



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:41 PM JST

PDB ID : 9X2B / pdb_00009x2b
EMDB ID : EMD-66476
Title : Cryo-EM structure of PsoA in apo state (PsoA-PKS-II)
Authors : Sun, L.; Bai, L.
Deposited on : 2025-10-04
Resolution : 3.39 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

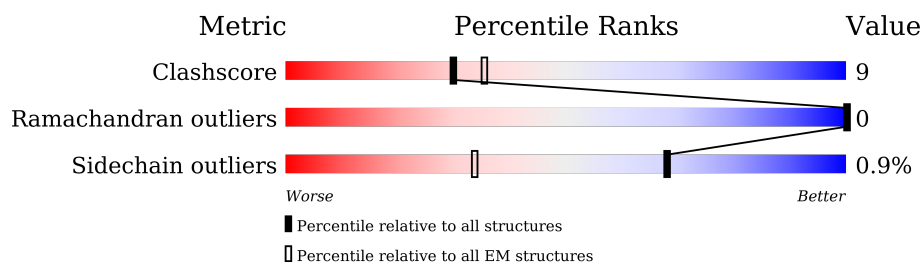
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.39 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	4007	
1	B	4007	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 72161 atoms, of which 35907 are hydrogens and 0 are deuteriums.

In the tables below, 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.

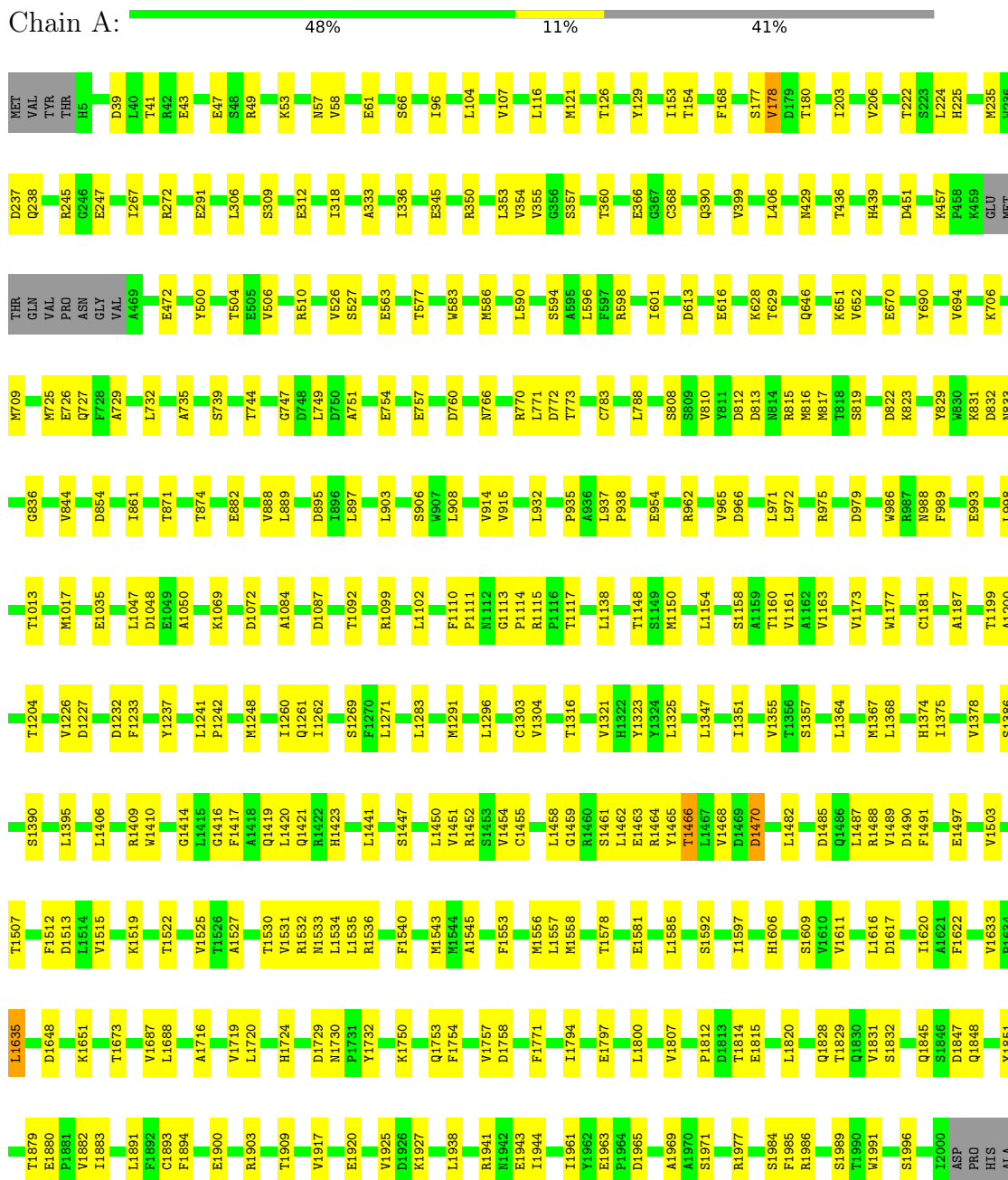
- Molecule 1 is a protein called PKS-NRPS hybrid synthetase psoA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2368	Total	C	H	N	O	S	0	0
			36099	11410	17963	3177	3468	81		
1	B	2365	Total	C	H	N	O	S	0	0
			36062	11399	17944	3174	3464	81		

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. 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. 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.

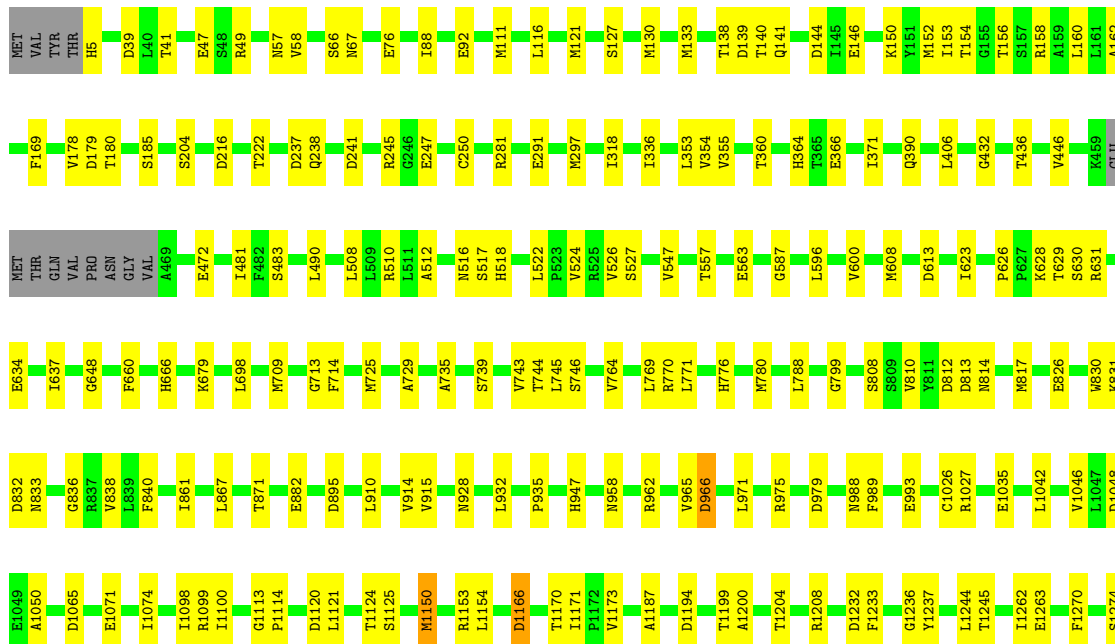
- Molecule 1: PKS-NRPS hybrid synthetase psoA





[illegible]

Chain B: 47% 12% 41%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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	0.13	0/18531	0.27	0/25201
1	B	0.13	0/18511	0.26	0/25170
All	All	0.13	0/37042	0.27	0/50371

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	18136	17963	17969	314	0
1	B	18118	17944	17948	344	0
All	All	36254	35907	35917	653	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 9.

All (653) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1455:CYS:O	1:A:1459:GLY:N	2.05	0.90
1:A:2258:PHE:O	1:A:2298:SER:OG	1.92	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:GLN:OE1	1:A:1447:SER:OG	1.93	0.87
1:B:510:ARG:NH2	1:B:935:PRO:O	2.12	0.83
1:B:512:ALA:O	1:B:516:ASN:ND2	2.12	0.83
1:A:1069:LYS:NZ	1:B:2030:CYS:SG	2.51	0.81
1:B:2217:MET:SD	1:B:2276:TYR:OH	2.39	0.80
1:A:47:GLU:O	1:A:962:ARG:NH2	2.13	0.80
1:B:2221:ASP:OD1	1:B:2272:THR:OG1	1.98	0.79
1:B:1849:VAL:O	1:B:2096:THR:OG1	2.01	0.79
1:A:808:SER:OG	1:A:829:TYR:OH	1.94	0.78
1:A:1716:ALA:O	1:A:1750:LYS:NZ	2.15	0.78
1:B:2248:GLU:OE1	1:B:2248:GLU:N	2.17	0.78
1:B:127:SER:OG	1:B:204:SER:OG	2.01	0.78
1:B:2127:SER:OG	1:B:2129:ASN:OD1	2.01	0.78
1:B:2258:PHE:O	1:B:2298:SER:OG	2.01	0.78
1:A:472:GLU:N	1:A:472:GLU:OE2	2.17	0.78
1:B:2324:GLU:OE2	1:B:2328:ARG:NH2	2.17	0.78
1:A:1532:ARG:NH2	1:A:1616:LEU:O	2.16	0.78
1:A:563:GLU:N	1:A:563:GLU:OE1	2.17	0.77
1:A:2313:ARG:NH1	1:A:2313:ARG:O	2.16	0.77
1:B:1421:GLN:OE1	1:B:1447:SER:OG	2.03	0.77
1:A:1148:THR:OG1	1:A:1160:THR:O	2.03	0.77
1:A:1578:THR:N	1:A:1581:GLU:OE2	2.17	0.77
1:B:1455:CYS:O	1:B:1459:GLY:N	2.17	0.77
1:B:1578:THR:N	1:B:1581:GLU:OE2	2.18	0.77
1:A:1533:ASN:OD1	1:A:1534:LEU:HD23	1.85	0.76
1:A:1347:LEU:HD21	1:A:1556:MET:SD	2.26	0.76
1:B:626:PRO:O	1:B:630:SER:OG	2.04	0.76
1:B:1624:ARG:O	1:B:1624:ARG:NE	2.18	0.76
1:B:291:GLU:OE1	1:B:291:GLU:N	2.19	0.76
1:A:1938:LEU:HD13	1:A:2080:PHE:CE1	2.21	0.76
1:A:1470:ASP:OD2	1:A:1519:LYS:NZ	2.17	0.76
1:A:690:TYR:O	1:A:694:VAL:HG23	1.87	0.75
1:A:1303:CYS:SG	1:A:1304:VAL:N	2.60	0.75
1:A:2236:MET:HE1	1:A:2279:ALA:HB2	1.68	0.75
1:A:291:GLU:N	1:A:291:GLU:OE1	2.20	0.75
1:A:670:GLU:OE1	1:A:833:ASN:ND2	2.20	0.75
1:B:1963:GLU:OE1	1:B:1989:SER:OG	2.04	0.75
1:A:1828:GLN:N	1:A:1828:GLN:OE1	2.19	0.74
1:A:577:THR:O	1:A:646:GLN:NE2	2.20	0.74
1:B:882:GLU:OE1	1:B:882:GLU:N	2.20	0.74
1:B:2197:ASP:OD2	1:B:2201:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1828:GLN:N	1:B:1828:GLN:OE1	2.20	0.74
1:B:1503:VAL:O	1:B:1507:THR:OG1	2.04	0.73
1:B:57:ASN:OD1	1:B:58:VAL:N	2.21	0.73
1:B:1532:ARG:NH2	1:B:1616:LEU:O	2.21	0.73
1:A:116:LEU:HD13	1:A:121:MET:HE3	1.70	0.73
1:A:235:MET:SD	1:A:357:SER:OG	2.45	0.72
1:B:1764:GLU:OE1	1:B:1764:GLU:N	2.23	0.72
1:B:993:GLU:OE1	1:B:993:GLU:N	2.21	0.72
1:A:1325:LEU:HD22	1:A:1351:ILE:HG21	1.70	0.72
1:B:318:ILE:HG22	1:B:353:LEU:HD21	1.72	0.72
1:A:1829:THR:O	1:A:2115:LEU:N	2.22	0.71
1:A:2199:ARG:NH2	1:A:2253:ASP:OD1	2.24	0.71
1:B:1482:LEU:HD13	1:B:1489:VAL:HG21	1.73	0.71
1:A:808:SER:HG	1:A:829:TYR:HH	1.18	0.71
1:A:57:ASN:OD1	1:A:58:VAL:N	2.23	0.71
1:A:1920:GLU:OE1	1:A:1920:GLU:N	2.23	0.71
1:A:1035:GLU:OE1	1:A:1099:ARG:NH2	2.24	0.71
1:B:116:LEU:HD13	1:B:121:MET:CE	2.21	0.70
1:B:1035:GLU:OE2	1:B:1208:ARG:NE	2.23	0.70
1:A:245:ARG:NE	1:A:366:GLU:OE2	2.24	0.70
1:B:988:ASN:OD1	1:B:989:PHE:N	2.25	0.70
1:A:345:GLU:N	1:A:345:GLU:OE1	2.24	0.70
1:A:1963:GLU:OE1	1:A:1989:SER:OG	2.09	0.70
1:B:47:GLU:OE1	1:B:47:GLU:N	2.24	0.70
1:B:1289:GLN:OE1	1:B:1290:GLU:N	2.25	0.70
1:B:1303:CYS:SG	1:B:1304:VAL:N	2.65	0.69
1:A:318:ILE:HG22	1:A:353:LEU:HD21	1.74	0.69
1:A:725:MET:O	1:A:729:ALA:N	2.26	0.69
1:A:1943:GLU:OE2	1:A:1977:ARG:NH2	2.26	0.69
1:A:126:THR:HG23	1:A:203:ILE:HG23	1.74	0.69
1:A:1150:MET:CE	1:A:1187:ALA:HB1	2.22	0.69
1:B:47:GLU:O	1:B:962:ARG:NH2	2.26	0.69
1:B:1496:VAL:HG13	1:B:1500:ILE:HD11	1.75	0.68
1:A:1729:ASP:OD1	1:A:1730:ASN:N	2.26	0.68
1:B:1431:ILE:HD12	1:B:1432:SER:N	2.08	0.68
1:B:1438:LEU:HD12	1:B:1458:LEU:HD21	1.76	0.68
1:B:1434:GLN:O	1:B:1809:ARG:NH2	2.27	0.68
1:B:1943:GLU:OE1	1:B:1977:ARG:NH2	2.27	0.68
1:A:1687:VAL:CG2	1:A:1719:VAL:HG22	2.23	0.68
1:B:1415:LEU:O	1:B:1419:GLN:NE2	2.26	0.68
1:B:1543:MET:N	1:B:1543:MET:SD	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ALA:HB3	1:A:1087:ASP:OD1	1.94	0.67
1:B:1473:GLN:NE2	1:B:1477:GLU:OE2	2.27	0.67
1:A:1048:ASP:OD1	1:A:1050:ALA:N	2.27	0.67
1:B:1422:ARG:O	1:B:1426:SER:N	2.26	0.67
1:B:2188:ASP:OD1	1:B:2189:VAL:N	2.28	0.67
1:B:1071:GLU:OE1	1:B:1071:GLU:N	2.28	0.67
1:B:1194:ASP:OD2	1:B:2336:SER:OG	2.08	0.67
1:A:988:ASN:OD1	1:A:989:PHE:N	2.27	0.67
1:B:158:ARG:NH1	1:B:179:ASP:OD2	2.28	0.66
1:B:1232:ASP:OD1	1:B:1233:PHE:N	2.29	0.66
1:A:1882:VAL:HG12	1:A:1941:ARG:HD2	1.78	0.66
1:B:1395:LEU:HD13	1:B:1557:LEU:HD22	1.76	0.66
1:B:2288:GLU:OE1	1:B:2291:ARG:NH2	2.29	0.66
1:A:1092:THR:OG1	1:B:1065:ASP:OD2	2.08	0.65
1:A:2284:VAL:HG22	1:A:2288:GLU:OE2	1.97	0.65
1:B:810:VAL:HG21	1:B:833:ASN:OD1	1.96	0.65
1:B:1581:GLU:N	1:B:1581:GLU:OE1	2.29	0.65
1:A:1321:VAL:HG22	1:A:1553:PHE:HD2	1.59	0.65
1:B:2183:VAL:HG23	1:B:2183:VAL:O	1.96	0.65
1:A:583:TRP:O	1:A:586:MET:HE2	1.96	0.65
1:A:1503:VAL:O	1:A:1507:THR:OG1	2.08	0.65
1:B:1386:SER:O	1:B:1390:SER:N	2.30	0.65
1:A:832:ASP:O	1:A:836:GLY:N	2.28	0.65
1:B:2315:GLN:OE1	1:B:2315:GLN:N	2.30	0.64
1:B:2259:LEU:HD11	1:B:2348:ILE:HD11	1.79	0.64
1:A:510:ARG:NH2	1:A:935:PRO:O	2.29	0.64
1:A:1648:ASP:OD1	1:A:1651:LYS:NZ	2.31	0.64
1:A:2236:MET:CE	1:A:2279:ALA:HB2	2.28	0.64
1:A:1903:ARG:HB2	1:A:1925:VAL:HG23	1.80	0.63
1:A:2013:VAL:HG22	1:A:2038:ALA:O	1.98	0.63
1:B:1921:TRP:CD1	1:B:2062:LEU:HD22	2.33	0.63
1:B:563:GLU:N	1:B:563:GLU:OE1	2.31	0.63
1:B:596:LEU:O	1:B:600:VAL:HG23	1.99	0.63
1:A:2150:VAL:HG22	1:A:2180:VAL:HG21	1.80	0.63
1:A:1325:LEU:HD22	1:A:1351:ILE:CG2	2.28	0.62
1:A:590:LEU:O	1:A:594:SER:N	2.30	0.62
1:A:2075:SER:O	1:A:2076:THR:OG1	2.12	0.62
1:A:1464:ARG:NE	1:A:1490:ASP:OD2	2.33	0.62
1:A:817:MET:SD	1:A:817:MET:N	2.72	0.62
1:B:141:GLN:NE2	1:B:152:MET:HE3	2.15	0.62
1:A:975:ARG:NH2	1:A:979:ASP:OD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2023:MET:O	1:A:2025:GLN:NE2	2.32	0.61
1:B:679:LYS:O	1:B:799:GLY:N	2.34	0.61
1:A:1592:SER:CB	1:A:1616:LEU:HD11	2.31	0.61
1:B:1451:VAL:HG12	1:B:1487:LEU:HD13	1.81	0.61
1:A:1150:MET:HE1	1:A:1187:ALA:HB1	1.82	0.61
1:B:1321:VAL:HG22	1:B:1553:PHE:HD2	1.64	0.61
1:A:237:ASP:OD1	1:A:238:GLN:N	2.34	0.60
1:B:2264:ILE:N	1:B:2301:ASP:OD1	2.34	0.60
1:A:66:SER:HA	1:A:222:THR:HG21	1.84	0.60
1:A:2031:GLU:OE1	1:A:2031:GLU:N	2.31	0.60
1:B:1150:MET:HE2	1:B:1187:ALA:HB1	1.83	0.60
1:A:819:SER:O	1:A:823:LYS:NZ	2.32	0.60
1:A:2158:VAL:HG23	1:A:2183:VAL:CG2	2.32	0.60
1:A:355:VAL:HG21	1:A:406:LEU:HD23	1.82	0.60
1:A:43:GLU:OE2	1:A:53:LYS:NZ	2.34	0.59
1:B:613:ASP:OD1	1:B:613:ASP:N	2.35	0.59
1:A:2264:ILE:O	1:A:2268:THR:HG22	2.02	0.59
1:A:1204:THR:O	1:A:1204:THR:HG22	2.00	0.59
1:A:1894:PHE:CE2	1:A:1917:VAL:HG21	2.37	0.59
1:B:2048:PHE:HA	1:B:2051:LEU:HD12	1.84	0.59
1:A:1072:ASP:O	1:A:1102:LEU:N	2.34	0.59
1:A:1316:THR:HG23	1:A:1367:MET:HE2	1.84	0.59
1:B:628:LYS:HG3	1:B:629:THR:HG23	1.84	0.59
1:B:364:HIS:O	1:B:364:HIS:ND1	2.36	0.59
1:B:965:VAL:HG23	1:B:966:ASP:OD1	2.02	0.59
1:A:706:LYS:O	1:A:749:LEU:N	2.35	0.58
1:A:903:LEU:O	1:A:906:SER:OG	2.16	0.58
1:A:1451:VAL:HG12	1:A:1487:LEU:HD13	1.83	0.58
1:B:2121:ASP:OD1	1:B:2122:THR:N	2.36	0.58
1:A:882:GLU:N	1:A:882:GLU:OE1	2.36	0.58
1:B:971:LEU:O	1:B:988:ASN:ND2	2.36	0.58
1:A:1724:HIS:ND1	1:A:1757:VAL:O	2.36	0.58
1:A:1925:VAL:HG22	1:A:1927:LYS:HG3	1.86	0.58
1:B:1321:VAL:HG22	1:B:1553:PHE:CD2	2.38	0.58
1:B:1840:LEU:HD11	1:B:1851:TYR:HB3	1.86	0.58
1:A:1617:ASP:OD1	1:A:1620:ILE:N	2.32	0.58
1:A:1883:ILE:HD11	1:A:2061:LEU:HD23	1.85	0.58
1:B:1150:MET:CE	1:B:1187:ALA:HB1	2.34	0.58
1:A:1463:GLU:O	1:A:1488:ARG:NH1	2.36	0.58
1:B:156:THR:HG22	1:B:156:THR:O	2.04	0.58
1:B:1758:ASP:OD1	1:B:1758:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:VAL:HG13	1:A:1173:VAL:O	2.04	0.57
1:B:1333:LEU:HD21	1:B:1387:LEU:HD22	1.85	0.57
1:A:1386:SER:O	1:A:1390:SER:N	2.37	0.57
1:A:2135:VAL:HG23	1:A:2160:THR:CG2	2.34	0.57
1:A:2301:ASP:N	1:A:2301:ASP:OD2	2.36	0.57
1:B:2136:GLY:N	1:B:2160:THR:O	2.36	0.57
1:A:954:GLU:OE2	1:A:962:ARG:NH1	2.35	0.57
1:B:245:ARG:NH2	1:B:366:GLU:OE1	2.37	0.57
1:B:1312:LYS:NZ	1:B:1316:THR:OG1	2.37	0.57
1:B:1829:THR:O	1:B:2115:LEU:N	2.33	0.57
1:A:1232:ASP:OD1	1:A:1233:PHE:N	2.37	0.57
1:A:500:TYR:CE1	1:A:504:THR:HG21	2.39	0.57
1:A:153:ILE:HG13	1:A:154:THR:HG23	1.87	0.57
1:B:1465:TYR:CE2	1:B:1489:VAL:HG13	2.40	0.57
1:A:613:ASP:N	1:A:613:ASP:OD1	2.38	0.57
1:B:1883:ILE:HD11	1:B:2061:LEU:HD23	1.86	0.57
1:B:1938:LEU:HD13	1:B:2080:PHE:CE2	2.39	0.57
1:A:596:LEU:HD21	1:A:651:LYS:HG2	1.88	0.56
1:A:2125:LEU:HD21	1:A:2348:ILE:HG21	1.87	0.56
1:A:1375:ILE:HD11	1:A:1406:LEU:HG	1.87	0.56
1:B:1278:ASP:OD1	1:B:1278:ASP:N	2.36	0.56
1:B:1935:ALA:HA	1:B:1938:LEU:HD12	1.87	0.56
1:B:608:MET:C	1:B:608:MET:HE3	2.30	0.56
1:A:2023:MET:SD	1:A:2023:MET:N	2.79	0.56
1:B:709:MET:HG3	1:B:771:LEU:HD13	1.88	0.56
1:B:1853:ALA:CB	1:B:2113:ILE:HD11	2.36	0.56
1:A:180:THR:HG21	1:A:436:THR:HG21	1.88	0.56
1:B:1425:VAL:CG2	1:B:1450:LEU:HD21	2.36	0.56
1:B:355:VAL:HG21	1:B:406:LEU:HD23	1.87	0.55
1:A:1592:SER:HB2	1:A:1616:LEU:HD11	1.87	0.55
1:A:116:LEU:HD13	1:A:121:MET:CE	2.36	0.55
1:A:816:MET:HE2	1:A:816:MET:HA	1.88	0.55
1:A:1512:PHE:O	1:A:1536:ARG:N	2.36	0.55
1:B:2133:LEU:HD23	1:B:2212:ILE:HG12	1.88	0.55
1:B:2288:GLU:O	1:B:2291:ARG:NH2	2.39	0.55
1:B:840:PHE:CZ	1:B:867:LEU:HD21	2.42	0.55
1:B:1291:MET:O	1:B:1296:LEU:HD11	2.07	0.55
1:B:1894:PHE:CE2	1:B:1917:VAL:HG21	2.41	0.55
1:B:2085:VAL:HG22	1:B:2104:VAL:HB	1.89	0.55
1:B:725:MET:O	1:B:729:ALA:N	2.40	0.55
1:A:1291:MET:CE	1:A:1296:LEU:HD22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1820:LEU:HD23	1:A:1820:LEU:O	2.07	0.55
1:B:2358:GLU:C	1:B:2359:LEU:HD12	2.32	0.55
1:B:1639:LEU:HD13	1:B:1664:TRP:CH2	2.42	0.54
1:B:1840:LEU:HD12	1:B:1852:THR:O	2.08	0.54
1:B:1944:ILE:HG23	1:B:2061:LEU:HD21	1.88	0.54
1:B:2023:MET:O	1:B:2025:GLN:NE2	2.41	0.54
1:B:1173:VAL:HG13	1:B:1173:VAL:O	2.06	0.54
1:B:1375:ILE:HD11	1:B:1406:LEU:HG	1.90	0.54
1:A:1465:TYR:CD2	1:A:1489:VAL:HG13	2.43	0.54
1:A:429:ASN:OD1	1:A:439:HIS:ND1	2.39	0.54
1:A:760:ASP:OD1	1:A:766:ASN:ND2	2.40	0.54
1:B:1875:GLU:C	1:B:1876:LEU:HD12	2.33	0.54
1:A:1543:MET:O	1:A:1611:VAL:N	2.41	0.53
1:B:1986:ARG:HG3	1:B:1986:ARG:HH11	1.74	0.53
1:A:61:GLU:OE2	1:A:225:HIS:NE2	2.33	0.53
1:B:297:MET:HE1	1:B:318:ILE:HD11	1.90	0.53
1:B:2022:HIS:O	1:B:2048:PHE:N	2.41	0.53
1:A:932:LEU:HD23	1:A:932:LEU:O	2.08	0.53
1:A:616:GLU:N	1:A:616:GLU:OE1	2.41	0.53
1:A:526:VAL:HG22	1:A:527:SER:H	1.73	0.53
1:B:832:ASP:O	1:B:836:GLY:N	2.38	0.53
1:A:1606:HIS:CE1	1:A:1609:SER:HG	2.24	0.53
1:A:2211:GLY:C	1:A:2212:ILE:HD13	2.34	0.53
1:B:353:LEU:HD23	1:B:354:VAL:N	2.24	0.53
1:B:2019:MET:HE2	1:B:2021:ILE:HD11	1.91	0.53
1:A:2262:SER:OG	1:A:2263:SER:N	2.42	0.53
1:B:1421:GLN:O	1:B:1425:VAL:HG23	2.09	0.53
1:B:1525:VAL:HG22	1:B:1585:LEU:HD21	1.91	0.53
1:A:2133:LEU:HD23	1:A:2212:ILE:HG23	1.91	0.53
1:A:1154:LEU:HD13	1:A:2337:GLU:OE2	2.09	0.52
1:A:1291:MET:HE3	1:A:1291:MET:O	2.09	0.52
1:B:1431:ILE:HD12	1:B:1431:ILE:C	2.34	0.52
1:B:1516:ILE:CD1	1:B:1542:LEU:HD22	2.39	0.52
1:B:1516:ILE:HD13	1:B:1542:LEU:HD22	1.89	0.52
1:B:2377:HIS:ND1	1:B:2386:ILE:HD12	2.24	0.52
1:A:312:GLU:N	1:A:312:GLU:OE1	2.42	0.52
1:B:483:SER:OG	1:B:522:LEU:N	2.38	0.52
1:A:506:VAL:HG21	1:A:937:LEU:HD11	1.90	0.52
1:A:1893:CYS:SG	1:A:1941:ARG:NH1	2.82	0.52
1:A:2236:MET:HE3	1:A:2236:MET:HA	1.90	0.52
1:A:1622:PHE:CD1	1:A:1622:PHE:C	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1452:ARG:NE	1:A:1485:ASP:OD1	2.42	0.52
1:A:2228:PRO:O	1:A:2231:SER:OG	2.26	0.52
1:B:817:MET:SD	1:B:817:MET:N	2.81	0.52
1:A:772:ASP:OD1	1:A:773:THR:N	2.42	0.52
1:B:153:ILE:HG13	1:B:154:THR:HG23	1.91	0.52
1:B:2021:ILE:CG2	1:B:2051:LEU:HD11	2.40	0.52
1:B:76:GLU:OE2	1:B:947:HIS:ND1	2.42	0.52
1:B:138:THR:HG21	1:B:156:THR:HG23	1.91	0.52
1:B:180:THR:HG21	1:B:436:THR:HG21	1.92	0.52
1:A:732:LEU:HD23	1:A:747:GLY:HA3	1.92	0.52
1:B:49:ARG:NH2	1:B:247:GLU:OE1	2.43	0.52
1:B:1542:LEU:C	1:B:1542:LEU:HD23	2.34	0.52
1:A:766:ASN:OD1	1:A:766:ASN:C	2.53	0.52
1:B:1244:LEU:O	1:B:1245:THR:OG1	2.25	0.52
1:B:1920:GLU:N	1:B:1920:GLU:OE1	2.42	0.52
1:B:2256:ASP:O	1:B:2352:GLN:NE2	2.43	0.52
1:A:813:ASP:OD2	1:A:815:ARG:NE	2.44	0.51
1:B:237:ASP:OD1	1:B:238:GLN:N	2.44	0.51
1:B:2031:GLU:OE1	1:B:2031:GLU:N	2.38	0.51
1:B:1872:ILE:HD11	1:B:1896:GLY:CA	2.41	0.51
1:A:368:CYS:SG	1:A:368:CYS:O	2.69	0.51
1:A:1831:VAL:HG12	1:A:1832:SER:N	2.25	0.51
1:B:587:GLY:N	1:B:895:ASP:OD2	2.40	0.51
1:B:1912:SER:OG	1:B:1914:VAL:O	2.25	0.51
1:A:1527:ALA:O	1:A:1531:VAL:HG23	2.10	0.51
1:B:1435:HIS:HB3	1:B:1438:LEU:HD21	1.92	0.51
1:B:472:GLU:OE2	1:B:928:ASN:ND2	2.44	0.51
1:B:1124:THR:HG22	1:B:1125:SER:H	1.75	0.51
1:B:1425:VAL:HA	1:B:1428:ALA:HB3	1.93	0.51
1:B:1458:LEU:HD22	1:B:1461:SER:HB3	1.92	0.51
1:A:2300:ILE:C	1:A:2300:ILE:HD12	2.36	0.51
1:B:1425:VAL:HG23	1:B:1450:LEU:HD21	1.92	0.51
1:A:971:LEU:O	1:A:988:ASN:ND2	2.41	0.51
1:A:1163:VAL:HG13	1:A:1177:TRP:CD1	2.46	0.51
1:B:1425:VAL:O	1:B:1429:LYS:N	2.32	0.51
1:B:1536:ARG:NE	1:B:1789:THR:O	2.40	0.51
1:B:2169:GLN:OE1	1:B:2172:ARG:NH2	2.41	0.51
1:B:2320:VAL:O	1:B:2320:VAL:HG13	2.09	0.51
1:B:154:THR:HG21	1:B:160:LEU:HD21	1.93	0.51
1:B:2066:LEU:HA	1:B:2069:ILE:HG22	1.92	0.51
1:B:1442:GLN:OE1	1:B:1465:TYR:OH	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ASP:OD1	1:A:823:LYS:N	2.44	0.50
1:A:2261:PHE:HD1	1:A:2300:ILE:HD11	1.77	0.50
1:B:1501:ASP:N	1:B:1501:ASP:OD1	2.44	0.50
1:A:360:THR:HG22	1:A:360:THR:O	2.12	0.50
1:A:1321:VAL:HG22	1:A:1553:PHE:CD2	2.44	0.50
1:A:168:PHE:O	1:B:281:ARG:NH1	2.45	0.50
1:B:1688:LEU:HD11	1:B:1767:ILE:CG2	2.42	0.50
1:B:2178:GLN:OE1	1:B:2180:VAL:HG23	2.11	0.50
1:B:1853:ALA:HB2	1:B:2113:ILE:HD11	1.92	0.50
1:A:1797:GLU:O	1:A:1807:VAL:HG12	2.12	0.50
1:A:2324:GLU:OE2	1:A:2325:ASN:N	2.45	0.50
1:B:1905:VAL:HG12	1:B:1923:ILE:O	2.12	0.50
1:A:1296:LEU:HD23	1:A:1597:ILE:HD13	1.93	0.50
1:B:1098:ILE:HG22	1:B:1099:ARG:N	2.27	0.50
1:A:2135:VAL:HG23	1:A:2160:THR:HG23	1.93	0.49
1:B:1841:SER:OG	1:B:1842:ARG:N	2.45	0.49
1:A:1395:LEU:HD13	1:A:1557:LEU:HD22	1.94	0.49
1:B:526:VAL:HG22	1:B:527:SER:H	1.76	0.49
1:B:1953:ILE:HD12	1:B:1980:THR:OG1	2.12	0.49
1:B:2120:VAL:CG1	1:B:2345:ALA:HB1	2.42	0.49
1:B:2135:VAL:HG22	1:B:2214:ASN:HA	1.92	0.49
1:A:1489:VAL:HG12	1:A:1490:ASP:H	1.76	0.49
1:A:914:VAL:HG23	1:A:915:VAL:HG23	1.95	0.49
1:B:490:LEU:HD22	1:B:524:VAL:HG12	1.94	0.49
1:B:1194:ASP:CG	1:B:2336:SER:HG	2.11	0.49
1:B:1512:PHE:HB2	1:B:1535:LEU:HA	1.94	0.49
1:A:1882:VAL:HB	1:A:1944:ILE:HG21	1.95	0.49
1:B:1497:GLU:OE1	1:B:1522:THR:N	2.45	0.49
1:B:1656:ILE:HD11	1:B:1767:ILE:HD13	1.95	0.49
1:A:336:ILE:HG21	1:A:406:LEU:HD21	1.95	0.49
1:A:1533:ASN:OD1	1:A:1533:ASN:C	2.55	0.49
1:B:517:SER:O	1:B:518:HIS:ND1	2.46	0.49
1:A:1622:PHE:HE2	1:A:1633:VAL:HG23	1.77	0.49
1:A:1879:THR:OG1	1:A:1880:GLU:OE2	2.23	0.49
1:A:2246:LEU:HD12	1:A:2247:GLU:N	2.27	0.49
1:A:1525:VAL:HG22	1:A:1585:LEU:HD21	1.95	0.49
1:B:1417:PHE:HA	1:B:1420:LEU:HD12	1.94	0.49
1:A:2085:VAL:HG22	1:A:2104:VAL:HB	1.95	0.49
1:A:726:GLU:OE1	1:A:726:GLU:N	2.45	0.49
1:A:727:GLN:NE2	1:A:754:GLU:OE2	2.46	0.49
1:A:1441:LEU:HB3	1:A:1515:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:HA	1:B:222:THR:HG21	1.94	0.49
1:B:808:SER:O	1:B:814:ASN:ND2	2.40	0.49
1:B:910:LEU:HD23	1:B:914:VAL:HG21	1.94	0.49
1:B:1204:THR:HG22	1:B:1204:THR:O	2.11	0.49
1:A:1416:GLY:O	1:A:1420:LEU:N	2.45	0.48
1:A:1758:ASP:OD1	1:A:1758:ASP:N	2.37	0.48
1:A:1984:SER:O	1:A:1996:SER:OG	2.17	0.48
1:B:1879:THR:HG22	1:B:2105:VAL:HG23	1.94	0.48
1:B:2316:ASN:ND2	1:B:2320:VAL:O	2.46	0.48
1:A:1283:LEU:HD23	1:A:1812:PRO:HA	1.94	0.48
1:A:1489:VAL:HG11	1:A:1491:PHE:CE1	2.47	0.48
1:B:1719:VAL:HG12	1:B:1720:LEU:N	2.28	0.48
1:B:1731:PRO:O	1:B:1734:ASN:N	2.46	0.48
1:A:1533:ASN:OD1	1:A:1534:LEU:N	2.46	0.48
1:B:660:PHE:CZ	1:B:861:ILE:HD11	2.49	0.48
1:A:965:VAL:HG13	1:A:966:ASP:N	2.28	0.48
1:A:2036:ARG:NH2	1:A:2045:VAL:HG23	2.29	0.48
1:B:975:ARG:NH2	1:B:979:ASP:OD2	2.36	0.48
1:B:2091:LEU:O	1:B:2095:GLY:N	2.46	0.48
1:B:1410:TRP:O	1:B:1414:GLY:N	2.46	0.48
1:B:1639:LEU:HD13	1:B:1664:TRP:CZ2	2.49	0.48
1:B:432:GLY:N	1:B:436:THR:O	2.40	0.48
1:A:1110:PHE:HB3	1:A:1111:PRO:HD2	1.96	0.48
1:B:1113:GLY:N	1:B:1114:PRO:CD	2.77	0.48
1:A:1847:ASP:OD1	1:A:1848:GLN:N	2.47	0.47
1:B:660:PHE:HZ	1:B:861:ILE:HD11	1.78	0.47
1:B:1113:GLY:N	1:B:1114:PRO:HD3	2.29	0.47
1:B:1946:SER:OG	1:B:1977:ARG:NH2	2.42	0.47
1:A:709:MET:CG	1:A:771:LEU:HD13	2.44	0.47
1:A:937:LEU:HD23	1:A:938:PRO:HD2	1.96	0.47
1:A:1158:SER:OG	1:A:1227:ASP:OD1	2.27	0.47
1:B:141:GLN:CD	1:B:152:MET:HE3	2.39	0.47
1:B:709:MET:SD	1:B:746:SER:OG	2.72	0.47
1:B:1712:LEU:C	1:B:1712:LEU:HD23	2.39	0.47
1:B:144:ASP:OD1	1:B:146:GLU:N	2.47	0.47
1:B:153:ILE:O	1:B:154:THR:OG1	2.24	0.47
1:A:788:LEU:HD22	1:A:831:LYS:HD3	1.95	0.47
1:A:1323:TYR:CG	1:A:1364:LEU:HD13	2.49	0.47
1:A:1961:ILE:O	1:A:1985:PHE:N	2.37	0.47
1:B:1314:ILE:HG21	1:B:1605:LYS:HD3	1.95	0.47
1:B:1603:PRO:O	1:B:1606:HIS:ND1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1679:ASP:OD1	1:B:1711:ARG:NH1	2.48	0.47
1:B:2275:ASN:OD1	1:B:2275:ASN:N	2.47	0.47
1:A:1515:VAL:HG23	1:A:1535:LEU:HD21	1.96	0.47
1:A:1687:VAL:HG21	1:A:1719:VAL:HG22	1.95	0.47
1:B:1291:MET:HE2	1:B:1540:PHE:CE2	2.50	0.47
1:B:1871:THR:O	1:B:1898:THR:HG22	2.14	0.47
1:B:2227:MET:HE1	1:B:2275:ASN:ND2	2.29	0.47
1:A:1367:MET:SD	1:A:1368:LEU:N	2.88	0.47
1:A:1489:VAL:HG11	1:A:1491:PHE:CZ	2.50	0.47
1:A:2301:ASP:OD2	1:A:2359:LEU:O	2.32	0.47
1:B:2300:ILE:HD12	1:B:2300:ILE:O	2.15	0.47
1:A:1513:ASP:O	1:A:1540:PHE:N	2.48	0.47
1:B:1199:THR:OG1	1:B:1200:ALA:N	2.48	0.47
1:A:1451:VAL:HG12	1:A:1487:LEU:CD1	2.45	0.46
1:A:2158:VAL:HG23	1:A:2183:VAL:HG23	1.97	0.46
1:A:1364:LEU:HA	1:A:1367:MET:HG3	1.98	0.46
1:B:2158:VAL:HG22	1:B:2183:VAL:CG2	2.44	0.46
1:A:810:VAL:HG21	1:A:833:ASN:OD1	2.15	0.46
1:A:1753:GLN:OE1	1:A:1754:PHE:N	2.49	0.46
1:A:972:LEU:HD22	1:A:986:TRP:CG	2.50	0.46
1:A:1374:HIS:O	1:A:1378:VAL:HG23	2.15	0.46
1:A:1633:VAL:O	1:A:1635:LEU:HD12	2.15	0.46
1:A:1986:ARG:NH1	1:A:1991:TRP:O	2.49	0.46
1:B:130:MET:HA	1:B:130:MET:HE3	1.97	0.46
1:B:245:ARG:NE	1:B:366:GLU:OE2	2.48	0.46
1:B:867:LEU:O	1:B:867:LEU:HD23	2.15	0.46
1:B:336:ILE:HG21	1:B:406:LEU:HD21	1.97	0.46
1:B:2066:LEU:HD22	1:B:2070:ARG:NE	2.31	0.46
1:B:1166:ASP:N	1:B:1166:ASP:OD1	2.46	0.46
1:B:2295:LEU:HD12	1:B:2295:LEU:H	1.81	0.46
1:B:1688:LEU:HD11	1:B:1767:ILE:HG22	1.98	0.46
1:B:1746:GLU:OE2	1:B:2272:THR:N	2.43	0.46
1:B:2021:ILE:HG23	1:B:2051:LEU:HD11	1.96	0.46
1:B:2246:LEU:HD11	1:B:2258:PHE:HZ	1.81	0.46
1:A:1482:LEU:HD13	1:A:1489:VAL:HG21	1.98	0.46
1:A:2259:LEU:HD22	1:A:2259:LEU:N	2.31	0.46
1:A:2354:ASP:OD1	1:A:2354:ASP:N	2.48	0.46
1:B:1814:THR:HG23	1:B:1815:GLU:N	2.31	0.46
1:B:914:VAL:HG23	1:B:915:VAL:HG23	1.96	0.46
1:B:1328:LEU:HD22	1:B:1333:LEU:HD22	1.98	0.46
1:B:1638:ASN:C	1:B:1639:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:VAL:HG21	1:A:1181:CYS:SG	2.55	0.45
1:A:1226:VAL:HG22	1:A:1227:ASP:N	2.32	0.45
1:A:2121:ASP:OD1	1:A:2122:THR:N	2.49	0.45
1:B:1512:PHE:C	1:B:1535:LEU:HD23	2.41	0.45
1:B:1974:ARG:NH1	1:B:2072:ASP:OD2	2.49	0.45
1:A:1417:PHE:HA	1:A:1420:LEU:HD12	1.97	0.45
1:A:2275:ASN:N	1:A:2275:ASN:OD1	2.50	0.45
1:B:1048:ASP:OD1	1:B:1050:ALA:N	2.45	0.45
1:B:1517:VAL:HG21	1:B:1543:MET:HB3	1.97	0.45
1:B:2106:ASP:O	1:B:2111:GLN:NE2	2.42	0.45
1:A:1688:LEU:HD12	1:A:1771:PHE:CD2	2.51	0.45
1:A:2281:ASN:HA	1:A:2284:VAL:HG12	1.97	0.45
1:B:1428:ALA:O	1:B:1432:SER:OG	2.28	0.45
1:B:1876:LEU:HD12	1:B:1876:LEU:N	2.31	0.45
1:B:2183:VAL:O	1:B:2183:VAL:CG2	2.63	0.45
1:A:1321:VAL:HG13	1:A:1553:PHE:HB3	1.99	0.45
1:B:2239:LYS:NZ	1:B:2280:ASN:OD1	2.46	0.45
1:A:1622:PHE:CE2	1:A:1633:VAL:HG23	2.51	0.45
1:B:1886:ILE:HD11	1:B:2058:PRO:HG3	1.99	0.45
1:A:628:LYS:CG	1:A:629:THR:HG23	2.46	0.45
1:A:1323:TYR:CE1	1:A:1364:LEU:HD22	2.51	0.45
1:B:1153:ARG:O	1:B:1154:LEU:C	2.60	0.45
1:B:1894:PHE:CZ	1:B:1917:VAL:HG21	2.52	0.45
1:A:628:LYS:HG3	1:A:629:THR:HG23	1.99	0.45
1:A:1113:GLY:N	1:A:1114:PRO:HD3	2.32	0.45
1:B:788:LEU:HD22	1:B:831:LYS:CE	2.47	0.45
1:B:1688:LEU:HD12	1:B:1771:PHE:CD2	2.52	0.45
1:A:129:TYR:HB2	1:A:206:VAL:HG12	1.98	0.45
1:A:180:THR:HG22	1:A:180:THR:O	2.16	0.45
1:A:399:VAL:HG12	1:A:399:VAL:O	2.17	0.45
1:B:1236:GLY:O	1:B:1237:TYR:CG	2.70	0.45
1:A:709:MET:HG3	1:A:771:LEU:HD13	1.98	0.45
1:A:735:ALA:HB3	1:A:744:THR:HG23	1.98	0.45
1:A:812:ASP:N	1:A:812:ASP:OD1	2.50	0.45
1:A:1113:GLY:N	1:A:1114:PRO:CD	2.80	0.45
1:A:1458:LEU:HD22	1:A:1461:SER:HB3	1.99	0.45
1:B:140:THR:HG23	1:B:958:ASN:ND2	2.32	0.45
1:A:1355:VAL:HG12	1:A:1357:SER:H	1.82	0.45
1:A:1578:THR:OG1	1:A:1581:GLU:OE1	2.34	0.45
1:A:224:LEU:HD21	1:B:150:LYS:O	2.16	0.44
1:A:333:ALA:CB	1:A:399:VAL:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:ALA:N	1:A:1609:SER:O	2.48	0.44
1:B:1614:GLN:NE2	1:B:1616:LEU:HD21	2.32	0.44
1:B:2141:ILE:HD11	1:B:2340:LEU:HD22	1.99	0.44
1:A:1237:TYR:O	1:A:1845:GLN:NE2	2.44	0.44
1:B:666:HIS:CD2	1:B:838:VAL:HG11	2.52	0.44
1:B:1328:LEU:HD22	1:B:1333:LEU:CD2	2.46	0.44
1:B:769:LEU:C	1:B:771:LEU:HD12	2.43	0.44
1:B:1752:LEU:HD12	1:B:1753:GLN:H	1.82	0.44
1:B:1793:THR:HB	1:B:1795:GLU:OE1	2.17	0.44
1:A:1965:ASP:O	1:A:1969:ALA:N	2.40	0.44
1:A:2358:GLU:OE1	1:A:2359:LEU:N	2.50	0.44
1:B:1652:LEU:O	1:B:1656:ILE:HG13	2.17	0.44
1:B:1763:VAL:O	1:B:1767:ILE:HD12	2.17	0.44
1:A:1199:THR:OG1	1:A:1200:ALA:N	2.51	0.44
1:B:1574:PHE:O	1:B:1577:ALA:N	2.50	0.44
1:A:360:THR:HG21	1:A:390:GLN:O	2.18	0.44
1:A:844:VAL:CG2	1:A:874:THR:HG21	2.48	0.44
1:A:993:GLU:OE1	1:A:993:GLU:N	2.48	0.44
1:A:1512:PHE:HB2	1:A:1535:LEU:HA	1.99	0.44
1:A:1800:LEU:C	1:A:1800:LEU:HD23	2.42	0.44
1:A:2239:LYS:CD	1:A:2279:ALA:HB1	2.48	0.44
1:B:1714:SER:O	1:B:1750:LYS:NZ	2.32	0.44
1:B:2247:GLU:OE2	1:B:2290:ARG:NH1	2.50	0.44
1:A:353:LEU:HD23	1:A:354:VAL:N	2.32	0.44
1:A:1851:TYR:CE2	1:A:2091:LEU:HD11	2.52	0.44
1:A:2195:LEU:HD12	1:A:2245:TYR:HB3	2.00	0.44
1:A:2214:ASN:OD1	1:A:2214:ASN:C	2.61	0.44
1:B:776:HIS:N	1:B:780:MET:SD	2.91	0.44
1:B:1124:THR:HG22	1:B:1125:SER:N	2.33	0.44
1:B:1262:ILE:HG22	1:B:1263:GLU:N	2.33	0.44
1:B:2288:GLU:O	1:B:2292:ALA:N	2.50	0.44
1:A:1160:THR:O	1:A:1160:THR:OG1	2.35	0.44
1:B:185:SER:OG	1:B:371:ILE:N	2.50	0.44
1:B:1990:THR:HG22	1:B:1999:LEU:HD11	1.99	0.44
1:A:1375:ILE:HD13	1:A:1409:ARG:CD	2.48	0.44
1:B:1656:ILE:HD13	1:B:1767:ILE:HB	2.00	0.44
1:B:1678:ASP:OD1	1:B:1680:GLU:HB3	2.18	0.44
1:A:732:LEU:HD21	1:A:751:ALA:CB	2.48	0.43
1:A:889:LEU:HD23	1:A:889:LEU:HA	1.89	0.43
1:A:1489:VAL:HG12	1:A:1490:ASP:N	2.33	0.43
1:B:547:VAL:O	1:B:547:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1547:THR:OG1	1:B:1609:SER:OG	2.12	0.43
1:A:451:ASP:OD2	1:A:457:LYS:NZ	2.42	0.43
1:A:770:ARG:C	1:A:771:LEU:HD12	2.42	0.43
1:A:2237:LYS:O	1:A:2241:GLN:CB	2.66	0.43
1:A:2323:MET:O	1:A:2326:SER:OG	2.33	0.43
1:B:116:LEU:HD13	1:B:121:MET:HE1	1.99	0.43
1:B:446:VAL:O	1:B:446:VAL:HG13	2.16	0.43
1:B:1421:GLN:HB3	1:B:1450:LEU:HD22	2.00	0.43
1:B:1404:GLY:O	1:B:1407:ILE:HG22	2.17	0.43
1:A:104:LEU:O	1:A:107:VAL:HG12	2.18	0.43
1:A:1115:ARG:NH2	1:A:1117:THR:O	2.51	0.43
1:A:1512:PHE:C	1:A:1535:LEU:HD23	2.43	0.43
1:A:1891:LEU:HA	1:A:1909:THR:HG22	2.00	0.43
1:A:1419:GLN:O	1:A:1423:HIS:CD2	2.71	0.43
1:A:1512:PHE:CE2	1:A:1534:LEU:HD13	2.54	0.43
1:A:2020:LEU:HD22	1:A:2045:VAL:HG22	2.01	0.43
1:A:2258:PHE:C	1:A:2259:LEU:HD22	2.43	0.43
1:A:2323:MET:O	1:A:2327:ILE:HG12	2.19	0.43
1:B:250:CYS:HB3	1:B:371:ILE:HG21	2.00	0.43
1:B:360:THR:O	1:B:360:THR:HG22	2.17	0.43
1:B:714:PHE:O	1:B:743:VAL:HG12	2.18	0.43
1:B:812:ASP:OD1	1:B:813:ASP:N	2.50	0.43
1:B:1026:CYS:SG	1:B:1027:ARG:N	2.92	0.43
1:B:1274:SER:O	1:B:1275:GLU:HB3	2.18	0.43
1:B:1344:LEU:HD11	1:B:1347:LEU:HD22	1.99	0.43
1:B:1688:LEU:HD23	1:B:1689:SER:N	2.34	0.43
1:A:272:ARG:CZ	1:A:306:LEU:HD11	2.48	0.43
1:A:1410:TRP:O	1:A:1414:GLY:N	2.51	0.43
1:A:2313:ARG:O	1:A:2313:ARG:CZ	2.67	0.43
1:B:1445:PRO:HB2	1:B:1474:THR:HG22	2.00	0.43
1:A:1260:ILE:HG22	1:A:1261:GLN:N	2.32	0.43
1:A:2237:LYS:O	1:A:2241:GLN:HB2	2.18	0.43
1:A:2390:ASP:OD1	1:A:2390:ASP:N	2.51	0.43
1:B:490:LEU:CD2	1:B:524:VAL:HG12	2.49	0.43
1:B:1938:LEU:HD22	1:B:2080:PHE:CE2	2.53	0.43
1:A:596:LEU:HD22	1:A:652:VAL:HG22	2.01	0.43
1:A:908:LEU:O	1:A:908:LEU:HD23	2.18	0.43
1:A:1794:ILE:HG22	1:A:1794:ILE:O	2.18	0.43
1:B:735:ALA:HB3	1:B:744:THR:HG23	2.01	0.43
1:B:771:LEU:HD12	1:B:771:LEU:N	2.34	0.43
1:B:1395:LEU:HD21	1:B:1557:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:OD1	1:A:41:THR:HG22	2.18	0.43
1:A:1351:ILE:O	1:A:1351:ILE:HG22	2.18	0.43
1:B:1993:ILE:HG23	1:B:1994:PRO:HD2	2.00	0.43
1:B:1439:ARG:NH2	1:B:1463:GLU:OE1	2.52	0.43
1:B:1948:VAL:HG13	1:B:2053:ALA:HA	2.01	0.43
1:A:1497:GLU:OE1	1:A:1522:THR:OG1	2.34	0.42
1:B:360:THR:HG21	1:B:390:GLN:O	2.19	0.42
1:B:788:LEU:HD22	1:B:831:LYS:HE2	2.00	0.42
1:B:1379:LEU:HD12	1:B:1403:MET:SD	2.59	0.42
1:B:1882:VAL:HB	1:B:1944:ILE:HG21	2.01	0.42
1:B:2344:LEU:N	1:B:2344:LEU:HD23	2.33	0.42
1:A:1291:MET:HE1	1:A:1296:LEU:HD22	2.01	0.42
1:A:2331:ASP:N	1:A:2331:ASP:OD1	2.52	0.42
1:B:1895:VAL:HG22	1:B:1905:VAL:HG23	2.00	0.42
1:A:1814:THR:HG23	1:A:1815:GLU:N	2.34	0.42
1:B:2013:VAL:HG22	1:B:2038:ALA:O	2.19	0.42
1:B:5:HIS:O	1:B:5:HIS:ND1	2.48	0.42
1:B:1542:LEU:HD21	1:B:1610:VAL:HG13	2.02	0.42
1:A:177:SER:O	1:A:177:SER:OG	2.36	0.42
1:A:1459:GLY:O	1:A:1462:LEU:N	2.53	0.42
1:A:1971:SER:O	1:A:1977:ARG:NH2	2.53	0.42
1:B:1321:VAL:HG13	1:B:1553:PHE:HB3	2.01	0.42
1:B:1443:VAL:HB	1:B:1517:VAL:HA	2.00	0.42
1:B:631:ARG:NH1	1:B:637:ILE:HD11	2.35	0.42
1:B:1961:ILE:HG12	1:B:2021:ILE:HD12	2.00	0.42
1:A:2266:VAL:HG13	1:A:2267:MET:N	2.34	0.42
1:B:826:GLU:O	1:B:830:TRP:NE1	2.52	0.42
1:A:1013:THR:O	1:A:1017:MET:HG3	2.20	0.42
1:A:1173:VAL:HG23	1:A:1177:TRP:CZ2	2.55	0.42
1:A:1241:LEU:HB3	1:A:1242:PRO:HD2	2.02	0.42
1:A:2377:HIS:O	1:A:2386:ILE:HD13	2.20	0.42
1:B:1438:LEU:CD1	1:B:1458:LEU:HD21	2.48	0.42
1:A:309:SER:O	1:A:350:ARG:NH2	2.52	0.42
1:A:2086:VAL:HG12	1:A:2087:LYS:N	2.35	0.42
1:B:336:ILE:CG2	1:B:406:LEU:HD21	2.49	0.42
1:B:709:MET:HB2	1:B:771:LEU:HD13	2.02	0.42
1:A:2125:LEU:O	1:A:2125:LEU:HD23	2.20	0.42
1:B:39:ASP:OD1	1:B:41:THR:HG22	2.20	0.42
1:B:139:ASP:OD2	1:B:216:ASP:OD2	2.37	0.42
1:B:600:VAL:HG11	1:B:648:GLY:HA2	2.00	0.42
1:B:1170:THR:HG23	1:B:1171:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1872:ILE:O	1:B:1914:VAL:HG13	2.20	0.42
1:B:2141:ILE:HD11	1:B:2340:LEU:CD2	2.50	0.42
1:B:67:ASN:OD1	1:B:222:THR:OG1	2.37	0.41
1:B:481:ILE:HD11	1:B:516:ASN:CB	2.50	0.41
1:B:1532:ARG:CZ	1:B:1615:ALA:HB1	2.49	0.41
1:B:1299:ALA:HB3	1:B:1597:ILE:HD12	2.02	0.41
1:B:1407:ILE:HG23	1:B:1408:SER:N	2.35	0.41
1:B:2350:VAL:O	1:B:2350:VAL:HG22	2.19	0.41
1:A:732:LEU:HD21	1:A:751:ALA:HB3	2.02	0.41
1:A:1199:THR:OG1	1:A:1271:LEU:HD13	2.20	0.41
1:A:1525:VAL:HG21	1:A:1585:LEU:HD11	2.01	0.41
1:B:1556:MET:SD	1:B:1556:MET:C	3.03	0.41
1:B:2086:VAL:HG12	1:B:2087:LYS:N	2.35	0.41
1:A:897:LEU:C	1:A:897:LEU:HD23	2.45	0.41
1:A:2088:ALA:N	1:A:2111:GLN:OE1	2.52	0.41
1:B:634:GLU:HB2	1:B:637:ILE:HD12	2.02	0.41
1:B:1046:VAL:O	1:B:1046:VAL:HG13	2.19	0.41
1:B:1465:TYR:CD2	1:B:1489:VAL:HG22	2.55	0.41
1:A:2300:ILE:HG21	1:A:2347:ALA:HB2	2.02	0.41
1:B:133:MET:O	1:B:158:ARG:NH2	2.54	0.41
1:B:139:ASP:OD1	1:B:139:ASP:C	2.63	0.41
1:B:1244:LEU:N	1:B:1244:LEU:HD12	2.36	0.41
1:B:1322:HIS:ND1	1:B:1351:ILE:O	2.53	0.41
1:B:1441:LEU:HD22	1:B:1515:VAL:HG13	2.01	0.41
1:B:1547:THR:HG1	1:B:1609:SER:CB	2.23	0.41
1:B:1527:ALA:O	1:B:1531:VAL:HG23	2.20	0.41
1:A:1466:THR:HG22	1:A:1468:VAL:HG23	2.02	0.41
1:A:2178:GLN:OE1	1:A:2180:VAL:HG23	2.20	0.41
1:B:241:ASP:OD1	1:B:241:ASP:N	2.53	0.41
1:B:2300:ILE:HG21	1:B:2347:ALA:HB2	2.03	0.41
1:A:998:LEU:HD13	1:A:1047:LEU:CD2	2.51	0.41
1:A:1406:LEU:HB3	1:A:1558:MET:HE1	2.01	0.41
1:B:180:THR:O	1:B:180:THR:HG22	2.20	0.41
1:B:744:THR:C	1:B:745:LEU:HD22	2.45	0.41
1:B:1839:SER:HB3	1:B:1856:VAL:HG22	2.03	0.41
1:A:49:ARG:NH2	1:A:247:GLU:OE1	2.50	0.41
1:A:178:VAL:HG12	1:B:178:VAL:HG12	2.02	0.41
1:A:1248:MET:HE2	1:A:1262:ILE:HD12	2.03	0.41
1:A:1829:THR:N	1:A:2115:LEU:O	2.49	0.41
1:A:2246:LEU:HD12	1:A:2246:LEU:C	2.46	0.41
1:A:2320:VAL:HG12	1:A:2321:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ILE:HG22	1:B:92:GLU:HB2	2.02	0.41
1:B:770:ARG:C	1:B:771:LEU:HD12	2.46	0.41
1:B:932:LEU:O	1:B:932:LEU:HD23	2.21	0.41
1:B:1963:GLU:OE2	1:B:1987:ALA:N	2.53	0.41
1:A:598:ARG:O	1:A:601:ILE:HG13	2.21	0.41
1:A:1482:LEU:O	1:A:1482:LEU:HD12	2.19	0.41
1:A:2123:ARG:HA	1:A:2123:ARG:NE	2.36	0.41
1:A:2245:TYR:O	1:A:2249:VAL:HG23	2.21	0.41
1:B:1382:THR:HB	1:B:1403:MET:HE1	2.03	0.40
1:A:1450:LEU:HG	1:A:1454:VAL:HG23	2.02	0.40
1:A:1720:LEU:C	1:A:1720:LEU:HD23	2.45	0.40
1:A:1894:PHE:CZ	1:A:1917:VAL:HG21	2.56	0.40
1:B:130:MET:HG2	1:B:162:ALA:HB2	2.03	0.40
1:B:714:PHE:CZ	1:B:764:VAL:HG12	2.56	0.40
1:B:1364:LEU:O	1:B:1367:MET:HG2	2.21	0.40
1:B:2036:ARG:NH2	1:B:2043:ALA:O	2.51	0.40
1:B:2240:VAL:HG23	1:B:2241:GLN:N	2.35	0.40
1:A:854:ASP:C	1:A:854:ASP:OD2	2.64	0.40
1:A:1530:THR:O	1:A:1534:LEU:HG	2.20	0.40
1:B:1823:LEU:HD21	1:B:2119:PRO:HG2	2.04	0.40
1:B:1859:HIS:HB2	1:B:1862:LEU:HD21	2.04	0.40
1:B:2320:VAL:O	1:B:2320:VAL:CG1	2.70	0.40
1:A:47:GLU:OE1	1:A:47:GLU:N	2.54	0.40
1:A:1732:TYR:CD1	1:A:1732:TYR:N	2.90	0.40
1:A:1831:VAL:HG12	1:A:1832:SER:H	1.86	0.40
1:B:111:MET:HE1	1:B:169:PHE:CE1	2.57	0.40
1:B:1120:ASP:O	1:B:1121:LEU:HD12	2.22	0.40
1:B:1270:PHE:CD2	1:B:1270:PHE:C	2.99	0.40
1:B:1490:ASP:OD2	1:B:1506:LEU:HD21	2.22	0.40
1:B:1875:GLU:O	1:B:2108:THR:HG23	2.22	0.40
1:A:861:ILE:HD12	1:A:888:VAL:HG21	2.04	0.40
1:A:889:LEU:HD21	1:A:895:ASP:CG	2.47	0.40
1:A:1138:LEU:HD11	1:A:1200:ALA:HB1	2.02	0.40
1:A:1241:LEU:HB3	1:A:1269:SER:HB3	2.04	0.40
1:A:2217:MET:O	1:A:2218:VAL:HG13	2.22	0.40
1:B:713:GLY:C	1:B:714:PHE:CG	2.99	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 PDB entries followed by that with respect to all EM entries.

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	2362/4007 (59%)	2218 (94%)	144 (6%)	0	100	100
1	B	2355/4007 (59%)	2217 (94%)	138 (6%)	0	100	100
All	All	4717/8014 (59%)	4435 (94%)	282 (6%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	1969/3338 (59%)	1953 (99%)	16 (1%)	73	77
1	B	1967/3338 (59%)	1949 (99%)	18 (1%)	70	76
All	All	3936/6676 (59%)	3902 (99%)	34 (1%)	68	76

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ILE
1	A	178	VAL
1	A	267	ILE
1	A	739	SER
1	A	757	GLU
1	A	783	CYS
1	A	871	THR
1	A	1466	THR

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Mol	Chain	Res	Type
1	A	1470	ASP
1	A	1635	LEU
1	A	1673	THR
1	A	1900	GLU
1	A	2113	ILE
1	A	2281	ASN
1	A	2323	MET
1	A	2358	GLU
1	B	508	LEU
1	B	557	THR
1	B	623	ILE
1	B	698	LEU
1	B	739	SER
1	B	871	THR
1	B	966	ASP
1	B	1042	LEU
1	B	1074	ILE
1	B	1100	ILE
1	B	1150	MET
1	B	1166	ASP
1	B	1965	ASP
1	B	1980	THR
1	B	2137	LEU
1	B	2196	LEU
1	B	2300	ILE
1	B	2344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	210	ASN
1	A	214	ASN
1	A	394	ASN
1	A	450	HIS
1	A	518	HIS
1	A	610	GLN
1	A	1070	HIS
1	A	1730	ASN
1	A	1933	GLN
1	A	2163	HIS
1	A	2169	GLN

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Mol	Chain	Res	Type
1	A	2281	ASN
1	B	293	GLN
1	B	394	ASN
1	B	516	ASN
1	B	599	GLN
1	B	960	ASN
1	B	1238	GLN
1	B	1285	ASN
1	B	1498	ASN
1	B	1518	HIS
1	B	1749	GLN
1	B	2233	GLN
1	B	2312	GLN
1	B	2325	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 oligosaccharides 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.