Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:03 PM GMT

PDB ID	:	1DTY
Title	:	CRYSTAL STRUCTURE OF ADENOSYLMETHIONINE-8-AMINO-7-OXONANOATE AMINOTRANSFERASE WITH PYRIDOXAL PHOSPHATE COFACTOR.
Authors	:	Alexeev, D.; Sawyer, L.; Baxter, R.L.; Alexeeva, M.V.; Campopiano, D.
Deposited on	:	2000-01-13
Resolution	:	2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

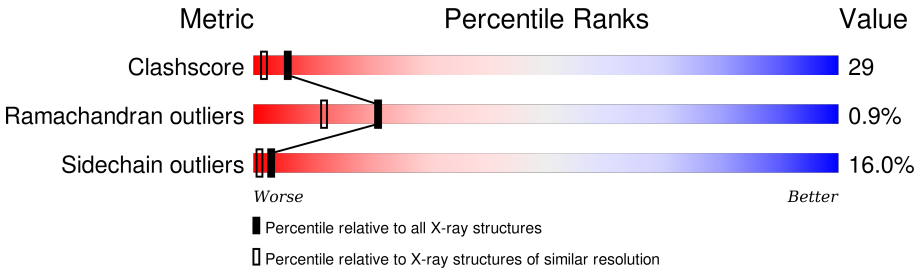
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.14 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))
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	429	44% 48% 7%
1	B	429	51% 41% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7006 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.

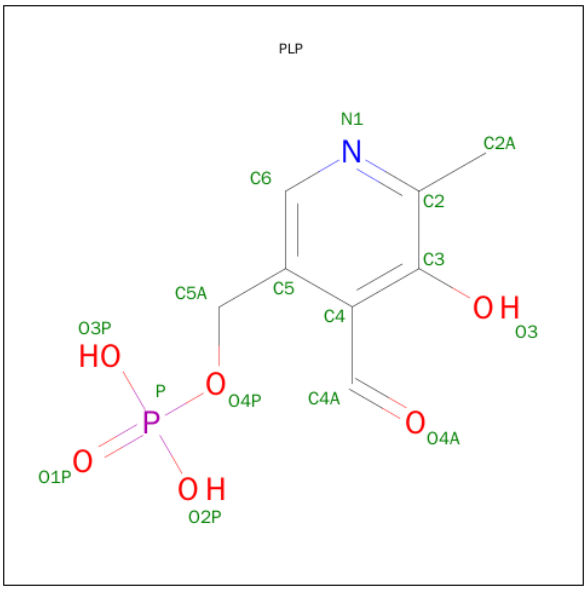
- Molecule 1 is a protein called ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3319	2104	573	610	32			
1	B	429	Total	C	N	O	S	0	0	0
			3319	2104	573	610	32			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		
4	B	169	Total	O	0	0
			169	169		

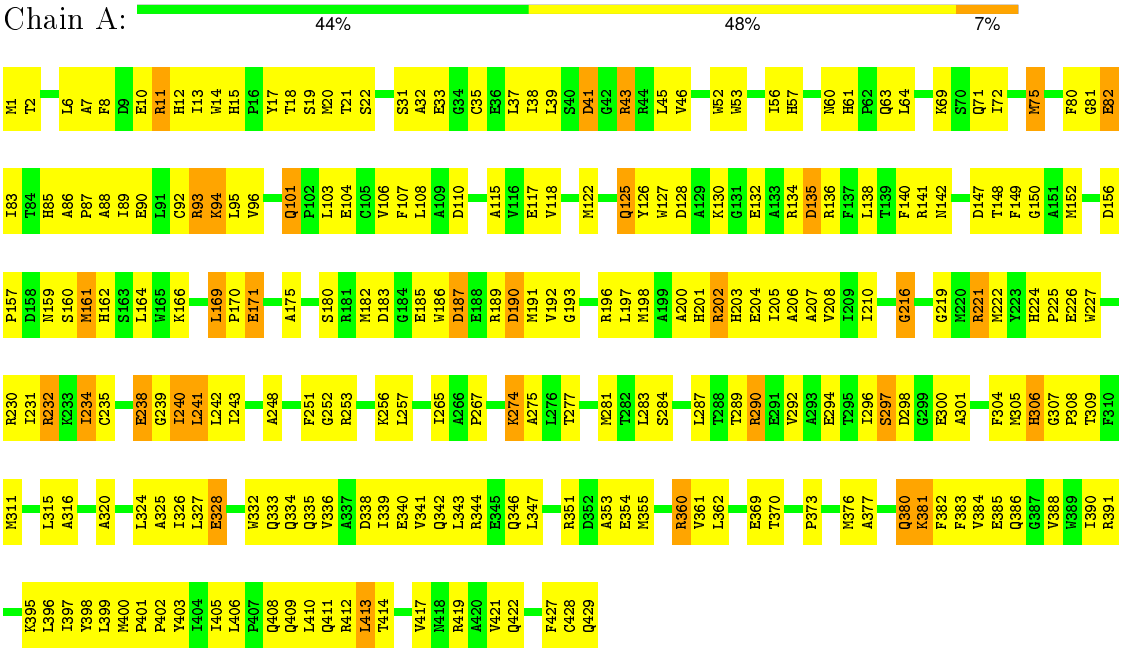
3 Residue-property plots (i)

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

Note EDS was not executed.

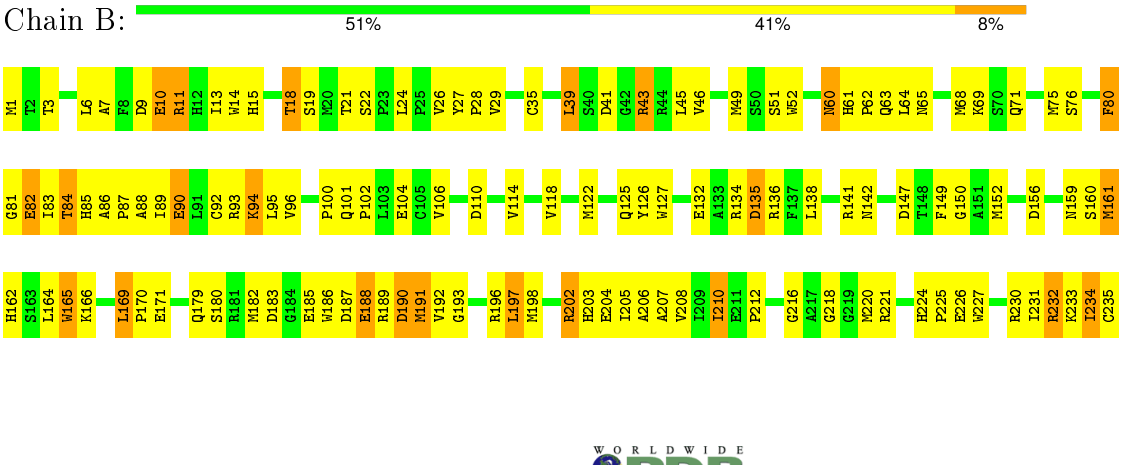
• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE

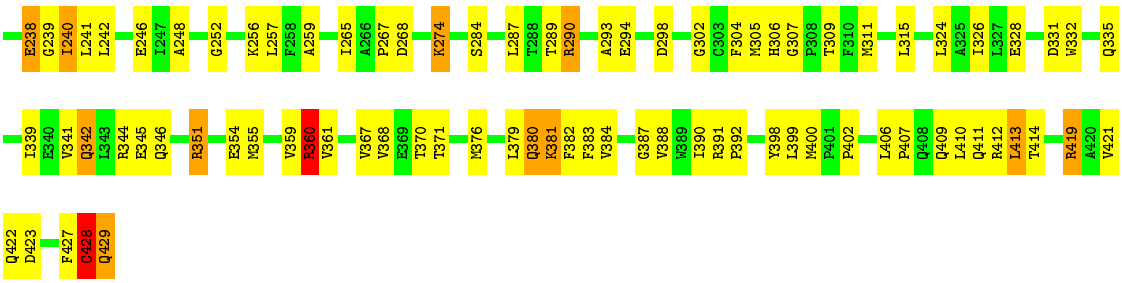
Chain A:



• Molecule 1: ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE

Chain B:




E238
G239
I240
L241
L242
E246
I247
A248
G252
K256
L257
F258
A259
I265
A266
P267
D268
K274
S284
L287
T288
T289
R290
A293
E294
D298
G302
C303
F304
M305
H306
G307
P308
T309
F310
M311
L315
L324
A325
I326
L327
E328
D331
W332
Q335
I339
E340
V341
Q342
L343
R344
E345
Q346
R351
E354
M355
V359
R360
V361
V367
V368
E369
T370
T371
M376
L379
Q380
K381
F382
F383
V384
G387
V388
W389
I390
R391
P392
Y398
L399
M400
P401
P402
L406
P407
Q408
Q409
L410
Q411
R412
L413
T414
R419
A420
V421
Q422
D423
F427
C428
Q429

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.28Å 56.27Å 121.93Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	10.00 – 2.14	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.14)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.196 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7006	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: NA, PLP

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	0.30	0/3399	0.79	1/4615 (0.0%)
1	B	0.30	0/3399	0.80	2/4615 (0.0%)
All	All	0.30	0/6798	0.79	3/9230 (0.0%)

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	B	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	428	CYS	CA-C-N	-7.10	101.59	117.20
1	A	82	GLU	C-N-CA	5.45	135.31	121.70
1	B	360	ARG	NE-CZ-NH1	5.31	122.96	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	428	CYS	Mainchain,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	A	3319	0	3253	209	0
1	B	3319	0	3255	202	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
4	A	165	0	0	18	0
4	B	169	0	0	17	0
All	All	7006	0	6522	380	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 29.

All (380) 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:B:429:GLN:CD	1:B:429:GLN:O	1.90	1.09
1:B:125:GLN:HE22	1:B:305:MET:H	1.20	0.90
1:B:76:SER:HB2	1:B:315:LEU:HD22	1.56	0.88
1:A:82:GLU:HB3	1:B:26:VAL:HG12	1.54	0.88
1:B:134:ARG:HH12	1:B:240:ILE:HG22	1.39	0.86
1:A:106:VAL:HG22	1:A:287:LEU:HG	1.61	0.83
1:B:428:CYS:O	1:B:429:GLN:HB3	1.80	0.81
1:B:406:LEU:H	1:B:409:GLN:HE21	1.27	0.79
1:A:238:GLU:HB3	1:A:240:ILE:HG23	1.63	0.79
1:B:46:VAL:HG22	1:B:388:VAL:HG12	1.65	0.79
1:B:429:GLN:OE1	1:B:429:GLN:O	2.00	0.78
1:B:248:ALA:HB2	3:B:450:PLP:O3	1.83	0.78
1:A:399:LEU:HD13	1:A:413:LEU:HB3	1.65	0.77
1:B:346:GLN:OE1	1:B:414:THR:HG21	1.84	0.77
1:B:252:GLY:HA2	1:B:256:LYS:O	1.85	0.76
1:B:179:GLN:HB2	1:B:190:ASP:OD2	1.86	0.76
1:B:39:LEU:HD12	1:B:43:ARG:HB3	1.66	0.75
1:B:406:LEU:H	1:B:409:GLN:NE2	1.86	0.74
1:A:21:THR:HG22	1:B:294:GLU:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:NH1	1:B:240:ILE:HG22	2.03	0.73
1:B:198:MET:SD	1:B:234:ILE:HD11	2.28	0.73
1:A:93:ARG:HD3	4:A:1109:HOH:O	1.88	0.73
1:A:227:TRP:O	1:A:231:ILE:HG13	1.89	0.73
1:A:11:ARG:HD3	4:A:1164:HOH:O	1.89	0.73
1:A:274:LYS:HE3	1:B:309:THR:OG1	1.89	0.72
1:A:169:LEU:HD12	1:A:170:PRO:HD2	1.71	0.72
1:A:346:GLN:OE1	1:A:414:THR:HG21	1.89	0.72
1:A:309:THR:OG1	1:B:274:LYS:HE3	1.89	0.72
1:A:206:ALA:O	1:A:241:LEU:HG	1.88	0.72
1:B:210:ILE:HD12	1:B:231:ILE:HD12	1.70	0.72
1:A:376:MET:O	1:A:380:GLN:HB3	1.89	0.71
1:B:429:GLN:CG	1:B:429:GLN:O	2.37	0.71
1:A:52:TRP:HA	1:A:400:MET:HE1	1.72	0.71
1:A:198:MET:SD	1:A:234:ILE:HD11	2.31	0.70
1:A:324:LEU:O	1:A:328:GLU:HG2	1.91	0.70
1:A:248:ALA:HB2	3:A:450:PLP:O3	1.92	0.68
1:A:192:VAL:O	1:A:196:ARG:HG2	1.94	0.68
1:A:56:ILE:HD13	1:A:275:ALA:HB1	1.74	0.68
1:A:207:ALA:HA	1:A:240:ILE:HD12	1.75	0.68
1:A:115:ALA:HB2	1:A:284:SER:OG	1.94	0.68
1:A:343:LEU:O	1:A:347:LEU:HB2	1.93	0.68
1:A:221:ARG:HA	1:A:360:ARG:HH21	1.58	0.68
1:A:370:THR:HG21	1:A:427:PHE:HE2	1.59	0.67
1:B:63:GLN:OE1	1:B:326:ILE:HG12	1.94	0.67
1:B:7:ALA:HA	1:B:10:GLU:OE1	1.94	0.67
1:A:150:GLY:HA3	1:B:149:PHE:HD1	1.60	0.67
1:B:341:VAL:O	1:B:345:GLU:HB2	1.96	0.66
1:B:230:ARG:O	1:B:234:ILE:HG22	1.96	0.65
1:A:224:HIS:HD2	1:A:226:GLU:H	1.44	0.65
1:B:64:LEU:O	1:B:68:MET:HG3	1.97	0.65
1:A:290:ARG:O	1:A:290:ARG:HG3	1.96	0.65
1:B:169:LEU:HD13	1:B:170:PRO:HD2	1.79	0.65
1:A:15:HIS:HB3	1:B:82:GLU:OE2	1.96	0.65
1:A:85:HIS:HD2	1:A:88:ALA:H	1.44	0.65
1:A:397:ILE:HG21	1:A:417:VAL:HG13	1.79	0.64
1:B:224:HIS:HD2	1:B:226:GLU:H	1.44	0.64
1:A:308:PRO:HD2	1:A:311:MET:HB2	1.80	0.64
1:B:52:TRP:HA	1:B:400:MET:HE1	1.80	0.64
1:A:39:LEU:HD11	1:A:45:LEU:HD11	1.81	0.63
1:A:148:THR:O	1:A:152:MET:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HD13	1:A:399:LEU:HD21	1.81	0.63
1:A:85:HIS:CD2	1:A:88:ALA:H	2.16	0.63
1:B:90:GLU:HB3	4:B:1097:HOH:O	1.98	0.63
1:B:242:LEU:HD12	1:B:267:PRO:HA	1.81	0.62
1:A:298:ASP:OD1	1:B:21:THR:HG21	1.99	0.62
1:B:376:MET:O	1:B:380:GLN:HB3	2.00	0.62
1:B:224:HIS:CD2	1:B:226:GLU:HB2	2.35	0.61
1:B:193:GLY:O	1:B:197:LEU:HD23	2.00	0.61
1:A:382:PHE:HZ	1:A:419:ARG:HD3	1.64	0.61
1:B:161:MET:O	1:B:164:LEU:HB2	2.00	0.61
1:B:344:ARG:HG2	1:B:361:VAL:HB	1.81	0.61
1:B:64:LEU:HB3	4:B:1240:HOH:O	2.01	0.61
1:B:126:TYR:CE2	1:B:241:LEU:HD21	2.34	0.61
1:B:136:ARG:HG3	1:B:204:GLU:HG2	1.83	0.61
1:A:61:HIS:HB3	1:A:64:LEU:HB2	1.83	0.61
1:B:156:ASP:HB3	1:B:159:ASN:HB2	1.82	0.61
1:B:3:THR:HG23	4:B:1248:HOH:O	2.00	0.61
1:A:301:ALA:HB2	1:B:164:LEU:HD11	1.83	0.60
1:A:63:GLN:OE1	1:A:326:ILE:HG12	2.01	0.60
1:A:332:TRP:O	1:A:336:VAL:HG23	2.01	0.60
1:A:283:LEU:HD13	1:A:316:ALA:HB3	1.82	0.60
1:A:43:ARG:HH21	1:A:385:GLU:HA	1.65	0.60
1:A:342:GLN:OE1	1:A:410:LEU:HB3	2.02	0.60
1:A:31:SER:OG	1:A:38:ILE:HD12	2.01	0.60
1:B:198:MET:O	1:B:202:ARG:HB2	2.02	0.59
1:B:52:TRP:HA	1:B:400:MET:CE	2.32	0.59
1:B:205:ILE:CG2	1:B:240:ILE:HD13	2.33	0.59
1:A:413:LEU:O	1:A:417:VAL:HG23	2.03	0.59
1:B:118:VAL:O	1:B:122:MET:HG3	2.02	0.59
1:B:324:LEU:O	1:B:328:GLU:HG3	2.02	0.58
1:A:221:ARG:HA	1:A:360:ARG:NH2	2.16	0.58
1:A:1:MET:HE1	1:B:84:THR:HG23	1.84	0.58
1:A:53:TRP:HE3	1:A:253:ARG:HD3	1.68	0.58
1:B:6:LEU:O	1:B:10:GLU:HG3	2.04	0.58
1:A:398:TYR:O	1:A:399:LEU:HD23	2.03	0.58
1:A:61:HIS:HD2	1:A:63:GLN:H	1.52	0.58
1:A:125:GLN:OE1	1:A:296:ILE:HG23	2.03	0.58
1:A:202:ARG:NH1	1:A:203:HIS:HA	2.18	0.57
1:B:85:HIS:CD2	1:B:88:ALA:H	2.23	0.57
1:A:43:ARG:HH22	1:A:384:VAL:HG12	1.68	0.57
1:A:187:ASP:O	1:A:190:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG12	4:A:1197:HOH:O	2.04	0.57
1:B:370:THR:HG21	1:B:427:PHE:CE2	2.39	0.57
1:A:157:PRO:HA	1:A:162:HIS:CD2	2.39	0.57
1:B:398:TYR:HE2	1:B:400:MET:HE2	1.70	0.57
1:A:19:SER:HB2	1:B:302:GLY:O	2.05	0.57
1:A:39:LEU:HD12	1:A:43:ARG:HB3	1.86	0.57
1:B:331:ASP:N	4:B:1120:HOH:O	2.37	0.57
1:A:383:PHE:CD1	1:A:390:ILE:HB	2.40	0.56
1:A:118:VAL:O	1:A:122:MET:HG3	2.04	0.56
1:B:11:ARG:HG3	1:B:11:ARG:O	2.04	0.56
1:A:140:PHE:CE1	1:A:210:ILE:HD12	2.39	0.56
1:B:370:THR:HG21	1:B:427:PHE:HE2	1.69	0.56
1:B:61:HIS:CD2	1:B:63:GLN:HB2	2.40	0.56
1:B:290:ARG:HD3	4:B:1075:HOH:O	2.06	0.56
1:A:46:VAL:CG2	1:A:388:VAL:HG12	2.35	0.56
1:A:61:HIS:CD2	1:A:63:GLN:HB2	2.41	0.56
1:B:335:GLN:O	1:B:339:ILE:HG13	2.06	0.56
1:A:161:MET:HE2	1:A:164:LEU:HG	1.88	0.56
1:A:43:ARG:NH2	1:A:385:GLU:HA	2.20	0.56
1:B:118:VAL:HG13	1:B:304:PHE:CZ	2.40	0.55
1:B:371:THR:HB	4:B:1321:HOH:O	2.06	0.55
1:A:138:LEU:HB3	1:A:208:VAL:HG22	1.87	0.55
1:A:80:PHE:HB2	1:A:311:MET:O	2.06	0.55
1:B:85:HIS:HD2	1:B:88:ALA:H	1.54	0.55
1:B:160:SER:HB2	1:B:162:HIS:CD2	2.42	0.55
1:B:35:CYS:SG	1:B:402:PRO:HD2	2.47	0.55
1:A:52:TRP:HA	1:A:400:MET:CE	2.35	0.55
1:B:399:LEU:CD1	1:B:413:LEU:HB3	2.37	0.55
1:B:399:LEU:HD11	1:B:413:LEU:HB3	1.89	0.55
1:B:238:GLU:HA	1:B:238:GLU:OE1	2.06	0.55
1:B:187:ASP:OD2	1:B:189:ARG:HB3	2.07	0.55
1:B:76:SER:CB	1:B:315:LEU:HD22	2.35	0.54
1:B:411:GLN:O	1:B:414:THR:HG22	2.07	0.54
1:A:43:ARG:NH2	1:A:384:VAL:HG12	2.22	0.54
1:B:202:ARG:NH1	1:B:203:HIS:HA	2.22	0.54
1:A:230:ARG:O	1:A:234:ILE:HG22	2.08	0.54
1:A:222:MET:SD	1:A:362:LEU:HB2	2.47	0.54
1:A:149:PHE:HD1	1:B:150:GLY:HA3	1.71	0.54
1:B:220:MET:HB3	1:B:367:VAL:HG21	1.89	0.54
1:A:8:PHE:CZ	1:B:93:ARG:HA	2.42	0.54
1:B:234:ILE:O	1:B:238:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TRP:HE1	1:A:230:ARG:NH2	2.05	0.53
1:A:46:VAL:HG22	1:A:388:VAL:HG12	1.89	0.53
1:A:118:VAL:HG13	1:A:304:PHE:CZ	2.43	0.53
1:B:150:GLY:HA2	4:B:1208:HOH:O	2.07	0.53
1:B:187:ASP:O	1:B:190:ASP:HB2	2.07	0.53
1:A:125:GLN:HE22	1:A:305:MET:H	1.55	0.53
1:A:125:GLN:NE2	1:A:305:MET:H	2.07	0.53
1:A:216:GLY:HA3	4:A:1136:HOH:O	2.09	0.53
1:A:419:ARG:HA	1:A:422:GLN:NE2	2.24	0.53
1:B:127:TRP:CE3	1:B:134:ARG:HD2	2.44	0.52
1:A:409:GLN:HG2	4:A:1197:HOH:O	2.10	0.52
1:A:15:HIS:HE1	1:B:83:ILE:O	1.92	0.52
1:B:94:LYS:HE3	1:B:324:LEU:HB2	1.90	0.52
1:A:53:TRP:CE3	1:A:253:ARG:HD3	2.44	0.52
1:B:161:MET:HE2	1:B:164:LEU:HD11	1.91	0.52
1:A:283:LEU:HD13	1:A:316:ALA:CB	2.39	0.52
1:B:381:LYS:HG2	4:B:1039:HOH:O	2.10	0.52
1:A:306:HIS:CE1	1:B:147:ASP:HB3	2.44	0.52
1:A:399:LEU:CD1	1:A:413:LEU:HB3	2.37	0.52
1:A:96:VAL:HB	4:A:1169:HOH:O	2.08	0.52
1:A:189:ARG:O	1:A:192:VAL:HG22	2.10	0.51
1:B:359:VAL:HG22	1:B:368:VAL:HG22	1.92	0.51
1:B:45:LEU:HA	1:B:387:GLY:O	2.09	0.51
1:B:46:VAL:CG2	1:B:388:VAL:HG12	2.39	0.51
1:A:193:GLY:O	1:A:196:ARG:HG3	2.10	0.51
1:A:147:ASP:HB3	1:B:306:HIS:CE1	2.46	0.51
1:A:373:PRO:HD3	1:A:395:LYS:NZ	2.26	0.51
1:A:57:HIS:HB2	4:A:1266:HOH:O	2.11	0.51
1:B:210:ILE:CD1	1:B:231:ILE:HD12	2.38	0.51
1:B:205:ILE:HG22	1:B:240:ILE:HD13	1.92	0.51
1:B:51:SER:O	1:B:52:TRP:HB2	2.10	0.51
1:B:141:ARG:O	1:B:142:ASN:HB2	2.10	0.51
1:B:216:GLY:HA3	4:B:1271:HOH:O	2.09	0.51
1:A:134:ARG:O	1:A:206:ALA:HB2	2.11	0.50
1:B:49:MET:HE3	1:B:398:TYR:CE2	2.46	0.50
1:B:9:ASP:HA	1:B:13:ILE:HD12	1.93	0.50
1:A:238:GLU:OE1	1:A:238:GLU:HA	2.09	0.50
1:B:183:ASP:OD1	1:B:183:ASP:O	2.30	0.50
1:B:368:VAL:O	1:B:368:VAL:HG12	2.11	0.50
1:A:411:GLN:O	1:A:414:THR:HG22	2.11	0.50
1:A:13:ILE:HD11	1:B:89:ILE:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PRO:O	1:A:160:SER:O	2.30	0.50
1:B:241:LEU:HA	1:B:268:ASP:OD2	2.12	0.50
1:A:183:ASP:OD1	1:A:183:ASP:O	2.30	0.50
1:B:186:TRP:CE3	1:B:226:GLU:HB3	2.47	0.50
1:A:157:PRO:HA	1:A:162:HIS:CG	2.46	0.50
1:A:71:GLN:OE1	1:A:75:MET:O	2.30	0.50
1:A:156:ASP:HB3	1:A:159:ASN:HB2	1.94	0.50
1:A:340:GLU:O	1:A:344:ARG:HG3	2.11	0.50
1:A:208:VAL:HG23	1:A:240:ILE:HD11	1.93	0.50
1:B:165:TRP:HB2	1:B:169:LEU:HD23	1.94	0.49
1:B:202:ARG:HH12	1:B:203:HIS:HA	1.76	0.49
1:B:165:TRP:CD1	1:B:169:LEU:HD23	2.47	0.49
1:A:69:LYS:HD3	1:B:69:LYS:HD3	1.94	0.49
1:A:118:VAL:HG13	1:A:304:PHE:CE2	2.48	0.49
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.94	0.49
1:B:390:ILE:O	1:B:392:PRO:HD3	2.12	0.49
1:A:72:ILE:HG12	1:B:68:MET:HE1	1.94	0.49
1:B:428:CYS:O	1:B:429:GLN:CB	2.57	0.49
1:B:100:PRO:HD3	4:B:1261:HOH:O	2.12	0.49
1:B:134:ARG:NH2	1:B:202:ARG:HH22	2.10	0.49
1:A:383:PHE:O	1:A:386:GLN:HB2	2.13	0.49
1:B:43:ARG:NH2	1:B:384:VAL:HG12	2.27	0.49
1:A:324:LEU:HA	1:A:327:LEU:HD12	1.94	0.49
1:B:27:TYR:OH	1:B:381:LYS:HE2	2.13	0.49
1:A:182:MET:O	1:A:183:ASP:HB3	2.13	0.48
1:B:207:ALA:HA	1:B:240:ILE:HD12	1.93	0.48
1:B:106:VAL:HG22	1:B:287:LEU:HG	1.95	0.48
1:B:15:HIS:O	1:B:18:THR:HB	2.13	0.48
1:B:186:TRP:HZ2	1:B:191:MET:HG3	1.78	0.48
1:A:61:HIS:CD2	1:A:63:GLN:H	2.30	0.48
1:A:7:ALA:HB1	4:A:1153:HOH:O	2.13	0.48
1:A:106:VAL:HG22	1:A:287:LEU:CG	2.40	0.48
1:B:406:LEU:N	1:B:409:GLN:HE21	2.04	0.47
1:A:200:ALA:O	1:A:203:HIS:HE1	1.97	0.47
1:B:1:MET:HE1	1:B:28:PRO:C	2.34	0.47
1:A:35:CYS:SG	1:A:402:PRO:HG2	2.54	0.47
1:B:381:LYS:O	1:B:381:LYS:HD3	2.14	0.47
1:B:205:ILE:HG21	1:B:240:ILE:HD13	1.95	0.47
1:B:232:ARG:HH22	1:B:268:ASP:CG	2.18	0.47
1:A:101:GLN:H	1:A:101:GLN:HG3	1.46	0.47
1:A:39:LEU:CD1	1:A:43:ARG:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:O	1:A:339:ILE:HG13	2.14	0.47
1:A:397:ILE:CG2	1:A:417:VAL:HG13	2.44	0.47
1:A:189:ARG:HG2	1:A:189:ARG:O	2.14	0.47
1:B:212:PRO:HG3	1:B:246:GLU:HG2	1.97	0.47
1:A:232:ARG:O	1:A:232:ARG:HD3	2.15	0.47
1:A:338:ASP:O	1:A:341:VAL:HB	2.13	0.47
1:A:193:GLY:O	1:A:197:LEU:HD23	2.15	0.47
1:A:53:TRP:HZ3	1:A:253:ARG:HG2	1.80	0.47
1:A:130:LYS:HG2	4:A:1206:HOH:O	2.15	0.47
1:B:186:TRP:CZ2	1:B:191:MET:HG3	2.50	0.46
1:B:421:VAL:O	1:B:421:VAL:HG23	2.14	0.46
1:A:61:HIS:HD2	1:A:63:GLN:N	2.11	0.46
1:A:290:ARG:O	1:A:294:GLU:HG3	2.16	0.46
1:B:411:GLN:HA	1:B:414:THR:HG22	1.98	0.46
1:B:138:LEU:O	1:B:208:VAL:HA	2.15	0.46
1:B:152:MET:HE2	1:B:169:LEU:HD21	1.97	0.46
1:A:12:HIS:CE1	1:B:104:GLU:HB2	2.51	0.46
1:B:3:THR:HB	4:B:1280:HOH:O	2.15	0.46
1:B:85:HIS:NE2	1:B:88:ALA:HB2	2.31	0.46
1:A:353:ALA:HB1	1:A:421:VAL:O	2.16	0.46
1:B:134:ARG:HH22	1:B:202:ARG:NH2	2.13	0.46
1:A:421:VAL:HG23	1:A:421:VAL:O	2.16	0.46
1:B:342:GLN:HE22	1:B:407:PRO:HA	1.82	0.45
1:B:135:ASP:OD1	1:B:135:ASP:N	2.50	0.45
1:A:400:MET:HG3	1:A:400:MET:O	2.17	0.45
1:A:135:ASP:OD1	1:A:135:ASP:N	2.50	0.45
1:B:165:TRP:HB2	1:B:169:LEU:HB2	1.99	0.45
1:A:381:LYS:HE3	4:A:1018:HOH:O	2.16	0.45
1:A:136:ARG:NH2	1:A:171:GLU:O	2.50	0.45
1:B:238:GLU:HB3	1:B:240:ILE:HG23	1.99	0.45
1:A:126:TYR:CD1	1:A:292:VAL:HG13	2.51	0.45
1:B:71:GLN:NE2	4:B:1104:HOH:O	2.50	0.45
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.99	0.45
1:A:252:GLY:HA2	1:A:256:LYS:O	2.17	0.45
1:B:24:LEU:N	1:B:24:LEU:HD23	2.32	0.45
1:B:344:ARG:NH2	1:B:361:VAL:O	2.50	0.45
1:B:189:ARG:O	1:B:189:ARG:HG2	2.17	0.45
1:B:161:MET:HE2	1:B:164:LEU:CD1	2.46	0.45
1:A:216:GLY:N	4:A:1082:HOH:O	2.50	0.45
1:B:379:LEU:O	1:B:382:PHE:N	2.50	0.45
1:B:161:MET:HE3	1:B:161:MET:HB3	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:O	1:A:409:GLN:N	2.49	0.45
1:B:182:MET:SD	1:B:225:PRO:HD3	2.56	0.45
1:A:198:MET:O	1:A:202:ARG:N	2.49	0.44
1:B:7:ALA:HA	1:B:10:GLU:CD	2.37	0.44
1:B:169:LEU:HA	1:B:170:PRO:HD2	1.87	0.44
1:B:192:VAL:HB	1:B:196:ARG:NH2	2.32	0.44
1:A:405:ILE:HG13	1:A:409:GLN:HE21	1.83	0.44
1:B:188:GLU:OE2	1:B:189:ARG:N	2.50	0.44
1:A:161:MET:HB3	1:A:161:MET:HE3	1.89	0.44
1:B:61:HIS:CD2	1:B:62:PRO:HD2	2.52	0.44
1:B:400:MET:O	1:B:400:MET:HG3	2.17	0.44
1:B:344:ARG:NH2	4:B:1108:HOH:O	2.50	0.44
1:A:108:LEU:HG	4:A:1037:HOH:O	2.17	0.44
1:A:373:PRO:HD3	1:A:395:LYS:HZ2	1.82	0.44
1:A:210:ILE:CD1	1:A:231:ILE:HD12	2.47	0.44
1:A:344:ARG:NH2	1:A:361:VAL:O	2.50	0.44
1:B:235:CYS:O	1:B:239:GLY:N	2.50	0.44
1:A:136:ARG:HG3	1:A:204:GLU:HG2	1.99	0.44
1:B:226:GLU:OE1	1:B:230:ARG:NE	2.50	0.44
1:B:212:PRO:CG	1:B:246:GLU:HG2	2.48	0.44
1:A:235:CYS:O	1:A:239:GLY:N	2.51	0.44
1:A:192:VAL:HG23	1:A:193:GLY:N	2.33	0.44
1:A:21:THR:HG21	1:B:298:ASP:OD1	2.18	0.43
1:A:370:THR:HG21	1:A:427:PHE:CE2	2.44	0.43
1:A:382:PHE:CZ	1:A:419:ARG:HD3	2.49	0.43
1:B:351:ARG:HG2	1:B:351:ARG:H	1.57	0.43
1:A:141:ARG:HG3	1:A:175:ALA:O	2.18	0.43
1:B:134:ARG:O	1:B:206:ALA:HB2	2.17	0.43
1:A:182:MET:SD	1:A:225:PRO:HD3	2.59	0.43
1:A:140:PHE:CZ	1:A:231:ILE:HD11	2.53	0.43
1:B:161:MET:HE2	1:B:164:LEU:HG	1.99	0.43
1:A:107:PHE:CZ	1:A:306:HIS:HB3	2.54	0.43
1:A:11:ARG:O	1:A:11:ARG:HG3	2.18	0.43
1:A:193:GLY:HA2	1:A:196:ARG:HG2	2.01	0.43
1:A:149:PHE:CD1	1:B:150:GLY:HA3	2.52	0.43
1:A:277:THR:HA	1:A:320:ALA:HA	2.01	0.43
1:A:238:GLU:HB3	1:A:240:ILE:CG2	2.41	0.43
1:B:165:TRP:CG	1:B:169:LEU:HD23	2.54	0.43
1:A:141:ARG:O	1:A:142:ASN:HB2	2.18	0.43
1:A:325:ALA:HA	1:A:328:GLU:HG3	2.00	0.43
1:A:192:VAL:HG23	1:A:193:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:HD3	1:B:69:LYS:CD	2.48	0.43
1:A:242:LEU:HD22	1:A:243:ILE:N	2.33	0.43
1:B:84:THR:HG23	1:B:85:HIS:N	2.33	0.43
1:B:191:MET:HB3	1:B:191:MET:HE2	1.84	0.42
1:A:41:ASP:OD2	1:A:43:ARG:HB2	2.19	0.42
1:B:161:MET:HE2	1:B:164:LEU:CG	2.48	0.42
1:B:161:MET:HB2	1:B:164:LEU:HG	2.00	0.42
1:A:71:GLN:NE2	4:A:1149:HOH:O	2.50	0.42
1:A:369:GLU:HA	1:A:396:LEU:HD23	2.02	0.42
1:A:138:LEU:HD13	1:A:198:MET:HE2	2.00	0.42
1:B:360:ARG:HH11	1:B:367:VAL:HG11	1.83	0.42
1:A:32:ALA:HB1	1:A:37:LEU:HD23	2.01	0.42
1:A:161:MET:HE2	1:A:164:LEU:CG	2.48	0.42
1:A:94:LYS:NZ	4:A:1232:HOH:O	2.50	0.42
1:A:82:GLU:HB2	1:B:391:ARG:NH2	2.35	0.42
1:A:170:PRO:HD3	4:A:1073:HOH:O	2.19	0.42
1:B:60:ASN:OD1	1:B:65:ASN:ND2	2.50	0.42
1:A:82:GLU:OE1	1:B:391:ARG:NH2	2.50	0.42
1:B:80:PHE:HB2	1:B:311:MET:O	2.20	0.42
1:B:233:LYS:HG3	4:B:1180:HOH:O	2.19	0.42
1:A:251:PHE:N	1:A:257:LEU:O	2.52	0.42
1:A:197:LEU:HD13	1:A:197:LEU:HA	1.96	0.42
1:A:17:TYR:OH	1:A:147:ASP:OD1	2.38	0.42
1:A:89:ILE:HA	1:B:13:ILE:HD11	2.01	0.42
1:A:103:LEU:HD11	1:A:267:PRO:HG2	2.01	0.42
1:B:221:ARG:HE	1:B:221:ARG:HB3	1.55	0.42
1:A:297:SER:HB2	1:B:21:THR:HG23	2.01	0.42
1:A:53:TRP:CZ3	1:A:253:ARG:HG2	2.55	0.42
1:A:20:MET:HG2	1:B:293:ALA:HB1	2.02	0.42
1:B:212:PRO:HG2	1:B:259:ALA:HB3	2.02	0.41
1:A:289:THR:OG1	1:A:292:VAL:HG23	2.20	0.41
1:A:201:HIS:O	1:A:205:ILE:HG13	2.20	0.41
1:A:127:TRP:CE3	1:A:134:ARG:HD2	2.55	0.41
1:B:332:TRP:HA	1:B:335:GLN:OE1	2.20	0.41
1:B:232:ARG:HH21	1:B:267:PRO:HA	1.85	0.41
1:A:335:GLN:OE1	1:A:403:TYR:HB3	2.19	0.41
1:A:202:ARG:HH12	1:A:203:HIS:HA	1.84	0.41
1:A:377:ALA:O	1:A:380:GLN:NE2	2.53	0.41
1:B:114:VAL:O	1:B:118:VAL:HG23	2.21	0.41
1:B:390:ILE:HD13	1:B:399:LEU:HD21	2.01	0.41
1:A:381:LYS:HD3	1:A:381:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:HG3	1:B:305:MET:CE	2.50	0.41
1:B:257:LEU:HA	1:B:257:LEU:HD12	1.91	0.41
1:B:419:ARG:HD3	4:B:1313:HOH:O	2.19	0.41
1:A:161:MET:O	1:A:164:LEU:HB2	2.21	0.41
1:A:117:GLU:OE2	1:A:148:THR:OG1	2.34	0.41
1:A:294:GLU:HG2	4:A:1210:HOH:O	2.20	0.41
1:B:81:GLY:HA2	1:B:82:GLU:HA	1.87	0.41
1:A:92:CYS:O	1:A:96:VAL:HG23	2.20	0.41
1:A:75:MET:CE	1:B:29:VAL:HG12	2.50	0.41
1:A:6:LEU:O	1:A:10:GLU:HG3	2.21	0.41
1:B:198:MET:SD	1:B:205:ILE:HD12	2.61	0.41
1:B:224:HIS:O	1:B:227:TRP:HB2	2.20	0.41
1:A:391:ARG:NH2	1:B:82:GLU:OE1	2.54	0.41
1:B:102:PRO:O	1:B:289:THR:HA	2.21	0.41
1:B:35:CYS:SG	1:B:402:PRO:HG2	2.60	0.40
1:B:379:LEU:HG	1:B:383:PHE:CE1	2.56	0.40
1:A:192:VAL:HG22	4:A:1081:HOH:O	2.21	0.40
1:B:192:VAL:HG23	1:B:193:GLY:N	2.36	0.40
1:B:142:ASN:O	1:B:218:GLY:HA3	2.20	0.40
1:B:218:GLY:N	4:B:1217:HOH:O	2.50	0.40
1:A:13:ILE:HG12	1:B:92:CYS:SG	2.60	0.40
1:B:342:GLN:O	1:B:346:GLN:HG3	2.21	0.40
1:A:115:ALA:HB2	1:A:284:SER:HG	1.84	0.40
1:B:169:LEU:CD1	1:B:170:PRO:HD2	2.50	0.40
1:B:335:GLN:HA	4:B:1195:HOH:O	2.20	0.40
1:A:81:GLY:HA2	1:A:82:GLU:HA	1.85	0.40
1:A:253:ARG:NH2	1:A:401:PRO:O	2.50	0.40
1:A:226:GLU:OE1	1:A:230:ARG:NE	2.54	0.40
1:A:240:ILE:HD12	1:A:241:LEU:O	2.22	0.40
1:B:28:PRO:O	1:B:39:LEU:HA	2.22	0.40
1:A:189:ARG:HG2	4:A:1254:HOH:O	2.21	0.40
1:B:96:VAL:HG22	1:B:104:GLU:HA	2.03	0.40
1:A:281:MET:SD	1:A:315:LEU:HG	2.61	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	427/429 (100%)	396 (93%)	26 (6%)	5 (1%)	16 8
1	B	427/429 (100%)	401 (94%)	23 (5%)	3 (1%)	26 17
All	All	854/858 (100%)	797 (93%)	49 (6%)	8 (1%)	21 12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	MET
1	A	75	MET
1	A	216	GLY
1	A	274	LYS
1	B	274	LYS
1	B	307	GLY
1	A	307	GLY
1	A	219	GLY

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	346/346 (100%)	290 (84%)	56 (16%)	3 1
1	B	346/346 (100%)	291 (84%)	55 (16%)	3 1
All	All	692/692 (100%)	581 (84%)	111 (16%)	3 1

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	11	ARG
1	A	14	TRP
1	A	18	THR
1	A	22	SER
1	A	33	GLU
1	A	41	ASP
1	A	43	ARG
1	A	60	ASN
1	A	83	ILE
1	A	90	GLU
1	A	93	ARG
1	A	94	LYS
1	A	95	LEU
1	A	101	GLN
1	A	104	GLU
1	A	110	ASP
1	A	125	GLN
1	A	128	ASP
1	A	132	GLU
1	A	135	ASP
1	A	161	MET
1	A	166	LYS
1	A	169	LEU
1	A	171	GLU
1	A	180	SER
1	A	185	GLU
1	A	187	ASP
1	A	190	ASP
1	A	191	MET
1	A	202	ARG
1	A	221	ARG
1	A	232	ARG
1	A	234	ILE
1	A	238	GLU
1	A	240	ILE
1	A	241	LEU
1	A	265	ILE
1	A	290	ARG
1	A	297	SER
1	A	300	GLU
1	A	306	HIS
1	A	328	GLU

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Mol	Chain	Res	Type
1	A	333	GLN
1	A	334	GLN
1	A	351	ARG
1	A	354	GLU
1	A	355	MET
1	A	360	ARG
1	A	380	GLN
1	A	381	LYS
1	A	408	GLN
1	A	412	ARG
1	A	413	LEU
1	A	428	CYS
1	A	429	GLN
1	B	10	GLU
1	B	11	ARG
1	B	14	TRP
1	B	18	THR
1	B	19	SER
1	B	22	SER
1	B	39	LEU
1	B	41	ASP
1	B	43	ARG
1	B	60	ASN
1	B	80	PHE
1	B	82	GLU
1	B	84	THR
1	B	90	GLU
1	B	94	LYS
1	B	95	LEU
1	B	101	GLN
1	B	110	ASP
1	B	132	GLU
1	B	135	ASP
1	B	161	MET
1	B	165	TRP
1	B	166	LYS
1	B	169	LEU
1	B	171	GLU
1	B	180	SER
1	B	185	GLU
1	B	188	GLU
1	B	190	ASP

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Mol	Chain	Res	Type
1	B	191	MET
1	B	197	LEU
1	B	202	ARG
1	B	210	ILE
1	B	232	ARG
1	B	234	ILE
1	B	238	GLU
1	B	240	ILE
1	B	265	ILE
1	B	284	SER
1	B	290	ARG
1	B	342	GLN
1	B	351	ARG
1	B	354	GLU
1	B	355	MET
1	B	360	ARG
1	B	380	GLN
1	B	381	LYS
1	B	410	LEU
1	B	412	ARG
1	B	413	LEU
1	B	419	ARG
1	B	422	GLN
1	B	423	ASP
1	B	428	CYS
1	B	429	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	71	GLN
1	A	85	HIS
1	A	125	GLN
1	A	142	ASN
1	A	162	HIS
1	A	179	GLN
1	A	201	HIS
1	A	224	HIS
1	A	333	GLN
1	A	372	HIS
1	A	380	GLN

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Mol	Chain	Res	Type
1	A	409	GLN
1	A	422	GLN
1	A	429	GLN
1	B	61	HIS
1	B	71	GLN
1	B	85	HIS
1	B	125	GLN
1	B	142	ASN
1	B	162	HIS
1	B	179	GLN
1	B	224	HIS
1	B	372	HIS
1	B	380	GLN
1	B	409	GLN
1	B	422	GLN
1	B	429	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\|>2$
3	PLP	A	450	1	15,15,16	1.53	3 (20%)	21,22,23	3.50	7 (33%)
3	PLP	B	450	1	15,15,16	1.48	4 (26%)	21,22,23	3.48	7 (33%)

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
3	PLP	A	450	1	-	0/6/6/8	0/1/1/1
3	PLP	B	450	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	PLP	C5-C4	-3.83	1.36	1.40
3	B	450	PLP	C5-C4	-3.58	1.36	1.40
3	A	450	PLP	C3-C2	-2.64	1.38	1.40
3	B	450	PLP	C3-C2	-2.43	1.39	1.40
3	B	450	PLP	P-O4P	-2.29	1.52	1.60
3	A	450	PLP	O3-C3	2.46	1.42	1.37
3	B	450	PLP	O3-C3	2.48	1.42	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	450	PLP	C5-C6-N1	-4.53	116.00	123.86
3	A	450	PLP	C5-C6-N1	-4.30	116.40	123.86
3	B	450	PLP	C4-C3-C2	-2.15	116.39	120.05
3	A	450	PLP	C4-C3-C2	-2.05	116.56	120.05
3	B	450	PLP	C6-C5-C4	2.21	120.02	118.15
3	B	450	PLP	O3-C3-C2	2.44	121.90	117.66
3	A	450	PLP	C6-C5-C4	2.67	120.41	118.15
3	A	450	PLP	O3-C3-C2	2.69	122.33	117.66
3	A	450	PLP	C3-C4-C5	3.09	122.15	118.78
3	A	450	PLP	C6-N1-C2	3.22	125.84	119.28
3	B	450	PLP	C6-N1-C2	3.60	126.62	119.28
3	B	450	PLP	C3-C4-C5	3.73	122.85	118.78
3	B	450	PLP	O4P-C5A-C5	13.19	130.79	108.99
3	A	450	PLP	O4P-C5A-C5	13.72	131.68	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	PLP	1	0
3	B	450	PLP	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.