Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2023 – 11:07 PM EDT

PDB ID	:	2WSY
Title	:	CRYSTAL STRUCTURE OF WILD-TYPE TRYPTOPHAN SYNTHASE
Authors	:	Schneider, T.R.; Gerhardt, E.; Lee, M.; Liang, P.-H.; Anderson, K.S.; Schlichting, I.
Deposited on	:	1998-02-18
Resolution	:	3.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

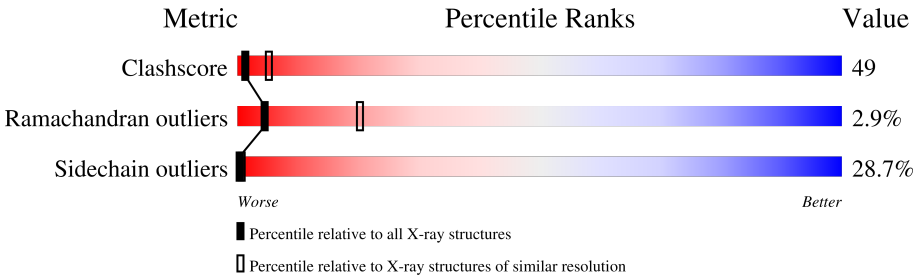
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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))
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	268	26% 45% 17% 12%
2	B	396	34% 46% 14% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4648 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 TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1787	1137	308	334	8	0	0	0

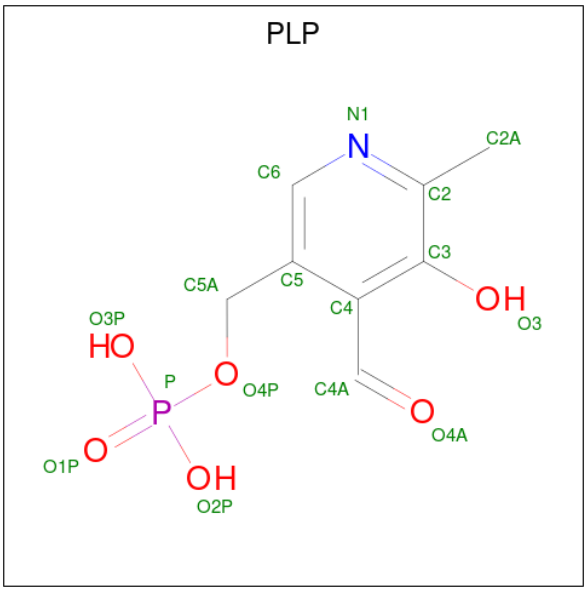
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	375	2845	1791	498	537	19	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	B	1	1	1	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

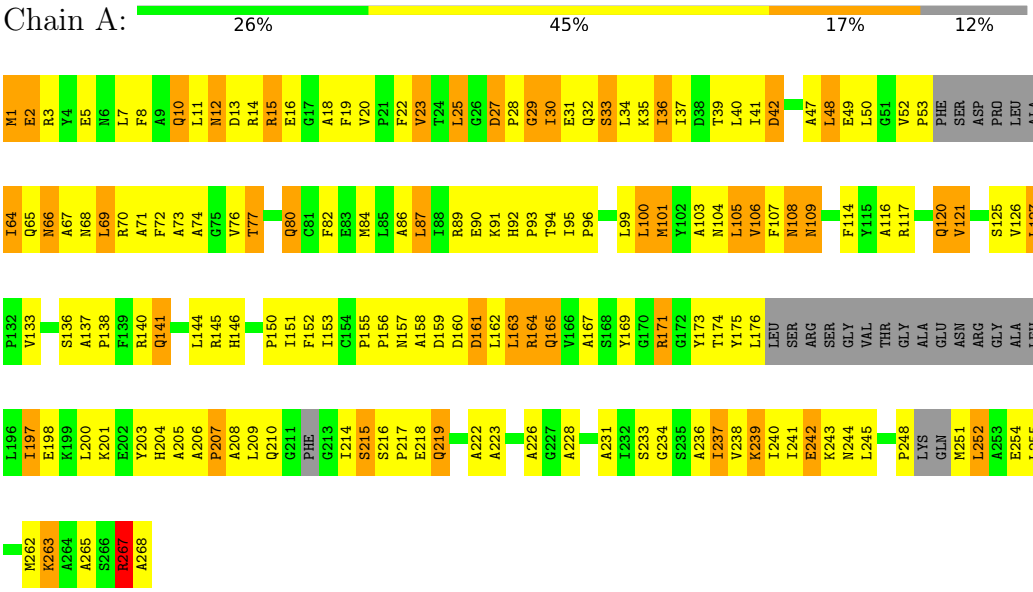
3 Residue-property plots (i)

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.

Note EDS was not executed.

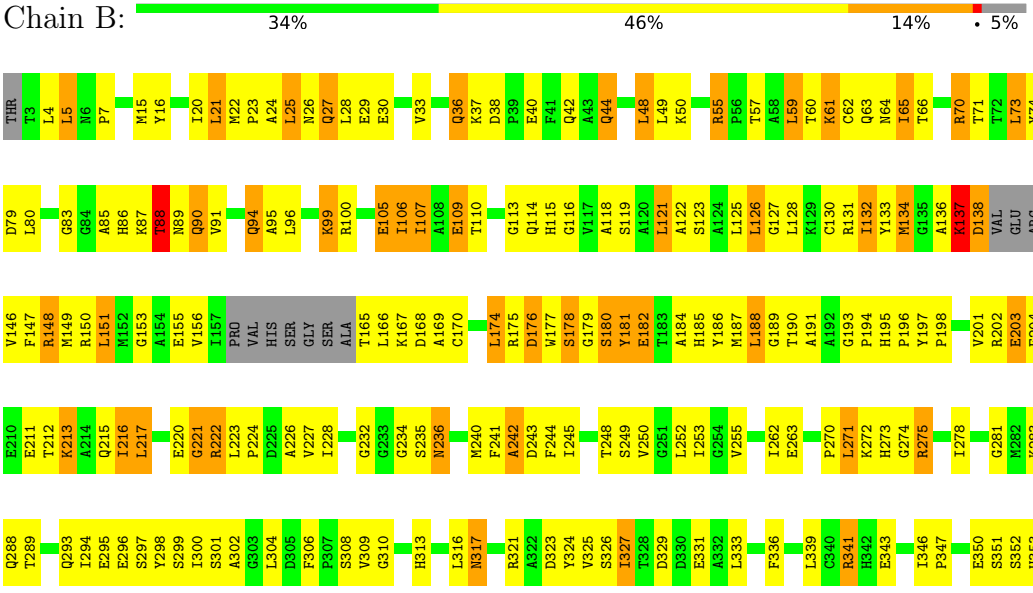
• Molecule 1: TRYPTOPHAN SYNTHASE

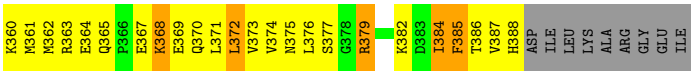
Chain A:



• Molecule 2: TRYPTOPHAN SYNTHASE

Chain B:




K360
M361
M362
R363
E364
Q365
P366
E367
K368
E369
Q370
L371
L372
V373
V374
N375
L376
S377
G378
R379
K382
D383
I384
F385
T386
V387
H388
ASP
ILE
LEU
LYS
ALA
ARG
GLY
GLU
ILE

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.10Å 61.20Å 67.60Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	10.00 – 3.05	Depositor
% Data completeness (in resolution range)	90.9 (10.00-3.05)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4648	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.23	0/1816	0.45	0/2461
2	B	0.24	0/2899	0.50	0/3912
All	All	0.24	0/4715	0.48	0/6373

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	1787	0	1802	190	0
2	B	2845	0	2819	277	0
3	B	1	0	0	0	0
4	B	15	0	7	3	0
All	All	4648	0	4628	458	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 49.

All (458) 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:52:VAL:HB	1:A:101:MET:HE2	1.36	1.06
2:B:222:ARG:HH11	2:B:222:ARG:HB3	1.15	1.03
1:A:27:ASP:HB3	1:A:28:PRO:HD3	1.41	1.02
1:A:137:ALA:HB3	1:A:138:PRO:HD3	1.41	1.01
2:B:191:ALA:HA	2:B:201:VAL:HG21	1.45	0.98
1:A:140:ARG:HD3	1:A:169:TYR:HB3	1.42	0.97
2:B:71:THR:HG21	2:B:362:MET:HB3	1.46	0.97
1:A:66:ASN:HD22	1:A:66:ASN:H	1.09	0.97
2:B:145:ASN:N	2:B:145:ASN:HD22	1.58	0.96
1:A:215:SER:H	1:A:219:GLN:HE21	1.05	0.94
2:B:301:SER:HB2	2:B:350:GLU:HG3	1.50	0.93
2:B:134:MET:HE3	2:B:138:ASP:HB2	1.52	0.91
2:B:372:LEU:H	2:B:372:LEU:HD22	1.37	0.90
2:B:222:ARG:HB3	2:B:222:ARG:NH1	1.86	0.90
2:B:274:GLY:O	2:B:275:ARG:HB2	1.70	0.88
1:A:66:ASN:H	1:A:66:ASN:ND2	1.73	0.86
2:B:134:MET:CE	2:B:138:ASP:HB2	2.04	0.85
1:A:101:MET:SD	1:A:105:LEU:HD21	2.17	0.85
1:A:109:ASN:ND2	1:A:109:ASN:H	1.75	0.85
2:B:191:ALA:CA	2:B:201:VAL:HG21	2.06	0.84
2:B:71:THR:HG21	2:B:362:MET:CB	2.08	0.83
2:B:188:LEU:HG	2:B:197:TYR:CD2	2.13	0.83
2:B:336:PHE:CE2	2:B:387:VAL:HG11	2.13	0.83
1:A:27:ASP:HB3	1:A:28:PRO:CD	2.09	0.82
2:B:145:ASN:N	2:B:145:ASN:ND2	2.22	0.82
2:B:143:SER:HB3	2:B:144:PRO:HD3	1.63	0.81
1:A:48:LEU:HD13	1:A:50:LEU:HD21	1.61	0.80
2:B:271:LEU:HD23	2:B:309:VAL:HG11	1.63	0.79
1:A:20:VAL:HG22	1:A:47:ALA:HB3	1.62	0.78
2:B:55:ARG:CG	2:B:55:ARG:HH11	1.97	0.76
2:B:105:GLU:O	2:B:106:ILE:HD13	1.85	0.76
2:B:61:LYS:HB2	2:B:74:TYR:CE1	2.20	0.76
1:A:10:GLN:O	1:A:14:ARG:HG3	1.86	0.76
1:A:176:LEU:HD22	1:A:208:ALA:HB1	1.67	0.76
1:A:41:ILE:HG12	1:A:95:ILE:HD13	1.68	0.75
2:B:346:ILE:HD13	2:B:384:ILE:HD11	1.70	0.74
1:A:108:ASN:HD21	2:B:275:ARG:HH12	1.34	0.74
2:B:186:TYR:CE2	2:B:188:LEU:HD23	2.22	0.74
2:B:301:SER:CB	2:B:350:GLU:HG3	2.18	0.73
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.16	0.73
1:A:215:SER:H	1:A:219:GLN:NE2	1.83	0.73
1:A:22:PHE:HA	1:A:49:GLU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLY:HA2	2:B:240:MET:HE3	1.71	0.72
1:A:30:ILE:CG2	1:A:31:GLU:N	2.51	0.72
1:A:109:ASN:H	1:A:109:ASN:HD22	1.37	0.72
2:B:99:LYS:HD3	2:B:128:LEU:HD21	1.70	0.72
2:B:21:LEU:HD11	2:B:178:SER:HA	1.73	0.71
2:B:347:PRO:HB3	2:B:376:LEU:HD11	1.72	0.70
1:A:7:LEU:O	1:A:11:LEU:HB2	1.91	0.70
2:B:91:VAL:HG13	2:B:187:MET:HE3	1.73	0.70
2:B:365:GLN:O	2:B:368:LYS:HB3	1.91	0.70
2:B:232:GLY:O	2:B:306:PHE:HB3	1.92	0.70
2:B:191:ALA:HA	2:B:201:VAL:CG2	2.22	0.70
2:B:242:ALA:HA	2:B:245:ILE:HD12	1.72	0.70
2:B:70:ARG:HG2	2:B:369:GLU:HG3	1.72	0.69
2:B:321:ARG:HD2	2:B:321:ARG:O	1.91	0.69
2:B:78:GLU:HB2	2:B:376:LEU:O	1.92	0.69
2:B:86:HIS:O	2:B:89:ASN:HB2	1.93	0.69
1:A:11:LEU:HD12	1:A:14:ARG:HH21	1.58	0.69
2:B:325:VAL:HG21	2:B:357:HIS:CE1	2.28	0.69
1:A:33:SER:HA	1:A:36:ILE:HG13	1.73	0.69
1:A:215:SER:N	1:A:219:GLN:HE21	1.86	0.69
1:A:242:GLU:HG2	1:A:242:GLU:O	1.92	0.68
2:B:55:ARG:NH1	2:B:55:ARG:HG3	2.09	0.68
1:A:133:VAL:HG21	1:A:165:GLN:HB3	1.76	0.68
2:B:22:MET:O	2:B:26:ASN:ND2	2.27	0.68
2:B:48:LEU:HD21	2:B:125:LEU:HD21	1.75	0.68
2:B:346:ILE:HG23	2:B:346:ILE:O	1.93	0.68
2:B:270:PRO:N	2:B:287:MET:HE3	2.08	0.68
1:A:52:VAL:CB	1:A:101:MET:HE2	2.21	0.67
2:B:71:THR:OG1	2:B:370:GLN:HG3	1.93	0.67
2:B:197:TYR:HB2	2:B:198:PRO:HD3	1.77	0.67
2:B:285:PRO:C	2:B:286:MET:HG2	2.13	0.67
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.30	0.66
1:A:128:VAL:CG1	1:A:131:VAL:HG23	2.26	0.66
2:B:91:VAL:HG13	2:B:187:MET:CE	2.25	0.66
2:B:29:GLU:O	2:B:33:VAL:HG23	1.96	0.66
2:B:274:GLY:O	2:B:275:ARG:CB	2.43	0.66
2:B:336:PHE:HE2	2:B:387:VAL:HG11	1.59	0.66
2:B:73:LEU:HD21	2:B:374:VAL:CG1	2.25	0.66
1:A:27:ASP:CB	1:A:28:PRO:HD3	2.22	0.65
1:A:242:GLU:HA	1:A:245:LEU:HD13	1.77	0.65
1:A:267:ARG:O	1:A:268:ALA:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HD13	1:A:173:TYR:CZ	2.31	0.65
2:B:327:ILE:CD1	2:B:357:HIS:HB2	2.27	0.65
2:B:360:LYS:O	2:B:364:GLU:HG3	1.97	0.65
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.32	0.65
2:B:271:LEU:CD2	2:B:309:VAL:HG11	2.27	0.65
2:B:136:ALA:C	2:B:138:ASP:H	2.00	0.64
2:B:105:GLU:HG3	2:B:184:ALA:HB2	1.80	0.64
1:A:105:LEU:HD12	1:A:105:LEU:O	1.98	0.64
1:A:109:ASN:ND2	1:A:109:ASN:N	2.47	0.63
1:A:11:LEU:CD2	1:A:18:ALA:HB2	2.29	0.63
1:A:137:ALA:O	1:A:141:GLN:HG2	1.98	0.63
2:B:40:GLU:O	2:B:44:GLN:HG2	1.99	0.63
1:A:108:ASN:ND2	2:B:275:ARG:HH12	1.95	0.63
2:B:22:MET:N	2:B:23:PRO:HD2	2.14	0.62
2:B:284:ALA:HB1	2:B:285:PRO:HD2	1.80	0.62
1:A:65:GLN:O	1:A:69:LEU:HD22	1.99	0.62
1:A:30:ILE:HG22	1:A:31:GLU:H	1.64	0.62
2:B:64:ASN:HB2	2:B:343:GLU:OE2	2.00	0.62
2:B:90:GLN:HA	2:B:204:PHE:HB3	1.81	0.62
2:B:83:GLY:HA3	2:B:88:THR:HG21	1.82	0.62
2:B:213:LYS:HG3	2:B:244:PHE:CE1	2.35	0.62
1:A:22:PHE:HD2	1:A:49:GLU:HG3	1.64	0.62
1:A:117:ARG:O	1:A:121:VAL:HG22	2.00	0.61
2:B:21:LEU:CD1	2:B:178:SER:HA	2.29	0.61
2:B:42:GLN:HA	2:B:42:GLN:NE2	2.16	0.61
2:B:88:THR:O	2:B:88:THR:OG1	2.15	0.61
2:B:371:LEU:HG	2:B:371:LEU:O	2.00	0.61
1:A:33:SER:O	1:A:37:ILE:HG13	2.00	0.61
2:B:309:VAL:HG22	2:B:310:GLY:N	2.14	0.61
2:B:284:ALA:HB1	2:B:285:PRO:CD	2.30	0.61
2:B:55:ARG:HH11	2:B:55:ARG:HG3	1.60	0.60
2:B:96:LEU:HD12	2:B:126:LEU:HD21	1.83	0.60
1:A:155:PRO:HB2	1:A:156:PRO:HD2	1.83	0.60
2:B:121:LEU:C	2:B:121:LEU:HD12	2.22	0.60
1:A:86:ALA:HB2	1:A:121:VAL:HG12	1.83	0.60
2:B:179:GLY:O	2:B:180:SER:HB3	2.02	0.60
2:B:145:ASN:HA	2:B:148:ARG:HB2	1.82	0.60
1:A:140:ARG:HG3	1:A:152:PHE:HZ	1.67	0.59
1:A:210:GLN:HG3	1:A:214:ILE:HD11	1.84	0.59
1:A:30:ILE:HG23	1:A:31:GLU:N	2.17	0.59
1:A:155:PRO:CB	1:A:156:PRO:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG12	2:B:122:ALA:CB	2.32	0.59
2:B:289:THR:CG2	2:B:293:GLN:HB2	2.32	0.59
1:A:20:VAL:CG2	1:A:47:ALA:HB3	2.32	0.59
2:B:217:LEU:O	2:B:221:GLY:HA2	2.02	0.59
2:B:55:ARG:CG	2:B:55:ARG:NH1	2.61	0.59
2:B:271:LEU:O	2:B:271:LEU:HD13	2.02	0.59
2:B:25:LEU:HD12	2:B:196:PRO:HD3	1.85	0.58
2:B:289:THR:HG23	2:B:293:GLN:HB2	1.84	0.58
1:A:27:ASP:CB	1:A:28:PRO:CD	2.80	0.58
1:A:72:PHE:C	1:A:74:ALA:H	2.06	0.58
1:A:174:THR:HB	1:A:208:ALA:HA	1.85	0.58
2:B:22:MET:HG3	2:B:26:ASN:HD21	1.68	0.58
1:A:37:ILE:HG23	1:A:48:LEU:HD11	1.85	0.58
2:B:227:VAL:HG11	2:B:240:MET:CG	2.34	0.58
2:B:309:VAL:HG22	2:B:310:GLY:H	1.68	0.58
2:B:85:ALA:HA	2:B:377:SER:O	2.03	0.57
2:B:357:HIS:HD2	2:B:361:MET:CE	2.16	0.57
1:A:12:ASN:C	1:A:14:ARG:H	2.07	0.57
2:B:136:ALA:C	2:B:138:ASP:N	2.56	0.57
2:B:165:THR:CG2	2:B:168:ASP:HB2	2.33	0.57
2:B:165:THR:HG22	2:B:168:ASP:HB2	1.84	0.57
1:A:77:THR:HG23	1:A:80:GLN:NE2	2.20	0.57
1:A:117:ARG:HH11	1:A:120:GLN:NE2	2.03	0.57
1:A:137:ALA:O	1:A:141:GLN:CG	2.53	0.57
2:B:372:LEU:H	2:B:372:LEU:CD2	2.11	0.57
2:B:38:ASP:OD2	2:B:100:ARG:NH2	2.37	0.57
1:A:150:PRO:HD2	1:A:171:ARG:HB3	1.86	0.57
2:B:29:GLU:HB2	2:B:196:PRO:HG3	1.87	0.57
2:B:262:ILE:HG21	2:B:273:HIS:CE1	2.39	0.57
1:A:15:ARG:O	1:A:268:ALA:HA	2.03	0.57
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.87	0.56
1:A:203:TYR:O	1:A:204:HIS:HB2	2.05	0.56
2:B:357:HIS:HD2	2:B:361:MET:HE3	1.70	0.56
1:A:16:GLU:HB2	1:A:267:ARG:HA	1.87	0.56
1:A:116:ALA:HB2	1:A:146:HIS:CE1	2.41	0.56
1:A:137:ALA:CB	1:A:138:PRO:HD3	2.26	0.56
2:B:73:LEU:HD21	2:B:374:VAL:HG12	1.87	0.56
2:B:286:MET:CE	2:B:294:ILE:HD12	2.36	0.56
1:A:25:LEU:HD22	1:A:50:LEU:HB3	1.87	0.56
1:A:71:ALA:O	1:A:74:ALA:HB3	2.06	0.56
2:B:55:ARG:NH1	2:B:211:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ASN:ND2	2:B:145:ASN:H	2.02	0.56
2:B:339:LEU:CD2	2:B:347:PRO:HG3	2.36	0.56
1:A:37:ILE:CG2	1:A:48:LEU:HD11	2.36	0.56
1:A:47:ALA:HA	1:A:96:PRO:HD2	1.88	0.55
1:A:11:LEU:CD1	1:A:14:ARG:HH21	2.20	0.55
2:B:204:PHE:O	2:B:207:MET:HE1	2.06	0.55
1:A:34:LEU:HD11	1:A:87:LEU:HD22	1.89	0.55
2:B:253:ILE:HA	2:B:323:ASP:O	2.07	0.55
1:A:105:LEU:HD12	1:A:105:LEU:C	2.25	0.55
2:B:212:THR:HG21	2:B:240:MET:HE1	1.88	0.55
1:A:104:ASN:HB2	2:B:278:ILE:O	2.07	0.55
2:B:87:LYS:O	2:B:89:ASN:N	2.37	0.55
1:A:101:MET:HB3	1:A:105:LEU:HD23	1.89	0.54
1:A:167:ALA:CB	1:A:205:ALA:HB2	2.37	0.54
1:A:163:LEU:HD13	1:A:200:LEU:HD23	1.89	0.54
2:B:377:SER:C	4:B:901:PLP:H2A2	2.27	0.54
1:A:3:ARG:NH1	1:A:89:ARG:CZ	2.71	0.54
1:A:164:ARG:CZ	1:A:164:ARG:HB2	2.37	0.54
2:B:285:PRO:O	2:B:286:MET:HG2	2.07	0.54
2:B:336:PHE:CD2	2:B:387:VAL:HG11	2.43	0.54
2:B:372:LEU:HD23	2:B:372:LEU:O	2.08	0.54
2:B:165:THR:HG23	2:B:168:ASP:H	1.73	0.54
2:B:213:LYS:O	2:B:217:LEU:HD22	2.08	0.54
1:A:71:ALA:O	1:A:74:ALA:N	2.40	0.54
2:B:175:ARG:O	2:B:178:SER:HB3	2.07	0.54
2:B:209:GLY:HA2	2:B:240:MET:CE	2.37	0.54
1:A:197:ILE:O	1:A:201:LYS:HG3	2.08	0.53
2:B:346:ILE:CD1	2:B:384:ILE:HD11	2.38	0.53
1:A:40:LEU:HD21	1:A:255:LEU:HD22	1.90	0.53
1:A:53:PRO:HA	1:A:68:ASN:OD1	2.08	0.53
2:B:339:LEU:HD23	2:B:347:PRO:HG3	1.89	0.53
1:A:252:LEU:HD13	1:A:252:LEU:N	2.22	0.53
2:B:59:LEU:HD23	2:B:75:LEU:O	2.09	0.53
1:A:87:LEU:O	1:A:90:GLU:HB2	2.08	0.53
1:A:238:VAL:HA	1:A:241:ILE:HD12	1.90	0.53
2:B:270:PRO:HB3	2:B:287:MET:HG2	1.90	0.53
2:B:145:ASN:O	2:B:149:MET:N	2.33	0.53
2:B:242:ALA:HA	2:B:245:ILE:CD1	2.38	0.53
1:A:12:ASN:ND2	1:A:13:ASP:N	2.57	0.52
2:B:77:ARG:HB3	2:B:80:LEU:HG	1.89	0.52
1:A:252:LEU:N	1:A:252:LEU:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:PHE:HE1	2:B:347:PRO:O	1.93	0.52
1:A:1:MET:SD	1:A:171:ARG:HG2	2.48	0.52
2:B:4:LEU:HD12	2:B:29:GLU:OE1	2.09	0.52
1:A:255:LEU:O	1:A:259:VAL:HG23	2.08	0.52
1:A:99:LEU:HB3	1:A:126:VAL:HG22	1.92	0.52
1:A:140:ARG:CD	1:A:169:TYR:HB3	2.29	0.52
1:A:173:TYR:CD1	1:A:173:TYR:C	2.82	0.52
1:A:223:ALA:O	1:A:226:ALA:HB3	2.10	0.52
2:B:288:GLN:HA	2:B:295:GLU:HG3	1.91	0.52
1:A:197:ILE:CG2	1:A:201:LYS:HE2	2.39	0.52
2:B:107:ILE:HG13	2:B:185:HIS:O	2.09	0.52
2:B:202:ARG:HG2	2:B:203:GLU:OE1	2.10	0.52
2:B:298:TYR:CG	2:B:299:SER:N	2.77	0.52
2:B:136:ALA:O	2:B:138:ASP:N	2.44	0.51
1:A:66:ASN:HD22	1:A:66:ASN:N	1.93	0.51
1:A:128:VAL:HG11	1:A:131:VAL:CG2	2.41	0.51
1:A:237:ILE:HG13	1:A:238:VAL:N	2.16	0.51
2:B:144:PRO:C	2:B:145:ASN:HD22	2.10	0.51
2:B:186:TYR:HB3	2:B:197:TYR:OH	2.11	0.51
1:A:3:ARG:NH1	1:A:93:PRO:O	2.43	0.51
1:A:11:LEU:HD23	1:A:18:ALA:HB2	1.93	0.51
1:A:30:ILE:CG2	1:A:31:GLU:H	2.20	0.51
2:B:131:ARG:HH21	2:B:176:ASP:CG	2.14	0.51
2:B:188:LEU:HG	2:B:197:TYR:CE2	2.46	0.51
2:B:228:ILE:N	2:B:228:ILE:HD12	2.26	0.51
1:A:47:ALA:O	1:A:48:LEU:HD23	2.10	0.51
1:A:267:ARG:O	1:A:268:ALA:CB	2.59	0.51
2:B:66:THR:HG21	2:B:73:LEU:H	1.75	0.51
2:B:286:MET:HE3	2:B:294:ILE:HD12	1.93	0.50
1:A:11:LEU:HD21	1:A:18:ALA:HB2	1.91	0.50
1:A:239:LYS:O	1:A:243:LYS:HG3	2.11	0.50
2:B:144:PRO:O	2:B:148:ARG:HB2	2.11	0.50
1:A:64:ILE:O	1:A:67:ALA:HB3	2.11	0.50
2:B:55:ARG:NH2	2:B:78:GLU:OE1	2.37	0.50
1:A:233:SER:OG	1:A:236:ALA:HB3	2.12	0.50
2:B:204:PHE:C	2:B:207:MET:CE	2.80	0.50
1:A:89:ARG:NH1	1:A:92:HIS:O	2.43	0.49
2:B:71:THR:O	2:B:71:THR:HG23	2.12	0.49
2:B:228:ILE:HD12	2:B:228:ILE:H	1.77	0.49
1:A:252:LEU:HD13	1:A:252:LEU:H	1.77	0.49
2:B:134:MET:HE3	2:B:138:ASP:CB	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HB3	1:A:109:ASN:ND2	2.28	0.49
2:B:372:LEU:CD2	2:B:372:LEU:N	2.73	0.49
2:B:119:SER:HA	2:B:187:MET:CE	2.42	0.49
2:B:123:SER:OG	2:B:130:CYS:HB2	2.11	0.49
2:B:145:ASN:HA	2:B:148:ARG:CB	2.43	0.49
1:A:8:PHE:CD2	1:A:207:PRO:HG2	2.48	0.49
1:A:117:ARG:HH11	1:A:120:GLN:HE22	1.61	0.49
1:A:125:SER:CB	1:A:151:ILE:HD11	2.42	0.49
1:A:133:VAL:HG23	1:A:169:TYR:HD2	1.78	0.49
1:A:197:ILE:HG22	1:A:201:LYS:HE2	1.95	0.49
2:B:130:CYS:SG	2:B:132:ILE:HD11	2.52	0.49
2:B:234:GLY:O	2:B:313:HIS:HE1	1.96	0.49
2:B:346:ILE:O	2:B:346:ILE:CG2	2.59	0.49
1:A:23:VAL:CG2	1:A:237:ILE:HD11	2.43	0.48
1:A:108:ASN:ND2	2:B:275:ARG:NH1	2.60	0.48
2:B:25:LEU:HD12	2:B:196:PRO:CD	2.43	0.48
2:B:110:THR:HG21	2:B:113:GLY:HA2	1.95	0.48
1:A:52:VAL:HB	1:A:101:MET:CE	2.25	0.48
1:A:136:SER:O	1:A:137:ALA:C	2.52	0.48
2:B:191:ALA:CB	2:B:201:VAL:HG21	2.43	0.48
2:B:71:THR:CB	2:B:370:GLN:HG3	2.44	0.48
2:B:197:TYR:CB	2:B:198:PRO:HD3	2.44	0.48
2:B:147:PHE:O	2:B:151:LEU:HB2	2.14	0.48
2:B:262:ILE:HG21	2:B:273:HIS:ND1	2.29	0.48
2:B:357:HIS:CD2	2:B:361:MET:CE	2.97	0.48
1:A:128:VAL:HG11	1:A:131:VAL:HG23	1.95	0.48
2:B:234:GLY:HA3	2:B:313:HIS:CE1	2.48	0.48
1:A:244:ASN:HB2	1:A:251:MET:HB2	1.96	0.48
1:A:52:VAL:CG2	1:A:101:MET:HE1	2.43	0.48
1:A:82:PHE:CE1	1:A:117:ARG:HG3	2.49	0.48
2:B:24:ALA:O	2:B:27:GLN:HG2	2.13	0.48
2:B:194:PRO:HB3	2:B:281:GLY:O	2.13	0.48
2:B:357:HIS:CD2	2:B:361:MET:HE2	2.50	0.47
1:A:66:ASN:ND2	1:A:66:ASN:N	2.47	0.47
1:A:92:HIS:HB3	1:A:95:ILE:HG22	1.96	0.47
1:A:41:ILE:HG22	1:A:42:ASP:N	2.29	0.47
2:B:105:GLU:HG3	2:B:184:ALA:CB	2.44	0.47
2:B:372:LEU:HD22	2:B:372:LEU:N	2.13	0.47
2:B:341:ARG:HE	2:B:341:ARG:HB3	1.45	0.47
2:B:236:ASN:HB3	4:B:901:PLP:O1P	2.15	0.47
2:B:255:VAL:HG22	2:B:325:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:GLY:HA3	2:B:149:MET:SD	2.54	0.47
1:A:156:PRO:C	1:A:158:ALA:H	2.18	0.47
1:A:165:GLN:HG2	1:A:169:TYR:CE2	2.50	0.47
2:B:272:LYS:C	2:B:273:HIS:CD2	2.88	0.47
2:B:313:HIS:CD2	2:B:324:TYR:OH	2.68	0.47
2:B:300:ILE:HG23	2:B:329:ASP:OD2	2.14	0.47
1:A:72:PHE:C	1:A:74:ALA:N	2.68	0.46
2:B:130:CYS:SG	2:B:132:ILE:CD1	3.03	0.46
1:A:12:ASN:C	1:A:14:ARG:N	2.68	0.46
1:A:125:SER:OG	1:A:151:ILE:HD11	2.14	0.46
2:B:44:GLN:HG2	2:B:44:GLN:H	1.38	0.46
2:B:105:GLU:C	2:B:106:ILE:HD13	2.34	0.46
2:B:109:GLU:HB2	2:B:133:TYR:HB2	1.96	0.46
1:A:127:LEU:HD11	1:A:153:ILE:HG13	1.97	0.46
1:A:156:PRO:O	1:A:158:ALA:N	2.44	0.46
2:B:190:THR:OG1	2:B:191:ALA:N	2.47	0.46
2:B:204:PHE:C	2:B:207:MET:HE1	2.36	0.46
2:B:137:LYS:NZ	2:B:302:ALA:HB1	2.30	0.46
2:B:220:GLU:O	2:B:222:ARG:N	2.48	0.46
2:B:386:THR:C	2:B:388:HIS:N	2.69	0.46
2:B:213:LYS:CG	2:B:244:PHE:CE1	2.98	0.46
1:A:167:ALA:HB2	1:A:205:ALA:HB2	1.97	0.46
1:A:237:ILE:O	1:A:241:ILE:HG13	2.15	0.46
2:B:36:GLN:HA	2:B:36:GLN:NE2	2.29	0.46
2:B:55:ARG:NH1	2:B:211:GLU:OE2	2.49	0.46
2:B:222:ARG:HD2	2:B:223:LEU:O	2.15	0.46
1:A:52:VAL:HG23	1:A:101:MET:HE1	1.98	0.45
1:A:72:PHE:O	1:A:74:ALA:N	2.49	0.45
1:A:216:SER:O	1:A:219:GLN:HG2	2.16	0.45
2:B:287:MET:O	2:B:295:GLU:N	2.39	0.45
2:B:313:HIS:HD2	2:B:324:TYR:OH	1.99	0.45
1:A:153:ILE:HA	1:A:175:TYR:HB3	1.99	0.45
1:A:219:GLN:HG2	1:A:219:GLN:H	1.39	0.45
2:B:22:MET:N	2:B:23:PRO:CD	2.79	0.45
2:B:55:ARG:NH1	2:B:211:GLU:CD	2.69	0.45
2:B:317:ASN:HB2	2:B:324:TYR:CD1	2.51	0.45
2:B:220:GLU:O	2:B:221:GLY:C	2.53	0.45
1:A:22:PHE:CG	1:A:23:VAL:N	2.85	0.45
1:A:127:LEU:HB2	1:A:151:ILE:HB	1.98	0.45
1:A:128:VAL:CG1	1:A:131:VAL:CG2	2.94	0.45
2:B:94:GLN:OE1	2:B:187:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:HD21	2:B:125:LEU:CD2	2.45	0.45
2:B:275:ARG:NH2	2:B:289:THR:O	2.50	0.45
2:B:352:SER:O	2:B:353:HIS:C	2.55	0.45
1:A:155:PRO:HB2	2:B:20:ILE:HD12	1.97	0.45
1:A:2:GLU:O	1:A:2:GLU:HG2	2.14	0.45
2:B:91:VAL:HG21	2:B:118:ALA:HB1	1.99	0.45
1:A:80:GLN:O	1:A:84:MET:HG3	2.17	0.45
1:A:258:PHE:O	1:A:262:MET:HG2	2.17	0.45
2:B:385:PHE:O	2:B:388:HIS:HB3	2.16	0.45
1:A:108:ASN:HD21	2:B:275:ARG:NH1	2.10	0.45
2:B:61:LYS:O	2:B:61:LYS:CD	2.65	0.44
2:B:96:LEU:CD1	2:B:126:LEU:HD21	2.46	0.44
2:B:226:ALA:HB1	2:B:253:ILE:HD12	1.99	0.44
2:B:310:GLY:O	2:B:313:HIS:HB2	2.18	0.44
1:A:125:SER:HB2	1:A:151:ILE:CD1	2.48	0.44
1:A:133:VAL:CG2	1:A:169:TYR:HD2	2.31	0.44
1:A:161:ASP:N	1:A:161:ASP:OD1	2.50	0.44
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.81	0.44
2:B:86:HIS:CD2	2:B:236:ASN:HB2	2.52	0.44
2:B:242:ALA:O	2:B:245:ILE:HD12	2.16	0.44
1:A:219:GLN:O	1:A:222:ALA:HB3	2.17	0.44
2:B:121:LEU:HD12	2:B:122:ALA:N	2.33	0.44
2:B:234:GLY:CA	2:B:313:HIS:HE1	2.31	0.44
2:B:94:GLN:OE1	2:B:187:MET:HA	2.18	0.44
2:B:150:ARG:O	2:B:153:GLY:N	2.47	0.44
1:A:27:ASP:HA	1:A:71:ALA:HB2	1.98	0.44
2:B:21:LEU:HD23	2:B:174:LEU:HD13	1.99	0.44
2:B:59:LEU:HB2	2:B:215:GLN:NE2	2.32	0.44
2:B:289:THR:HG23	2:B:293:GLN:O	2.18	0.44
2:B:362:MET:HG3	2:B:363:ARG:N	2.33	0.44
1:A:16:GLU:CB	1:A:267:ARG:HA	2.47	0.44
2:B:95:ALA:CB	2:B:126:LEU:HD23	2.48	0.44
2:B:188:LEU:HD11	2:B:193:GLY:HA3	2.00	0.44
1:A:263:LYS:HE3	1:A:267:ARG:HH21	1.82	0.44
2:B:126:LEU:HD12	2:B:126:LEU:HA	1.74	0.43
1:A:29:GLY:HA2	1:A:74:ALA:CB	2.48	0.43
2:B:16:TYR:CE2	2:B:278:ILE:HD13	2.52	0.43
2:B:336:PHE:CE1	2:B:347:PRO:O	2.69	0.43
1:A:52:VAL:CG2	1:A:101:MET:CE	2.96	0.43
1:A:217:PRO:HB3	1:A:265:ALA:HB2	2.00	0.43
2:B:138:ASP:OD1	2:B:138:ASP:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:VAL:HG13	2:B:156:VAL:HG21	2.00	0.43
2:B:166:LEU:O	2:B:170:CYS:N	2.47	0.43
2:B:270:PRO:CA	2:B:287:MET:HE3	2.49	0.43
2:B:327:ILE:HG22	2:B:353:HIS:CD2	2.53	0.43
1:A:216:SER:O	1:A:219:GLN:CG	2.66	0.43
2:B:109:GLU:HG2	2:B:110:THR:N	2.32	0.43
1:A:130:ASP:OD1	1:A:130:ASP:N	2.41	0.43
2:B:180:SER:O	2:B:182:GLU:N	2.51	0.43
2:B:234:GLY:CA	2:B:313:HIS:CE1	3.01	0.43
2:B:132:ILE:H	2:B:132:ILE:HG12	1.71	0.43
2:B:384:ILE:HG22	2:B:385:PHE:N	2.32	0.43
2:B:166:LEU:O	2:B:169:ALA:N	2.52	0.43
1:A:107:PHE:O	1:A:108:ASN:C	2.56	0.42
2:B:216:ILE:HG22	2:B:217:LEU:N	2.34	0.42
2:B:27:GLN:CG	2:B:28:LEU:N	2.82	0.42
2:B:66:THR:HB	2:B:71:THR:O	2.19	0.42
2:B:90:GLN:HE21	2:B:90:GLN:HB3	1.57	0.42
1:A:197:ILE:CD1	1:A:228:ALA:N	2.82	0.42
2:B:123:SER:O	2:B:127:GLY:N	2.53	0.42
2:B:191:ALA:CB	2:B:201:VAL:CG2	2.97	0.42
2:B:99:LYS:HD2	2:B:99:LYS:HA	1.80	0.42
2:B:177:TRP:O	2:B:178:SER:C	2.58	0.42
2:B:376:LEU:HD12	2:B:376:LEU:HA	1.92	0.42
1:A:19:PHE:HE2	1:A:259:VAL:HG13	1.83	0.42
1:A:214:ILE:HG12	1:A:231:ALA:HB1	2.02	0.42
2:B:5:LEU:O	2:B:7:PRO:HD3	2.20	0.42
2:B:37:LYS:HE3	2:B:37:LYS:HB2	1.90	0.42
2:B:176:ASP:OD1	2:B:176:ASP:C	2.58	0.42
2:B:351:SER:HB3	2:B:376:LEU:HD12	2.01	0.42
2:B:365:GLN:NE2	2:B:368:LYS:HZ2	2.18	0.42
2:B:386:THR:O	2:B:388:HIS:N	2.52	0.42
1:A:82:PHE:CD1	1:A:121:VAL:HG21	2.55	0.42
1:A:155:PRO:O	1:A:158:ALA:HB2	2.19	0.42
1:A:22:PHE:HD2	1:A:49:GLU:CG	2.29	0.42
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.75	0.42
1:A:206:ALA:O	1:A:207:PRO:C	2.57	0.42
2:B:227:VAL:CG1	2:B:240:MET:HG2	2.50	0.42
2:B:374:VAL:HG23	2:B:375:ASN:N	2.35	0.42
1:A:22:PHE:CA	1:A:49:GLU:HB3	2.47	0.42
2:B:55:ARG:HH11	2:B:55:ARG:HG2	1.82	0.42
2:B:270:PRO:CA	2:B:287:MET:CE	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:C	1:A:101:MET:HG2	2.39	0.42
2:B:95:ALA:HB1	2:B:126:LEU:HD23	2.02	0.42
2:B:181:TYR:HA	2:B:184:ALA:O	2.20	0.41
1:A:141:GLN:HB2	1:A:145:ARG:NH2	2.35	0.41
2:B:62:CYS:SG	2:B:65:ILE:HD11	2.60	0.41
2:B:79:ASP:HB2	2:B:379:ARG:HG2	2.01	0.41
2:B:271:LEU:HD13	2:B:271:LEU:C	2.40	0.41
1:A:252:LEU:HA	1:A:255:LEU:HD12	2.02	0.41
2:B:62:CYS:SG	2:B:75:LEU:HD22	2.60	0.41
2:B:298:TYR:CD2	2:B:299:SER:N	2.88	0.41
1:A:104:ASN:HD21	2:B:288:GLN:HE22	1.66	0.41
1:A:104:ASN:HD22	2:B:278:ILE:H	1.67	0.41
1:A:106:VAL:HB	1:A:114:PHE:CD2	2.54	0.41
2:B:91:VAL:HG12	2:B:122:ALA:HB2	2.02	0.41
1:A:239:LYS:HE2	1:A:243:LYS:HD2	2.03	0.41
2:B:60:THR:OG1	2:B:77:ARG:HD3	2.20	0.41
2:B:195:HIS:CG	2:B:196:PRO:HA	2.55	0.41
2:B:316:LEU:HD23	2:B:316:LEU:HA	1.91	0.41
1:A:39:THR:HA	1:A:42:ASP:OD1	2.20	0.41
2:B:191:ALA:HB2	2:B:201:VAL:CG2	2.50	0.41
1:A:248:PRO:O	1:A:252:LEU:HD22	2.21	0.41
2:B:55:ARG:NH2	2:B:78:GLU:CD	2.74	0.41
2:B:204:PHE:C	2:B:207:MET:HE3	2.41	0.41
2:B:212:THR:CB	2:B:240:MET:HE3	2.51	0.41
2:B:368:LYS:HZ2	2:B:368:LYS:HG2	1.63	0.41
1:A:36:ILE:O	1:A:40:LEU:HG	2.21	0.41
1:A:163:LEU:HD13	1:A:200:LEU:CD2	2.49	0.41
2:B:372:LEU:HD23	2:B:372:LEU:C	2.42	0.41
2:B:62:CYS:HB3	2:B:65:ILE:HD11	2.03	0.41
2:B:87:LYS:NZ	4:B:901:PLP:O3	2.53	0.41
2:B:346:ILE:HD13	2:B:384:ILE:CD1	2.46	0.41
1:A:103:ALA:CB	2:B:278:ILE:HG21	2.51	0.40
1:A:160:ASP:OD1	1:A:203:TYR:OH	2.35	0.40
2:B:21:LEU:CD2	2:B:174:LEU:HD13	2.51	0.40
2:B:325:VAL:HG11	2:B:357:HIS:CE1	2.56	0.40
1:A:116:ALA:HA	1:A:146:HIS:ND1	2.37	0.40
2:B:333:LEU:HD23	2:B:333:LEU:HA	1.83	0.40
1:A:65:GLN:C	1:A:69:LEU:HD22	2.42	0.40
1:A:146:HIS:CD2	1:A:146:HIS:N	2.90	0.40
1:A:171:ARG:HE	1:A:171:ARG:HB2	1.48	0.40
1:A:14:ARG:O	1:A:15:ARG:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:CZ	1:A:15:ARG:HB2	2.47	0.40
1:A:19:PHE:HE1	1:A:233:SER:HB2	1.86	0.40
2:B:241:PHE:O	2:B:242:ALA:C	2.60	0.40
1:A:163:LEU:HD22	1:A:163:LEU:HA	1.78	0.40
2:B:59:LEU:HD12	2:B:215:GLN:HB3	2.03	0.40
2:B:387:VAL:O	2:B:387:VAL:HG12	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	A	227/268 (85%)	187 (82%)	31 (14%)	9 (4%)	3	14
2	B	369/396 (93%)	319 (86%)	42 (11%)	8 (2%)	6	25
All	All	596/664 (90%)	506 (85%)	73 (12%)	17 (3%)	4	20

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	108	ASN
2	B	180	SER
2	B	242	ALA
2	B	275	ARG
1	A	73	ALA
1	A	234	GLY
2	B	181	TYR
1	A	267	ARG
1	A	207	PRO
2	B	137	LYS
2	B	221	GLY

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Mol	Chain	Res	Type
1	A	27	ASP
1	A	157	ASN
2	B	176	ASP
1	A	29	GLY
2	B	88	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	184/208 (88%)	127 (69%)	57 (31%)	0 0
2	B	293/310 (94%)	213 (73%)	80 (27%)	0 1
All	All	477/518 (92%)	340 (71%)	137 (29%)	0 1

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	5	GLU
1	A	10	GLN
1	A	12	ASN
1	A	15	ARG
1	A	23	VAL
1	A	25	LEU
1	A	32	GLN
1	A	33	SER
1	A	35	LYS
1	A	36	ILE
1	A	42	ASP
1	A	48	LEU
1	A	64	ILE
1	A	66	ASN
1	A	69	LEU
1	A	70	ARG

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Mol	Chain	Res	Type
1	A	76	VAL
1	A	77	THR
1	A	80	GLN
1	A	87	LEU
1	A	91	LYS
1	A	94	THR
1	A	100	LEU
1	A	101	MET
1	A	105	LEU
1	A	106	VAL
1	A	109	ASN
1	A	120	GLN
1	A	121	VAL
1	A	127	LEU
1	A	130	ASP
1	A	141	GLN
1	A	144	LEU
1	A	159	ASP
1	A	161	ASP
1	A	162	LEU
1	A	163	LEU
1	A	164	ARG
1	A	165	GLN
1	A	171	ARG
1	A	197	ILE
1	A	198	GLU
1	A	209	LEU
1	A	215	SER
1	A	218	GLU
1	A	219	GLN
1	A	237	ILE
1	A	239	LYS
1	A	240	ILE
1	A	242	GLU
1	A	252	LEU
1	A	254	GLU
1	A	257	SER
1	A	263	LYS
1	A	267	ARG
2	B	5	LEU
2	B	15	MET
2	B	21	LEU

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Mol	Chain	Res	Type
2	B	25	LEU
2	B	27	GLN
2	B	30	GLU
2	B	36	GLN
2	B	44	GLN
2	B	48	LEU
2	B	49	LEU
2	B	50	LYS
2	B	55	ARG
2	B	57	THR
2	B	59	LEU
2	B	61	LYS
2	B	63	GLN
2	B	65	ILE
2	B	70	ARG
2	B	73	LEU
2	B	75	LEU
2	B	78	GLU
2	B	88	THR
2	B	90	GLN
2	B	94	GLN
2	B	99	LYS
2	B	105	GLU
2	B	106	ILE
2	B	107	ILE
2	B	109	GLU
2	B	114	GLN
2	B	121	LEU
2	B	126	LEU
2	B	132	ILE
2	B	134	MET
2	B	137	LYS
2	B	138	ASP
2	B	145	ASN
2	B	148	ARG
2	B	151	LEU
2	B	155	GLU
2	B	167	LYS
2	B	174	LEU
2	B	178	SER
2	B	182	GLU
2	B	188	LEU

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Mol	Chain	Res	Type
2	B	203	GLU
2	B	207	MET
2	B	213	LYS
2	B	216	ILE
2	B	217	LEU
2	B	222	ARG
2	B	235	SER
2	B	236	ASN
2	B	243	ASP
2	B	248	THR
2	B	249	SER
2	B	250	VAL
2	B	252	LEU
2	B	263	GLU
2	B	271	LEU
2	B	283	LYS
2	B	286	MET
2	B	296	GLU
2	B	297	SER
2	B	304	LEU
2	B	308	SER
2	B	317	ASN
2	B	326	SER
2	B	327	ILE
2	B	331	GLU
2	B	341	ARG
2	B	359	LEU
2	B	367	GLU
2	B	368	LYS
2	B	372	LEU
2	B	373	VAL
2	B	379	ARG
2	B	382	LYS
2	B	384	ILE
2	B	385	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	12	ASN
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	66	ASN
1	A	80	GLN
1	A	92	HIS
1	A	104	ASN
1	A	108	ASN
1	A	109	ASN
1	A	120	GLN
1	A	157	ASN
1	A	219	GLN
1	A	244	ASN
2	B	26	ASN
2	B	36	GLN
2	B	42	GLN
2	B	64	ASN
2	B	82	HIS
2	B	90	GLN
2	B	94	GLN
2	B	115	HIS
2	B	145	ASN
2	B	171	ASN
2	B	195	HIS
2	B	215	GLN
2	B	267	HIS
2	B	273	HIS
2	B	288	GLN
2	B	313	HIS
2	B	357	HIS
2	B	365	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PLP	B	901	2	15,15,16	1.67	3 (20%)	20,22,23	1.20	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	B	901	2	-	3/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	PLP	C3-C2	-3.57	1.37	1.40
4	B	901	PLP	C5-C4	-2.32	1.37	1.40
4	B	901	PLP	C4A-C4	2.18	1.56	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	901	PLP	C5-C6-N1	-2.25	120.07	123.82
4	B	901	PLP	C6-C5-C4	2.22	119.91	118.16
4	B	901	PLP	O3P-P-O2P	2.05	115.47	107.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	PLP	C5A-O4P-P-O1P
4	B	901	PLP	C5A-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
4	B	901	PLP	C5A-O4P-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	PLP	3	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.