



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2017 – 01:02 AM EDT

PDB ID : 4LL8  
Title : Complex of carboxy terminal domain of Myo4p and She3p middle fragment  
Authors : Shi, H.; Singh, N.; Esselborn, F.; Blobel, G.  
Deposited on : unknown  
Resolution : 3.58 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

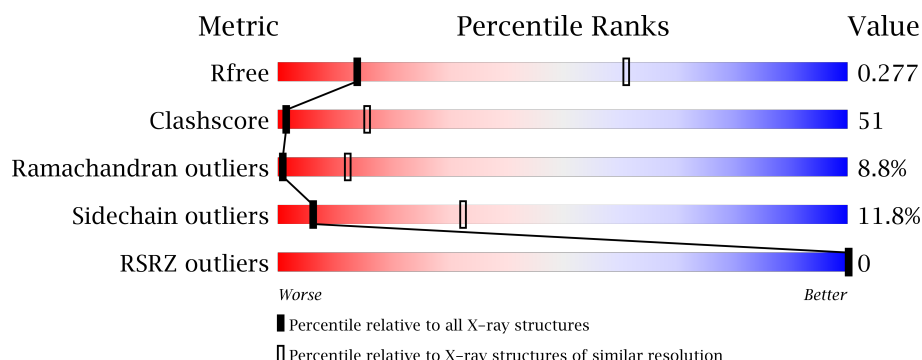
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.58 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))
$R_{free}$	100719	1009 (3.70-3.46)
Clashscore	112137	1128 (3.70-3.46)
Ramachandran outliers	110173	1088 (3.70-3.46)
Sidechain outliers	110143	1088 (3.70-3.46)
RSRZ outliers	101464	1034 (3.70-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	539	
2	B	235	
2	E	235	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5337 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 Myosin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3421	2203	568	639	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1018	ALA	LYS	ENGINEERED MUTATION	UNP P32492
A	1019	ALA	LYS	ENGINEERED MUTATION	UNP P32492
A	1020	ALA	LYS	ENGINEERED MUTATION	UNP P32492
A	1113	SER	CYS	ENGINEERED MUTATION	UNP P32492
A	1288	SER	CYS	ENGINEERED MUTATION	UNP P32492
A	1320	SER	CYS	ENGINEERED MUTATION	UNP P32492

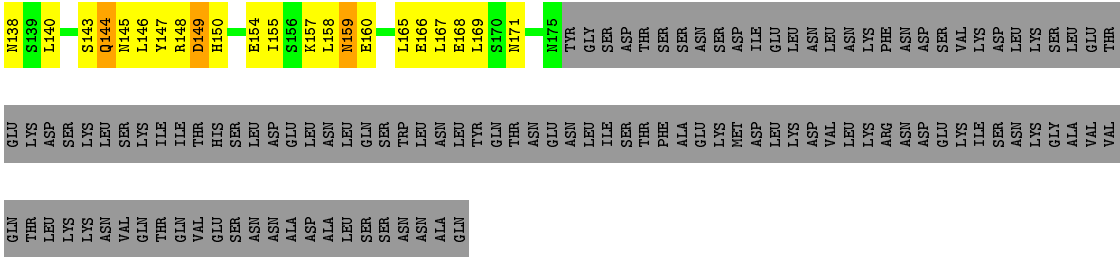
- Molecule 2 is a protein called SWI5-dependent HO expression protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	119	Total	C	N	O	S	0	0	0
			982	602	170	206	4			
2	B	113	Total	C	N	O	S	0	0	0
			934	574	159	197	4			

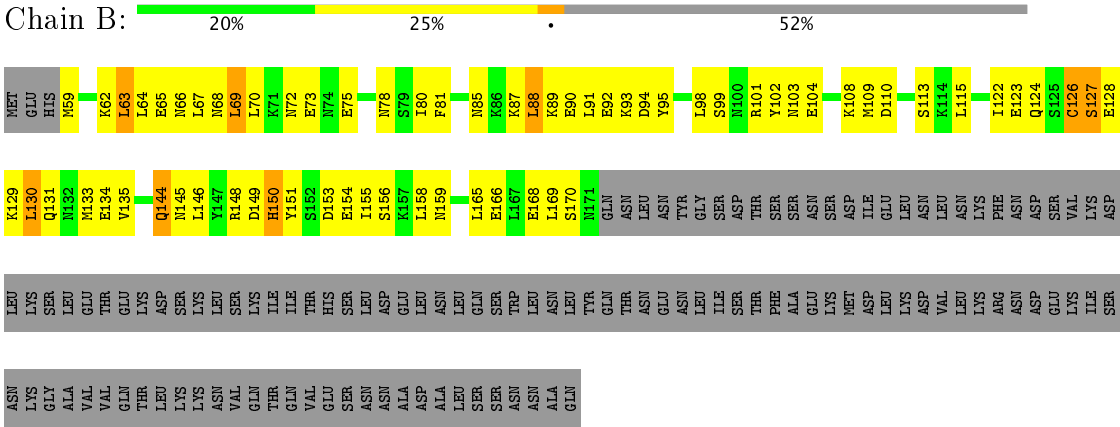
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	56	MET	-	EXPRESSION TAG	UNP P38272
E	57	GLU	-	EXPRESSION TAG	UNP P38272
E	58	HIS	-	EXPRESSION TAG	UNP P38272
E	59	MET	-	EXPRESSION TAG	UNP P38272
B	56	MET	-	EXPRESSION TAG	UNP P38272
B	57	GLU	-	EXPRESSION TAG	UNP P38272
B	58	HIS	-	EXPRESSION TAG	UNP P38272
B	59	MET	-	EXPRESSION TAG	UNP P38272





• Molecule 2: SWI5-dependent HO expression protein 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	272.01Å 38.12Å 183.99Å 90.00° 125.24° 90.00°	Depositor
Resolution (Å)	50.00 – 3.58 44.15 – 3.58	Depositor EDS
% Data completeness (in resolution range)	75.5 (50.00-3.58) 89.8 (44.15-3.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.268 0.233 , 0.277	Depositor DCC
$R_{free}$ test set	1641 reflections (9.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 72.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.48	0/3479	0.78	1/4702 (0.0%)
2	B	0.39	0/940	0.60	0/1253
2	E	0.41	0/989	0.62	0/1320
All	All	0.45	0/5408	0.73	1/7275 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1320	SER	N-CA-C	6.59	128.80	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	3421	0	3515	443	0
2	B	934	0	928	84	0
2	E	982	0	968	76	0
All	All	5337	0	5411	545	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 51.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:LEU:HD23	2:B:91:LEU:HD22	1.37	1.05
2:E:123:GLU:HG3	2:B:122:ILE:HG21	1.42	1.02
1:A:1163:ILE:HD13	1:A:1226:LEU:HD11	1.40	1.01
1:A:1343:GLU:HB2	1:A:1344:PRO:HD3	1.40	1.00
2:E:166:GLU:HG2	2:B:165:LEU:HD13	1.46	0.97
1:A:1384:ASN:OD1	1:A:1387:GLN:HG2	1.65	0.95
1:A:1137:LEU:HD11	1:A:1291:GLN:HB2	1.48	0.94
1:A:1114:TYR:HA	1:A:1459:LEU:HD23	1.49	0.94
1:A:1207:TYR:HD2	1:A:1219:THR:HG21	1.32	0.93
1:A:1443:LEU:O	1:A:1444:ARG:HG2	1.68	0.93
1:A:1039:LYS:HE3	1:A:1419:ARG:HH22	1.34	0.92
1:A:1208:GLU:HG2	1:A:1220:LEU:HD21	1.54	0.89
1:A:1207:TYR:CD2	1:A:1219:THR:HG21	2.07	0.89
2:E:84:LYS:HE3	2:B:85:ASN:OD1	1.72	0.89
1:A:1178:PRO:HD2	1:A:1181:GLU:HB3	1.53	0.88
1:A:1039:LYS:HE3	1:A:1419:ARG:NH2	1.88	0.88
1:A:1127:ASN:HD22	1:A:1130:GLU:HB3	1.39	0.87
1:A:1319:LYS:O	1:A:1321:PRO:HA	1.75	0.87
1:A:1420:GLU:HG2	1:A:1428:MET:HE3	1.54	0.87
1:A:1346:ILE:HD11	1:A:1349:VAL:HG13	1.54	0.86
1:A:1321:PRO:HG2	1:A:1322:ALA:H	1.39	0.86
1:A:1360:VAL:HA	1:A:1363:LEU:HD13	1.57	0.86
1:A:1206:LEU:HG	1:A:1207:TYR:CD1	2.11	0.86
1:A:1420:GLU:HG2	1:A:1428:MET:CE	2.05	0.85
1:A:1309:ASN:HD21	1:A:1355:GLN:HB2	1.41	0.85
2:E:158:LEU:HB3	2:B:158:LEU:HD21	1.59	0.84
1:A:1167:LEU:HG	1:A:1233:VAL:HG11	1.58	0.84
1:A:1187:ILE:HD12	1:A:1286:VAL:HG11	1.58	0.84
1:A:1260:LEU:HD11	1:A:1316:LEU:HD13	1.59	0.84
1:A:1096:ARG:HD2	1:A:1097:GLU:N	1.94	0.82
1:A:1305:LEU:HD11	1:A:1349:VAL:HG12	1.61	0.81
1:A:1359:ALA:HB1	1:A:1391:ILE:HD11	1.63	0.80
1:A:1379:PHE:CE2	2:E:143:SER:HB2	2.17	0.79
1:A:1406:PRO:HG3	1:A:1409:ILE:HD12	1.65	0.78
1:A:1376:LEU:O	1:A:1379:PHE:HB2	1.84	0.78
1:A:1029:MET:HG2	1:A:1056:PHE:CE2	2.19	0.77
1:A:1299:LYS:HG2	1:A:1303:ASP:OD2	1.84	0.77
1:A:1167:LEU:HD23	1:A:1233:VAL:HG21	1.66	0.76
1:A:1456:THR:HG21	1:A:1464:LYS:HZ2	1.51	0.76
1:A:1216:ASP:O	1:A:1220:LEU:HB2	1.86	0.76
1:A:1153:ASN:N	1:A:1153:ASN:HD22	1.84	0.76
1:A:1412:TYR:O	1:A:1416:VAL:HG23	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:LEU:HD22	1:A:1230:THR:HG21	1.68	0.75
1:A:1308:LEU:O	1:A:1312:LEU:HB2	1.86	0.75
1:A:1145:THR:HG21	1:A:1464:LYS:HG2	1.66	0.75
2:E:91:LEU:CD2	2:B:91:LEU:HD22	2.15	0.75
1:A:1187:ILE:HD12	1:A:1286:VAL:CG1	2.16	0.75
1:A:1259:VAL:HG23	1:A:1312:LEU:HD21	1.68	0.75
1:A:1251:ALA:O	1:A:1254:GLU:HG3	1.87	0.74
1:A:1321:PRO:CG	1:A:1322:ALA:H	2.00	0.74
1:A:1108:LEU:HD13	1:A:1155:LEU:HD12	1.68	0.73
1:A:1337:ARG:O	1:A:1340:SER:HB3	1.87	0.73
1:A:1137:LEU:O	1:A:1140:ILE:HG22	1.86	0.73
1:A:1137:LEU:HD23	1:A:1450:ILE:HD13	1.71	0.72
1:A:1280:LEU:HD13	1:A:1341:TRP:CE3	2.24	0.72
1:A:1309:ASN:HD21	1:A:1355:GLN:CB	2.03	0.72
1:A:1050:MET:SD	2:E:158:LEU:HD23	2.30	0.72
1:A:1101:ASN:CG	1:A:1102:PRO:HD2	2.11	0.71
2:E:157:LYS:O	2:E:160:GLU:HB3	1.88	0.71
1:A:1050:MET:SD	2:B:158:LEU:HD23	2.30	0.71
1:A:1457:GLU:HG3	1:A:1458:GLY:H	1.55	0.71
1:A:1147:VAL:O	1:A:1151:VAL:HG23	1.91	0.70
2:E:77:LEU:HD21	2:B:78:ASN:HA	1.72	0.70
1:A:1169:THR:O	1:A:1173:ILE:HG13	1.91	0.70
1:A:1151:VAL:HG12	1:A:1207:TYR:HE2	1.56	0.70
1:A:1460:ALA:O	1:A:1463:SER:N	2.24	0.70
2:E:102:TYR:CZ	2:E:106:LYS:HD2	2.27	0.70
1:A:1309:ASN:HB2	1:A:1353:LEU:HD23	1.74	0.70
1:A:1115:THR:HG23	1:A:1162:PHE:CD1	2.27	0.69
1:A:1310:VAL:HG13	1:A:1432:LEU:HB3	1.74	0.69
1:A:1439:ALA:O	1:A:1443:LEU:HG	1.92	0.69
1:A:1266:LYS:C	1:A:1268:SER:H	1.96	0.69
1:A:1353:LEU:O	1:A:1357:ILE:HG22	1.91	0.69
1:A:1207:TYR:HD2	1:A:1219:THR:CG2	2.04	0.69
1:A:1156:LEU:C	1:A:1158:GLN:H	1.94	0.68
1:A:1456:THR:HG21	1:A:1464:LYS:NZ	2.07	0.68
1:A:1333:ARG:HA	1:A:1336:GLU:HG2	1.76	0.68
1:A:1026:GLN:HG3	2:B:170:SER:OG	1.92	0.68
2:E:87:LYS:HB3	2:B:88:LEU:HD12	1.75	0.68
1:A:1264:LEU:HD21	1:A:1268:SER:HB2	1.76	0.67
1:A:1122:TYR:O	1:A:1126:VAL:HG23	1.94	0.67
1:A:1346:ILE:HD11	1:A:1349:VAL:CG1	2.24	0.67
1:A:1093:VAL:CG2	1:A:1154:GLY:HA3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:TYR:N	1:A:1445:TYR:CD1	2.61	0.67
1:A:1100:GLY:HA2	1:A:1104:LEU:HD13	1.77	0.66
1:A:1114:TYR:O	1:A:1118:VAL:HG23	1.96	0.66
1:A:1360:VAL:HA	1:A:1363:LEU:CD1	2.25	0.66
2:B:150:HIS:HD1	2:B:150:HIS:C	1.98	0.66
1:A:1406:PRO:HG2	1:A:1409:ILE:HB	1.78	0.66
1:A:1457:GLU:HG3	1:A:1458:GLY:N	2.10	0.66
1:A:1309:ASN:HD21	1:A:1355:GLN:CG	2.09	0.65
1:A:1108:LEU:O	1:A:1110:ASP:N	2.30	0.65
1:A:1258:MET:HE1	1:A:1273:PHE:HA	1.79	0.65
1:A:1399:ASN:O	1:A:1400:LYS:HB2	1.96	0.65
1:A:1276:LEU:O	1:A:1279:PHE:HB3	1.96	0.65
2:E:83:ARG:C	2:E:85:ASN:H	1.99	0.65
2:E:87:LYS:HB3	2:B:88:LEU:CD1	2.27	0.65
2:E:88:LEU:HD12	2:B:88:LEU:HA	1.78	0.65
1:A:1212:GLY:O	1:A:1216:ASP:HB2	1.98	0.64
1:A:1386:ALA:HA	1:A:1417:ILE:HD11	1.78	0.64
2:E:159:ASN:HA	2:B:158:LEU:HD11	1.77	0.64
1:A:1379:PHE:HE2	2:E:143:SER:HB2	1.59	0.64
1:A:1111:LEU:HD23	1:A:1112:ASN:N	2.13	0.64
1:A:1149:SER:OG	1:A:1467:LYS:HG3	1.98	0.64
2:E:109:MET:HE1	2:B:108:LYS:HB2	1.79	0.64
1:A:1115:THR:HG23	1:A:1162:PHE:HD1	1.62	0.64
1:A:1208:GLU:CG	1:A:1220:LEU:HD21	2.27	0.64
1:A:1163:ILE:HD13	1:A:1226:LEU:CD1	2.24	0.64
1:A:1198:ALA:C	1:A:1200:ALA:H	2.00	0.64
1:A:1456:THR:CG2	1:A:1464:LYS:NZ	2.61	0.64
1:A:1331:VAL:O	1:A:1335:ILE:HG13	1.97	0.64
2:B:130:LEU:C	2:B:130:LEU:HD23	2.19	0.64
1:A:1114:TYR:HA	1:A:1459:LEU:CD2	2.26	0.63
1:A:1456:THR:CG2	1:A:1464:LYS:HZ2	2.11	0.63
1:A:1108:LEU:HD22	1:A:1150:LEU:HD23	1.78	0.63
1:A:1152:ARG:HA	1:A:1207:TYR:OH	1.98	0.63
1:A:1346:ILE:CD1	1:A:1349:VAL:HG13	2.27	0.63
1:A:1139:PRO:O	1:A:1143:ILE:HD12	1.98	0.63
1:A:1259:VAL:CG2	1:A:1312:LEU:HD21	2.27	0.63
1:A:1381:TYR:CD2	2:E:150:HIS:ND1	2.66	0.63
1:A:1414:ALA:O	1:A:1417:ILE:HB	1.98	0.63
1:A:1180:ASP:C	1:A:1182:THR:H	2.02	0.62
1:A:1091:VAL:HB	1:A:1218:LEU:HD13	1.82	0.62
2:E:91:LEU:HB3	2:B:91:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:ILE:HD11	2:B:166:GLU:CG	2.29	0.62
1:A:1384:ASN:HD21	1:A:1386:ALA:HB3	1.62	0.62
2:B:133:MET:O	2:B:134:GLU:C	2.38	0.62
1:A:1057:ILE:HG22	2:E:165:LEU:HD23	1.82	0.62
1:A:1425:PRO:HD2	1:A:1426:GLY:H	1.64	0.62
2:B:129:LYS:O	2:B:133:MET:HG2	1.98	0.62
1:A:1164:SER:O	1:A:1168:LEU:HG	2.00	0.61
2:E:77:LEU:HD21	2:B:78:ASN:CA	2.29	0.61
2:B:85:ASN:O	2:B:89:LYS:HG2	2.00	0.61
1:A:1375:LEU:C	1:A:1375:LEU:HD23	2.20	0.61
1:A:1146:VAL:HG12	1:A:1150:LEU:CD1	2.30	0.61
1:A:1258:MET:CE	1:A:1273:PHE:HA	2.30	0.61
2:B:126:CYS:O	2:B:128:GLU:N	2.33	0.61
1:A:1026:GLN:HE22	1:A:1030:GLN:HB2	1.65	0.61
1:A:1250:SER:HB3	1:A:1255:ILE:HD11	1.83	0.60
1:A:1160:SER:HA	1:A:1222:TYR:OH	2.00	0.60
2:E:101:ARG:O	2:E:105:GLN:HG2	2.02	0.60
2:E:76:ASN:O	2:E:80:ILE:HG12	2.02	0.60
1:A:1095:ARG:HG3	1:A:1096:ARG:H	1.67	0.60
1:A:1174:VAL:HA	1:A:1177:LEU:HD11	1.84	0.60
1:A:1413:LEU:O	1:A:1414:ALA:C	2.39	0.60
1:A:1424:LEU:CB	1:A:1425:PRO:HD3	2.31	0.60
1:A:1090:LEU:HD12	1:A:1090:LEU:O	2.02	0.60
1:A:1321:PRO:CG	1:A:1322:ALA:N	2.64	0.60
1:A:1384:ASN:OD1	1:A:1387:GLN:CG	2.46	0.60
1:A:1061:ILE:HD12	2:E:169:LEU:HD12	1.82	0.60
1:A:1345:ARG:HH11	1:A:1345:ARG:HG2	1.65	0.60
1:A:1446:ASP:OD1	1:A:1446:ASP:O	2.20	0.59
1:A:1369:ASN:HB3	1:A:1371:ASN:OD1	2.01	0.59
1:A:1042:ARG:NH2	1:A:1412:TYR:OH	2.26	0.59
1:A:1108:LEU:C	1:A:1110:ASP:H	2.05	0.59
2:E:168:GLU:HG2	2:E:168:GLU:O	2.03	0.59
1:A:1092:ASN:HD21	1:A:1157:ILE:HB	1.68	0.59
1:A:1253:ILE:HD11	1:A:1279:PHE:CD2	2.38	0.59
2:B:95:TYR:O	2:B:99:SER:HB2	2.03	0.59
2:E:166:GLU:CG	2:B:165:LEU:HD13	2.29	0.59
1:A:1457:GLU:CG	1:A:1458:GLY:N	2.66	0.58
2:E:123:GLU:CG	2:B:122:ILE:HG21	2.27	0.58
1:A:1029:MET:O	1:A:1033:ALA:HB2	2.02	0.58
1:A:1145:THR:O	1:A:1148:SER:HB3	2.02	0.58
1:A:1278:THR:O	1:A:1282:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:LEU:HD12	1:A:1327:TYR:OH	2.03	0.58
1:A:1144:THR:O	1:A:1145:THR:C	2.42	0.58
1:A:1324:ASN:OD1	1:A:1397:PRO:HA	2.03	0.58
1:A:1273:PHE:CD2	1:A:1337:ARG:HD2	2.39	0.58
1:A:1258:MET:HE2	1:A:1273:PHE:CD1	2.38	0.58
1:A:1174:VAL:HA	1:A:1177:LEU:CD1	2.34	0.58
1:A:1309:ASN:OD1	1:A:1353:LEU:HA	2.03	0.58
1:A:1397:PRO:HG3	1:A:1403:ALA:C	2.24	0.58
1:A:1135:ASN:HA	1:A:1453:ASN:O	2.04	0.58
1:A:1174:VAL:O	1:A:1177:LEU:HD12	2.04	0.58
1:A:1359:ALA:HB1	1:A:1391:ILE:CD1	2.34	0.58
1:A:1387:GLN:O	1:A:1390:ALA:HB3	2.04	0.58
1:A:1206:LEU:HG	1:A:1207:TYR:CE1	2.38	0.57
1:A:1091:VAL:HB	1:A:1218:LEU:CD1	2.34	0.57
1:A:1204:LYS:O	1:A:1208:GLU:HG3	2.04	0.57
1:A:1157:ILE:HG22	1:A:1157:ILE:O	2.04	0.57
1:A:1176:SER:O	1:A:1177:LEU:O	2.22	0.57
2:B:72:ASN:O	2:B:75:GLU:HB3	2.04	0.57
1:A:1141:HIS:CD2	1:A:1464:LYS:HZ3	2.22	0.57
1:A:1127:ASN:ND2	1:A:1130:GLU:HB3	2.15	0.57
1:A:1363:LEU:HD12	1:A:1363:LEU:H	1.70	0.57
1:A:1131:VAL:O	1:A:1133:GLY:N	2.39	0.56
1:A:1256:PHE:CD1	1:A:1256:PHE:C	2.79	0.56
1:A:1405:VAL:HG23	1:A:1406:PRO:HD2	1.86	0.56
2:B:115:LEU:O	2:B:115:LEU:HD23	2.04	0.56
2:B:150:HIS:ND1	2:B:150:HIS:C	2.58	0.56
1:A:1057:ILE:HD11	2:B:166:GLU:HG2	1.86	0.56
1:A:1135:ASN:HA	1:A:1453:ASN:C	2.26	0.56
1:A:1296:MET:CE	1:A:1296:MET:HA	2.36	0.56
2:E:109:MET:HE3	2:B:109:MET:HG2	1.87	0.56
1:A:1239:SER:O	1:A:1243:VAL:HG23	2.05	0.56
1:A:1321:PRO:HG2	1:A:1322:ALA:N	2.15	0.56
1:A:1177:LEU:HB3	1:A:1181:GLU:O	2.06	0.56
1:A:1323:LEU:HD22	1:A:1363:LEU:HD21	1.87	0.56
1:A:1393:LEU:HD23	1:A:1410:LEU:HD11	1.88	0.56
1:A:1423:SER:O	1:A:1424:LEU:HG	2.06	0.56
1:A:1343:GLU:HB2	1:A:1344:PRO:CD	2.27	0.55
1:A:1430:ILE:HG22	1:A:1431:MET:N	2.20	0.55
1:A:1268:SER:O	1:A:1271:GLU:HB2	2.06	0.55
1:A:1288:SER:C	1:A:1290:PHE:N	2.60	0.55
2:E:159:ASN:CA	2:B:158:LEU:HD11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1282:GLU:O	1:A:1285:ALA:HB3	2.07	0.55
2:B:165:LEU:O	2:B:169:LEU:HD13	2.06	0.55
1:A:1057:ILE:O	1:A:1061:ILE:HG12	2.07	0.55
1:A:1309:ASN:HD21	1:A:1355:GLN:HG3	1.72	0.55
1:A:1309:ASN:ND2	1:A:1355:GLN:HB2	2.16	0.55
1:A:1424:LEU:HB2	1:A:1425:PRO:HD3	1.88	0.55
1:A:1128:VAL:C	1:A:1130:GLU:H	2.09	0.55
1:A:1136:VAL:HG11	1:A:1290:PHE:HA	1.87	0.55
1:A:1457:GLU:OE2	1:A:1457:GLU:HA	2.06	0.55
1:A:1166:VAL:O	1:A:1170:VAL:HG23	2.07	0.54
1:A:1095:ARG:O	1:A:1096:ARG:CB	2.55	0.54
1:A:1135:ASN:OD1	1:A:1135:ASN:C	2.46	0.54
1:A:1163:ILE:CD1	1:A:1226:LEU:HD21	2.36	0.54
1:A:1386:ALA:HA	1:A:1417:ILE:CD1	2.37	0.54
1:A:1159:SER:O	1:A:1160:SER:C	2.45	0.54
1:A:1140:ILE:HG23	1:A:1141:HIS:N	2.23	0.54
1:A:1152:ARG:NH1	1:A:1152:ARG:HG2	2.23	0.54
1:A:1136:VAL:O	1:A:1188:PHE:HE1	1.90	0.54
1:A:1153:ASN:N	1:A:1153:ASN:ND2	2.54	0.54
1:A:1196:LEU:HB3	1:A:1197:PRO:HD3	1.88	0.54
1:A:1202:ASN:C	1:A:1204:LYS:H	2.11	0.54
1:A:1171:GLU:HB2	1:A:1237:ILE:HD11	1.89	0.54
1:A:1288:SER:C	1:A:1290:PHE:H	2.10	0.54
1:A:1413:LEU:O	1:A:1415:ASN:N	2.41	0.54
1:A:1445:TYR:N	1:A:1445:TYR:HD1	2.02	0.54
2:B:69:LEU:HD12	2:B:73:GLU:OE2	2.08	0.54
2:B:90:GLU:O	2:B:93:LYS:HB3	2.08	0.54
1:A:1197:PRO:HG3	1:A:1230:THR:HB	1.90	0.54
1:A:1425:PRO:CD	1:A:1426:GLY:H	2.20	0.54
2:B:66:ASN:O	2:B:70:LEU:HD13	2.08	0.54
1:A:1384:ASN:ND2	1:A:1386:ALA:HB3	2.22	0.53
1:A:1399:ASN:HD22	1:A:1399:ASN:N	2.06	0.53
1:A:1115:THR:O	1:A:1118:VAL:N	2.40	0.53
1:A:1155:LEU:O	1:A:1158:GLN:HB3	2.08	0.53
1:A:1151:VAL:HG12	1:A:1207:TYR:CE2	2.39	0.53
1:A:1319:LYS:O	1:A:1321:PRO:CA	2.53	0.53
1:A:1153:ASN:O	1:A:1155:LEU:HG	2.08	0.53
1:A:1156:LEU:C	1:A:1158:GLN:N	2.62	0.53
1:A:1375:LEU:HD23	1:A:1375:LEU:O	2.07	0.53
1:A:1221:ILE:O	1:A:1225:ASP:HB2	2.08	0.53
1:A:1267:ASN:O	1:A:1270:ASP:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:TRP:CZ3	2:E:132:ASN:HA	2.44	0.53
1:A:1420:GLU:HG2	1:A:1428:MET:HE1	1.88	0.53
1:A:1104:LEU:HD23	1:A:1104:LEU:C	2.28	0.53
1:A:1114:TYR:OH	1:A:1150:LEU:HD21	2.09	0.53
1:A:1188:PHE:HB2	1:A:1290:PHE:CE2	2.43	0.53
1:A:1397:PRO:C	1:A:1399:ASN:H	2.11	0.53
1:A:1323:LEU:HD22	1:A:1363:LEU:CD2	2.39	0.53
1:A:1093:VAL:HG22	1:A:1154:GLY:HA3	1.91	0.53
1:A:1324:ASN:HA	1:A:1395:TYR:HE1	1.73	0.53
2:E:67:LEU:HB2	2:B:67:LEU:HD12	1.90	0.53
1:A:1253:ILE:HD13	1:A:1276:LEU:HD13	1.91	0.53
1:A:1095:ARG:CG	1:A:1096:ARG:N	2.72	0.52
2:E:91:LEU:HD21	2:B:92:GLU:HA	1.92	0.52
1:A:1269:GLY:O	1:A:1273:PHE:N	2.34	0.52
1:A:1306:LYS:O	1:A:1309:ASN:HB3	2.08	0.52
1:A:1095:ARG:CG	1:A:1096:ARG:H	2.21	0.52
2:B:80:ILE:O	2:B:80:ILE:HG22	2.08	0.52
1:A:1356:ILE:O	1:A:1360:VAL:HG23	2.09	0.52
1:A:1117:GLU:OE1	1:A:1459:LEU:HB2	2.09	0.52
1:A:1381:TYR:CD2	2:E:150:HIS:CE1	2.97	0.52
1:A:1350:ARG:NH1	1:A:1357:ILE:HD13	2.25	0.52
2:B:123:GLU:O	2:B:127:SER:HB3	2.10	0.52
1:A:1137:LEU:O	1:A:1140:ILE:CG2	2.57	0.52
1:A:1156:LEU:O	1:A:1158:GLN:N	2.43	0.52
1:A:1358:GLN:O	1:A:1359:ALA:C	2.49	0.52
1:A:1129:THR:HG22	1:A:1129:THR:O	2.10	0.52
1:A:1256:PHE:HD1	1:A:1257:ASP:N	2.08	0.52
1:A:1443:LEU:C	1:A:1444:ARG:HG2	2.28	0.52
2:B:126:CYS:C	2:B:128:GLU:H	2.13	0.52
2:E:98:LEU:HD23	2:B:98:LEU:O	2.10	0.52
1:A:1092:ASN:ND2	1:A:1157:ILE:HB	2.25	0.51
1:A:1319:LYS:N	1:A:1319:LYS:HD2	2.26	0.51
1:A:1029:MET:HG3	1:A:1029:MET:O	2.10	0.51
1:A:1285:ALA:O	1:A:1288:SER:N	2.39	0.51
1:A:1026:GLN:O	1:A:1028:HIS:N	2.43	0.51
1:A:1029:MET:HG2	1:A:1056:PHE:CZ	2.45	0.51
1:A:1193:LEU:HB3	1:A:1234:PHE:HD1	1.75	0.51
1:A:1370:LEU:HD23	1:A:1370:LEU:C	2.31	0.51
2:B:144:GLN:O	2:B:145:ASN:C	2.47	0.51
1:A:1090:LEU:HD13	1:A:1157:ILE:HD13	1.92	0.51
1:A:1162:PHE:O	1:A:1166:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:ASP:O	1:A:1220:LEU:N	2.40	0.51
1:A:1359:ALA:O	1:A:1362:ILE:HB	2.10	0.51
2:B:101:ARG:HA	2:B:104:GLU:OE1	2.10	0.51
1:A:1436:PHE:N	1:A:1436:PHE:CD1	2.77	0.51
1:A:1359:ALA:O	1:A:1363:LEU:HD12	2.10	0.51
1:A:1389:GLN:NE2	1:A:1417:ILE:HG13	2.26	0.51
1:A:1246:MET:CE	1:A:1308:LEU:HD12	2.40	0.51
1:A:1365:LEU:O	1:A:1366:LYS:C	2.49	0.51
1:A:1449:ALA:HA	1:A:1452:GLN:HG3	1.93	0.51
2:B:122:ILE:C	2:B:124:GLN:N	2.64	0.51
2:E:143:SER:O	2:E:145:ASN:N	2.44	0.51
1:A:1239:SER:HG	1:A:1436:PHE:HD1	1.58	0.51
1:A:1026:GLN:C	1:A:1028:HIS:H	2.14	0.50
1:A:1093:VAL:HG23	1:A:1154:GLY:HA3	1.93	0.50
1:A:1092:ASN:OD1	1:A:1155:LEU:HA	2.11	0.50
1:A:1090:LEU:HD13	1:A:1157:ILE:CD1	2.41	0.50
1:A:1180:ASP:C	1:A:1182:THR:N	2.64	0.50
1:A:1151:VAL:CG1	1:A:1207:TYR:HE2	2.23	0.50
1:A:1266:LYS:C	1:A:1268:SER:N	2.64	0.50
1:A:1095:ARG:O	1:A:1096:ARG:HB2	2.10	0.50
1:A:1306:LYS:HE2	1:A:1352:ASN:OD1	2.11	0.50
2:E:81:PHE:HB2	2:B:81:PHE:HD2	1.75	0.50
2:B:59:MET:CE	2:B:59:MET:HA	2.42	0.50
1:A:1146:VAL:HG12	1:A:1150:LEU:HD11	1.93	0.50
1:A:1451:THR:HA	1:A:1454:SER:OG	2.11	0.50
1:A:1026:GLN:C	1:A:1028:HIS:N	2.64	0.50
1:A:1057:ILE:HD11	2:B:166:GLU:HG3	1.94	0.50
1:A:1061:ILE:CD1	2:E:169:LEU:HD12	2.42	0.50
2:E:83:ARG:O	2:E:85:ASN:N	2.45	0.50
1:A:1152:ARG:HH11	1:A:1152:ARG:HG2	1.77	0.50
1:A:1303:ASP:OD1	1:A:1436:PHE:HB3	2.11	0.50
1:A:1155:LEU:O	1:A:1158:GLN:CB	2.60	0.49
1:A:1293:VAL:HG12	1:A:1294:ASP:N	2.27	0.49
1:A:1146:VAL:HG12	1:A:1150:LEU:HD12	1.92	0.49
2:E:123:GLU:OE1	2:B:122:ILE:HD13	2.11	0.49
2:E:83:ARG:C	2:E:85:ASN:N	2.64	0.49
1:A:1026:GLN:CD	1:A:1026:GLN:C	2.70	0.49
1:A:1137:LEU:CD2	1:A:1450:ILE:HD13	2.40	0.49
1:A:1096:ARG:O	1:A:1097:GLU:O	2.30	0.49
1:A:1119:THR:HG23	1:A:1169:THR:HG21	1.94	0.49
1:A:1163:ILE:HG21	1:A:1226:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:PHE:HE2	1:A:1319:LYS:HB2	1.75	0.49
1:A:1097:GLU:O	1:A:1098:SER:C	2.51	0.49
1:A:1384:ASN:ND2	1:A:1428:MET:HB2	2.27	0.49
1:A:1128:VAL:C	1:A:1130:GLU:N	2.66	0.49
1:A:1296:MET:C	1:A:1298:THR:N	2.64	0.49
2:B:149:ASP:O	2:B:150:HIS:C	2.51	0.49
1:A:1174:VAL:C	1:A:1176:SER:H	2.14	0.49
1:A:1358:GLN:NE2	1:A:1381:TYR:CE1	2.70	0.49
2:E:64:LEU:HD12	2:B:63:LEU:HD21	1.95	0.49
1:A:1137:LEU:N	1:A:1137:LEU:HD12	2.27	0.49
2:E:91:LEU:HB3	2:B:91:LEU:CD1	2.43	0.49
2:E:95:TYR:O	2:E:99:SER:HB2	2.13	0.48
1:A:1393:LEU:HD21	1:A:1410:LEU:HD21	1.95	0.48
1:A:1222:TYR:CD2	1:A:1223:LEU:HD23	2.48	0.48
2:E:134:GLU:HA	2:B:133:MET:HE1	1.95	0.48
2:B:156:SER:HA	2:B:159:ASN:HD22	1.77	0.48
2:E:83:ARG:O	2:E:86:LYS:N	2.46	0.48
1:A:1111:LEU:O	1:A:1113:SER:N	2.47	0.48
1:A:1138:GLY:N	1:A:1139:PRO:HD2	2.27	0.48
1:A:1246:MET:HE1	1:A:1308:LEU:HD12	1.95	0.48
2:B:151:TYR:O	2:B:155:ILE:N	2.38	0.48
1:A:1169:THR:O	1:A:1173:ILE:CG1	2.62	0.48
1:A:1091:VAL:HB	1:A:1218:LEU:HD22	1.95	0.48
2:E:134:GLU:HA	2:B:133:MET:CE	2.42	0.48
1:A:1111:LEU:HD11	1:A:1161:LYS:HB3	1.94	0.48
1:A:1109:MET:HA	1:A:1158:GLN:NE2	2.29	0.48
1:A:1170:VAL:O	1:A:1174:VAL:HG23	2.14	0.48
1:A:1399:ASN:ND2	1:A:1399:ASN:N	2.61	0.48
2:E:148:ARG:O	2:E:149:ASP:C	2.50	0.48
1:A:1122:TYR:CD1	1:A:1123:LEU:N	2.81	0.48
1:A:1288:SER:O	1:A:1290:PHE:N	2.46	0.48
1:A:1085:ALA:O	1:A:1086:ASN:ND2	2.46	0.48
1:A:1057:ILE:CG2	2:E:165:LEU:HD23	2.43	0.48
1:A:1384:ASN:HB2	1:A:1385:PRO:HD2	1.95	0.48
1:A:1096:ARG:C	1:A:1096:ARG:HD2	2.32	0.48
1:A:1095:ARG:HD3	1:A:1105:LEU:CD2	2.44	0.47
1:A:1316:LEU:O	1:A:1316:LEU:HG	2.14	0.47
1:A:1354:ILE:HG23	1:A:1355:GLN:N	2.30	0.47
1:A:1186:GLY:O	1:A:1187:ILE:C	2.51	0.47
1:A:1354:ILE:HA	1:A:1357:ILE:CG2	2.44	0.47
1:A:1197:PRO:HG3	1:A:1230:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:PRO:HG2	1:A:1428:MET:SD	2.54	0.47
1:A:1439:ALA:CB	1:A:1443:LEU:HD21	2.44	0.47
2:B:155:ILE:O	2:B:159:ASN:ND2	2.48	0.47
2:E:132:ASN:ND2	2:E:136:ASN:ND2	2.61	0.47
1:A:1292:VAL:O	1:A:1293:VAL:O	2.32	0.47
1:A:1114:TYR:HD1	1:A:1115:THR:N	2.12	0.47
1:A:1435:GLN:HG2	1:A:1436:PHE:N	2.30	0.47
1:A:1085:ALA:O	1:A:1086:ASN:CG	2.53	0.47
2:B:88:LEU:HD23	2:B:88:LEU:C	2.35	0.47
2:B:88:LEU:O	2:B:92:GLU:HG3	2.14	0.47
1:A:1455:ASN:O	1:A:1456:THR:HG23	2.14	0.47
2:E:109:MET:CE	2:B:108:LYS:HB2	2.43	0.47
1:A:1097:GLU:O	1:A:1100:GLY:N	2.48	0.47
1:A:1346:ILE:CG1	1:A:1349:VAL:HG13	2.45	0.47
1:A:1156:LEU:HD23	1:A:1156:LEU:N	2.31	0.46
1:A:1301:PHE:HE2	1:A:1341:TRP:CH2	2.33	0.46
1:A:1142:VAL:O	1:A:1146:VAL:HG23	2.16	0.46
1:A:1170:VAL:HA	1:A:1173:ILE:HD12	1.98	0.46
1:A:1345:ARG:NH1	1:A:1345:ARG:HG2	2.29	0.46
1:A:1196:LEU:HD23	1:A:1196:LEU:O	2.15	0.46
1:A:1280:LEU:HD13	1:A:1341:TRP:CD2	2.50	0.46
2:E:109:MET:CE	2:B:109:MET:HG2	2.45	0.46
2:B:98:LEU:HD12	2:B:101:ARG:HD2	1.96	0.46
2:E:143:SER:C	2:E:145:ASN:N	2.69	0.46
1:A:1152:ARG:C	1:A:1153:ASN:HD22	2.19	0.46
1:A:1272:LYS:CE	1:A:1275:LYS:HD2	2.46	0.46
1:A:1393:LEU:C	1:A:1395:TYR:H	2.19	0.46
1:A:1397:PRO:C	1:A:1399:ASN:N	2.69	0.46
1:A:1411:ASN:O	1:A:1413:LEU:N	2.49	0.46
2:B:130:LEU:HD23	2:B:131:GLN:N	2.31	0.46
2:B:145:ASN:HA	2:B:148:ARG:HH11	1.81	0.46
1:A:1373:PHE:HD2	1:A:1409:ILE:HD13	1.80	0.46
1:A:1379:PHE:HZ	2:E:144:GLN:HB2	1.80	0.46
1:A:1294:ASP:C	1:A:1296:MET:H	2.18	0.45
1:A:1183:MET:HG3	1:A:1184:LEU:N	2.31	0.45
1:A:1056:PHE:O	1:A:1060:VAL:HG23	2.17	0.45
1:A:1091:VAL:HB	1:A:1218:LEU:CD2	2.46	0.45
2:B:110:ASP:O	2:B:113:SER:HB3	2.15	0.45
2:B:126:CYS:C	2:B:128:GLU:N	2.70	0.45
2:B:62:LYS:C	2:B:64:LEU:H	2.20	0.45
1:A:1137:LEU:O	1:A:1138:GLY:C	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1373:PHE:C	1:A:1373:PHE:CD1	2.90	0.45
1:A:1144:THR:O	1:A:1147:VAL:N	2.50	0.45
1:A:1121:GLY:O	1:A:1125:LYS:HD2	2.16	0.45
1:A:1445:TYR:O	1:A:1446:ASP:CG	2.55	0.45
1:A:1046:GLU:O	1:A:1049:SER:HB2	2.16	0.45
1:A:1219:THR:C	1:A:1221:ILE:N	2.70	0.45
1:A:1301:PHE:CE2	1:A:1341:TRP:CH2	3.05	0.45
1:A:1039:LYS:O	1:A:1041:SER:N	2.42	0.45
1:A:1108:LEU:C	1:A:1110:ASP:N	2.71	0.45
1:A:1350:ARG:HH11	1:A:1357:ILE:HD13	1.82	0.44
1:A:1392:LEU:HD23	1:A:1392:LEU:O	2.17	0.44
2:B:150:HIS:O	2:B:154:GLU:HB2	2.16	0.44
1:A:1194:SER:O	1:A:1443:LEU:HB3	2.17	0.44
1:A:1096:ARG:CD	1:A:1096:ARG:C	2.86	0.44
1:A:1309:ASN:ND2	1:A:1355:GLN:HG3	2.32	0.44
1:A:1387:GLN:H	1:A:1387:GLN:HG2	1.40	0.44
1:A:1132:ASN:C	1:A:1134:ASP:H	2.18	0.44
1:A:1159:SER:O	1:A:1162:PHE:N	2.51	0.44
1:A:1093:VAL:HG21	1:A:1215:LYS:HG3	1.99	0.44
1:A:1231:LEU:HD11	1:A:1440:LYS:HA	2.00	0.44
1:A:1335:ILE:O	1:A:1339:VAL:HG23	2.17	0.44
1:A:1111:LEU:HA	1:A:1114:TYR:CE1	2.52	0.44
1:A:1301:PHE:CE2	1:A:1341:TRP:CZ3	3.06	0.44
1:A:1159:SER:OG	1:A:1160:SER:N	2.50	0.44
1:A:1198:ALA:C	1:A:1200:ALA:N	2.70	0.44
1:A:1217:LYS:O	1:A:1221:ILE:HG12	2.18	0.44
1:A:1313:PHE:O	1:A:1316:LEU:HB3	2.17	0.44
2:E:91:LEU:CG	2:B:91:LEU:HD22	2.47	0.44
1:A:1366:LYS:HE2	2:E:132:ASN:HD21	1.82	0.44
1:A:1030:GLN:HA	1:A:1033:ALA:HB3	2.00	0.44
1:A:1128:VAL:O	1:A:1130:GLU:N	2.51	0.44
2:E:88:LEU:HD21	2:B:87:LYS:HE3	2.00	0.44
1:A:1357:ILE:O	1:A:1361:LYS:HG2	2.17	0.43
1:A:1386:ALA:HB2	1:A:1428:MET:SD	2.57	0.43
1:A:1184:LEU:C	1:A:1184:LEU:HD12	2.39	0.43
1:A:1193:LEU:HA	1:A:1193:LEU:HD23	1.91	0.43
1:A:1342:PHE:HB2	1:A:1349:VAL:HG11	1.99	0.43
1:A:1305:LEU:CD1	1:A:1349:VAL:HG12	2.40	0.43
1:A:1373:PHE:C	1:A:1373:PHE:HD1	2.21	0.43
1:A:1202:ASN:C	1:A:1204:LYS:N	2.71	0.43
1:A:1362:ILE:HG22	1:A:1363:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:MET:CE	1:A:1273:PHE:CD1	3.01	0.43
1:A:1402:GLU:HG2	1:A:1403:ALA:N	2.33	0.43
2:E:101:ARG:O	2:B:102:TYR:HE1	2.01	0.43
1:A:1139:PRO:HG2	1:A:1192:ASN:OD1	2.17	0.43
1:A:1371:ASN:N	1:A:1371:ASN:OD1	2.48	0.43
1:A:1411:ASN:O	1:A:1412:TYR:C	2.57	0.43
2:E:167:LEU:O	2:E:171:ASN:HB2	2.19	0.43
1:A:1349:VAL:C	1:A:1351:PRO:CD	2.87	0.43
1:A:1176:SER:O	1:A:1177:LEU:C	2.57	0.43
1:A:1196:LEU:HD23	1:A:1196:LEU:C	2.39	0.43
1:A:1362:ILE:O	1:A:1365:LEU:HD12	2.19	0.43
1:A:1095:ARG:HG3	1:A:1096:ARG:N	2.33	0.43
2:E:158:LEU:O	2:E:159:ASN:C	2.57	0.43
1:A:1343:GLU:CB	1:A:1344:PRO:HD3	2.22	0.42
1:A:1399:ASN:O	1:A:1400:LYS:CB	2.65	0.42
2:B:145:ASN:OD1	2:B:148:ARG:NH1	2.52	0.42
2:E:77:LEU:HD11	2:B:78:ASN:ND2	2.34	0.42
1:A:1024:LEU:C	1:A:1026:GLN:N	2.72	0.42
1:A:1057:ILE:HG22	2:E:165:LEU:CD2	2.48	0.42
1:A:1323:LEU:HB3	1:A:1363:LEU:HD23	2.01	0.42
2:E:145:ASN:O	2:E:146:LEU:C	2.57	0.42
2:E:155:ILE:HD13	2:E:155:ILE:HA	1.80	0.42
2:B:65:GLU:O	2:B:68:ASN:N	2.53	0.42
1:A:1365:LEU:HA	2:E:136:ASN:OD1	2.18	0.42
1:A:1060:VAL:HG12	1:A:1060:VAL:O	2.20	0.42
1:A:1117:GLU:O	1:A:1121:GLY:HA3	2.19	0.42
1:A:1177:LEU:HA	1:A:1178:PRO:HD3	1.85	0.42
1:A:1246:MET:HE1	1:A:1308:LEU:CD1	2.50	0.42
1:A:1292:VAL:O	1:A:1293:VAL:C	2.58	0.42
1:A:1439:ALA:HB1	1:A:1443:LEU:HD21	2.01	0.42
1:A:1123:LEU:HD11	1:A:1143:ILE:HD11	2.00	0.42
2:E:77:LEU:CD1	2:B:78:ASN:ND2	2.83	0.42
1:A:1140:ILE:O	1:A:1141:HIS:C	2.58	0.42
1:A:1270:ASP:OD2	1:A:1337:ARG:NH2	2.53	0.42
1:A:1443:LEU:C	1:A:1444:ARG:CG	2.86	0.42
1:A:1093:VAL:HG12	1:A:1214:GLU:HG2	2.02	0.42
1:A:1282:GLU:O	1:A:1286:VAL:HG23	2.19	0.42
1:A:1324:ASN:O	1:A:1327:TYR:N	2.53	0.42
1:A:1350:ARG:N	1:A:1351:PRO:CD	2.83	0.42
1:A:1107:LEU:HA	1:A:1107:LEU:HD23	1.96	0.42
1:A:1312:LEU:HB3	1:A:1356:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:PHE:O	1:A:1343:GLU:C	2.58	0.42
1:A:1390:ALA:O	1:A:1391:ILE:C	2.57	0.42
1:A:1123:LEU:CD1	1:A:1143:ILE:HD11	2.49	0.42
2:E:105:GLN:HG3	2:B:102:TYR:CE1	2.55	0.42
1:A:1085:ALA:O	1:A:1086:ASN:CB	2.68	0.41
1:A:1135:ASN:OD1	1:A:1138:GLY:CA	2.68	0.41
1:A:1178:PRO:O	1:A:1182:THR:HB	2.20	0.41
1:A:1342:PHE:CB	1:A:1349:VAL:HG11	2.49	0.41
2:B:99:SER:O	2:B:103:ASN:ND2	2.53	0.41
1:A:1115:THR:O	1:A:1116:LEU:C	2.57	0.41
1:A:1255:ILE:O	1:A:1256:PHE:C	2.59	0.41
1:A:1406:PRO:HG3	1:A:1409:ILE:CD1	2.45	0.41
1:A:1420:GLU:O	1:A:1423:SER:HB3	2.20	0.41
1:A:1256:PHE:CD1	1:A:1257:ASP:N	2.88	0.41
2:E:155:ILE:HD11	2:B:155:ILE:CD1	2.50	0.41
1:A:1095:ARG:HD3	1:A:1105:LEU:HD21	2.02	0.41
1:A:1160:SER:HB2	1:A:1222:TYR:CE1	2.54	0.41
1:A:1462:VAL:O	1:A:1466:ILE:HG13	2.21	0.41
2:E:147:TYR:CE2	2:B:144:GLN:NE2	2.88	0.41
1:A:1108:LEU:HD22	1:A:1150:LEU:CD2	2.46	0.41
2:E:98:LEU:HD21	2:B:99:SER:HA	2.03	0.41
1:A:1051:LYS:HE3	2:E:154:GLU:OE1	2.21	0.41
2:B:150:HIS:ND1	2:B:150:HIS:O	2.52	0.41
2:E:89:LYS:HE2	2:E:89:LYS:HB3	1.86	0.41
1:A:1219:THR:O	1:A:1221:ILE:N	2.54	0.41
1:A:1262:GLU:OE2	1:A:1321:PRO:HG3	2.21	0.41
1:A:1371:ASN:O	1:A:1372:GLU:C	2.58	0.41
2:B:88:LEU:O	2:B:88:LEU:HG	2.20	0.41
2:E:137:TYR:O	2:E:140:LEU:HB3	2.21	0.41
1:A:1377:PHE:O	1:A:1379:PHE:N	2.54	0.41
1:A:1408:GLU:HG2	1:A:1408:GLU:H	1.48	0.41
1:A:1413:LEU:O	1:A:1416:VAL:N	2.54	0.41
2:E:131:GLN:O	2:E:132:ASN:C	2.59	0.41
1:A:1159:SER:C	1:A:1161:LYS:N	2.71	0.41
1:A:1409:ILE:O	1:A:1411:ASN:N	2.54	0.41
2:E:118:ASN:O	2:E:122:ILE:HG13	2.21	0.41
1:A:1137:LEU:HB3	1:A:1140:ILE:CG2	2.51	0.40
1:A:1253:ILE:HD13	1:A:1276:LEU:CD1	2.50	0.40
1:A:1417:ILE:HG22	1:A:1418:LYS:N	2.36	0.40
1:A:1425:PRO:CD	1:A:1426:GLY:N	2.84	0.40
2:B:155:ILE:HA	2:B:155:ILE:HD13	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:PRO:HG3	1:A:1230:THR:CB	2.51	0.40
1:A:1362:ILE:O	1:A:1363:LEU:C	2.57	0.40
2:E:95:TYR:CG	2:E:95:TYR:O	2.73	0.40
1:A:1180:ASP:O	1:A:1182:THR:N	2.42	0.40
1:A:1228:ASN:C	1:A:1230:THR:H	2.24	0.40
1:A:1167:LEU:HA	1:A:1167:LEU:HD12	1.86	0.40
1:A:1277:PHE:CE1	1:A:1341:TRP:HB2	2.57	0.40
1:A:1360:VAL:HG12	1:A:1364:GLN:HE21	1.87	0.40
1:A:1422:LEU:HD12	1:A:1423:SER:N	2.37	0.40
1:A:1446:ASP:O	1:A:1447:THR:C	2.60	0.40
2:B:91:LEU:C	2:B:93:LYS:N	2.73	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	422/539 (78%)	262 (62%)	110 (26%)	50 (12%)	0	7
2	B	111/235 (47%)	95 (86%)	13 (12%)	3 (3%)	6	42
2	E	117/235 (50%)	104 (89%)	9 (8%)	4 (3%)	4	37
All	All	650/1009 (64%)	461 (71%)	132 (20%)	57 (9%)	1	12

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1086	ASN
1	A	1096	ARG
1	A	1097	GLU
1	A	1098	SER
1	A	1109	MET
1	A	1119	THR

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Mol	Chain	Res	Type
1	A	1132	ASN
1	A	1177	LEU
1	A	1187	ILE
1	A	1293	VAL
1	A	1320	SER
1	A	1321	PRO
1	A	1425	PRO
1	A	1427	LYS
1	A	1445	TYR
1	A	1448	SER
1	A	1112	ASN
1	A	1157	ILE
1	A	1209	ALA
1	A	1210	ASN
1	A	1213	ASP
1	A	1266	LYS
1	A	1286	VAL
1	A	1400	LYS
1	A	1437	ASP
2	E	84	LYS
2	E	144	GLN
2	B	127	SER
1	A	1145	THR
1	A	1263	LYS
1	A	1291	GLN
1	A	1412	TYR
1	A	1424	LEU
1	A	1467	LYS
2	E	125	SER
2	B	126	CYS
1	A	1027	SER
1	A	1095	ARG
1	A	1285	ALA
1	A	1378	ASP
1	A	1394	LYS
1	A	1414	ALA
1	A	1041	SER
1	A	1115	THR
1	A	1129	THR
1	A	1186	GLY
1	A	1348	ASP
1	A	1362	ILE

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Mol	Chain	Res	Type
1	A	1175	MET
1	A	1232	LYS
2	E	138	ASN
1	A	1310	VAL
2	B	135	VAL
1	A	1138	GLY
1	A	1450	ILE
1	A	1350	ARG
1	A	1243	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	385/488 (79%)	336 (87%)	49 (13%)	5	29
2	B	110/225 (49%)	100 (91%)	10 (9%)	11	45
2	E	115/225 (51%)	102 (89%)	13 (11%)	7	35
All	All	610/938 (65%)	538 (88%)	72 (12%)	6	32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1045	ASP
1	A	1054	LEU
1	A	1096	ARG
1	A	1111	LEU
1	A	1112	ASN
1	A	1114	TYR
1	A	1115	THR
1	A	1122	TYR
1	A	1132	ASN
1	A	1135	ASN
1	A	1143	ILE
1	A	1144	THR
1	A	1153	ASN

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Mol	Chain	Res	Type
1	A	1161	LYS
1	A	1167	LEU
1	A	1168	LEU
1	A	1169	THR
1	A	1175	MET
1	A	1184	LEU
1	A	1199	PHE
1	A	1231	LEU
1	A	1239	SER
1	A	1255	ILE
1	A	1256	PHE
1	A	1262	GLU
1	A	1265	PHE
1	A	1267	ASN
1	A	1273	PHE
1	A	1308	LEU
1	A	1345	ARG
1	A	1349	VAL
1	A	1365	LEU
1	A	1371	ASN
1	A	1373	PHE
1	A	1375	LEU
1	A	1377	PHE
1	A	1379	PHE
1	A	1387	GLN
1	A	1392	LEU
1	A	1399	ASN
1	A	1410	LEU
1	A	1422	LEU
1	A	1428	MET
1	A	1436	PHE
1	A	1437	ASP
1	A	1441	ASN
1	A	1445	TYR
1	A	1448	SER
1	A	1453	ASN
2	E	67	LEU
2	E	68	ASN
2	E	69	LEU
2	E	73	GLU
2	E	74	ASN
2	E	88	LEU

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Mol	Chain	Res	Type
2	E	104	GLU
2	E	115	LEU
2	E	129	LYS
2	E	132	ASN
2	E	133	MET
2	E	149	ASP
2	E	159	ASN
2	B	63	LEU
2	B	69	LEU
2	B	88	LEU
2	B	94	ASP
2	B	130	LEU
2	B	144	GLN
2	B	146	LEU
2	B	150	HIS
2	B	153	ASP
2	B	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1026	GLN
1	A	1052	GLN
1	A	1086	ASN
1	A	1092	ASN
1	A	1112	ASN
1	A	1127	ASN
1	A	1153	ASN
1	A	1267	ASN
1	A	1309	ASN
1	A	1334	ASN
1	A	1364	GLN
1	A	1389	GLN
1	A	1399	ASN
1	A	1411	ASN
1	A	1415	ASN
1	A	1421	ASN
1	A	1435	GLN
2	E	72	ASN
2	E	132	ASN
2	B	78	ASN
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	136	ASN
2	B	159	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](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	428/539 (79%)	-0.45	0 100 100	39, 98, 162, 190	1 (0%)
2	B	113/235 (48%)	-0.36	0 100 100	59, 119, 161, 184	0
2	E	119/235 (50%)	-0.36	0 100 100	54, 125, 159, 186	0
All	All	660/1009 (65%)	-0.42	0 100 100	39, 106, 161, 190	1 (0%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no 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.