



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:18 PM GMT

PDB ID : 1A3G
Title : BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE FROM ES-
CHERICHIA COLI
Authors : Okada, K.; Hirotsu, K.; Sato, M.; Hayashi, H.; Kagamiyama, H.
Deposited on : 1998-01-21
Resolution : 2.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

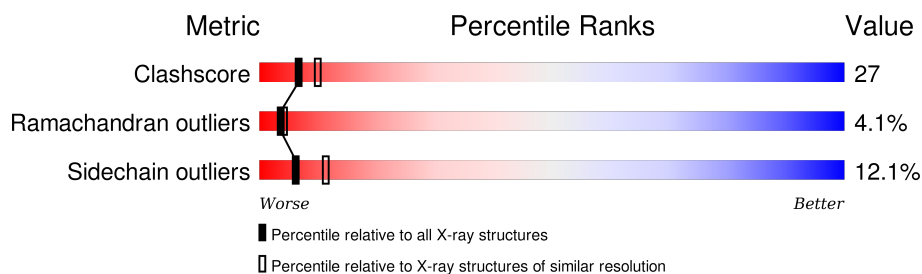
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 $\leq 5\%$. 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	308	
1	B	308	
1	C	308	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	B	413	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	413	-	X	-	-

2 Entry composition [i](#)

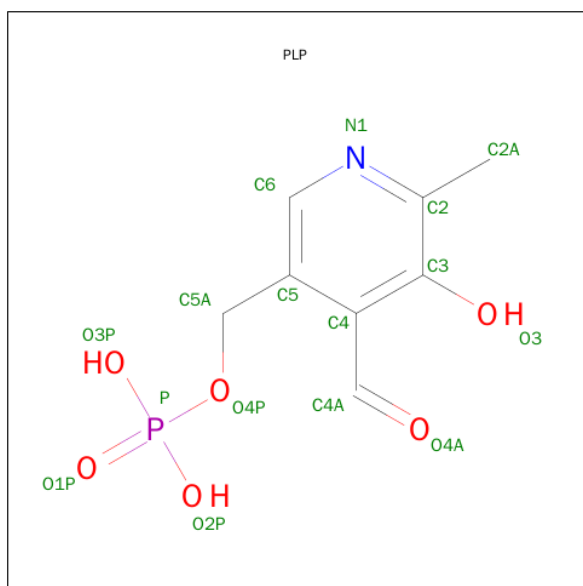
There are 3 unique types of molecules in this entry. The entry contains 7474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2303	1460	402	431	10			
1	B	295	Total	C	N	O	S	0	0	0
			2303	1460	402	431	10			
1	C	295	Total	C	N	O	S	0	0	0
			2303	1460	402	431	10			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is water.

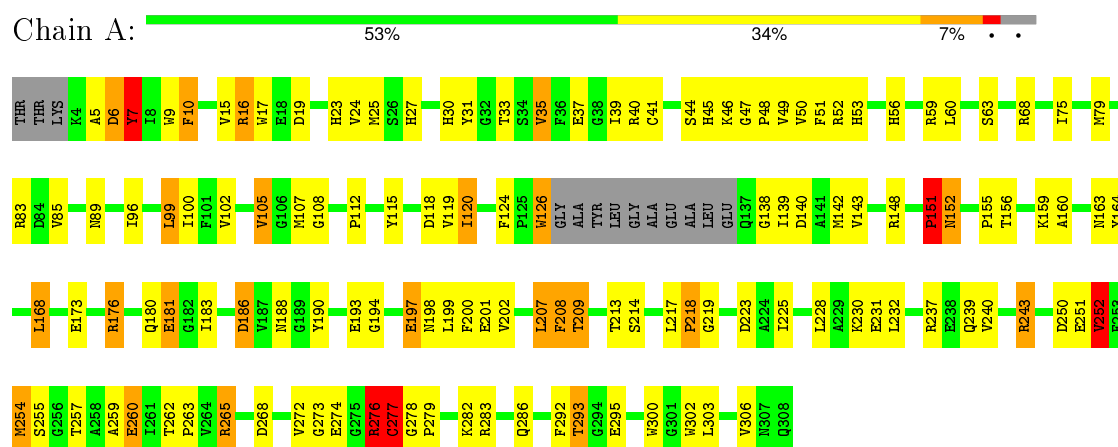
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total 155	O 155	0	0
3	B	191	Total 191	O 191	0	0
3	C	174	Total 174	O 174	0	0

3 Residue-property plots

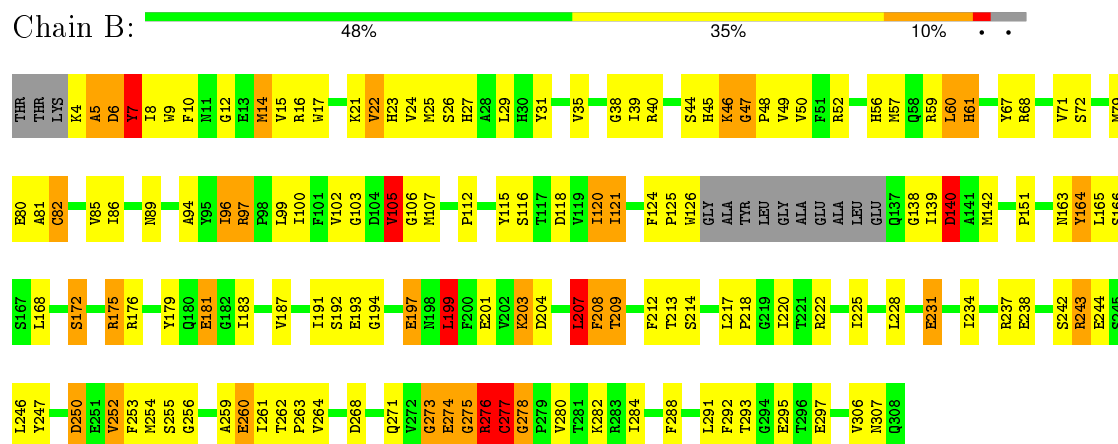
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

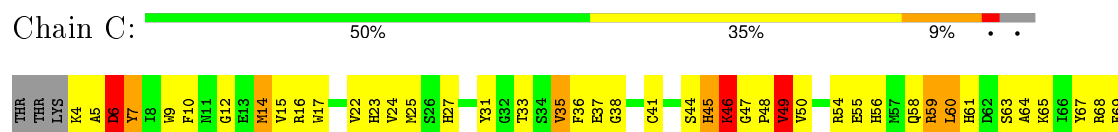
• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE

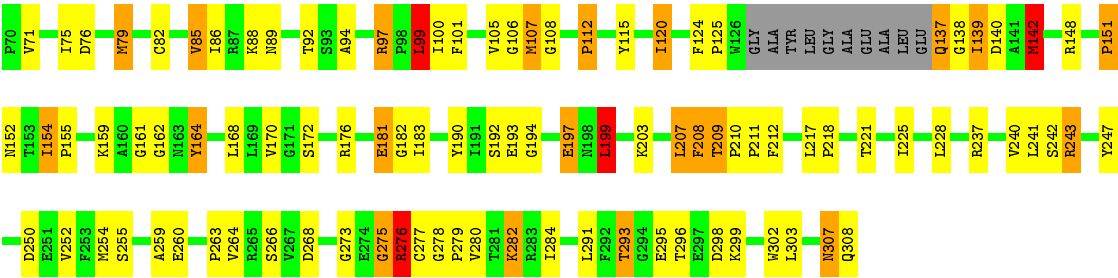


• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE



• Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.10Å 144.00Å 102.90Å 90.00° 136.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.6 (10.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.188 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7474	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.22	4/2357 (0.2%)	1.26	18/3193 (0.6%)
1	B	1.36	12/2357 (0.5%)	1.35	23/3193 (0.7%)
1	C	1.30	4/2357 (0.2%)	1.32	16/3193 (0.5%)
All	All	1.30	20/7071 (0.3%)	1.31	57/9579 (0.6%)

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	A	0	3
1	B	0	3
1	C	0	2
All	All	0	8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLU	CD-OE2	11.14	1.38	1.25
1	A	181	GLU	CD-OE1	9.06	1.35	1.25
1	B	181	GLU	CD-OE2	8.45	1.34	1.25
1	B	24	VAL	CB-CG1	-7.53	1.37	1.52
1	B	80	GLU	CG-CD	6.70	1.61	1.51
1	A	252	VAL	CB-CG1	-6.69	1.38	1.52
1	C	31	TYR	CE2-CZ	-6.67	1.29	1.38
1	A	277	CYS	CB-SG	6.66	1.93	1.82
1	B	277	CYS	CB-SG	6.27	1.93	1.82
1	B	100	ILE	CA-CB	-5.90	1.41	1.54
1	B	243	ARG	CG-CD	-5.67	1.37	1.51
1	B	82	CYS	CB-SG	-5.66	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	GLU	CG-CD	5.45	1.60	1.51
1	A	173	GLU	CB-CG	-5.30	1.42	1.52
1	B	225	ILE	CA-CB	-5.26	1.42	1.54
1	B	175	ARG	CG-CD	5.20	1.65	1.51
1	C	50	VAL	CB-CG1	-5.19	1.42	1.52
1	B	187	VAL	CB-CG1	-5.18	1.42	1.52
1	B	252	VAL	CB-CG1	-5.17	1.42	1.52
1	C	49	VAL	CB-CG1	-5.17	1.42	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ARG	NE-CZ-NH1	-11.47	114.56	120.30
1	C	97	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	C	97	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	C	199	LEU	CA-CB-CG	9.46	137.07	115.30
1	B	199	LEU	CA-CB-CG	8.08	133.88	115.30
1	A	176	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	250	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	A	186	ASP	CB-CG-OD1	7.89	125.40	118.30
1	A	168	LEU	CA-CB-CG	7.81	133.27	115.30
1	B	97	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	105	VAL	N-CA-C	-7.27	91.37	111.00
1	C	308	GLN	N-CA-C	-7.12	91.79	111.00
1	C	307	ASN	CA-C-N	-6.99	101.82	117.20
1	B	105	VAL	N-CA-C	-6.88	92.43	111.00
1	B	151	PRO	N-CA-C	6.66	129.41	112.10
1	C	99	LEU	CA-CB-CG	6.64	130.58	115.30
1	B	151	PRO	C-N-CA	-6.61	105.19	121.70
1	C	151	PRO	N-CA-C	6.57	129.17	112.10
1	B	29	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	151	PRO	N-CA-C	6.43	128.82	112.10
1	A	250	ASP	CB-CG-OD1	6.27	123.94	118.30
1	C	16	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	176	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	16	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	275	GLY	N-CA-C	6.03	128.17	113.10
1	B	22	VAL	CG1-CB-CG2	6.00	120.50	110.90
1	B	97	ARG	CG-CD-NE	-5.99	99.21	111.80
1	A	243	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	142	MET	CG-SD-CE	5.96	109.73	100.20
1	A	152	ASN	N-CA-CB	-5.95	99.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	208	PHE	CB-CA-C	-5.83	98.73	110.40
1	C	16	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	140	ASP	CB-CA-C	-5.77	98.86	110.40
1	B	57	MET	CG-SD-CE	5.67	109.28	100.20
1	C	59	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	118	ASP	N-CA-C	-5.63	95.78	111.00
1	B	207	LEU	N-CA-C	5.60	126.13	111.00
1	B	204	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	152	ASN	CB-CA-C	5.45	121.29	110.40
1	B	59	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	B	208	PHE	N-CA-C	5.44	125.68	111.00
1	A	99	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	203	LYS	C-N-CA	-5.41	108.18	121.70
1	B	291	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	276	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	208	PHE	CB-CA-C	-5.27	99.85	110.40
1	C	79	MET	CG-SD-CE	-5.27	91.76	100.20
1	B	47	GLY	N-CA-C	-5.25	99.99	113.10
1	C	97	ARG	CG-CD-NE	-5.21	100.86	111.80
1	B	250	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	76	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	19	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	6	ASP	N-CA-C	-5.05	97.37	111.00
1	A	243	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	5	ALA	N-CA-C	-5.03	97.42	111.00
1	B	118	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	TYR	Sidechain
1	A	31	TYR	Sidechain
1	A	7	TYR	Sidechain
1	B	247	TYR	Sidechain
1	B	260	GLU	Mainchain
1	B	7	TYR	Sidechain
1	C	164	TYR	Sidechain
1	C	307	ASN	Mainchain

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	2303	0	2243	124	0
1	B	2303	0	2242	136	0
1	C	2303	0	2243	118	0
2	A	15	0	7	2	0
2	B	15	0	6	2	0
2	C	15	0	6	3	0
3	A	155	0	0	8	0
3	B	191	0	0	16	0
3	C	174	0	0	15	0
All	All	7474	0	6747	371	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 27.

All (371) 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:49:VAL:HG11	1:A:303:LEU:HB3	1.27	1.14
1:B:120:ILE:HG21	3:B:1621:HOH:O	1.51	1.10
1:C:105:VAL:HG13	1:C:112:PRO:HD2	1.49	0.95
1:A:7:TYR:HA	1:A:15:VAL:O	1.68	0.94
1:A:282:LYS:O	1:A:286:GLN:HG3	1.67	0.93
1:C:41:CYS:SG	3:C:1961:HOH:O	2.25	0.93
1:A:265:ARG:HG2	1:A:265:ARG:HH11	1.31	0.92
1:A:47:GLY:CA	1:A:49:VAL:HG23	2.01	0.90
1:B:264:VAL:HG23	3:B:1780:HOH:O	1.72	0.89
1:C:293:THR:HG21	1:C:295:GLU:OE1	1.73	0.89
1:C:7:TYR:HA	1:C:15:VAL:O	1.73	0.89
1:C:137:GLN:HG3	1:C:276:ARG:HB3	1.52	0.88
1:B:276:ARG:HD3	1:B:277:CYS:N	1.88	0.88
1:A:208:PHE:HA	1:A:237:ARG:O	1.74	0.86
1:A:47:GLY:HA2	1:A:49:VAL:HG23	1.56	0.86
1:A:27:HIS:HE1	1:A:108:GLY:O	1.58	0.84
1:A:183:ILE:HD12	3:A:1901:HOH:O	1.78	0.83
1:C:92:THR:HG22	3:C:1927:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HG22	1:A:79:MET:CE	2.09	0.81
1:A:183:ILE:HB	3:A:1901:HOH:O	1.80	0.80
1:A:197:GLU:HB2	1:A:255:SER:O	1.81	0.80
1:B:27:HIS:CE1	1:B:31:TYR:HD2	2.01	0.78
1:A:100:ILE:HG12	1:A:119:VAL:HG22	1.65	0.78
1:C:293:THR:HG22	1:C:295:GLU:H	1.49	0.78
1:B:199:LEU:O	1:B:209:THR:HG22	1.84	0.77
1:A:265:ARG:NH1	1:A:265:ARG:HG2	2.00	0.76
1:C:105:VAL:CG1	1:C:112:PRO:HD2	2.15	0.75
1:A:265:ARG:HB3	1:A:276:ARG:HB2	1.68	0.75
1:C:210:PRO:HD3	1:C:241:LEU:HD12	1.67	0.75
1:B:86:ILE:HG21	1:B:306:VAL:HG21	1.68	0.74
1:B:96:ILE:HD12	1:B:96:ILE:N	2.03	0.73
1:A:202:VAL:HB	1:A:251:GLU:HB2	1.69	0.73
1:A:199:LEU:O	1:A:209:THR:HG22	1.88	0.73
1:C:302:TRP:HZ3	3:C:1985:HOH:O	1.72	0.72
1:B:44:SER:OG	1:B:47:GLY:N	2.21	0.72
1:B:94:ALA:HB1	1:B:124:PHE:O	1.88	0.72
1:A:139:ILE:HD13	1:A:262:THR:CG2	2.20	0.72
1:C:199:LEU:O	1:C:209:THR:HG22	1.88	0.71
1:A:207:LEU:O	1:A:208:PHE:HB2	1.90	0.71
1:B:27:HIS:CE1	1:B:31:TYR:CD2	2.77	0.71
1:A:126:TRP:HA	1:A:126:TRP:CE3	2.24	0.71
1:A:139:ILE:HD13	1:A:262:THR:HG21	1.72	0.70
1:B:47:GLY:HA2	1:B:49:VAL:HB	1.74	0.69
1:C:208:PHE:HA	1:C:237:ARG:O	1.93	0.69
1:B:21:LYS:HD2	3:B:1651:HOH:O	1.93	0.69
1:B:208:PHE:HA	1:B:237:ARG:O	1.94	0.68
1:B:7:TYR:HB3	1:B:14:MET:HE2	1.75	0.68
1:A:303:LEU:N	1:A:303:LEU:HD23	2.09	0.68
1:C:137:GLN:HG3	1:C:276:ARG:CB	2.22	0.67
1:A:200:PHE:CD1	1:A:209:THR:HG23	2.28	0.67
1:B:256:GLY:HA3	3:B:1769:HOH:O	1.94	0.67
1:A:47:GLY:HA3	1:A:49:VAL:HG23	1.77	0.67
1:B:201:GLU:O	1:B:207:LEU:O	2.13	0.67
1:B:8:ILE:HD11	1:B:17:TRP:CE3	2.30	0.66
1:C:45:HIS:CD2	1:C:45:HIS:H	2.12	0.66
1:B:276:ARG:HE	1:B:278:GLY:N	1.94	0.66
1:A:37:GLU:OE1	1:A:56:HIS:HD2	1.79	0.65
1:B:44:SER:C	1:B:46:LYS:H	1.97	0.65
1:A:274:GLU:HB2	1:A:277:CYS:SG	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:HG22	1:C:264:VAL:HB	1.77	0.65
1:C:291:LEU:HD11	3:C:1985:HOH:O	1.94	0.65
1:C:255:SER:HA	1:C:260:GLU:O	1.96	0.65
1:B:268:ASP:O	1:C:68:ARG:NH2	2.30	0.64
1:A:274:GLU:CB	1:A:277:CYS:SG	2.86	0.64
1:B:8:ILE:HG22	1:B:9:TRP:O	1.96	0.64
1:C:139:ILE:O	1:C:140:ASP:HB2	1.98	0.64
1:B:253:PHE:HA	3:B:1780:HOH:O	1.98	0.63
1:B:139:ILE:O	1:B:140:ASP:CB	2.44	0.63
1:A:75:ILE:HG22	1:A:79:MET:HE3	1.80	0.63
1:A:75:ILE:HG22	1:A:79:MET:HE2	1.80	0.63
1:C:45:HIS:O	1:C:46:LYS:HB3	1.98	0.63
1:B:120:ILE:HG23	1:B:121:ILE:N	2.13	0.62
1:A:268:ASP:O	1:B:68:ARG:NH2	2.32	0.62
1:B:207:LEU:O	1:B:208:PHE:HB2	1.99	0.62
1:C:60:LEU:HD13	1:C:100:ILE:HD11	1.82	0.62
1:C:37:GLU:HG3	1:C:38:GLY:N	2.14	0.62
1:A:49:VAL:HG11	1:A:303:LEU:CB	2.17	0.62
1:A:190:TYR:CE1	1:B:213:THR:HB	2.35	0.61
1:B:139:ILE:O	1:B:140:ASP:HB2	2.00	0.61
1:B:6:ASP:O	1:B:7:TYR:HB2	2.01	0.61
1:B:96:ILE:H	1:B:96:ILE:HD12	1.65	0.60
1:C:209:THR:HB	3:C:1506:HOH:O	2.00	0.60
1:C:37:GLU:HG3	1:C:38:GLY:H	1.66	0.60
1:A:159:LYS:NZ	2:A:413:PLP:O3	2.32	0.60
1:C:139:ILE:O	1:C:140:ASP:CB	2.47	0.60
1:A:75:ILE:N	1:A:75:ILE:HD12	2.17	0.60
1:C:45:HIS:CD2	1:C:45:HIS:N	2.69	0.60
1:C:154:ILE:O	1:C:154:ILE:HG22	2.02	0.60
1:B:276:ARG:HE	1:B:278:GLY:HA3	1.67	0.59
1:A:201:GLU:O	1:A:207:LEU:O	2.20	0.59
1:B:271:GLN:CD	1:B:275:GLY:H	2.05	0.59
1:B:26:SER:HA	1:B:103:GLY:O	2.02	0.59
1:B:27:HIS:ND1	1:B:31:TYR:HD2	1.98	0.59
1:C:49:VAL:CG1	1:C:303:LEU:HD22	2.33	0.59
1:A:207:LEU:O	1:A:208:PHE:CB	2.50	0.58
1:B:164:TYR:OH	2:B:413:PLP:O3	2.14	0.58
1:A:47:GLY:HA2	1:A:49:VAL:CG2	2.32	0.58
1:A:44:SER:OG	1:A:47:GLY:N	2.36	0.58
1:C:291:LEU:HD23	1:C:296:THR:HB	1.84	0.58
1:C:228:LEU:HD11	3:C:1985:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HG2	1:A:257:THR:CG2	2.33	0.58
1:C:159:LYS:NZ	2:C:413:PLP:O3	2.33	0.58
1:A:252:VAL:HG12	1:A:272:VAL:HG11	1.85	0.57
1:C:148:ARG:HD3	1:C:192:SER:OG	2.04	0.57
1:B:181:GLU:HG2	1:B:254:MET:CE	2.34	0.57
1:B:6:ASP:O	1:B:7:TYR:CB	2.52	0.57
1:C:75:ILE:HG22	1:C:79:MET:CE	2.35	0.57
1:A:23:HIS:CD2	1:A:25:MET:H	2.22	0.57
1:C:207:LEU:O	1:C:208:PHE:HB2	2.05	0.57
1:C:164:TYR:OH	2:C:413:PLP:O3	2.23	0.57
1:C:302:TRP:CZ3	3:C:1985:HOH:O	2.53	0.57
1:A:209:THR:HB	3:A:1501:HOH:O	2.03	0.56
1:C:217:LEU:HD23	1:C:217:LEU:C	2.26	0.56
1:B:112:PRO:HG2	3:B:1878:HOH:O	2.04	0.56
1:B:191:ILE:HD11	1:B:246:LEU:HG	1.86	0.56
1:A:75:ILE:H	1:A:75:ILE:HD12	1.69	0.56
1:C:6:ASP:O	1:C:89:ASN:OD1	2.24	0.56
1:C:293:THR:CG2	1:C:295:GLU:HG3	2.35	0.56
1:B:276:ARG:HE	1:B:278:GLY:CA	2.18	0.56
1:B:45:HIS:O	1:B:46:LYS:HB3	2.05	0.56
1:B:6:ASP:HA	1:B:17:TRP:HB2	1.88	0.55
1:A:274:GLU:HB3	1:A:277:CYS:SG	2.46	0.55
1:B:261:ILE:HG22	1:B:261:ILE:O	2.06	0.55
1:C:7:TYR:H	1:C:17:TRP:H	1.53	0.55
1:B:105:VAL:HA	3:B:1878:HOH:O	2.07	0.55
1:A:217:LEU:O	1:A:219:GLY:N	2.39	0.55
1:C:86:ILE:HD13	3:C:1961:HOH:O	2.05	0.55
1:B:15:VAL:HG12	1:B:16:ARG:O	2.06	0.55
1:C:36:PHE:HB3	1:C:99:LEU:HD23	1.89	0.55
1:C:27:HIS:HE1	1:C:108:GLY:O	1.89	0.55
1:B:106:GLY:N	3:B:1878:HOH:O	2.40	0.55
1:B:47:GLY:CA	1:B:49:VAL:HB	2.36	0.55
1:B:273:GLY:O	1:B:274:GLU:HB2	2.07	0.54
1:B:197:GLU:HG3	1:B:254:MET:HB3	1.89	0.54
1:A:112:PRO:O	1:A:115:TYR:HB3	2.07	0.54
1:A:156:THR:O	1:A:217:LEU:HD12	2.08	0.54
1:A:276:ARG:HH12	1:A:282:LYS:HE2	1.72	0.54
1:C:164:TYR:HE1	3:C:1592:HOH:O	1.89	0.54
1:A:293:THR:HG22	1:A:295:GLU:H	1.73	0.54
1:A:199:LEU:HD23	1:A:254:MET:SD	2.47	0.54
1:B:259:ALA:O	1:B:260:GLU:C	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:CD2	1:A:79:MET:HG2	2.43	0.54
1:C:44:SER:OG	1:C:47:GLY:N	2.41	0.54
1:C:54:ARG:HG3	1:C:79:MET:HE1	1.89	0.54
1:B:280:VAL:O	1:B:284:ILE:HG12	2.09	0.53
1:B:175:ARG:HG3	3:B:1648:HOH:O	2.08	0.53
1:A:302:TRP:C	1:A:303:LEU:HD23	2.29	0.53
1:B:255:SER:HA	1:B:260:GLU:O	2.09	0.53
1:A:259:ALA:O	1:A:260:GLU:HB2	2.08	0.53
1:C:23:HIS:HD2	1:C:25:MET:H	1.56	0.53
1:A:24:VAL:O	1:A:30:HIS:HE1	1.91	0.53
1:B:181:GLU:CG	1:B:254:MET:HE1	2.38	0.53
1:C:49:VAL:HG11	1:C:303:LEU:HD22	1.89	0.53
1:C:94:ALA:HB1	1:C:124:PHE:O	2.09	0.53
1:A:23:HIS:HD2	1:A:25:MET:H	1.56	0.53
1:A:138:GLY:HA2	1:A:263:PRO:O	2.08	0.53
1:B:44:SER:C	1:B:46:LYS:N	2.62	0.52
1:B:67:TYR:O	1:B:68:ARG:HB2	2.08	0.52
1:A:68:ARG:NH2	1:C:268:ASP:O	2.43	0.52
1:B:203:LYS:O	1:B:250:ASP:OD2	2.27	0.52
1:A:6:ASP:N	1:A:6:ASP:OD1	2.42	0.52
1:B:212:PHE:CE1	1:B:218:PRO:HA	2.44	0.52
1:A:181:GLU:HG2	1:A:254:MET:CE	2.39	0.52
1:A:37:GLU:OE2	1:A:59:ARG:HB3	2.09	0.52
1:C:45:HIS:O	1:C:46:LYS:CB	2.57	0.52
1:C:99:LEU:HD13	1:C:101:PHE:CD1	2.44	0.52
1:A:255:SER:HA	1:A:260:GLU:O	2.10	0.52
1:C:6:ASP:O	1:C:7:TYR:HB2	2.10	0.52
1:B:46:LYS:C	1:B:47:GLY:O	2.45	0.52
1:C:75:ILE:HG22	1:C:79:MET:HE2	1.90	0.52
1:A:252:VAL:CG1	1:A:272:VAL:HG11	2.40	0.51
1:A:213:THR:HB	1:C:190:TYR:CE1	2.44	0.51
1:A:9:TRP:HZ3	1:A:119:VAL:HG12	1.75	0.51
1:C:209:THR:CG2	3:C:1506:HOH:O	2.57	0.51
1:A:75:ILE:HD13	3:A:1777:HOH:O	2.10	0.51
1:B:60:LEU:HA	3:B:1649:HOH:O	2.09	0.51
1:B:81:ALA:O	1:B:85:VAL:HG23	2.09	0.51
1:B:179:TYR:CD1	1:B:179:TYR:N	2.79	0.51
1:C:27:HIS:HD2	1:C:33:THR:OG1	1.94	0.50
1:A:41:CYS:HA	1:A:50:VAL:HA	1.93	0.50
1:C:71:VAL:HG22	1:C:100:ILE:HD13	1.94	0.50
1:B:197:GLU:HB2	1:B:255:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:PRO:O	1:C:282:LYS:HB2	2.12	0.50
1:B:242:SER:HB2	1:B:244:GLU:OE1	2.11	0.50
1:A:176:ARG:NH2	3:A:1697:HOH:O	2.44	0.50
1:C:170:VAL:O	1:C:170:VAL:HG12	2.10	0.50
1:C:35:VAL:CG2	1:C:63:SER:HB3	2.41	0.50
1:C:280:VAL:O	1:C:284:ILE:HG13	2.12	0.50
1:C:105:VAL:CG2	1:C:115:TYR:HB2	2.42	0.50
1:B:276:ARG:CD	1:B:277:CYS:N	2.70	0.50
1:A:105:VAL:HG13	1:A:112:PRO:CD	2.42	0.50
1:C:259:ALA:O	1:C:260:GLU:C	2.48	0.50
1:B:217:LEU:HD23	1:B:218:PRO:N	2.27	0.50
1:B:94:ALA:HA	1:B:126:TRP:H	1.77	0.49
1:A:27:HIS:HD2	1:A:33:THR:OG1	1.95	0.49
1:B:45:HIS:CE1	1:B:46:LYS:HD3	2.47	0.49
1:C:46:LYS:C	1:C:47:GLY:O	2.47	0.49
1:C:35:VAL:HG21	1:C:63:SER:HB3	1.93	0.49
1:A:96:ILE:HD12	1:A:96:ILE:N	2.28	0.49
1:A:139:ILE:O	1:A:140:ASP:CB	2.55	0.49
1:B:27:HIS:HB3	1:B:102:VAL:HB	1.93	0.49
1:B:61:HIS:CE1	1:B:71:VAL:HG11	2.48	0.49
1:B:172:SER:O	1:B:176:ARG:HB2	2.11	0.49
1:A:44:SER:H	1:A:47:GLY:HA3	1.77	0.49
1:A:75:ILE:H	1:A:75:ILE:CD1	2.25	0.49
1:A:126:TRP:HE3	1:A:126:TRP:HA	1.74	0.49
1:B:181:GLU:HG2	1:B:254:MET:HE3	1.94	0.49
1:B:254:MET:HG2	3:B:1780:HOH:O	2.13	0.49
1:C:37:GLU:OE2	1:C:56:HIS:HD2	1.95	0.49
1:B:14:MET:HE3	1:B:14:MET:HA	1.94	0.48
1:B:271:GLN:CG	1:B:275:GLY:H	2.26	0.48
1:A:6:ASP:O	1:A:89:ASN:OD1	2.31	0.48
1:A:52:ARG:HH12	1:A:223:ASP:HB3	1.77	0.48
1:C:293:THR:HG22	1:C:295:GLU:N	2.25	0.48
1:A:138:GLY:HA3	1:A:265:ARG:N	2.29	0.48
1:B:6:ASP:HB3	3:B:1681:HOH:O	2.12	0.48
1:B:181:GLU:HG2	1:B:254:MET:HE1	1.95	0.48
1:B:260:GLU:HG2	1:B:288:PHE:HE2	1.79	0.48
1:A:10:PHE:CG	1:A:120:ILE:HD11	2.49	0.48
1:C:65:LYS:NZ	3:C:1568:HOH:O	2.46	0.48
1:A:293:THR:CG2	1:A:295:GLU:HG3	2.44	0.47
1:B:23:HIS:CD2	1:B:25:MET:H	2.32	0.47
1:A:39:ILE:HB	1:A:96:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:O	1:B:165:LEU:N	2.47	0.47
1:B:276:ARG:NH2	1:B:282:LYS:HG2	2.30	0.47
1:B:207:LEU:O	1:B:208:PHE:CB	2.60	0.47
1:B:56:HIS:HE1	3:B:1505:HOH:O	1.95	0.47
1:A:5:ALA:O	1:A:17:TRP:HB2	2.15	0.47
1:A:15:VAL:HG12	1:A:16:ARG:O	2.15	0.47
1:C:217:LEU:HD23	1:C:218:PRO:N	2.30	0.47
1:B:274:GLU:O	1:B:276:ARG:N	2.48	0.47
1:C:23:HIS:CD2	1:C:25:MET:H	2.33	0.47
1:C:176:ARG:NH1	3:C:1685:HOH:O	2.48	0.47
1:C:197:GLU:HB2	1:C:255:SER:O	2.15	0.47
1:A:27:HIS:CE1	1:A:108:GLY:O	2.51	0.47
1:C:45:HIS:O	1:C:45:HIS:CG	2.64	0.47
1:C:61:HIS:CE1	1:C:71:VAL:HG11	2.50	0.47
1:A:240:VAL:HG12	1:B:213:THR:HG21	1.97	0.46
1:C:228:LEU:HD21	3:C:1985:HOH:O	2.14	0.46
1:B:228:LEU:O	1:B:231:GLU:N	2.48	0.46
1:A:75:ILE:CG2	1:A:79:MET:HE2	2.43	0.46
1:B:6:ASP:HB3	3:B:1873:HOH:O	2.15	0.46
1:C:44:SER:H	1:C:47:GLY:HA3	1.80	0.46
1:A:105:VAL:HG13	1:A:112:PRO:HD3	1.95	0.46
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.81	0.46
1:A:152:ASN:N	3:A:1547:HOH:O	2.42	0.46
1:B:9:TRP:CZ2	1:B:12:GLY:HA2	2.51	0.46
1:A:142:MET:HG2	1:A:143:VAL:N	2.30	0.46
1:C:203:LYS:O	1:C:250:ASP:OD2	2.34	0.46
1:C:107:MET:HA	1:C:107:MET:CE	2.46	0.46
1:B:96:ILE:CD1	1:B:96:ILE:H	2.29	0.46
1:A:181:GLU:HG2	1:A:254:MET:HE3	1.97	0.46
1:B:7:TYR:HB3	1:B:14:MET:CE	2.44	0.46
1:A:96:ILE:N	1:A:96:ILE:CD1	2.79	0.46
1:C:4:LYS:HG2	1:C:5:ALA:N	2.31	0.46
1:B:276:ARG:HD3	1:B:277:CYS:CA	2.46	0.46
1:B:96:ILE:CD1	1:B:96:ILE:N	2.73	0.46
1:B:7:TYR:HA	1:B:15:VAL:O	2.16	0.46
1:B:23:HIS:HD2	1:B:25:MET:H	1.64	0.46
1:C:9:TRP:HB2	1:C:85:VAL:HG23	1.98	0.46
1:C:124:PHE:HB2	1:C:125:PRO:HD2	1.97	0.45
1:B:124:PHE:N	1:B:124:PHE:CD1	2.84	0.45
1:C:140:ASP:HA	1:C:266:SER:O	2.15	0.45
1:B:38:GLY:O	1:B:56:HIS:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ALA:HA	1:B:126:TRP:N	2.31	0.45
1:C:199:LEU:O	1:C:209:THR:CG2	2.63	0.45
1:C:44:SER:C	1:C:46:LYS:H	2.20	0.45
1:C:193:GLU:OE1	2:C:413:PLP:N1	2.50	0.45
1:C:181:GLU:HG2	1:C:254:MET:CE	2.45	0.45
1:C:45:HIS:CD2	1:C:46:LYS:HG2	2.51	0.45
1:C:9:TRP:CZ2	1:C:12:GLY:HA2	2.52	0.45
1:B:27:HIS:ND1	1:B:31:TYR:CD2	2.82	0.45
1:A:193:GLU:OE1	2:A:413:PLP:N1	2.49	0.45
1:B:199:LEU:O	1:B:209:THR:CG2	2.59	0.44
1:C:45:HIS:HD2	1:C:45:HIS:H	1.61	0.44
1:B:6:ASP:O	1:B:89:ASN:OD1	2.35	0.44
1:C:64:ALA:HB1	1:C:69:PHE:HB2	1.99	0.44
1:A:160:ALA:O	1:A:163:ASN:HB2	2.17	0.44
1:A:276:ARG:HD3	1:A:277:CYS:N	2.33	0.44
1:B:45:HIS:CD2	1:B:45:HIS:H	2.35	0.44
1:B:120:ILE:CG2	1:B:121:ILE:N	2.71	0.44
1:A:75:ILE:N	1:A:75:ILE:CD1	2.81	0.44
1:B:193:GLU:OE1	2:B:413:PLP:N1	2.51	0.44
1:B:115:TYR:H	1:B:115:TYR:HD1	1.65	0.44
1:C:45:HIS:HD2	1:C:45:HIS:N	2.16	0.44
1:C:60:LEU:HD13	1:C:100:ILE:CD1	2.47	0.44
1:A:303:LEU:N	1:A:303:LEU:CD2	2.81	0.43
1:C:37:GLU:OE2	1:C:56:HIS:CD2	2.70	0.43
1:B:105:VAL:CA	3:B:1878:HOH:O	2.65	0.43
1:B:139:ILE:HD13	1:B:262:THR:HG21	2.00	0.43
1:A:139:ILE:HD13	1:A:262:THR:HG22	1.99	0.43
1:B:142:MET:HB3	1:B:179:TYR:CG	2.53	0.43
1:C:209:THR:HG22	3:C:1506:HOH:O	2.17	0.43
1:A:45:HIS:HD2	1:A:292:PHE:O	2.00	0.43
1:B:39:ILE:HB	1:B:96:ILE:HB	2.01	0.43
1:C:181:GLU:HG2	1:C:254:MET:HE2	2.01	0.43
1:B:168:LEU:C	1:B:168:LEU:HD13	2.39	0.43
1:B:120:ILE:HA	1:B:120:ILE:HD12	1.61	0.43
1:B:181:GLU:CG	1:B:254:MET:CE	2.95	0.43
1:C:58:GLN:O	1:C:61:HIS:N	2.51	0.43
1:A:213:THR:HG21	1:C:240:VAL:HG12	2.00	0.43
1:B:97:ARG:HG3	1:B:97:ARG:O	2.19	0.43
1:B:183:ILE:HA	1:B:194:GLY:HA2	2.00	0.43
1:C:138:GLY:N	1:C:276:ARG:HG3	2.34	0.43
1:A:23:HIS:HD2	1:A:25:MET:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:HA	1:C:211:PRO:HD3	1.75	0.43
1:C:67:TYR:OH	1:C:155:PRO:HG2	2.19	0.43
1:B:192:SER:O	1:B:193:GLU:HB3	2.18	0.43
1:A:9:TRP:O	1:A:120:ILE:HD13	2.19	0.42
1:A:251:GLU:CD	1:A:278:GLY:HA2	2.39	0.42
1:C:58:GLN:O	1:C:59:ARG:C	2.57	0.42
1:A:279:PRO:O	1:A:283:ARG:HG3	2.19	0.42
1:A:68:ARG:NH1	3:A:1752:HOH:O	2.48	0.42
1:B:293:THR:HG22	1:B:295:GLU:H	1.84	0.42
1:A:75:ILE:CG2	1:A:79:MET:CE	2.91	0.42
1:B:86:ILE:HG21	1:B:306:VAL:CG2	2.44	0.42
1:A:272:VAL:O	1:A:272:VAL:HG12	2.18	0.42
1:B:181:GLU:HA	1:B:181:GLU:OE1	2.18	0.42
1:A:183:ILE:HA	1:A:194:GLY:HA2	2.00	0.42
1:A:51:PHE:CZ	1:A:52:ARG:HD2	2.54	0.42
1:C:221:THR:O	1:C:225:ILE:HD12	2.19	0.42
1:B:124:PHE:HB2	1:B:125:PRO:HD2	2.01	0.42
1:A:148:ARG:NH1	3:A:1604:HOH:O	2.48	0.42
1:B:138:GLY:HA2	1:B:263:PRO:O	2.20	0.42
1:A:120:ILE:HD13	1:A:120:ILE:HA	1.81	0.42
1:C:9:TRP:O	1:C:120:ILE:HA	2.20	0.42
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.68	0.42
1:A:208:PHE:H	1:A:237:ARG:H	1.67	0.42
1:B:94:ALA:CB	1:B:124:PHE:O	2.63	0.42
1:B:293:THR:CG2	1:B:295:GLU:HG3	2.50	0.42
1:A:35:VAL:HG22	1:A:63:SER:HB3	2.01	0.42
1:A:138:GLY:HA3	1:A:265:ARG:H	1.85	0.42
1:B:243:ARG:HH11	1:B:243:ARG:CG	2.33	0.42
1:C:212:PHE:CE1	1:C:218:PRO:HB3	2.55	0.41
1:C:142:MET:O	1:C:182:GLY:HA2	2.20	0.41
1:A:276:ARG:C	1:A:276:ARG:HD3	2.40	0.41
1:A:139:ILE:O	1:A:140:ASP:HB2	2.20	0.41
1:C:207:LEU:O	1:C:208:PHE:O	2.38	0.41
1:A:40:ARG:HG2	1:A:257:THR:HG22	2.02	0.41
1:B:79:MET:O	1:B:82:CYS:HB3	2.20	0.41
1:A:27:HIS:HB3	1:A:102:VAL:HB	2.02	0.41
1:C:88:LYS:CG	1:C:88:LYS:O	2.69	0.41
1:A:186:ASP:OD1	1:A:188:ASN:HB2	2.20	0.41
1:B:253:PHE:HB2	1:B:262:THR:O	2.20	0.41
1:B:139:ILE:HD13	1:B:262:THR:CG2	2.51	0.41
1:C:14:MET:HE2	1:C:14:MET:HB3	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LYS:HG2	1:C:5:ALA:H	1.86	0.41
1:C:243:ARG:NH1	1:C:247:TYR:OH	2.54	0.41
1:C:7:TYR:HB3	1:C:14:MET:HE2	2.03	0.41
1:B:276:ARG:HD3	1:B:276:ARG:C	2.41	0.41
1:B:293:THR:HG22	1:B:295:GLU:HG3	2.03	0.41
1:C:152:ASN:CG	1:C:152:ASN:O	2.59	0.41
1:B:52:ARG:HD3	1:B:220:ILE:HG22	2.02	0.41
1:C:183:ILE:HA	1:C:194:GLY:HA2	2.02	0.41
1:B:181:GLU:HG3	1:B:254:MET:HE1	2.03	0.41
1:B:259:ALA:O	1:B:261:ILE:N	2.54	0.41
1:A:83:ARG:HD3	1:A:306:VAL:HA	2.03	0.41
1:A:198:ASN:HD21	1:A:219:GLY:HA3	1.86	0.40
1:C:263:PRO:HB3	3:C:1583:HOH:O	2.20	0.40
1:B:40:ARG:HD2	1:B:40:ARG:HA	1.84	0.40
1:A:9:TRP:HB2	1:A:85:VAL:CG2	2.51	0.40
1:A:51:PHE:CZ	1:A:52:ARG:HG3	2.56	0.40
1:C:55:GLU:N	1:C:55:GLU:OE1	2.43	0.40
1:B:307:ASN:ND2	3:B:1933:HOH:O	2.54	0.40
1:A:44:SER:C	1:A:46:LYS:N	2.75	0.40
1:B:209:THR:O	1:B:238:GLU:HA	2.21	0.40
1:B:45:HIS:HD2	1:B:292:PHE:O	2.04	0.40
1:C:242:SER:O	1:C:243:ARG:C	2.59	0.40
1:C:17:TRP:C	1:C:17:TRP:CD1	2.94	0.40
1:B:45:HIS:N	1:B:292:PHE:O	2.50	0.40
1:A:230:LYS:O	1:A:231:GLU:C	2.59	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	291/308 (94%)	256 (88%)	25 (9%)	10 (3%)	5 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	291/308 (94%)	245 (84%)	32 (11%)	14 (5%)	3	3
1	C	291/308 (94%)	251 (86%)	28 (10%)	12 (4%)	3	4
All	All	873/924 (94%)	752 (86%)	85 (10%)	36 (4%)	3	4

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	PRO
1	B	46	LYS
1	B	275	GLY
1	C	46	LYS
1	C	275	GLY
1	C	277	CYS
1	A	7	TYR
1	A	155	PRO
1	A	260	GLU
1	A	273	GLY
1	B	7	TYR
1	B	278	GLY
1	C	273	GLY
1	C	278	GLY
1	A	277	CYS
1	B	5	ALA
1	B	121	ILE
1	B	274	GLU
1	C	161	GLY
1	C	208	PHE
1	A	48	PRO
1	A	207	LEU
1	A	218	PRO
1	B	140	ASP
1	B	164	TYR
1	B	276	ARG
1	B	277	CYS
1	C	276	ARG
1	C	298	ASP
1	A	276	ARG
1	B	207	LEU
1	C	7	TYR
1	C	106	GLY
1	C	162	GLY

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Mol	Chain	Res	Type
1	B	273	GLY
1	B	48	PRO

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	242/250 (97%)	215 (89%)	27 (11%)	7	14
1	B	242/250 (97%)	215 (89%)	27 (11%)	7	14
1	C	242/250 (97%)	208 (86%)	34 (14%)	4	8
All	All	726/750 (97%)	638 (88%)	88 (12%)	6	11

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	10	PHE
1	A	35	VAL
1	A	60	LEU
1	A	99	LEU
1	A	107	MET
1	A	120	ILE
1	A	124	PHE
1	A	126	TRP
1	A	151	PRO
1	A	168	LEU
1	A	180	GLN
1	A	197	GLU
1	A	209	THR
1	A	214	SER
1	A	218	PRO
1	A	225	ILE
1	A	232	LEU
1	A	239	GLN
1	A	243	ARG

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Mol	Chain	Res	Type
1	A	252	VAL
1	A	254	MET
1	A	265	ARG
1	A	276	ARG
1	A	277	CYS
1	A	293	THR
1	A	300	TRP
1	B	4	LYS
1	B	6	ASP
1	B	10	PHE
1	B	14	MET
1	B	22	VAL
1	B	35	VAL
1	B	50	VAL
1	B	60	LEU
1	B	61	HIS
1	B	72	SER
1	B	96	ILE
1	B	99	LEU
1	B	105	VAL
1	B	107	MET
1	B	116	SER
1	B	120	ILE
1	B	166	SER
1	B	172	SER
1	B	197	GLU
1	B	199	LEU
1	B	207	LEU
1	B	209	THR
1	B	214	SER
1	B	231	GLU
1	B	234	ILE
1	B	252	VAL
1	B	276	ARG
1	C	6	ASP
1	C	10	PHE
1	C	14	MET
1	C	22	VAL
1	C	24	VAL
1	C	35	VAL
1	C	45	HIS
1	C	46	LYS

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Mol	Chain	Res	Type
1	C	48	PRO
1	C	49	VAL
1	C	60	LEU
1	C	82	CYS
1	C	85	VAL
1	C	97	ARG
1	C	99	LEU
1	C	107	MET
1	C	112	PRO
1	C	120	ILE
1	C	137	GLN
1	C	139	ILE
1	C	142	MET
1	C	151	PRO
1	C	154	ILE
1	C	168	LEU
1	C	172	SER
1	C	197	GLU
1	C	199	LEU
1	C	207	LEU
1	C	209	THR
1	C	243	ARG
1	C	276	ARG
1	C	282	LYS
1	C	293	THR
1	C	299	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	27	HIS
1	A	30	HIS
1	A	45	HIS
1	A	56	HIS
1	A	89	ASN
1	A	198	ASN
1	B	23	HIS
1	B	30	HIS
1	B	45	HIS
1	B	56	HIS
1	B	61	HIS

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Mol	Chain	Res	Type
1	C	23	HIS
1	C	27	HIS
1	C	45	HIS
1	C	56	HIS
1	C	58	GLN
1	C	61	HIS
1	C	147	ASN
1	C	198	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	PLP	A	413	1	15,15,16	2.33	5 (33%)	21,22,23	2.83	11 (52%)
2	PLP	B	413	1	15,15,16	3.89	9 (60%)	21,22,23	2.43	9 (42%)
2	PLP	C	413	1	15,15,16	4.34	10 (66%)	21,22,23	2.92	11 (52%)

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
2	PLP	A	413	1	-	0/6/6/8	0/1/1/1
2	PLP	B	413	1	-	0/6/6/8	0/1/1/1
2	PLP	C	413	1	-	0/6/6/8	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	413	PLP	C3-C2	-11.50	1.32	1.40
2	B	413	PLP	C3-C2	-10.75	1.33	1.40
2	C	413	PLP	C5-C4	-7.86	1.31	1.40
2	A	413	PLP	C3-C4	-5.06	1.27	1.40
2	C	413	PLP	O3-C3	-4.38	1.26	1.37
2	C	413	PLP	C3-C4	-4.18	1.29	1.40
2	C	413	PLP	C2-N1	-3.37	1.26	1.34
2	A	413	PLP	C2A-C2	-3.33	1.43	1.50
2	B	413	PLP	P-O1P	-3.06	1.41	1.51
2	B	413	PLP	P-O3P	-2.98	1.44	1.54
2	B	413	PLP	O4P-C5A	-2.84	1.32	1.44
2	A	413	PLP	P-O3P	-2.69	1.45	1.54
2	C	413	PLP	P-O1P	-2.64	1.42	1.51
2	B	413	PLP	P-O4P	-2.44	1.52	1.60
2	C	413	PLP	P-O2P	-2.43	1.46	1.54
2	A	413	PLP	C6-C5	-2.02	1.33	1.37
2	C	413	PLP	C2A-C2	2.13	1.54	1.50
2	B	413	PLP	C5-C4	2.37	1.43	1.40
2	C	413	PLP	C5A-C5	2.48	1.58	1.50
2	B	413	PLP	C2-N1	2.83	1.40	1.34
2	C	413	PLP	C6-N1	3.35	1.41	1.34
2	A	413	PLP	C6-N1	4.09	1.43	1.34
2	B	413	PLP	C6-N1	4.12	1.43	1.34
2	B	413	PLP	C2A-C2	5.88	1.62	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	413	PLP	O2P-P-O4P	-8.23	82.88	106.56
2	C	413	PLP	O2P-P-O4P	-4.53	93.51	106.56
2	C	413	PLP	O4P-P-O1P	-3.99	96.99	107.14
2	B	413	PLP	C2A-C2-C3	-3.98	116.24	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	413	PLP	O2P-P-O1P	-3.26	100.10	110.58
2	A	413	PLP	O2P-P-O1P	-3.21	100.26	110.58
2	C	413	PLP	C6-C5-C4	-3.12	115.50	118.15
2	B	413	PLP	O3P-P-O2P	-2.96	96.09	107.38
2	A	413	PLP	C4A-C4-C3	-2.74	115.40	120.36
2	B	413	PLP	C4A-C4-C3	-2.64	115.57	120.36
2	C	413	PLP	C3-C2-N1	-2.36	117.35	120.61
2	A	413	PLP	C5-C6-N1	-2.20	120.03	123.86
2	B	413	PLP	C5-C6-N1	-2.09	120.23	123.86
2	A	413	PLP	C3-C4-C5	2.07	121.03	118.78
2	B	413	PLP	O3P-P-O1P	2.29	117.97	110.58
2	C	413	PLP	C3-C4-C5	2.31	121.30	118.78
2	A	413	PLP	C4A-C4-C5	2.33	123.31	120.88
2	A	413	PLP	O3P-P-O2P	2.38	116.43	107.38
2	A	413	PLP	O3-C3-C2	2.85	122.62	117.66
2	B	413	PLP	O2P-P-O4P	2.90	114.92	106.56
2	B	413	PLP	C5A-C5-C4	2.97	125.58	121.65
2	C	413	PLP	C4-C3-C2	3.00	125.17	120.05
2	C	413	PLP	O3P-P-O4P	3.17	115.70	106.56
2	A	413	PLP	O4P-C5A-C5	3.50	114.78	108.99
2	B	413	PLP	C2A-C2-N1	3.52	125.75	117.95
2	C	413	PLP	O3P-P-O2P	3.58	121.03	107.38
2	A	413	PLP	O3P-P-O1P	3.80	122.81	110.58
2	C	413	PLP	O3P-P-O1P	3.96	123.31	110.58
2	A	413	PLP	O4P-P-O1P	4.53	118.67	107.14
2	B	413	PLP	O4P-C5A-C5	6.03	118.97	108.99
2	C	413	PLP	O4P-C5A-C5	7.27	121.00	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	413	PLP	2	0
2	B	413	PLP	2	0
2	C	413	PLP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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