



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:31 am BST

PDB ID : 2VYF
Title : Crystal Structure of the DnaC
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Deposited on : 2008-07-23
Resolution : 3.60 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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

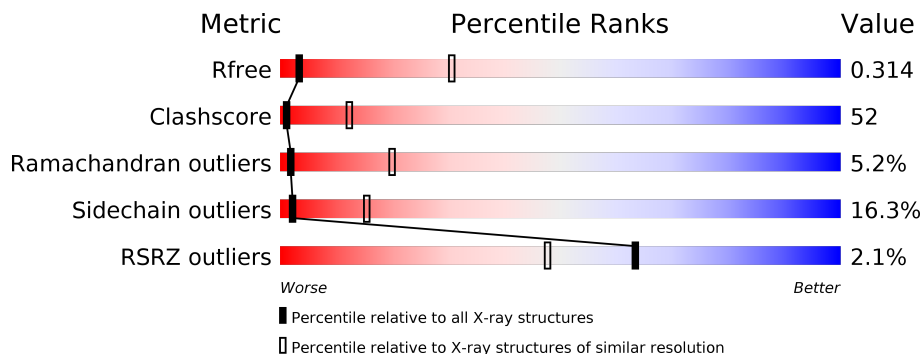
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	454	 % 33% 42% 11% • 12%
1	B	454	 3% 34% 37% 10% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5946 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 REPLICATIVE DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3062	1912	539	599	12	0	0	4
1	B	377	2880	1798	506	564	12	0	0	6

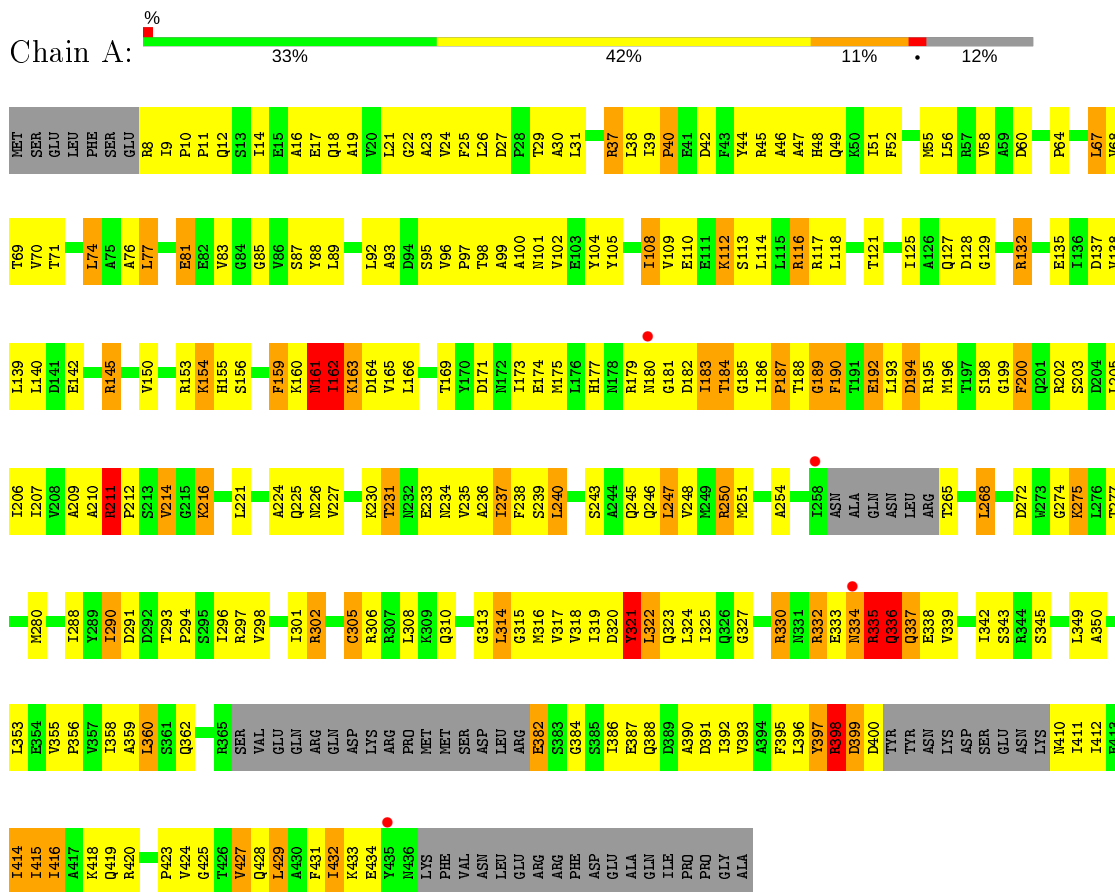
- Molecule 2 is GOLD ION (three-letter code: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Au	0	0
			2	2		
2	A	2	Total	Au	0	0
			2	2		

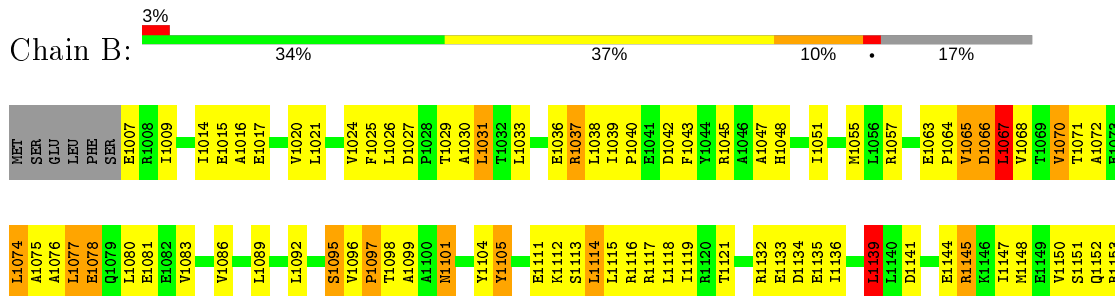
3 Residue-property plots [i](#)

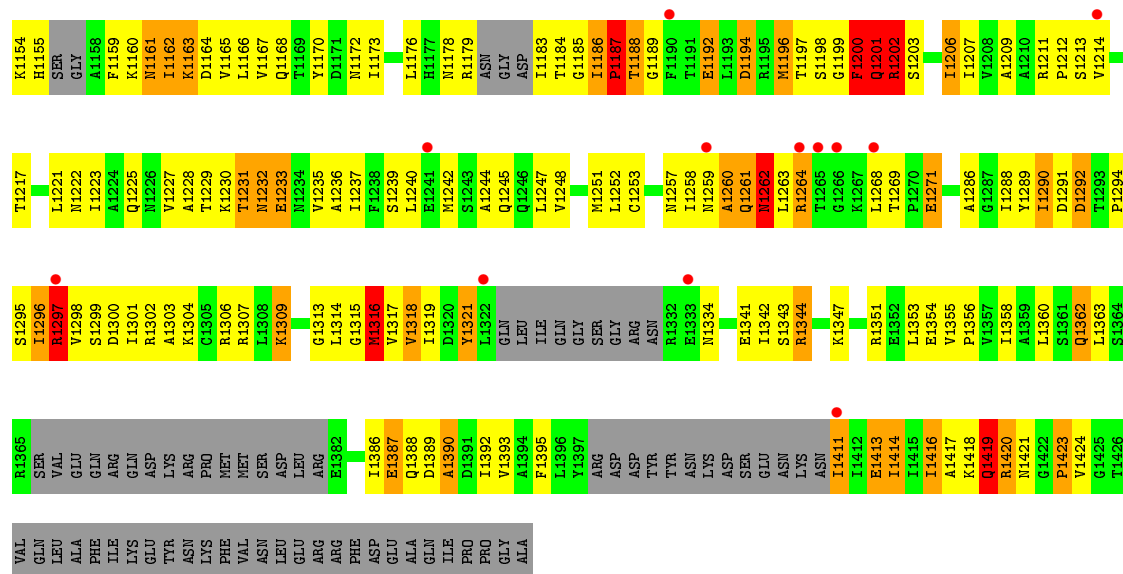
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: REPLICATIVE DNA HELICASE



- Molecule 1: REPLICATIVE DNA HELICASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	176.97Å 176.97Å 108.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.87 – 3.60 24.87 – 3.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.87-3.60) 91.9 (24.87-3.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.64Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.324 0.290 , 0.314	Depositor DCC
R_{free} test set	1770 reflections (7.86%)	wwPDB-VP
Wilson B-factor (Å ²)	142.8	Xtrriage
Anisotropy	0.540	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5946	wwPDB-VP
Average B, all atoms (Å ²)	167.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
AU

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	0.40	0/3096	0.77	3/4184 (0.1%)
1	B	0.43	0/2908	0.95	18/3930 (0.5%)
All	All	0.42	0/6004	0.86	21/8114 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1297	ARG	N-CA-C	9.29	136.08	111.00
1	B	1260	ALA	N-CA-C	9.18	135.79	111.00
1	A	162	ILE	CG1-CB-CG2	-8.29	93.16	111.40
1	B	1411	ILE	N-CA-C	8.28	133.36	111.00
1	B	1419	GLN	N-CA-C	7.66	131.68	111.00
1	B	1202	ARG	N-CA-C	6.96	129.79	111.00
1	B	1390	ALA	C-N-CA	6.79	138.68	121.70
1	B	1262	ASN	N-CA-C	-6.51	93.41	111.00
1	B	1139	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	1316	MET	N-CA-C	-6.22	94.19	111.00
1	B	1416	ILE	C-N-CA	6.08	136.90	121.70
1	A	268	LEU	N-CA-C	5.88	126.89	111.00
1	B	1067	LEU	N-CA-C	5.83	126.74	111.00
1	B	1313	GLY	N-CA-C	-5.61	99.08	113.10
1	B	1067	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	327	GLY	N-CA-C	-5.42	99.56	113.10
1	B	1201	GLN	N-CA-C	5.41	125.60	111.00
1	B	1200	PHE	N-CA-C	-5.40	96.42	111.00
1	B	1065	VAL	N-CA-C	5.31	125.35	111.00
1	B	1260	ALA	CA-C-N	-5.12	105.95	117.20
1	B	1066	ASP	N-CA-C	5.00	124.51	111.00

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	3062	0	3098	343	2
1	B	2880	0	2922	299	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	5946	0	6020	621	2

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 52.

All (621) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HD3	1:A:212:PRO:CD	1.49	1.41
1:A:297:ARG:HH22	1:B:1154:LYS:N	1.15	1.39
1:A:145:ARG:NH2	1:A:145:ARG:HB3	1.35	1.37
1:B:1145:ARG:NH2	1:B:1145:ARG:HB2	1.41	1.34
1:A:297:ARG:NH2	1:B:1154:LYS:H	1.24	1.33
1:B:1076:ALA:O	1:B:1077:LEU:HD22	1.35	1.21
1:A:211:ARG:CD	1:A:212:PRO:HD3	1.71	1.19
1:B:1290:ILE:N	1:B:1290:ILE:HD12	1.38	1.18
1:A:193:LEU:HD13	1:A:200:PHE:CZ	1.80	1.17
1:B:1201:GLN:NE2	1:B:1201:GLN:H	1.41	1.17
1:B:1227:VAL:O	1:B:1231:THR:CG2	1.98	1.11
1:A:186:ILE:HD11	1:A:231:THR:HB	1.17	1.11
1:A:332:ARG:HD3	1:A:332:ARG:C	1.71	1.10
1:B:1227:VAL:O	1:B:1231:THR:HG22	1.51	1.10
1:A:193:LEU:HD13	1:A:200:PHE:HZ	1.10	1.09
1:A:240:LEU:H	1:A:240:LEU:HD23	1.16	1.09
1:A:214:VAL:HG21	1:A:216:LYS:HE3	1.29	1.09
1:A:211:ARG:CD	1:A:212:PRO:CD	2.27	1.08
1:A:81:GLU:HA	1:A:81:GLU:OE1	1.53	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:CG2	1:A:216:LYS:HE3	1.82	1.08
1:B:1196:MET:HG2	1:B:1416:ILE:HD12	1.25	1.07
1:A:192:GLU:HG2	1:A:193:LEU:N	1.69	1.04
1:A:414:ILE:HD13	1:A:427:VAL:O	1.57	1.04
1:A:192:GLU:HG2	1:A:193:LEU:H	0.92	1.04
1:A:398:ARG:NE	1:A:398:ARG:HA	1.74	1.03
1:B:1231:THR:CG2	1:B:1233:GLU:H	1.72	1.02
1:A:99:ALA:O	1:A:102:VAL:HG23	1.59	1.02
1:B:1413:GLU:OE2	1:B:1413:GLU:HA	1.53	1.02
1:B:1211:ARG:HG2	1:B:1363:LEU:O	1.58	1.01
1:A:210:ALA:HB2	1:A:216:LYS:HD3	1.41	1.01
1:B:1201:GLN:HE21	1:B:1201:GLN:H	1.02	1.00
1:B:1203:SER:HB3	1:B:1354:GLU:HA	1.44	1.00
1:A:332:ARG:HD3	1:A:332:ARG:O	1.60	0.99
1:A:298:VAL:HA	1:A:301:ILE:HD13	1.43	0.98
1:B:1393:VAL:O	1:B:1417:ALA:HB3	1.63	0.98
1:A:332:ARG:NH2	1:A:336:GLN:H	1.62	0.97
1:A:145:ARG:HH21	1:A:145:ARG:HB3	1.15	0.97
1:A:333:GLU:OE1	1:A:337:GLN:HG3	1.64	0.97
1:B:1201:GLN:HE21	1:B:1201:GLN:N	1.60	0.97
1:B:1145:ARG:HH21	1:B:1145:ARG:CB	1.78	0.97
1:A:414:ILE:HD12	1:A:429:LEU:HD21	1.44	0.96
1:A:305:CYS:SG	1:A:317:VAL:HG21	2.05	0.96
1:B:1290:ILE:HD12	1:B:1290:ILE:H	1.19	0.94
1:B:1161:ASN:O	1:B:1163:LYS:N	2.01	0.93
1:A:145:ARG:CZ	1:A:145:ARG:HB3	1.96	0.93
1:A:414:ILE:HD12	1:A:429:LEU:CD2	1.98	0.93
1:A:171:ASP:HA	1:A:174:GLU:HG2	1.50	0.93
1:B:1261:GLN:HE22	1:B:1264:ARG:HB2	1.31	0.93
1:B:1392:ILE:HD11	1:B:1420:ARG:HB2	1.49	0.93
1:A:297:ARG:NH2	1:B:1154:LYS:N	1.94	0.92
1:A:214:VAL:HG21	1:A:216:LYS:CE	2.00	0.91
1:B:1201:GLN:HG2	1:B:1202:ARG:HG2	1.53	0.91
1:B:1211:ARG:HG3	1:B:1363:LEU:HB2	1.55	0.89
1:B:1253:CYS:SG	1:B:1260:ALA:HB2	2.12	0.89
1:B:1299:SER:HA	1:B:1302:ARG:HE	1.38	0.88
1:A:160:LYS:O	1:A:161:ASN:O	1.91	0.88
1:B:1299:SER:O	1:B:1302:ARG:HG3	1.72	0.88
1:A:145:ARG:NH2	1:A:145:ARG:CB	2.31	0.87
1:B:1039:ILE:HG23	1:B:1040:PRO:HD2	1.56	0.87
1:B:1290:ILE:N	1:B:1290:ILE:CD1	2.28	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:O	1:A:49:GLN:HG2	1.75	0.87
1:A:211:ARG:CD	1:A:212:PRO:HD2	2.03	0.86
1:A:414:ILE:CD1	1:A:429:LEU:HD21	2.06	0.86
1:A:235:VAL:CG1	1:A:288:ILE:HG12	2.05	0.86
1:A:211:ARG:HH11	1:A:212:PRO:HG2	1.38	0.86
1:A:192:GLU:CG	1:A:193:LEU:H	1.73	0.85
1:B:1145:ARG:HB2	1:B:1145:ARG:HH21	1.11	0.85
1:B:1185:GLY:HA3	1:B:1201:GLN:HB3	1.56	0.85
1:A:332:ARG:HH22	1:A:336:GLN:N	1.74	0.85
1:A:332:ARG:HH22	1:A:336:GLN:H	0.88	0.85
1:A:411:ILE:HD11	1:A:428:GLN:HB2	1.58	0.84
1:B:1145:ARG:NH2	1:B:1145:ARG:CB	2.32	0.84
1:B:1392:ILE:H	1:B:1392:ILE:HD12	1.41	0.84
1:A:121:THR:O	1:A:125:ILE:HD13	1.77	0.83
1:B:1416:ILE:O	1:B:1424:VAL:HG22	1.78	0.83
1:B:1211:ARG:CG	1:B:1363:LEU:O	2.27	0.83
1:B:1007:GLU:O	1:B:1007:GLU:CD	2.17	0.83
1:A:296:ILE:HG23	1:A:301:ILE:HD11	1.60	0.83
1:B:1145:ARG:HB2	1:B:1145:ARG:CZ	2.07	0.82
1:B:1201:GLN:N	1:B:1201:GLN:NE2	2.20	0.82
1:B:1231:THR:CG2	1:B:1232:ASN:N	2.42	0.82
1:B:1231:THR:HG21	1:B:1233:GLU:HB2	1.61	0.82
1:B:1067:LEU:O	1:B:1071:THR:HB	1.80	0.81
1:B:1200:PHE:H	1:B:1201:GLN:HE21	1.28	0.81
1:A:297:ARG:NH2	1:B:1153:ARG:HA	1.96	0.81
1:B:1236:ALA:HB3	1:B:1317:VAL:HG22	1.62	0.81
1:A:236:ALA:HB3	1:A:317:VAL:HG22	1.61	0.81
1:B:1231:THR:HG22	1:B:1233:GLU:H	1.46	0.80
1:A:216:LYS:HG3	1:A:360:LEU:HB3	1.64	0.80
1:A:40:PRO:HD3	1:A:56:LEU:HD11	1.62	0.80
1:B:1024:VAL:HG23	1:B:1031:LEU:HB2	1.64	0.80
1:A:240:LEU:H	1:A:240:LEU:CD2	1.94	0.80
1:B:1200:PHE:HE1	1:B:1206:ILE:HG21	1.46	0.79
1:A:297:ARG:HH12	1:B:1154:LYS:HB3	1.48	0.79
1:A:301:ILE:O	1:A:305:CYS:HB2	1.82	0.79
1:A:188:THR:HG21	1:A:192:GLU:OE2	1.82	0.79
1:A:186:ILE:CD1	1:A:231:THR:HB	2.08	0.78
1:A:166:LEU:O	1:A:169:THR:HG22	1.83	0.78
1:A:235:VAL:HG13	1:A:288:ILE:HG12	1.64	0.78
1:B:1231:THR:CG2	1:B:1233:GLU:N	2.47	0.78
1:A:210:ALA:CB	1:A:216:LYS:HD3	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:HB2	1:A:356:PRO:HG2	1.66	0.77
1:A:171:ASP:CA	1:A:174:GLU:HG2	2.13	0.77
1:A:399:ASP:CG	1:A:400:ASP:N	2.38	0.77
1:B:1309:LYS:CG	1:B:1314:LEU:HB2	2.15	0.77
1:B:1315:GLY:O	1:B:1355:VAL:HG23	1.83	0.77
1:A:211:ARG:HD2	1:A:212:PRO:HD2	1.65	0.77
1:A:382:GLU:OE2	1:A:382:GLU:N	2.17	0.77
1:A:424:VAL:HG22	1:A:425:GLY:H	1.50	0.77
1:A:22:GLY:O	1:A:26:LEU:HD23	1.85	0.76
1:B:1184:THR:HB	1:B:1201:GLN:CD	2.06	0.76
1:A:297:ARG:HH21	1:B:1153:ARG:HA	1.47	0.76
1:A:211:ARG:HH11	1:A:212:PRO:CG	1.99	0.75
1:A:414:ILE:HD13	1:A:414:ILE:H	1.47	0.75
1:A:21:LEU:HG	1:A:92:LEU:HD21	1.66	0.75
1:B:1047:ALA:HB1	1:B:1083:VAL:HG13	1.69	0.75
1:A:302:ARG:HH12	1:A:349:LEU:HB2	1.51	0.75
1:B:1067:LEU:HA	1:B:1070:VAL:HG13	1.66	0.75
1:A:192:GLU:HG2	1:A:193:LEU:HG	1.68	0.74
1:A:211:ARG:NH1	1:A:212:PRO:HG2	2.02	0.74
1:B:1200:PHE:H	1:B:1201:GLN:NE2	1.84	0.74
1:A:101:ASN:HB2	1:A:104:TYR:HD1	1.51	0.74
1:A:24:VAL:HG11	1:A:55:MET:SD	2.27	0.74
1:A:12:GLN:HE21	1:A:14:ILE:HG23	1.50	0.74
1:B:1414:ILE:H	1:B:1414:ILE:HD13	1.51	0.74
1:A:145:ARG:HH21	1:A:145:ARG:CB	1.99	0.73
1:B:1068:VAL:HA	1:B:1071:THR:HG22	1.68	0.73
1:A:290:ILE:HD13	1:A:291:ASP:N	2.03	0.73
1:A:237:ILE:HG12	1:A:318:VAL:HB	1.70	0.73
1:A:414:ILE:HD11	1:A:427:VAL:HG23	1.70	0.73
1:B:1014:ILE:HA	1:B:1017:GLU:HB2	1.71	0.73
1:B:1021:LEU:O	1:B:1024:VAL:HG12	1.88	0.72
1:B:1037:ARG:HH11	1:B:1037:ARG:HB2	1.55	0.72
1:A:416:ILE:HD13	1:A:419:GLN:NE2	2.05	0.72
1:B:1231:THR:HG22	1:B:1232:ASN:N	2.04	0.72
1:A:25:PHE:HZ	1:A:89:LEU:HD12	1.55	0.71
1:B:1262:ASN:O	1:B:1263:LEU:HB2	1.90	0.71
1:B:1314:LEU:HG	1:B:1315:GLY:H	1.56	0.70
1:B:1203:SER:HB2	1:B:1351:ARG:HA	1.73	0.70
1:A:211:ARG:HD3	1:A:212:PRO:HD3	0.75	0.70
1:A:315:GLY:O	1:A:356:PRO:HD2	1.91	0.70
1:B:1227:VAL:O	1:B:1231:THR:HG21	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:CD1	1:A:429:LEU:CD2	2.67	0.69
1:A:121:THR:HG21	1:A:150:VAL:HG21	1.75	0.69
1:B:1309:LYS:HG2	1:B:1314:LEU:HB2	1.72	0.69
1:A:162:ILE:HG22	1:A:162:ILE:O	1.93	0.69
1:B:1076:ALA:C	1:B:1077:LEU:HD22	2.12	0.68
1:B:1196:MET:HG2	1:B:1416:ILE:CD1	2.16	0.68
1:B:1290:ILE:H	1:B:1290:ILE:CD1	2.00	0.68
1:B:1392:ILE:HA	1:B:1418:LYS:O	1.93	0.68
1:B:1231:THR:HG23	1:B:1233:GLU:N	2.09	0.68
1:A:145:ARG:CZ	1:A:145:ARG:CB	2.67	0.67
1:A:216:LYS:HD2	1:A:360:LEU:HB3	1.76	0.67
1:A:22:GLY:HA3	1:A:92:LEU:O	1.93	0.67
1:A:187:PRO:HG2	1:A:194:ASP:OD1	1.95	0.67
1:A:297:ARG:O	1:A:301:ILE:HD12	1.95	0.67
1:B:1051:ILE:HD11	1:B:1083:VAL:HG11	1.75	0.67
1:A:16:ALA:CB	1:A:108:ILE:HD11	2.24	0.67
1:B:1161:ASN:CB	1:B:1164:ASP:HB2	2.24	0.67
1:A:238:PHE:HE1	1:A:301:ILE:HA	1.58	0.67
1:A:67:LEU:HD13	1:A:67:LEU:H	1.59	0.67
1:B:1024:VAL:HG21	1:B:1055:MET:HE3	1.77	0.67
1:A:297:ARG:NH2	1:B:1153:ARG:CA	2.58	0.67
1:B:1217:THR:O	1:B:1221:LEU:HD23	1.94	0.67
1:B:1344:ARG:HG2	1:B:1344:ARG:O	1.94	0.67
1:B:1057:ARG:HH22	1:B:1077:LEU:HD11	1.61	0.66
1:A:414:ILE:CD1	1:A:427:VAL:O	2.39	0.66
1:B:1188:THR:HB	1:B:1223:ILE:CD1	2.26	0.66
1:A:214:VAL:HG23	1:A:216:LYS:HE3	1.71	0.66
1:A:160:LYS:O	1:A:160:LYS:HG3	1.96	0.66
1:A:265:THR:N	1:A:268:LEU:HD13	2.10	0.66
1:A:67:LEU:HD13	1:A:67:LEU:N	2.11	0.66
1:B:1221:LEU:HD12	1:B:1251:MET:SD	2.36	0.66
1:A:185:GLY:O	1:A:186:ILE:HG13	1.96	0.66
1:B:1161:ASN:HB2	1:B:1164:ASP:HB2	1.78	0.65
1:A:113:SER:HA	1:A:116:ARG:HB3	1.78	0.65
1:A:162:ILE:CG2	1:A:162:ILE:O	2.44	0.65
1:B:1185:GLY:CA	1:B:1201:GLN:HB3	2.25	0.65
1:B:1066:ASP:C	1:B:1067:LEU:HD13	2.17	0.65
1:A:297:ARG:HH21	1:B:1153:ARG:CA	2.10	0.65
1:A:169:THR:O	1:A:173:ILE:HG12	1.96	0.65
1:A:414:ILE:CD1	1:A:427:VAL:HG23	2.27	0.65
1:B:1024:VAL:HG11	1:B:1055:MET:SD	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TYR:O	1:A:398:ARG:HB2	1.97	0.65
1:B:1039:ILE:O	1:B:1042:ASP:HB2	1.97	0.65
1:B:1067:LEU:HA	1:B:1070:VAL:CG1	2.26	0.65
1:A:105:TYR:O	1:A:109:VAL:HG23	1.97	0.64
1:A:193:LEU:HD13	1:A:200:PHE:CE1	2.32	0.64
1:A:393:VAL:HG22	1:A:418:LYS:H	1.61	0.64
1:A:322:LEU:O	1:A:325:ILE:HD13	1.97	0.64
1:A:99:ALA:O	1:A:102:VAL:CG2	2.41	0.64
1:B:1211:ARG:O	1:B:1213:SER:N	2.26	0.64
1:B:1192:GLU:O	1:B:1196:MET:HB2	1.98	0.64
1:A:101:ASN:HB2	1:A:104:TYR:CD1	2.31	0.64
1:A:183:ILE:CD1	1:A:184:THR:OG1	2.46	0.64
1:B:1299:SER:HA	1:B:1302:ARG:NE	2.10	0.64
1:A:349:LEU:C	1:A:349:LEU:HD23	2.18	0.64
1:A:45:ARG:HD3	1:A:48:HIS:CD2	2.33	0.63
1:A:19:ALA:O	1:A:96:VAL:HG22	1.98	0.63
1:B:1321:TYR:CE1	1:B:1362:GLN:HG2	2.32	0.63
1:A:110:GLU:O	1:A:114:LEU:HB2	1.98	0.63
1:A:117:ARG:NH1	1:A:153:ARG:HD2	2.13	0.63
1:B:1024:VAL:CG2	1:B:1031:LEU:HB2	2.28	0.63
1:B:1141:ASP:O	1:B:1144:GLU:HG2	1.98	0.63
1:B:1162:ILE:O	1:B:1166:LEU:HD23	1.98	0.63
1:A:85:GLY:O	1:A:89:LEU:HD23	1.98	0.62
1:A:24:VAL:CG2	1:A:31:LEU:HB2	2.29	0.62
1:B:1298:VAL:HG13	1:B:1299:SER:N	2.13	0.62
1:A:297:ARG:NH1	1:B:1154:LYS:HB3	2.14	0.62
1:B:1253:CYS:SG	1:B:1260:ALA:CB	2.87	0.62
1:B:1170:TYR:O	1:B:1173:ILE:HG22	2.00	0.62
1:B:1014:ILE:HD12	1:B:1015:GLU:N	2.15	0.62
1:B:1014:ILE:HD12	1:B:1015:GLU:H	1.65	0.62
1:B:1225:GLN:O	1:B:1229:THR:HG22	2.00	0.62
1:A:40:PRO:HD3	1:A:56:LEU:CD1	2.29	0.62
1:A:192:GLU:CG	1:A:193:LEU:N	2.44	0.62
1:A:240:LEU:N	1:A:240:LEU:HD23	2.00	0.62
1:A:416:ILE:HG13	1:A:416:ILE:O	1.99	0.62
1:A:192:GLU:HA	1:A:427:VAL:HG21	1.81	0.62
1:B:1299:SER:CA	1:B:1302:ARG:HE	2.10	0.62
1:A:238:PHE:CE1	1:A:301:ILE:HA	2.35	0.61
1:A:387:GLU:HG3	1:A:388:GLN:N	2.16	0.61
1:A:431:PHE:C	1:A:432:ILE:HG13	2.21	0.61
1:B:1188:THR:HB	1:B:1223:ILE:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:CG	1:A:360:LEU:HB3	2.30	0.61
1:A:171:ASP:HA	1:A:174:GLU:CG	2.28	0.61
1:A:183:ILE:HD12	1:A:184:THR:OG1	1.99	0.61
1:B:1068:VAL:O	1:B:1071:THR:HG22	2.01	0.61
1:B:1258:ILE:O	1:B:1260:ALA:N	2.34	0.61
1:B:1152:GLN:NE2	1:B:1152:GLN:HA	2.16	0.61
1:B:1211:ARG:HG3	1:B:1363:LEU:CB	2.30	0.61
1:A:398:ARG:HE	1:A:398:ARG:HA	1.61	0.60
1:A:247:LEU:HD22	1:A:290:ILE:HG13	1.83	0.60
1:A:428:GLN:O	1:A:429:LEU:HD13	2.01	0.60
1:A:185:GLY:HA3	1:A:199:GLY:O	2.01	0.60
1:A:297:ARG:HH12	1:B:1154:LYS:CB	2.14	0.60
1:A:102:VAL:HA	1:A:105:TYR:HD1	1.66	0.60
1:B:1057:ARG:NH2	1:B:1077:LEU:HD11	2.17	0.60
1:B:1113:SER:HA	1:B:1116:ARG:CZ	2.31	0.60
1:A:321:TYR:HB3	1:A:324:LEU:HG	1.82	0.59
1:B:1321:TYR:CZ	1:B:1362:GLN:HG2	2.37	0.59
1:B:1392:ILE:CD1	1:B:1420:ARG:HB2	2.28	0.59
1:A:52:PHE:O	1:A:56:LEU:HG	2.01	0.59
1:A:391:ASP:C	1:A:392:ILE:HD12	2.23	0.59
1:B:1038:LEU:C	1:B:1039:ILE:HD12	2.22	0.59
1:A:214:VAL:HG13	1:A:214:VAL:O	2.01	0.59
1:A:21:LEU:CG	1:A:92:LEU:HD21	2.31	0.59
1:B:1068:VAL:CA	1:B:1071:THR:HG22	2.31	0.59
1:A:113:SER:O	1:A:116:ARG:HG2	2.01	0.59
1:A:24:VAL:HG23	1:A:31:LEU:HB2	1.83	0.59
1:B:1039:ILE:CG2	1:B:1040:PRO:HD2	2.29	0.59
1:A:335:ARG:H	1:A:335:ARG:HD2	1.68	0.59
1:A:227:VAL:HG12	1:A:227:VAL:O	2.02	0.59
1:A:207:ILE:HD13	1:A:359:ALA:HB3	1.84	0.59
1:B:1015:GLU:HG2	1:B:1016:ALA:N	2.17	0.59
1:A:239:SER:HA	1:A:320:ASP:HB3	1.84	0.59
1:A:296:ILE:HG12	1:A:301:ILE:HD12	1.83	0.59
1:A:225:GLN:HA	1:A:288:ILE:HD11	1.85	0.59
1:B:1016:ALA:O	1:B:1020:VAL:HG23	2.03	0.59
1:A:25:PHE:CZ	1:A:89:LEU:HD12	2.38	0.59
1:A:332:ARG:NH2	1:A:336:GLN:N	2.43	0.58
1:A:332:ARG:CD	1:A:332:ARG:C	2.60	0.58
1:A:188:THR:O	1:A:194:ASP:OD1	2.20	0.58
1:A:319:ILE:O	1:A:360:LEU:HG	2.03	0.58
1:A:322:LEU:HD13	1:A:322:LEU:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HA	1:A:30:ALA:HB3	1.85	0.58
1:A:51:ILE:HG22	1:A:55:MET:HE3	1.86	0.57
1:B:1162:ILE:HA	1:B:1165:VAL:HB	1.86	0.57
1:B:1347:LYS:HD2	1:B:1389:ASP:HB3	1.86	0.57
1:A:188:THR:HG21	1:A:192:GLU:CD	2.23	0.57
1:A:216:LYS:CD	1:A:360:LEU:HB3	2.34	0.57
1:A:70:VAL:O	1:A:74:LEU:HB2	2.04	0.57
1:A:187:PRO:HG2	1:A:194:ASP:CG	2.24	0.57
1:B:1168:GLN:O	1:B:1172:ASN:HB2	2.04	0.57
1:A:320:ASP:O	1:A:321:TYR:HB2	2.03	0.57
1:A:38:LEU:C	1:A:39:ILE:HD12	2.24	0.57
1:A:12:GLN:OE1	1:A:44:TYR:CE1	2.57	0.57
1:A:392:ILE:HG13	1:A:419:GLN:HA	1.87	0.57
1:B:1068:VAL:HA	1:B:1071:THR:CG2	2.35	0.57
1:B:1144:GLU:O	1:B:1148:MET:HG2	2.05	0.57
1:B:1261:GLN:NE2	1:B:1264:ARG:HD3	2.19	0.57
1:B:1413:GLU:OE2	1:B:1413:GLU:CA	2.37	0.57
1:A:81:GLU:CA	1:A:81:GLU:OE1	2.41	0.57
1:B:1147:ILE:O	1:B:1150:VAL:HG12	2.05	0.57
1:A:429:LEU:N	1:A:429:LEU:HD22	2.19	0.57
1:B:1063:GLU:HB3	1:B:1064:PRO:HD2	1.86	0.57
1:B:1268:LEU:HD12	1:B:1268:LEU:C	2.24	0.57
1:A:12:GLN:NE2	1:A:14:ILE:HG23	2.18	0.57
1:A:51:ILE:O	1:A:55:MET:HG2	2.05	0.57
1:B:1314:LEU:HG	1:B:1315:GLY:N	2.18	0.57
1:A:132:ARG:HH11	1:A:135:GLU:H	1.51	0.56
1:A:382:GLU:CD	1:A:382:GLU:N	2.58	0.56
1:A:67:LEU:H	1:A:67:LEU:HD22	1.71	0.56
1:A:214:VAL:CG2	1:A:216:LYS:CE	2.66	0.56
1:B:1086:VAL:HA	1:B:1089:LEU:HD12	1.87	0.56
1:A:183:ILE:O	1:A:184:THR:HG23	2.04	0.56
1:B:1392:ILE:N	1:B:1392:ILE:HD12	2.18	0.56
1:A:104:TYR:O	1:A:108:ILE:HG23	2.05	0.56
1:A:250:ARG:HA	1:A:250:ARG:NE	2.20	0.56
1:B:1228:ALA:HB2	1:B:1235:VAL:HG12	1.86	0.56
1:A:398:ARG:CG	1:A:412:ILE:HA	2.36	0.56
1:B:1207:ILE:HD13	1:B:1386:ILE:HB	1.88	0.56
1:A:237:ILE:HD13	1:A:237:ILE:C	2.26	0.55
1:A:211:ARG:HH11	1:A:212:PRO:CD	2.18	0.55
1:B:1070:VAL:O	1:B:1074:LEU:HB2	2.07	0.55
1:B:1154:LYS:O	1:B:1154:LYS:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PHE:CD2	1:A:159:PHE:O	2.59	0.55
1:A:297:ARG:NH2	1:B:1153:ARG:C	2.60	0.55
1:B:1164:ASP:O	1:B:1167:VAL:HB	2.07	0.55
1:B:1196:MET:CG	1:B:1416:ILE:HD12	2.18	0.55
1:A:27:ASP:OD2	1:A:29:THR:HB	2.07	0.55
1:A:265:THR:HA	1:A:268:LEU:HD22	1.87	0.55
1:A:414:ILE:CG1	1:A:427:VAL:HG23	2.37	0.55
1:A:358:ILE:HD12	1:A:358:ILE:H	1.71	0.55
1:A:248:VAL:HG21	1:B:1165:VAL:HG11	1.89	0.55
1:A:97:PRO:HB2	1:B:1066:ASP:OD2	2.07	0.55
1:B:1319:ILE:O	1:B:1360:LEU:HD13	2.07	0.55
1:B:1025:PHE:CD1	1:B:1067:LEU:HB3	2.42	0.54
1:B:1392:ILE:CD1	1:B:1392:ILE:H	2.19	0.54
1:B:1416:ILE:HB	1:B:1423:PRO:O	2.07	0.54
1:B:1024:VAL:HG13	1:B:1025:PHE:N	2.22	0.54
1:B:1118:LEU:HA	1:B:1121:THR:HG22	1.89	0.54
1:B:1211:ARG:HG2	1:B:1212:PRO:CD	2.37	0.54
1:B:1229:THR:HG23	1:B:1230:LYS:N	2.23	0.54
1:A:175:MET:HG2	1:A:423:PRO:HG3	1.88	0.54
1:A:200:PHE:HD2	1:A:206:ILE:HG12	1.72	0.54
1:A:358:ILE:HD12	1:A:358:ILE:N	2.22	0.54
1:A:412:ILE:HG12	1:A:431:PHE:HB2	1.89	0.54
1:A:231:THR:HG23	1:A:233:GLU:H	1.71	0.54
1:A:185:GLY:O	1:A:186:ILE:CG1	2.56	0.54
1:A:237:ILE:HG23	1:A:290:ILE:HG12	1.88	0.54
1:B:1096:VAL:HG12	1:B:1098:THR:O	2.08	0.54
1:A:338:GLU:O	1:A:342:ILE:HD13	2.07	0.54
1:A:333:GLU:HG2	1:A:333:GLU:O	2.07	0.54
1:A:209:ALA:HB3	1:A:395:PHE:CD1	2.43	0.54
1:A:118:LEU:O	1:A:121:THR:HG22	2.08	0.53
1:A:415:ILE:HD13	1:A:415:ILE:C	2.29	0.53
1:A:414:ILE:HG12	1:A:427:VAL:HG23	1.91	0.53
1:B:1186:ILE:HD12	1:B:1186:ILE:N	2.23	0.53
1:A:206:ILE:N	1:A:206:ILE:HD12	2.22	0.53
1:B:1117:ARG:HH12	1:B:1155:HIS:N	2.06	0.53
1:B:1207:ILE:CD1	1:B:1386:ILE:HB	2.39	0.53
1:A:180:ASN:HB3	1:A:195:ARG:NH1	2.23	0.53
1:A:302:ARG:NH1	1:A:349:LEU:HB2	2.23	0.53
1:B:1183:ILE:O	1:B:1183:ILE:HD12	2.07	0.53
1:A:190:PHE:HA	1:A:194:ASP:CG	2.29	0.53
1:B:1289:TYR:C	1:B:1290:ILE:HD12	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:HD11	1:A:207:ILE:HD11	1.89	0.53
1:A:216:LYS:HG3	1:A:360:LEU:HD13	1.89	0.53
1:A:183:ILE:C	1:A:183:ILE:HD13	2.28	0.53
1:A:77:LEU:N	1:A:77:LEU:HD13	2.24	0.53
1:B:1245:GLN:HA	1:B:1248:VAL:HG22	1.91	0.53
1:A:298:VAL:HA	1:A:301:ILE:CD1	2.30	0.53
1:A:332:ARG:HH12	1:A:339:VAL:HB	1.73	0.53
1:A:207:ILE:CD1	1:A:359:ALA:HB3	2.39	0.53
1:B:1200:PHE:CE1	1:B:1206:ILE:HG21	2.35	0.53
1:B:1300:ASP:O	1:B:1304:LYS:HG3	2.08	0.53
1:A:296:ILE:CG2	1:A:301:ILE:HD11	2.37	0.52
1:A:272:ASP:HB3	1:A:275:LYS:HB2	1.92	0.52
1:B:1051:ILE:HD11	1:B:1083:VAL:CG1	2.39	0.52
1:A:68:VAL:HA	1:A:71:THR:CG2	2.38	0.52
1:B:1288:ILE:HD12	1:B:1288:ILE:N	2.25	0.52
1:B:1291:ASP:OD2	1:B:1304:LYS:NZ	2.42	0.52
1:B:1390:ALA:HB1	1:B:1393:VAL:CG2	2.39	0.52
1:B:1197:THR:HG23	1:B:1199:GLY:O	2.10	0.52
1:A:418:LYS:HE2	1:A:420:ARG:HG2	1.92	0.52
1:A:64:PRO:O	1:A:69:THR:HG21	2.10	0.52
1:B:1025:PHE:HB3	1:B:1067:LEU:HD12	1.91	0.52
1:B:1152:GLN:HE21	1:B:1152:GLN:HA	1.75	0.52
1:A:288:ILE:O	1:B:1162:ILE:HG22	2.10	0.51
1:A:302:ARG:NH2	1:A:349:LEU:HA	2.24	0.51
1:A:315:GLY:O	1:A:355:VAL:HB	2.10	0.51
1:B:1237:ILE:HG23	1:B:1290:ILE:HG23	1.92	0.51
1:A:397:TYR:O	1:A:398:ARG:CB	2.58	0.51
1:B:1231:THR:HG23	1:B:1232:ASN:N	2.18	0.51
1:A:424:VAL:HG22	1:A:425:GLY:N	2.22	0.51
1:B:1136:ILE:HA	1:B:1139:LEU:HD13	1.93	0.51
1:B:1247:LEU:HD12	1:B:1248:VAL:N	2.25	0.51
1:B:1184:THR:HG22	1:B:1201:GLN:HG3	1.92	0.51
1:B:1024:VAL:HG21	1:B:1055:MET:CE	2.40	0.51
1:B:1290:ILE:HG22	1:B:1291:ASP:N	2.25	0.51
1:B:1200:PHE:O	1:B:1200:PHE:CD1	2.63	0.51
1:A:210:ALA:HB2	1:A:216:LYS:HB3	1.93	0.51
1:A:398:ARG:HG3	1:A:411:ILE:O	2.11	0.51
1:B:1024:VAL:HA	1:B:1030:ALA:HB3	1.93	0.51
1:A:226:ASN:O	1:A:230:LYS:HB2	2.11	0.50
1:A:296:ILE:HG12	1:A:301:ILE:CD1	2.42	0.50
1:B:1026:LEU:HD12	1:B:1099:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1133:GLU:OE2	1:B:1136:ILE:HD11	2.11	0.50
1:B:1198:SER:O	1:B:1201:GLN:NE2	2.45	0.50
1:A:236:ALA:O	1:A:317:VAL:HA	2.11	0.50
1:A:193:LEU:CD1	1:A:200:PHE:HZ	2.02	0.50
1:B:1007:GLU:C	1:B:1007:GLU:CD	2.70	0.50
1:B:1229:THR:HA	1:B:1286:ALA:HB2	1.93	0.50
1:A:431:PHE:O	1:A:432:ILE:HG13	2.12	0.50
1:B:1007:GLU:O	1:B:1007:GLU:OE1	2.29	0.50
1:A:9:ILE:O	1:A:9:ILE:HG23	2.11	0.50
1:B:1299:SER:O	1:B:1302:ARG:CG	2.54	0.50
1:A:297:ARG:HG3	1:B:1153:ARG:NH1	2.26	0.50
1:A:67:LEU:O	1:A:71:THR:HG22	2.11	0.49
1:B:1066:ASP:HB2	1:B:1067:LEU:HD13	1.94	0.49
1:B:1163:LYS:O	1:B:1166:LEU:HB2	2.12	0.49
1:B:1037:ARG:CB	1:B:1037:ARG:HH11	2.22	0.49
1:B:1239:SER:OG	1:B:1242:MET:HG2	2.12	0.49
1:B:1231:THR:HG22	1:B:1232:ASN:H	1.75	0.49
1:B:1414:ILE:N	1:B:1414:ILE:HD13	2.25	0.49
1:A:290:ILE:O	1:B:1160:LYS:HB2	2.12	0.49
1:A:171:ASP:C	1:A:174:GLU:HG2	2.33	0.49
1:A:183:ILE:HG23	1:A:184:THR:N	2.27	0.49
1:A:24:VAL:CG1	1:A:25:PHE:N	2.76	0.49
1:A:26:LEU:HD21	1:A:93:ALA:O	2.12	0.49
1:B:1290:ILE:HG22	1:B:1291:ASP:H	1.77	0.49
1:A:139:LEU:HA	1:A:142:GLU:HB3	1.93	0.49
1:B:1236:ALA:O	1:B:1317:VAL:HG13	2.12	0.49
1:A:243:SER:OG	1:A:246:GLN:HB2	2.12	0.49
1:A:308:LEU:HD23	1:A:308:LEU:O	2.11	0.49
1:B:1170:TYR:HA	1:B:1173:ILE:HG22	1.95	0.49
1:A:132:ARG:HH12	1:A:138:VAL:HG21	1.77	0.49
1:A:432:ILE:HD12	1:A:433:LYS:N	2.28	0.49
1:B:1211:ARG:CG	1:B:1363:LEU:HB2	2.36	0.49
1:A:16:ALA:O	1:A:19:ALA:HB3	2.13	0.48
1:B:1043:PHE:CD2	1:B:1048:HIS:HB3	2.48	0.48
1:A:251:MET:O	1:A:254:ALA:HB3	2.13	0.48
1:A:288:ILE:O	1:B:1162:ILE:CG2	2.61	0.48
1:A:183:ILE:HD13	1:A:183:ILE:O	2.13	0.48
1:A:216:LYS:HD2	1:A:360:LEU:CB	2.42	0.48
1:A:51:ILE:HD11	1:A:83:VAL:HB	1.95	0.48
1:B:1244:ALA:N	1:B:1292:ASP:OD2	2.46	0.48
1:A:21:LEU:O	1:A:24:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:O	1:A:237:ILE:HG23	2.13	0.48
1:B:1178:ASN:OD1	1:B:1179:ARG:N	2.46	0.48
1:B:1297:ARG:O	1:B:1301:ILE:HG13	2.13	0.48
1:B:1163:LYS:HD3	1:B:1163:LYS:C	2.34	0.48
1:A:332:ARG:NH2	1:A:335:ARG:HA	2.29	0.48
1:A:349:LEU:HD21	1:A:353:LEU:HD22	1.95	0.48
1:B:1200:PHE:O	1:B:1200:PHE:CG	2.66	0.48
1:B:1231:THR:CG2	1:B:1233:GLU:HB2	2.40	0.48
1:B:1207:ILE:HD12	1:B:1390:ALA:HB2	1.94	0.48
1:A:238:PHE:CE1	1:A:301:ILE:HG13	2.49	0.48
1:A:108:ILE:HD12	1:A:108:ILE:O	2.14	0.48
1:A:166:LEU:HD22	1:A:166:LEU:O	2.13	0.48
1:A:192:GLU:CG	1:A:193:LEU:HG	2.41	0.48
1:A:338:GLU:N	1:A:338:GLU:OE2	2.47	0.48
1:B:1089:LEU:O	1:B:1092:LEU:HB2	2.14	0.48
1:B:1214:VAL:O	1:B:1214:VAL:HG12	2.13	0.47
1:B:1231:THR:O	1:B:1232:ASN:CB	2.62	0.47
1:B:1188:THR:HB	1:B:1223:ILE:HD11	1.96	0.47
1:B:1199:GLY:O	1:B:1200:PHE:CB	2.61	0.47
1:A:161:ASN:HD21	1:A:164:ASP:HB2	1.80	0.47
1:B:1132:ARG:O	1:B:1132:ARG:HG3	2.13	0.47
1:A:14:ILE:O	1:A:18:GLN:HG3	2.14	0.47
1:A:293:THR:O	1:A:293:THR:HG23	2.14	0.47
1:B:1184:THR:CG2	1:B:1201:GLN:HG3	2.45	0.47
1:A:382:GLU:C	1:A:384:GLY:H	2.17	0.47
1:B:1067:LEU:N	1:B:1067:LEU:HD13	2.29	0.47
1:B:1203:SER:HA	1:B:1355:VAL:O	2.15	0.47
1:A:117:ARG:CZ	1:A:153:ARG:HD2	2.44	0.47
1:A:56:LEU:O	1:A:60:ASP:HB2	2.15	0.47
1:A:88:TYR:HE1	1:A:92:LEU:HD13	1.78	0.47
1:A:386:ILE:HG13	1:A:387:GLU:N	2.30	0.47
1:B:1112:LYS:N	1:B:1112:LYS:HD3	2.30	0.47
1:B:1207:ILE:CD1	1:B:1390:ALA:HB2	2.45	0.47
1:B:1150:VAL:HG13	1:B:1151:SER:N	2.29	0.47
1:B:1117:ARG:HG3	1:B:1150:VAL:HG23	1.95	0.47
1:A:183:ILE:HD13	1:A:184:THR:OG1	2.14	0.47
1:A:25:PHE:CE1	1:A:70:VAL:HG21	2.50	0.47
1:A:302:ARG:HH22	1:A:349:LEU:HA	1.79	0.47
1:B:1039:ILE:O	1:B:1042:ASP:N	2.42	0.47
1:A:415:ILE:O	1:A:415:ILE:HG23	2.15	0.46
1:A:333:GLU:OE1	1:A:337:GLN:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1386:ILE:HG13	1:B:1387:GLU:N	2.31	0.46
1:A:314:LEU:HB3	1:A:315:GLY:H	1.42	0.46
1:B:1200:PHE:N	1:B:1201:GLN:NE2	2.59	0.46
1:A:240:LEU:N	1:A:240:LEU:CD2	2.68	0.46
1:A:39:ILE:O	1:A:42:ASP:N	2.33	0.46
1:B:1031:LEU:HD12	1:B:1055:MET:HE3	1.98	0.46
1:B:1154:LYS:C	1:B:1154:LYS:HD3	2.36	0.46
1:B:1223:ILE:O	1:B:1227:VAL:HG23	2.15	0.46
1:B:1235:VAL:HG23	1:B:1316:MET:O	2.16	0.46
1:A:132:ARG:HD2	1:A:132:ARG:HA	1.57	0.46
1:A:188:THR:OG1	1:A:189:GLY:N	2.49	0.46
1:A:214:VAL:HG21	1:A:216:LYS:NZ	2.30	0.46
1:B:1303:ALA:O	1:B:1307:ARG:HG3	2.16	0.46
1:A:248:VAL:HG21	1:B:1165:VAL:CG1	2.46	0.46
1:B:1298:VAL:O	1:B:1302:ARG:HG2	2.16	0.46
1:B:1362:GLN:N	1:B:1362:GLN:OE1	2.48	0.46
1:A:159:PHE:CD2	1:A:159:PHE:N	2.84	0.46
1:A:200:PHE:CD2	1:A:206:ILE:HG12	2.51	0.46
1:A:46:ALA:O	1:A:47:ALA:C	2.53	0.46
1:A:68:VAL:HA	1:A:71:THR:HG22	1.96	0.46
1:B:1227:VAL:O	1:B:1231:THR:CB	2.63	0.46
1:B:1039:ILE:HG23	1:B:1040:PRO:CD	2.38	0.46
1:B:1353:LEU:O	1:B:1354:GLU:C	2.53	0.46
1:A:322:LEU:HD12	1:A:323:GLN:NE2	2.31	0.45
1:A:396:LEU:CD2	1:A:414:ILE:HG22	2.46	0.45
1:B:1111:GLU:O	1:B:1115:LEU:HD23	2.16	0.45
1:A:205:LEU:HD12	1:A:390:ALA:HA	1.98	0.45
1:A:183:ILE:HG22	1:A:198:SER:HB2	1.98	0.45
1:B:1033:LEU:O	1:B:1036:GLU:HB3	2.16	0.45
1:B:1298:VAL:CG1	1:B:1299:SER:N	2.79	0.45
1:B:1390:ALA:CB	1:B:1393:VAL:CG2	2.94	0.45
1:A:171:ASP:O	1:A:174:GLU:HG2	2.17	0.45
1:A:290:ILE:C	1:A:290:ILE:HD13	2.36	0.45
1:A:238:PHE:CE2	1:B:1159:PHE:HE1	2.34	0.45
1:B:1309:LYS:HG3	1:B:1314:LEU:HB2	1.96	0.45
1:A:127:GLN:C	1:A:129:GLY:H	2.20	0.45
1:A:137:ASP:O	1:A:140:LEU:HB3	2.17	0.45
1:A:293:THR:HA	1:A:294:PRO:HD3	1.68	0.45
1:A:98:THR:O	1:A:100:ALA:O	2.34	0.45
1:A:316:MET:CB	1:A:356:PRO:HG2	2.42	0.45
1:A:234:ASN:HB2	1:A:313:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1043:PHE:HD2	1:B:1048:HIS:HB3	1.82	0.45
1:B:1297:ARG:HH11	1:B:1297:ARG:HG3	1.82	0.45
1:B:1353:LEU:HB3	1:B:1355:VAL:HG12	1.97	0.45
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.85	0.44
1:A:23:ALA:N	1:A:96:VAL:HG21	2.32	0.44
1:A:274:GLY:O	1:A:277:THR:N	2.48	0.44
1:A:308:LEU:HD23	1:A:308:LEU:C	2.38	0.44
1:A:306:ARG:HG2	1:A:310:GLN:OE1	2.16	0.44
1:B:1024:VAL:CG1	1:B:1025:PHE:N	2.81	0.44
1:A:154:LYS:HE2	1:A:156:SER:O	2.18	0.44
1:A:206:ILE:O	1:A:207:ILE:HD13	2.18	0.44
1:A:24:VAL:HG13	1:A:25:PHE:N	2.32	0.44
1:B:1221:LEU:H	1:B:1221:LEU:HD23	1.82	0.44
1:A:37:ARG:HH22	1:A:156:SER:HB2	1.82	0.44
1:B:1184:THR:HB	1:B:1201:GLN:CG	2.47	0.44
1:A:332:ARG:CZ	1:A:335:ARG:HA	2.48	0.44
1:B:1318:VAL:HA	1:B:1358:ILE:O	2.18	0.44
1:A:186:ILE:O	1:A:186:ILE:HG13	2.17	0.44
1:A:342:ILE:O	1:A:345:SER:HB2	2.18	0.44
1:B:1392:ILE:HD11	1:B:1420:ARG:CB	2.35	0.44
1:A:98:THR:C	1:A:100:ALA:N	2.71	0.44
1:A:410:ASN:O	1:A:431:PHE:N	2.42	0.44
1:B:1161:ASN:HB3	1:B:1164:ASP:HB2	1.99	0.44
1:A:162:ILE:HG23	1:A:162:ILE:HD12	1.37	0.44
1:B:1227:VAL:HG21	1:B:1316:MET:SD	2.58	0.44
1:B:1206:ILE:O	1:B:1358:ILE:HA	2.18	0.43
1:B:1187:PRO:HG3	1:B:1194:ASP:HA	1.99	0.43
1:B:1027:ASP:OD1	1:B:1029:THR:N	2.49	0.43
1:A:25:PHE:HZ	1:A:89:LEU:CD1	2.27	0.43
1:B:1211:ARG:HG2	1:B:1212:PRO:HD3	1.99	0.43
1:A:245:GLN:HG2	1:B:1419:GLN:NE2	2.33	0.43
1:A:398:ARG:HG3	1:A:412:ILE:HA	2.00	0.43
1:B:1009:ILE:O	1:B:1009:ILE:HG23	2.18	0.43
1:B:1240:LEU:N	1:B:1240:LEU:HD12	2.34	0.43
1:B:1261:GLN:NE2	1:B:1264:ARG:HB2	2.15	0.43
1:A:37:ARG:NH2	1:A:156:SER:HB2	2.34	0.43
1:B:1057:ARG:HH22	1:B:1077:LEU:CD1	2.30	0.43
1:B:1114:LEU:O	1:B:1117:ARG:HB3	2.19	0.43
1:A:166:LEU:C	1:A:166:LEU:HD22	2.39	0.43
1:A:330:ARG:H	1:A:330:ARG:HG2	1.41	0.43
1:B:1314:LEU:CG	1:B:1315:GLY:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1298:VAL:HG13	1:B:1299:SER:H	1.80	0.42
1:A:254:ALA:HA	1:A:434:GLU:HG3	2.01	0.42
1:B:1033:LEU:HA	1:B:1036:GLU:HB2	2.01	0.42
1:A:387:GLU:HG3	1:A:388:GLN:H	1.81	0.42
1:B:1206:ILE:O	1:B:1206:ILE:HG13	2.20	0.42
1:A:38:LEU:O	1:A:39:ILE:HD12	2.19	0.42
1:A:277:THR:HA	1:A:280:MET:HB2	2.01	0.42
1:A:414:ILE:HD13	1:A:414:ILE:N	2.26	0.42
1:B:1072:ALA:O	1:B:1075:ALA:HB3	2.19	0.42
1:B:1209:ALA:HB3	1:B:1395:PHE:HD2	1.84	0.42
1:A:161:ASN:HB2	1:A:162:ILE:H	1.63	0.42
1:A:334:ASN:O	1:A:335:ARG:C	2.58	0.42
1:A:163:LYS:HG3	1:A:164:ASP:N	2.31	0.42
1:A:22:GLY:O	1:A:26:LEU:CD2	2.63	0.42
1:A:325:ILE:HD12	1:A:325:ILE:N	2.34	0.42
1:B:1119:ILE:C	1:B:1119:ILE:HD12	2.39	0.42
1:B:1296:ILE:HG23	1:B:1297:ARG:N	2.35	0.42
1:A:10:PRO:HA	1:A:11:PRO:HD3	1.68	0.42
1:B:1076:ALA:C	1:B:1078:GLU:N	2.72	0.42
1:B:1101:ASN:O	1:B:1105:TYR:HB2	2.20	0.42
1:B:1261:GLN:HE22	1:B:1264:ARG:CB	2.18	0.42
1:A:39:ILE:O	1:A:42:ASP:HB2	2.18	0.42
1:B:1185:GLY:H	1:B:1199:GLY:HA3	1.85	0.42
1:B:1342:ILE:HG13	1:B:1343:SER:N	2.35	0.42
1:B:1411:ILE:HD12	1:B:1411:ILE:C	2.40	0.42
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.40	0.41
1:A:76:ALA:C	1:A:77:LEU:HD13	2.40	0.41
1:A:132:ARG:HH11	1:A:135:GLU:N	2.18	0.41
1:A:424:VAL:HG13	1:A:425:GLY:N	2.35	0.41
1:A:52:PHE:CE1	1:A:56:LEU:HD11	2.55	0.41
1:A:414:ILE:HG12	1:A:414:ILE:O	2.19	0.41
1:B:1042:ASP:OD1	1:B:1154:LYS:HE2	2.21	0.41
1:A:398:ARG:CA	1:A:398:ARG:NE	2.62	0.41
1:B:1188:THR:OG1	1:B:1189:GLY:N	2.51	0.41
1:B:1197:THR:O	1:B:1197:THR:OG1	2.37	0.41
1:A:17:GLU:OE2	1:A:44:TYR:N	2.51	0.41
1:A:227:VAL:CG1	1:A:227:VAL:O	2.67	0.41
1:B:1066:ASP:HB2	1:B:1067:LEU:CD1	2.51	0.41
1:A:203:SER:HA	1:A:350:ALA:O	2.20	0.41
1:B:1092:LEU:O	1:B:1095:SER:HB2	2.21	0.41
1:B:1166:LEU:HA	1:B:1166:LEU:HD13	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:THR:HB	1:B:1201:GLN:OE1	2.19	0.41
1:B:1212:PRO:HD3	1:B:1363:LEU:O	2.20	0.41
1:B:1065:VAL:O	1:B:1070:VAL:HG12	2.21	0.41
1:B:1237:ILE:CG2	1:B:1290:ILE:HG13	2.51	0.41
1:B:1114:LEU:HA	1:B:1114:LEU:HD12	1.82	0.41
1:B:1269:THR:HG22	1:B:1271:GLU:HG3	2.03	0.41
1:B:1209:ALA:HB3	1:B:1395:PHE:CD2	2.56	0.41
1:A:298:VAL:O	1:A:301:ILE:HB	2.21	0.41
1:B:1025:PHE:HE1	1:B:1070:VAL:HG11	1.87	0.41
1:B:1039:ILE:N	1:B:1039:ILE:HD12	2.35	0.41
1:B:1096:VAL:HA	1:B:1097:PRO:HD3	1.85	0.41
1:B:1248:VAL:O	1:B:1252:LEU:HD13	2.22	0.41
1:B:1086:VAL:O	1:B:1089:LEU:HB2	2.21	0.40
1:B:1199:GLY:O	1:B:1200:PHE:HB3	2.21	0.40
1:B:1245:GLN:HA	1:B:1248:VAL:CG2	2.50	0.40
1:A:221:LEU:O	1:A:224:ALA:HB3	2.22	0.40
1:A:343:SER:HB2	1:A:386:ILE:HG22	2.03	0.40
1:B:1104:TYR:CD1	1:B:1104:TYR:N	2.89	0.40
1:B:1321:TYR:CE1	1:B:1362:GLN:CG	3.03	0.40
1:B:1314:LEU:HD23	1:B:1355:VAL:HB	2.03	0.40
1:A:221:LEU:C	1:A:221:LEU:HD12	2.42	0.40
1:B:1021:LEU:HD23	1:B:1021:LEU:HA	1.90	0.40
1:B:1101:ASN:N	1:B:1101:ASN:HD22	2.18	0.40
1:B:1039:ILE:CG2	1:B:1040:PRO:CD	2.96	0.40
1:B:1074:LEU:HB3	1:B:1080:LEU:HD23	2.02	0.40
1:B:1392:ILE:HG12	1:B:1421:ASN:HD21	1.87	0.40
1:A:294:PRO:HG2	1:B:1388:GLN:CD	2.42	0.40
1:B:1211:ARG:HG2	1:B:1212:PRO:HD2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:O	1:B:1307:ARG:NH1[2_655]	1.77	0.43
1:A:87:SER:OG	1:B:1163:LYS:NZ[4_665]	1.89	0.31

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	390/454 (86%)	319 (82%)	54 (14%)	17 (4%)	2	23
1	B	365/454 (80%)	305 (84%)	38 (10%)	22 (6%)	1	17
All	All	755/908 (83%)	624 (83%)	92 (12%)	39 (5%)	2	20

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	161	ASN
1	A	190	PHE
1	A	192	GLU
1	A	211	ARG
1	A	334	ASN
1	A	398	ARG
1	B	1067	LEU
1	B	1161	ASN
1	B	1162	ILE
1	B	1188	THR
1	B	1200	PHE
1	B	1202	ARG
1	B	1297	ARG
1	B	1423	PRO
1	A	187	PRO
1	A	189	GLY
1	A	200	PHE
1	A	335	ARG
1	A	336	GLN
1	B	1078	GLU
1	B	1097	PRO
1	B	1187	PRO
1	B	1259	ASN
1	B	1261	GLN

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Mol	Chain	Res	Type
1	B	1296	ILE
1	B	1186	ILE
1	B	1295	SER
1	A	321	TYR
1	A	432	ILE
1	B	1232	ASN
1	B	1257	ASN
1	B	1294	PRO
1	B	1356	PRO
1	B	1135	GLU
1	B	1264	ARG
1	A	314	LEU
1	A	181	GLY
1	A	214	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/388 (86%)	274 (82%)	58 (18%)	2	12
1	B	313/388 (81%)	266 (85%)	47 (15%)	3	19
All	All	645/776 (83%)	540 (84%)	105 (16%)	2	15

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

Mol	Chain	Res	Type
1	A	8	ARG
1	A	37	ARG
1	A	58	VAL
1	A	67	LEU
1	A	74	LEU
1	A	77	LEU
1	A	81	GLU
1	A	95	SER
1	A	108	ILE

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Mol	Chain	Res	Type
1	A	112	LYS
1	A	116	ARG
1	A	128	ASP
1	A	132	ARG
1	A	145	ARG
1	A	154	LYS
1	A	155	HIS
1	A	159	PHE
1	A	161	ASN
1	A	162	ILE
1	A	163	LYS
1	A	165	VAL
1	A	177	HIS
1	A	179	ARG
1	A	182	ASP
1	A	183	ILE
1	A	184	THR
1	A	194	ASP
1	A	196	MET
1	A	202	ARG
1	A	211	ARG
1	A	216	LYS
1	A	231	THR
1	A	237	ILE
1	A	240	LEU
1	A	247	LEU
1	A	250	ARG
1	A	275	LYS
1	A	290	ILE
1	A	302	ARG
1	A	305	CYS
1	A	321	TYR
1	A	322	LEU
1	A	330	ARG
1	A	332	ARG
1	A	335	ARG
1	A	336	GLN
1	A	337	GLN
1	A	360	LEU
1	A	362	GLN
1	A	382	GLU
1	A	397	TYR

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Mol	Chain	Res	Type
1	A	398	ARG
1	A	399	ASP
1	A	414	ILE
1	A	415	ILE
1	A	416	ILE
1	A	427	VAL
1	A	429	LEU
1	B	1031	LEU
1	B	1037	ARG
1	B	1045	ARG
1	B	1067	LEU
1	B	1070	VAL
1	B	1074	LEU
1	B	1077	LEU
1	B	1081	GLU
1	B	1095	SER
1	B	1101	ASN
1	B	1105	TYR
1	B	1114	LEU
1	B	1134	ASP
1	B	1139	LEU
1	B	1145	ARG
1	B	1163	LYS
1	B	1176	LEU
1	B	1187	PRO
1	B	1192	GLU
1	B	1194	ASP
1	B	1196	MET
1	B	1200	PHE
1	B	1201	GLN
1	B	1202	ARG
1	B	1206	ILE
1	B	1222	ASN
1	B	1231	THR
1	B	1233	GLU
1	B	1262	ASN
1	B	1271	GLU
1	B	1290	ILE
1	B	1292	ASP
1	B	1297	ARG
1	B	1306	ARG
1	B	1309	LYS

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Mol	Chain	Res	Type
1	B	1316	MET
1	B	1318	VAL
1	B	1321	TYR
1	B	1334	ASN
1	B	1341	GLU
1	B	1344	ARG
1	B	1362	GLN
1	B	1387	GLU
1	B	1413	GLU
1	B	1414	ILE
1	B	1419	GLN
1	B	1420	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	18	GLN
1	A	79	GLN
1	A	101	ASN
1	A	161	ASN
1	A	222	ASN
1	A	225	GLN
1	A	336	GLN
1	A	428	GLN
1	B	1012	GLN
1	B	1101	ASN
1	B	1127	GLN
1	B	1152	GLN
1	B	1201	GLN
1	B	1222	ASN
1	B	1225	GLN
1	B	1234	ASN
1	B	1261	GLN
1	B	1262	ASN
1	B	1285	ASN
1	B	1334	ASN
1	B	1336	GLN
1	B	1419	GLN
1	B	1421	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	398/454 (87%)	-0.18	4 (1%) 82 70	112, 165, 187, 187	0
1	B	377/454 (83%)	-0.12	12 (3%) 47 32	96, 175, 187, 187	0
All	All	775/908 (85%)	-0.15	16 (2%) 63 48	96, 171, 187, 187	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1265	THR	5.4
1	B	1266	GLY	3.1
1	B	1322	LEU	2.9
1	B	1259	ASN	2.9
1	B	1214	VAL	2.9
1	A	435	TYR	2.8
1	B	1268	LEU	2.7
1	B	1411	ILE	2.6
1	B	1190	PHE	2.6
1	B	1241	GLU	2.5
1	B	1333	GLU	2.5
1	A	180	ASN	2.4
1	A	334	ASN	2.4
1	A	258	ILE	2.2
1	B	1264	ARG	2.1
1	B	1297	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AU	A	1437	1/1	0.97	0.09	186,186,186,186	0
2	AU	B	2426	1/1	0.97	0.11	186,186,186,186	0
2	AU	B	2427	1/1	0.98	0.05	186,186,186,186	0
2	AU	A	1436	1/1	0.99	0.04	186,186,186,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.