



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:45 AM UTC

PDB ID : 1DTY / pdb_00001dtY
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

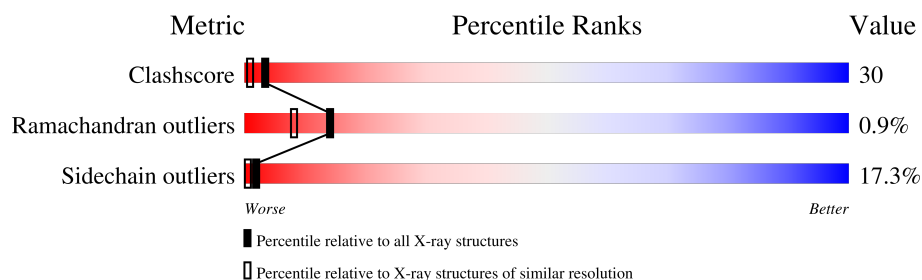
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	429	43% 48% 9%
1	B	429	49% 40% 10%

2 Entry composition [i](#)

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.

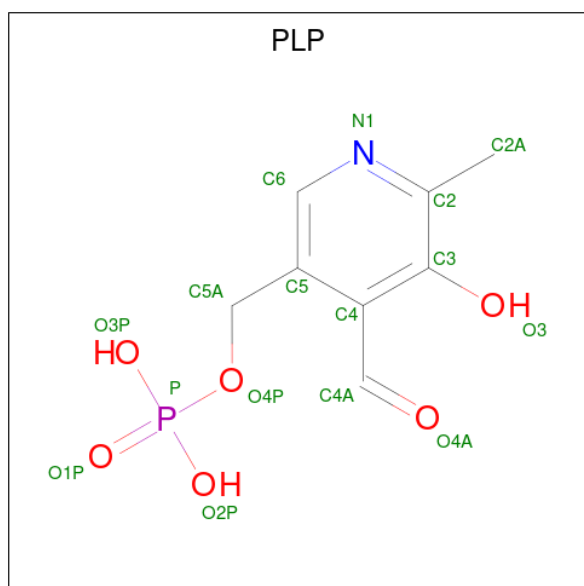
- Molecule 1 is a protein called ADENOSYLMETHIONINE-8-AMINO-7-OXONONANOATE AMINOTRANSFERASE.

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 (CCD ID: NA) (formula: Na).

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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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.

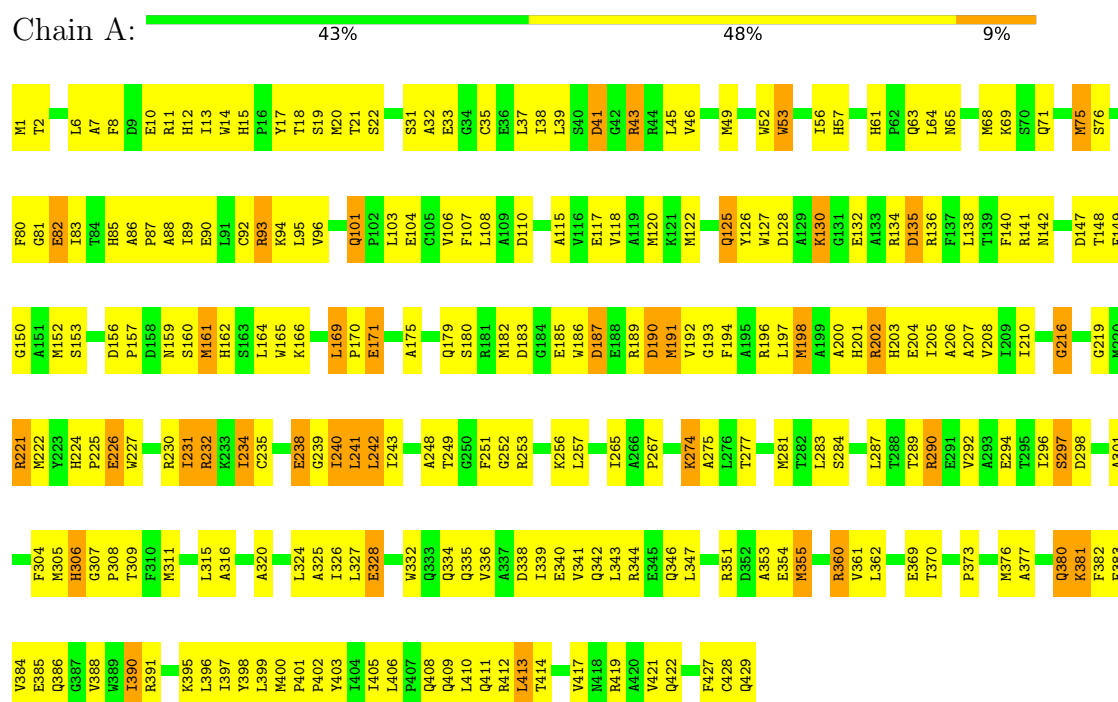
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		
4	B	169	Total	O	0	0
			169	169		

3 Residue-property plots

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.

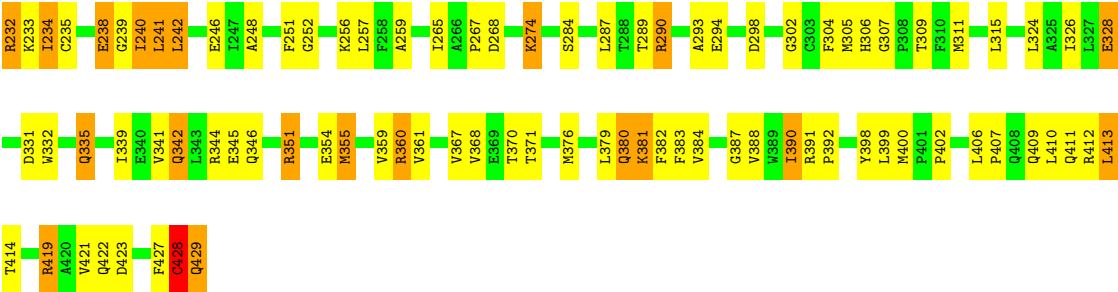
Note EDS was not executed.

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



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





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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: 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	0.37	0/3399	1.19	6/4615 (0.1%)
1	B	0.37	0/3399	1.18	7/4615 (0.2%)
All	All	0.37	0/6798	1.19	13/9230 (0.1%)

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 (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	53	TRP	CA-C-N	7.75	130.52	120.44
1	B	53	TRP	C-N-CA	7.75	130.52	120.44
1	A	82	GLU	CA-C-N	7.72	135.31	122.57
1	A	82	GLU	C-N-CA	7.72	135.31	122.57
1	A	53	TRP	CA-C-N	6.65	129.52	120.54
1	A	53	TRP	C-N-CA	6.65	129.52	120.54
1	B	54	ALA	N-CA-C	6.14	117.64	111.07
1	B	328	GLU	CA-C-N	5.44	128.32	120.38
1	B	328	GLU	C-N-CA	5.44	128.32	120.38
1	A	249	THR	CA-C-N	5.20	125.28	120.34
1	A	249	THR	C-N-CA	5.20	125.28	120.34
1	B	251	PHE	CA-C-N	5.11	130.92	120.80
1	B	251	PHE	C-N-CA	5.11	130.92	120.80

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 ⓘ

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	218	0
1	B	3319	0	3255	209	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	7	2	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	396	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 30.

All (396) 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:O	1:B:429:GLN:CD	1.90	1.14
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:161:MET:HG3	1:B:305:MET:HE2	1.58	0.85
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:O	1:B:429:GLN:OE1	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1:MET:HE1	1:B:84:THR:HG23	1.67	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
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:11:ARG:HD3	4:A:1164:HOH:O	1.89	0.73
1:A:227:TRP:O	1:A:231:ILE:HG13	1.89	0.73
1:A:169:LEU:HD12	1:A:170:PRO:HD2	1.71	0.72
1:A:274:LYS:HE3	1:B:309:THR:OG1	1.89	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:O	1:B:429:GLN:CG	2.37	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:52:TRP:HA	1:A:400:MET:HE1	1.73	0.69
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:115:ALA:HB2	1:A:284:SER:OG	1.94	0.68
1:A:207:ALA:HA	1:A:240:ILE:HD12	1.75	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:355:MET:HE3	1:B:355:MET:HA	1.76	0.67
1:A:150:GLY:HA3	1:B:149:PHE:HD1	1.60	0.67
1:B:7:ALA:HA	1:B:10:GLU:OE1	1.94	0.67
1:B:341:VAL:O	1:B:345:GLU:HB2	1.96	0.66
1:A:355:MET:HE3	1:A:355:MET:HA	1.78	0.66
1:A:224:HIS:HD2	1:A:226:GLU:H	1.44	0.65
1:B:230:ARG:O	1:B:234:ILE:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:75:MET:HE1	1:B:29:VAL:HG12	1.78	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: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
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:52:TRP:HA	1:B:400:MET:HE1	1.82	0.62
1:B:376:MET:O	1:B:380:GLN:HB3	2.00	0.62
3:A:450:PLP:H2A2	4:A:1146:HOH:O	2.00	0.62
1:B:224:HIS:CD2	1:B:226:GLU:HB2	2.35	0.61
1:A:305:MET:HE2	1:B:161:MET:HG3	1.83	0.61
1:A:382:PHE:HZ	1:A:419:ARG:HD3	1.64	0.61
1:B:193:GLY:O	1:B:197:LEU:HD23	2.00	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:A:61:HIS:HB3	1:A:64:LEU:HB2	1.83	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: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:63:GLN:OE1	1:A:326:ILE:HG12	2.01	0.60
1:A:301:ALA:HB2	1:B:164:LEU:HD11	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:TRP:HE3	1:A:253:ARG:HD3	1.68	0.58
1:A:221:ARG:HA	1:A:360:ARG:NH2	2.16	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
1:A:46:VAL:HG12	4:A:1197:HOH:O	2.04	0.57
1:A:157:PRO:HA	1:A:162:HIS:CD2	2.39	0.57
1:B:370:THR:HG21	1:B:427:PHE:CE2	2.39	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:118:VAL:O	1:A:122:MET:HG3	2.04	0.56
1:A:383:PHE:CD1	1:A:390:ILE:HB	2.40	0.56
1:B:11:ARG:O	1:B:11:ARG:HG3	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:398:TYR:HE2	1:B:400:MET:HE2	1.70	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: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:80:PHE:HB2	1:A:311:MET:O	2.06	0.55
1:A:138:LEU:HB3	1:A:208:VAL:HG22	1.87	0.55
1:B:161:MET:HE2	1:B:164:LEU:HD11	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LEU:HD11	1:B:413:LEU:HB3	1.89	0.55
1:B:187:ASP:OD2	1:B:189:ARG:HB3	2.07	0.55
1:B:238:GLU:HA	1:B:238:GLU:OE1	2.06	0.55
1:A:43:ARG:NH2	1:A:384:VAL:HG12	2.22	0.54
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:222:MET:SD	1:A:362:LEU:HB2	2.47	0.54
1:A:230:ARG:O	1:A:234:ILE:HG22	2.08	0.54
1:B:202:ARG:NH1	1:B:203:HIS:HA	2.22	0.54
1:B:152:MET:HE2	1:B:169:LEU:HD21	1.90	0.54
1:A:149:PHE:HD1	1:B:150:GLY:HA3	1.71	0.54
1:A:8:PHE:CZ	1:B:93:ARG:HA	2.42	0.54
1:B:220:MET:HB3	1:B:367:VAL:HG21	1.89	0.54
1:B:49:MET:HE3	1:B:400:MET:CE	2.38	0.54
1:B:234:ILE:O	1:B:238:GLU:HB2	2.08	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:A:186:TRP:HE1	1:A:230:ARG:NH2	2.05	0.53
1:B:79:MET:HE2	1:B:81:GLY:O	2.08	0.53
1:B:150:GLY:HA2	4:B:1208:HOH:O	2.07	0.53
1:A:125:GLN:NE2	1:A:305:MET:H	2.07	0.53
1:A:125:GLN:HE22	1:A:305:MET:H	1.55	0.53
1:B:187:ASP:O	1:B:190:ASP:HB2	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:A:409:GLN:HG2	4:A:1197:HOH:O	2.10	0.52
1:B:127:TRP:CE3	1:B:134:ARG:HD2	2.44	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:49:MET:HE1	1:B:398:TYR:CE2	2.44	0.52
1:B:232:ARG:HH22	1:B:268:ASP:CG	2.18	0.52
1:A:283:LEU:HD13	1:A:316:ALA:CB	2.39	0.52
1:A:306:HIS:CE1	1:B:147:ASP:HB3	2.44	0.52
1:B:381:LYS:HG2	4:B:1039:HOH:O	2.10	0.52
1:A:96:VAL:HB	4:A:1169:HOH:O	2.08	0.52
1:A:399:LEU:CD1	1:A:413:LEU:HB3	2.37	0.52
1:A:189:ARG:O	1:A:192:VAL:HG22	2.10	0.51
1:B:45:LEU:HA	1:B:387:GLY:O	2.09	0.51
1:B:359:VAL:HG22	1:B:368:VAL:HG22	1.92	0.51
1:A:193:GLY:O	1:A:196:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:VAL:CG2	1:B:388:VAL:HG12	2.39	0.51
1:A:147:ASP:HB3	1:B:306:HIS:CE1	2.46	0.51
1:A:57:HIS:HB2	4:A:1266:HOH:O	2.11	0.51
1:A:373:PRO:HD3	1:A:395:LYS:NZ	2.26	0.51
1:B:210:ILE:CD1	1:B:231:ILE:HD12	2.38	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:205:ILE:HG22	1:B:240:ILE:HD13	1.92	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: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:13:ILE:HD11	1:B:89:ILE:HA	1.92	0.50
1:A:411:GLN:O	1:A:414:THR:HG22	2.11	0.50
1:A:157:PRO:O	1:A:160:SER:O	2.30	0.50
1:A:183:ASP:OD1	1:A:183:ASP:O	2.30	0.50
1:B:241:LEU:HA	1:B:268:ASP:OD2	2.12	0.50
1:A:71:GLN:OE1	1:A:75:MET:O	2.30	0.50
1:A:157:PRO:HA	1:A:162:HIS:CG	2.46	0.50
1:B:186:TRP:CE3	1:B:226:GLU:HB3	2.47	0.50
1:A:156:ASP:HB3	1:A:159:ASN:HB2	1.94	0.50
1:A:191:MET:HE3	1:A:194:PHE:HB3	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:A:69:LYS:HD3	1:B:69:LYS:HD3	1.94	0.49
1:B:165:TRP:CD1	1:B:169:LEU:HD23	2.47	0.49
1:B:202:ARG:HH12	1:B:203:HIS:HA	1.76	0.49
1:A:86:ALA:HB3	1:A:87:PRO:HD3	1.94	0.49
1:A:118:VAL:HG13	1:A:304:PHE:CE2	2.48	0.49
1:B:390:ILE:O	1:B:392:PRO:HD3	2.12	0.49
1:A:152:MET:HE2	1:A:169:LEU:HD21	1.95	0.49
1:B:7:ALA:HA	1:B:10:GLU:CD	2.37	0.49
1:B:428:CYS:O	1:B:429:GLN:CB	2.57	0.49
1:A:120:MET:HE1	1:A:150:GLY:O	2.13	0.49
1:B:100:PRO:HD3	4:B:1261:HOH:O	2.12	0.49
1:A:324:LEU:HA	1:A:327:LEU:HD12	1.94	0.49
1:A:383:PHE:O	1:A:386:GLN:HB2	2.13	0.49
1:B:27:TYR:OH	1:B:381:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:NH2	1:B:384:VAL:HG12	2.27	0.49
1:B:134:ARG:NH2	1:B:202:ARG:HH22	2.10	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:1:MET:HE2	1:B:30:VAL:HG12	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:7:ALA:HB1	4:A:1153:HOH:O	2.13	0.48
1:A:61:HIS:CD2	1:A:63:GLN:H	2.30	0.48
1:A:106:VAL:HG22	1:A:287:LEU:CG	2.40	0.48
1:A:35:CYS:SG	1:A:402:PRO:HG2	2.54	0.47
1:A:200:ALA:O	1:A:203:HIS:HE1	1.97	0.47
1:B:406:LEU:N	1:B:409:GLN:HE21	2.04	0.47
1:B:381:LYS:HD3	1:B:381:LYS:O	2.14	0.47
1:B:205:ILE:HG21	1:B:240:ILE:HD13	1.95	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
1:A:335:GLN:O	1:A:339:ILE:HG13	2.14	0.47
1:A:189:ARG:O	1:A:189:ARG:HG2	2.14	0.47
1:A:397:ILE:CG2	1:A:417:VAL:HG13	2.44	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:53:TRP:HZ3	1:A:253:ARG:HG2	1.80	0.47
1:A:150:GLY:O	1:A:153:SER:OG	2.30	0.47
1:A:193:GLY:O	1:A:197:LEU:HD23	2.15	0.47
1:A:130:LYS:HG2	4:A:1206:HOH:O	2.15	0.47
1:A:152:MET:HE1	1:A:165:TRP:CE2	2.51	0.46
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:65:ASN:HA	1:A:68:MET:HE3	1.97	0.46
1:A:290:ARG:O	1:A:294:GLU:HG3	2.16	0.46
1:B:138:LEU:O	1:B:208:VAL:HA	2.15	0.46
1:B:411:GLN:HA	1:B:414:THR:HG22	1.98	0.46
1:A:12:HIS:CE1	1:B:104:GLU:HB2	2.51	0.46
1:A:353:ALA:HB1	1:A:421:VAL:O	2.16	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:421:VAL:O	1:A:421:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:HH22	1:B:202:ARG:NH2	2.13	0.46
1:B:135:ASP:N	1:B:135:ASP:OD1	2.50	0.45
1:B:198:MET:HE2	1:B:198:MET:HB2	1.68	0.45
1:B:342:GLN:HE22	1:B:407:PRO:HA	1.82	0.45
1:A:400:MET:O	1:A:400:MET:HG3	2.17	0.45
1:B:49:MET:HE3	1:B:400:MET:HE3	1.97	0.45
1:B:161:MET:HB3	1:B:161:MET:HE3	1.74	0.45
1:A:135:ASP:OD1	1:A:135:ASP:N	2.50	0.45
1:A:161:MET:HB3	1:A:161:MET:HE3	1.69	0.45
1:B:165:TRP:HB2	1:B:169:LEU:HB2	1.99	0.45
1:A:136:ARG:NH2	1:A:171:GLU:O	2.50	0.45
1:A:381:LYS:HE3	4:A:1018:HOH:O	2.16	0.45
1:A:126:TYR:CD1	1:A:292:VAL:HG13	2.51	0.45
1:A:252:GLY:HA2	1:A:256:LYS:O	2.17	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:B:238:GLU:HB3	1:B:240:ILE:HG23	1.99	0.45
1:B:24:LEU:HD23	1:B:24:LEU:N	2.32	0.45
1:B:344:ARG:NH2	1:B:361:VAL:O	2.50	0.45
1:A:216:GLY:N	4:A:1082:HOH:O	2.50	0.45
1:B:189:ARG:O	1:B:189:ARG:HG2	2.17	0.45
1:B:379:LEU:O	1:B:382:PHE:N	2.50	0.45
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:A:405:ILE:HG13	1:A:409:GLN:HE21	1.83	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:B:188:GLU:OE2	1:B:189:ARG:N	2.50	0.44
1:A:108:LEU:HG	4:A:1037:HOH:O	2.17	0.44
1:A:136:ARG:HD2	1:A:204:GLU:CD	2.42	0.44
1:B:61:HIS:CD2	1:B:62:PRO:HD2	2.52	0.44
1:B:344:ARG:NH2	4:B:1108:HOH:O	2.50	0.44
1:B:400:MET:HG3	1:B:400:MET: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:A:398:TYR:C	1:A:399:LEU:HD23	2.43	0.44
1:A:235:CYS:O	1:A:239:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:CG	1:B:246:GLU:HG2	2.48	0.44
1:B:226:GLU:OE1	1:B:230:ARG:NE	2.50	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:H	1:B:351:ARG:HG2	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:49:MET:HE3	1:A:400:MET:CE	2.47	0.43
1:A:182:MET:SD	1:A:225:PRO:HD3	2.59	0.43
1:A:107:PHE:CZ	1:A:306:HIS:HB3	2.54	0.43
1:A:140:PHE:CZ	1:A:231:ILE:HD11	2.53	0.43
1:A:11:ARG:HG3	1:A:11:ARG:O	2.18	0.43
1:A:149:PHE:CD1	1:B:150:GLY:HA3	2.52	0.43
1:A:193:GLY:HA2	1:A:196:ARG:HG2	2.01	0.43
1:A:277:THR:HA	1:A:320:ALA:HA	2.01	0.43
1:A:141:ARG:O	1:A:142:ASN:HB2	2.18	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:69:LYS:HD3	1:B:69:LYS:CD	2.48	0.43
1:A:192:VAL:HG23	1:A:193:GLY:H	1.83	0.43
1:A:242:LEU:HD22	1:A:243:ILE:N	2.33	0.43
1:A:325:ALA:HA	1:A:328:GLU:HG3	2.00	0.43
1:B:84:THR:HG23	1:B:85:HIS:N	2.33	0.43
1:A:41:ASP:OD2	1:A:43:ARG:HB2	2.19	0.42
1:A:49:MET:HE3	1:A:400:MET:HE3	2.01	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:B:161:MET:HB2	1:B:164:LEU:HG	2.00	0.42
1:A:32:ALA:HB1	1:A:37:LEU:HD23	2.01	0.42
1:B:360:ARG:HH11	1:B:367:VAL:HG11	1.83	0.42
1:B:49:MET:HE3	1:B:400:MET:HE2	2.01	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:A:251:PHE:N	1:A:257:LEU:O	2.52	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:17:TYR:OH	1:A:147:ASP:OD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD13	1:A:197:LEU:HA	1.96	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:20:MET:HG2	1:B:293:ALA:HB1	2.02	0.42
1:A:53:TRP:CZ3	1:A:253:ARG:HG2	2.55	0.42
1:A:191:MET:HB3	1:A:191:MET:HE2	1.76	0.41
1:A:201:HIS:O	1:A:205:ILE:HG13	2.20	0.41
1:A:289:THR:OG1	1:A:292:VAL:HG23	2.20	0.41
1:B:212:PRO:HG2	1:B:259:ALA:HB3	2.02	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:411:GLN:C	1:B:414:THR:HG22	2.44	0.41
1:A:335:GLN:OE1	1:A:403:TYR:HB3	2.19	0.41
1:B:232:ARG:HH21	1:B:267:PRO:HA	1.85	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:A:381:LYS:O	1:A:381:LYS:HD3	2.21	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:B:257:LEU:HD12	1:B:257:LEU:HA	1.91	0.41
1:B:419:ARG:HD3	4:B:1313:HOH:O	2.19	0.41
1:A:117:GLU:OE2	1:A:148:THR:OG1	2.34	0.41
1:A:138:LEU:HD13	1:A:198:MET:HE2	2.02	0.41
1:A:161:MET:O	1:A:164:LEU:HB2	2.21	0.41
1:A:6:LEU:O	1:A:10:GLU:HG3	2.21	0.41
1:A:92:CYS:O	1:A:96:VAL:HG23	2.20	0.41
1:A:294:GLU:HG2	4:A:1210:HOH:O	2.20	0.41
1:B:1:MET:HE1	1:B:28:PRO:C	2.46	0.41
1:B:1:MET:HE3	1:B:28:PRO:HB2	2.02	0.41
1:B:81:GLY:HA2	1:B:82:GLU:HA	1.87	0.41
1:A:76:SER:HB3	1:B:68:MET:HE1	2.03	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: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: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:13:ILE:HG12	1:B:92:CYS:SG	2.60	0.40
1:A:192:VAL:HG22	4:A:1081:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASN:O	1:B:218:GLY:HA3	2.20	0.40
1:B:192:VAL:HG23	1:B:193:GLY:N	2.36	0.40
1:B:218:GLY:N	4:B:1217:HOH:O	2.50	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:B:342:GLN:O	1:B:346:GLN:HG3	2.21	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:B:50:SER:OG	1:B:400:MET:O	2.31	0.40
1:A:189:ARG:HG2	4:A:1254:HOH:O	2.21	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:A:281:MET:SD	1:A:315:LEU:HG	2.61	0.40
1:B:28:PRO:O	1:B:39:LEU:HA	2.22	0.40
1:B:96:VAL:HG22	1:B:104:GLU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	427/429 (100%)	396 (93%)	26 (6%)	5 (1%)	10	5
1	B	427/429 (100%)	401 (94%)	23 (5%)	3 (1%)	18	13
All	All	854/858 (100%)	797 (93%)	49 (6%)	8 (1%)	14	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	MET
1	A	75	MET
1	A	216	GLY

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Mol	Chain	Res	Type
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 ⓘ

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%)	287 (83%)	59 (17%)	2	0
1	B	346/346 (100%)	285 (82%)	61 (18%)	2	0
All	All	692/692 (100%)	572 (83%)	120 (17%)	2	0

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
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	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	130	LYS

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Mol	Chain	Res	Type
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	179	GLN
1	A	180	SER
1	A	185	GLU
1	A	187	ASP
1	A	190	ASP
1	A	191	MET
1	A	198	MET
1	A	202	ARG
1	A	221	ARG
1	A	226	GLU
1	A	231	ILE
1	A	232	ARG
1	A	234	ILE
1	A	238	GLU
1	A	240	ILE
1	A	241	LEU
1	A	242	LEU
1	A	265	ILE
1	A	290	ARG
1	A	297	SER
1	A	306	HIS
1	A	328	GLU
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	390	ILE
1	A	408	GLN
1	A	412	ARG
1	A	413	LEU
1	A	428	CYS
1	A	429	GLN
1	B	10	GLU

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Mol	Chain	Res	Type
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	82	GLU
1	B	83	ILE
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
1	B	191	MET
1	B	197	LEU
1	B	202	ARG
1	B	210	ILE
1	B	221	ARG
1	B	226	GLU
1	B	231	ILE
1	B	232	ARG
1	B	234	ILE
1	B	238	GLU
1	B	240	ILE
1	B	241	LEU
1	B	242	LEU
1	B	265	ILE
1	B	284	SER

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Mol	Chain	Res	Type
1	B	290	ARG
1	B	335	GLN
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	390	ILE
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

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	61	HIS
1	A	71	GLN
1	A	85	HIS
1	A	125	GLN
1	A	142	ASN
1	A	179	GLN
1	A	203	HIS
1	A	224	HIS
1	A	372	HIS
1	A	380	GLN
1	A	409	GLN
1	A	422	GLN
1	A	429	GLN
1	B	61	HIS
1	B	71	GLN
1	B	125	GLN
1	B	142	ASN
1	B	162	HIS
1	B	179	GLN
1	B	215	GLN

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Mol	Chain	Res	Type
1	B	224	HIS
1	B	372	HIS
1	B	409	GLN
1	B	411	GLN
1	B	422	GLN
1	B	429	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.52	3 (20%)	21,22,23	3.23	8 (38%)
3	PLP	B	450	1	15,15,16	1.49	3 (20%)	21,22,23	3.25	9 (42%)

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	-	2/6/6/8	0/1/1/1
3	PLP	B	450	1	-	2/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	PLP	C5-C4	-3.95	1.36	1.40
3	B	450	PLP	C5-C4	-3.69	1.36	1.40
3	B	450	PLP	O3-C3	2.62	1.42	1.36
3	A	450	PLP	O3-C3	2.60	1.42	1.36
3	B	450	PLP	P-O4P	-2.45	1.52	1.60
3	A	450	PLP	P-O4P	-2.08	1.53	1.60

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	PLP	O4P-C5A-C5	11.91	131.68	109.36
3	B	450	PLP	O4P-C5A-C5	11.43	130.79	109.36
3	B	450	PLP	C5-C6-N1	-4.81	116.00	123.83
3	A	450	PLP	C5-C6-N1	-4.57	116.40	123.83
3	B	450	PLP	C6-N1-C2	4.09	126.62	119.20
3	A	450	PLP	C6-N1-C2	3.66	125.84	119.20
3	B	450	PLP	C3-C4-C5	3.55	122.85	118.59
3	A	450	PLP	C3-C4-C5	2.97	122.15	118.59
3	A	450	PLP	C6-C5-C4	2.82	120.41	118.10
3	B	450	PLP	C2A-C2-N1	2.39	122.14	117.64
3	B	450	PLP	C6-C5-C4	2.35	120.02	118.10
3	B	450	PLP	C4-C3-C2	-2.34	116.39	119.89
3	A	450	PLP	O3-C3-C2	2.29	122.33	117.58
3	B	450	PLP	C3-C2-N1	-2.25	118.12	120.96
3	A	450	PLP	C4-C3-C2	-2.23	116.56	119.89
3	B	450	PLP	O3-C3-C2	2.08	121.90	117.58
3	A	450	PLP	C2A-C2-N1	2.04	121.49	117.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	450	PLP	C5A-O4P-P-O1P
3	B	450	PLP	C5A-O4P-P-O2P
3	A	450	PLP	C5A-O4P-P-O1P
3	A	450	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	PLP	2	0
3	B	450	PLP	1	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.