILE:N	1:A:525:ILE:HD12	2.23	0.50
2:B:1172:GLU:H	2:B:1174:HIS:N	2.09	0.50
2:B:1:MET:HG2	2:B:2:ASN:H	1.76	0.50
2:B:227:ILE:O	2:B:230:LEU:HB2	2.12	0.50
1:A:688:LYS:HD3	1:A:833:GLN:NE2	2.27	0.50
1:A:172:VAL:HG23	1:A:173:LEU:N	2.26	0.49
2:B:874:ASN:HB2	2:B:1036:VAL:HG13	1.94	0.49
2:B:212:ASP:HB3	2:B:213:GLU:OE2	2.12	0.49
1:A:1269:ARG:CZ	2:B:850:VAL:HG11	2.42	0.49
2:B:374:ILE:HD12	2:B:375:ASN:N	2.27	0.49
2:B:227:ILE:HD11	2:B:339:PHE:HE2	1.77	0.49
2:B:864:SER:HB2	2:B:867:ILE:HG13	1.93	0.49
1:A:1096:ILE:O	1:A:1098:LYS:HE3	2.11	0.49
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.95	0.49
2:B:1115:SER:HB2	2:B:1123:TYR:CD2	2.48	0.49
2:B:326:ILE:HG23	2:B:327:ASN:N	2.28	0.49
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.94	0.49
1:A:172:VAL:HG23	1:A:173:LEU:H	1.77	0.49
1:A:634:ILE:N	1:A:634:ILE:HD12	2.27	0.49
1:A:954:ASN:OD1	1:A:956:ILE:HG12	2.13	0.49
2:B:633:GLU:HA	2:B:633:GLU:OE1	2.12	0.49
2:B:243:VAL:HG11	2:B:259:GLN:CD	2.33	0.49
2:B:407:ASN:OD1	2:B:411:VAL:HG12	2.13	0.48
1:A:45:ILE:HB	1:A:154:ILE:HG22	1.94	0.48
2:B:259:GLN:OE1	2:B:426:THR:O	2.31	0.48
1:A:532:PRO:O	1:A:534:ILE:HD12	2.14	0.48
2:B:615:ILE:O	2:B:615:ILE:HG13	2.12	0.48
2:B:528:ASP:CB	2:B:530:SER:N	2.61	0.48
1:A:1164:LYS:NZ	1:A:1170:LYS:HA	2.29	0.48
2:B:944:ILE:HB	2:B:950:GLU:HG3	1.95	0.47
1:A:177:ARG:HD3	1:A:238:ASN:HA	1.95	0.47
2:B:1123:TYR:HE1	2:B:1138:LYS:HB2	1.77	0.47
2:B:238:PRO:HD2	2:B:263:VAL:CG2	2.45	0.47
2:B:902:PHE:HE1	2:B:904:ILE:HD11	1.80	0.47
1:A:1186:VAL:HB	1:A:1191:TYR:CE1	2.49	0.47
1:A:97:ARG:HA	1:A:386:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:ILE:HG22	2:B:317:LYS:N	2.29	0.47
2:B:914:ASP:OD2	2:B:916:ILE:HG23	2.14	0.47
1:A:179:GLY:CA	1:A:234:GLY:HA3	2.44	0.47
1:A:565:ARG:HB2	1:A:749:TYR:CE2	2.50	0.47
2:B:761:ILE:HD12	2:B:761:ILE:N	2.30	0.47
1:A:858:ASP:N	1:A:858:ASP:OD1	2.47	0.47
1:A:1:MET:H2	1:A:2:PRO:HD3	1.78	0.46
2:B:272:ASP:N	2:B:273:PRO:HD2	2.29	0.46
1:A:1014:TRP:CH2	1:A:1068:TRP:HB3	2.49	0.46
1:A:1122:TYR:CE2	1:A:1156:ARG:NE	2.83	0.46
1:A:590:TYR:O	1:A:594:VAL:HG12	2.15	0.46
2:B:1172:GLU:N	2:B:1173:ASN:HA	2.29	0.46
2:B:1166:CYS:HB3	2:B:1188:TYR:CD1	2.51	0.46
2:B:892:ASP:O	2:B:895:GLU:HG2	2.15	0.46
2:B:1039:ASN:O	2:B:1040:SER:CB	2.63	0.46
2:B:1129:ASP:OD1	2:B:1129:ASP:N	2.49	0.46
2:B:17:ASN:HD22	2:B:34:LYS:HE3	1.81	0.46
2:B:426:THR:CG2	2:B:428:ASP:OD2	2.58	0.46
1:A:334:ASP:HB3	1:A:337:LYS:HB2	1.98	0.46
1:A:930:ASN:O	1:A:933:VAL:HG13	2.16	0.46
2:B:1115:SER:HB2	2:B:1123:TYR:CE2	2.50	0.46
2:B:528:ASP:CB	2:B:529:LYS:HA	2.40	0.46
2:B:435:LYS:HA	2:B:628:ILE:HG23	1.98	0.46
2:B:569:TYR:CE2	2:B:734:ILE:HG23	2.51	0.46
1:A:1125:VAL:HG22	1:A:1134:MET:HG2	1.98	0.46
1:A:1134:MET:HB2	1:A:1134:MET:HE3	1.77	0.46
2:B:528:ASP:HB2	2:B:529:LYS:C	2.35	0.46
2:B:636:ASN:HA	2:B:639:LEU:CD1	2.46	0.46
2:B:92:THR:HB	2:B:343:PHE:CZ	2.51	0.46
2:B:966:ILE:HD12	2:B:966:ILE:N	2.30	0.46
1:A:1268:ASN:HB2	2:B:843:PHE:CE2	2.51	0.46
2:B:1123:TYR:HD1	2:B:1138:LYS:HA	1.80	0.46
2:B:1167:LEU:HA	2:B:1167:LEU:HD12	1.81	0.45
2:B:842:ALA:HA	2:B:850:VAL:O	2.16	0.45
2:B:261:ASN:OD1	2:B:263:VAL:HG23	2.16	0.45
1:A:421:GLY:H	1:A:424:GLU:CG	2.18	0.45
2:B:1080:THR:OG1	2:B:1081:ILE:N	2.49	0.45
2:B:368:TYR:HA	2:B:369:PRO:HA	1.62	0.45
1:A:1209:LEU:HD11	1:A:1217:LEU:HD13	1.99	0.45
1:A:125:THR:O	1:A:301:LYS:N	2.48	0.45
1:A:1271:ILE:HG13	2:B:854:ALA:HB3	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:HIS:CE1	1:A:264:ARG:HD3	2.51	0.45
2:B:774:ASN:O	2:B:778:ILE:HG12	2.16	0.45
1:A:135:ILE:HD13	1:A:149:LEU:HD23	1.99	0.45
2:B:587:LYS:HE2	2:B:587:LYS:HB3	1.67	0.45
1:A:26:ASN:HD21	1:A:54:PRO:HD3	1.81	0.45
2:B:155:TYR:HA	2:B:165:TYR:O	2.16	0.45
1:A:49:ASP:HB2	1:A:154:ILE:HD12	1.98	0.44
2:B:1114:ILE:HB	2:B:1124:ILE:HD12	1.98	0.44
2:B:314:ASN:O	2:B:318:LEU:HB2	2.16	0.44
2:B:184:VAL:CG2	2:B:200:GLU:HB2	2.47	0.44
1:A:257:GLU:HG3	1:A:534:ILE:HG21	1.98	0.44
1:A:22:ILE:HD11	1:A:45:ILE:HD11	1.99	0.44
2:B:406:LEU:HD11	2:B:494:ASN:HB3	1.99	0.44
1:A:773:LEU:O	1:A:777:ILE:HG13	2.17	0.44
2:B:798:LEU:HD23	2:B:798:LEU:HA	1.87	0.44
1:A:1097:LEU:HD12	1:A:1225:SER:HB3	2.00	0.44
1:A:481:ILE:O	1:A:682:VAL:HG12	2.18	0.44
2:B:293:LYS:HB2	2:B:293:LYS:NZ	2.32	0.44
1:A:1135:TYR:HB2	1:A:1259:ALA:O	2.18	0.44
1:A:1202:VAL:HG13	1:A:1203:GLU:OE2	2.18	0.44
2:B:426:THR:HB	2:B:428:ASP:HA	2.00	0.44
2:B:967:THR:HB	2:B:980:PHE:HB2	2.00	0.44
1:A:128:LYS:HG2	1:A:304:VAL:HB	1.99	0.44
2:B:1156:LEU:HD21	2:B:1192:PHE:CD2	2.53	0.43
2:B:841:TYR:CZ	2:B:852:GLY:HA3	2.53	0.43
2:B:306:ILE:HG23	2:B:312:ILE:HD12	1.99	0.43
2:B:762:TYR:O	2:B:765:PHE:HB3	2.18	0.43
1:A:43:TRP:CD1	1:A:149:LEU:HD22	2.53	0.43
2:B:1123:TYR:CD1	2:B:1138:LYS:HA	2.53	0.43
2:B:154:ASN:HB2	2:B:167:SER:O	2.18	0.43
1:A:1275:SER:CA	2:B:827:LEU:HD21	2.42	0.43
1:A:1122:TYR:CD1	1:A:1157:GLY:HA2	2.53	0.43
1:A:118:TRP:HB3	1:A:128:LYS:O	2.17	0.43
2:B:1122:LYS:HB3	2:B:1134:LEU:HB3	2.00	0.43
2:B:105:ALA:HB3	2:B:233:LEU:HD13	2.00	0.43
2:B:427:VAL:HA	2:B:428:ASP:HA	1.68	0.43
2:B:859:THR:HA	2:B:890:SER:O	2.18	0.43
2:B:1084:THR:HB	2:B:1087:LEU:HB2	2.01	0.43
2:B:34:LYS:HB2	2:B:40:TRP:CZ3	2.53	0.43
1:A:164:GLU:OE2	1:A:166:LYS:HE2	2.19	0.43
1:A:195:GLY:HA2	1:A:213:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:ASP:HB3	1:A:910:ASP:O	2.19	0.43
2:B:554:THR:OG1	2:B:557:LYS:HG3	2.19	0.43
2:B:715:ILE:HB	2:B:720:LEU:CD2	2.49	0.43
1:A:1277:THR:CG2	1:A:1277:THR:O	2.67	0.43
1:A:149:LEU:HD11	1:A:183:THR:HG21	2.00	0.43
1:A:10:TYR:CE1	1:A:84:LYS:HD3	2.53	0.43
1:A:881:LEU:HD11	1:A:898:ILE:HG12	2.01	0.43
2:B:20:VAL:HG13	2:B:29:VAL:HG13	2.01	0.43
2:B:313:GLY:H	2:B:317:LYS:NZ	2.17	0.43
1:A:322:LEU:HA	1:A:322:LEU:HD23	1.90	0.42
2:B:40:TRP:HD1	2:B:167:SER:HB2	1.84	0.42
2:B:314:ASN:HB3	2:B:318:LEU:CD1	2.42	0.42
2:B:340:SER:HB2	2:B:347:MET:HE3	2.00	0.42
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.76	0.42
2:B:993:GLU:H	2:B:993:GLU:HG3	1.45	0.42
1:A:1265:ASN:ND2	2:B:845:GLU:HG3	2.33	0.42
1:A:600:ALA:HA	1:A:754:TYR:CZ	2.54	0.42
2:B:1172:GLU:HB2	2:B:1173:ASN:C	2.39	0.42
2:B:1071:VAL:CG1	2:B:1176:TRP:HZ3	2.33	0.42
2:B:185:PHE:HB2	2:B:197:THR:HG21	2.01	0.42
1:A:1155:TYR:CD2	1:A:1293:GLU:HG3	2.53	0.42
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	2.01	0.42
1:A:178:ASN:OD1	1:A:180:TYR:HB2	2.19	0.42
1:A:1030:TYR:O	1:A:1031:ILE:HD13	2.19	0.42
2:B:871:TYR:CE2	2:B:1049:ARG:HD3	2.55	0.42
2:B:1173:ASN:O	2:B:1174:HIS:CD2	2.72	0.42
2:B:636:ASN:HA	2:B:639:LEU:HD13	2.01	0.42
1:A:1293:GLU:O	1:A:1295:PRO:HD3	2.19	0.42
1:A:135:ILE:CD1	1:A:149:LEU:HD23	2.49	0.42
1:A:67:GLN:HA	1:A:425:PHE:CZ	2.54	0.42
2:B:648:GLU:HG2	2:B:648:GLU:O	2.19	0.42
2:B:1052:TYR:CE1	2:B:1098:SER:HB2	2.55	0.42
1:A:1169:ASN:HB3	2:B:1111:GLU:HG3	2.01	0.42
1:A:980:TYR:OH	1:A:1148:ILE:O	2.28	0.42
1:A:1193:LEU:HD11	1:A:1206:LEU:HD13	2.00	0.42
2:B:1108:LYS:O	2:B:1109:LEU:HB2	2.19	0.42
1:A:1228:ASP:H	1:A:1232:THR:HA	1.85	0.42
1:A:97:ARG:HD2	1:A:386:ILE:O	2.20	0.42
2:B:426:THR:CB	2:B:427:VAL:CG2	2.98	0.42
2:B:639:LEU:CD1	2:B:783:PHE:HE1	2.32	0.42
1:A:987:LEU:HD23	1:A:987:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:ARG:NH1	2:B:973:LEU:O	2.52	0.42
2:B:911:LEU:HG	2:B:911:LEU:H	1.68	0.42
1:A:242:VAL:HG13	1:A:258:VAL:O	2.20	0.41
2:B:249:ARG:NH1	2:B:256:GLU:OE2	2.52	0.41
2:B:504:LEU:HD12	2:B:504:LEU:HA	1.82	0.41
1:A:1023:ARG:HB3	1:A:1023:ARG:NH1	2.34	0.41
2:B:1039:ASN:O	2:B:1040:SER:OG	2.33	0.41
2:B:237:LYS:HA	2:B:238:PRO:HD3	1.87	0.41
2:B:184:VAL:HG22	2:B:200:GLU:HB2	2.01	0.41
2:B:224:LYS:HB2	2:B:336:LEU:HD11	2.03	0.41
2:B:674:THR:HG22	2:B:675:GLN:N	2.35	0.41
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.95	0.41
1:A:313:MET:HE1	1:A:515:ILE:HD13	2.03	0.41
1:A:711:LYS:HB3	1:A:711:LYS:HE2	1.80	0.41
1:A:471:PHE:CE2	1:A:720:LYS:HE3	2.54	0.41
1:A:964:ILE:HD13	1:A:978:LEU:HG	2.03	0.41
2:B:1031:SER:O	2:B:1035:GLU:CG	2.64	0.41
2:B:343:PHE:HB3	2:B:345:ILE:HG13	2.03	0.41
2:B:838:LEU:HD13	2:B:859:THR:HG21	2.01	0.41
1:A:788:LEU:HD23	1:A:788:LEU:HA	1.82	0.41
2:B:355:LEU:HD23	2:B:355:LEU:HA	1.85	0.41
2:B:638:MET:HA	2:B:641:LEU:HD13	2.01	0.41
2:B:754:ILE:O	2:B:758:GLU:HG3	2.21	0.41
1:A:688:LYS:HB2	1:A:688:LYS:HE3	1.79	0.41
2:B:1070:GLU:CD	2:B:1077:ILE:HD11	2.40	0.41
2:B:330:ASP:HB3	2:B:453:SER:HB3	2.02	0.41
1:A:1271:ILE:HD11	2:B:839:VAL:HG11	2.03	0.41
2:B:11:SER:HA	2:B:12:PRO:HD3	1.96	0.41
2:B:211:TYR:O	2:B:212:ASP:HB2	2.21	0.41
2:B:528:ASP:N	2:B:528:ASP:OD1	2.54	0.41
1:A:1023:ARG:NH2	1:A:1045:GLY:O	2.54	0.41
2:B:177:ASN:ND2	2:B:180:GLU:HB2	2.36	0.41
2:B:579:ILE:O	2:B:585:ILE:HA	2.21	0.41
1:A:985:TRP:CE2	1:A:1019:ILE:HG21	2.55	0.41
1:A:266:PHE:CE1	1:A:366:PHE:HB3	2.56	0.41
2:B:853:ASP:OD1	2:B:859:THR:HB	2.22	0.40
2:B:906:PHE:HB3	2:B:1017:LEU:HA	2.02	0.40
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.56	0.40
1:A:179:GLY:HA2	1:A:234:GLY:HA3	2.02	0.40
2:B:306:ILE:HG23	2:B:312:ILE:HD13	2.03	0.40
1:A:275:ASP:OD2	1:A:275:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ARG:HD2	1:A:749:TYR:CE1	2.55	0.40
1:A:578:ASN:HA	1:A:579:PRO:HD3	1.80	0.40
2:B:1152:ILE:CG2	2:B:1155:CYS:HB2	2.52	0.40
2:B:511:ASN:HB3	2:B:513:LYS:O	2.21	0.40
1:A:48:ARG:HG2	1:A:78:LEU:HB3	2.04	0.40
2:B:1127:SER:OG	2:B:1128:GLU:N	2.54	0.40
2:B:346:MET:CE	2:B:832:GLU:HG3	2.52	0.40
1:A:1099:ASP:O	1:A:1233:ASN:OD1	2.39	0.40
1:A:688:LYS:O	1:A:692:VAL:HG23	2.21	0.40
2:B:328:ILE:HA	2:B:328:ILE:HD13	1.84	0.40
2:B:368:TYR:N	2:B:368:TYR:CD2	2.89	0.40
2:B:695:GLU:OE2	2:B:735:SER:HA	2.22	0.40

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:GLY:CA	2:B:925:GLU:OE1[4_655]	1.34	0.86
1:A:832:GLY:C	2:B:925:GLU:OE1[4_655]	1.35	0.85
1:A:1187:LYS:N	2:B:793:ASP:OD1[10_555]	1.42	0.78
1:A:832:GLY:N	2:B:925:GLU:OE2[4_655]	1.53	0.67
1:A:825:ASP:N	2:B:718:ASP:CB[4_655]	1.53	0.67
1:A:825:ASP:CA	2:B:718:ASP:CA[4_655]	1.67	0.53
1:A:824:TYR:C	2:B:718:ASP:CB[4_655]	1.74	0.46
1:A:825:ASP:N	2:B:718:ASP:CA[4_655]	1.83	0.37
1:A:832:GLY:N	2:B:925:GLU:OE1[4_655]	1.84	0.36
1:A:832:GLY:N	2:B:925:GLU:CD[4_655]	1.86	0.34
1:A:1153:SER:CB	2:B:644:ASN:OD1[10_555]	1.87	0.33
1:A:825:ASP:O	2:B:721:ALA:CB[4_655]	1.88	0.32
1:A:1143:VAL:CG1	2:B:644:ASN:ND2[10_555]	1.89	0.31
1:A:825:ASP:OD2	2:B:717:SER:CB[4_655]	1.90	0.30
1:A:825:ASP:OD1	2:B:717:SER:O[4_655]	1.91	0.29
1:A:1153:SER:OG	2:B:644:ASN:OD1[10_555]	1.91	0.29
1:A:1186:VAL:C	2:B:793:ASP:OD1[10_555]	1.92	0.28
2:B:409:ASN:O	2:B:491:ARG:NE[12_545]	1.96	0.24
1:A:1156:ARG:NH2	2:B:789:ASN:ND2[10_555]	1.97	0.23
1:A:835:ASP:OD1	2:B:926:ASP:N[4_655]	2.01	0.19
1:A:1156:ARG:NH2	2:B:789:ASN:O[10_555]	2.03	0.17
1:A:1156:ARG:NH1	2:B:642:PRO:CB[10_555]	2.04	0.16
1:A:825:ASP:CB	2:B:717:SER:OG[4_655]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:GLY:O	2:B:925:GLU:OE1[4_655]	2.09	0.11
1:A:832:GLY:CA	2:B:925:GLU:CD[4_655]	2.11	0.09
1:A:833:GLN:N	2:B:925:GLU:OE1[4_655]	2.11	0.09
1:A:1156:ARG:NH2	2:B:789:ASN:CG[10_555]	2.11	0.09
1:A:956:ILE:CD1	1:A:1294:ARG:CD[10_555]	2.11	0.09
1:A:835:ASP:OD1	2:B:926:ASP:CA[4_655]	2.14	0.06
1:A:825:ASP:OD2	2:B:717:SER:OG[4_655]	2.14	0.06
1:A:825:ASP:CA	2:B:718:ASP:N[4_655]	2.15	0.05
2:B:409:ASN:O	2:B:491:ARG:CZ[12_545]	2.17	0.03

## 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	1276/1296 (98%)	1242 (97%)	34 (3%)	0	100	100
2	B	1144/1196 (96%)	1105 (97%)	38 (3%)	1 (0%)	53	86
All	All	2420/2492 (97%)	2347 (97%)	72 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	429	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1162/1176 (99%)	1126 (97%)	36 (3%)	43	71
2	B	1076/1114 (97%)	1007 (94%)	69 (6%)	19	53
All	All	2238/2290 (98%)	2133 (95%)	105 (5%)	29	62

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	55	GLU
1	A	58	ASP
1	A	97	ARG
1	A	240	ASN
1	A	482	THR
1	A	484	ASP
1	A	507	ASN
1	A	510	ASN
1	A	520	LEU
1	A	525	ILE
1	A	541	LYS
1	A	546	ASP
1	A	608	GLU
1	A	645	ASN
1	A	682	VAL
1	A	690	LEU
1	A	757	GLU
1	A	770	SER
1	A	806	LYS
1	A	819	LEU
1	A	858	ASP
1	A	871	LYS
1	A	933	VAL
1	A	948	ARG
1	A	958	LEU
1	A	1027	SER
1	A	1065	ARG
1	A	1087	LEU
1	A	1146	THR
1	A	1169	ASN
1	A	1170	LYS
1	A	1188	ASN
1	A	1226	LYS
1	A	1272	GLU

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Mol	Chain	Res	Type
1	A	1274	SER
2	B	7	LEU
2	B	29	VAL
2	B	50	SER
2	B	186	TYR
2	B	230	LEU
2	B	250	SER
2	B	251	GLU
2	B	253	GLU
2	B	279	ASP
2	B	284	THR
2	B	310	ASN
2	B	320	LEU
2	B	326	ILE
2	B	329	ASN
2	B	359	TYR
2	B	406	LEU
2	B	409	ASN
2	B	469	ILE
2	B	487	ILE
2	B	492	GLU
2	B	493	ILE
2	B	504	LEU
2	B	509	THR
2	B	511	ASN
2	B	528	ASP
2	B	550	SER
2	B	553	ASP
2	B	554	THR
2	B	583	CYS
2	B	585	ILE
2	B	611	ASN
2	B	621	LYS
2	B	624	LEU
2	B	648	GLU
2	B	674	THR
2	B	703	GLN
2	B	709	LEU
2	B	712	ASN
2	B	716	SER
2	B	718	ASP
2	B	720	LEU

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Mol	Chain	Res	Type
2	B	724	ASN
2	B	745	VAL
2	B	796	LEU
2	B	797	GLN
2	B	800	ASN
2	B	830	LYS
2	B	834	TRP
2	B	865	LYS
2	B	913	LYS
2	B	916	ILE
2	B	924	LYS
2	B	927	ASN
2	B	978	LEU
2	B	993	GLU
2	B	1024	THR
2	B	1026	SER
2	B	1077	ILE
2	B	1083	ASN
2	B	1086	ASN
2	B	1089	LEU
2	B	1115	SER
2	B	1117	LEU
2	B	1128	GLU
2	B	1129	ASP
2	B	1136	ASP
2	B	1142	LYS
2	B	1144	MET
2	B	1167	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	913	GLN
1	A	1265	ASN
2	B	961	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

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

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	1280/1296 (98%)	0.34	77 (6%)	22	16	106, 184, 268, 448	10 (0%)
2	B	1150/1196 (96%)	0.35	75 (6%)	19	13	92, 159, 251, 587	14 (1%)
All	All	2430/2492 (97%)	0.34	152 (6%)	20	14	92, 173, 263, 587	24 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	12.1
2	B	451	ASP	8.7
2	B	150	TYR	7.6
1	A	1227	ASN	7.3
2	B	43	PRO	6.4
1	A	169	GLY	6.2
2	B	17	ASN	6.0
1	A	1232	THR	5.7
1	A	131	ASP	5.2
1	A	118	TRP	5.2
2	B	552	ILE	5.1
2	B	2	ASN	5.0
1	A	698	ALA	4.9
2	B	149	GLY	4.9
1	A	1228	ASP	4.8
2	B	110	TYR	4.7
2	B	44	GLU	4.2
1	A	515	ILE	4.2
2	B	18	VAL	4.1
2	B	306	ILE	4.0
1	A	1295	PRO	4.0
2	B	314	ASN	3.9
1	A	1229	GLN	3.8
1	A	825	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1294	ARG	3.7
1	A	168	PHE	3.7
2	B	165	TYR	3.7
2	B	152	GLU	3.6
1	A	17	VAL	3.5
2	B	636	ASN	3.5
1	A	160	ILE	3.4
1	A	1293	GLU	3.4
1	A	300	ALA	3.3
2	B	65	ASP	3.3
2	B	9	ILE	3.3
2	B	308	GLY	3.3
1	A	764	PHE	3.2
2	B	1142	LYS	3.2
2	B	33	PHE	3.2
1	A	758	GLU	3.2
2	B	307	GLU	3.2
2	B	718	ASP	3.2
2	B	84	THR	3.2
1	A	524	ILE	3.1
1	A	138	ILE	3.1
2	B	80	GLN	3.1
1	A	559	PHE	3.1
2	B	73	SER	3.0
2	B	76	ASP	3.0
2	B	81	ALA	3.0
2	B	452	SER	3.0
1	A	16	GLY	3.0
1	A	36	PHE	3.0
2	B	555	ASP	2.9
1	A	762	ILE	2.9
1	A	59	LEU	2.9
1	A	1195	THR	2.9
1	A	34	LYS	2.9
1	A	548	TYR	2.9
2	B	1126	ILE	2.9
2	B	1086	ASN	2.9
1	A	434	ILE	2.9
1	A	19	ILE	2.8
2	B	19	VAL	2.8
1	A	481	ILE	2.8
1	A	18	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	763	ASN	2.8
1	A	761	ASN	2.8
1	A	493	ASN	2.8
1	A	563	LYS	2.8
2	B	1077	ILE	2.7
1	A	119	GLY	2.7
1	A	565	ARG	2.7
2	B	1135	ILE	2.7
1	A	136	ASN	2.7
2	B	112	TYR	2.7
1	A	525	ILE	2.7
2	B	41	VAL	2.7
2	B	31	LYS	2.7
2	B	23	ALA	2.7
1	A	527	GLN	2.6
1	A	753	GLN	2.6
2	B	1079	LEU	2.6
2	B	74	GLU	2.6
2	B	186	TYR	2.6
2	B	553	ASP	2.6
2	B	166	ALA	2.6
1	A	1206	LEU	2.6
2	B	844	LYS	2.5
1	A	332	SER	2.5
1	A	661	ALA	2.5
1	A	127	LEU	2.5
1	A	1193	LEU	2.5
1	A	185	TYR	2.5
1	A	8	PHE	2.5
2	B	477	ASN	2.5
2	B	1124	ILE	2.5
1	A	72	TYR	2.5
2	B	77	LYS	2.5
2	B	1167	LEU	2.5
2	B	1177	MET	2.5
1	A	1203	GLU	2.5
2	B	441	ALA	2.4
2	B	1143	LYS	2.4
1	A	297	LEU	2.4
1	A	685	ILE	2.4
1	A	1053	ILE	2.4
2	B	558	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	705	LYS	2.4
1	A	568	LEU	2.3
2	B	1130	ASN	2.3
2	B	109	PRO	2.3
2	B	843	PHE	2.3
2	B	1134	LEU	2.3
1	A	139	GLN	2.3
2	B	721	ALA	2.3
2	B	845	GLU	2.2
1	A	43	TRP	2.2
1	A	932	ILE	2.2
2	B	632	TYR	2.2
1	A	170	HIS	2.2
1	A	1219	GLN	2.2
1	A	1225	SER	2.2
2	B	108	PHE	2.2
1	A	146	SER	2.2
1	A	681	LEU	2.2
1	A	566	ILE	2.2
2	B	35	VAL	2.2
2	B	1133	GLN	2.1
2	B	491	ARG	2.1
1	A	1239	LEU	2.1
2	B	1116	VAL	2.1
2	B	199	THR	2.1
1	A	137	VAL	2.1
1	A	323	LEU	2.1
1	A	73	TYR	2.1
2	B	822	SER	2.1
2	B	481	PHE	2.1
1	A	755	THR	2.1
1	A	560	GLU	2.1
1	A	1199	GLN	2.1
1	A	694	THR	2.1
2	B	710	ILE	2.1
2	B	1057	GLN	2.1
1	A	182	SER	2.0
2	B	850	VAL	2.0
1	A	492	GLU	2.0
2	B	889	PHE	2.0
2	B	151	ARG	2.0
2	B	1068	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1240	GLN	2.0
2	B	69	LEU	2.0

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

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. 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
3	ZN	A	1297	1/1	0.75	0.43	550,550,550,550	0
4	CA	A	1298	1/1	0.84	0.12	169,169,169,169	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.