



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3LXU  
Title : Crystal Structure of Tripeptidyl Peptidase 2 (TPP II)  
Authors : Chuang, C.K.  
Deposited on : 2010-02-25  
Resolution : 3.14 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

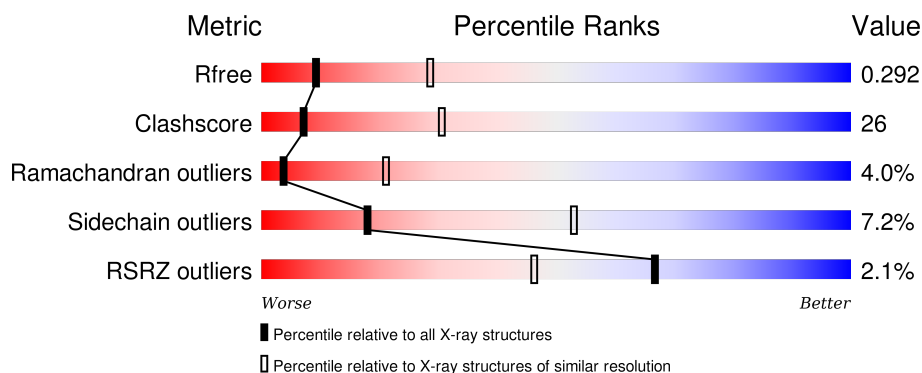
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 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))
$R_{free}$	91344	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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	X	1354	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9464 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.

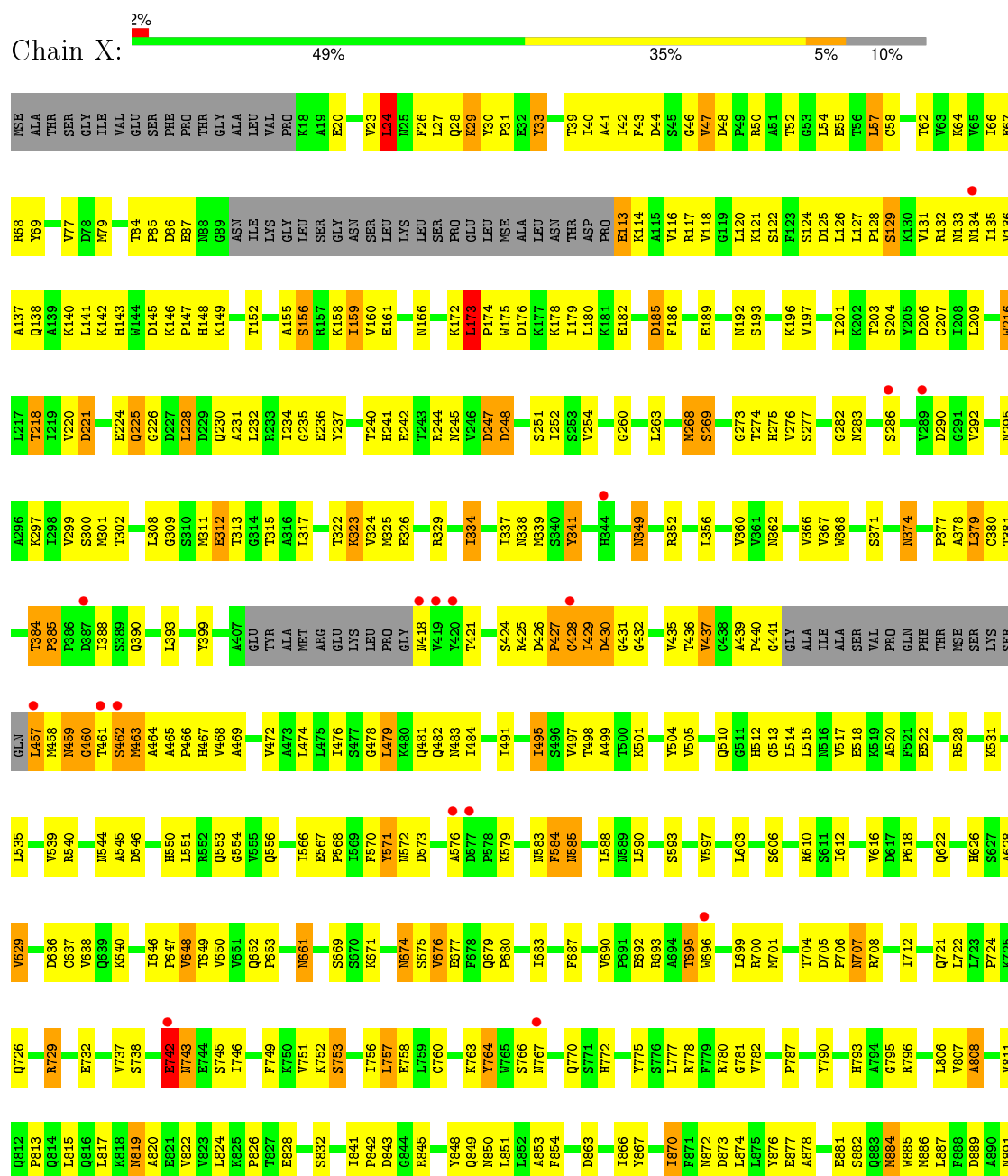
- Molecule 1 is a protein called Tripeptidyl-peptidase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	X	1217	9464	5958	1648	1816	17	25	0	0	0

### 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 errors 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: Tripeptidyl-peptidase 2



I1311	T1239	L1160	ALA	G1010	K892
H1319	L1240	P1161	ALA	R1011	A893
F1320	I1241	L1162	GLY	R1012	
E1321	E1242	T1163	ASP	V1013	T897
V1322	A1243		GLY	A1014	G898
L1323	L1244	T1170	ILE	F1018	K908
	S1245	S1171	SER	T1019	
I1326	K1246	P1172	VAL	Y1020	Y914
	K1247	P1173	GLN	I1021	T915
L1330	G1248	E1174	ASN	L1022	I916
G1331	I1249	A1175	ASP	E1026	R917
H1332	A1250	S1178	PRO	LYS	L918
E1333	V1251		VAL	LYS	
H1334	L1254	Q1186	ASP	LYS	R921
I1335			SER	SER	H922
	L1257	V1189	GLY	HIS	R925
V1338	L1260	R1190	GLY	THR	
I1339	I1261	S1191	SER	ASN	
N1340	K1262	A1192	PRO	GLY	L928
R1341	D1263		ALA	SER	E929
M1342	S1264	I1196	SER	K930	
M1343	L1265	V1197	PRO	ASN	I931
I1344	A1266	K1198	LYS	GLY	
T1345	E1267	L1199	SER	LYS	A934
A1346	I1268	A1200	ALA	SER	
F1347	N1269	D1201	ALA	K941	
P1348	E1270	K1202	ALA	L942	
	L1271	V1203	GLY		
R1352	Y1272	I1204	SER	L948	
I1353	T1273	Q1205	THR		Q956
F1354	E1274	E1206	ALA	THR	
	K1277	T1207	ALA	THR	
		D1208	ALA	ALA	G961
A1281	A1281	L1212	ALA	ALA	R962
N1282	N1282	L1213	ALA	ALA	K963
	K1285	Y1216	VAL	VAL	
A1286	A1286	G1217	THR	THR	L969
I1287	I1287	V1119	ALA	ALA	R970
Q1288	Q1288	K1120	ASN	ALA	L971
F1289	F1289	C1121	GLY	ASN	
		E1122	ALA	LYS	I978
	W1292	N1220	LYS	LYS	Q983
		D1221	PRO	PRO	
		T1222	LYS	LYS	T987
			ALA	ALA	
H1297	H1297	A1226	PRO	ALA	A993
G1298	G1298	A1227	ALA	ALA	Q994
H1299	H1299	K1228	THR	THR	C995
Y1300	Y1300	I1229	PRO	PRO	
		K1230	GLN	GLN	L998
M1303	M1303	T1231	ALA	ALA	
Y1304	Y1304	N1232	ALA	ALA	V1003
K1305	K1305	M1233	THR	THR	F1004
Y1306	Y1306	D1234	SER	SER	P1005
V1307	V1307	K1235	VAL	VAL	Q1006
V1308	V1308	Q1236	THR	THR	D1007
K1309	K1309	K1237	ASN	ASN	E1008
L1310	L1310	N1238	PRO	PRO	V1009

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.37Å 126.37Å 213.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.14 49.97 – 3.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.14) 99.2 (49.97-3.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.241 , 0.293 0.246 , 0.292	Depositor DCC
$R_{free}$ test set	1548 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30700 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage'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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	X	0.22	0/9621	0.41	0/12999

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	384	THR	Peptide
1	X	462	SER	Peptide

### 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	X	9464	0	9342	492	0
All	All	9464	0	9342	492	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 26.

All (492) 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:X:429:ILE:CD1	1:X:722:LEU:HD13	1.87	1.03
1:X:457:LEU:HD13	1:X:458:MSE:H	1.30	0.97
1:X:729:ARG:HG2	1:X:729:ARG:HH11	1.31	0.94
1:X:793:HIS:HD2	1:X:795:GLY:H	1.10	0.90
1:X:116:VAL:HG22	1:X:117:ARG:H	1.35	0.88
1:X:79:MSE:HE1	1:X:207:CYS:HB3	1.55	0.88
1:X:1160:LEU:HB2	1:X:1322:GLU:HG3	1.56	0.87
1:X:39:THR:HG22	1:X:297:LYS:HB2	1.54	0.87
1:X:338:ASN:HD22	1:X:469:ALA:HB2	1.38	0.86
1:X:275:HIS:HB2	1:X:463:MSE:HE1	1.57	0.86
1:X:1205:GLN:HG2	1:X:1207:THR:HG22	1.58	0.86
1:X:457:LEU:HD22	1:X:458:MSE:HG3	1.56	0.84
1:X:553:GLN:HB3	1:X:554:GLY:CA	2.09	0.83
1:X:429:ILE:CD1	1:X:722:LEU:CD1	2.56	0.83
1:X:1197:VAL:HG11	1:X:1247:LYS:HB2	1.60	0.82
1:X:143:HIS:HE1	1:X:146:LYS:HE2	1.47	0.79
1:X:637:CYS:HB3	1:X:640:LYS:HE3	1.64	0.79
1:X:1151:ILE:HG22	1:X:1189:VAL:HG13	1.64	0.79
1:X:24:LEU:HD23	1:X:27:LEU:H	1.47	0.79
1:X:439:ALA:HB3	1:X:464:ALA:HB1	1.64	0.79
1:X:461:THR:HG21	1:X:466:PRO:HD3	1.65	0.78
1:X:50:ARG:HD2	1:X:244:ARG:HD3	1.64	0.78
1:X:1231:THR:O	1:X:1235:LYS:HB2	1.82	0.78
1:X:33:TYR:CE2	1:X:478:GLY:HA3	2.19	0.78
1:X:429:ILE:HD11	1:X:722:LEU:CD1	2.13	0.78
1:X:235:GLY:H	1:X:241:HIS:HD2	1.31	0.78
1:X:583:ASN:HD21	1:X:606:SER:HB2	1.48	0.78
1:X:970:ARG:HG2	1:X:971:LEU:HD23	1.66	0.77
1:X:140:LYS:HD2	1:X:1352:ARG:HH12	1.48	0.77
1:X:553:GLN:HB3	1:X:554:GLY:HA3	1.68	0.76
1:X:113:GLU:HG3	1:X:133:ASN:ND2	2.01	0.76
1:X:201:ILE:HD11	1:X:1342:MSE:HE2	1.68	0.76
1:X:766:SER:O	1:X:767:ASN:HB2	1.86	0.75
1:X:457:LEU:CD2	1:X:458:MSE:HG3	2.14	0.75
1:X:27:LEU:HD13	1:X:517:VAL:HG12	1.67	0.75
1:X:146:LYS:HG3	1:X:148:HIS:CE1	2.22	0.75
1:X:478:GLY:HA2	1:X:481:GLN:HG2	1.68	0.75
1:X:135:ILE:HD11	1:X:1344:ILE:HG23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:349:ASN:H	1:X:349:ASN:HD22	1.34	0.74
1:X:922:HIS:HB3	1:X:928:LEU:HD11	1.69	0.74
1:X:1304:TYR:HD1	1:X:1323:LEU:HD11	1.51	0.73
1:X:24:LEU:HG	1:X:517:VAL:HB	1.69	0.73
1:X:143:HIS:CE1	1:X:146:LYS:HB2	2.24	0.73
1:X:540:ARG:HB2	1:X:545:ALA:HA	1.72	0.72
1:X:461:THR:HG22	1:X:464:ALA:H	1.53	0.72
1:X:349:ASN:H	1:X:349:ASN:ND2	1.88	0.72
1:X:465:ALA:HB3	1:X:466:PRO:HD3	1.71	0.71
1:X:235:GLY:H	1:X:241:HIS:CD2	2.07	0.71
1:X:484:ILE:HD12	1:X:528:ARG:HD2	1.71	0.71
1:X:377:PRO:O	1:X:425:ARG:HD3	1.90	0.71
1:X:457:LEU:HD13	1:X:458:MSE:N	2.04	0.71
1:X:1186:GLN:HB3	1:X:1190:ARG:CZ	2.20	0.71
1:X:429:ILE:HD13	1:X:722:LEU:HD13	1.70	0.70
1:X:882:SER:HB3	1:X:921:ARG:H	1.56	0.70
1:X:380:CYS:SG	1:X:427:PRO:HB2	2.31	0.70
1:X:793:HIS:HB3	1:X:796:ARG:HG3	1.73	0.70
1:X:323:LYS:HA	1:X:323:LYS:HE2	1.73	0.70
1:X:884:MSE:HG2	1:X:1354:PHE:HE2	1.55	0.70
1:X:143:HIS:CE1	1:X:146:LYS:HE2	2.27	0.69
1:X:870:ILE:H	1:X:870:ILE:HD13	1.57	0.69
1:X:793:HIS:CD2	1:X:795:GLY:H	2.02	0.69
1:X:380:CYS:H	1:X:427:PRO:HD2	1.58	0.69
1:X:1297:HIS:HB3	1:X:1299:HIS:CE1	2.28	0.69
1:X:1310:LEU:HB3	1:X:1319:HIS:HE2	1.58	0.69
1:X:367:VAL:HG11	1:X:472:VAL:HG11	1.74	0.69
1:X:145:ASP:C	1:X:147:PRO:HD3	2.13	0.68
1:X:700:ARG:HE	1:X:778:ARG:HD3	1.58	0.68
1:X:700:ARG:HH21	1:X:778:ARG:HD3	1.57	0.68
1:X:173:LEU:H	1:X:174:PRO:HD3	1.58	0.68
1:X:173:LEU:N	1:X:174:PRO:HD3	2.08	0.68
1:X:339:MSE:HE3	1:X:368:TRP:HZ2	1.59	0.68
1:X:1241:ILE:HD12	1:X:1242:GLU:N	2.09	0.68
1:X:793:HIS:CE1	1:X:1021:ILE:HD11	2.28	0.67
1:X:696:TRP:CZ2	1:X:780:ARG:HD3	2.30	0.67
1:X:491:ILE:O	1:X:495:ILE:HG22	1.95	0.67
1:X:1190:ARG:HH11	1:X:1257:LEU:HD11	1.58	0.67
1:X:311:MSE:SE	1:X:457:LEU:HB3	2.45	0.67
1:X:752:LYS:HD3	1:X:753:SER:N	2.09	0.67
1:X:326:GLU:O	1:X:329:ARG:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:142:LYS:HE3	1:X:146:LYS:HD2	1.77	0.67
1:X:23:VAL:O	1:X:24:LEU:HB3	1.92	0.67
1:X:312:GLU:HG2	1:X:341:TYR:CD1	2.29	0.66
1:X:275:HIS:HB2	1:X:463:MSE:CE	2.24	0.66
1:X:956:GLN:HE21	1:X:962:ARG:H	1.39	0.66
1:X:120:LEU:O	1:X:121:LYS:HB2	1.94	0.66
1:X:1151:ILE:CG2	1:X:1189:VAL:HG13	2.26	0.65
1:X:1339:ILE:HG22	1:X:1343:MSE:HE2	1.78	0.65
1:X:315:THR:HG22	1:X:921:ARG:HD3	1.78	0.65
1:X:431:GLY:HA2	1:X:550:HIS:HB2	1.77	0.65
1:X:1308:VAL:O	1:X:1311:ILE:HG22	1.97	0.65
1:X:461:THR:HG21	1:X:466:PRO:CD	2.26	0.65
1:X:79:MSE:HE1	1:X:207:CYS:CB	2.26	0.65
1:X:1245:SER:O	1:X:1249:ILE:HG22	1.97	0.65
1:X:311:MSE:HE2	1:X:457:LEU:HG	1.78	0.65
1:X:1186:GLN:HB3	1:X:1190:ARG:NH1	2.11	0.65
1:X:729:ARG:HG2	1:X:729:ARG:NH1	2.07	0.64
1:X:142:LYS:HE3	1:X:146:LYS:CD	2.27	0.64
1:X:499:ALA:HB3	1:X:512:HIS:O	1.97	0.64
1:X:749:PHE:HA	1:X:1013:VAL:HG11	1.79	0.64
1:X:116:VAL:HG22	1:X:117:ARG:N	2.11	0.64
1:X:700:ARG:HG2	1:X:746:ILE:HG12	1.78	0.64
1:X:819:ASN:HB3	1:X:941:LYS:HA	1.77	0.64
1:X:1198:LYS:O	1:X:1202:LYS:HG3	1.98	0.64
1:X:1111:ARG:HG3	1:X:1112:ASP:N	2.13	0.64
1:X:324:VAL:HG13	1:X:334:ILE:HG12	1.79	0.64
1:X:234:ILE:HD11	1:X:245:ASN:HB2	1.80	0.63
1:X:426:ASP:HB2	1:X:435:VAL:HG23	1.79	0.63
1:X:381:THR:HG23	1:X:424:SER:HB2	1.79	0.63
1:X:237:TYR:O	1:X:242:GLU:HG2	1.99	0.63
1:X:79:MSE:HE2	1:X:263:LEU:HD22	1.80	0.63
1:X:437:VAL:HG21	1:X:495:ILE:HD11	1.80	0.63
1:X:701:MSE:HB3	1:X:775:TYR:HB3	1.80	0.63
1:X:1281:ALA:O	1:X:1287:ILE:HA	1.98	0.63
1:X:956:GLN:NE2	1:X:962:ARG:H	1.96	0.63
1:X:1155:GLN:HB3	1:X:1189:VAL:HG21	1.80	0.63
1:X:441:GLY:HA3	1:X:462:SER:O	2.00	0.62
1:X:156:SER:O	1:X:159:ILE:HD12	1.98	0.62
1:X:29:LYS:C	1:X:31:PRO:HD3	2.20	0.62
1:X:501:LYS:HA	1:X:513:GLY:HA3	1.81	0.62
1:X:77:VAL:HB	1:X:263:LEU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1160:LEU:HB3	1:X:1161:PRO:HD2	1.81	0.62
1:X:1248:GLY:HA3	1:X:1289:PHE:CE1	2.35	0.61
1:X:158:LYS:HG3	1:X:1334:HIS:CE1	2.36	0.61
1:X:1192:ALA:O	1:X:1196:ILE:HG12	1.99	0.61
1:X:721:GLN:HG3	1:X:757:LEU:HD23	1.83	0.61
1:X:457:LEU:HD22	1:X:458:MSE:N	2.16	0.61
1:X:384:THR:HG22	1:X:385:PRO:CD	2.31	0.61
1:X:956:GLN:HE21	1:X:961:GLY:HA3	1.66	0.60
1:X:819:ASN:HA	1:X:942:LEU:HG	1.83	0.60
1:X:1311:ILE:HD11	1:X:1320:PHE:CE1	2.35	0.60
1:X:956:GLN:HE21	1:X:962:ARG:N	1.99	0.60
1:X:218:THR:HG21	1:X:254:VAL:HG11	1.83	0.60
1:X:468:VAL:O	1:X:472:VAL:HG23	2.00	0.60
1:X:158:LYS:O	1:X:161:GLU:HG3	2.01	0.60
1:X:1160:LEU:H	1:X:1160:LEU:HD12	1.65	0.60
1:X:1322:GLU:O	1:X:1326:ILE:HG13	2.02	0.59
1:X:50:ARG:CD	1:X:244:ARG:HD3	2.32	0.59
1:X:743:ASN:ND2	1:X:743:ASN:H	2.01	0.59
1:X:66:ILE:HG12	1:X:67:GLU:HG2	1.83	0.59
1:X:863:ASP:OD2	1:X:908:LYS:HD2	2.01	0.59
1:X:1162:LEU:HD13	1:X:1303:MSE:HE1	1.84	0.59
1:X:603:LEU:HD11	1:X:610:ARG:HG2	1.84	0.59
1:X:85:PRO:C	1:X:87:GLU:H	2.06	0.59
1:X:505:VAL:HB	1:X:510:GLN:HE22	1.67	0.59
1:X:1304:TYR:O	1:X:1308:VAL:HG13	2.02	0.58
1:X:1206:GLU:HB2	1:X:1240:LEU:HD21	1.84	0.58
1:X:1340:ASN:HA	1:X:1343:MSE:HE3	1.85	0.58
1:X:1190:ARG:NH1	1:X:1257:LEU:HD11	2.19	0.58
1:X:142:LYS:HE2	1:X:149:LYS:HG2	1.85	0.58
1:X:1155:GLN:CB	1:X:1189:VAL:HG21	2.33	0.58
1:X:884:MSE:HG2	1:X:1354:PHE:CE2	2.36	0.58
1:X:757:LEU:HD22	1:X:758:GLU:N	2.18	0.58
1:X:146:LYS:N	1:X:147:PRO:HD3	2.19	0.58
1:X:1204:ILE:O	1:X:1204:ILE:HD13	2.04	0.58
1:X:322:THR:HA	1:X:325:MSE:HE3	1.86	0.58
1:X:113:GLU:HB3	1:X:206:ASP:OD1	2.04	0.58
1:X:1212:LEU:HD13	1:X:1233:MSE:HG3	1.86	0.58
1:X:311:MSE:HG3	1:X:312:GLU:H	1.68	0.57
1:X:28:GLN:HA	1:X:28:GLN:OE1	2.05	0.57
1:X:867:TYR:HB2	1:X:872:ASN:HD22	1.68	0.57
1:X:886:MSE:HG2	1:X:897:THR:HB	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:50:ARG:HD2	1:X:244:ARG:CD	2.33	0.57
1:X:1249:ILE:HG13	1:X:1292:TRP:NE1	2.20	0.57
1:X:514:LEU:HD23	1:X:515:LEU:N	2.19	0.57
1:X:429:ILE:HD11	1:X:722:LEU:HD11	1.86	0.57
1:X:743:ASN:HD22	1:X:743:ASN:N	2.03	0.57
1:X:729:ARG:CG	1:X:729:ARG:HH11	2.11	0.56
1:X:159:ILE:HD13	1:X:160:VAL:H	1.69	0.56
1:X:885:TRP:HB3	1:X:918:LEU:HD23	1.85	0.56
1:X:1163:THR:OG1	1:X:1322:GLU:HG2	2.05	0.56
1:X:23:VAL:HG21	1:X:467:HIS:NE2	2.20	0.56
1:X:381:THR:HG23	1:X:424:SER:CB	2.36	0.56
1:X:1121:CYS:HB3	1:X:1125:MSE:HE2	1.87	0.56
1:X:622:GLN:O	1:X:626:HIS:HE1	1.88	0.56
1:X:47:VAL:HG23	1:X:274:THR:HA	1.88	0.56
1:X:848:TYR:CE2	1:X:925:ARG:HD3	2.40	0.56
1:X:427:PRO:O	1:X:428:CYS:HB3	2.06	0.56
1:X:553:GLN:HB3	1:X:554:GLY:HA2	1.87	0.55
1:X:884:MSE:HA	1:X:898:GLY:O	2.06	0.55
1:X:158:LYS:HG3	1:X:1334:HIS:HE1	1.68	0.55
1:X:1147:LEU:O	1:X:1151:ILE:HG13	2.06	0.55
1:X:216:TRP:HB2	1:X:236:GLU:OE2	2.07	0.55
1:X:1197:VAL:HG13	1:X:1243:ALA:HB1	1.88	0.55
1:X:692:GLU:O	1:X:693:ARG:HB2	2.06	0.55
1:X:436:THR:O	1:X:437:VAL:HG13	2.07	0.55
1:X:676:VAL:HG11	1:X:775:TYR:HE2	1.72	0.54
1:X:204:SER:OG	1:X:1345:THR:HG22	2.07	0.54
1:X:540:ARG:HA	1:X:546:ASP:O	2.06	0.54
1:X:1118:ILE:HG22	1:X:1129:ILE:HG21	1.88	0.54
1:X:276:VAL:HG13	1:X:466:PRO:HG3	1.89	0.54
1:X:679:GLN:HB3	1:X:680:PRO:HD2	1.90	0.54
1:X:428:CYS:O	1:X:430:ASP:N	2.36	0.54
1:X:763:LYS:HE2	1:X:766:SER:HB2	1.89	0.54
1:X:120:LEU:C	1:X:122:SER:H	2.10	0.54
1:X:234:ILE:HG12	1:X:245:ASN:ND2	2.22	0.54
1:X:1267:GLU:O	1:X:1270:GLU:HG2	2.07	0.54
1:X:1170:THR:HG22	1:X:1172:PRO:HD3	1.89	0.54
1:X:826:PRO:HG3	1:X:934:ALA:O	2.08	0.54
1:X:1009:VAL:HA	1:X:1012:ARG:HE	1.73	0.54
1:X:743:ASN:ND2	1:X:743:ASN:N	2.56	0.54
1:X:505:VAL:HB	1:X:510:GLN:NE2	2.23	0.54
1:X:622:GLN:O	1:X:626:HIS:CE1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1152:GLU:HB2	1:X:1156:LEU:HD11	1.90	0.54
1:X:457:LEU:CD1	1:X:457:LEU:N	2.71	0.54
1:X:426:ASP:HB2	1:X:435:VAL:CG2	2.38	0.54
1:X:362:ASN:HD21	1:X:390:GLN:HE22	1.54	0.54
1:X:125:ASP:C	1:X:127:LEU:H	2.11	0.54
1:X:132:ARG:HB2	1:X:209:LEU:HD23	1.89	0.53
1:X:113:GLU:HG3	1:X:133:ASN:HD21	1.73	0.53
1:X:20:GLU:O	1:X:24:LEU:O	2.26	0.53
1:X:334:ILE:HG13	1:X:334:ILE:O	2.08	0.53
1:X:339:MSE:HE3	1:X:368:TRP:CZ2	2.42	0.53
1:X:26:PHE:O	1:X:29:LYS:HB2	2.08	0.53
1:X:1241:ILE:HD13	1:X:1285:LYS:CB	2.39	0.53
1:X:1175:ALA:HB3	1:X:1178:SER:HB3	1.91	0.53
1:X:841:ILE:O	1:X:845:ARG:HB2	2.09	0.53
1:X:311:MSE:HG3	1:X:312:GLU:N	2.23	0.53
1:X:597:VAL:HG21	1:X:648:VAL:HG21	1.90	0.53
1:X:790:TYR:HA	1:X:1018:PHE:CD2	2.44	0.53
1:X:1227:ALA:C	1:X:1229:ILE:H	2.10	0.53
1:X:813:PRO:HA	1:X:1003:VAL:O	2.08	0.53
1:X:427:PRO:O	1:X:428:CYS:CB	2.56	0.52
1:X:136:VAL:HG22	1:X:137:ALA:O	2.09	0.52
1:X:695:THR:HB	1:X:781:GLY:HA2	1.90	0.52
1:X:374:ASN:H	1:X:374:ASN:HD22	1.56	0.52
1:X:1305:LYS:O	1:X:1308:VAL:HG22	2.09	0.52
1:X:1303:MSE:O	1:X:1307:VAL:HG12	2.08	0.52
1:X:701:MSE:HE3	1:X:737:VAL:HG11	1.92	0.52
1:X:1272:TYR:HA	1:X:1289:PHE:HE2	1.75	0.52
1:X:874:LEU:HB3	1:X:878:ALA:HB2	1.91	0.52
1:X:891:ASN:O	1:X:892:LYS:HB2	2.09	0.52
1:X:1004:PHE:HB2	1:X:1005:PRO:HD3	1.91	0.52
1:X:970:ARG:HH11	1:X:970:ARG:HB2	1.74	0.52
1:X:1233:MSE:HE2	1:X:1233:MSE:HA	1.90	0.52
1:X:1172:PRO:N	1:X:1173:PRO:CD	2.73	0.52
1:X:1021:ILE:HD12	1:X:1022:LEU:O	2.09	0.52
1:X:472:VAL:O	1:X:476:ILE:HG13	2.10	0.52
1:X:113:GLU:N	1:X:133:ASN:HD21	2.08	0.51
1:X:42:ILE:O	1:X:42:ILE:HG22	2.11	0.51
1:X:1274:GLU:HA	1:X:1277:LYS:HE2	1.92	0.51
1:X:971:LEU:HD23	1:X:971:LEU:H	1.75	0.51
1:X:1310:LEU:HB3	1:X:1319:HIS:NE2	2.23	0.51
1:X:388:ILE:HD11	1:X:393:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:225:GLN:HG3	1:X:226:GLY:H	1.75	0.51
1:X:700:ARG:NH2	1:X:778:ARG:HD3	2.25	0.51
1:X:676:VAL:HG11	1:X:775:TYR:CE2	2.45	0.51
1:X:576:ALA:HA	1:X:579:LYS:O	2.10	0.51
1:X:584:PHE:O	1:X:585:ASN:C	2.49	0.51
1:X:138:GLN:HG2	1:X:141:LEU:HD11	1.91	0.51
1:X:247:ASP:O	1:X:248:ASP:HB2	2.11	0.51
1:X:143:HIS:CD2	1:X:269:SER:HB3	2.46	0.51
1:X:69:TYR:CE1	1:X:323:LYS:HD3	2.45	0.51
1:X:1287:ILE:HD13	1:X:1287:ILE:O	2.11	0.51
1:X:690:VAL:HG11	1:X:751:VAL:CG1	2.41	0.50
1:X:628:ALA:HB3	1:X:648:VAL:CG2	2.41	0.50
1:X:371:SER:HB3	1:X:461:THR:OG1	2.12	0.50
1:X:377:PRO:HB2	1:X:760:CYS:SG	2.51	0.50
1:X:700:ARG:HA	1:X:745:SER:O	2.12	0.50
1:X:292:VAL:O	1:X:474:LEU:HD21	2.10	0.50
1:X:460:GLY:O	1:X:461:THR:HB	2.11	0.50
1:X:24:LEU:CG	1:X:517:VAL:HB	2.38	0.50
1:X:143:HIS:HE1	1:X:146:LYS:HB2	1.75	0.50
1:X:854:PHE:HB2	1:X:916:ILE:HB	1.93	0.50
1:X:616:VAL:O	1:X:618:PRO:HD3	2.11	0.50
1:X:185:ASP:O	1:X:189:GLU:HG3	2.11	0.50
1:X:24:LEU:HD23	1:X:27:LEU:N	2.23	0.50
1:X:819:ASN:N	1:X:819:ASN:OD1	2.44	0.50
1:X:1249:ILE:HG13	1:X:1292:TRP:CD1	2.47	0.49
1:X:743:ASN:HD22	1:X:743:ASN:H	1.58	0.49
1:X:1274:GLU:HG3	1:X:1277:LYS:HE2	1.93	0.49
1:X:172:LYS:O	1:X:173:LEU:HB2	2.12	0.49
1:X:752:LYS:HD3	1:X:753:SER:H	1.76	0.49
1:X:33:TYR:N	1:X:33:TYR:CD1	2.81	0.49
1:X:234:ILE:HG12	1:X:245:ASN:HD22	1.77	0.49
1:X:925:ARG:HA	1:X:928:LEU:HD13	1.95	0.49
1:X:54:LEU:HA	1:X:64:LYS:NZ	2.28	0.49
1:X:1307:VAL:HG11	1:X:1323:LEU:HD13	1.95	0.49
1:X:1307:VAL:HG22	1:X:1307:VAL:O	2.13	0.49
1:X:461:THR:HG21	1:X:465:ALA:HB3	1.95	0.49
1:X:425:ARG:HH21	1:X:683:ILE:CD1	2.26	0.49
1:X:653:PRO:HG3	1:X:756:ILE:CD1	2.43	0.49
1:X:518:GLU:O	1:X:522:GLU:HG3	2.13	0.48
1:X:729:ARG:CG	1:X:729:ARG:NH1	2.74	0.48
1:X:1003:VAL:HG11	1:X:1011:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:806:LEU:HG	1:X:807:VAL:HG12	1.95	0.48
1:X:457:LEU:HD13	1:X:457:LEU:N	2.28	0.48
1:X:1232:ASN:O	1:X:1236:GLN:HG3	2.13	0.48
1:X:956:GLN:HG2	1:X:962:ARG:HB2	1.96	0.48
1:X:1007:ASP:OD1	1:X:1009:VAL:HG22	2.14	0.48
1:X:1347:PHE:N	1:X:1348:PRO:HD3	2.29	0.48
1:X:628:ALA:HB3	1:X:648:VAL:HG22	1.95	0.48
1:X:220:VAL:O	1:X:231:ALA:HB1	2.13	0.48
1:X:193:SER:O	1:X:197:VAL:HG23	2.13	0.48
1:X:1204:ILE:HG23	1:X:1204:ILE:O	2.13	0.48
1:X:134:ASN:ND2	1:X:135:ILE:H	2.11	0.48
1:X:700:ARG:NE	1:X:778:ARG:HD3	2.27	0.48
1:X:57:LEU:H	1:X:57:LEU:HD23	1.79	0.48
1:X:152:THR:HB	1:X:155:ALA:HB3	1.96	0.48
1:X:866:ILE:HD13	1:X:916:ILE:HD11	1.95	0.48
1:X:1207:THR:HG23	1:X:1208:ASP:N	2.29	0.47
1:X:1307:VAL:CG1	1:X:1323:LEU:HD13	2.45	0.47
1:X:179:ILE:HG13	1:X:180:LEU:N	2.29	0.47
1:X:457:LEU:C	1:X:457:LEU:HD22	2.34	0.47
1:X:850:ASN:HB2	1:X:928:LEU:HD23	1.96	0.47
1:X:41:ALA:HA	1:X:299:VAL:HG23	1.97	0.47
1:X:700:ARG:HH21	1:X:778:ARG:CD	2.26	0.47
1:X:40:ILE:O	1:X:299:VAL:HG22	2.15	0.47
1:X:872:ASN:O	1:X:873:ASP:CB	2.63	0.47
1:X:216:TRP:CZ2	1:X:260:GLY:HA3	2.50	0.47
1:X:138:GLN:HG2	1:X:141:LEU:CD1	2.45	0.47
1:X:712:ILE:HG21	1:X:738:SER:HB3	1.97	0.47
1:X:922:HIS:HB3	1:X:928:LEU:CD1	2.43	0.47
1:X:866:ILE:HD13	1:X:916:ILE:CD1	2.45	0.47
1:X:842:PRO:HA	1:X:843:ASP:HA	1.53	0.47
1:X:593:SER:HB3	1:X:629:VAL:H	1.78	0.47
1:X:828:GLU:HG2	1:X:853:ALA:HB3	1.97	0.47
1:X:30:TYR:HB3	1:X:33:TYR:CD1	2.50	0.46
1:X:158:LYS:CG	1:X:1334:HIS:HE1	2.28	0.46
1:X:1198:LYS:HA	1:X:1201:ASP:HB2	1.97	0.46
1:X:132:ARG:HB2	1:X:209:LEU:CD2	2.45	0.46
1:X:232:LEU:HG	1:X:245:ASN:HB3	1.97	0.46
1:X:140:LYS:C	1:X:142:LYS:H	2.19	0.46
1:X:356:LEU:O	1:X:360:VAL:HG13	2.14	0.46
1:X:551:LEU:HD13	1:X:650:VAL:HG22	1.97	0.46
1:X:1102:ASN:H	1:X:1105:ASP:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1229:ILE:HG23	1:X:1231:THR:HB	1.96	0.46
1:X:590:LEU:N	1:X:590:LEU:HD12	2.31	0.46
1:X:140:LYS:HD2	1:X:1352:ARG:NH1	2.23	0.46
1:X:201:ILE:HG12	1:X:1338:VAL:CG1	2.45	0.46
1:X:338:ASN:HD21	1:X:465:ALA:C	2.19	0.46
1:X:1340:ASN:O	1:X:1344:ILE:HD13	2.16	0.46
1:X:499:ALA:CB	1:X:512:HIS:O	2.64	0.46
1:X:43:PHE:CD1	1:X:43:PHE:N	2.84	0.45
1:X:970:ARG:NH1	1:X:970:ARG:HB2	2.31	0.45
1:X:315:THR:HG22	1:X:882:SER:HB2	1.97	0.45
1:X:1156:LEU:O	1:X:1156:LEU:HD12	2.15	0.45
1:X:352:ARG:NH2	1:X:881:GLU:OE1	2.49	0.45
1:X:317:LEU:HG	1:X:339:MSE:HE1	1.98	0.45
1:X:311:MSE:HB2	1:X:311:MSE:HE3	1.84	0.45
1:X:312:GLU:OE2	1:X:457:LEU:HA	2.16	0.45
1:X:531:LYS:HG2	1:X:584:PHE:CE2	2.52	0.45
1:X:135:ILE:CD1	1:X:1344:ILE:HG23	2.41	0.45
1:X:700:ARG:HE	1:X:778:ARG:CD	2.27	0.45
1:X:1121:CYS:SG	1:X:1125:MSE:HE2	2.57	0.45
1:X:128:PRO:O	1:X:129:SER:HB3	2.16	0.45
1:X:817:LEU:HD13	1:X:998:LEU:HD12	1.99	0.45
1:X:41:ALA:C	1:X:42:ILE:HD12	2.36	0.45
1:X:808:ALA:HA	1:X:969:LEU:O	2.16	0.45
1:X:742:GLU:HB2	1:X:743:ASN:HD22	1.82	0.45
1:X:1237:LYS:HG3	1:X:1238:ASN:N	2.31	0.45
1:X:993:ALA:HA	1:X:994:GLN:HA	1.49	0.45
1:X:24:LEU:CD2	1:X:27:LEU:HB3	2.47	0.45
1:X:27:LEU:HD13	1:X:517:VAL:CG1	2.43	0.45
1:X:1297:HIS:HB3	1:X:1299:HIS:ND1	2.31	0.45
1:X:961:GLY:O	1:X:963:LYS:HD2	2.17	0.45
1:X:54:LEU:HD21	1:X:277:SER:HB2	1.98	0.45
1:X:24:LEU:C	1:X:24:LEU:HD22	2.37	0.45
1:X:268:MSE:HG3	1:X:269:SER:N	2.30	0.45
1:X:33:TYR:N	1:X:33:TYR:HD1	2.15	0.45
1:X:84:THR:HA	1:X:85:PRO:HD3	1.86	0.45
1:X:47:VAL:HG22	1:X:48:ASP:H	1.81	0.45
1:X:876:TYR:O	1:X:878:ALA:N	2.50	0.45
1:X:570:PHE:O	1:X:571:TYR:C	2.55	0.45
1:X:671:LYS:NZ	1:X:671:LYS:HB2	2.32	0.45
1:X:429:ILE:HD12	1:X:722:LEU:HD13	1.92	0.45
1:X:460:GLY:C	1:X:462:SER:H	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:240:THR:HA	1:X:242:GLU:CG	2.47	0.44
1:X:1200:ALA:O	1:X:1204:ILE:HG21	2.16	0.44
1:X:24:LEU:HD23	1:X:27:LEU:HB3	1.99	0.44
1:X:476:ILE:HA	1:X:479:LEU:HB2	1.99	0.44
1:X:1334:HIS:CE1	1:X:1335:ILE:HG13	2.52	0.44
1:X:539:VAL:HG22	1:X:566:ILE:HD12	1.99	0.44
1:X:380:CYS:HB3	1:X:429:ILE:HG12	2.00	0.44
1:X:122:SER:C	1:X:124:SER:H	2.21	0.44
1:X:1260:CYS:C	1:X:1262:LYS:N	2.70	0.44
1:X:1229:ILE:HG22	1:X:1232:ASN:H	1.83	0.44
1:X:201:ILE:HG12	1:X:1338:VAL:HG13	1.99	0.44
1:X:47:VAL:HG12	1:X:300:SER:HB2	2.00	0.44
1:X:57:LEU:HD21	1:X:62:THR:HG22	1.99	0.44
1:X:399:TYR:HE1	1:X:504:TYR:HH	1.63	0.44
1:X:887:LEU:HD11	1:X:914:TYR:HB3	2.00	0.44
1:X:175:TRP:HA	1:X:176:ASP:HA	1.49	0.44
1:X:117:ARG:O	1:X:118:VAL:HG23	2.17	0.44
1:X:299:VAL:CG2	1:X:301:MSE:HE3	2.48	0.44
1:X:679:GLN:HB3	1:X:679:GLN:HE21	1.67	0.44
1:X:140:LYS:CD	1:X:1352:ARG:HH12	2.23	0.44
1:X:1269:ASN:ND2	1:X:1297:HIS:NE2	2.66	0.44
1:X:567:GLU:HA	1:X:568:PRO:HD3	1.83	0.44
1:X:690:VAL:HB	1:X:753:SER:O	2.17	0.44
1:X:889:ASP:HB2	1:X:893:ALA:HB3	2.00	0.44
1:X:707:ASN:O	1:X:708:ARG:HB2	2.18	0.44
1:X:427:PRO:O	1:X:432:GLY:O	2.36	0.43
1:X:459:ASN:O	1:X:461:THR:N	2.51	0.43
1:X:1254:LEU:HD12	1:X:1254:LEU:HA	1.82	0.43
1:X:41:ALA:HB2	1:X:334:ILE:HD13	2.00	0.43
1:X:1123:LEU:HD23	1:X:1154:ASN:HB2	2.00	0.43
1:X:677:GLU:HB2	1:X:772:HIS:CD2	2.52	0.43
1:X:498:THR:HG21	1:X:520:ALA:N	2.33	0.43
1:X:228:LEU:H	1:X:228:LEU:HD12	1.81	0.43
1:X:313:THR:HG22	1:X:315:THR:H	1.83	0.43
1:X:669:SER:HA	1:X:674:ASN:HB3	2.01	0.43
1:X:1263:ASP:OD1	1:X:1263:ASP:N	2.44	0.43
1:X:251:SER:O	1:X:252:ILE:HD13	2.17	0.43
1:X:52:THR:HA	1:X:55:GLU:OE1	2.18	0.43
1:X:428:CYS:C	1:X:430:ASP:H	2.19	0.43
1:X:186:PHE:CE1	1:X:1305:LYS:HE2	2.53	0.43
1:X:377:PRO:O	1:X:378:ALA:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:440:PRO:O	1:X:464:ALA:HB2	2.18	0.43
1:X:384:THR:O	1:X:385:PRO:O	2.37	0.43
1:X:1162:LEU:HB2	1:X:1322:GLU:OE1	2.18	0.43
1:X:553:GLN:CB	1:X:554:GLY:HA3	2.36	0.43
1:X:337:ILE:HG13	1:X:366:VAL:HG11	2.01	0.43
1:X:931:ILE:HG22	1:X:931:ILE:O	2.18	0.43
1:X:872:ASN:O	1:X:873:ASP:HB2	2.19	0.43
1:X:695:THR:CG2	1:X:1014:ALA:HB1	2.49	0.43
1:X:47:VAL:CG1	1:X:300:SER:HB2	2.49	0.43
1:X:418:ASN:N	1:X:764:TYR:HH	2.17	0.43
1:X:1009:VAL:HG12	1:X:1012:ARG:HH21	1.84	0.42
1:X:807:VAL:O	1:X:807:VAL:HG22	2.19	0.42
1:X:192:ASN:O	1:X:196:LYS:HG3	2.19	0.42
1:X:85:PRO:C	1:X:87:GLU:N	2.71	0.42
1:X:571:TYR:CG	1:X:572:ASN:N	2.88	0.42
1:X:948:LEU:HD23	1:X:978:ILE:HG21	2.00	0.42
1:X:1021:ILE:O	1:X:1021:ILE:HG13	2.18	0.42
1:X:1304:TYR:CD1	1:X:1323:LEU:HD11	2.42	0.42
1:X:178:LYS:O	1:X:182:GLU:HG3	2.20	0.42
1:X:276:VAL:HA	1:X:463:MSE:SE	2.69	0.42
1:X:67:GLU:HB2	1:X:299:VAL:HG12	2.01	0.42
1:X:556:GLN:N	1:X:652:GLN:HE22	2.17	0.42
1:X:478:GLY:O	1:X:482:GLN:HB2	2.20	0.42
1:X:1282:ASN:HA	1:X:1287:ILE:HG12	2.01	0.42
1:X:885:TRP:HA	1:X:917:ARG:O	2.18	0.42
1:X:849:GLN:HG3	1:X:849:GLN:O	2.19	0.42
1:X:553:GLN:CB	1:X:554:GLY:CA	2.82	0.42
1:X:33:TYR:CD2	1:X:478:GLY:HA3	2.53	0.42
1:X:135:ILE:HD11	1:X:1344:ILE:CG2	2.44	0.42
1:X:499:ALA:HB1	1:X:514:LEU:O	2.20	0.42
1:X:690:VAL:HG11	1:X:751:VAL:HG13	2.02	0.42
1:X:43:PHE:N	1:X:43:PHE:HD1	2.16	0.42
1:X:1254:LEU:HD12	1:X:1257:LEU:HD12	2.01	0.42
1:X:687:PHE:CE1	1:X:758:GLU:HG3	2.55	0.42
1:X:68:ARG:HA	1:X:300:SER:O	2.19	0.42
1:X:777:LEU:HD23	1:X:777:LEU:HA	1.88	0.42
1:X:46:GLY:O	1:X:273:GLY:HA3	2.20	0.42
1:X:465:ALA:N	1:X:466:PRO:CD	2.83	0.42
1:X:724:PRO:O	1:X:726:GLN:HG3	2.20	0.42
1:X:459:ASN:O	1:X:460:GLY:C	2.58	0.41
1:X:142:LYS:HE2	1:X:149:LYS:CG	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:374:ASN:H	1:X:374:ASN:ND2	2.18	0.41
1:X:58:CYS:HA	1:X:283:ASN:OD1	2.20	0.41
1:X:1160:LEU:HD13	1:X:1322:GLU:HG3	2.02	0.41
1:X:113:GLU:HB2	1:X:114:LYS:H	1.55	0.41
1:X:69:TYR:CZ	1:X:323:LYS:HD3	2.55	0.41
1:X:152:THR:CB	1:X:155:ALA:HB3	2.51	0.41
1:X:1300:TYR:HB2	1:X:1330:LEU:HD21	2.03	0.41
1:X:583:ASN:ND2	1:X:585:ASN:HD22	2.19	0.41
1:X:429:ILE:HD13	1:X:722:LEU:CD1	2.39	0.41
1:X:29:LYS:HD3	1:X:29:LYS:HA	1.69	0.41
1:X:638:VAL:O	1:X:638:VAL:HG12	2.21	0.41
1:X:646:ILE:HA	1:X:647:PRO:HD3	1.83	0.41
1:X:815:LEU:HD12	1:X:948:LEU:HD22	2.01	0.41
1:X:1174:GLU:HG2	1:X:1174:GLU:H	1.61	0.41
1:X:705:ASP:HA	1:X:706:PRO:HD3	1.75	0.41
1:X:44:ASP:O	1:X:302:THR:HA	2.20	0.41
1:X:276:VAL:N	1:X:463:MSE:SE	3.04	0.41
1:X:149:LYS:HE2	1:X:248:ASP:O	2.21	0.41
1:X:793:HIS:HD2	1:X:795:GLY:N	1.94	0.41
1:X:1227:ALA:C	1:X:1229:ILE:N	2.74	0.41
1:X:201:ILE:HG22	1:X:201:ILE:O	2.20	0.41
1:X:742:GLU:H	1:X:742:GLU:HG2	1.66	0.41
1:X:374:ASN:N	1:X:374:ASN:HD22	2.13	0.41
1:X:983:GLN:HE21	1:X:987:THR:HG23	1.85	0.41
1:X:379:LEU:O	1:X:380:CYS:HB2	2.21	0.41
1:X:182:GLU:HB3	1:X:186:PHE:CE2	2.56	0.41
1:X:1248:GLY:HA2	1:X:1251:VAL:HG12	2.03	0.41
1:X:1114:GLN:O	1:X:1118:ILE:HG23	2.21	0.40
1:X:820:ALA:HB1	1:X:995:CYS:SG	2.61	0.40
1:X:1145:LEU:HD12	1:X:1242:GLU:HG2	2.02	0.40
1:X:159:ILE:HD13	1:X:160:VAL:N	2.36	0.40
1:X:384:THR:HG22	1:X:385:PRO:HD3	2.00	0.40
1:X:704:THR:O	1:X:705:ASP:C	2.59	0.40
1:X:311:MSE:CE	1:X:457:LEU:HG	2.47	0.40
1:X:461:THR:CG2	1:X:465:ALA:H	2.34	0.40
1:X:20:GLU:HA	1:X:467:HIS:HE1	1.85	0.40
1:X:1118:ILE:HD11	1:X:1146:LEU:HB2	2.02	0.40
1:X:1123:LEU:HD12	1:X:1123:LEU:C	2.42	0.40
1:X:1116:SER:O	1:X:1120:LYS:HE3	2.21	0.40
1:X:379:LEU:HG	1:X:427:PRO:HG2	2.02	0.40
1:X:464:ALA:O	1:X:467:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:54:LEU:HA	1:X:64:LYS:CE	2.52	0.40
1:X:228:LEU:C	1:X:230:GLN:H	2.25	0.40
1:X:221:ASP:OD1	1:X:224:GLU:HA	2.22	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	X	1207/1354 (89%)	1001 (83%)	158 (13%)	48 (4%)	4	21

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	129	SER
1	X	225	GLN
1	X	385	PRO
1	X	429	ILE
1	X	571	TYR
1	X	636	ASP
1	X	742	GLU
1	X	884	MSE
1	X	1260	CYS
1	X	309	GLY
1	X	427	PRO
1	X	428	CYS
1	X	459	ASN
1	X	463	MSE
1	X	497	VAL
1	X	585	ASN
1	X	674	ASN
1	X	753	SER

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Mol	Chain	Res	Type
1	X	24	LEU
1	X	86	ASP
1	X	248	ASP
1	X	269	SER
1	X	421	THR
1	X	661	ASN
1	X	787	PRO
1	X	877	GLU
1	X	1100	LYS
1	X	1161	PRO
1	X	126	LEU
1	X	282	GLY
1	X	286	SER
1	X	770	GLN
1	X	1174	GLU
1	X	1203	VAL
1	X	1204	ILE
1	X	1332	HIS
1	X	228	LEU
1	X	675	SER
1	X	764	TYR
1	X	1216	TYR
1	X	173	LEU
1	X	221	ASP
1	X	782	VAL
1	X	808	ALA
1	X	1004	PHE
1	X	1217	GLY
1	X	1261	ILE
1	X	460	GLY

### 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	X	1027/1116 (92%)	953 (93%)	74 (7%)	18 53

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	24	LEU
1	X	29	LYS
1	X	33	TYR
1	X	47	VAL
1	X	57	LEU
1	X	113	GLU
1	X	131	VAL
1	X	156	SER
1	X	159	ILE
1	X	166	ASN
1	X	173	LEU
1	X	185	ASP
1	X	203	THR
1	X	216	TRP
1	X	218	THR
1	X	247	ASP
1	X	268	MSE
1	X	290	ASP
1	X	295	ASN
1	X	308	LEU
1	X	312	GLU
1	X	323	LYS
1	X	334	ILE
1	X	341	TYR
1	X	349	ASN
1	X	374	ASN
1	X	379	LEU
1	X	430	ASP
1	X	437	VAL
1	X	457	LEU
1	X	479	LEU
1	X	483	ASN
1	X	495	ILE
1	X	535	LEU
1	X	544	ASN
1	X	573	ASP
1	X	584	PHE
1	X	588	LEU
1	X	612	ILE
1	X	629	VAL
1	X	648	VAL
1	X	649	THR

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Mol	Chain	Res	Type
1	X	661	ASN
1	X	676	VAL
1	X	695	THR
1	X	699	LEU
1	X	707	ASN
1	X	729	ARG
1	X	732	GLU
1	X	742	GLU
1	X	743	ASN
1	X	757	LEU
1	X	811	VAL
1	X	819	ASN
1	X	822	VAL
1	X	824	LEU
1	X	832	SER
1	X	851	LEU
1	X	870	ILE
1	X	897	THR
1	X	930	LYS
1	X	971	LEU
1	X	1019	THR
1	X	1021	ILE
1	X	1026	GLU
1	X	1118	ILE
1	X	1123	LEU
1	X	1147	LEU
1	X	1204	ILE
1	X	1206	GLU
1	X	1254	LEU
1	X	1265	LEU
1	X	1287	ILE
1	X	1299	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	25	ASN
1	X	133	ASN
1	X	143	HIS
1	X	241	HIS
1	X	295	ASN
1	X	338	ASN

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Mol	Chain	Res	Type
1	X	349	ASN
1	X	374	ASN
1	X	390	GLN
1	X	403	GLN
1	X	483	ASN
1	X	523	HIS
1	X	553	GLN
1	X	563	ASN
1	X	583	ASN
1	X	585	ASN
1	X	626	HIS
1	X	652	GLN
1	X	654	HIS
1	X	660	GLN
1	X	661	ASN
1	X	679	GLN
1	X	707	ASN
1	X	743	ASN
1	X	770	GLN
1	X	772	HIS
1	X	788	ASN
1	X	793	HIS
1	X	812	GLN
1	X	849	GLN
1	X	857	ASN
1	X	903	HIS
1	X	956	GLN
1	X	983	GLN
1	X	1006	GLN
1	X	1117	GLN
1	X	1131	ASN
1	X	1142	GLN
1	X	1144	ASN
1	X	1150	ASN
1	X	1182	GLN
1	X	1220	ASN
1	X	1269	ASN
1	X	1288	GLN
1	X	1293	HIS
1	X	1327	ASN
1	X	1334	HIS



### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	X	1192/1354 (88%)	0.15	25 (2%) 67 46	53, 86, 137, 179	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	462	SER	5.3
1	X	286	SER	4.2
1	X	577	ASP	4.1
1	X	576	ALA	4.1
1	X	1227	ALA	3.5
1	X	420	TYR	3.3
1	X	418	ASN	3.3
1	X	1222	THR	3.2
1	X	461	THR	3.0
1	X	1221	ASP	3.0
1	X	428	CYS	2.9
1	X	1216	TYR	2.9
1	X	767	ASN	2.7
1	X	1226	ALA	2.7
1	X	387	ASP	2.7
1	X	742	GLU	2.5
1	X	696	TRP	2.4
1	X	289	VAL	2.4
1	X	1220	ASN	2.3
1	X	419	VAL	2.3
1	X	1219	LYS	2.2
1	X	457	LEU	2.2
1	X	134	ASN	2.1
1	X	1213	LEU	2.1
1	X	344	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.