



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:55 AM UTC

PDB ID : 3RMX / pdb_00003rmx
Title : Crystal structure of HCR/D F1240A mutant
Authors : Fu, Z.; Karalewitz, A.; Kroken, A.; Kim, J.-J.P.; Barbieri, J.T.
Deposited on : 2011-04-21
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

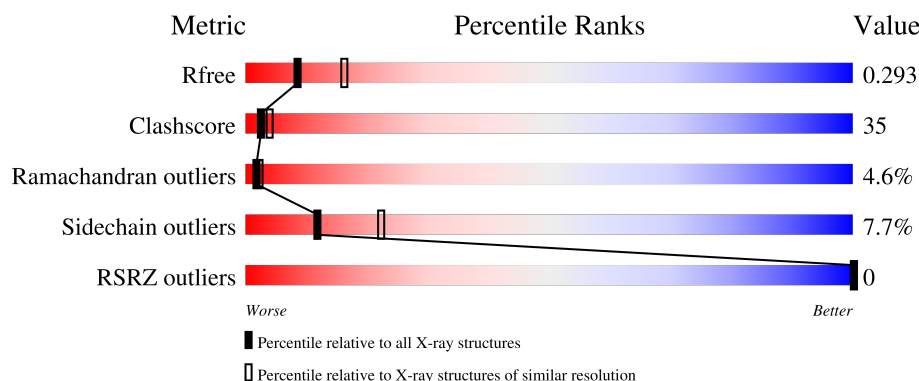
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

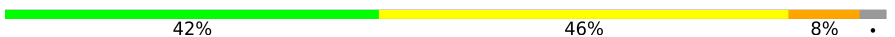
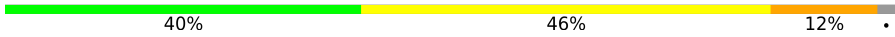
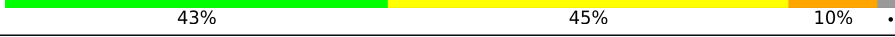
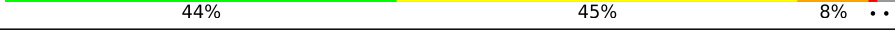
The reported resolution of this entry is 2.75 Å.

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	415	
1	B	415	
1	C	415	
1	D	415	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13363 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 D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3317	2119	548	640	10			
1	B	407	Total	C	N	O	S	0	0	0
			3336	2131	551	644	10			
1	C	403	Total	C	N	O	S	0	0	0
			3304	2111	547	636	10			
1	D	406	Total	C	N	O	S	0	0	0
			3333	2131	550	642	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	ALA	PHE	engineered mutation	UNP P19321
B	1240	ALA	PHE	engineered mutation	UNP P19321
C	1240	ALA	PHE	engineered mutation	UNP P19321
D	1240	ALA	PHE	engineered mutation	UNP P19321

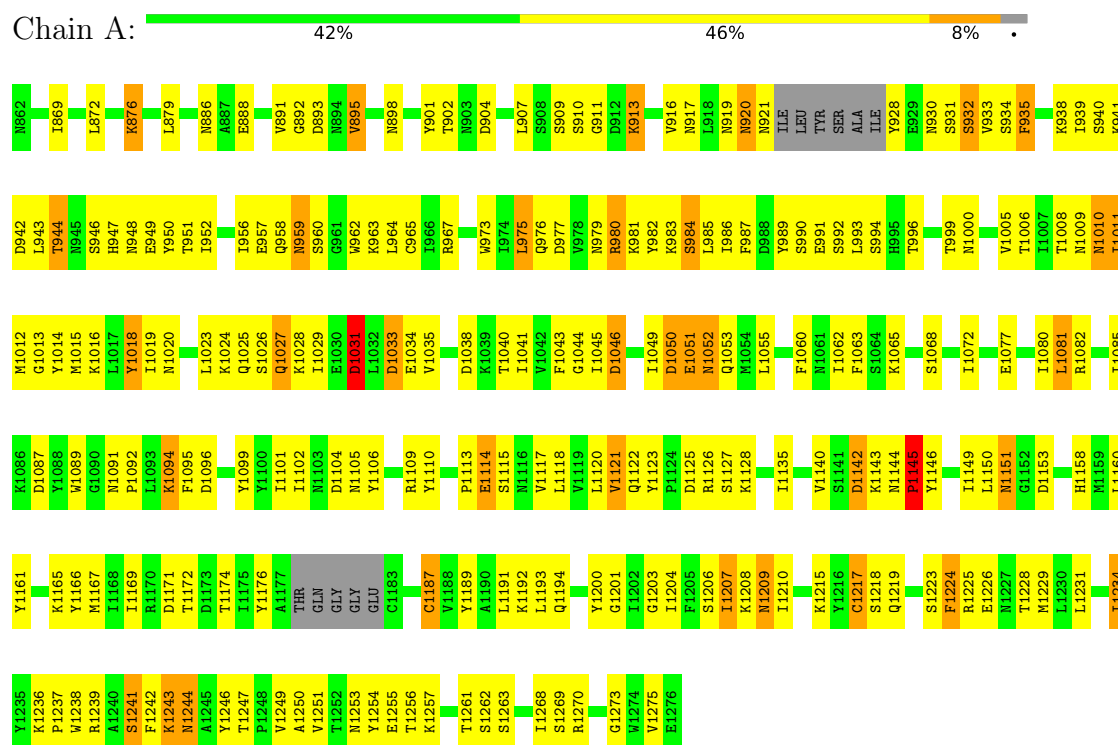
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	18	Total	O	0	0
			18	18		
2	C	17	Total	O	0	0
			17	17		
2	D	19	Total	O	0	0
			19	19		

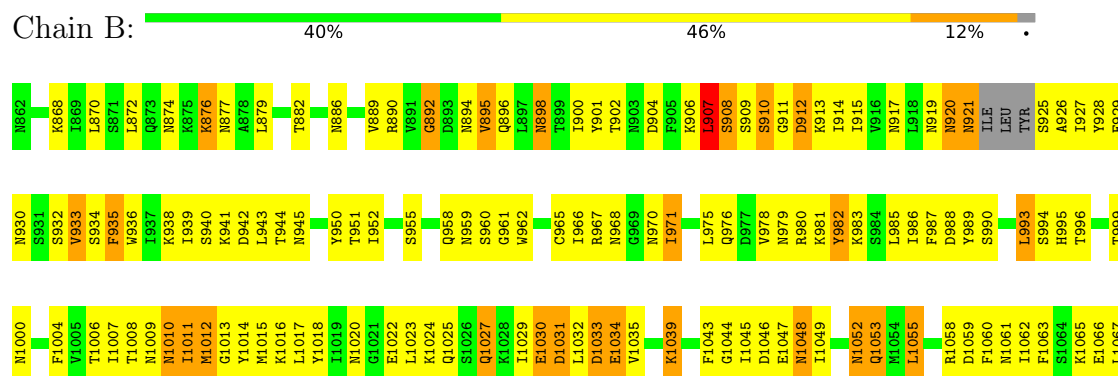
3 Residue-property plots

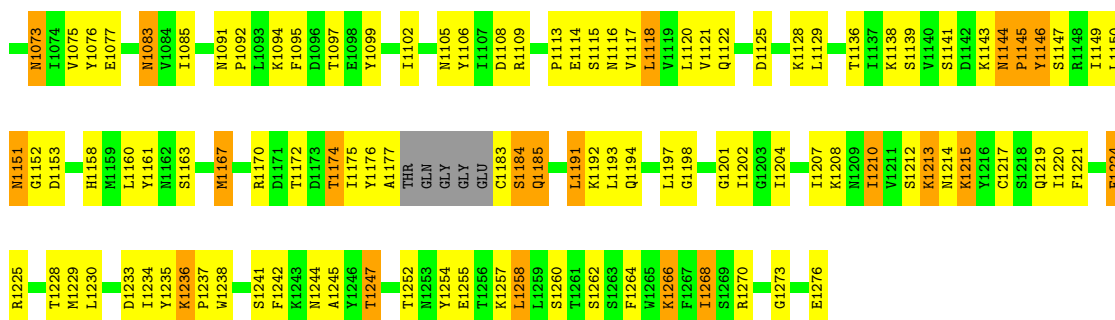
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 D

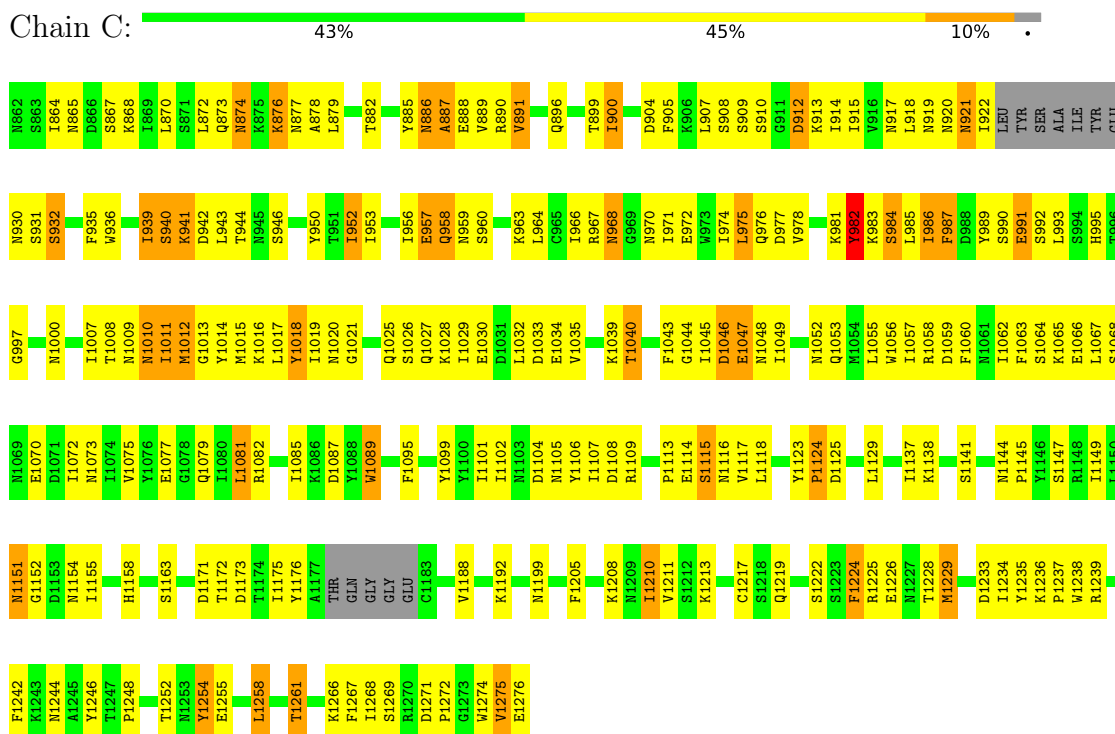


• Molecule 1: Botulinum neurotoxin type D

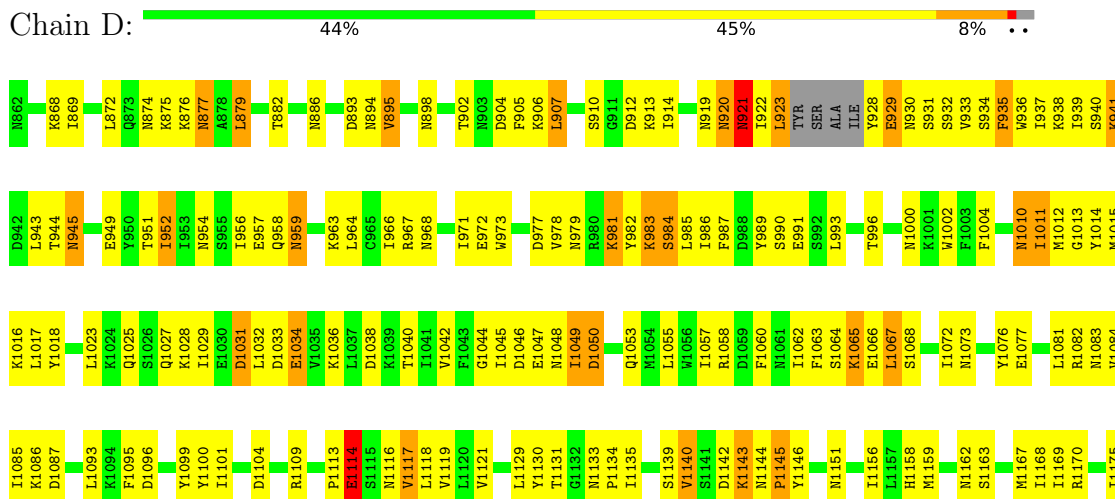


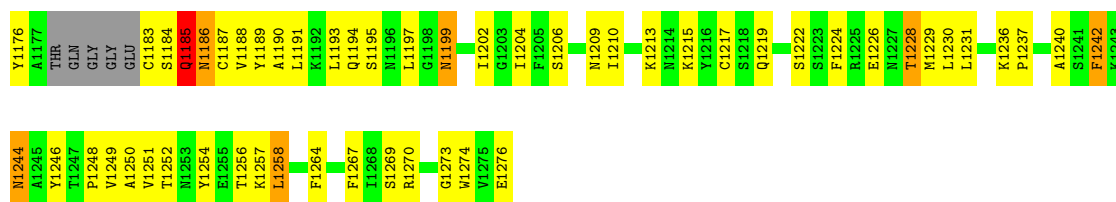


• Molecule 1: Botulinum neurotoxin type D



• Molecule 1: Botulinum neurotoxin type D





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.57Å 115.63Å 107.24Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	36.61 – 2.75 36.61 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.3 (36.61-2.75) 96.3 (36.61-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.03 (at 2.72Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.293 0.238 , 0.293	Depositor DCC
R_{free} test set	5885 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13363	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.49	0/3385	0.99	16/4583 (0.3%)
1	B	0.51	0/3404	1.00	15/4609 (0.3%)
1	C	0.46	0/3371	0.95	12/4564 (0.3%)
1	D	0.50	0/3401	0.96	14/4605 (0.3%)
All	All	0.49	0/13561	0.97	57/18361 (0.3%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1252	THR	N-CA-C	9.19	124.03	113.01
1	B	1039	LYS	N-CA-C	-8.63	101.52	114.64
1	C	1152	GLY	N-CA-C	-8.46	103.70	114.37
1	D	1236	LYS	CA-C-N	7.19	127.03	119.05
1	D	1236	LYS	C-N-CA	7.19	127.03	119.05
1	C	1252	THR	N-CA-C	7.17	122.12	113.23
1	A	1242	PHE	N-CA-C	-7.00	105.08	112.93
1	B	1083	ASN	N-CA-C	6.67	120.40	112.93
1	A	1270	ARG	N-CA-C	-6.66	100.03	109.96
1	B	1152	GLY	N-CA-C	-6.58	105.70	114.25
1	C	982	TYR	N-CA-C	6.50	120.14	109.94
1	D	1144	ASN	CA-C-N	6.49	127.96	119.84
1	D	1144	ASN	C-N-CA	6.49	127.96	119.84
1	A	984	SER	N-CA-C	6.30	118.13	108.42
1	A	886	ASN	N-CA-C	6.30	119.94	111.24
1	D	1195	SER	N-CA-C	6.28	118.12	111.28
1	C	891	VAL	N-CA-C	6.23	117.09	107.99
1	C	984	SER	N-CA-C	6.18	119.61	109.85
1	B	1091	ASN	CA-C-N	-6.17	113.16	120.13
1	B	1091	ASN	C-N-CA	-6.17	113.16	120.13
1	A	1144	ASN	CA-C-N	6.12	127.49	119.84
1	A	1144	ASN	C-N-CA	6.12	127.49	119.84
1	C	1242	PHE	N-CA-C	-6.09	105.16	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	982	TYR	N-CA-C	6.06	118.17	109.14
1	A	1121	VAL	N-CA-C	6.01	117.67	108.71
1	D	1251	VAL	N-CA-C	6.01	116.94	108.17
1	B	1144	ASN	CA-C-N	5.98	127.31	119.84
1	B	1144	ASN	C-N-CA	5.98	127.31	119.84
1	C	1246	TYR	N-CA-C	-5.88	100.40	109.76
1	C	1268	ILE	N-CA-C	5.84	116.09	107.15
1	B	1236	LYS	CA-C-N	5.84	127.14	119.84
1	B	1236	LYS	C-N-CA	5.84	127.14	119.84
1	D	1246	TYR	N-CA-C	-5.83	101.02	109.59
1	A	1239	ARG	N-CA-C	-5.78	106.39	113.50
1	B	1147	SER	N-CA-C	5.66	117.37	110.41
1	A	1275	VAL	N-CA-C	5.52	116.93	108.71
1	D	984	SER	N-CA-C	5.51	117.56	109.24
1	C	939	ILE	N-CA-C	5.48	115.98	107.99
1	D	983	LYS	N-CA-C	-5.42	99.26	108.26
1	D	996	THR	N-CA-C	-5.37	105.36	112.94
1	B	907	LEU	N-CA-C	-5.36	101.14	109.72
1	C	1040	THR	N-CA-C	5.36	118.18	108.69
1	C	1275	VAL	N-CA-C	5.32	117.37	109.17
1	A	891	VAL	N-CA-C	5.30	115.59	108.17
1	A	1241	SER	N-CA-C	5.27	117.42	109.41
1	D	886	ASN	N-CA-C	5.22	117.02	110.91
1	D	1082	ARG	N-CA-C	5.20	116.95	111.28
1	A	1246	TYR	N-CA-C	-5.18	100.07	108.41
1	B	1258	LEU	N-CA-C	5.13	117.61	111.71
1	D	982	TYR	N-CA-C	5.13	118.08	110.14
1	A	895	VAL	N-CA-C	5.09	115.42	107.99
1	C	1229	MET	N-CA-C	-5.07	101.49	109.50
1	A	1236	LYS	CA-C-N	5.05	126.15	119.84
1	A	1236	LYS	C-N-CA	5.05	126.15	119.84
1	B	1210	ILE	N-CA-C	-5.04	101.15	108.36
1	D	893	ASP	N-CA-C	5.03	117.88	111.69
1	A	1094	LYS	N-CA-C	5.02	117.44	109.50

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	3317	0	3260	210	0
1	B	3336	0	3281	269	0
1	C	3304	0	3256	242	0
1	D	3333	0	3282	199	0
2	A	19	0	0	0	0
2	B	18	0	0	2	0
2	C	17	0	0	1	0
2	D	19	0	0	1	0
All	All	13363	0	13079	911	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 35.

All (911) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:SER:HB3	1:B:1048:ASN:HA	1.36	1.08
1:B:1114:GLU:HG3	1:B:1115:SER:H	1.10	1.07
1:B:943:LEU:HD13	1:B:1053:GLN:HE22	1.17	1.05
1:B:927:ILE:HG22	1:B:1029:ILE:HD13	1.37	1.05
1:C:958:GLN:HG2	1:C:959:ASN:H	1.19	1.04
1:B:993:LEU:HD13	1:B:999:THR:HG21	1.40	1.03
1:C:958:GLN:HE21	1:C:960:SER:H	1.04	1.03
1:B:958:GLN:HG2	1:B:959:ASN:H	1.23	1.00
1:B:1029:ILE:HG23	1:B:1032:LEU:HD12	1.47	0.97
1:B:1010:ASN:HD21	1:B:1014:TYR:H	1.12	0.97
1:D:983:LYS:HZ1	1:D:1031:ASP:HB2	1.29	0.97
1:B:907:LEU:HD12	1:B:1044:GLY:HA2	1.44	0.95
1:C:1028:LYS:HD3	1:C:1029:ILE:N	1.81	0.95
1:B:976:GLN:HB3	1:B:982:TYR:HB3	1.48	0.95
1:B:958:GLN:HE21	1:B:960:SER:H	1.11	0.94
1:C:985:LEU:HD13	1:C:1017:LEU:HB2	1.52	0.91
1:C:1114:GLU:HG2	1:C:1238:TRP:HZ2	1.36	0.91
1:A:933:VAL:HG12	1:A:1062:ILE:HG12	1.51	0.90
1:D:983:LYS:HG3	1:D:1027:GLN:HE21	1.36	0.89
1:A:958:GLN:HG2	1:A:959:ASN:H	1.35	0.89
1:B:943:LEU:HD13	1:B:1053:GLN:NE2	1.87	0.89
1:B:966:ILE:HG22	1:B:971:ILE:HG13	1.55	0.88
1:A:977:ASP:HA	1:A:1035:VAL:HG22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:ILE:HD11	1:C:1151:ASN:HB3	1.53	0.88
1:D:1116:ASN:HD21	1:D:1193:LEU:H	1.21	0.87
1:B:944:THR:HG22	1:B:989:TYR:OH	1.75	0.87
1:D:923:LEU:HG	1:D:929:GLU:HG2	1.56	0.87
1:C:986:ILE:HG12	1:C:987:PHE:H	1.39	0.87
1:B:1254:TYR:HD1	1:B:1258:LEU:HD11	1.38	0.86
1:D:985:LEU:HA	1:D:1025:GLN:NE2	1.92	0.85
1:D:1210:ILE:HD11	1:D:1219:GLN:HG3	1.59	0.85
1:B:940:SER:O	1:B:944:THR:HG23	1.77	0.84
1:B:942:ASP:OD1	1:B:1052:ASN:HB2	1.77	0.84
1:D:1083:ASN:HA	1:D:1151:ASN:ND2	1.91	0.84
1:B:1114:GLU:HG3	1:B:1115:SER:N	1.87	0.84
1:A:940:SER:O	1:A:944:THR:HG22	1.76	0.83
1:B:1010:ASN:HD21	1:B:1014:TYR:N	1.76	0.83
1:D:1014:TYR:HA	1:D:1028:LYS:HA	1.61	0.82
1:D:983:LYS:HG3	1:D:1027:GLN:NE2	1.95	0.82
1:B:1049:ILE:HD13	1:B:1053:GLN:HB2	1.60	0.82
1:A:932:SER:HB3	1:A:1008:THR:HG22	1.61	0.81
1:C:1102:ILE:HD12	1:C:1107:ILE:HA	1.62	0.80
1:A:1228:THR:HA	1:A:1251:VAL:O	1.81	0.80
1:C:1010:ASN:HD21	1:C:1014:TYR:H	1.27	0.80
1:C:1011:ILE:HD13	1:C:1011:ILE:H	1.46	0.80
1:C:1105:ASN:OD1	1:C:1261:THR:HB	1.81	0.80
1:C:958:GLN:CG	1:C:959:ASN:H	1.96	0.79
1:C:940:SER:O	1:C:944:THR:HG23	1.82	0.78
1:D:985:LEU:HA	1:D:1025:GLN:HE22	1.48	0.78
1:B:958:GLN:CD	1:B:958:GLN:H	1.91	0.78
1:B:1065:LYS:HZ2	1:B:1067:LEU:HD23	1.48	0.78
1:A:985:LEU:HA	1:A:1025:GLN:NE2	1.98	0.78
1:C:910:SER:CB	1:C:1048:ASN:HA	2.14	0.78
1:C:1114:GLU:HG2	1:C:1238:TRP:CZ2	2.19	0.77
1:A:952:ILE:HG22	1:A:1045:ILE:HG12	1.66	0.77
1:D:876:LYS:O	1:D:877:ASN:HB2	1.85	0.77
1:D:1183:CYS:HB3	1:D:1189:TYR:OH	1.83	0.77
1:D:983:LYS:NZ	1:D:1031:ASP:HB2	1.99	0.77
1:C:910:SER:HB2	1:C:1048:ASN:HA	1.67	0.76
1:B:1049:ILE:HB	1:B:1053:GLN:CB	2.15	0.76
1:A:1110:TYR:HB3	1:A:1123:TYR:HE2	1.51	0.76
1:B:917:ASN:HA	1:B:1039:LYS:O	1.85	0.76
1:B:1138:LYS:HG3	1:B:1158:HIS:CD2	2.21	0.76
1:A:1117:VAL:HG11	1:A:1237:PRO:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:ILE:HD11	1:B:966:ILE:HG12	1.67	0.76
1:D:1010:ASN:ND2	1:D:1013:GLY:H	1.83	0.76
1:C:972:GLU:HG3	1:C:974:ILE:HD11	1.68	0.76
1:B:945:ASN:ND2	1:B:993:LEU:HD21	2.01	0.76
1:B:945:ASN:HD21	1:B:993:LEU:HD21	1.51	0.75
1:C:1015:MET:HE3	1:C:1029:ILE:HD11	1.68	0.75
1:B:993:LEU:CD1	1:B:999:THR:HG21	2.16	0.75
1:A:1016:LYS:HB3	1:A:1023:LEU:HD11	1.69	0.75
1:C:1032:LEU:HB3	1:C:1035:VAL:HG21	1.67	0.75
1:B:1146:TYR:HD2	1:B:1146:TYR:N	1.85	0.74
1:A:1228:THR:HB	1:A:1250:ALA:HB1	1.69	0.74
1:C:1233:ASP:OD1	1:C:1234:ILE:N	2.18	0.74
1:D:940:SER:O	1:D:944:THR:HG23	1.88	0.74
1:C:930:ASN:HD21	1:C:1011:ILE:HD13	1.52	0.74
1:B:874:ASN:HD21	1:B:879:LEU:HD23	1.52	0.73
1:B:1117:VAL:HG11	1:B:1237:PRO:HB2	1.70	0.73
1:C:865:ASN:O	1:C:868:LYS:HG3	1.89	0.73
1:B:994:SER:C	1:B:996:THR:H	1.95	0.72
1:D:1226:GLU:O	1:D:1228:THR:HG22	1.89	0.72
1:B:1114:GLU:CG	1:B:1115:SER:H	1.92	0.72
1:B:1254:TYR:CD1	1:B:1258:LEU:HD11	2.24	0.72
1:D:978:VAL:HG13	1:D:1034:GLU:O	1.89	0.72
1:A:1210:ILE:HD13	1:A:1219:GLN:HG3	1.71	0.72
1:B:1065:LYS:NZ	1:B:1067:LEU:HD23	2.05	0.72
1:C:1117:VAL:HG11	1:C:1237:PRO:HB2	1.71	0.72
1:A:981:LYS:HZ3	1:A:1031:ASP:C	1.98	0.72
1:A:981:LYS:HZ3	1:A:1031:ASP:HB2	1.54	0.72
1:D:1215:LYS:HG2	1:D:1217:CYS:SG	2.30	0.72
1:B:927:ILE:HD12	1:B:927:ILE:O	1.89	0.72
1:C:918:LEU:O	1:C:1039:LYS:HE3	1.90	0.72
1:C:1073:ASN:HD21	1:C:1213:LYS:NZ	1.87	0.72
1:C:943:LEU:HD13	1:C:1053:GLN:HB3	1.72	0.71
1:C:958:GLN:HG2	1:C:959:ASN:N	2.01	0.71
1:B:983:LYS:NZ	1:B:1030:GLU:HB2	2.06	0.71
1:C:939:ILE:HG23	1:C:943:LEU:HD23	1.71	0.71
1:D:933:VAL:HG22	1:D:1062:ILE:HG12	1.73	0.70
1:B:1010:ASN:ND2	1:B:1014:TYR:H	1.86	0.70
1:B:1170:ARG:NH1	1:B:1224:PHE:HB3	2.07	0.70
1:D:958:GLN:O	1:D:959:ASN:HB2	1.92	0.70
1:B:958:GLN:HE21	1:B:960:SER:N	1.88	0.70
1:B:1146:TYR:N	1:B:1146:TYR:CD2	2.58	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1233:ASP:HB3	1:B:1235:TYR:CE1	2.27	0.70
1:B:907:LEU:HD12	1:B:1044:GLY:CA	2.20	0.69
1:C:1229:MET:HE2	1:C:1254:TYR:HB2	1.73	0.69
1:C:1254:TYR:HD1	1:C:1258:LEU:HD13	1.58	0.69
1:D:1116:ASN:ND2	1:D:1193:LEU:H	1.90	0.69
1:C:974:ILE:HA	1:C:984:SER:HB3	1.73	0.69
1:D:1064:SER:O	1:D:1065:LYS:HB3	1.90	0.69
1:A:1201:GLY:HA2	1:A:1204:ILE:HG12	1.75	0.69
1:A:943:LEU:HD13	1:A:1053:GLN:HB3	1.74	0.69
1:C:1073:ASN:HD21	1:C:1213:LYS:HZ1	1.41	0.69
1:D:1083:ASN:HA	1:D:1151:ASN:HD21	1.57	0.69
1:B:959:ASN:HB3	1:B:980:ARG:HG3	1.74	0.69
1:A:981:LYS:NZ	1:A:1031:ASP:HB2	2.06	0.68
1:C:907:LEU:HD11	1:C:1045:ILE:H	1.57	0.68
1:C:919:ASN:HD22	1:C:921:ASN:ND2	1.91	0.68
1:B:921:ASN:N	1:B:921:ASN:HD22	1.89	0.68
1:B:898:ASN:ND2	1:B:902:THR:HA	2.07	0.68
1:B:933:VAL:HG12	1:B:1062:ILE:HG12	1.74	0.68
1:B:1150:LEU:O	1:B:1153:ASP:HB2	1.94	0.68
1:C:1029:ILE:HG23	1:C:1032:LEU:HD12	1.76	0.68
1:A:980:ARG:O	1:A:980:ARG:HG2	1.92	0.68
1:B:1055:LEU:O	1:B:1055:LEU:HG	1.93	0.68
1:A:958:GLN:CG	1:A:959:ASN:H	2.06	0.68
1:B:900:ILE:HG22	1:B:901:TYR:CD1	2.28	0.67
1:B:985:LEU:HA	1:B:1025:GLN:NE2	2.09	0.67
1:A:1256:THR:HG23	1:A:1257:LYS:H	1.60	0.67
1:B:1006:THR:HB	1:B:1018:TYR:HB2	1.74	0.67
1:B:979:ASN:O	1:B:980:ARG:HB2	1.93	0.67
1:B:1114:GLU:HG2	1:B:1238:TRP:HZ2	1.59	0.67
1:C:944:THR:HG22	1:C:989:TYR:OH	1.95	0.67
1:D:1117:VAL:HG11	1:D:1237:PRO:HB2	1.74	0.67
1:B:1049:ILE:HD12	1:B:1049:ILE:O	1.94	0.67
1:B:1102:ILE:HD13	1:B:1268:ILE:HD11	1.77	0.66
1:C:907:LEU:HG	1:C:1044:GLY:HA2	1.75	0.66
1:C:1010:ASN:HB3	1:C:1066:GLU:OE2	1.94	0.66
1:C:1210:ILE:HG21	1:C:1217:CYS:SG	2.34	0.66
1:A:898:ASN:ND2	1:A:902:THR:HA	2.10	0.66
1:A:1231:LEU:HD22	1:A:1257:LYS:HD3	1.78	0.66
1:D:930:ASN:ND2	1:D:1010:ASN:HA	2.10	0.66
1:B:909:SER:HA	1:B:1049:ILE:HD11	1.77	0.66
1:D:1228:THR:OG1	1:D:1250:ALA:HB1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:894:ASN:HB2	1:D:912:ASP:CG	2.21	0.66
1:B:898:ASN:HD21	1:B:902:THR:HA	1.59	0.66
1:B:930:ASN:OD1	1:B:1011:ILE:HG23	1.96	0.65
1:B:1102:ILE:CD1	1:B:1268:ILE:HD11	2.26	0.65
1:A:944:THR:HB	1:A:989:TYR:OH	1.95	0.65
1:D:1029:ILE:HG23	1:D:1032:LEU:HD12	1.78	0.65
1:D:907:LEU:HG	1:D:1044:GLY:HA2	1.78	0.65
1:D:1118:LEU:HD11	1:D:1193:LEU:HD21	1.78	0.65
1:A:983:LYS:HZ3	1:A:1029:ILE:HA	1.60	0.64
1:A:932:SER:CB	1:A:1008:THR:HG22	2.27	0.64
1:B:927:ILE:HG23	1:B:1035:VAL:HG21	1.79	0.64
1:B:1201:GLY:HA2	1:B:1204:ILE:HG12	1.79	0.64
1:C:1234:ILE:HD11	1:C:1244:ASN:HB3	1.78	0.64
1:D:1000:ASN:ND2	1:D:1273:GLY:HA3	2.13	0.64
1:A:1174:THR:HG23	1:A:1176:TYR:O	1.97	0.64
1:D:1050:ASP:H	1:D:1053:GLN:HE21	1.44	0.64
1:D:1000:ASN:HD21	1:D:1273:GLY:HA3	1.62	0.64
1:D:1184:SER:O	1:D:1185:GLN:HB2	1.97	0.64
1:B:932:SER:OG	1:B:1008:THR:HG22	1.98	0.64
1:C:990:SER:O	1:C:992:SER:N	2.31	0.64
1:D:958:GLN:H	1:D:958:GLN:NE2	1.96	0.64
1:B:1011:ILE:HG12	1:B:1012:MET:N	2.12	0.63
1:C:873:GLN:O	1:C:879:LEU:HD22	1.98	0.63
1:B:872:LEU:HD13	1:B:1060:PHE:HB3	1.81	0.63
1:C:977:ASP:HA	1:C:1035:VAL:HG22	1.80	0.63
1:A:1026:SER:O	1:A:1027:GLN:HB2	1.98	0.63
1:C:930:ASN:HD21	1:C:1011:ILE:CD1	2.10	0.63
1:A:888:GLU:HB3	1:A:917:ASN:HB2	1.80	0.63
1:D:1010:ASN:C	1:D:1010:ASN:HD22	2.06	0.63
1:B:1229:MET:HE2	1:B:1254:TYR:HB2	1.79	0.62
1:D:957:GLU:HB2	1:D:1038:ASP:OD2	1.98	0.62
1:A:983:LYS:NZ	1:A:1029:ILE:HA	2.14	0.62
1:A:1046:ASP:OD2	1:A:1046:ASP:N	2.31	0.62
1:C:1101:ILE:HG12	1:C:1267:PHE:CD2	2.34	0.62
1:A:907:LEU:HD23	1:A:1055:LEU:CD1	2.29	0.62
1:A:956:ILE:HG21	1:A:976:GLN:OE1	1.98	0.62
1:D:1229:MET:HE2	1:D:1254:TYR:HB2	1.81	0.62
1:A:991:GLU:HB2	1:A:994:SER:OG	1.99	0.62
1:C:908:SER:O	1:C:1049:ILE:HD11	1.98	0.62
1:A:907:LEU:HD23	1:A:1055:LEU:HD12	1.82	0.62
1:A:1113:PRO:HG3	1:A:1161:TYR:CZ	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:SER:O	1:C:993:LEU:HB2	2.00	0.62
1:B:911:GLY:O	1:B:912:ASP:C	2.43	0.62
1:C:1099:TYR:CE1	1:C:1269:SER:HB3	2.35	0.62
1:A:931:SER:HA	1:A:1065:LYS:H	1.64	0.62
1:A:1085:ILE:HA	1:A:1209:ASN:OD1	2.00	0.62
1:C:974:ILE:N	1:C:974:ILE:HD12	2.15	0.62
1:C:986:ILE:HG23	1:C:987:PHE:N	2.14	0.62
1:C:952:ILE:HD13	1:C:952:ILE:H	1.65	0.61
1:D:945:ASN:OD1	1:D:993:LEU:HD11	1.99	0.61
1:B:958:GLN:HG2	1:B:959:ASN:N	2.06	0.61
1:B:1151:ASN:CB	1:B:1208:LYS:HA	2.30	0.61
1:A:943:LEU:HB2	1:A:1053:GLN:HA	1.80	0.61
1:A:1050:ASP:CG	1:A:1053:GLN:HE21	2.08	0.61
1:A:1118:LEU:HD23	1:A:1191:LEU:O	2.00	0.61
1:B:1073:ASN:HD21	1:B:1213:LYS:NZ	1.99	0.61
1:D:1049:ILE:HB	1:D:1053:GLN:HB2	1.82	0.61
1:D:1175:ILE:HG23	1:D:1176:TYR:HD1	1.66	0.61
1:A:1160:LEU:HB2	1:A:1165:LYS:HE2	1.81	0.61
1:A:1229:MET:O	1:A:1250:ALA:HA	2.00	0.61
1:A:913:LYS:HG3	1:A:1044:GLY:HA3	1.82	0.61
1:A:1167:MET:HE1	1:A:1200:TYR:HB2	1.82	0.61
1:D:936:TRP:HB2	1:D:1058:ARG:HG3	1.81	0.61
1:D:1093:LEU:HD12	1:D:1099:TYR:CZ	2.36	0.61
1:A:1228:THR:HG22	1:A:1251:VAL:O	2.00	0.61
1:B:1113:PRO:HG3	1:B:1161:TYR:CZ	2.36	0.61
1:B:1017:LEU:O	1:B:1023:LEU:HD12	2.01	0.61
1:B:1125:ASP:OD2	1:B:1128:LYS:HG2	2.01	0.61
1:C:958:GLN:HE21	1:C:960:SER:N	1.88	0.61
1:C:1009:ASN:OD1	1:C:1015:MET:HB3	2.01	0.61
1:B:967:ARG:NH1	1:B:967:ARG:HB3	2.16	0.60
1:A:958:GLN:HG2	1:A:959:ASN:N	2.12	0.60
1:B:958:GLN:CG	1:B:959:ASN:H	1.99	0.60
1:C:1188:VAL:HG11	1:C:1235:TYR:CE2	2.37	0.60
1:A:1113:PRO:HG3	1:A:1161:TYR:CE1	2.37	0.60
1:A:1207:ILE:HG13	1:A:1218:SER:HB3	1.83	0.60
1:C:952:ILE:HD11	1:C:964:LEU:HG	1.84	0.60
1:A:930:ASN:HB3	1:A:1065:LYS:HA	1.83	0.60
1:A:907:LEU:HD12	1:A:1044:GLY:HA2	1.82	0.60
1:C:1138:LYS:HB3	2:C:12:HOH:O	2.02	0.60
1:B:1255:GLU:OE2	1:B:1255:GLU:HA	2.00	0.60
1:D:1048:ASN:HD22	1:D:1048:ASN:C	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:TRP:HB2	1:B:1058:ARG:HG2	1.84	0.59
1:B:1094:LYS:HE2	2:B:62:HOH:O	2.02	0.59
1:B:1118:LEU:HD23	1:B:1191:LEU:HB3	1.84	0.59
1:D:1010:ASN:HD21	1:D:1014:TYR:N	2.00	0.59
1:A:938:LYS:NZ	1:A:1000:ASN:HD21	2.01	0.59
1:A:1256:THR:HG23	1:A:1257:LYS:N	2.17	0.59
1:C:942:ASP:HB3	1:C:1053:GLN:HE21	1.66	0.59
1:A:1110:TYR:HB3	1:A:1123:TYR:CE2	2.37	0.59
1:C:950:TYR:HB3	1:C:1045:ILE:HD13	1.84	0.59
1:B:983:LYS:HG3	1:B:1027:GLN:HG2	1.85	0.59
1:B:1254:TYR:HD1	1:B:1258:LEU:CD1	2.13	0.59
1:A:958:GLN:H	1:A:958:GLN:CD	2.10	0.59
1:C:936:TRP:O	1:C:1057:ILE:HA	2.03	0.59
1:C:995:HIS:CE1	1:C:1129:LEU:HD13	2.38	0.59
1:B:894:ASN:O	1:B:895:VAL:C	2.46	0.59
1:B:896:GLN:NE2	1:B:906:LYS:HD2	2.18	0.59
1:D:934:SER:O	1:D:935:PHE:HB3	2.02	0.59
1:B:930:ASN:HA	1:B:1009:ASN:O	2.02	0.59
1:B:876:LYS:C	1:B:877:ASN:HD22	2.11	0.58
1:B:970:ASN:HD21	1:B:988:ASP:HB2	1.68	0.58
1:D:1184:SER:O	1:D:1185:GLN:CB	2.51	0.58
1:B:1151:ASN:HB3	1:B:1208:LYS:HA	1.85	0.58
1:D:1029:ILE:CG2	1:D:1032:LEU:HB2	2.33	0.58
1:A:959:ASN:C	1:A:959:ASN:HD22	2.12	0.58
1:B:1016:LYS:HB3	1:B:1023:LEU:HD11	1.85	0.58
1:B:1024:LYS:O	1:B:1025:GLN:HB2	2.04	0.58
1:A:1102:ILE:HD13	1:A:1268:ILE:HD11	1.86	0.58
1:C:1028:LYS:C	1:C:1029:ILE:HD12	2.29	0.58
1:C:1239:ARG:H	1:C:1239:ARG:HD3	1.67	0.58
1:C:896:GLN:HB3	1:C:899:THR:HG21	1.84	0.58
1:D:895:VAL:HG11	1:D:914:ILE:HD11	1.86	0.58
1:D:920:ASN:O	1:D:922:ILE:N	2.36	0.58
1:B:909:SER:O	1:B:910:SER:C	2.45	0.58
1:B:966:ILE:CG2	1:B:971:ILE:HG13	2.32	0.58
1:C:1222:SER:HB3	1:C:1228:THR:OG1	2.04	0.58
1:D:894:ASN:HB2	1:D:912:ASP:OD2	2.04	0.58
1:A:1011:ILE:HD13	1:A:1011:ILE:H	1.69	0.58
1:A:973:TRP:O	1:A:984:SER:HB2	2.04	0.57
1:A:956:ILE:HD13	1:A:976:GLN:OE1	2.04	0.57
1:A:1104:ASP:OD1	1:A:1215:LYS:HE3	2.04	0.57
1:B:1257:LYS:O	1:B:1260:SER:HB3	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:LYS:HB3	1:A:1023:LEU:CD1	2.33	0.57
1:A:1126:ARG:O	1:A:1128:LYS:N	2.37	0.57
1:B:920:ASN:HD22	1:B:1039:LYS:NZ	2.03	0.57
1:B:1006:THR:C	1:B:1007:ILE:HD12	2.29	0.57
1:C:1255:GLU:HA	1:C:1255:GLU:OE2	2.03	0.57
1:C:870:LEU:HD23	1:C:1062:ILE:HD12	1.85	0.57
1:C:1018:TYR:N	1:C:1018:TYR:CD2	2.72	0.57
1:C:1010:ASN:OD1	1:C:1012:MET:HB2	2.05	0.57
1:C:1099:TYR:HE1	1:C:1269:SER:HB3	1.69	0.57
1:B:926:ALA:HB3	1:B:1035:VAL:HG11	1.85	0.57
1:B:1083:ASN:ND2	1:B:1151:ASN:HD21	2.03	0.57
1:D:1118:LEU:HD23	1:D:1191:LEU:HB3	1.86	0.57
1:A:1096:ASP:OD2	1:A:1145:PRO:O	2.23	0.57
1:B:1049:ILE:HB	1:B:1053:GLN:HB3	1.86	0.57
1:B:1233:ASP:HB3	1:B:1235:TYR:HE1	1.69	0.57
1:C:879:LEU:O	1:C:889:VAL:HG11	2.05	0.57
1:C:1073:ASN:ND2	1:C:1213:LYS:NZ	2.51	0.57
1:B:934:SER:O	1:B:935:PHE:HB3	2.03	0.57
1:B:983:LYS:HE3	1:B:1030:GLU:H	1.69	0.57
1:C:882:THR:HG22	1:C:882:THR:O	2.04	0.57
1:C:986:ILE:HG22	1:C:1025:GLN:OE1	2.05	0.57
1:A:1010:ASN:C	1:A:1010:ASN:HD22	2.12	0.56
1:D:1100:TYR:OH	1:D:1270:ARG:NH1	2.38	0.56
1:D:1101:ILE:HG12	1:D:1267:PHE:CD2	2.40	0.56
1:B:1245:ALA:O	1:B:1247:THR:HG22	2.05	0.56
1:D:1156:ILE:HD11	1:D:1199:ASN:HA	1.88	0.56
1:B:1113:PRO:HB3	1:B:1193:LEU:HD11	1.87	0.56
1:A:944:THR:HG21	1:A:999:THR:HG23	1.88	0.56
1:B:966:ILE:HA	1:B:970:ASN:O	2.06	0.56
1:B:1176:TYR:O	1:B:1177:ALA:O	2.24	0.56
1:C:1081:LEU:HD23	1:C:1081:LEU:N	2.21	0.56
1:B:1167:MET:HE2	1:B:1197:LEU:HA	1.86	0.56
1:C:952:ILE:HD12	1:C:966:ILE:HG23	1.87	0.56
1:C:971:ILE:HG23	1:C:971:ILE:O	2.05	0.56
1:C:868:LYS:HG2	1:C:1063:PHE:CE1	2.40	0.56
1:B:1011:ILE:HD13	1:B:1011:ILE:H	1.70	0.56
1:C:986:ILE:HG12	1:C:987:PHE:N	2.16	0.56
1:C:1271:ASP:OD1	1:C:1272:PRO:HD2	2.06	0.56
1:B:1215:LYS:HZ1	1:B:1264:PHE:HD2	1.54	0.56
1:D:1135:ILE:HG23	1:D:1158:HIS:O	2.05	0.56
1:A:1089:TRP:HB2	1:A:1091:ASN:ND2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:974:ILE:HG22	1:C:975:LEU:N	2.20	0.55
1:D:1095:PHE:CE1	1:D:1139:SER:HB3	2.40	0.55
1:C:913:LYS:HD2	1:C:913:LYS:N	2.21	0.55
1:C:1073:ASN:ND2	1:C:1213:LYS:HZ1	2.04	0.55
1:A:901:TYR:CZ	1:A:1092:PRO:HD3	2.41	0.55
1:B:1183:CYS:SG	1:B:1184:SER:N	2.66	0.55
1:C:874:ASN:HA	1:C:878:ALA:O	2.07	0.55
1:A:957:GLU:CD	1:A:1038:ASP:HB3	2.31	0.55
1:C:1018:TYR:N	1:C:1018:TYR:HD2	2.05	0.55
1:D:956:ILE:HD12	1:D:963:LYS:HD3	1.89	0.55
1:A:977:ASP:OD2	1:A:981:LYS:HB3	2.06	0.55
1:B:910:SER:HB3	1:B:1048:ASN:CA	2.25	0.55
1:B:921:ASN:HD22	1:B:921:ASN:H	1.55	0.55
1:D:1045:ILE:HB	1:D:1047:GLU:OE2	2.07	0.55
1:D:1183:CYS:HB3	1:D:1189:TYR:HH	1.70	0.55
1:B:892:GLY:N	1:B:913:LYS:O	2.40	0.55
1:C:1075:VAL:O	1:C:1079:GLN:HG3	2.07	0.55
1:D:985:LEU:HG	1:D:1015:MET:HE3	1.88	0.55
1:B:1030:GLU:O	1:B:1032:LEU:N	2.40	0.54
1:B:1045:ILE:HD12	1:B:1049:ILE:HG21	1.88	0.54
1:D:1276:GLU:HG3	1:D:1276:GLU:O	2.07	0.54
1:B:1007:ILE:HD12	1:B:1007:ILE:N	2.22	0.54
1:B:1008:THR:O	1:B:1015:MET:HA	2.07	0.54
1:B:1095:PHE:CE1	1:B:1139:SER:HB3	2.43	0.54
1:C:963:LYS:NZ	1:C:974:ILE:HG12	2.21	0.54
1:C:1000:ASN:O	1:C:1089:TRP:HB3	2.07	0.54
1:A:994:SER:C	1:A:996:THR:H	2.15	0.54
1:C:978:VAL:HG13	1:C:1034:GLU:O	2.07	0.54
1:C:904:ASP:HA	1:C:1057:ILE:O	2.07	0.54
1:D:952:ILE:HD11	1:D:964:LEU:HG	1.90	0.54
1:A:1055:LEU:HD12	1:A:1055:LEU:C	2.32	0.54
1:B:952:ILE:N	1:B:952:ILE:HD12	2.23	0.54
1:B:985:LEU:HD13	1:B:1017:LEU:HB2	1.88	0.54
1:B:1095:PHE:CE2	1:B:1149:ILE:HG12	2.43	0.54
1:D:910:SER:HB2	1:D:1046:ASP:O	2.08	0.54
1:C:919:ASN:ND2	1:C:921:ASN:ND2	2.55	0.54
1:C:1029:ILE:CG2	1:C:1032:LEU:HD12	2.37	0.54
1:D:958:GLN:OE1	1:D:1036:LYS:HD3	2.08	0.54
1:D:1169:ILE:HD13	1:D:1194:GLN:HB2	1.90	0.54
1:B:968:ASN:ND2	1:B:968:ASN:O	2.40	0.54
1:C:872:LEU:HD13	1:C:1060:PHE:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:937:ILE:HD11	1:D:1055:LEU:HD13	1.90	0.54
1:D:1175:ILE:HG23	1:D:1176:TYR:CD1	2.43	0.54
1:C:1233:ASP:OD1	1:C:1234:ILE:HG22	2.08	0.54
1:D:1050:ASP:H	1:D:1053:GLN:NE2	2.06	0.54
1:A:904:ASP:C	1:A:904:ASP:OD1	2.51	0.54
1:A:990:SER:C	1:A:992:SER:H	2.16	0.54
1:B:879:LEU:HD12	1:B:889:VAL:HG11	1.88	0.53
1:B:913:LYS:NZ	1:B:1046:ASP:HB3	2.22	0.53
1:B:1106:TYR:HB3	1:B:1109:ARG:HD2	1.90	0.53
1:D:1064:SER:O	1:D:1065:LYS:CB	2.55	0.53
1:C:936:TRP:HB2	1:C:1058:ARG:HG2	1.91	0.53
1:C:1010:ASN:HD21	1:C:1014:TYR:N	2.03	0.53
1:A:1113:PRO:HA	1:A:1118:LEU:HD13	1.90	0.53
1:B:920:ASN:HA	1:B:1039:LYS:HZ2	1.74	0.53
1:C:956:ILE:C	1:C:958:GLN:H	2.16	0.53
1:C:957:GLU:OE2	1:C:1040:THR:HB	2.09	0.53
1:D:1068:SER:O	1:D:1072:ILE:HG13	2.07	0.53
1:C:1224:PHE:CE1	1:C:1225:ARG:HG2	2.43	0.53
1:D:876:LYS:HD3	1:D:876:LYS:N	2.22	0.53
1:A:951:THR:HA	1:A:965:CYS:HB3	1.89	0.53
1:B:970:ASN:ND2	1:B:988:ASP:HB2	2.23	0.53
1:D:894:ASN:HB2	1:D:912:ASP:OD1	2.08	0.53
1:A:876:LYS:HD2	1:A:876:LYS:N	2.23	0.53
1:C:1085:ILE:CD1	1:C:1151:ASN:HB3	2.35	0.53
1:C:1151:ASN:HB2	1:C:1208:LYS:HA	1.90	0.53
1:D:1190:ALA:HA	1:D:1249:VAL:HG12	1.89	0.53
1:B:914:ILE:HB	1:B:1043:PHE:HB2	1.90	0.53
1:B:983:LYS:HZ2	1:B:1030:GLU:HB2	1.71	0.53
1:D:1029:ILE:CG2	1:D:1032:LEU:HD12	2.39	0.53
1:A:1005:VAL:HG12	1:A:1006:THR:N	2.24	0.53
1:A:1101:ILE:CD1	1:A:1135:ILE:HB	2.39	0.53
1:A:1010:ASN:C	1:A:1010:ASN:ND2	2.67	0.52
1:C:986:ILE:O	1:C:987:PHE:CB	2.58	0.52
1:C:991:GLU:OE1	1:C:997:GLY:HA2	2.09	0.52
1:A:919:ASN:O	1:A:921:ASN:N	2.42	0.52
1:A:952:ILE:HG21	1:A:1055:LEU:HD21	1.91	0.52
1:B:951:THR:O	1:B:1045:ILE:HG22	2.09	0.52
1:B:1022:GLU:O	1:B:1024:LYS:HG2	2.08	0.52
1:D:1095:PHE:CZ	1:D:1139:SER:HB3	2.44	0.52
1:A:934:SER:O	1:A:935:PHE:HB3	2.09	0.52
1:B:1276:GLU:HG3	1:B:1276:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:THR:HA	1:A:965:CYS:CB	2.39	0.52
1:A:994:SER:C	1:A:996:THR:N	2.68	0.52
1:D:985:LEU:HG	1:D:1015:MET:CE	2.39	0.52
1:D:1067:LEU:HD23	1:D:1067:LEU:H	1.74	0.52
1:B:952:ILE:CD1	1:B:966:ILE:HG12	2.38	0.52
1:D:919:ASN:O	1:D:920:ASN:C	2.52	0.52
1:B:1073:ASN:HD21	1:B:1213:LYS:HZ1	1.56	0.52
1:A:1087:ASP:C	1:A:1087:ASP:OD2	2.53	0.52
1:B:890:ARG:HB2	1:B:915:ILE:HB	1.91	0.52
1:C:986:ILE:O	1:C:987:PHE:HB2	2.09	0.52
1:C:1026:SER:O	1:C:1027:GLN:HG3	2.10	0.52
1:D:1118:LEU:O	1:D:1248:PRO:HD2	2.10	0.52
1:A:1113:PRO:O	1:A:1114:GLU:HB3	2.10	0.52
1:B:958:GLN:CD	1:B:958:GLN:N	2.66	0.52
1:C:1124:PRO:HG2	1:C:1125:ASP:H	1.75	0.52
1:A:985:LEU:HD22	1:A:1025:GLN:HG2	1.92	0.52
1:B:928:TYR:N	1:B:928:TYR:CD2	2.75	0.52
1:B:1217:CYS:HB3	1:B:1266:LYS:HG3	1.91	0.52
1:C:1029:ILE:O	1:C:1029:ILE:HG22	2.10	0.52
1:C:1175:ILE:HG23	1:C:1176:TYR:CD1	2.45	0.52
1:C:1275:VAL:HG12	1:C:1276:GLU:N	2.25	0.52
1:C:1008:THR:O	1:C:1015:MET:HA	2.10	0.51
1:B:1010:ASN:ND2	1:B:1014:TYR:N	2.51	0.51
1:B:1143:LYS:O	1:B:1144:ASN:C	2.51	0.51
1:C:1118:LEU:O	1:C:1248:PRO:HD2	2.10	0.51
1:A:940:SER:HB2	1:A:1273:GLY:O	2.10	0.51
1:A:1109:ARG:HA	1:A:1121:VAL:O	2.09	0.51
1:B:913:LYS:HZ1	1:B:1046:ASP:HB3	1.74	0.51
1:B:938:LYS:NZ	1:B:1000:ASN:HD21	2.09	0.51
1:B:945:ASN:HD21	1:B:993:LEU:CD2	2.20	0.51
1:C:1030:GLU:C	1:C:1032:LEU:H	2.18	0.51
1:C:1254:TYR:CD1	1:C:1258:LEU:HD13	2.44	0.51
1:D:939:ILE:HD12	1:D:989:TYR:CZ	2.45	0.51
1:D:1187:CYS:HB2	1:D:1252:THR:HG23	1.92	0.51
1:A:935:PHE:HB3	1:A:1060:PHE:HA	1.91	0.51
1:C:1010:ASN:ND2	1:C:1010:ASN:H	2.08	0.51
1:D:990:SER:O	1:D:991:GLU:HB2	2.11	0.51
1:D:1066:GLU:O	1:D:1066:GLU:HG2	2.11	0.51
1:B:961:GLY:O	1:B:975:LEU:HD12	2.11	0.51
1:B:994:SER:C	1:B:996:THR:N	2.64	0.51
1:B:928:TYR:HA	1:B:1010:ASN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:ASN:O	1:B:968:ASN:CG	2.53	0.51
1:C:1058:ARG:HG3	1:C:1059:ASP:OD1	2.11	0.51
1:C:1113:PRO:O	1:C:1117:VAL:O	2.29	0.51
1:D:921:ASN:H	1:D:921:ASN:ND2	2.07	0.51
1:D:1185:GLN:O	1:D:1186:ASN:C	2.53	0.51
1:A:1171:ASP:CG	1:A:1192:LYS:HD2	2.35	0.51
1:B:868:LYS:HE3	1:B:1063:PHE:CE1	2.46	0.51
1:B:1004:PHE:HB3	1:B:1020:ASN:HA	1.93	0.50
1:C:1104:ASP:OD2	1:C:1266:LYS:HE3	2.11	0.50
1:C:910:SER:HB3	1:C:1049:ILE:H	1.76	0.50
1:C:1224:PHE:O	1:D:882:THR:O	2.29	0.50
1:B:1113:PRO:HG3	1:B:1161:TYR:CE2	2.46	0.50
1:C:1046:ASP:O	1:C:1047:GLU:C	2.54	0.50
1:A:1150:LEU:O	1:A:1153:ASP:HB2	2.11	0.50
1:B:1049:ILE:HD12	1:B:1049:ILE:C	2.36	0.50
1:C:920:ASN:O	1:C:922:ILE:N	2.45	0.50
1:C:1171:ASP:OD2	1:C:1172:THR:N	2.45	0.50
1:D:868:LYS:HG2	1:D:1063:PHE:CE1	2.46	0.50
1:B:950:TYR:O	1:B:965:CYS:HA	2.11	0.50
1:C:1192:LYS:HZ3	1:C:1239:ARG:HH22	1.59	0.50
1:D:958:GLN:H	1:D:958:GLN:CD	2.19	0.50
1:D:1016:LYS:HB3	1:D:1023:LEU:HD11	1.92	0.50
1:B:909:SER:CA	1:B:1049:ILE:HD11	2.42	0.50
1:C:1015:MET:CE	1:C:1029:ILE:HD11	2.39	0.50
1:C:1068:SER:O	1:C:1072:ILE:HG13	2.11	0.50
1:D:937:ILE:HD12	1:D:1057:ILE:HG12	1.94	0.50
1:A:956:ILE:HD13	1:A:976:GLN:CD	2.37	0.50
1:B:872:LEU:HG	1:B:879:LEU:HD11	1.93	0.50
1:B:927:ILE:CG2	1:B:1029:ILE:HD13	2.25	0.50
1:B:1011:ILE:C	1:B:1013:GLY:N	2.69	0.50
1:B:1242:PHE:HD1	1:B:1242:PHE:O	1.94	0.50
1:C:974:ILE:CG2	1:C:975:LEU:N	2.74	0.50
1:D:932:SER:HB2	1:D:1067:LEU:HD21	1.94	0.50
1:D:1113:PRO:O	1:D:1114:GLU:HB2	2.12	0.50
1:A:1140:VAL:C	1:A:1142:ASP:H	2.20	0.50
1:B:913:LYS:HG2	1:B:1043:PHE:O	2.12	0.50
1:B:950:TYR:HB2	1:B:966:ILE:HG13	1.94	0.50
1:C:872:LEU:HB3	1:C:879:LEU:HD11	1.94	0.50
1:C:913:LYS:NZ	1:C:1046:ASP:HA	2.26	0.50
1:D:1222:SER:HB3	1:D:1228:THR:HG23	1.93	0.50
1:A:1158:HIS:HA	1:A:1166:TYR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1113:PRO:HB3	1:D:1193:LEU:HD11	1.93	0.50
1:A:1077:GLU:OE1	1:A:1082:ARG:NH1	2.44	0.49
1:A:1231:LEU:C	1:A:1231:LEU:HD12	2.37	0.49
1:A:1241:SER:C	1:A:1243:LYS:H	2.19	0.49
1:B:1049:ILE:CD1	1:B:1053:GLN:HB2	2.36	0.49
1:A:957:GLU:OE1	1:A:1038:ASP:HB3	2.12	0.49
1:A:1009:ASN:OD1	1:A:1015:MET:HB2	2.12	0.49
1:C:1010:ASN:H	1:C:1010:ASN:HD22	1.58	0.49
1:C:990:SER:O	1:C:991:GLU:C	2.55	0.49
1:C:1085:ILE:HD11	1:C:1151:ASN:CB	2.35	0.49
1:C:1113:PRO:O	1:C:1115:SER:N	2.43	0.49
1:D:1085:ILE:HA	1:D:1209:ASN:HD21	1.78	0.49
1:D:1104:ASP:OD2	1:D:1215:LYS:HD3	2.12	0.49
1:A:1085:ILE:HG21	1:A:1207:ILE:CD1	2.42	0.49
1:B:1170:ARG:HH22	1:B:1225:ARG:HB2	1.77	0.49
1:C:1224:PHE:CD1	1:C:1225:ARG:HG2	2.48	0.49
1:A:931:SER:HA	1:A:1065:LYS:N	2.28	0.49
1:A:1095:PHE:CZ	1:A:1149:ILE:HG12	2.48	0.49
1:C:930:ASN:HB3	1:C:1066:GLU:H	1.78	0.49
1:C:976:GLN:HA	1:C:982:TYR:HA	1.93	0.49
1:B:1113:PRO:O	1:B:1114:GLU:HB3	2.13	0.49
1:B:1170:ARG:O	1:B:1202:ILE:HD11	2.13	0.49
1:C:1115:SER:O	1:C:1116:ASN:HB2	2.12	0.49
1:B:1049:ILE:HB	1:B:1053:GLN:HB2	1.93	0.49
1:C:983:LYS:HG3	1:C:1027:GLN:NE2	2.28	0.49
1:D:874:ASN:HB2	1:D:902:THR:O	2.13	0.49
1:A:930:ASN:HD22	1:A:1010:ASN:HA	1.77	0.49
1:A:1113:PRO:HG2	1:A:1114:GLU:H	1.76	0.49
1:C:1017:LEU:C	1:C:1018:TYR:HD2	2.20	0.49
1:C:1068:SER:C	1:C:1070:GLU:H	2.20	0.49
1:A:973:TRP:O	1:A:984:SER:CB	2.61	0.49
1:A:1169:ILE:HD13	1:A:1194:GLN:HB2	1.95	0.49
1:B:939:ILE:HD12	1:B:989:TYR:CE1	2.48	0.49
1:B:1016:LYS:HB3	1:B:1023:LEU:CD1	2.43	0.49
1:D:1010:ASN:HD21	1:D:1014:TYR:H	1.60	0.49
1:D:1014:TYR:CE1	1:D:1028:LYS:HD2	2.47	0.49
1:A:909:SER:C	1:A:1049:ILE:HD11	2.38	0.48
1:C:1028:LYS:HD3	1:C:1029:ILE:C	2.38	0.48
1:B:1010:ASN:C	1:B:1010:ASN:HD22	2.20	0.48
1:B:1083:ASN:CG	1:B:1151:ASN:HD21	2.21	0.48
1:B:925:SER:O	1:B:929:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1154:ASN:HA	1:C:1205:PHE:O	2.13	0.48
1:A:958:GLN:CG	1:A:959:ASN:N	2.74	0.48
1:A:1207:ILE:HG13	1:A:1218:SER:CB	2.43	0.48
1:B:901:TYR:CZ	1:B:1092:PRO:HD3	2.48	0.48
1:B:913:LYS:HG2	1:B:1044:GLY:HA3	1.94	0.48
1:C:1226:GLU:HG3	1:D:876:LYS:NZ	2.29	0.48
1:B:920:ASN:HD22	1:B:1039:LYS:HZ1	1.61	0.48
1:B:920:ASN:HA	1:B:1039:LYS:NZ	2.28	0.48
1:C:1017:LEU:C	1:C:1018:TYR:CD2	2.92	0.48
1:C:1237:PRO:HG2	1:C:1238:TRP:H	1.78	0.48
1:D:923:LEU:C	1:D:923:LEU:HD13	2.39	0.48
1:D:939:ILE:CG2	1:D:944:THR:HG22	2.44	0.48
1:A:1040:THR:CG2	1:A:1041:ILE:N	2.76	0.48
1:B:1011:ILE:O	1:B:1013:GLY:N	2.47	0.48
1:B:1031:ASP:O	1:B:1032:LEU:HD23	2.12	0.48
1:B:1085:ILE:HD11	1:B:1151:ASN:CA	2.44	0.48
1:C:930:ASN:O	1:C:1064:SER:O	2.31	0.48
1:C:876:LYS:C	1:C:877:ASN:HD22	2.22	0.48
1:C:941:LYS:HE3	1:C:1274:TRP:CE2	2.48	0.48
1:C:956:ILE:HD13	1:C:976:GLN:OE1	2.14	0.48
1:C:967:ARG:HG3	1:C:967:ARG:HH11	1.78	0.48
1:D:928:TYR:OH	1:D:1029:ILE:HG22	2.14	0.48
1:A:892:GLY:O	1:A:895:VAL:HG23	2.14	0.48
1:B:1151:ASN:HB2	1:B:1208:LYS:HA	1.95	0.48
1:C:1019:ILE:C	1:C:1021:GLY:N	2.70	0.48
1:D:875:LYS:C	1:D:877:ASN:H	2.21	0.48
1:C:1068:SER:C	1:C:1070:GLU:N	2.72	0.47
1:D:1109:ARG:HA	1:D:1121:VAL:O	2.14	0.47
1:D:1242:PHE:N	1:D:1242:PHE:CD2	2.81	0.47
1:A:1040:THR:HG22	1:A:1041:ILE:N	2.29	0.47
1:D:879:LEU:HD11	1:D:905:PHE:CD2	2.48	0.47
1:B:1151:ASN:HA	1:B:1207:ILE:O	2.15	0.47
1:B:1236:LYS:NZ	1:B:1244:ASN:HD21	2.12	0.47
1:D:910:SER:HB3	1:D:1047:GLU:O	2.14	0.47
1:B:1049:ILE:HD13	1:B:1053:GLN:CB	2.37	0.47
1:C:1144:ASN:HB2	1:C:1147:SER:HB3	1.95	0.47
1:C:1199:ASN:N	1:C:1199:ASN:HD22	2.12	0.47
1:D:949:GLU:HG3	1:D:967:ARG:HB2	1.96	0.47
1:D:951:THR:O	1:D:1045:ILE:HG22	2.13	0.47
1:D:1034:GLU:O	1:D:1034:GLU:HG3	2.15	0.47
1:D:1057:ILE:HG22	1:D:1058:ARG:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1135:ILE:HG12	1:D:1159:MET:HG3	1.96	0.47
1:A:1114:GLU:HG3	1:A:1115:SER:N	2.29	0.47
1:C:890:ARG:HH11	1:C:915:ILE:HG21	1.78	0.47
1:C:952:ILE:CD1	1:C:966:ILE:HG23	2.44	0.47
1:D:921:ASN:ND2	1:D:921:ASN:N	2.58	0.47
1:D:981:LYS:HE2	2:D:72:HOH:O	2.14	0.47
1:D:1084:VAL:O	1:D:1086:LYS:HE3	2.13	0.47
1:B:1113:PRO:O	1:B:1117:VAL:O	2.33	0.47
1:B:1212:SER:O	1:B:1214:ASN:N	2.48	0.47
1:C:873:GLN:C	1:C:879:LEU:HD22	2.39	0.47
1:C:1043:PHE:HZ	1:C:1060:PHE:CE1	2.33	0.47
1:A:1118:LEU:O	1:A:1247:THR:OG1	2.31	0.47
1:C:912:ASP:C	1:C:913:LYS:HD2	2.39	0.47
1:A:1011:ILE:HG12	1:A:1012:MET:N	2.28	0.47
1:B:1105:ASN:ND2	1:B:1262:SER:HB3	2.30	0.47
1:C:867:SER:OG	1:C:1065:LYS:HG2	2.13	0.47
1:D:941:LYS:NZ	1:D:1274:TRP:CE2	2.83	0.47
1:D:1229:MET:O	1:D:1250:ALA:HA	2.15	0.47
1:A:1012:MET:O	1:A:1028:LYS:HE3	2.14	0.47
1:A:1229:MET:HE2	1:A:1254:TYR:HB2	1.97	0.47
1:A:1224:PHE:O	1:B:882:THR:O	2.32	0.47
1:B:1045:ILE:HG13	1:B:1045:ILE:O	2.15	0.47
1:C:950:TYR:HB2	1:C:966:ILE:CG1	2.45	0.47
1:C:982:TYR:O	1:C:983:LYS:HE2	2.15	0.47
1:A:958:GLN:HE21	1:A:960:SER:H	1.63	0.46
1:A:1125:ASP:OD2	1:A:1128:LYS:HG2	2.15	0.46
1:B:1046:ASP:N	1:B:1046:ASP:OD2	2.48	0.46
1:B:1254:TYR:O	1:B:1258:LEU:HD13	2.14	0.46
1:C:1210:ILE:HG22	1:C:1210:ILE:O	2.14	0.46
1:A:910:SER:N	1:A:1049:ILE:HD11	2.30	0.46
1:A:1187:CYS:HB2	1:A:1189:TYR:CE1	2.50	0.46
1:A:1234:ILE:HG12	1:D:1197:LEU:HD12	1.97	0.46
1:B:874:ASN:ND2	1:B:879:LEU:HD23	2.26	0.46
1:D:1010:ASN:ND2	1:D:1010:ASN:O	2.38	0.46
1:D:1011:ILE:HD13	1:D:1012:MET:H	1.80	0.46
1:D:1229:MET:CE	1:D:1257:LYS:HB2	2.44	0.46
1:D:1230:LEU:HA	1:D:1249:VAL:O	2.16	0.46
1:D:1242:PHE:N	1:D:1242:PHE:HD2	2.13	0.46
1:A:944:THR:CB	1:A:989:TYR:OH	2.63	0.46
1:A:1011:ILE:C	1:A:1013:GLY:H	2.23	0.46
1:A:1215:LYS:HD2	1:A:1217:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:ASN:O	1:A:1256:THR:HG22	2.15	0.46
1:B:1116:ASN:O	1:B:1192:LYS:HG2	2.15	0.46
1:C:966:ILE:HA	1:C:970:ASN:O	2.15	0.46
1:D:938:LYS:HD3	1:D:1002:TRP:CE2	2.50	0.46
1:A:907:LEU:N	1:A:907:LEU:HD22	2.31	0.46
1:A:1015:MET:O	1:A:1015:MET:HG3	2.14	0.46
1:B:921:ASN:N	1:B:921:ASN:ND2	2.61	0.46
1:B:966:ILE:HG13	1:B:966:ILE:O	2.14	0.46
1:C:864:ILE:O	1:C:867:SER:HB3	2.15	0.46
1:A:1237:PRO:HG2	1:A:1238:TRP:CE3	2.50	0.46
1:B:909:SER:HA	1:B:1049:ILE:CD1	2.45	0.46
1:B:1158:HIS:CE1	1:B:1197:LEU:HD22	2.50	0.46
1:C:1175:ILE:HD11	1:C:1236:LYS:C	2.40	0.46
1:D:1010:ASN:ND2	1:D:1010:ASN:C	2.73	0.46
1:D:1016:LYS:HB3	1:D:1023:LEU:CD1	2.46	0.46
1:B:1167:MET:HE1	1:B:1198:GLY:O	2.15	0.46
1:B:1184:SER:C	1:B:1185:GLN:HG3	2.41	0.46
1:D:1038:ASP:C	1:D:1040:THR:H	2.23	0.46
1:D:1215:LYS:CG	1:D:1217:CYS:SG	3.02	0.46
1:A:1085:ILE:HG21	1:A:1207:ILE:HD13	1.97	0.46
1:C:913:LYS:HE3	1:C:1046:ASP:OD2	2.16	0.46
1:B:1270:ARG:NH2	1:B:1270:ARG:HG2	2.31	0.46
1:C:985:LEU:HB3	1:C:1017:LEU:HD22	1.98	0.46
1:A:962:TRP:HB3	1:A:975:LEU:HD23	1.98	0.46
1:A:1113:PRO:O	1:A:1117:VAL:O	2.34	0.46
1:B:1010:ASN:ND2	1:B:1014:TYR:O	2.49	0.46
1:B:1058:ARG:O	1:B:1059:ASP:HB2	2.15	0.46
1:B:1219:GLN:HB3	1:B:1221:PHE:CE2	2.51	0.46
1:C:942:ASP:OD2	1:C:1052:ASN:HB3	2.16	0.46
1:D:1114:GLU:CA	1:D:1114:GLU:OE2	2.63	0.46
1:A:1109:ARG:NH1	1:A:1122:GLN:N	2.64	0.46
1:B:1136:THR:HG21	1:B:1138:LYS:NZ	2.31	0.46
1:D:1140:VAL:CG2	1:D:1204:ILE:HD12	2.46	0.46
1:B:933:VAL:CG2	1:B:1007:ILE:HB	2.47	0.45
1:B:983:LYS:CG	1:B:1027:GLN:HG2	2.46	0.45
1:B:1191:LEU:HD21	1:B:1230:LEU:HD22	1.98	0.45
1:C:907:LEU:C	1:C:907:LEU:HD13	2.41	0.45
1:C:1055:LEU:C	1:C:1055:LEU:HD12	2.40	0.45
1:D:931:SER:HA	1:D:1065:LYS:H	1.80	0.45
1:D:1004:PHE:CD2	1:D:1076:TYR:HB2	2.50	0.45
1:D:1199:ASN:N	1:D:1199:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:GLU:HA	1:A:967:ARG:HB2	1.97	0.45
1:B:941:LYS:HG3	1:B:993:LEU:HD11	1.97	0.45
1:D:936:TRP:HB2	1:D:1058:ARG:CG	2.44	0.45
1:D:1113:PRO:HB3	1:D:1193:LEU:CD1	2.46	0.45
1:A:913:LYS:HB3	1:A:1043:PHE:O	2.16	0.45
1:B:908:SER:OG	1:B:909:SER:N	2.47	0.45
1:B:932:SER:CB	1:B:1008:THR:HG22	2.47	0.45
1:C:1087:ASP:C	1:C:1087:ASP:OD2	2.60	0.45
1:B:1114:GLU:CG	1:B:1115:SER:N	2.62	0.45
1:C:946:SER:O	1:C:968:ASN:HA	2.16	0.45
1:C:956:ILE:HG23	1:C:960:SER:N	2.31	0.45
1:C:972:GLU:HA	1:C:985:LEU:O	2.17	0.45
1:D:930:ASN:HD22	1:D:1010:ASN:HA	1.80	0.45
1:D:1085:ILE:HA	1:D:1209:ASN:ND2	2.31	0.45
1:B:950:TYR:HB2	1:B:966:ILE:CG1	2.47	0.45
1:B:982:TYR:CD1	1:B:982:TYR:C	2.95	0.45
1:B:1000:ASN:ND2	1:B:1273:GLY:HA3	2.31	0.45
1:C:1016:LYS:CB	1:C:1018:TYR:HE2	2.29	0.45
1:C:1045:ILE:HG22	1:C:1045:ILE:O	2.16	0.45
1:A:976:GLN:HA	1:A:981:LYS:O	2.17	0.45
1:A:1225:ARG:O	1:A:1226:GLU:HG3	2.16	0.45
1:B:1085:ILE:HD11	1:B:1151:ASN:HA	1.99	0.45
1:C:964:LEU:HD11	1:C:971:ILE:HG12	1.99	0.45
1:C:1010:ASN:HD22	1:C:1010:ASN:N	2.13	0.45
1:D:904:ASP:HA	1:D:1057:ILE:O	2.15	0.45
1:D:1048:ASN:C	1:D:1048:ASN:ND2	2.72	0.45
1:A:1126:ARG:C	1:A:1128:LYS:H	2.25	0.45
1:B:872:LEU:CG	1:B:879:LEU:HD11	2.47	0.45
1:C:1275:VAL:O	1:C:1276:GLU:HB3	2.15	0.45
1:D:934:SER:HB2	1:D:1004:PHE:CZ	2.51	0.45
1:D:973:TRP:O	1:D:984:SER:HB2	2.16	0.45
1:D:1087:ASP:HB2	1:D:1267:PHE:O	2.17	0.45
1:A:1109:ARG:HD3	1:A:1120:LEU:O	2.16	0.45
1:A:1201:GLY:HA2	1:A:1204:ILE:CG1	2.45	0.45
1:B:981:LYS:HE3	1:B:1031:ASP:HB2	1.99	0.45
1:B:1202:ILE:HB	2:B:61:HOH:O	2.16	0.45
1:B:1233:ASP:CB	1:B:1235:TYR:HE1	2.30	0.45
1:C:907:LEU:CG	1:C:1044:GLY:HA2	2.45	0.45
1:D:921:ASN:N	1:D:921:ASN:HD22	2.13	0.45
1:D:1002:TRP:CZ3	1:D:1058:ARG:HG2	2.51	0.45
1:C:919:ASN:ND2	1:C:921:ASN:HD22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:LEU:HD23	1:B:1062:ILE:HD12	1.99	0.45
1:B:1167:MET:HE3	1:B:1194:GLN:NE2	2.32	0.45
1:C:977:ASP:OD2	1:C:981:LYS:HB3	2.16	0.45
1:C:1095:PHE:CE2	1:C:1149:ILE:HG12	2.52	0.45
1:D:1175:ILE:HG22	1:D:1188:VAL:O	2.17	0.45
1:D:1231:LEU:HD12	1:D:1231:LEU:C	2.42	0.45
1:B:874:ASN:HD21	1:B:879:LEU:CD2	2.25	0.44
1:B:874:ASN:ND2	1:B:879:LEU:CD2	2.80	0.44
1:B:981:LYS:CE	1:B:1031:ASP:HB2	2.47	0.44
1:C:1095:PHE:CZ	1:C:1149:ILE:HG12	2.52	0.44
1:A:1106:TYR:HA	1:D:1163:SER:HB3	1.99	0.44
1:B:995:HIS:CE1	1:B:1129:LEU:HD13	2.53	0.44
1:D:986:ILE:HG12	1:D:987:PHE:N	2.32	0.44
1:A:1231:LEU:HD21	1:A:1251:VAL:HG11	2.00	0.44
1:C:899:THR:C	1:C:900:ILE:HG13	2.41	0.44
1:C:963:LYS:HZ2	1:C:974:ILE:HG12	1.82	0.44
1:A:1033:ASP:HB3	1:A:1034:GLU:H	1.64	0.44
1:B:901:TYR:CE1	1:B:1092:PRO:HD3	2.51	0.44
1:B:1212:SER:C	1:B:1214:ASN:H	2.26	0.44
1:C:953:ILE:HB	1:C:964:LEU:HB3	2.00	0.44
1:D:898:ASN:C	1:D:898:ASN:HD22	2.25	0.44
1:D:1073:ASN:O	1:D:1077:GLU:HB3	2.18	0.44
1:A:1050:ASP:OD1	1:A:1053:GLN:NE2	2.49	0.44
1:A:1261:THR:C	1:A:1263:SER:H	2.25	0.44
1:B:938:LYS:HZ3	1:B:1000:ASN:HD21	1.63	0.44
1:A:952:ILE:HG22	1:A:1045:ILE:CG1	2.42	0.44
1:B:939:ILE:HD12	1:B:989:TYR:CZ	2.52	0.44
1:B:981:LYS:HD3	1:B:1031:ASP:O	2.18	0.44
1:B:1241:SER:OG	1:B:1242:PHE:N	2.51	0.44
1:C:886:ASN:C	1:C:887:ALA:O	2.60	0.44
1:C:1019:ILE:O	1:C:1020:ASN:C	2.60	0.44
1:C:1028:LYS:HD3	1:C:1028:LYS:C	2.42	0.44
1:D:1185:GLN:HB2	1:D:1185:GLN:HE21	1.58	0.44
1:B:1270:ARG:HG2	1:B:1270:ARG:HH21	1.82	0.44
1:D:879:LEU:HD23	1:D:879:LEU:HA	1.83	0.44
1:D:958:GLN:O	1:D:959:ASN:CB	2.65	0.44
1:A:1167:MET:HE3	1:A:1203:GLY:HA3	1.99	0.44
1:C:918:LEU:O	1:C:1039:LYS:HG3	2.17	0.44
1:D:920:ASN:C	1:D:920:ASN:ND2	2.73	0.44
1:D:1135:ILE:HD13	1:D:1168:ILE:HD11	2.00	0.44
1:A:1143:LYS:HE2	1:A:1143:LYS:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:PHE:HE1	1:B:1024:LYS:HE2	1.83	0.44
1:B:1160:LEU:HD22	1:C:1105:ASN:ND2	2.31	0.44
1:A:956:ILE:HD12	1:A:963:LYS:HD3	2.00	0.43
1:B:967:ARG:HB3	1:B:967:ARG:CZ	2.48	0.43
1:B:1236:LYS:NZ	1:B:1244:ASN:ND2	2.66	0.43
1:C:972:GLU:HG3	1:C:974:ILE:CD1	2.42	0.43
1:C:982:TYR:CD1	1:C:982:TYR:C	2.96	0.43
1:D:977:ASP:C	1:D:979:ASN:H	2.26	0.43
1:D:1011:ILE:HD13	1:D:1011:ILE:N	2.33	0.43
1:D:1099:TYR:CE1	1:D:1269:SER:HB3	2.53	0.43
1:A:942:ASP:OD1	1:A:1052:ASN:HB3	2.18	0.43
1:A:958:GLN:NE2	1:A:960:SER:H	2.15	0.43
1:A:1051:GLU:O	1:A:1052:ASN:C	2.61	0.43
1:A:1068:SER:O	1:A:1072:ILE:HG13	2.18	0.43
1:B:1174:THR:HG21	1:B:1177:ALA:HB3	2.00	0.43
1:D:1133:ASN:HA	1:D:1134:PRO:HD2	1.88	0.43
1:A:931:SER:HB2	1:A:1063:PHE:O	2.19	0.43
1:B:1000:ASN:HD21	1:B:1273:GLY:HA3	1.84	0.43
1:B:1017:LEU:HD12	1:B:1018:TYR:H	1.83	0.43
1:B:1046:ASP:O	1:B:1047:GLU:C	2.62	0.43
1:C:953:ILE:HD12	1:C:964:LEU:HD23	2.00	0.43
1:C:1082:ARG:NH1	1:C:1211:VAL:HG13	2.34	0.43
1:A:941:LYS:O	1:A:944:THR:HG23	2.18	0.43
1:A:1171:ASP:O	1:A:1189:TYR:HD2	2.00	0.43
1:B:1121:VAL:HG12	1:B:1122:GLN:N	2.32	0.43
1:C:1010:ASN:ND2	1:C:1013:GLY:H	2.16	0.43
1:A:939:ILE:O	1:A:1000:ASN:HA	2.18	0.43
1:A:1024:LYS:O	1:A:1025:GLN:HB2	2.17	0.43
1:C:891:VAL:HG22	1:C:914:ILE:HG23	2.00	0.43
1:C:930:ASN:HA	1:C:1010:ASN:HA	1.99	0.43
1:A:1208:LYS:O	1:A:1209:ASN:C	2.62	0.43
1:C:905:PHE:CE1	1:C:1057:ILE:HB	2.53	0.43
1:C:1210:ILE:O	1:C:1210:ILE:CG2	2.65	0.43
1:A:1126:ARG:C	1:A:1128:LYS:N	2.76	0.43
1:A:1231:LEU:HA	1:A:1262:SER:O	2.19	0.43
1:B:1108:ASP:OD2	1:B:1108:ASP:C	2.60	0.43
1:A:986:ILE:HG12	1:A:987:PHE:N	2.34	0.43
1:B:925:SER:O	1:B:929:GLU:CB	2.66	0.43
1:B:1075:VAL:O	1:B:1076:TYR:C	2.61	0.43
1:B:1097:THR:HB	1:B:1099:TYR:CE2	2.54	0.43
1:C:974:ILE:N	1:C:974:ILE:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:898:ASN:C	1:D:898:ASN:ND2	2.75	0.43
1:D:928:TYR:CE1	1:D:1013:GLY:HA2	2.54	0.43
1:D:966:ILE:HG22	1:D:971:ILE:HG13	2.00	0.43
1:D:977:ASP:OD1	1:D:979:ASN:HB2	2.19	0.43
1:A:1231:LEU:HD22	1:A:1257:LYS:CD	2.45	0.43
1:C:939:ILE:N	1:C:939:ILE:HD12	2.34	0.43
1:C:958:GLN:NE2	1:C:960:SER:O	2.52	0.43
1:D:1129:LEU:O	1:D:1131:THR:N	2.46	0.43
1:B:933:VAL:HG23	1:B:1007:ILE:HB	2.00	0.43
1:B:1201:GLY:CA	1:B:1204:ILE:HG12	2.48	0.43
1:C:870:LEU:HB3	1:C:1062:ILE:HB	2.00	0.43
1:C:1210:ILE:HD13	1:C:1219:GLN:HG2	1.99	0.43
1:D:1096:ASP:HB2	1:D:1146:TYR:CD1	2.54	0.43
1:A:869:ILE:CG1	1:A:1062:ILE:HG22	2.49	0.42
1:A:1051:GLU:O	1:A:1053:GLN:N	2.52	0.42
1:B:987:PHE:CE2	1:B:989:TYR:HA	2.54	0.42
1:B:1109:ARG:HA	1:B:1121:VAL:O	2.18	0.42
1:C:888:GLU:HB3	1:C:917:ASN:HB2	2.01	0.42
1:C:1028:LYS:HD3	1:C:1029:ILE:H	1.71	0.42
1:C:1109:ARG:C	1:C:1123:TYR:HE2	2.27	0.42
1:D:1170:ARG:O	1:D:1202:ILE:HD11	2.19	0.42
1:B:870:LEU:O	1:B:1061:ASN:HA	2.19	0.42
1:B:986:ILE:H	1:B:1025:GLN:NE2	2.17	0.42
1:D:919:ASN:O	1:D:921:ASN:N	2.52	0.42
1:D:1018:TYR:N	1:D:1018:TYR:CD2	2.87	0.42
1:A:1113:PRO:HG3	1:A:1161:TYR:CE2	2.54	0.42
1:A:1223:SER:O	1:A:1224:PHE:O	2.37	0.42
1:B:1010:ASN:HD21	1:B:1014:TYR:CA	2.32	0.42
1:B:1015:MET:HE3	1:B:1015:MET:HB2	1.86	0.42
1:C:985:LEU:HD22	1:C:1025:GLN:HB3	2.02	0.42
1:C:1141:SER:HB2	1:D:920:ASN:OD1	2.19	0.42
1:D:1264:PHE:N	1:D:1264:PHE:CD1	2.87	0.42
1:A:1244:ASN:HD22	1:A:1244:ASN:HA	1.63	0.42
1:C:1106:TYR:HB3	1:C:1109:ARG:HD2	2.01	0.42
1:A:907:LEU:HD23	1:A:1055:LEU:HD11	1.99	0.42
1:A:1255:GLU:OE2	1:A:1255:GLU:N	2.48	0.42
1:B:939:ILE:HD11	1:B:971:ILE:HD12	2.01	0.42
1:C:885:TYR:CD1	1:C:885:TYR:N	2.87	0.42
1:C:935:PHE:HB3	1:C:1060:PHE:HA	2.01	0.42
1:C:1029:ILE:HG23	1:C:1032:LEU:CD1	2.47	0.42
1:C:1039:LYS:O	1:C:1039:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1167:MET:HE3	1:D:1169:ILE:CG2	2.50	0.42
1:B:1017:LEU:HD12	1:B:1018:TYR:N	2.34	0.42
1:C:905:PHE:O	1:C:1056:TRP:HA	2.19	0.42
1:C:920:ASN:C	1:C:922:ILE:N	2.76	0.42
1:D:1038:ASP:C	1:D:1040:THR:N	2.76	0.42
1:A:1101:ILE:HD13	1:A:1135:ILE:HD12	2.01	0.42
1:A:1257:LYS:HD2	1:D:1146:TYR:OH	2.19	0.42
1:B:955:SER:HB3	1:B:962:TRP:O	2.20	0.42
1:B:1033:ASP:HB3	1:B:1034:GLU:H	1.66	0.42
1:B:1109:ARG:NH1	1:B:1120:LEU:O	2.53	0.42
1:C:920:ASN:C	1:C:922:ILE:H	2.27	0.42
1:D:876:LYS:O	1:D:877:ASN:CB	2.61	0.42
1:D:935:PHE:HB3	1:D:1060:PHE:HA	2.01	0.42
1:A:932:SER:HB3	1:A:1008:THR:HA	2.02	0.42
1:C:867:SER:HG	1:C:1065:LYS:HG2	1.84	0.42
1:C:1007:ILE:N	1:C:1007:ILE:HD12	2.35	0.42
1:D:1142:ASP:O	1:D:1143:LYS:HB3	2.19	0.42
1:A:1019:ILE:O	1:A:1020:ASN:C	2.63	0.42
1:B:1175:ILE:HD13	1:B:1237:PRO:HA	2.01	0.42
1:C:1210:ILE:HD13	1:C:1219:GLN:CG	2.50	0.42
1:D:920:ASN:C	1:D:920:ASN:HD22	2.28	0.42
1:D:1073:ASN:ND2	1:D:1213:LYS:HZ1	2.18	0.42
1:A:1094:LYS:HD2	1:A:1146:TYR:O	2.20	0.42
1:B:986:ILE:H	1:B:1025:GLN:HE22	1.67	0.42
1:D:1057:ILE:CG2	1:D:1058:ARG:N	2.82	0.42
1:A:938:LYS:HZ3	1:A:1000:ASN:HD21	1.68	0.41
1:A:980:ARG:O	1:A:980:ARG:CG	2.60	0.41
1:A:1011:ILE:H	1:A:1011:ILE:CD1	2.33	0.41
1:A:1113:PRO:O	1:A:1114:GLU:CB	2.68	0.41
1:D:932:SER:CB	1:D:1067:LEU:HD21	2.49	0.41
1:A:982:TYR:C	1:A:982:TYR:CD1	2.98	0.41
1:A:1118:LEU:N	1:A:1118:LEU:HD22	2.35	0.41
1:B:909:SER:N	1:B:1049:ILE:HD11	2.36	0.41
1:B:942:ASP:HB2	1:B:1052:ASN:O	2.20	0.41
1:C:941:LYS:HE3	1:C:1274:TRP:CD2	2.55	0.41
1:C:1029:ILE:N	1:C:1029:ILE:HD12	2.35	0.41
1:C:1032:LEU:HB3	1:C:1035:VAL:CG2	2.44	0.41
1:D:1199:ASN:N	1:D:1199:ASN:ND2	2.68	0.41
1:A:919:ASN:O	1:A:920:ASN:C	2.63	0.41
1:A:1241:SER:OG	1:A:1243:LYS:HB2	2.20	0.41
1:B:920:ASN:ND2	1:B:1039:LYS:NZ	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:SER:HB3	1:C:912:ASP:OD1	2.19	0.41
1:C:931:SER:O	1:C:932:SER:HB3	2.20	0.41
1:C:1138:LYS:HG3	1:C:1158:HIS:NE2	2.35	0.41
1:A:975:LEU:HD23	1:A:975:LEU:HA	1.89	0.41
1:A:1113:PRO:HB3	1:A:1193:LEU:HD11	2.03	0.41
1:B:1011:ILE:HD13	1:B:1011:ILE:N	2.34	0.41
1:A:1166:TYR:HB3	1:A:1193:LEU:HB3	2.01	0.41
1:A:1201:GLY:CA	1:A:1204:ILE:HG12	2.47	0.41
1:A:1238:TRP:CZ3	1:A:1243:LYS:HG2	2.56	0.41
1:C:1137:ILE:CG2	1:C:1155:ILE:HB	2.51	0.41
1:C:930:ASN:HB3	1:C:1066:GLU:N	2.35	0.41
1:D:1228:THR:OG1	1:D:1229:MET:N	2.54	0.41
1:A:1010:ASN:HD21	1:A:1014:TYR:H	1.68	0.41
1:C:1063:PHE:CD2	1:C:1067:LEU:HD11	2.56	0.41
1:D:954:ASN:HD21	1:D:956:ILE:HB	1.86	0.41
1:D:1116:ASN:O	1:D:1117:VAL:HG23	2.21	0.41
1:A:990:SER:C	1:A:992:SER:N	2.75	0.41
1:C:982:TYR:C	1:C:982:TYR:HD1	2.28	0.41
1:C:1192:LYS:NZ	1:C:1239:ARG:HH22	2.18	0.41
1:D:964:LEU:HD11	1:D:971:ILE:HG12	2.03	0.41
1:A:916:VAL:O	1:A:1040:THR:HA	2.21	0.41
1:A:948:ASN:HB2	1:A:950:TYR:CE2	2.56	0.41
1:A:964:LEU:HB2	1:A:973:TRP:CZ3	2.55	0.41
1:A:1099:TYR:CE1	1:A:1269:SER:HB3	2.56	0.41
1:B:1234:ILE:O	1:B:1234:ILE:HG23	2.21	0.41
1:C:1271:ASP:CG	1:C:1272:PRO:HD2	2.45	0.41
1:A:930:ASN:O	1:A:931:SER:HB3	2.21	0.41
1:A:994:SER:O	1:A:996:THR:N	2.54	0.41
1:A:1080:ILE:O	1:A:1081:LEU:HB2	2.21	0.41
1:A:1229:MET:HE2	1:A:1254:TYR:CB	2.51	0.41
1:B:960:SER:HA	1:B:976:GLN:O	2.21	0.41
1:B:983:LYS:HB2	1:B:983:LYS:HE2	1.90	0.41
1:B:1163:SER:CB	1:C:1108:ASP:OD2	2.68	0.41
1:C:872:LEU:N	1:C:872:LEU:HD12	2.35	0.41
1:C:1016:LYS:HB3	1:C:1018:TYR:CE2	2.56	0.41
1:B:1102:ILE:HD11	1:B:1268:ILE:HD11	2.03	0.40
1:B:1220:ILE:HB	1:B:1230:LEU:HD12	2.02	0.40
1:C:930:ASN:ND2	1:C:1010:ASN:HA	2.36	0.40
1:D:937:ILE:HG13	1:D:938:LYS:N	2.35	0.40
1:D:939:ILE:O	1:D:1000:ASN:N	2.52	0.40
1:D:987:PHE:HB2	1:D:1017:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1117:VAL:O	1:D:1119:VAL:HG13	2.21	0.40
1:A:977:ASP:OD1	1:A:979:ASN:N	2.53	0.40
1:C:966:ILE:HG13	1:C:966:ILE:O	2.21	0.40
1:C:1229:MET:SD	1:C:1258:LEU:HD12	2.61	0.40
1:D:983:LYS:CE	1:D:1032:LEU:HG	2.51	0.40
1:D:1073:ASN:ND2	1:D:1213:LYS:NZ	2.70	0.40
1:D:1118:LEU:HD22	1:D:1118:LEU:H	1.86	0.40
1:D:1244:ASN:HD22	1:D:1244:ASN:HA	1.73	0.40
1:A:928:TYR:CD1	1:A:928:TYR:N	2.89	0.40
1:A:1016:LYS:HB2	1:A:1018:TYR:CE2	2.56	0.40
1:B:1095:PHE:CE2	1:B:1143:LYS:HD2	2.55	0.40
1:C:1059:ASP:OD1	1:C:1059:ASP:N	2.54	0.40
1:D:894:ASN:O	1:D:895:VAL:C	2.63	0.40
1:A:911:GLY:C	1:A:913:LYS:HD3	2.46	0.40
1:A:1011:ILE:C	1:A:1013:GLY:N	2.79	0.40
1:A:1151:ASN:ND2	1:A:1208:LYS:HG2	2.36	0.40
1:B:907:LEU:N	1:B:907:LEU:CD2	2.84	0.40
1:B:1047:GLU:O	1:B:1049:ILE:HG23	2.21	0.40
1:B:1167:MET:HE3	1:B:1194:GLN:HE21	1.87	0.40
1:C:1082:ARG:CZ	1:C:1211:VAL:HG13	2.52	0.40
1:D:913:LYS:HD3	1:D:1042:VAL:CG1	2.51	0.40
1:D:972:GLU:HA	1:D:986:ILE:HA	2.03	0.40
1:A:913:LYS:CB	1:A:1043:PHE:O	2.70	0.40
1:A:986:ILE:CG1	1:A:987:PHE:N	2.85	0.40
1:A:1105:ASN:ND2	1:A:1262:SER:HB3	2.37	0.40
1:C:1010:ASN:ND2	1:C:1010:ASN:N	2.69	0.40
1:D:939:ILE:HG22	1:D:944:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/415 (96%)	328 (82%)	53 (13%)	17 (4%)	2	3
1	B	401/415 (97%)	327 (82%)	57 (14%)	17 (4%)	2	3
1	C	397/415 (96%)	326 (82%)	52 (13%)	19 (5%)	2	2
1	D	400/415 (96%)	340 (85%)	39 (10%)	21 (5%)	1	2
All	All	1596/1660 (96%)	1321 (83%)	201 (13%)	74 (5%)	2	2

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	LYS
1	A	920	ASN
1	A	1127	SER
1	A	1142	ASP
1	A	1224	PHE
1	B	895	VAL
1	B	1031	ASP
1	B	1145	PRO
1	B	1213	LYS
1	B	1224	PHE
1	C	876	LYS
1	C	958	GLN
1	C	987	PHE
1	C	991	GLU
1	C	1145	PRO
1	C	1224	PHE
1	D	921	ASN
1	D	959	ASN
1	D	1065	LYS
1	D	1145	PRO
1	D	1185	GLN
1	D	1224	PHE
1	D	1258	LEU
1	A	980	ARG
1	A	1031	ASP
1	A	1052	ASN
1	B	892	GLY
1	B	908	SER
1	B	912	ASP
1	B	1012	MET
1	C	887	ALA
1	C	921	ASN
1	C	940	SER

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Mol	Chain	Res	Type
1	D	920	ASN
1	D	1033	ASP
1	D	1130	TYR
1	A	935	PHE
1	A	946	SER
1	A	1033	ASP
1	B	910	SER
1	B	919	ASN
1	B	935	PHE
1	B	1048	ASN
1	B	1184	SER
1	C	1033	ASP
1	C	1047	GLU
1	C	1115	SER
1	C	1254	TYR
1	D	895	VAL
1	D	1081	LEU
1	D	1114	GLU
1	D	1143	LYS
1	D	1240	ALA
1	A	1027	GLN
1	A	1114	GLU
1	A	1145	PRO
1	B	876	LYS
1	C	886	ASN
1	C	932	SER
1	D	929	GLU
1	D	935	PHE
1	D	1186	ASN
1	D	1199	ASN
1	A	1051	GLU
1	A	1081	LEU
1	A	1209	ASN
1	B	886	ASN
1	B	1030	GLU
1	C	900	ILE
1	C	1124	PRO
1	D	877	ASN
1	C	957	GLU
1	C	986	ILE
1	D	1117	VAL

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	378/386 (98%)	351 (93%)	27 (7%)	13	25
1	B	380/386 (98%)	343 (90%)	37 (10%)	8	15
1	C	377/386 (98%)	356 (94%)	21 (6%)	19	36
1	D	380/386 (98%)	349 (92%)	31 (8%)	10	20
All	All	1515/1544 (98%)	1399 (92%)	116 (8%)	12	22

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	872	LEU
1	A	879	LEU
1	A	893	ASP
1	A	913	LYS
1	A	932	SER
1	A	944	THR
1	A	947	HIS
1	A	959	ASN
1	A	975	LEU
1	A	993	LEU
1	A	1010	ASN
1	A	1011	ILE
1	A	1018	TYR
1	A	1031	ASP
1	A	1046	ASP
1	A	1050	ASP
1	A	1145	PRO
1	A	1151	ASN
1	A	1172	THR
1	A	1187	CYS
1	A	1206	SER
1	A	1207	ILE
1	A	1217	CYS
1	A	1234	ILE

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Mol	Chain	Res	Type
1	A	1243	LYS
1	A	1244	ASN
1	A	1249	VAL
1	B	898	ASN
1	B	904	ASP
1	B	907	LEU
1	B	920	ASN
1	B	921	ASN
1	B	933	VAL
1	B	971	ILE
1	B	978	VAL
1	B	990	SER
1	B	993	LEU
1	B	1010	ASN
1	B	1011	ILE
1	B	1027	GLN
1	B	1033	ASP
1	B	1034	GLU
1	B	1052	ASN
1	B	1053	GLN
1	B	1055	LEU
1	B	1066	GLU
1	B	1073	ASN
1	B	1077	GLU
1	B	1118	LEU
1	B	1141	SER
1	B	1145	PRO
1	B	1146	TYR
1	B	1151	ASN
1	B	1167	MET
1	B	1172	THR
1	B	1174	THR
1	B	1185	GLN
1	B	1191	LEU
1	B	1210	ILE
1	B	1215	LYS
1	B	1228	THR
1	B	1247	THR
1	B	1266	LYS
1	B	1268	ILE
1	C	874	ASN
1	C	912	ASP

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Mol	Chain	Res	Type
1	C	941	LYS
1	C	952	ILE
1	C	968	ASN
1	C	975	LEU
1	C	982	TYR
1	C	1010	ASN
1	C	1011	ILE
1	C	1012	MET
1	C	1018	TYR
1	C	1046	ASP
1	C	1077	GLU
1	C	1081	LEU
1	C	1089	TRP
1	C	1151	ASN
1	C	1163	SER
1	C	1173	ASP
1	C	1210	ILE
1	C	1258	LEU
1	C	1261	THR
1	D	869	ILE
1	D	872	LEU
1	D	879	LEU
1	D	906	LYS
1	D	907	LEU
1	D	921	ASN
1	D	923	LEU
1	D	941	LYS
1	D	943	LEU
1	D	945	ASN
1	D	952	ILE
1	D	968	ASN
1	D	981	LYS
1	D	1010	ASN
1	D	1011	ILE
1	D	1031	ASP
1	D	1034	GLU
1	D	1049	ILE
1	D	1050	ASP
1	D	1067	LEU
1	D	1114	GLU
1	D	1140	VAL
1	D	1145	PRO

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Mol	Chain	Res	Type
1	D	1162	ASN
1	D	1185	GLN
1	D	1206	SER
1	D	1228	THR
1	D	1242	PHE
1	D	1244	ASN
1	D	1256	THR
1	D	1258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	873	GLN
1	A	886	ASN
1	A	896	GLN
1	A	898	ASN
1	A	919	ASN
1	A	920	ASN
1	A	921	ASN
1	A	930	ASN
1	A	958	GLN
1	A	959	ASN
1	A	968	ASN
1	A	1000	ASN
1	A	1010	ASN
1	A	1025	GLN
1	A	1048	ASN
1	A	1069	ASN
1	A	1105	ASN
1	A	1116	ASN
1	A	1151	ASN
1	A	1162	ASN
1	A	1199	ASN
1	A	1219	GLN
1	A	1244	ASN
1	B	874	ASN
1	B	896	GLN
1	B	898	ASN
1	B	919	ASN
1	B	920	ASN
1	B	921	ASN
1	B	945	ASN

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Mol	Chain	Res	Type
1	B	958	GLN
1	B	959	ASN
1	B	968	ASN
1	B	970	ASN
1	B	976	GLN
1	B	995	HIS
1	B	1000	ASN
1	B	1010	ASN
1	B	1048	ASN
1	B	1053	GLN
1	B	1061	ASN
1	B	1073	ASN
1	B	1083	ASN
1	B	1116	ASN
1	B	1151	ASN
1	B	1158	HIS
1	B	1185	GLN
1	B	1199	ASN
1	B	1219	GLN
1	B	1244	ASN
1	C	865	ASN
1	C	877	ASN
1	C	898	ASN
1	C	919	ASN
1	C	921	ASN
1	C	930	ASN
1	C	948	ASN
1	C	958	GLN
1	C	968	ASN
1	C	995	HIS
1	C	1000	ASN
1	C	1010	ASN
1	C	1027	GLN
1	C	1053	GLN
1	C	1069	ASN
1	C	1073	ASN
1	C	1079	GLN
1	C	1185	GLN
1	C	1199	ASN
1	C	1219	GLN
1	C	1227	ASN
1	C	1244	ASN

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Mol	Chain	Res	Type
1	D	862	ASN
1	D	877	ASN
1	D	898	ASN
1	D	919	ASN
1	D	921	ASN
1	D	930	ASN
1	D	954	ASN
1	D	968	ASN
1	D	976	GLN
1	D	1000	ASN
1	D	1010	ASN
1	D	1025	GLN
1	D	1027	GLN
1	D	1048	ASN
1	D	1053	GLN
1	D	1073	ASN
1	D	1105	ASN
1	D	1116	ASN
1	D	1158	HIS
1	D	1185	GLN
1	D	1186	ASN
1	D	1199	ASN
1	D	1209	ASN
1	D	1219	GLN
1	D	1244	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/415 (97%)	-1.35	0 100 100	28, 60, 94, 106	0
1	B	407/415 (98%)	-1.36	0 100 100	29, 55, 91, 104	0
1	C	403/415 (97%)	-1.26	0 100 100	33, 68, 107, 120	0
1	D	406/415 (97%)	-1.35	0 100 100	31, 60, 96, 105	0
All	All	1620/1660 (97%)	-1.33	0 100 100	28, 61, 100, 120	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.