



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 04:47 pm GMT

PDB ID : 3RMX
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

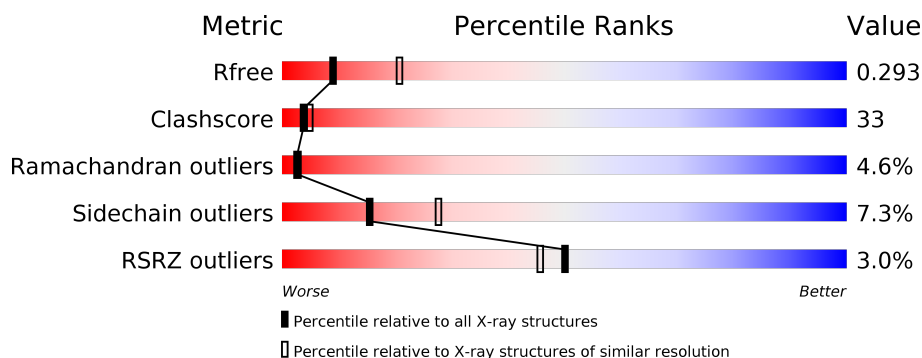
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	4013 (2.80-2.72)
Clashscore	122126	1029 (2.78-2.74)
Ramachandran outliers	120053	1013 (2.78-2.74)
Sidechain outliers	120020	1013 (2.78-2.74)
RSRZ outliers	108989	3920 (2.80-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	415	<div> <div>6%</div> <div>46%</div> <div>44%</div> <div>7%</div> <div>•</div> </div>
1	B	415	<div> <div>42%</div> <div>46%</div> <div>9%</div> <div>•</div> </div>
1	C	415	<div> <div>6%</div> <div>45%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>
1	D	415	<div> <div>3%</div> <div>48%</div> <div>43%</div> <div>6%</div> <div>••</div> </div>

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

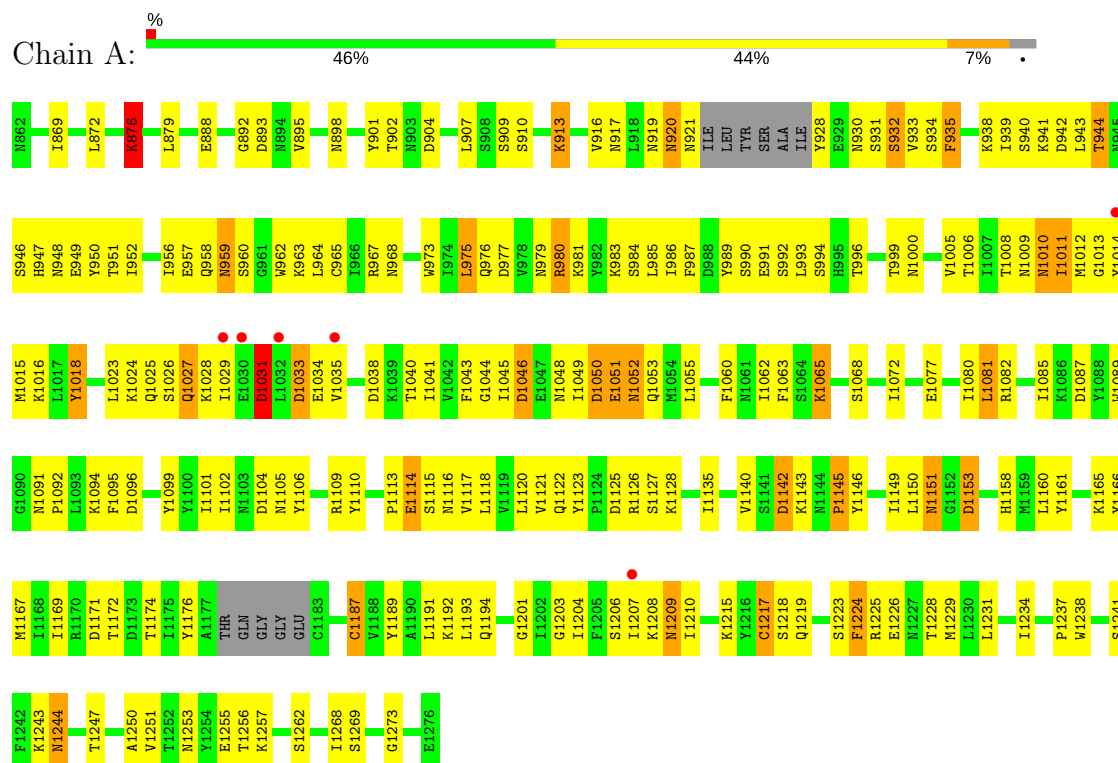
- Molecule 2 is water.

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		

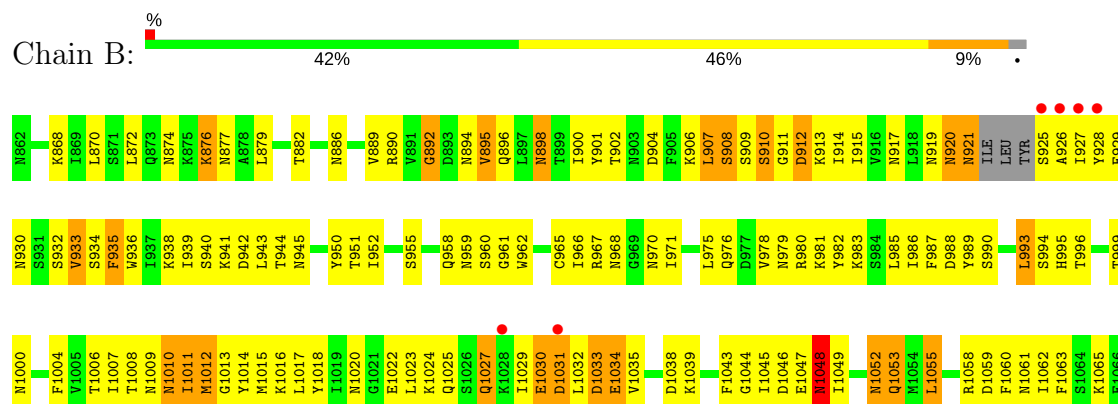
3 Residue-property plots

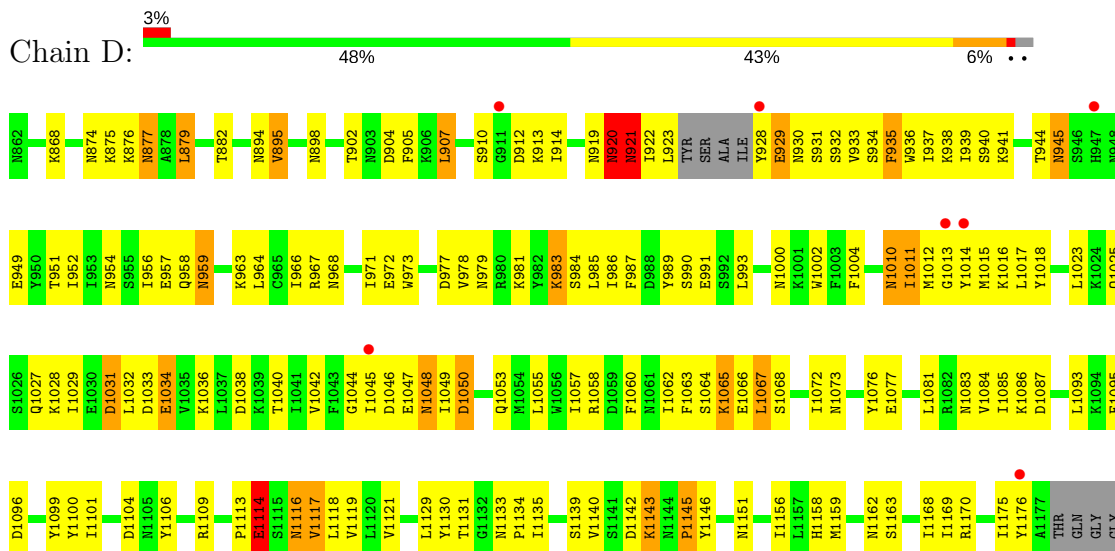
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Botulinum neurotoxin type 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 – 2.74	Depositor EDS
% Data completeness (in resolution range)	96.3 (36.61-2.75) 95.8 (36.61-2.74)	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)	0.31 , 31.9	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	0.90	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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	0/3385	0.66	0/4583
1	B	0.45	0/3404	0.67	0/4609
1	C	0.41	0/3371	0.65	0/4564
1	D	0.43	0/3401	0.65	0/4605
All	All	0.43	0/13561	0.66	0/18361

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 [i](#)

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	196	0
1	B	3336	0	3281	259	0
1	C	3304	0	3256	231	0
1	D	3333	0	3282	188	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	865	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 33.

All (865) 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: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:B:1114:GLU:HG3	1:B:1115:SER:N	1.87	0.90
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LYS:HZ3	1:A:1031:ASP:HB2	1.45	0.80
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:1011:ILE:HD13	1:C:1011:ILE:H	1.46	0.80
1:C:1010:ASN:HD21	1:C:1014:TYR:H	1.27	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: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:1183:CYS:HB3	1:D:1189:TYR:OH	1.83	0.77
1:D:876:LYS:O	1:D:877:ASN:HB2	1.85	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
1:B:952:ILE:HD11	1:B:966:ILE:HG12	1.67	0.76
1:D:983:LYS:HZ1	1:D:1031:ASP:HB2	1.49	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: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:N	1:B:1146:TYR:HD2	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:B:958:GLN:H	1:B:958:GLN:CD	1.91	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:B:1065:LYS:HZ2	1:B:1067:LEU:HD23	1.54	0.73
1:C:865:ASN:O	1:C:868:LYS:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1146:TYR:N	1:B:1146:TYR:CD2	2.58	0.70
1:B:1233:ASP:HB3	1:B:1235:TYR:CE1	2.27	0.70
1:B:958:GLN:HE21	1:B:960:SER:N	1.88	0.70
1:B:907:LEU:HD12	1:B:1044:GLY:CA	2.20	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: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: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:B:898:ASN:ND2	1:B:902:THR:HA	2.07	0.68
1:C:1029:ILE:HG23	1:C:1032:LEU:HD12	1.76	0.68
1:A:980:ARG:HG2	1:A:980:ARG:O	1.92	0.68
1:B:1055:LEU:HG	1:B:1055:LEU:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:994:SER:C	1:B:996:THR:H	1.95	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:1231:LEU:HD22	1:A:1257:LYS:HD3	1.78	0.66
1:A:898:ASN:ND2	1:A:902:THR:HA	2.10	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
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:1183:CYS:SG	1:B:1184:SER:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:957:GLU:HB2	1:D:1038:ASP:OD2	1.98	0.62
1:A:1046:ASP:OD2	1:A:1046:ASP:N	2.31	0.62
1:A:983:LYS:NZ	1:A:1029:ILE:HA	2.14	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: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
1:C:992:SER:O	1:C:993:LEU:HB2	2.00	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:A:981:LYS:HZ3	1:A:1031:ASP:C	2.04	0.61
1:C:952:ILE:H	1:C:952:ILE:HD13	1.65	0.61
1:D:945:ASN:OD1	1:D:993:LEU:HD11	1.99	0.61
1:B:1151:ASN:CB	1:B:1208:LYS:HA	2.30	0.61
1:B:958:GLN:HG2	1:B:959:ASN:N	2.06	0.61
1:A:943:LEU:HB2	1:A:1053:GLN:HA	1.80	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:D:894:ASN:HB2	1:D:912:ASP:CG	2.21	0.61
1:A:913:LYS:HG3	1:A:1044:GLY:HA3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1009:ASN:OD1	1:C:1015:MET:HB3	2.01	0.61
1:C:958:GLN:HE21	1:C:960:SER:N	1.88	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:A:1167:MET:HE3	1:A:1203:GLY:HA3	1.83	0.60
1:B:1255:GLU:OE2	1:B:1255:GLU:HA	2.00	0.60
1:D:934:SER:O	1:D:935:PHE:HB3	2.02	0.60
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:B:936:TRP:HB2	1:B:1058:ARG:HG2	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: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:896:GLN:NE2	1:B:906:LYS:HD2	2.18	0.59
1:B:930:ASN:HA	1:B:1009:ASN:O	2.02	0.59
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: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:1239:ARG:HD3	1:C:1239:ARG:H	1.67	0.58
1:D:1010:ASN:HD22	1:D:1010:ASN:C	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:A:1011:ILE:HD13	1.69	0.58
1:A:973:TRP:O	1:A:984:SER:HB2	2.04	0.57
1:A:1104:ASP:OD1	1:A:1215:LYS:HE3	2.04	0.57
1:A:956:ILE:HD13	1:A:976:GLN:OE1	2.04	0.57
1:B:1257:LYS:O	1:B:1260:SER:HB3	2.02	0.57
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:C:1073:ASN:HD21	1:C:1213:LYS:HZ3	1.53	0.57
1:C:1255:GLU:OE2	1:C:1255:GLU:HA	2.03	0.57
1:C:1018:TYR:N	1:C:1018:TYR:CD2	2.72	0.57
1:C:870:LEU:HD23	1:C:1062:ILE:HD12	1.85	0.57
1:C:882:THR:O	1:C:882:THR:HG22	2.04	0.57
1:B:911:GLY:O	1:B:912:ASP:C	2.43	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:1073:ASN:ND2	1:C:1213:LYS:NZ	2.51	0.57
1:C:879:LEU:O	1:C:889:VAL:HG11	2.05	0.57
1:B:983:LYS:HE3	1:B:1030:GLU:H	1.69	0.57
1:B:934:SER:O	1:B:935:PHE:HB3	2.03	0.57
1:C:986:ILE:HG22	1:C:1025:GLN:OE1	2.05	0.57
1:A:1050:ASP:CG	1:A:1053:GLN:HE21	2.08	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1271:ASP:OD1	1:C:1272:PRO:HD2	2.06	0.56
1:C:986:ILE:HG12	1:C:987:PHE:N	2.16	0.56
1:D:1048:ASN:HD22	1:D:1048:ASN:C	2.09	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
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:A:901:TYR:CZ	1:A:1092:PRO:HD3	2.41	0.55
1:C:874:ASN:HA	1:C:878:ALA:O	2.07	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:H	1:B:921:ASN:HD22	1.55	0.55
1:C:1073:ASN:ND2	1:C:1213:LYS:HZ3	2.04	0.55
1:D:1045:ILE:HB	1:D:1047:GLU:OE2	2.07	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: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:O	1:D:1276:GLU:HG3	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:1000:ASN:O	1:C:1089:TRP:HB3	2.07	0.54
1:C:963:LYS:NZ	1:C:974:ILE:HG12	2.21	0.54
1:C:978:VAL:HG13	1:C:1034:GLU:O	2.07	0.54
1:B:894:ASN:O	1:B:895:VAL:C	2.46	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: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:B:952:ILE:N	1:B:952:ILE:HD12	2.23	0.54
1:D:910:SER:HB2	1:D:1046:ASP:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1029:ILE:CG2	1:C:1032:LEU:HD12	2.37	0.54
1:C:919:ASN:ND2	1:C:921:ASN:ND2	2.55	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:A:958:GLN:CD	1:A:958:GLN:H	2.10	0.54
1:B:876:LYS:C	1:B:877:ASN:HD22	2.11	0.54
1:B:968:ASN:O	1:B:968:ASN:ND2	2.40	0.54
1:C:872:LEU:HD13	1:C:1060:PHE:HD2	1.71	0.54
1:D:1175:ILE:HG23	1:D:1176:TYR:CD1	2.43	0.54
1:D:937:ILE:HD11	1:D:1055:LEU:HD13	1.90	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:959:ASN:HD22	1:A:959:ASN:C	2.12	0.54
1:B:1106:TYR:HB3	1:B:1109:ARG:HD2	1.90	0.53
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:D:1064:SER:O	1:D:1065:LYS:CB	2.55	0.53
1:C:1010:ASN:HD21	1:C:1014:TYR:N	2.03	0.53
1:C:936:TRP:HB2	1:C:1058:ARG:HG2	1.91	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: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:1028:LYS:C	1:C:1029:ILE:HD12	2.29	0.53
1:C:1073:ASN:HD21	1:C:1213:LYS:HZ1	1.56	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:909:SER:O	1:B:910:SER:C	2.45	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:N	1:A:876:LYS:HD2	2.23	0.53
1:C:1151:ASN:HB2	1:C:1208:LYS:HA	1.90	0.53
1:C:1085:ILE:CD1	1:C:1151:ASN:HB3	2.35	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:C:1015:MET:CE	1:C:1029:ILE:HD11	2.39	0.53
1:B:1006:THR:C	1:B:1007:ILE:HD12	2.29	0.53
1:D:1029:ILE:CG2	1:D:1032:LEU:HD12	2.39	0.53
1:A:934:SER:O	1:A:935:PHE:HB3	2.09	0.53
1:A:1005:VAL:HG12	1:A:1006:THR:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:ILE:CD1	1:A:1135:ILE:HB	2.39	0.53
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:952:ILE:HG21	1:A:1055:LEU:HD21	1.91	0.52
1:A:919:ASN:O	1:A:921:ASN:N	2.42	0.52
1:B:1022:GLU:O	1:B:1024:LYS:HG2	2.08	0.52
1:B:951:THR:O	1:B:1045:ILE:HG22	2.09	0.52
1:D:1095:PHE:CZ	1:D:1139:SER:HB3	2.44	0.52
1:B:1276:GLU:HG3	1:B:1276:GLU:O	2.10	0.52
1:A:951:THR:HA	1:A:965:CYS:CB	2.39	0.52
1:D:1067:LEU:H	1:D:1067:LEU:HD23	1.74	0.52
1:D:985:LEU:HG	1:D:1015:MET:CE	2.39	0.52
1:B:952:ILE:CD1	1:B:966:ILE:HG12	2.38	0.52
1:A:1010:ASN:C	1:A:1010:ASN:HD22	2.12	0.52
1:A:1113:PRO:O	1:A:1114:GLU:HB3	2.10	0.52
1:B:890:ARG:HB2	1:B:915:ILE:HB	1.91	0.52
1:C:1026:SER:O	1:C:1027:GLN:HG3	2.10	0.52
1:C:986:ILE:O	1:C:987:PHE:HB2	2.09	0.52
1:D:1118:LEU:O	1:D:1248:PRO:HD2	2.10	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:D:921:ASN:N	1:D:921:ASN:ND2	2.58	0.52
1:B:1217:CYS:HB3	1:B:1266:LYS:HG3	1.91	0.52
1:C:1029:ILE:HG22	1:C:1029:ILE:O	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:B:983:LYS:HZ2	1:B:1030:GLU:HB2	1.73	0.51
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:C:1118:LEU:O	1:C:1248:PRO:HD2	2.10	0.51
1:A:1109:ARG:HA	1:A:1121:VAL:O	2.09	0.51
1:A:940:SER:HB2	1:A:1273:GLY:O	2.10	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:1254:TYR:CD1	1:C:1258:LEU:HD13	2.44	0.51
1:D:1187:CYS:HB2	1:D:1252:THR:HG23	1.92	0.51
1:D:939:ILE:HD12	1:D:989:TYR:CZ	2.45	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:1066:GLU:O	1:D:1066:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:990:SER:O	1:D:991:GLU:HB2	2.11	0.51
1:B:961:GLY:O	1:B:975:LEU:HD12	2.11	0.51
1:B:928:TYR:HA	1:B:1010:ASN:O	2.10	0.51
1:B:1215:LYS:HZ1	1:B:1264:PHE:HD2	1.59	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:B:868:LYS:HE3	1:B:1063:PHE:CE1	2.46	0.51
1:D:985:LEU:HG	1:D:1015:MET:HE3	1.93	0.51
1:B:1004:PHE:HB3	1:B:1020:ASN:HA	1.93	0.50
1:B:958:GLN:CG	1:B:959:ASN:N	2.69	0.50
1:C:1104:ASP:OD2	1:C:1266:LYS:HE3	2.11	0.50
1:A:957:GLU:CD	1:A:1038:ASP:HB3	2.31	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:A:1150:LEU:O	1:A:1153:ASP:HB2	2.11	0.50
1:C:1171:ASP:OD2	1:C:1172:THR:N	2.45	0.50
1:C:920:ASN:O	1:C:922:ILE: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: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: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:B:927:ILE:CG2	1:B:1029:ILE:HD13	2.25	0.50
1:B:1242:PHE:HD1	1:B:1242:PHE:O	1.94	0.50
1:B:872:LEU:HG	1:B:879:LEU:HD11	1.93	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: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
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:B:1049:ILE:CD1	1:B:1053:GLN:HB2	2.36	0.49
1:A:1009:ASN:OD1	1:A:1015:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:GLU:OE1	1:A:1038:ASP:HB3	2.12	0.49
1:C:1010:ASN:H	1:C:1010:ASN:HD22	1.58	0.49
1:A:1055:LEU:C	1:A:1055:LEU:HD12	2.32	0.49
1:A:994:SER:C	1:A:996:THR:H	2.15	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:1095:PHE:CZ	1:A:1149:ILE:HG12	2.48	0.49
1:A:931:SER:HA	1:A:1065:LYS:N	2.28	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:A:904:ASP:OD1	1:A:904:ASP:C	2.51	0.49
1:A:990:SER:C	1:A:992:SER:H	2.16	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:A:1169:ILE:HD13	1:A:1194:GLN:HB2	1.95	0.49
1:A:973:TRP:O	1:A:984:SER:CB	2.61	0.49
1:B:1016:LYS:HB3	1:B:1023:LEU:CD1	2.43	0.49
1:B:939:ILE:HD12	1:B:989:TYR:CE1	2.48	0.49
1:C:956:ILE:C	1:C:958:GLN:H	2.16	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:B:925:SER:O	1:B:929:GLU:HB3	2.13	0.48
1:C:1154:ASN:HA	1:C:1205:PHE:O	2.13	0.48
1:A:1010:ASN:C	1:A:1010:ASN:ND2	2.67	0.48
1:A:1207:ILE:HG13	1:A:1218:SER:CB	2.43	0.48
1:A:958:GLN:CG	1:A:959:ASN:N	2.74	0.48
1:B:913:LYS:HG2	1:B:1044:GLY:HA3	1.94	0.48
1:B:901:TYR:CZ	1:B:1092:PRO:HD3	2.48	0.48
1:C:1226:GLU:HG3	1:D:876:LYS:NZ	2.29	0.48
1:A:1011:ILE:HG12	1:A:1012:MET:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1237:PRO:HG2	1:C:1238:TRP:H	1.78	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:941:LYS:HE3	1:C:1274:TRP:CE2	2.48	0.48
1:C:967:ARG:HH11	1:C:967:ARG:HG3	1.78	0.48
1:C:956:ILE:HD13	1:C:976:GLN:OE1	2.14	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: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:B:968:ASN:CG	1:B:968:ASN:O	2.53	0.47
1:D:910:SER:HB3	1:D:1047:GLU:O	2.14	0.47
1:D:919:ASN:O	1:D:920:ASN:C	2.52	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:1034:GLU:HG3	1:D:1034:GLU:O	2.15	0.47
1:D:951:THR:O	1:D:1045:ILE:HG22	2.13	0.47
1:D:1057:ILE:HG22	1:D:1058:ARG:N	2.28	0.47
1:D:1135:ILE:HG12	1:D:1159:MET:HG3	1.96	0.47
1:D:949:GLU:HG3	1:D:967:ARG:HB2	1.96	0.47
1:A:1087:ASP:OD2	1:A:1087:ASP:C	2.53	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:1084:VAL:O	1:D:1086:LYS:HE3	2.13	0.47
1:D:981:LYS:HE2	2:D:72:HOH:O	2.14	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:1043:PHE:HZ	1:C:1060:PHE:CE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:LEU:O	1:A:1247:THR:OG1	2.31	0.47
1:B:1167:MET:HE3	1:B:1200:TYR:CD1	2.49	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:1229:MET:O	1:D:1250:ALA:HA	2.15	0.47
1:D:941:LYS:NZ	1:D:1274:TRP:CE2	2.83	0.47
1:A:1012:MET:O	1:A:1028:LYS:HE3	2.14	0.47
1:B:1143:LYS:O	1:B:1144:ASN:C	2.51	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:1030:GLU:C	1:C:1032:LEU:H	2.18	0.47
1:C:1275:VAL:O	1:C:1276:GLU:HB3	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:1125:ASP:OD2	1:A:1128:LYS:HG2	2.15	0.46
1:A:958:GLN:HE21	1:A:960:SER:H	1.63	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:B:994:SER:C	1:B:996:THR:N	2.64	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: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:A:1234:ILE:HG12	1:D:1197:LEU:HD12	1.97	0.46
1:D:1229:MET:CE	1:D:1257:LYS:HB2	2.44	0.46
1:D:1242:PHE:HD2	1:D:1242:PHE:N	2.13	0.46
1:D:1230:LEU:HA	1:D:1249:VAL:O	2.16	0.46
1:A:1215:LYS:HD2	1:A:1217:CYS:SG	2.55	0.46
1:A:1253:ASN:O	1:A:1256:THR:HG22	2.15	0.46
1:A:944:THR:CB	1:A:989:TYR:OH	2.63	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:D:1114:GLU:CA	1:D:1114:GLU:OE2	2.63	0.46
1:A:1015:MET:O	1:A:1015:MET:HG3	2.14	0.46
1:A:907:LEU:HD22	1:A:907:LEU:N	2.31	0.46
1:B:921:ASN:ND2	1:B:921:ASN:N	2.61	0.46
1:B:966:ILE:O	1:B:966:ILE:HG13	2.14	0.46
1:C:1015:MET:HE3	1:C:1029:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1158:HIS:CE1	1:B:1197:LEU:HD22	2.50	0.46
1:B:909:SER:HA	1:B:1049:ILE:CD1	2.45	0.46
1:D:1016:LYS:HB3	1:D:1023:LEU:CD1	2.46	0.46
1:D:1185:GLN:O	1:D:1186:ASN:C	2.53	0.46
1:A:1171:ASP:CG	1:A:1192:LYS:HD2	2.35	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:HG2	1:B:1270:ARG:NH2	2.31	0.46
1:C:985:LEU:HB3	1:C:1017:LEU:HD22	1.98	0.46
1:A:1113:PRO:O	1:A:1117:VAL:O	2.34	0.46
1:A:962:TRP:HB3	1:A:975:LEU:HD23	1.98	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:A:1109:ARG:NH1	1:A:1122:GLN:N	2.64	0.46
1:B:1049:ILE:HD12	1:B:1049:ILE:C	2.36	0.46
1:B:1136:THR:HG21	1:B:1138:LYS:NZ	2.31	0.46
1:C:1046:ASP:O	1:C:1047:GLU:C	2.54	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:1191:LEU:HD21	1:B:1230:LEU:HD22	1.98	0.45
1:B:983:LYS:CG	1:B:1027:GLN:HG2	2.46	0.45
1:D:1004:PHE:CD2	1:D:1076:TYR:HB2	2.50	0.45
1:D:931:SER:HA	1:D:1065:LYS:H	1.80	0.45
1:D:1199:ASN:HD22	1:D:1199:ASN:N	2.14	0.45
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:1113:PRO:HB3	1:D:1193:LEU:CD1	2.46	0.45
1:D:936:TRP:HB2	1:D:1058:ARG:CG	2.44	0.45
1:A:913:LYS:HB3	1:A:1043:PHE:O	2.16	0.45
1:B:932:SER:CB	1:B:1008:THR:HG22	2.47	0.45
1:B:908:SER:OG	1:B:909:SER:N	2.47	0.45
1:B:1011:ILE:C	1:B:1013:GLY:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1140:VAL:C	1:A:1142:ASP:H	2.20	0.45
1:A:1241:SER:C	1:A:1243:LYS:H	2.19	0.45
1:B:1000:ASN:ND2	1:B:1273:GLY:HA3	2.31	0.45
1:B:950:TYR:HB2	1:B:966:ILE:CG1	2.47	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:1225:ARG:O	1:A:1226:GLU:HG3	2.16	0.45
1:A:956:ILE:HD13	1:A:976:GLN:CD	2.37	0.45
1:A:976:GLN:HA	1:A:981:LYS:O	2.17	0.45
1:A:994:SER:C	1:A:996:THR:N	2.68	0.45
1:B:1085:ILE:HD11	1:B:1151:ASN:HA	1.99	0.45
1:C:1010:ASN:HD22	1:C:1010:ASN:N	2.13	0.45
1:C:964:LEU:HD11	1:C:971:ILE:HG12	1.99	0.45
1:D:904:ASP:HA	1:D:1057:ILE:O	2.15	0.45
1:B:872:LEU:CG	1:B:879:LEU:HD11	2.47	0.45
1:D:934:SER:HB2	1:D:1004:PHE:CZ	2.51	0.45
1:D:1087:ASP:HB2	1:D:1267:PHE:O	2.17	0.45
1:D:973:TRP:O	1:D:984:SER:HB2	2.16	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: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:B:981:LYS:HE3	1:B:1031:ASP:HB2	1.99	0.45
1:C:1019:ILE:C	1:C:1021:GLY:N	2.70	0.45
1:C:907:LEU:CG	1:C:1044:GLY:HA2	2.45	0.45
1:D:1002:TRP:CZ3	1:D:1058:ARG:HG2	2.51	0.45
1:D:921:ASN:HD22	1:D:921:ASN:N	2.13	0.45
1:D:958:GLN:H	1:D:958:GLN:CD	2.19	0.45
1:C:919:ASN:ND2	1:C:921:ASN:HD22	2.15	0.45
1:C:990:SER:O	1:C:991:GLU:C	2.55	0.45
1:B:870:LEU:HD23	1:B:1062:ILE:HD12	1.99	0.45
1:C:1095:PHE:CE2	1:C:1149:ILE:HG12	2.52	0.45
1:C:977:ASP:OD2	1:C:981:LYS:HB3	2.16	0.45
1:D:1175:ILE:HG22	1:D:1188:VAL:O	2.17	0.45
1:B:981:LYS:CE	1:B:1031:ASP:HB2	2.47	0.44
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:C:1095:PHE:CZ	1:C:1149:ILE:HG12	2.52	0.44
1:C:958:GLN:CG	1:C:959:ASN:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:HIS:CE1	1:B:1129:LEU:HD13	2.53	0.44
1:A:1106:TYR:HA	1:D:1163:SER:HB3	1.99	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: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:A:1231:LEU:C	1:A:1231:LEU:HD12	2.37	0.44
1:B:901:TYR:CE1	1:B:1092:PRO:HD3	2.51	0.44
1:C:1068:SER:C	1:C:1070:GLU:H	2.20	0.44
1:C:953:ILE:HB	1:C:964:LEU:HB3	2.00	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:B:938:LYS:HZ3	1:B:1000:ASN:HD21	1.63	0.44
1:C:1017:LEU:C	1:C:1018:TYR:HD2	2.20	0.44
1:A:952:ILE:HG22	1:A:1045:ILE:CG1	2.42	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:B:939:ILE:HD12	1:B:989:TYR:CZ	2.52	0.44
1:C:1210:ILE:CG2	1:C:1210:ILE:O	2.65	0.44
1:D:1185:GLN:HE21	1:D:1185:GLN:HB2	1.58	0.44
1:B:1270:ARG:HG2	1:B:1270:ARG:HH21	1.82	0.44
1:C:1028:LYS:HD3	1:C:1029:ILE:C	2.38	0.44
1:D:879:LEU:HA	1:D:879:LEU:HD23	1.83	0.44
1:D:958:GLN:O	1:D:959:ASN:CB	2.65	0.44
1:A:909:SER:C	1:A:1049:ILE:HD11	2.38	0.44
1:B:1121:VAL:HG12	1:B:1122:GLN:N	2.32	0.44
1:B:1083:ASN:CG	1:B:1151:ASN:HD21	2.21	0.44
1:C:918:LEU:O	1:C:1039:LYS:HG3	2.17	0.44
1:D:1135:ILE:HD13	1:D:1168:ILE:HD11	2.00	0.44
1:A:1143:LYS:HB3	1:A:1143:LYS:HE2	1.83	0.44
1:B:1160:LEU:HD22	1:C:1105:ASN:ND2	2.31	0.44
1:B:987:PHE:HE1	1:B:1024:LYS:HE2	1.83	0.44
1:D:923:LEU:HD13	1:D:923:LEU:C	2.39	0.44
1:A:956:ILE:HD12	1:A:963:LYS:HD3	2.00	0.43
1:B:1236:LYS:NZ	1:B:1244:ASN:ND2	2.66	0.43
1:B:967:ARG:CZ	1:B:967:ARG:HB3	2.48	0.43
1:C:972:GLU:HG3	1:C:974:ILE:CD1	2.42	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:1068:SER:O	1:A:1072:ILE:HG13	2.18	0.43
1:A:942:ASP:OD1	1:A:1052:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:GLN:NE2	1:A:960:SER:H	2.15	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:C:1017:LEU:C	1:C:1018:TYR:CD2	2.92	0.43
1:C:1082:ARG:NH1	1:C:1211:VAL:HG13	2.34	0.43
1:C:953:ILE:HD12	1:C:964:LEU:HD23	2.00	0.43
1:A:1171:ASP:O	1:A:1189:TYR:HD2	2.00	0.43
1:A:941:LYS:O	1:A:944:THR:HG23	2.18	0.43
1:B:1010:ASN:C	1:B:1010:ASN:HD22	2.20	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:930:ASN:HA	1:C:1010:ASN:HA	1.99	0.43
1:C:876:LYS:C	1:C:877:ASN:HD22	2.22	0.43
1:C:891:VAL:HG22	1:C:914:ILE:HG23	2.00	0.43
1:C:905:PHE:CE1	1:C:1057:ILE:HB	2.53	0.43
1:A:1231:LEU:HA	1:A:1262:SER:O	2.19	0.43
1:C:1068:SER:C	1:C:1070:GLU:N	2.72	0.43
1:D:875:LYS:C	1:D:877:ASN:H	2.21	0.43
1:A:986:ILE:HG12	1:A:987:PHE:N	2.34	0.43
1:B:1097:THR:HB	1:B:1099:TYR:CE2	2.54	0.43
1:B:925:SER:O	1:B:929:GLU:CB	2.66	0.43
1:C:974:ILE:CD1	1:C:974:ILE:N	2.81	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:HD12	1:C:939:ILE:N	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:B:1229:MET:HE1	1:B:1254:TYR:HB2	2.00	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:1051:GLU:O	1:A:1053:GLN:N	2.52	0.42
1:A:869:ILE:CG1	1:A:1062:ILE:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:ARG:HA	1:B:1121:VAL:O	2.18	0.42
1:B:987:PHE:CE2	1:B:989:TYR:HA	2.54	0.42
1:C:1028:LYS:HD3	1:C:1029:ILE:H	1.71	0.42
1:C:912:ASP:C	1:C:913:LYS:HD2	2.39	0.42
1:C:888:GLU:HB3	1:C:917:ASN:HB2	2.01	0.42
1:D:1170:ARG:O	1:D:1202:ILE:HD11	2.19	0.42
1:B:986:ILE:H	1:B:1025:GLN:NE2	2.17	0.42
1:B:870:LEU:O	1:B:1061:ASN:HA	2.19	0.42
1:D:1018:TYR:N	1:D:1018:TYR:CD2	2.87	0.42
1:D:919:ASN:O	1:D:921:ASN:N	2.52	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:C:985:LEU:HD22	1:C:1025:GLN:HB3	2.02	0.42
1:D:1264:PHE:N	1:D:1264:PHE:CD1	2.87	0.42
1:C:1141:SER:HB2	1:D:920:ASN:OD1	2.19	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:C:873:GLN:C	1:C:879:LEU:HD22	2.39	0.42
1:A:1255:GLU:OE2	1:A:1255:GLU:N	2.48	0.42
1:A:907:LEU:HD23	1:A:1055:LEU:HD11	1.99	0.42
1:B:939:ILE:HD11	1:B:971:ILE:HD12	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
1:C:935:PHE:HB3	1:C:1060:PHE:HA	2.01	0.42
1:C:885:TYR:CD1	1:C:885:TYR:N	2.87	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:A:1101:ILE:HD13	1:A:1135:ILE:HD12	2.01	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:B:955:SER:HB3	1:B:962:TRP:O	2.20	0.42
1:D:935:PHE:HB3	1:D:1060:PHE:HA	2.01	0.42
1:A:1257:LYS:HD2	1:D:1146:TYR:OH	2.19	0.42
1:D:876:LYS:O	1:D:877:ASN:CB	2.61	0.42
1:A:932:SER:HB3	1:A:1008:THR:HA	2.02	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: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:A:1011:ILE:C	1:A:1013:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:980:ARG:O	1:A:980:ARG:CG	2.60	0.41
1:C:1055:LEU:HD12	1:C:1055:LEU:C	2.40	0.41
1:C:1192:LYS:NZ	1:C:1239:ARG:HH22	2.18	0.41
1:D:1048:ASN:ND2	1:D:1048:ASN:C	2.72	0.41
1:D:932:SER:CB	1:D:1067:LEU:HD21	2.49	0.41
1:A:1118:LEU:HD22	1:A:1118:LEU:N	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:1029:ILE:HD12	1:C:1029:ILE:N	2.35	0.41
1:C:1032:LEU:HB3	1:C:1035:VAL:CG2	2.44	0.41
1:C:1175:ILE:HD11	1:C:1236:LYS:C	2.40	0.41
1:C:941:LYS:HE3	1:C:1274:TRP:CD2	2.55	0.41
1:D:1199:ASN:N	1:D:1199:ASN:ND2	2.68	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
1:C:1138:LYS:HG3	1:C:1158:HIS:NE2	2.35	0.41
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:A:1113:PRO:HB3	1:A:1193:LEU:HD11	2.03	0.41
1:A:975:LEU:HA	1:A:975:LEU:HD23	1.89	0.41
1:B:1011:ILE:HD13	1:B:1011:ILE:N	2.34	0.41
1:D:1010:ASN:ND2	1:D:1010:ASN:C	2.73	0.41
1:D:1038:ASP:C	1:D:1040:THR:H	2.23	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:B:1184:SER:C	1:B:1185:GLN:HG3	2.41	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:1116:ASN:O	1:D:1117:VAL:HG23	2.21	0.41
1:D:954:ASN:HD21	1:D:956:ILE:HB	1.86	0.41
1:C:907:LEU:C	1:C:907:LEU:HD13	2.41	0.41
1:D:964:LEU:HD11	1:D:971:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:TYR:CE1	1:A:1269:SER:HB3	2.56	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:B:1234:ILE:HG23	1:B:1234:ILE:O	2.21	0.41
1:A:916:VAL:O	1:A:1040:THR:HA	2.21	0.41
1:D:1231:LEU:HD12	1:D:1231:LEU:C	2.42	0.41
1:D:937:ILE:HG13	1:D:938:LYS:N	2.35	0.41
1:A:1080:ILE:O	1:A:1081:LEU:HB2	2.21	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:B:960:SER:HA	1:B:976:GLN:O	2.21	0.41
1:B:983:LYS:HE2	1:B:983:LYS:HB2	1.90	0.41
1:C:1016:LYS:HB3	1:C:1018:TYR:CE2	2.56	0.41
1:C:1087:ASP:C	1:C:1087:ASP:OD2	2.60	0.41
1:B:1163:SER:CB	1:C:1108:ASP:OD2	2.68	0.41
1:C:872:LEU:HD12	1:C:872:LEU:N	2.35	0.41
1:B:1220:ILE:HB	1:B:1230:LEU:HD12	2.02	0.40
1:B:1102:ILE:HD11	1:B:1268:ILE:HD11	2.03	0.40
1:C:930:ASN:ND2	1:C:1010:ASN:HA	2.36	0.40
1:D:1117:VAL:O	1:D:1119:VAL:HG13	2.21	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
1:A:977:ASP:OD1	1:A:979:ASN:N	2.53	0.40
1:B:982:TYR:C	1:B:982:TYR:CD1	2.95	0.40
1:C:1229:MET:SD	1:C:1258:LEU:HD12	2.61	0.40
1:C:966:ILE:HG13	1:C:966:ILE:O	2.21	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:H	1:D:1118:LEU:HD22	1.86	0.40
1:D:1244:ASN:HA	1:D:1244:ASN:HD22	1.73	0.40
1:A:1016:LYS:HB2	1:A:1018:TYR:CE2	2.56	0.40
1:A:928:TYR:CD1	1:A:928:TYR:N	2.89	0.40
1:B:1095:PHE:CE2	1:B:1143:LYS:HD2	2.55	0.40
1:C:1059:ASP:N	1:C:1059:ASP:OD1	2.54	0.40
1:A:1126:ARG:C	1:A:1128:LYS:H	2.25	0.40
1:A:1151:ASN:ND2	1:A:1208:LYS:HG2	2.36	0.40
1:B:1047:GLU:O	1:B:1049:ILE:HG23	2.21	0.40
1:B:907:LEU:N	1:B:907:LEU:CD2	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:ASN:ND2	1:A:1262:SER:HB3	2.37	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: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 [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	398/415 (96%)	328 (82%)	53 (13%)	17 (4%)	3	3
1	B	401/415 (97%)	327 (82%)	57 (14%)	17 (4%)	3	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%)	2	2
All	All	1596/1660 (96%)	1321 (83%)	201 (13%)	74 (5%)	2	3

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	349 (92%)	29 (8%)	14	25
1	B	380/386 (98%)	346 (91%)	34 (9%)	11	20
1	C	377/386 (98%)	355 (94%)	22 (6%)	22	40
1	D	380/386 (98%)	354 (93%)	26 (7%)	17	31
All	All	1515/1544 (98%)	1404 (93%)	111 (7%)	15	28

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	872	LEU
1	A	876	LYS
1	A	879	LEU
1	A	893	ASP
1	A	913	LYS
1	A	920	ASN
1	A	932	SER
1	A	944	THR
1	A	947	HIS
1	A	959	ASN
1	A	968	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	1048	ASN
1	A	1050	ASP
1	A	1065	LYS
1	A	1116	ASN
1	A	1151	ASN
1	A	1153	ASP
1	A	1172	THR
1	A	1187	CYS
1	A	1206	SER
1	A	1217	CYS
1	A	1244	ASN
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	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

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Mol	Chain	Res	Type
1	B	1038	ASP
1	B	1048	ASN
1	B	1052	ASN
1	B	1053	GLN
1	B	1055	LEU
1	B	1077	GLU
1	B	1116	ASN
1	B	1118	LEU
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	1228	THR
1	B	1233	ASP
1	B	1247	THR
1	B	1266	LYS
1	C	874	ASN
1	C	912	ASP
1	C	941	LYS
1	C	952	ILE
1	C	967	ARG
1	C	968	ASN
1	C	975	LEU
1	C	977	ASP
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	1059	ASP
1	C	1077	GLU
1	C	1081	LEU
1	C	1089	TRP
1	C	1151	ASN
1	C	1173	ASP
1	C	1239	ARG
1	C	1261	THR

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Mol	Chain	Res	Type
1	D	879	LEU
1	D	898	ASN
1	D	907	LEU
1	D	920	ASN
1	D	921	ASN
1	D	945	ASN
1	D	968	ASN
1	D	983	LYS
1	D	1010	ASN
1	D	1011	ILE
1	D	1031	ASP
1	D	1034	GLU
1	D	1048	ASN
1	D	1050	ASP
1	D	1067	LEU
1	D	1106	TYR
1	D	1114	GLU
1	D	1116	ASN
1	D	1145	PRO
1	D	1162	ASN
1	D	1185	GLN
1	D	1206	SER
1	D	1228	THR
1	D	1231	LEU
1	D	1244	ASN
1	D	1256	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	873	GLN
1	A	898	ASN
1	A	920	ASN
1	A	930	ASN
1	A	958	GLN
1	A	959	ASN
1	A	968	ASN
1	A	970	ASN
1	A	1000	ASN
1	A	1010	ASN
1	A	1025	GLN
1	A	1048	ASN

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Mol	Chain	Res	Type
1	A	1073	ASN
1	A	1105	ASN
1	A	1116	ASN
1	A	1151	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
1	B	958	GLN
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	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	874	ASN
1	C	877	ASN
1	C	898	ASN
1	C	919	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

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Mol	Chain	Res	Type
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	1244	ASN
1	D	862	ASN
1	D	865	ASN
1	D	898	ASN
1	D	919	ASN
1	D	921	ASN
1	D	930	ASN
1	D	954	ASN
1	D	959	ASN
1	D	968	ASN
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	1116	ASN
1	D	1151	ASN
1	D	1185	GLN
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 [i](#)

There are no carbohydrates 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, 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%)	-0.03	6 (1%) 73 71	28, 60, 94, 106	0
1	B	407/415 (98%)	0.01	6 (1%) 73 71	29, 55, 91, 104	0
1	C	403/415 (97%)	0.27	26 (6%) 19 14	33, 68, 107, 120	0
1	D	406/415 (97%)	0.07	11 (2%) 54 50	31, 60, 96, 105	0
All	All	1620/1660 (97%)	0.08	49 (3%) 50 46	28, 61, 100, 120	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1183	CYS	7.9
1	C	1034	GLU	7.5
1	C	916	VAL	5.6
1	D	1184	SER	5.5
1	B	927	ILE	5.1
1	C	1014	TYR	4.9
1	D	1013	GLY	4.5
1	C	1029	ILE	4.2
1	D	1176	TYR	4.1
1	C	1030	GLU	4.1
1	B	928	TYR	3.8
1	C	1183	CYS	3.8
1	D	928	TYR	3.8
1	D	1241	SER	3.8
1	A	1029	ILE	3.7
1	C	1011	ILE	3.7
1	D	911	GLY	3.6
1	C	1049	ILE	3.5
1	A	1032	LEU	3.4
1	C	879	LEU	3.4
1	C	974	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	925	SER	3.1
1	C	1032	LEU	3.1
1	C	978	VAL	3.0
1	C	973	TRP	2.9
1	D	1237	PRO	2.9
1	C	1033	ASP	2.9
1	A	1030	GLU	2.8
1	B	926	ALA	2.8
1	C	907	LEU	2.8
1	D	1014	TYR	2.7
1	C	1045	ILE	2.6
1	B	1031	ASP	2.5
1	C	918	LEU	2.5
1	D	1045	ILE	2.4
1	C	947	HIS	2.4
1	C	1012	MET	2.4
1	C	961	GLY	2.3
1	C	963	LYS	2.2
1	C	1050	ASP	2.2
1	C	959	ASN	2.1
1	A	1014	TYR	2.1
1	C	975	LEU	2.1
1	A	1035	VAL	2.1
1	C	976	GLN	2.1
1	A	1207	ILE	2.0
1	B	1028	LYS	2.0
1	C	890	ARG	2.0
1	D	947	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.