Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 11:53 AM EDT

PDB ID	:	5VID
Title	:	Receptor binding domain of BoNT/B in complex with mini-protein binder Bot.0671.2
Authors	:	Jin, R.; Lam, K.; Yao, G.
Deposited on	:	2017-04-15
Resolution	:	2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

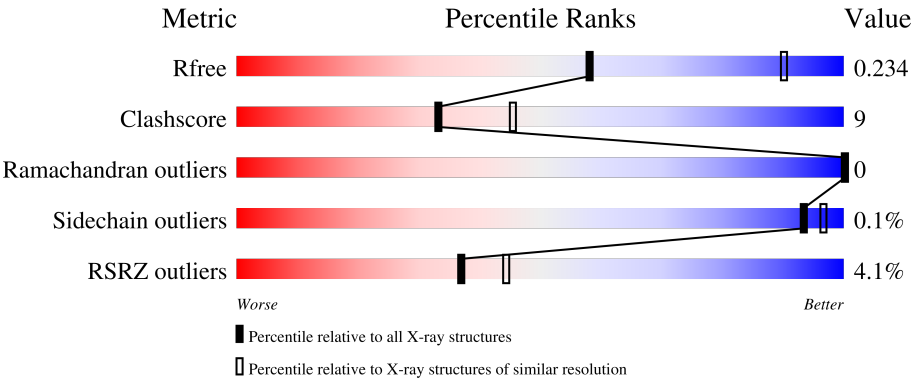
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	438	2% 80% 15% 5%
1	B	438	% 77% 17% 6%
1	C	438	3% 80% 17% .
1	D	438	% 81% 15% .
1	E	438	8% 74% 18% 8%

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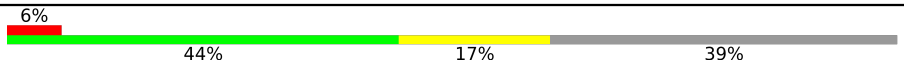
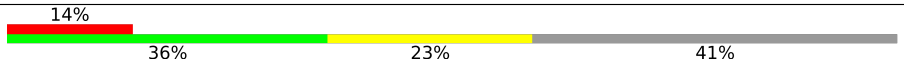
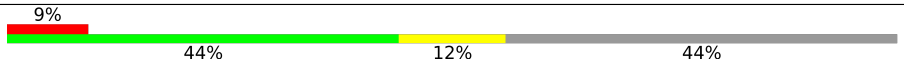
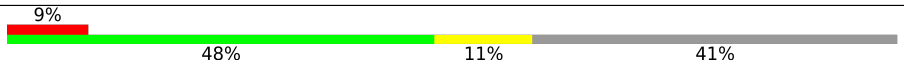
Mol	Chain	Length	Quality of chain
2	F	66	
2	G	66	
2	H	66	
2	I	66	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19064 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 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	420	Total	C	N	O	S	0	2	0
			3596	2326	587	675	8			
1	B	412	Total	C	N	O	S	0	1	0
			3527	2278	578	663	8			
1	C	426	Total	C	N	O	S	0	2	0
			3631	2342	596	685	8			
1	A	415	Total	C	N	O	S	0	2	0
			3543	2294	577	664	8			
1	E	405	Total	C	N	O	S	0	2	0
			3442	2233	560	641	8			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	854	GLY	-	expression tag	UNP P10844
D	855	PRO	-	expression tag	UNP P10844
D	856	LEU	-	expression tag	UNP P10844
D	857	GLY	-	expression tag	UNP P10844
D	858	SER	-	expression tag	UNP P10844
B	854	GLY	-	expression tag	UNP P10844
B	855	PRO	-	expression tag	UNP P10844
B	856	LEU	-	expression tag	UNP P10844
B	857	GLY	-	expression tag	UNP P10844
B	858	SER	-	expression tag	UNP P10844
C	854	GLY	-	expression tag	UNP P10844
C	855	PRO	-	expression tag	UNP P10844
C	856	LEU	-	expression tag	UNP P10844
C	857	GLY	-	expression tag	UNP P10844
C	858	SER	-	expression tag	UNP P10844
A	854	GLY	-	expression tag	UNP P10844
A	855	PRO	-	expression tag	UNP P10844
A	856	LEU	-	expression tag	UNP P10844
A	857	GLY	-	expression tag	UNP P10844

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Chain	Residue	Modelled	Actual	Comment	Reference
A	858	SER	-	expression tag	UNP P10844
E	854	GLY	-	expression tag	UNP P10844
E	855	PRO	-	expression tag	UNP P10844
E	856	LEU	-	expression tag	UNP P10844
E	857	GLY	-	expression tag	UNP P10844
E	858	SER	-	expression tag	UNP P10844

- Molecule 2 is a protein called Bot.0671.2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	40	Total C N O S 336 213 60 62 1	0	1	0
2	G	39	Total C N O 318 202 59 57	0	0	0
2	H	37	Total C N O 282 180 50 52	0	0	0
2	I	39	Total C N O 315 198 59 58	0	0	0

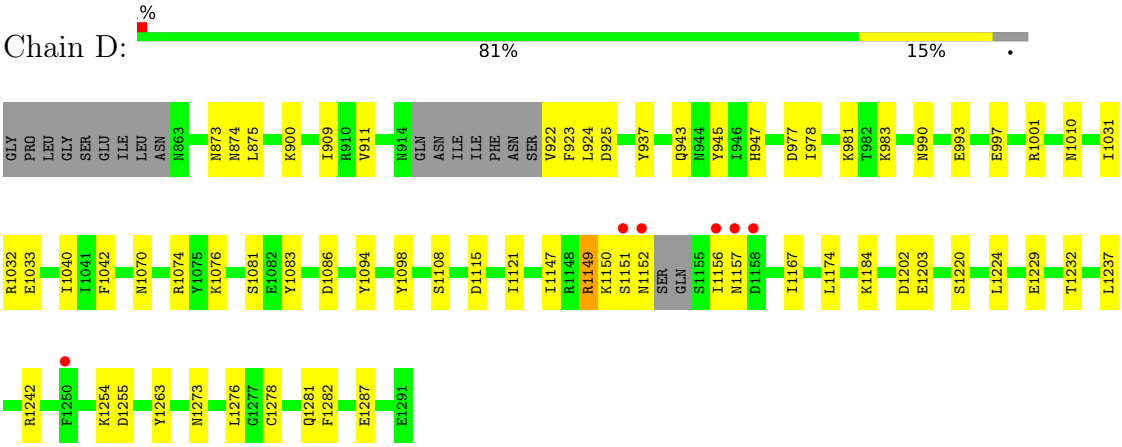
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	25	Total O 25 25	0	0
3	B	11	Total O 11 11	0	0
3	C	15	Total O 15 15	0	0
3	A	22	Total O 22 22	0	0
3	E	1	Total O 1 1	0	0

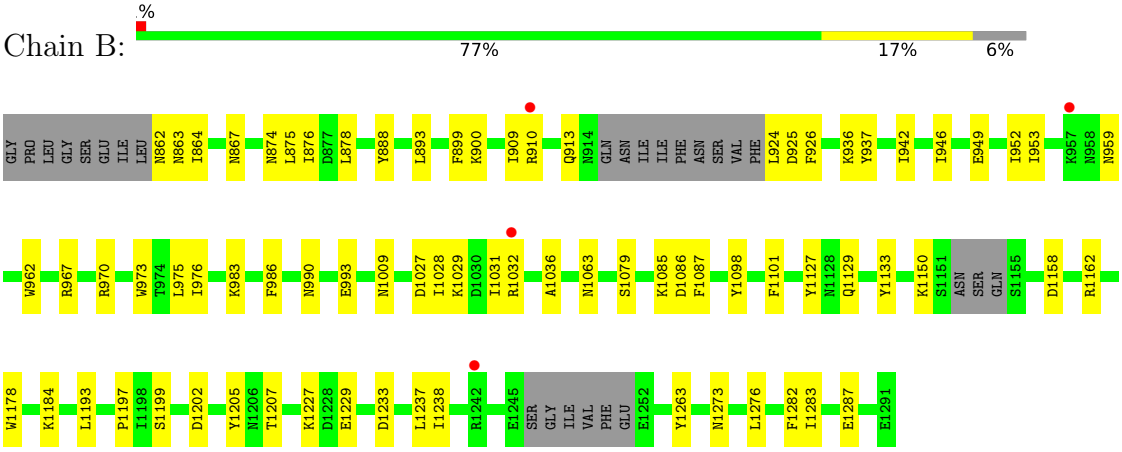
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

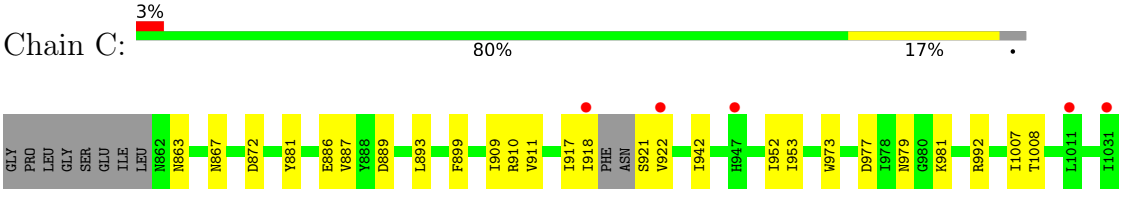
• Molecule 1: Botulinum neurotoxin type B

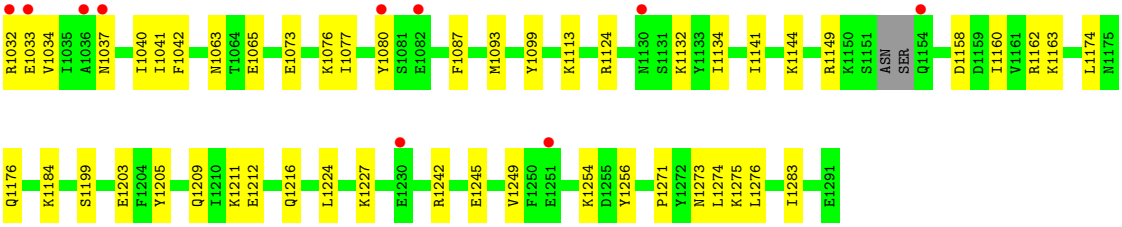


• Molecule 1: Botulinum neurotoxin type B



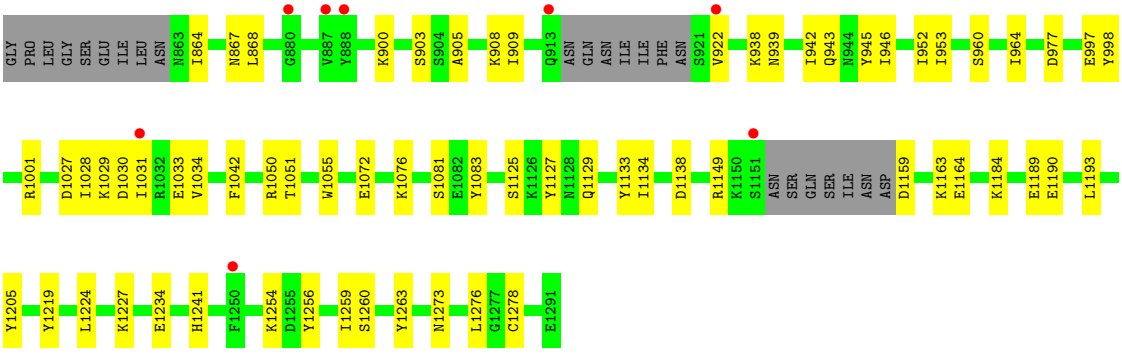
• Molecule 1: Botulinum neurotoxin type B





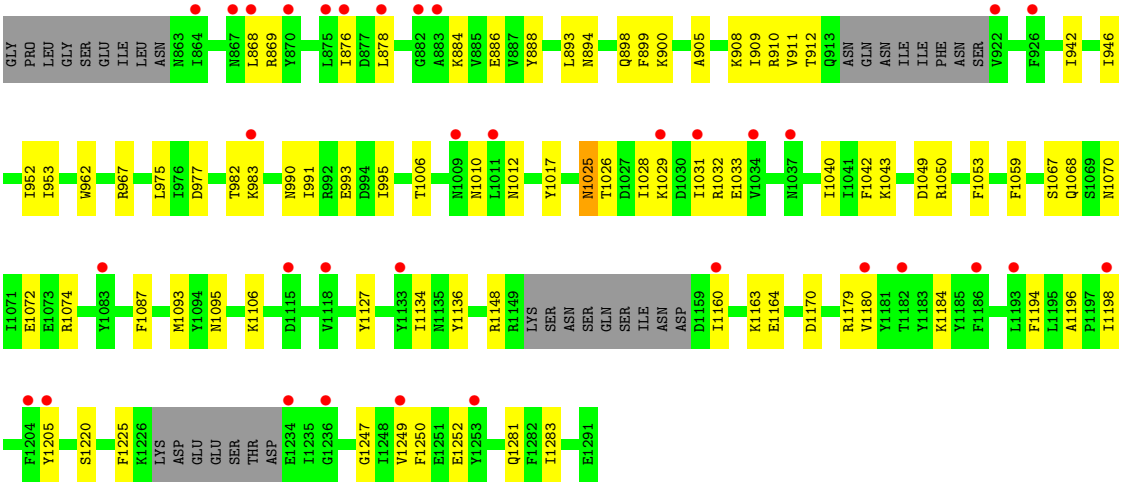
• Molecule 1: Botulinum neurotoxin type B

Chain A:



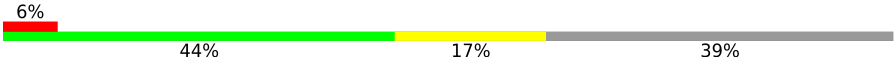
• Molecule 1: Botulinum neurotoxin type B

Chain E:



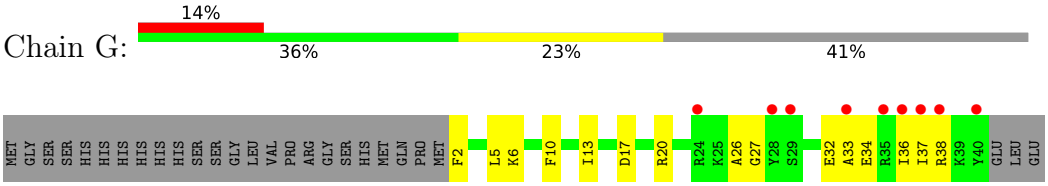
• Molecule 2: Bot.0671.2

Chain F:



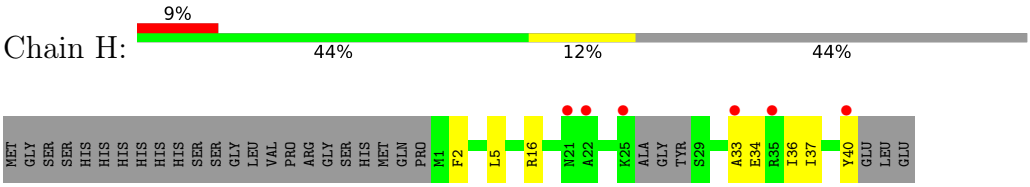
• Molecule 2: Bot.0671.2

Chain G:



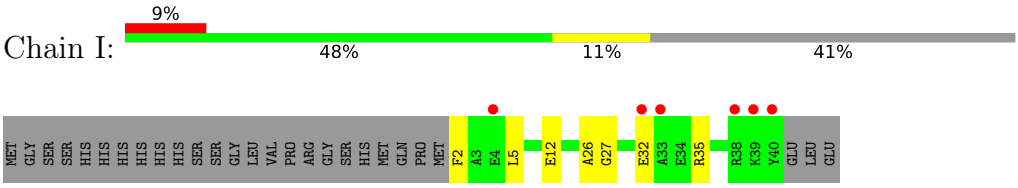
• Molecule 2: Bot.0671.2

Chain H:



• Molecule 2: Bot.0671.2

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	140.89Å 87.31Å 148.46Å 90.00° 114.53° 90.00°	Depositor
Resolution (Å)	67.53 – 2.75 67.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (67.53-2.75) 99.9 (67.53-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.219 , 0.232 0.222 , 0.234	Depositor DCC
R_{free} test set	4279 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19064	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.52	0/3627	0.65	0/4888
1	B	0.50	0/3609	0.67	0/4861
1	C	0.51	0/3714	0.66	0/5006
1	D	0.60	0/3681	0.70	0/4960
1	E	0.35	0/3524	0.58	0/4753
2	F	0.44	0/343	0.65	0/454
2	G	0.39	0/322	0.58	0/427
2	H	0.47	0/284	0.62	0/378
2	I	0.39	0/318	0.59	0/421
All	All	0.50	0/19422	0.65	0/26148

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	3543	0	3452	70	0
1	B	3527	0	3438	58	0
1	C	3631	0	3536	64	0
1	D	3596	0	3503	59	0
1	E	3442	0	3334	64	0
2	F	336	0	339	7	0
2	G	318	0	317	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	282	0	267	5	0
2	I	315	0	314	5	0
3	A	22	0	0	0	0
3	B	11	0	0	0	0
3	C	15	0	0	1	0
3	D	25	0	0	2	0
3	E	1	0	0	0	0
All	All	19064	0	18500	323	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 9.

All (323) 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:1184:LYS:HE3	1:A:1205:TYR:CE1	1.82	1.13
1:D:983:LYS:HG2	1:D:1031:ILE:HD11	1.29	1.13
1:A:942:ILE:HG12	1:A:1134:ILE:CD1	1.83	1.07
1:A:942:ILE:HG12	1:A:1134:ILE:HD11	1.13	1.07
1:E:1170:ASP:OD1	1:E:1179:ARG:HG2	1.54	1.06
1:E:1249:VAL:HG12	1:E:1250:PHE:CD2	1.90	1.05
1:D:1094:TYR:CE2	1:D:1149:ARG:NH1	2.24	1.04
1:E:1249:VAL:HG12	1:E:1250:PHE:HD2	1.20	1.04
1:E:908:LYS:HE2	1:E:1043:LYS:HD2	1.40	1.03
1:A:939:ASN:O	1:A:942:ILE:HD12	1.65	0.95
1:E:1028:ILE:O	1:E:1031:ILE:HG22	1.69	0.91
1:E:977:ASP:HB2	1:E:1033:GLU:O	1.71	0.90
1:E:977:ASP:OD2	1:E:1031:ILE:O	1.90	0.88
1:A:1184:LYS:HE3	1:A:1205:TYR:CZ	2.10	0.87
1:D:983:LYS:CG	1:D:1031:ILE:HD11	2.04	0.86
1:A:942:ILE:CG1	1:A:1134:ILE:HD11	2.04	0.84
1:B:864:ILE:HD11	1:B:867:ASN:HB3	1.61	0.82
1:A:997:GLU:OE2	1:A:998:TYR:CE2	2.39	0.76
1:A:938:LYS:NZ	1:A:1051:THR:HG21	2.02	0.75
1:A:1184:LYS:CE	1:A:1205:TYR:CE1	2.67	0.74
1:A:939:ASN:O	1:A:942:ILE:CD1	2.35	0.74
1:B:983:LYS:HG3	1:B:1028:ILE:HG22	1.70	0.74
1:A:1133:TYR:HB2	1:A:1134:ILE:HD12	1.70	0.73
1:C:918:ILE:HB	1:C:1063:ASN:OD1	1.90	0.71
1:A:1273:ASN:HB3	1:A:1276:LEU:HG	1.71	0.71
1:B:1199:SER:HB3	2:H:2:PHE:CE1	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:THR:O	1:A:1051:THR:HG22	1.89	0.71
1:C:881:TYR:CD2	1:C:917:ILE:HG22	2.25	0.70
1:E:1012:ASN:HB3	1:E:1029:LYS:HG2	1.72	0.70
1:C:1158:ASP:OD2	1:C:1162:ARG:NH2	2.24	0.70
2:I:32:GLU:HA	2:I:35:ARG:HD3	1.73	0.70
1:E:977:ASP:CB	1:E:1033:GLU:O	2.39	0.70
1:D:1174:LEU:HD21	1:A:1050:ARG:O	1.92	0.69
1:E:1028:ILE:O	1:E:1031:ILE:CG2	2.40	0.69
1:C:1076:LYS:HE2	1:C:1216:GLN:OE1	1.93	0.69
1:C:1245:GLU:OE1	1:C:1254:LYS:HG2	1.93	0.68
1:E:995:ILE:HG13	1:E:1106:LYS:HB2	1.75	0.68
2:G:17:ASP:OD1	2:G:20:ARG:NH2	2.26	0.68
1:D:1031:ILE:HG22	1:D:1032:ARG:N	2.07	0.68
1:A:1189:GLU:HG3	1:A:1190:GLU:OE1	1.94	0.68
1:A:864:ILE:HG21	1:A:867:ASN:ND2	2.10	0.67
1:A:1125:SER:OG	1:A:1138:ASP:OD2	2.09	0.67
1:A:1149:ARG:HH21	1:A:1159:ASP:HB3	1.60	0.67
1:B:942:ILE:HG13	1:B:946:ILE:HD12	1.77	0.66
1:E:908:LYS:HE2	1:E:1043:LYS:CD	2.23	0.66
1:B:973:TRP:HE1	1:B:975:LEU:HD11	1.59	0.66
1:A:1184:LYS:HE3	1:A:1205:TYR:HE1	1.55	0.65
1:B:924:LEU:HD12	1:B:924:LEU:O	1.96	0.65
1:C:921:SER:HB2	1:C:1037:ASN:ND2	2.12	0.65
1:A:942:ILE:CG1	1:A:1134:ILE:CD1	2.70	0.65
1:E:946:ILE:O	1:E:967:ARG:NH2	2.30	0.65
1:B:990:ASN:HD22	1:B:993:GLU:HG3	1.61	0.65
1:E:1163:LYS:HG2	1:E:1164:GLU:HG2	1.79	0.65
1:D:978:ILE:HG23	1:D:1033:GLU:O	1.96	0.64
1:E:1025:ASN:HD22	1:E:1026:THR:N	1.93	0.64
1:D:1150:LYS:HG2	1:D:1229:GLU:OE2	1.98	0.63
1:D:1149:ARG:CZ	3:D:1303:HOH:O	2.47	0.62
1:B:1158:ASP:OD2	1:B:1162:ARG:NH2	2.32	0.62
1:A:938:LYS:HZ3	1:A:1051:THR:HG21	1.64	0.62
1:E:869:ARG:HB2	1:E:878:LEU:HD13	1.80	0.62
1:D:1273:ASN:HB3	1:D:1276:LEU:HG	1.83	0.61
2:H:16:ARG:NH2	2:H:34:GLU:OE2	2.34	0.61
1:C:881:TYR:CE2	1:C:917:ILE:HG22	2.37	0.60
1:D:1149:ARG:HB3	1:D:1151:SER:O	2.02	0.59
1:D:1149:ARG:HH21	1:C:1077:ILE:HG12	1.67	0.59
1:E:962:TRP:HB3	1:E:975:LEU:HD23	1.84	0.59
1:A:1027:ASP:OD1	1:A:1029:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:GLN:NE2	1:B:1036:ALA:O	2.36	0.58
1:E:876:ILE:HG13	1:E:878:LEU:CD1	2.33	0.58
1:D:937:TYR:HB3	1:D:945:TYR:CD1	2.38	0.58
1:E:884:LYS:N	1:E:912:THR:O	2.34	0.58
1:E:1049:ASP:OD1	1:E:1050:ARG:N	2.36	0.58
1:A:903:SER:OG	1:A:1050:ARG:HG3	2.03	0.58
1:C:979:ASN:OD1	1:C:981:LYS:NZ	2.36	0.58
2:G:26:ALA:N	2:G:27:GLY:HA2	2.17	0.58
1:D:900:LYS:NZ	1:D:1287:GLU:OE2	2.29	0.57
1:B:949:GLU:HB2	1:B:967:ARG:HE	1.68	0.57
1:D:1156:ILE:HG22	1:D:1157:ASN:N	2.18	0.57
1:B:990:ASN:ND2	1:B:993:GLU:HG3	2.18	0.57
1:E:1012:ASN:CG	1:E:1029:LYS:HA	2.25	0.57
1:C:909:ILE:HG22	1:C:910:ARG:N	2.20	0.57
1:E:1247:GLY:HA3	1:E:1252:GLU:OE1	2.05	0.57
1:E:884:LYS:HB3	1:E:912:THR:HB	1.87	0.56
1:E:1012:ASN:HB3	1:E:1029:LYS:CG	2.34	0.56
1:D:1157:ASN:CB	1:C:867:ASN:HD21	2.17	0.56
1:D:1149:ARG:NH2	3:D:1303:HOH:O	2.37	0.56
1:A:997:GLU:HA	1:A:1001:ARG:NH1	2.21	0.56
1:A:1001:ARG:HH21	1:A:1219:TYR:HD2	1.53	0.56
1:E:1067:SER:OG	1:E:1070:ASN:OD1	2.17	0.56
1:B:888:TYR:OH	1:B:910:ARG:NH2	2.39	0.55
1:C:992:ARG:NH2	1:C:1132:LYS:O	2.40	0.55
1:E:1068[A]:GLN:NE2	1:E:1072:GLU:OE1	2.40	0.55
2:H:33:ALA:O	2:H:37:ILE:HG13	2.07	0.55
1:C:1113:LYS:NZ	2:I:12:GLU:OE2	2.37	0.55
1:C:886:GLU:HB2	1:C:910:ARG:HB3	1.89	0.55
1:A:997:GLU:HA	1:A:1001:ARG:HH11	1.71	0.54
2:H:36:ILE:CG2	2:H:40:TYR:CZ	2.90	0.54
1:B:1184:LYS:HD2	1:B:1205:TYR:CZ	2.43	0.54
1:A:945:TYR:CD2	1:A:946:ILE:CD1	2.90	0.54
1:E:869:ARG:HG3	1:E:878:LEU:HD22	1.89	0.54
1:E:909:ILE:HB	1:E:1042:PHE:HB2	1.90	0.54
1:C:1076:LYS:O	1:C:1080:TYR:CE1	2.60	0.54
1:A:864:ILE:HG21	1:A:867:ASN:HD21	1.72	0.54
1:D:1151:SER:HB3	1:C:1073:GLU:HG3	1.90	0.54
1:B:874:ASN:OD1	1:B:875:LEU:N	2.35	0.53
1:B:975:LEU:HD11	1:B:1009:ASN:OD1	2.08	0.53
1:E:1093:MET:SD	1:E:1160:ILE:HG12	2.49	0.53
1:B:1101:PHE:HB2	1:B:1283:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ILE:HG13	1:A:953:ILE:HG13	1.91	0.53
1:A:997:GLU:OE2	1:A:998:TYR:HE2	1.91	0.53
1:C:1254:LYS:HG3	1:C:1256:TYR:CE1	2.43	0.53
2:F:33:ALA:O	2:F:37:ILE:HG13	2.08	0.53
1:D:1202:ASP:HA	1:B:1032:ARG:HH21	1.73	0.53
2:I:26:ALA:N	2:I:27:GLY:HA2	2.22	0.53
1:C:911:VAL:HB	1:C:1040:ILE:HB	1.91	0.53
1:A:945:TYR:HD2	1:A:946:ILE:CD1	2.22	0.53
1:C:909:ILE:HG22	1:C:910:ARG:H	1.72	0.53
1:C:1245:GLU:HG2	1:C:1249:VAL:HG11	1.89	0.53
1:A:1163:LYS:HG2	1:A:1164:GLU:HG2	1.90	0.53
1:E:952:ILE:HG13	1:E:953:ILE:HG13	1.91	0.53
1:D:1094:TYR:HE2	1:D:1149:ARG:HH12	1.54	0.53
1:A:1051:THR:O	1:A:1051:THR:CG2	2.56	0.53
1:E:942:ILE:HD11	1:E:1134:ILE:HD13	1.89	0.52
1:E:1127:TYR:CE2	1:E:1134:ILE:HD11	2.44	0.52
1:C:1093:MET:SD	1:C:1160:ILE:HG12	2.49	0.52
1:C:1273:ASN:HB3	1:C:1276:LEU:HG	1.91	0.52
1:A:909:ILE:HB	1:A:1042:PHE:HB2	1.91	0.52
1:E:1127:TYR:CZ	1:E:1134:ILE:HD11	2.44	0.52
1:C:1245:GLU:OE1	1:C:1254:LYS:CG	2.55	0.52
1:D:1151:SER:O	1:D:1152:ASN:HB2	2.08	0.51
1:E:1127:TYR:HB2	1:E:1136:TYR:CE2	2.45	0.51
2:F:4[A]:GLU:OE2	2:F:40:TYR:OH	2.28	0.51
1:E:884:LYS:HE2	1:E:886:GLU:OE2	2.10	0.51
1:B:946:ILE:HD13	1:B:1133:TYR:CD2	2.45	0.51
1:C:1132:LYS:O	1:C:1132:LYS:HG3	2.10	0.51
1:A:1184:LYS:HG2	1:A:1205:TYR:CE1	2.45	0.51
2:H:2:PHE:O	2:H:5:LEU:N	2.44	0.51
1:D:990:ASN:HB3	1:D:993:GLU:HG2	1.92	0.51
1:A:938:LYS:HZ1	1:A:1051:THR:HG21	1.74	0.51
1:B:1150:LYS:NZ	1:B:1207:THR:OG1	2.32	0.51
1:C:921:SER:HB2	1:C:1037:ASN:HD22	1.75	0.51
1:E:1006:THR:HB	1:E:1017:TYR:HB2	1.93	0.50
1:D:1031:ILE:HG22	1:D:1032:ARG:H	1.75	0.50
1:D:1242:ARG:HG2	1:D:1255:ASP:OD1	2.12	0.50
1:D:909:ILE:HB	1:D:1042:PHE:HB2	1.92	0.50
1:C:1124:ARG:HG2	1:C:1141:ILE:HD11	1.94	0.50
1:A:1184:LYS:HG2	1:A:1205:TYR:CZ	2.47	0.50
1:D:1031:ILE:CG2	1:D:1032:ARG:N	2.73	0.50
1:A:942:ILE:O	1:A:946:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:905:ALA:O	1:E:908:LYS:HE3	2.12	0.49
1:C:1274:LEU:HD12	1:C:1274:LEU:C	2.32	0.49
1:D:1156:ILE:CG2	1:D:1157:ASN:N	2.75	0.49
1:B:952:ILE:HG13	1:B:953:ILE:HG13	1.94	0.49
1:C:1099:TYR:CZ	1:C:1144:LYS:HD3	2.47	0.49
1:B:862:ASN:OD1	1:B:863:ASN:N	2.45	0.49
1:A:922:VAL:HG13	1:A:1034:VAL:O	2.12	0.49
1:E:894:ASN:HD21	1:E:898:GLN:HB2	1.77	0.49
1:A:1263:TYR:CD2	1:A:1278:CYS:HB3	2.48	0.48
1:A:945:TYR:CD2	1:A:946:ILE:HD13	2.48	0.48
2:G:33:ALA:O	2:G:37:ILE:HG13	2.13	0.48
1:C:1174:LEU:O	1:C:1176:GLN:HG3	2.13	0.48
1:C:1254:LYS:HG3	1:C:1256:TYR:HE1	1.77	0.48
1:A:1224:LEU:HD11	1:A:1234:GLU:HB3	1.95	0.48
1:E:876:ILE:HG13	1:E:878:LEU:HD11	1.95	0.48
1:E:888:TYR:OH	1:E:910:ARG:NH2	2.47	0.48
1:D:1232:THR:HG22	1:D:1232:THR:O	2.13	0.48
1:B:1227:LYS:NZ	1:B:1233:ASP:OD2	2.36	0.48
1:C:1149:ARG:NH2	1:C:1158:ASP:O	2.44	0.48
1:D:873:ASN:ND2	1:C:872:ASP:OD1	2.37	0.48
1:D:943[B]:GLN:O	1:D:947:HIS:ND1	2.27	0.48
1:A:938:LYS:NZ	1:A:1051:THR:CG2	2.76	0.48
1:E:1012:ASN:OD1	1:E:1029:LYS:HA	2.14	0.48
1:D:923:PHE:HE1	1:D:1033:GLU:HA	1.79	0.47
1:B:1193:LEU:HD11	1:B:1238:ILE:HG23	1.95	0.47
1:A:1081:SER:HB2	1:A:1083:TYR:CE2	2.48	0.47
2:F:2:PHE:HE2	2:F:6:LYS:HE3	1.79	0.47
1:D:1070:ASN:OD1	1:D:1074:ARG:NH1	2.44	0.47
1:B:1087:PHE:CB	1:B:1283:ILE:HG12	2.44	0.47
1:D:1115:ASP:OD1	1:A:905:ALA:HB2	2.14	0.47
1:D:1151:SER:CB	1:C:1073:GLU:HG3	2.45	0.47
1:C:981:LYS:HZ1	1:C:1032:ARG:HG3	1.79	0.47
1:B:924:LEU:HD12	1:B:924:LEU:C	2.34	0.47
1:B:986:PHE:CZ	1:C:1271:PRO:HD2	2.49	0.47
1:B:1127:TYR:CZ	1:B:1129:GLN:HB2	2.50	0.47
1:D:1108:SER:HB3	1:D:1121:ILE:CG2	2.45	0.47
1:B:1079:SER:O	1:B:1085:LYS:NZ	2.48	0.47
1:D:1149:ARG:NH2	1:C:1077:ILE:HG12	2.30	0.46
1:C:1087:PHE:CB	1:C:1283:ILE:HG12	2.44	0.46
1:D:923:PHE:CE1	1:D:1033:GLU:HA	2.50	0.46
1:C:1184:LYS:HG3	1:C:1203:GLU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1008:THR:HB	1:C:1065:GLU:HG3	1.97	0.46
1:B:959:ASN:O	1:B:976:ILE:CG2	2.63	0.46
1:E:1087:PHE:CB	1:E:1283:ILE:HG12	2.45	0.46
2:G:10:PHE:HA	2:G:13:ILE:HG12	1.98	0.46
1:E:991:ILE:HD12	1:E:1134:ILE:HG22	1.98	0.46
1:E:1070:ASN:HD22	1:E:1074:ARG:HH22	1.64	0.46
1:D:1202:ASP:OD1	1:B:1032:ARG:NE	2.39	0.46
1:D:925:ASP:OD1	1:D:1010:ASN:HA	2.16	0.46
1:C:1274:LEU:HD12	1:C:1275:LYS:HG2	1.98	0.46
1:A:1241:HIS:HE1	1:A:1260:SER:CB	2.29	0.46
1:D:922:VAL:HG12	1:D:924:LEU:HG	1.98	0.46
1:D:1081:SER:HB2	1:D:1083:TYR:CE2	2.51	0.46
1:D:1254:LYS:HE2	1:D:1254:LYS:HB3	1.66	0.46
1:B:925:ASP:O	1:B:926:PHE:HB3	2.16	0.46
1:B:1086:ASP:HB2	1:B:1282:PHE:O	2.16	0.46
1:D:943[A]:GLN:O	1:D:947:HIS:ND1	2.27	0.45
1:C:922:VAL:HG11	1:C:1033:GLU:HG2	1.97	0.45
1:C:1205:TYR:CZ	1:C:1227:LYS:HG2	2.51	0.45
1:B:878:LEU:HG	1:B:878:LEU:O	2.16	0.45
1:A:1028:ILE:O	1:A:1031:ILE:HG22	2.16	0.45
1:E:893:LEU:HD23	1:E:899:PHE:HB3	1.98	0.45
1:D:997:GLU:HA	1:D:1001:ARG:HH11	1.82	0.45
1:A:1127:TYR:CZ	1:A:1129:GLN:HB2	2.50	0.45
1:E:900:LYS:HE3	1:E:1053:PHE:CD1	2.52	0.45
1:B:986:PHE:HZ	1:C:1271:PRO:HD2	1.80	0.45
1:A:942:ILE:HG21	1:A:1134:ILE:HD11	1.98	0.45
1:A:997:GLU:OE1	1:A:997:GLU:N	2.49	0.45
1:B:1028:ILE:HB	1:B:1031:ILE:CG1	2.47	0.45
1:C:1163:LYS:HE2	1:C:1212:GLU:HB3	1.99	0.45
1:A:1241:HIS:HE1	1:A:1260:SER:OG	2.00	0.45
1:B:893:LEU:HD23	1:B:899:PHE:HB3	1.98	0.45
1:B:1027:ASP:OD1	1:B:1029:LYS:HG3	2.17	0.45
1:B:1273:ASN:HB3	1:B:1276:LEU:HG	1.99	0.45
1:C:1245:GLU:OE1	1:C:1254:LYS:CD	2.65	0.44
2:G:5:LEU:HD23	2:G:5:LEU:HA	1.81	0.44
1:D:874:ASN:OD1	1:D:875:LEU:N	2.47	0.44
1:B:926:PHE:HZ	1:B:975:LEU:HD21	1.82	0.44
1:B:1150:LYS:HE2	1:B:1229:GLU:OE2	2.16	0.44
1:B:863:ASN:HB3	1:B:1063:ASN:OD1	2.17	0.44
1:C:1209:GLN:OE1	1:C:1211:LYS:NZ	2.38	0.44
2:F:26:ALA:N	2:F:27:GLY:HA2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:LYS:HE3	1:A:1205:TYR:OH	2.16	0.44
1:E:1249:VAL:O	1:E:1250:PHE:CD2	2.70	0.44
1:E:1025:ASN:HD22	1:E:1025:ASN:C	2.20	0.44
1:E:1184:LYS:HA	1:E:1205:TYR:CE2	2.52	0.44
1:B:962:TRP:HB3	1:B:975:LEU:HD23	1.99	0.44
1:C:942:ILE:HD11	1:C:1134:ILE:HD13	2.00	0.44
1:E:911:VAL:HB	1:E:1040:ILE:HB	1.99	0.44
1:A:900:LYS:HD2	1:A:1055:TRP:CZ2	2.53	0.44
1:E:1194:PHE:CE2	1:E:1196:ALA:HB2	2.53	0.44
1:A:1072:GLU:HG2	1:A:1076:LYS:HE3	1.99	0.44
1:E:1220:SER:HA	1:E:1281:GLN:HG2	1.99	0.44
1:D:1224:LEU:HA	1:D:1237:LEU:HD23	1.99	0.44
1:C:977:ASP:HA	1:C:1034:VAL:HG22	2.00	0.43
1:B:1229:GLU:OE1	1:B:1229:GLU:N	2.48	0.43
1:A:1189:GLU:CG	1:A:1190:GLU:OE1	2.65	0.43
1:B:1098:TYR:CG	1:B:1282:PHE:HB3	2.54	0.43
1:C:909:ILE:HB	1:C:1042:PHE:HB2	2.00	0.43
1:A:977:ASP:HA	1:A:1033:GLU:O	2.18	0.43
1:A:1205:TYR:CZ	1:A:1227:LYS:HG2	2.53	0.43
1:E:990:ASN:HD21	1:E:993:GLU:HG3	1.83	0.43
1:D:911:VAL:HB	1:D:1040:ILE:HB	2.00	0.43
1:A:942:ILE:CD1	1:A:1134:ILE:HD13	2.48	0.43
1:E:1010:ASN:OD1	1:E:1012:ASN:N	2.42	0.43
1:D:1220:SER:HA	1:D:1281:GLN:HG2	2.00	0.43
1:A:1193:LEU:HD21	1:A:1259:ILE:HB	2.01	0.43
1:D:983:LYS:HG2	1:D:1031:ILE:CD1	2.22	0.43
1:B:1129:GLN:O	1:C:1242:ARG:HD3	2.19	0.43
1:C:1205:TYR:CE1	1:C:1227:LYS:HA	2.53	0.43
1:A:1254:LYS:HG3	1:A:1256:TYR:CE1	2.54	0.43
1:B:1184:LYS:NZ	1:B:1202:ASP:O	2.50	0.42
1:A:977:ASP:HB3	1:A:1031:ILE:HG13	2.01	0.42
1:D:1086:ASP:HB2	1:D:1282:PHE:O	2.19	0.42
1:B:936:LYS:HG2	1:B:937:TYR:O	2.18	0.42
1:A:1241:HIS:CE1	1:A:1260:SER:HB2	2.54	0.42
1:A:868:LEU:HD23	1:A:868:LEU:HA	1.83	0.42
1:B:900:LYS:NZ	1:B:1287:GLU:OE2	2.46	0.42
1:D:1076:LYS:HE2	1:D:1076:LYS:HB3	1.79	0.42
1:B:875:LEU:O	1:B:876:ILE:HD13	2.19	0.42
1:C:1199:SER:HB3	2:I:2:PHE:CE1	2.54	0.42
1:C:953:ILE:HA	1:C:1041:ILE:O	2.20	0.42
1:E:868:LEU:HA	1:E:868:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:LEU:HD12	1:B:909:ILE:HD13	2.00	0.42
1:B:924:LEU:O	1:B:924:LEU:CD1	2.66	0.42
1:C:1211:LYS:HZ3	1:C:1224:LEU:HD23	1.85	0.42
1:E:908:LYS:HA	1:E:1042:PHE:O	2.20	0.42
1:B:936:LYS:HE2	1:B:937:TYR:CE1	2.54	0.41
1:B:970:ARG:HG3	1:B:986:PHE:CD1	2.55	0.41
1:C:889:ASP:CG	3:C:1301:HOH:O	2.57	0.41
1:C:981:LYS:NZ	1:C:1032:ARG:HG3	2.35	0.41
1:D:977:ASP:OD2	1:D:981:LYS:HB3	2.19	0.41
1:D:1147:ILE:HG23	1:D:1167:ILE:HD12	2.01	0.41
1:D:1184:LYS:HG3	1:D:1203:GLU:C	2.41	0.41
1:C:952:ILE:HG13	1:C:953:ILE:HG13	2.02	0.41
1:C:887:VAL:HG11	1:C:893:LEU:HD11	2.01	0.41
1:A:1184:LYS:HG2	1:A:1205:TYR:CD1	2.55	0.41
1:E:982:THR:O	1:E:983:LYS:HD3	2.20	0.41
1:C:909:ILE:CG2	1:C:910:ARG:N	2.82	0.41
1:E:1012:ASN:HA	1:E:1028:ILE:HG13	2.01	0.41
2:F:23:LEU:O	2:F:27:GLY:HA2	2.19	0.41
2:G:32:GLU:O	2:G:36:ILE:HG13	2.20	0.41
2:I:5:LEU:HD23	2:I:5:LEU:HA	1.83	0.41
1:D:1202:ASP:HA	1:B:1032:ARG:NH2	2.34	0.41
1:C:973:TRP:CG	1:C:1007:ILE:HG21	2.56	0.41
1:C:909:ILE:CG2	1:C:910:ARG:H	2.34	0.41
2:F:11:LEU:CD2	2:F:37:ILE:HG23	2.50	0.41
1:A:1029:LYS:HG3	1:A:1030:ASP:OD1	2.21	0.41
1:D:937:TYR:HB3	1:D:945:TYR:CE1	2.55	0.41
1:D:1094:TYR:CZ	1:D:1149:ARG:NH1	2.85	0.41
1:B:942:ILE:CG1	1:B:946:ILE:HD12	2.47	0.41
1:C:863:ASN:OD1	1:C:863:ASN:N	2.53	0.41
1:C:973:TRP:CD2	1:C:1007:ILE:HG21	2.55	0.41
1:A:943[B]:GLN:H	1:A:943[B]:GLN:CD	2.24	0.41
1:A:960:SER:OG	1:A:977:ASP:O	2.37	0.41
2:G:2:PHE:HE2	2:G:6:LYS:HE3	1.85	0.41
1:D:1263:TYR:CG	1:D:1278:CYS:HB3	2.56	0.41
1:E:1031:ILE:HG23	1:E:1032:ARG:N	2.36	0.41
1:E:1095:ASN:OD1	1:E:1148:ARG:NH1	2.46	0.41
1:A:1050:ARG:HH11	1:A:1050:ARG:HD3	1.76	0.40
1:C:893:LEU:HD23	1:C:899:PHE:HB3	2.03	0.40
1:A:953:ILE:HD12	1:A:964:ILE:HD12	2.03	0.40
1:E:1042:PHE:HZ	1:E:1059:PHE:CD2	2.39	0.40
1:E:1179:ARG:CZ	1:E:1198:ILE:HG23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:LEU:HA	2:F:5:LEU:HD23	1.88	0.40
1:A:908:LYS:HA	1:A:1042:PHE:O	2.22	0.40
1:E:1017:TYR:HE2	1:E:1068[A]:GLN:HA	1.87	0.40
1:D:1031:ILE:CG2	1:D:1032:ARG:H	2.34	0.40
1:D:1098:TYR:CG	1:D:1282:PHE:HB3	2.56	0.40
1:B:1178:TRP:CE2	1:B:1197:PRO:HG3	2.56	0.40
1:B:1184:LYS:HD2	1:B:1205:TYR:CE1	2.57	0.40
1:B:1237:LEU:HD12	1:B:1263:TYR:CB	2.51	0.40
2:G:34:GLU:HG2	2:G:38:ARG:HH21	1.86	0.40
1:E:1180:VAL:O	1:E:1225:PHE:HZ	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	411/438 (94%)	397 (97%)	14 (3%)	0	100	100
1	B	405/438 (92%)	389 (96%)	16 (4%)	0	100	100
1	C	422/438 (96%)	409 (97%)	13 (3%)	0	100	100
1	D	416/438 (95%)	401 (96%)	15 (4%)	0	100	100
1	E	399/438 (91%)	386 (97%)	13 (3%)	0	100	100
2	F	39/66 (59%)	38 (97%)	1 (3%)	0	100	100
2	G	37/66 (56%)	36 (97%)	1 (3%)	0	100	100
2	H	33/66 (50%)	31 (94%)	2 (6%)	0	100	100
2	I	37/66 (56%)	34 (92%)	3 (8%)	0	100	100
All	All	2199/2454 (90%)	2121 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	389/411 (95%)	389 (100%)	0	100 100
1	B	389/411 (95%)	389 (100%)	0	100 100
1	C	400/411 (97%)	400 (100%)	0	100 100
1	D	396/411 (96%)	395 (100%)	1 (0%)	92 95
1	E	374/411 (91%)	373 (100%)	1 (0%)	92 95
2	F	32/54 (59%)	32 (100%)	0	100 100
2	G	29/54 (54%)	29 (100%)	0	100 100
2	H	24/54 (44%)	24 (100%)	0	100 100
2	I	29/54 (54%)	29 (100%)	0	100 100
All	All	2062/2271 (91%)	2060 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1149	ARG
1	E	1025	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	415/438 (94%)	0.11	8 (1%) 66 75	23, 46, 99, 124	0
1	B	412/438 (94%)	0.04	4 (0%) 82 87	31, 48, 87, 118	0
1	C	426/438 (97%)	0.11	15 (3%) 44 52	28, 50, 101, 127	0
1	D	420/438 (95%)	-0.07	6 (1%) 75 82	17, 34, 78, 127	0
1	E	405/438 (92%)	0.64	34 (8%) 11 13	51, 87, 124, 142	0
2	F	40/66 (60%)	0.49	4 (10%) 7 7	31, 64, 135, 146	0
2	G	39/66 (59%)	0.86	9 (23%) 0 0	34, 89, 127, 141	0
2	H	37/66 (56%)	0.94	6 (16%) 1 1	44, 80, 131, 146	0
2	I	39/66 (59%)	0.99	6 (15%) 2 2	43, 85, 128, 136	0
All	All	2233/2454 (90%)	0.21	92 (4%) 37 44	17, 54, 114, 146	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	40	TYR	5.5
1	E	1031	ILE	4.9
1	E	1180	VAL	4.8
2	G	38	ARG	4.7
1	A	1031	ILE	4.4
1	E	1249	VAL	4.3
1	D	1152	ASN	4.1
1	E	1198	ILE	4.1
1	D	1151	SER	4.0
1	B	1242	ARG	4.0
2	F	24	ARG	4.0
1	E	1037	ASN	3.9
1	A	880	GLY	3.6
2	I	40	TYR	3.4
2	G	37	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	882	GLY	3.3
1	A	913	GLN	3.3
1	C	922	VAL	3.3
1	E	1083	TYR	3.3
1	E	868	LEU	3.2
1	C	918	ILE	3.2
1	E	864	ILE	3.2
2	G	35	ARG	3.2
1	E	1133	TYR	3.2
2	I	4	GLU	3.1
1	A	1250	PHE	3.1
2	F	32	GLU	3.0
1	D	1156	ILE	3.0
1	C	1130	ASN	2.9
1	C	1080	TYR	2.9
1	C	1033	GLU	2.9
1	B	957	LYS	2.9
2	G	40	TYR	2.9
1	E	1205	TYR	2.8
1	A	1151	SER	2.8
1	C	1031	ILE	2.7
1	E	1186	PHE	2.7
1	C	1082	GLU	2.7
1	E	1204	PHE	2.6
2	G	33	ALA	2.6
1	C	1230	GLU	2.6
2	G	28	TYR	2.6
1	E	1193	LEU	2.6
1	E	1009	ASN	2.5
2	I	32	GLU	2.5
1	C	1037	ASN	2.5
1	E	878	LEU	2.5
1	E	1115	ASP	2.5
1	E	1118	VAL	2.5
2	H	33	ALA	2.4
2	I	33	ALA	2.4
1	D	1157	ASN	2.4
1	E	876	ILE	2.4
2	G	36	ILE	2.4
1	A	887	VAL	2.4
1	E	1029	LYS	2.3
2	F	28	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	1034	VAL	2.3
2	G	24	ARG	2.3
2	I	38	ARG	2.3
1	E	867	ASN	2.3
1	E	1011	LEU	2.3
2	H	21	ASN	2.3
1	A	922	VAL	2.3
1	C	1011	LEU	2.2
2	H	35	ARG	2.2
1	C	1036	ALA	2.2
1	E	1160	ILE	2.2
2	H	25	LYS	2.2
1	C	1251	GLU	2.2
1	E	1234	GLU	2.2
2	F	31	GLU	2.2
1	D	1158	ASP	2.2
2	H	22	ALA	2.2
1	D	1250	PHE	2.2
1	E	926	PHE	2.2
1	E	1253	TYR	2.2
1	E	1236	GLY	2.2
1	C	1032	ARG	2.2
1	E	922	VAL	2.1
1	E	883	ALA	2.1
1	C	947	HIS	2.1
1	E	875	LEU	2.1
1	B	910	ARG	2.1
1	A	888	TYR	2.1
2	I	39	LYS	2.1
1	C	1154	GLN	2.0
2	G	29	SER	2.0
1	E	870	TYR	2.0
1	E	1182	THR	2.0
1	B	1032	ARG	2.0
1	E	983	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.