Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 06:57 AM EDT

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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39
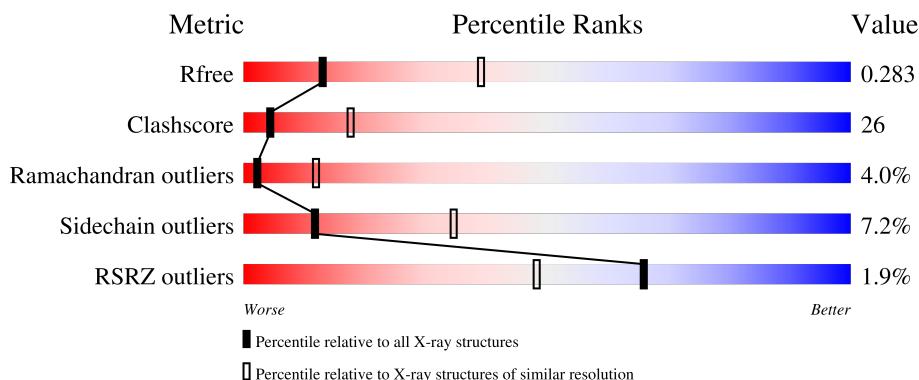
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
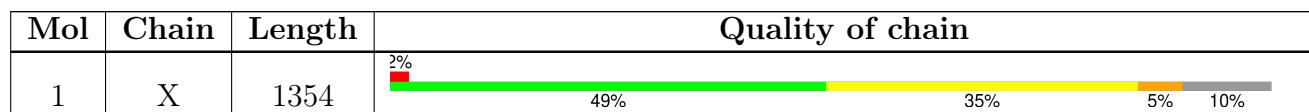
The reported resolution of this entry is 3.14 Å.

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}	164625	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.
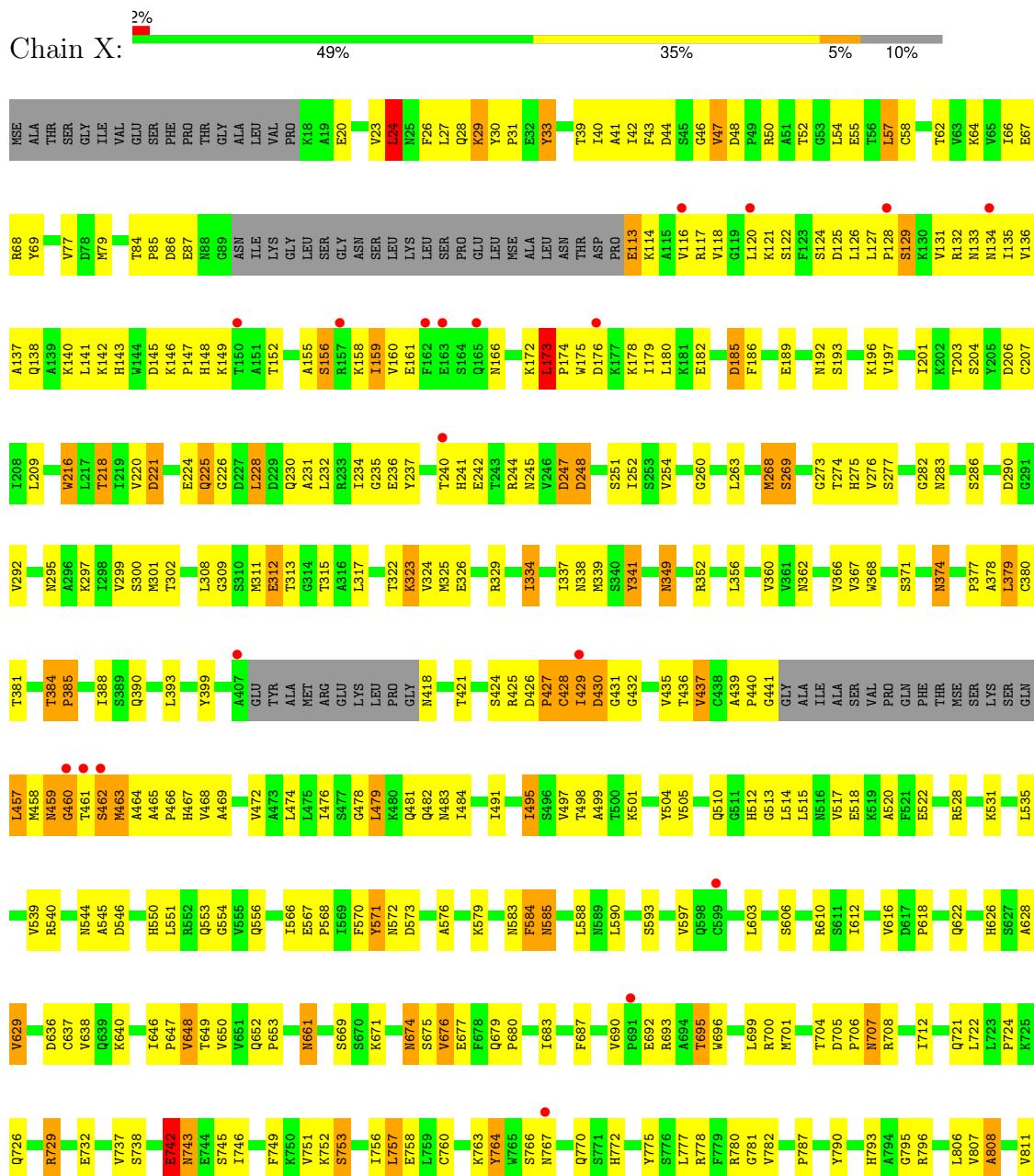
- Molecule 1 is a protein called Tripeptidyl-peptidase 2.
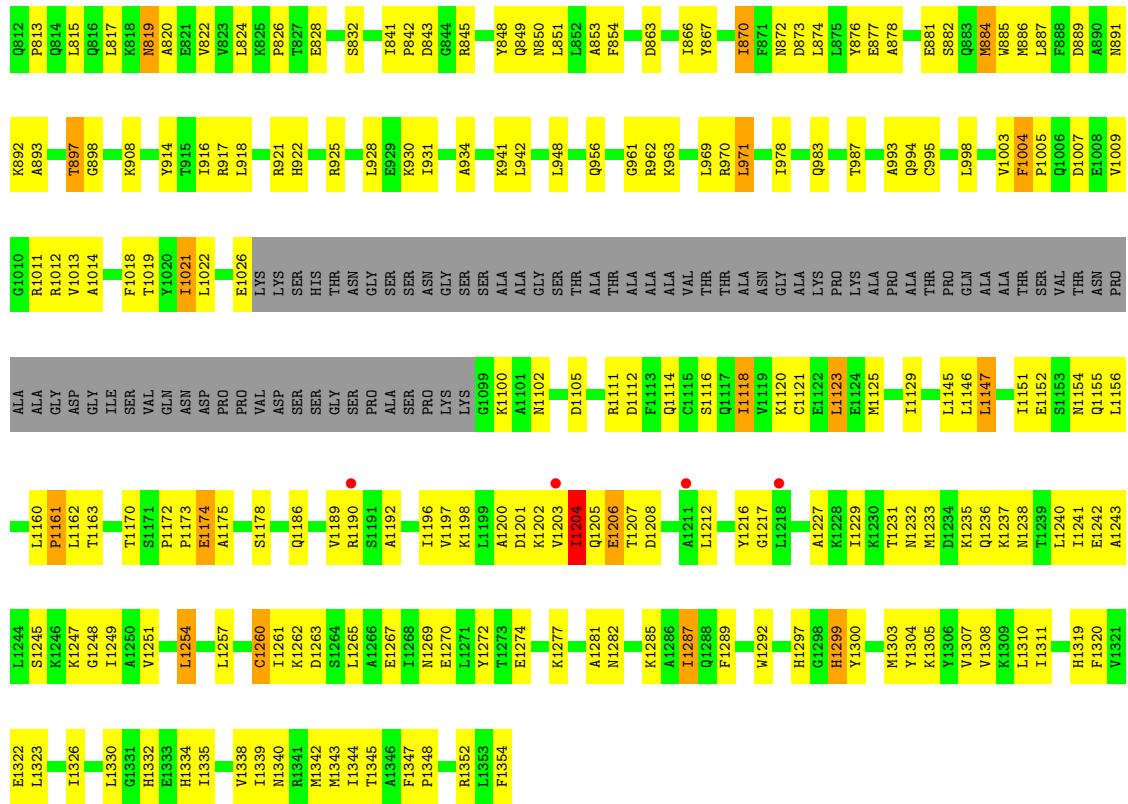
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	X	1217	Total 9464	C 5958	N 1648	O 1816	S 17	Se 25	0	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Tripeptidyl-peptidase 2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.37Å 126.37Å 213.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.14 50.00 – 3.14	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.14) 99.2 (50.00-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.241 , 0.293 0.240 , 0.283	Depositor DCC
R_{free} test set	1548 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	88.1	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9464	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:HH11	1:X:729:ARG:HG2	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:27:LEU:HD13	1:X:517:VAL:HG12	1.67	0.75
1:X:457:LEU:CD2	1:X:458:MSE:HG3	2.14	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:24:LEU:HG	1:X:517:VAL:HB	1.69	0.73
1:X:1304:TYR:HD1	1:X:1323:LEU:HD11	1.51	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:349:ASN:H	1:X:349:ASN:ND2	1.88	0.72
1:X:461:THR:HG22	1:X:464:ALA:H	1.53	0.72
1:X:235:GLY:H	1:X:241:HIS:CD2	2.07	0.71
1:X:377:PRO:O	1:X:425:ARG:HD3	1.90	0.71
1:X:465:ALA:HB3	1:X:466:PRO:HD3	1.71	0.71
1:X:484:ILE:HD12	1:X:528:ARG:HD2	1.71	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:HE2	1:X:323:LYS:HA	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:HD13	1:X:870:ILE:H	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:367:VAL:HG11	1:X:472:VAL:HG11	1.74	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: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: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: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:461:THR:HG21	1:X:466:PRO:CD	2.26	0.65
1:X:1308:VAL:O	1:X:1311:ILE:HG22	1.97	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: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:729:ARG:HG2	1:X:729:ARG:NH1	2.07	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:324:VAL:HG13	1:X:334:ILE:HG12	1.79	0.64
1:X:1111:ARG:HG3	1:X:1112:ASP:N	2.13	0.64
1:X:1198:LYS:O	1:X:1202:LYS:HG3	1.98	0.64
1:X:234:ILE:HD11	1:X:245:ASN:HB2	1.80	0.63
1:X:381:THR:HG23	1:X:424:SER:HB2	1.79	0.63
1:X:426:ASP:HB2	1:X:435:VAL:HG23	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:29:LYS:C	1:X:31:PRO:HD3	2.20	0.62
1:X:156:SER:O	1:X:159:ILE:HD12	1.98	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:158:LYS:HG3	1:X:1334:HIS:CE1	2.36	0.61
1:X:1248:GLY:HA3	1:X:1289:PHE:CE1	2.35	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:384:THR:HG22	1:X:385:PRO:CD	2.31	0.61
1:X:457:LEU:HD22	1:X:458:MSE:N	2.16	0.61
1:X:819:ASN:HA	1:X:942:LEU:HG	1.83	0.60
1:X:956:GLN:HE21	1:X:961:GLY:HA3	1.66	0.60
1:X:1311:ILE:HD11	1:X:1320:PHE:CE1	2.35	0.60
1:X:218:THR:HG21	1:X:254:VAL:HG11	1.83	0.60
1:X:956:GLN:HE21	1:X:962:ARG:N	1.99	0.60
1:X:158:LYS:O	1:X:161:GLU:HG3	2.01	0.60
1:X:468:VAL:O	1:X:472:VAL:HG23	2.00	0.60
1:X:1160:LEU:HD12	1:X:1160:LEU:H	1.65	0.60
1:X:50:ARG:CD	1:X:244:ARG:HD3	2.32	0.59
1:X:1322:GLU:O	1:X:1326:ILE:HG13	2.02	0.59
1:X:743:ASN:H	1:X:743:ASN:ND2	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: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:603:LEU:HD11	1:X:610:ARG:HG2	1.84	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:1190:ARG:NH1	1:X:1257:LEU:HD11	2.19	0.58
1:X:1340:ASN:HA	1:X:1343:MSE:HE3	1.85	0.58
1:X:142:LYS:HE2	1:X:149:LYS:HG2	1.85	0.58
1:X:757:LEU:HD22	1:X:758:GLU:N	2.18	0.58
1:X:884:MSE:HG2	1:X:1354:PHE:CE2	2.36	0.58
1:X:1155:GLN:CB	1:X:1189:VAL:HG21	2.33	0.58
1:X:146:LYS:N	1:X:147:PRO:HD3	2.19	0.58
1:X:1204:ILE:HD13	1:X:1204:ILE:O	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:OE1	1:X:28:GLN:HA	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:N	1:X:743:ASN:HD22	2.03	0.57
1:X:159:ILE:HD13	1:X:160:VAL:H	1.69	0.56
1:X:729:ARG:HH11	1:X:729:ARG:CG	2.11	0.56
1:X:885:TRP:HB3	1:X:918:LEU:HD23	1.85	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:622:GLN:O	1:X:626:HIS:HE1	1.88	0.56
1:X:1121:CYS:HB3	1:X:1125:MSE:HE2	1.87	0.56
1:X:1163:THR:OG1	1:X:1322:GLU:HG2	2.05	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:158:LYS:HG3	1:X:1334:HIS:HE1	1.68	0.55
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:216:TRP:HB2	1:X:236:GLU:OE2	2.07	0.55
1:X:1147:LEU:O	1:X:1151:ILE:HG13	2.06	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:204:SER:OG	1:X:1345:THR:HG22	2.07	0.54
1:X:676:VAL:HG11	1:X:775:TYR:HE2	1.72	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: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: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:1267:GLU:O	1:X:1270:GLU:HG2	2.07	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:1170:THR:HG22	1:X:1172:PRO:HD3	1.89	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
1:X:743:ASN:ND2	1:X:743:ASN:N	2.56	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:362:ASN:HD21	1:X:390:GLN:HE22	1.54	0.54
1:X:426:ASP:HB2	1:X:435:VAL:CG2	2.38	0.54
1:X:457:LEU:CD1	1:X:457:LEU:N	2.71	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:O	1:X:334:ILE:HG13	2.08	0.53
1:X:26:PHE:O	1:X:29:LYS:HB2	2.08	0.53
1:X:339:MSE:HE3	1:X:368:TRP:CZ2	2.42	0.53
1:X:1175:ALA:HB3	1:X:1178:SER:HB3	1.91	0.53
1:X:1241:ILE:HD13	1:X:1285:LYS:CB	2.39	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:813:PRO:HA	1:X:1003:VAL:O	2.08	0.53
1:X:1227:ALA:C	1:X:1229:ILE:H	2.10	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:374:ASN:HD22	1:X:374:ASN:H	1.56	0.52
1:X:695:THR:HB	1:X:781:GLY:HA2	1.90	0.52
1:X:1303:MSE:O	1:X:1307:VAL:HG12	2.08	0.52
1:X:1305:LYS:O	1:X:1308:VAL:HG22	2.09	0.52
1:X:701:MSE:HE3	1:X:737:VAL:HG11	1.92	0.52
1:X:874:LEU:HB3	1:X:878:ALA:HB2	1.91	0.52
1:X:1272:TYR:HA	1:X:1289:PHE:HE2	1.75	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:1172:PRO:N	1:X:1173:PRO:CD	2.73	0.52
1:X:1233:MSE:HE2	1:X:1233:MSE:HA	1.90	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:HG22	1:X:42:ILE:O	2.11	0.51
1:X:1274:GLU:HA	1:X:1277:LYS:HE2	1.92	0.51
1:X:225:GLN:HG3	1:X:226:GLY:H	1.75	0.51
1:X:388:ILE:HD11	1:X:393:LEU:HD13	1.91	0.51
1:X:971:LEU:HD23	1:X:971:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1310:LEU:HB3	1:X:1319:HIS:NE2	2.23	0.51
1:X:576:ALA:HA	1:X:579:LYS:O	2.10	0.51
1:X:676:VAL:HG11	1:X:775:TYR:CE2	2.45	0.51
1:X:700:ARG:NH2	1:X:778:ARG:HD3	2.25	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:69:TYR:CE1	1:X:323:LYS:HD3	2.45	0.51
1:X:143:HIS:CD2	1:X:269:SER:HB3	2.46	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:185:ASP:O	1:X:189:GLU:HG3	2.11	0.50
1:X:616:VAL:O	1:X:618:PRO:HD3	2.11	0.50
1:X:854:PHE:HB2	1:X:916:ILE:HB	1.93	0.50
1:X:24:LEU:HD23	1:X:27:LEU:N	2.23	0.50
1:X:819:ASN:OD1	1:X:819:ASN:N	2.44	0.50
1:X:743:ASN:H	1:X:743:ASN:HD22	1.58	0.49
1:X:1249:ILE:HG13	1:X:1292:TRP:CD1	2.47	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:425:ARG:HH21	1:X:683:ILE:CD1	2.26	0.49
1:X:461:THR:HG21	1:X:465:ALA:HB3	1.95	0.49
1:X:653:PRO:HG3	1:X:756:ILE:CD1	2.43	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:518:GLU:O	1:X:522:GLU:HG3	2.13	0.48
1:X:729:ARG:NH1	1:X:729:ARG:CG	2.74	0.48
1:X:806:LEU:HG	1:X:807:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1003:VAL:HG11	1:X:1011:ARG:HG2	1.94	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:193:SER:O	1:X:197:VAL:HG23	2.13	0.48
1:X:220:VAL:O	1:X:231:ALA:HB1	2.13	0.48
1:X:628:ALA:HB3	1:X:648:VAL:HG22	1.95	0.48
1:X:1204:ILE:O	1:X:1204:ILE:HG23	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:179:ILE:HG13	1:X:180:LEU:N	2.29	0.47
1:X:1307:VAL:CG1	1:X:1323:LEU:HD13	2.45	0.47
1:X:457:LEU:HD22	1:X:457:LEU:C	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:40:ILE:O	1:X:299:VAL:HG22	2.15	0.47
1:X:138:GLN:HG2	1:X:141:LEU:CD1	2.45	0.47
1:X:216:TRP:CZ2	1:X:260:GLY:HA3	2.50	0.47
1:X:700:ARG:HH21	1:X:778:ARG:CD	2.26	0.47
1:X:712:ILE:HG21	1:X:738:SER:HB3	1.97	0.47
1:X:872:ASN:O	1:X:873:ASP:CB	2.63	0.47
1:X:593:SER:HB3	1:X:629:VAL:H	1.78	0.47
1:X:842:PRO:HA	1:X:843:ASP:HA	1.53	0.47
1:X:866:ILE:HD13	1:X:916:ILE:CD1	2.45	0.47
1:X:922:HIS:HB3	1:X:928:LEU:CD1	2.43	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:132:ARG:HB2	1:X:209:LEU:CD2	2.45	0.46
1:X:1198:LYS:HA	1:X:1201:ASP:HB2	1.97	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:499:ALA:CB	1:X:512:HIS:O	2.64	0.46
1:X:1340:ASN:O	1:X:1344:ILE:HD13	2.16	0.46
1:X:43:PHE:CD1	1:X:43:PHE:N	2.84	0.45
1:X:970:ARG:HB2	1:X:970:ARG:NH1	2.31	0.45
1:X:315:THR:HG22	1:X:882:SER:HB2	1.97	0.45
1:X:352:ARG:NH2	1:X:881:GLU:OE1	2.49	0.45
1:X:1156:LEU:HD12	1:X:1156:LEU:O	2.15	0.45
1:X:317:LEU:HG	1:X:339:MSE:HE1	1.98	0.45
1:X:128:PRO:O	1:X:129:SER:HB3	2.16	0.45
1:X:135:ILE:CD1	1:X:1344:ILE:HG23	2.41	0.45
1:X:311:MSE:HE3	1:X:311:MSE:HB2	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:700:ARG:HE	1:X:778:ARG:CD	2.27	0.45
1:X:817:LEU:HD13	1:X:998:LEU:HD12	1.99	0.45
1:X:1121:CYS:SG	1:X:1125:MSE:HE2	2.57	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:993:ALA:HA	1:X:994:GLN:HA	1.49	0.45
1:X:1237:LYS:HG3	1:X:1238:ASN:N	2.31	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:54:LEU:HD21	1:X:277:SER:HB2	1.98	0.45
1:X:961:GLY:O	1:X:963:LYS:HD2	2.17	0.45
1:X:1297:HIS:HB3	1:X:1299:HIS:ND1	2.31	0.45
1:X:24:LEU:C	1:X:24:LEU:HD22	2.37	0.45
1:X:33:TYR:N	1:X:33:TYR:HD1	2.15	0.45
1:X:47:VAL:HG22	1:X:48:ASP:H	1.81	0.45
1:X:84:THR:HA	1:X:85:PRO:HD3	1.86	0.45
1:X:268:MSE:HG3	1:X:269:SER:N	2.30	0.45
1:X:570:PHE:O	1:X:571:TYR:C	2.55	0.45
1:X:671:LYS:HB2	1:X:671:LYS:NZ	2.32	0.45
1:X:876:TYR:O	1:X:878:ALA:N	2.50	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:539:VAL:HG22	1:X:566:ILE:HD12	1.99	0.44
1:X:1334:HIS:CE1	1:X:1335:ILE:HG13	2.52	0.44
1:X:122:SER:C	1:X:124:SER:H	2.21	0.44
1:X:380:CYS:HB3	1:X:429:ILE:HG12	2.00	0.44
1:X:1260:CYS:C	1:X:1262:LYS:N	2.70	0.44
1:X:201:ILE:HG12	1:X:1338:VAL:HG13	1.99	0.44
1:X:1229:ILE:HG22	1:X:1232:ASN:H	1.83	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:175:TRP:HA	1:X:176:ASP:HA	1.49	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: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:567:GLU:HA	1:X:568:PRO:HD3	1.83	0.44
1:X:1269:ASN:ND2	1:X:1297:HIS:NE2	2.66	0.44
1:X:690:VAL:HB	1:X:753:SER:O	2.17	0.44
1:X:707:ASN:O	1:X:708:ARG:HB2	2.18	0.44
1:X:889:ASP:HB2	1:X:893:ALA:HB3	2.00	0.44
1:X:41:ALA:HB2	1:X:334:ILE:HD13	2.00	0.43
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:677:GLU:HB2	1:X:772:HIS:CD2	2.52	0.43
1:X:1123:LEU:HD23	1:X:1154:ASN:HB2	2.00	0.43
1:X:1254:LEU:HD12	1:X:1254:LEU:HA	1.82	0.43
1:X:228:LEU:HD12	1:X:228:LEU:H	1.81	0.43
1:X:498:THR:HG21	1:X:520:ALA:N	2.33	0.43
1:X:52:THR:HA	1:X:55:GLU:OE1	2.18	0.43
1:X:251:SER:O	1:X:252:ILE:HD13	2.17	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: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:384:THR:O	1:X:385:PRO:O	2.37	0.43
1:X:440:PRO:O	1:X:464:ALA:HB2	2.18	0.43
1:X:337:ILE:HG13	1:X:366:VAL:HG11	2.01	0.43
1:X:553:GLN:CB	1:X:554:GLY:HA3	2.36	0.43
1:X:931:ILE:O	1:X:931:ILE:HG22	2.18	0.43
1:X:1162:LEU:HB2	1:X:1322:GLU:OE1	2.18	0.43
1:X:695:THR:CG2	1:X:1014:ALA:HB1	2.49	0.43
1:X:872:ASN:O	1:X:873:ASP:HB2	2.19	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:192:ASN:O	1:X:196:LYS:HG3	2.19	0.42
1:X:807:VAL:O	1:X:807:VAL:HG22	2.19	0.42
1:X:1009:VAL:HG12	1:X:1012:ARG:HH21	1.84	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:67:GLU:HB2	1:X:299:VAL:HG12	2.01	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: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: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:849:GLN:O	1:X:849:GLN:HG3	2.19	0.42
1:X:885:TRP:HA	1:X:917:ARG:O	2.18	0.42
1:X:1282:ASN:HA	1:X:1287:ILE:HG12	2.01	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:553:GLN:CB	1:X:554:GLY:CA	2.82	0.42
1:X:43:PHE:N	1:X:43:PHE:HD1	2.16	0.42
1:X:690:VAL:HG11	1:X:751:VAL:HG13	2.02	0.42
1:X:46:GLY:O	1:X:273:GLY:HA3	2.20	0.42
1:X:68:ARG:HA	1:X:300:SER:O	2.19	0.42
1:X:687:PHE:CE1	1:X:758:GLU:HG3	2.55	0.42
1:X:777:LEU:HD23	1:X:777:LEU:HA	1.88	0.42
1:X:1254:LEU:HD12	1:X:1257:LEU:HD12	2.01	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:142:LYS:HE2	1:X:149:LYS:CG	2.48	0.41
1:X:374:ASN:H	1:X:374:ASN:ND2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:459:ASN:O	1:X:460:GLY:C	2.58	0.41
1:X:58:CYS:HA	1:X:283:ASN:OD1	2.20	0.41
1:X:69:TYR:CZ	1:X:323:LYS:HD3	2.55	0.41
1:X:113:GLU:HB2	1:X:114:LYS:H	1.55	0.41
1:X:152:THR:CB	1:X:155:ALA:HB3	2.51	0.41
1:X:1160:LEU:HD13	1:X:1322:GLU:HG3	2.02	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:29:LYS:HD3	1:X:29:LYS:HA	1.69	0.41
1:X:429:ILE:HD13	1:X:722:LEU:CD1	2.39	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:H	1:X:1174:GLU:HG2	1.61	0.41
1:X:44:ASP:O	1:X:302:THR:HA	2.20	0.41
1:X:705:ASP:HA	1:X:706:PRO:HD3	1.75	0.41
1:X:149:LYS:HE2	1:X:248:ASP:O	2.21	0.41
1:X:276:VAL:N	1:X:463:MSE:SE	3.04	0.41
1:X:201:ILE:O	1:X:201:ILE:HG22	2.20	0.41
1:X:374:ASN:HD22	1:X:374:ASN:N	2.13	0.41
1:X:742:GLU:H	1:X:742:GLU:HG2	1.66	0.41
1:X:793:HIS:HD2	1:X:795:GLY:N	1.94	0.41
1:X:983:GLN:HE21	1:X:987:THR:HG23	1.85	0.41
1:X:1227:ALA:C	1:X:1229:ILE:N	2.74	0.41
1:X:182:GLU:HB3	1:X:186:PHE:CE2	2.56	0.41
1:X:379:LEU:O	1:X:380:CYS:HB2	2.21	0.41
1:X:1248:GLY:HA2	1:X:1251:VAL:HG12	2.03	0.41
1:X:820:ALA:HB1	1:X:995:CYS:SG	2.61	0.40
1:X:1114:GLN:O	1:X:1118:ILE:HG23	2.21	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:1145:LEU:HD12	1:X:1242:GLU:HG2	2.02	0.40
1:X:20:GLU:HA	1:X:467:HIS:HE1	1.85	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:1116:SER:O	1:X:1120:LYS:HE3	2.21	0.40
1:X:1118:ILE:HD11	1:X:1146:LEU:HB2	2.02	0.40
1:X:1123:LEU:C	1:X:1123:LEU:HD12	2.42	0.40
1:X:54:LEU:HA	1:X:64:LYS:CE	2.52	0.40
1:X:221:ASP:OD1	1:X:224:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:228:LEU:C	1:X:230:GLN:H	2.25	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

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	1207/1354 (89%)	1001 (83%)	158 (13%)	48 (4%)	2 12

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%)	12	34

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

Sometimes 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	X	1192/1354 (88%)	-0.04	23 (1%)	66	48	53, 86, 137, 179	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	150	THR	3.8
1	X	462	SER	3.2
1	X	767	ASN	3.2
1	X	407	ALA	3.1
1	X	134	ASN	2.9
1	X	461	THR	2.8
1	X	165	GLN	2.7
1	X	116	VAL	2.6
1	X	120	LEU	2.6
1	X	1203	VAL	2.5
1	X	240	THR	2.5
1	X	429	ILE	2.4
1	X	460	GLY	2.4
1	X	599	CYS	2.4
1	X	128	PRO	2.3
1	X	1218	LEU	2.3
1	X	163	GLU	2.3
1	X	157	ARG	2.2
1	X	162	PHE	2.1
1	X	1190	ARG	2.0
1	X	176	ASP	2.0
1	X	691	PRO	2.0
1	X	1211	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.