



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:30 PM GMT

PDB ID : 2E21
Title : Crystal structure of TilS in a complex with AMPPNP from Aquifex aeolicus.
Authors : Kuratani, M.; Yoshikawa, Y.; Sekine, S.; Ishii, T.; Shibata, R.; Bessho, Y.;
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-11-06
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

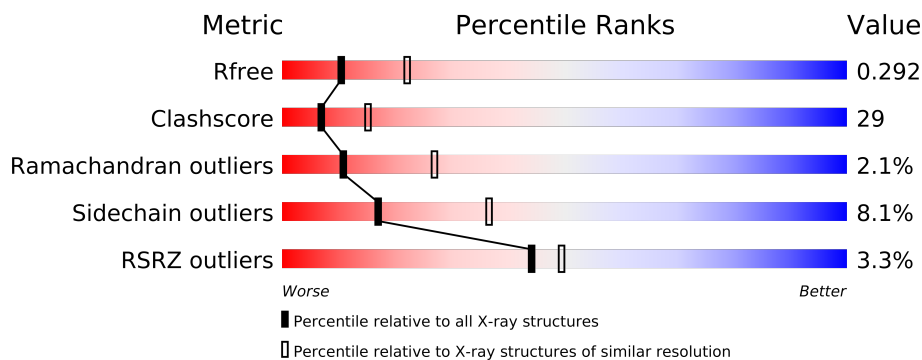
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	

2 Entry composition i

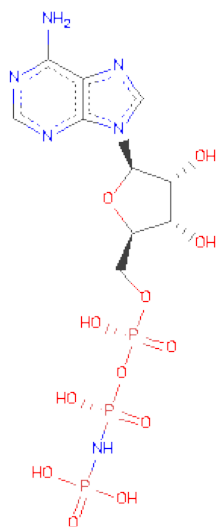
There are 3 unique types of molecules in this entry. The entry contains 10690 atoms, of which 0 are hydrogen and 0 are deuterium.

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 tRNA(Ile)-lysidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2630	1682	467	472	9			
1	B	314	Total	C	N	O	S	0	0	0
			2606	1667	464	466	9			
1	C	314	Total	C	N	O	S	0	0	0
			2606	1667	464	466	9			
1	D	314	Total	C	N	O	S	0	0	0
			2606	1667	464	466	9			

- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is water.

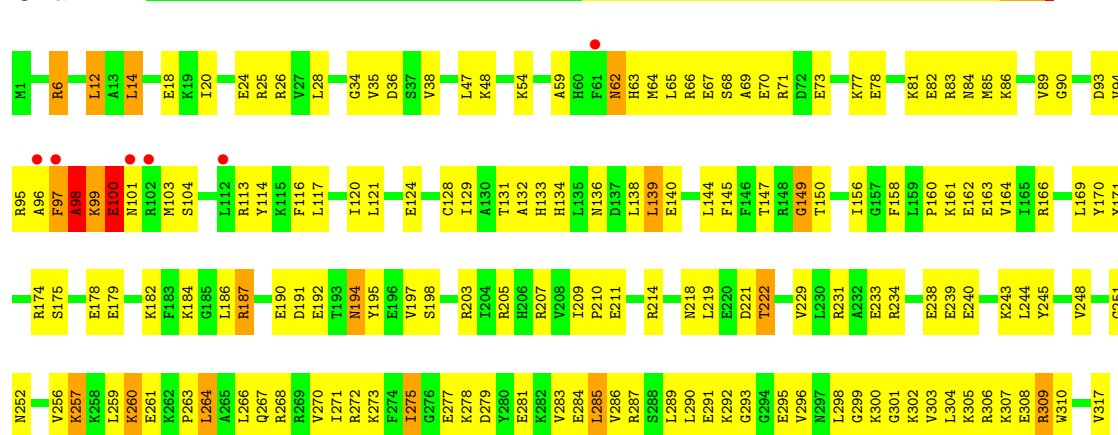
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	43	Total 43	O 43	0	0
3	C	59	Total 59	O 59	0	0
3	D	29	Total 29	O 29	0	0

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.

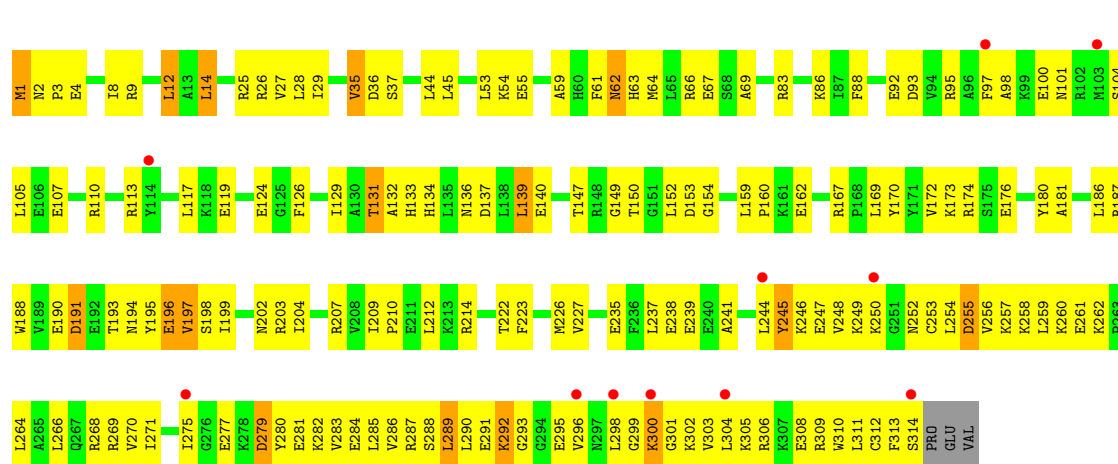
• Molecule 1: tRNA(Ile)-lysine synthase

Chain A:



• Molecule 1: tRNA(Ile)-lysine synthase

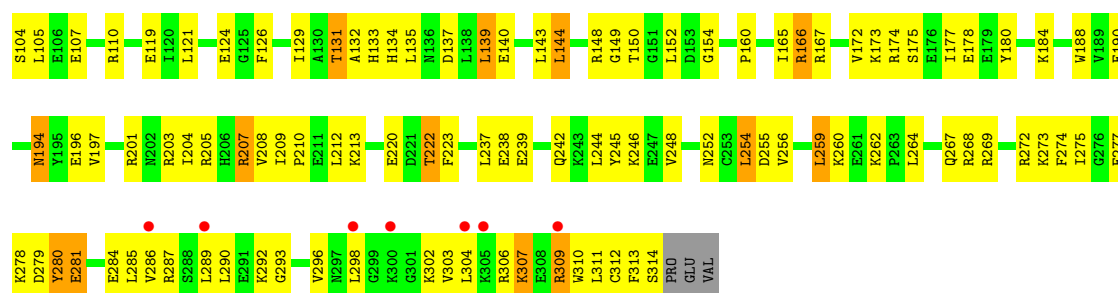
Chain B:



• Molecule 1: tRNA(Ile)-lysine synthase

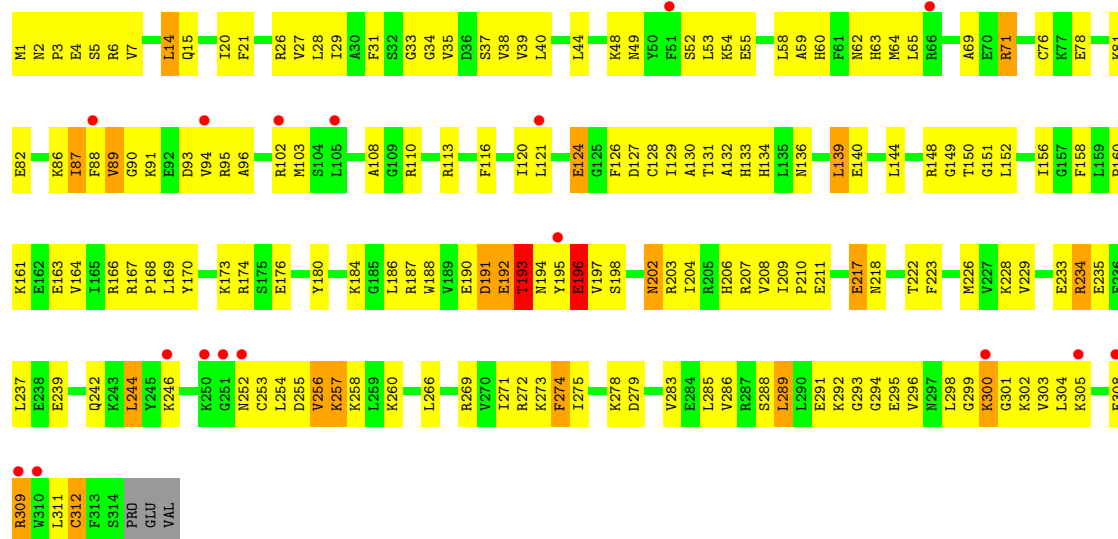
Chain C:





• Molecule 1: tRNA(Ile)-lysine synthase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.46Å 82.23Å 109.43Å 90.00° 105.85° 90.00°	Depositor
Resolution (Å)	49.01 – 2.70 49.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.01-2.70) 93.1 (49.01-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.294 0.221 , 0.292	Depositor DCC
R_{free} test set	2199 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 46212 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10690	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.56	1/2672 (0.0%)	0.70	5/3569 (0.1%)
1	B	0.44	0/2647	0.63	1/3535 (0.0%)
1	C	0.45	0/2647	0.68	1/3535 (0.0%)
1	D	0.38	0/2647	0.57	0/3535
All	All	0.46	1/10613 (0.0%)	0.65	7/14174 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ALA	CA-CB	-16.04	1.18	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLU	N-CA-C	-8.12	89.08	111.00
1	B	196	GLU	N-CA-C	-6.99	92.12	111.00
1	A	97	PHE	N-CA-C	-6.86	92.47	111.00
1	A	98	ALA	CB-CA-C	-6.86	99.82	110.10
1	C	307	LYS	N-CA-C	-5.55	96.02	111.00
1	A	97	PHE	CA-C-O	5.19	130.99	120.10
1	A	97	PHE	CA-C-N	-5.13	105.92	117.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2722	182	0
1	B	2606	0	2700	163	0
1	C	2606	0	2700	152	0
1	D	2606	0	2700	160	0
2	A	31	0	12	3	0
2	C	31	0	13	0	0
3	A	49	0	0	7	0
3	B	43	0	0	6	0
3	C	59	0	0	7	0
3	D	29	0	0	3	0
All	All	10690	0	10847	614	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (614) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:LYS:HG2	1:A:103:MET:H	1.09	1.18
1:A:95:ARG:C	1:A:98:ALA:HB2	1.64	1.16
1:A:95:ARG:O	1:A:98:ALA:CB	1.93	1.16
1:B:105:LEU:HD21	3:B:359:HOH:O	1.51	1.11
1:D:121:LEU:HD21	1:D:164:VAL:HG21	1.32	1.10
1:B:95:ARG:HA	3:B:359:HOH:O	1.60	1.00
1:A:6:ARG:HH11	1:A:6:ARG:HG2	1.27	1.00
1:B:295:GLU:HB3	1:B:305:LYS:HG3	1.41	0.99
1:C:131:THR:HG21	1:C:133:HIS:ND1	1.77	0.99
1:C:194:ASN:H	1:C:194:ASN:HD22	1.02	0.96
1:C:292:LYS:HG2	1:C:293:GLY:H	1.33	0.93
1:A:131:THR:HG22	1:A:133:HIS:H	1.33	0.93
1:C:252:ASN:HD21	1:C:313:PHE:HB2	1.32	0.93
1:C:62:ASN:ND2	1:C:64:MET:H	1.68	0.92
1:C:254:LEU:O	1:C:310:TRP:CE3	2.23	0.92
1:A:99:LYS:HG3	1:A:103:MET:O	1.71	0.90
1:B:181:ALA:HA	1:B:186:LEU:HD12	1.53	0.89
1:B:244:LEU:HD11	1:B:262:LYS:HG3	1.56	0.88
1:C:254:LEU:O	1:C:310:TRP:HE3	1.58	0.86
1:B:139:LEU:HD13	1:B:209:ILE:HD12	1.57	0.86
1:C:256:VAL:CG2	1:C:290:LEU:HD23	2.07	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:14:LEU:HD13	1:D:20:ILE:HD11	1.59	0.83
1:C:20:ILE:HG23	1:C:166:ARG:HG3	1.61	0.83
1:D:14:LEU:HD11	1:D:170:TYR:HB3	1.61	0.83
1:C:194:ASN:HD22	1:C:194:ASN:N	1.74	0.83
1:A:96:ALA:C	1:A:98:ALA:N	2.22	0.83
1:C:256:VAL:HG22	1:C:290:LEU:HD23	1.61	0.82
1:D:131:THR:HG22	1:D:133:HIS:H	1.45	0.81
1:A:190:GLU:HB3	1:D:71:ARG:HH12	1.43	0.81
1:A:131:THR:HG21	1:A:133:HIS:CE1	2.15	0.81
1:D:29:ILE:HD11	1:D:44:LEU:HD12	1.64	0.80
1:B:26:ARG:HG3	1:B:55:GLU:HB3	1.61	0.79
1:A:99:LYS:CG	1:A:103:MET:H	1.92	0.79
1:A:97:PHE:HE2	1:A:103:MET:HE1	1.45	0.79
1:A:6:ARG:HH11	1:A:6:ARG:CG	1.93	0.79
1:A:95:ARG:C	1:A:98:ALA:CB	2.39	0.79
1:B:62:ASN:HD21	1:B:69:ALA:HB1	1.48	0.79
1:D:257:LYS:N	1:D:257:LYS:HE2	1.97	0.78
1:C:256:VAL:O	1:C:260:LYS:HB2	1.82	0.78
1:D:202:ASN:HD22	1:D:202:ASN:N	1.82	0.78
1:B:191:ASP:HB3	1:B:194:ASN:HD22	1.49	0.78
1:A:65:LEU:HA	1:A:95:ARG:NH1	1.99	0.77
1:C:292:LYS:HG2	1:C:293:GLY:N	1.98	0.77
1:B:275:ILE:HG23	1:B:277:GLU:H	1.50	0.77
1:A:302:LYS:HG2	3:A:546:HOH:O	1.85	0.77
1:A:162:GLU:OE1	3:A:544:HOH:O	2.02	0.76
1:B:303:VAL:HG13	1:B:314:SER:HB3	1.67	0.76
1:B:266:LEU:O	1:B:269:ARG:HB2	1.86	0.76
1:A:260:LYS:HD2	1:A:261:GLU:HG3	1.68	0.76
1:A:197:VAL:HG11	1:A:207:ARG:NH2	2.01	0.76
1:A:131:THR:HG21	1:A:133:HIS:ND1	2.02	0.75
1:C:275:ILE:HG21	1:C:286:VAL:HG21	1.69	0.75
1:A:95:ARG:O	1:A:98:ALA:HB3	1.88	0.74
1:C:254:LEU:HD23	1:C:311:LEU:HD23	1.70	0.74
1:D:272:ARG:HD3	1:D:278:LYS:NZ	2.04	0.73
1:A:234:ARG:HD3	1:A:238:GLU:OE1	1.89	0.73
1:D:1:MET:HB2	1:D:5:SER:OG	1.88	0.73
1:C:306:ARG:HG2	1:C:307:LYS:O	1.88	0.73
1:A:305:LYS:HE2	1:A:307:LYS:HE3	1.69	0.73
1:D:257:LYS:H	1:D:257:LYS:HE2	1.52	0.73
1:A:99:LYS:HG2	1:A:103:MET:N	1.95	0.72
1:B:187:ARG:HG2	1:C:196:GLU:HG2	1.69	0.72
1:B:255:ASP:OD1	1:B:257:LYS:HB3	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:298:LEU:HB2	1:C:302:LYS:HB2	1.72	0.71
1:A:197:VAL:HG23	1:A:203:ARG:HA	1.72	0.71
1:C:256:VAL:HG22	1:C:290:LEU:CD2	2.20	0.71
1:C:62:ASN:HD22	1:C:64:MET:H	1.36	0.71
1:A:94:VAL:O	1:A:98:ALA:HB2	1.91	0.70
1:A:229:VAL:HA	1:B:268:ARG:NH1	2.06	0.70
1:B:191:ASP:CB	1:B:194:ASN:HD22	2.04	0.70
1:C:205:ARG:HA	1:C:209:ILE:HD13	1.72	0.70
1:B:93:ASP:OD1	1:B:95:ARG:HB3	1.91	0.70
1:C:131:THR:HG23	1:C:133:HIS:H	1.55	0.70
1:B:275:ILE:HD12	1:B:286:VAL:HG21	1.73	0.70
1:C:14:LEU:HD13	1:C:20:ILE:HG13	1.74	0.70
1:A:139:LEU:HD13	1:A:209:ILE:HD12	1.73	0.70
1:D:139:LEU:HD13	1:D:209:ILE:HD12	1.74	0.69
1:B:35:VAL:HG13	1:B:188:TRP:CE2	2.27	0.69
1:C:36:ASP:HB2	1:C:132:ALA:HB1	1.74	0.69
1:B:14:LEU:HD11	1:B:170:TYR:HB3	1.73	0.69
1:C:306:ARG:CG	1:C:307:LYS:O	2.41	0.69
1:D:134:HIS:HD2	1:D:136:ASN:H	1.40	0.69
1:C:296:VAL:O	1:C:303:VAL:HA	1.93	0.69
1:B:29:ILE:HD11	1:B:44:LEU:HD12	1.75	0.69
1:C:255:ASP:HA	1:C:309:ARG:O	1.92	0.68
1:A:131:THR:HG22	1:A:133:HIS:N	2.07	0.68
1:B:131:THR:HG21	1:B:133:HIS:ND1	2.09	0.68
1:C:194:ASN:ND2	1:C:194:ASN:H	1.80	0.68
1:D:257:LYS:HD2	1:D:309:ARG:HB2	1.75	0.68
1:A:95:ARG:O	1:A:98:ALA:HB2	1.68	0.68
1:C:207:ARG:HG2	1:D:211:GLU:CD	2.13	0.68
1:D:209:ILE:HB	1:D:210:PRO:HD3	1.74	0.68
1:A:209:ILE:HB	1:A:210:PRO:HD3	1.75	0.67
1:A:66:ARG:HD2	1:D:187:ARG:NH1	2.08	0.67
1:C:35:VAL:HG23	3:C:551:HOH:O	1.94	0.67
1:A:77:LYS:O	1:A:81:LYS:HG3	1.95	0.67
1:D:197:VAL:HG21	1:D:207:ARG:NH2	2.10	0.67
1:A:293:GLY:HA2	1:A:306:ARG:HD3	1.76	0.67
1:A:121:LEU:HD11	1:A:164:VAL:HG21	1.75	0.67
1:A:128:CYS:HA	1:A:164:VAL:HG22	1.76	0.67
1:B:62:ASN:ND2	1:B:64:MET:H	1.93	0.67
1:B:88:PHE:CZ	1:B:124:GLU:HG2	2.29	0.67
1:C:104:SER:OG	1:C:107:GLU:HG2	1.95	0.67
1:C:62:ASN:ND2	1:C:69:ALA:HB1	2.10	0.67
1:B:253:CYS:O	1:B:254:LEU:HD12	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:121:LEU:CD2	1:D:164:VAL:HG21	2.18	0.66
1:C:131:THR:CG2	1:C:133:HIS:H	2.09	0.66
1:A:100:GLU:C	1:A:100:GLU:OE2	2.33	0.66
1:C:296:VAL:HB	1:C:304:LEU:H	1.60	0.66
1:D:308:GLU:HG3	1:D:309:ARG:H	1.59	0.66
1:B:248:VAL:HG11	1:B:259:LEU:HG	1.76	0.66
1:A:65:LEU:HD21	1:A:94:VAL:HB	1.78	0.66
1:A:260:LYS:HD3	1:A:291:GLU:OE1	1.96	0.66
1:D:49:ASN:O	1:D:52:SER:N	2.27	0.65
1:D:292:LYS:HG2	1:D:293:GLY:H	1.62	0.65
1:B:305:LYS:HB3	1:B:305:LYS:NZ	2.12	0.65
1:D:14:LEU:HB3	1:D:20:ILE:HD11	1.78	0.65
1:A:266:LEU:O	1:A:270:VAL:HG23	1.97	0.65
1:A:156:ILE:HD12	1:A:234:ARG:NE	2.13	0.64
1:D:63:HIS:HB3	1:D:65:LEU:HG	1.80	0.64
1:B:25:ARG:HG3	1:B:54:LYS:NZ	2.12	0.64
1:A:275:ILE:CD1	1:A:286:VAL:HG21	2.27	0.64
1:A:86:LYS:HB2	1:A:86:LYS:NZ	2.12	0.64
1:A:96:ALA:C	1:A:98:ALA:H	1.93	0.64
1:A:275:ILE:HD11	1:A:286:VAL:HG21	1.78	0.64
1:D:289:LEU:HD23	1:D:311:LEU:HD11	1.78	0.64
1:D:121:LEU:HD12	1:D:126:PHE:HB2	1.80	0.64
1:D:110:ARG:NH1	1:D:113:ARG:HH22	1.96	0.64
1:C:222:THR:HG22	3:D:345:HOH:O	1.97	0.63
1:B:196:GLU:HG2	1:B:198:SER:OG	1.99	0.63
1:B:260:LYS:HG3	1:B:291:GLU:OE1	1.98	0.63
1:A:285:LEU:HD12	1:A:296:VAL:CG1	2.29	0.63
1:C:204:ILE:HG22	1:C:209:ILE:CD1	2.28	0.63
1:A:78:GLU:O	1:A:82:GLU:HG3	1.98	0.63
1:C:256:VAL:HG21	1:C:290:LEU:HA	1.81	0.62
1:B:281:GLU:OE2	1:B:281:GLU:HA	1.98	0.62
1:B:300:LYS:HG3	1:B:300:LYS:O	1.97	0.62
1:B:190:GLU:HG3	1:C:207:ARG:NH2	2.14	0.62
1:A:248:VAL:HG11	1:A:259:LEU:HB2	1.80	0.62
1:D:272:ARG:HD3	1:D:278:LYS:HZ2	1.65	0.62
1:A:99:LYS:HG3	1:A:103:MET:C	2.19	0.62
1:C:131:THR:CG2	1:C:133:HIS:ND1	2.58	0.62
1:B:159:LEU:HB2	1:B:162:GLU:HG3	1.81	0.62
1:A:28:LEU:HD11	1:A:59:ALA:HB2	1.81	0.62
1:C:306:ARG:HB3	3:C:559:HOH:O	2.00	0.61
1:B:55:GLU:OE1	1:B:86:LYS:HE2	2.01	0.61
1:D:234:ARG:HB3	1:D:234:ARG:HH11	1.66	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:62:ASN:C	1:C:62:ASN:HD22	2.03	0.61
1:A:203:ARG:HH12	1:B:214:ARG:HH11	1.46	0.61
1:B:35:VAL:HG13	1:B:188:TRP:CD2	2.36	0.61
1:A:257:LYS:HE3	1:A:306:ARG:NH1	2.15	0.61
1:C:259:LEU:HD22	1:C:267:GLN:HG2	1.82	0.61
1:B:62:ASN:ND2	1:B:69:ALA:HB1	2.15	0.61
1:D:161:LYS:HG3	1:D:166:ARG:HD3	1.81	0.61
1:A:218:ASN:ND2	3:A:549:HOH:O	2.32	0.61
1:C:256:VAL:CG2	1:C:290:LEU:HA	2.31	0.61
1:D:14:LEU:HD11	1:D:170:TYR:CB	2.30	0.61
1:C:20:ILE:CG2	1:C:166:ARG:HG3	2.30	0.61
1:C:149:GLY:HA2	1:D:222:THR:HG23	1.82	0.61
1:D:65:LEU:HA	1:D:95:ARG:HH22	1.66	0.60
1:A:222:THR:HG23	1:B:149:GLY:HA2	1.83	0.60
1:C:304:LEU:HA	1:C:312:CYS:O	2.01	0.60
1:A:267:GLN:O	1:A:271:ILE:HG12	2.01	0.60
1:B:289:LEU:HD12	1:B:292:LYS:O	2.00	0.60
1:A:36:ASP:HB3	1:A:132:ALA:HB1	1.84	0.60
1:D:15:GLN:HE22	1:D:21:PHE:HB2	1.65	0.60
1:C:14:LEU:HD13	1:C:20:ILE:CG1	2.31	0.60
1:B:139:LEU:CD1	1:B:209:ILE:HD12	2.30	0.60
1:D:63:HIS:O	1:D:64:MET:HB2	2.02	0.60
1:B:173:LYS:HG2	1:B:176:GLU:HG3	1.84	0.60
1:C:306:ARG:HG3	1:C:310:TRP:O	2.02	0.59
1:C:7:VAL:O	1:C:11:VAL:HG23	2.03	0.59
1:B:271:ILE:O	1:B:275:ILE:HG22	2.02	0.59
1:D:271:ILE:O	1:D:275:ILE:HG12	2.02	0.59
1:B:194:ASN:O	1:B:195:TYR:HB2	2.01	0.59
1:A:93:ASP:HB3	1:A:96:ALA:HB3	1.84	0.59
1:C:62:ASN:HD22	1:C:63:HIS:N	2.01	0.59
1:D:65:LEU:HD21	1:D:94:VAL:HB	1.84	0.59
1:C:268:ARG:HD2	3:C:553:HOH:O	2.01	0.59
1:A:131:THR:HG21	1:A:133:HIS:CG	2.38	0.59
1:C:204:ILE:HG22	1:C:209:ILE:HD11	1.85	0.59
1:A:26:ARG:HH22	1:A:54:LYS:HD2	1.67	0.59
1:D:173:LYS:HG2	1:D:176:GLU:OE1	2.02	0.59
1:A:150:THR:O	1:B:226:MET:HG3	2.02	0.59
1:A:190:GLU:CD	1:A:190:GLU:H	2.03	0.58
1:B:83:ARG:HG3	1:B:83:ARG:HH11	1.67	0.58
1:A:95:ARG:O	1:A:98:ALA:HB1	1.99	0.58
1:C:62:ASN:ND2	1:C:64:MET:N	2.47	0.58
1:D:29:ILE:CD1	1:D:44:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:296:VAL:O	1:B:303:VAL:HG23	2.03	0.58
1:B:62:ASN:C	1:B:62:ASN:HD22	2.05	0.58
1:B:83:ARG:NE	3:B:351:HOH:O	2.32	0.58
1:A:97:PHE:HE2	1:A:103:MET:CE	2.16	0.58
1:C:194:ASN:ND2	1:C:194:ASN:N	2.46	0.58
1:A:174:ARG:O	1:A:178:GLU:HG3	2.04	0.58
1:A:131:THR:HG23	2:A:500:ANP:O2'	2.03	0.58
1:A:83:ARG:HB2	1:A:85:MET:HG3	1.85	0.58
1:A:99:LYS:CG	1:A:103:MET:O	2.49	0.58
1:D:298:LEU:HB2	1:D:302:LYS:HB3	1.86	0.58
1:D:93:ASP:OD2	1:D:96:ALA:HB3	2.03	0.58
1:A:289:LEU:O	1:A:306:ARG:HD2	2.04	0.58
1:A:6:ARG:HG2	1:A:6:ARG:NH1	2.05	0.57
1:C:62:ASN:HD21	1:C:69:ALA:HB1	1.68	0.57
1:B:66:ARG:NE	1:B:66:ARG:HA	2.19	0.57
1:A:233:GLU:HB3	1:B:237:LEU:HD11	1.87	0.57
1:B:209:ILE:HB	1:B:210:PRO:HD3	1.87	0.57
1:A:121:LEU:HD12	1:A:129:ILE:HG13	1.85	0.57
1:D:86:LYS:HD3	1:D:87:ILE:H	1.69	0.57
1:A:191:ASP:O	1:A:192:GLU:HB2	2.05	0.57
1:A:275:ILE:HG22	1:A:277:GLU:H	1.69	0.57
1:A:275:ILE:HD11	1:A:286:VAL:CG2	2.34	0.57
1:B:124:GLU:HB3	1:B:126:PHE:CE1	2.40	0.57
1:C:281:GLU:N	1:C:281:GLU:OE1	2.38	0.57
1:C:173:LYS:HE3	3:C:525:HOH:O	2.04	0.56
1:C:149:GLY:CA	1:D:222:THR:HG23	2.35	0.56
1:C:256:VAL:O	1:C:260:LYS:CB	2.53	0.56
1:A:187:ARG:N	1:A:187:ARG:HD2	2.20	0.56
1:A:64:MET:O	1:A:65:LEU:HD23	2.06	0.56
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.70	0.56
1:A:257:LYS:HD2	1:A:309:ARG:HB2	1.86	0.56
1:B:134:HIS:HD2	1:B:136:ASN:H	1.52	0.56
1:D:131:THR:HG21	1:D:133:HIS:ND1	2.20	0.56
1:B:197:VAL:HG22	1:B:203:ARG:HA	1.88	0.56
1:A:285:LEU:HD12	1:A:296:VAL:HG11	1.88	0.56
1:D:161:LYS:HG3	1:D:166:ARG:CD	2.36	0.56
1:B:280:TYR:CZ	1:B:284:GLU:HG3	2.41	0.56
1:C:28:LEU:HD11	1:C:59:ALA:HB2	1.87	0.56
1:D:292:LYS:HG2	1:D:293:GLY:N	2.21	0.56
1:D:86:LYS:HD3	1:D:87:ILE:N	2.20	0.56
1:C:280:TYR:CZ	1:C:284:GLU:HG3	2.41	0.56
1:D:38:VAL:HG12	1:D:186:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:248:VAL:HG22	1:B:258:LYS:HB2	1.89	0.55
1:A:190:GLU:CB	1:D:71:ARG:HH12	2.18	0.55
1:B:190:GLU:HG3	1:C:207:ARG:CZ	2.36	0.55
1:C:140:GLU:OE2	1:C:174:ARG:NH2	2.36	0.55
1:B:187:ARG:CZ	1:C:66:ARG:HD3	2.37	0.55
1:C:134:HIS:HD2	1:C:137:ASP:H	1.54	0.55
1:B:150:THR:OG1	1:B:154:GLY:HA3	2.07	0.55
1:A:66:ARG:HD2	1:D:187:ARG:CZ	2.37	0.55
1:B:279:ASP:O	1:B:283:VAL:HG23	2.07	0.55
1:B:308:GLU:OE1	1:B:308:GLU:HA	2.06	0.55
1:C:254:LEU:HB2	1:C:311:LEU:HB3	1.88	0.55
1:D:204:ILE:O	1:D:209:ILE:HG12	2.06	0.55
1:C:135:LEU:HD21	1:C:220:GLU:O	2.06	0.55
1:B:25:ARG:HG3	1:B:54:LYS:HZ3	1.71	0.55
1:B:199:ILE:HB	1:B:202:ASN:ND2	2.21	0.55
1:B:25:ARG:NH2	3:B:319:HOH:O	2.39	0.55
1:D:254:LEU:HD13	1:D:274:PHE:CE1	2.41	0.55
1:A:94:VAL:O	1:A:98:ALA:CA	2.56	0.54
1:A:67:GLU:OE1	1:D:81:LYS:HG2	2.07	0.54
1:D:235:GLU:O	1:D:239:GLU:HG3	2.06	0.54
1:B:287:ARG:O	1:B:290:LEU:HG	2.08	0.54
1:D:29:ILE:HG12	1:D:130:ALA:HB3	1.88	0.54
1:B:304:LEU:HA	1:B:313:PHE:HA	1.89	0.54
1:D:255:ASP:HB3	1:D:258:LYS:HE3	1.90	0.54
1:D:255:ASP:OD2	1:D:258:LYS:HE2	2.07	0.54
1:C:86:LYS:HD2	1:C:87:ILE:H	1.74	0.53
1:C:152:LEU:HD21	1:D:152:LEU:HD21	1.89	0.53
1:A:190:GLU:HB3	1:D:71:ARG:NH1	2.19	0.53
1:A:83:ARG:CB	1:A:85:MET:HG3	2.38	0.53
1:C:88:PHE:CZ	1:C:124:GLU:HG2	2.43	0.53
1:B:187:ARG:HG2	1:C:196:GLU:CG	2.39	0.53
1:D:87:ILE:C	1:D:87:ILE:HD13	2.29	0.53
1:C:292:LYS:CG	1:C:293:GLY:H	2.16	0.53
1:A:178:GLU:O	1:A:182:LYS:HG3	2.09	0.53
1:D:308:GLU:HA	1:D:308:GLU:OE2	2.08	0.53
1:B:300:LYS:O	1:B:302:LYS:N	2.42	0.53
1:C:207:ARG:NH1	3:C:550:HOH:O	2.22	0.53
1:C:248:VAL:HG13	1:C:255:ASP:HB3	1.91	0.53
1:C:1:MET:HG3	1:C:5:SER:OG	2.09	0.53
1:A:194:ASN:ND2	1:D:190:GLU:CG	2.71	0.53
1:C:287:ARG:HG3	1:C:290:LEU:HD12	1.90	0.53
1:A:275:ILE:HG23	1:A:277:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:238:GLU:O	1:C:242:GLN:HG2	2.09	0.53
1:D:60:HIS:CD2	1:D:76:CYS:SG	3.01	0.53
1:A:6:ARG:NH1	1:A:6:ARG:CG	2.63	0.53
1:C:204:ILE:O	1:C:209:ILE:HD12	2.08	0.53
1:B:253:CYS:HA	1:B:311:LEU:O	2.09	0.53
1:B:235:GLU:HG2	1:B:239:GLU:OE2	2.09	0.53
1:D:308:GLU:HG3	1:D:309:ARG:N	2.22	0.52
1:B:139:LEU:HD13	1:B:209:ILE:CD1	2.34	0.52
1:C:222:THR:HG23	1:D:149:GLY:CA	2.39	0.52
1:B:308:GLU:HG3	1:B:309:ARG:H	1.74	0.52
1:A:116:PHE:O	1:A:120:ILE:HG12	2.09	0.52
1:D:39:VAL:HG13	1:D:180:TYR:CD2	2.45	0.52
1:A:73:GLU:CD	1:A:89:VAL:HG21	2.29	0.52
1:A:244:LEU:HD23	1:A:266:LEU:HB3	1.90	0.52
1:B:104:SER:OG	1:B:107:GLU:HG2	2.10	0.52
1:B:173:LYS:CG	1:B:176:GLU:HG3	2.40	0.52
1:A:175:SER:O	1:A:179:GLU:HG3	2.09	0.52
1:B:223:PHE:O	1:B:227:VAL:HG23	2.10	0.52
1:A:134:HIS:HD2	1:A:136:ASN:H	1.58	0.52
1:C:296:VAL:HG21	1:C:304:LEU:HB2	1.92	0.52
1:B:35:VAL:HG22	3:B:322:HOH:O	2.09	0.52
1:B:160:PRO:HD3	1:B:170:TYR:CE1	2.45	0.52
1:A:131:THR:HG22	1:A:132:ALA:N	2.24	0.52
1:C:209:ILE:HB	1:C:210:PRO:HD3	1.91	0.52
1:C:222:THR:HG22	1:C:223:PHE:N	2.25	0.51
1:D:254:LEU:HD22	1:D:274:PHE:CD1	2.45	0.51
1:D:40:LEU:HB2	1:D:169:LEU:HD11	1.92	0.51
1:B:61:PHE:HB3	1:B:113:ARG:HG3	1.92	0.51
1:A:161:LYS:HG3	1:A:166:ARG:HD3	1.93	0.51
1:D:272:ARG:HD3	1:D:278:LYS:HZ3	1.75	0.51
1:A:139:LEU:HD11	1:A:219:LEU:HD23	1.92	0.51
1:C:124:GLU:HB3	1:C:126:PHE:CE1	2.45	0.51
1:C:303:VAL:CG1	1:C:314:SER:HB2	2.40	0.51
1:B:131:THR:CG2	1:B:133:HIS:H	2.24	0.51
1:A:275:ILE:CG2	1:A:277:GLU:H	2.23	0.51
1:D:260:LYS:HE3	1:D:291:GLU:OE2	2.11	0.51
1:D:59:ALA:HA	1:D:88:PHE:O	2.10	0.51
1:B:309:ARG:HG3	1:B:310:TRP:CD1	2.45	0.51
1:C:306:ARG:HG3	1:C:307:LYS:O	2.11	0.51
1:D:14:LEU:HB3	1:D:20:ILE:CD1	2.41	0.51
1:B:2:ASN:HB2	1:B:3:PRO:CD	2.41	0.51
1:D:192:GLU:O	1:D:193:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:300:LYS:O	1:D:300:LYS:HG3	2.11	0.51
1:A:147:THR:OG1	1:B:212:LEU:HD22	2.10	0.51
1:A:121:LEU:C	1:A:121:LEU:HD23	2.32	0.50
1:A:272:ARG:HD3	1:A:278:LYS:HD2	1.93	0.50
1:A:156:ILE:HD12	1:A:234:ARG:HE	1.76	0.50
1:B:308:GLU:HG3	1:B:309:ARG:N	2.26	0.50
1:C:144:LEU:HD22	1:C:148:ARG:HD2	1.93	0.50
1:A:131:THR:CG2	1:A:132:ALA:N	2.75	0.50
1:A:281:GLU:O	1:A:285:LEU:HB2	2.12	0.50
1:A:68:SER:O	1:A:70:GLU:N	2.44	0.50
1:A:251:GLY:C	1:A:252:ASN:HD22	2.15	0.50
1:B:254:LEU:HD23	1:B:259:LEU:HD11	1.94	0.50
1:D:253:CYS:O	1:D:254:LEU:HD12	2.11	0.50
1:B:207:ARG:CZ	1:D:195:TYR:HB3	2.41	0.50
1:A:138:LEU:HD13	1:A:158:PHE:CE1	2.46	0.50
1:A:222:THR:HG23	1:B:149:GLY:CA	2.42	0.50
1:A:14:LEU:HD13	1:A:20:ILE:CG1	2.42	0.49
1:D:237:LEU:HD13	1:D:269:ARG:HH21	1.77	0.49
1:C:81:LYS:HD3	1:C:81:LYS:O	2.12	0.49
1:B:2:ASN:HB2	1:B:3:PRO:HD2	1.94	0.49
1:A:34:GLY:O	1:A:38:VAL:HG23	2.12	0.49
1:D:128:CYS:HA	1:D:164:VAL:HG22	1.95	0.49
1:D:164:VAL:HG22	1:D:164:VAL:O	2.13	0.49
1:C:222:THR:HG23	1:D:149:GLY:HA2	1.93	0.49
1:B:124:GLU:HB3	1:B:126:PHE:HE1	1.76	0.49
1:A:287:ARG:HG3	1:A:290:LEU:HD12	1.94	0.49
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.27	0.49
1:A:205:ARG:O	1:A:210:PRO:HD3	2.12	0.49
1:D:257:LYS:HD2	1:D:309:ARG:CB	2.43	0.49
1:D:87:ILE:HD13	1:D:88:PHE:N	2.27	0.49
1:A:194:ASN:HD21	1:D:190:GLU:HG2	1.76	0.49
1:A:256:VAL:HG13	1:A:290:LEU:HA	1.95	0.49
1:A:257:LYS:HA	1:A:257:LYS:HE2	1.94	0.49
1:A:214:ARG:HD2	1:B:203:ARG:NH2	2.27	0.49
1:C:134:HIS:CD2	1:C:137:ASP:H	2.31	0.49
1:C:303:VAL:HG13	1:C:314:SER:HB2	1.95	0.48
1:D:131:THR:CG2	1:D:133:HIS:H	2.22	0.48
1:D:191:ASP:O	1:D:193:THR:HG23	2.13	0.48
1:D:2:ASN:HB2	1:D:3:PRO:CD	2.43	0.48
1:B:26:ARG:HB3	1:B:126:PHE:CD2	2.48	0.48
1:C:86:LYS:HD2	1:C:87:ILE:N	2.27	0.48
1:A:97:PHE:CE2	1:A:103:MET:HE1	2.36	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:197:VAL:HG12	1:D:203:ARG:CZ	2.43	0.48
1:A:306:ARG:HG3	1:A:310:TRP:O	2.14	0.48
1:B:254:LEU:O	1:B:256:VAL:N	2.46	0.48
1:A:86:LYS:HB2	1:A:86:LYS:HZ3	1.76	0.48
1:A:94:VAL:O	1:A:98:ALA:CB	2.60	0.48
1:C:296:VAL:CG2	1:C:304:LEU:HB2	2.44	0.48
1:A:156:ILE:CD1	1:A:231:ARG:HA	2.43	0.48
1:B:260:LYS:HD3	1:B:261:GLU:N	2.28	0.48
1:B:245:TYR:HD1	1:B:270:VAL:HG13	1.78	0.48
1:C:4:GLU:OE2	1:C:184:LYS:NZ	2.44	0.48
1:A:194:ASN:ND2	1:D:190:GLU:HG3	2.27	0.48
1:D:140:GLU:OE2	1:D:174:ARG:NH2	2.46	0.48
1:A:190:GLU:OE2	1:A:190:GLU:N	2.36	0.48
1:A:203:ARG:NH1	1:B:214:ARG:HH11	2.11	0.48
1:D:144:LEU:HD21	1:D:148:ARG:NE	2.28	0.48
1:B:95:ARG:HG3	3:B:359:HOH:O	2.14	0.48
1:B:191:ASP:HB3	1:B:194:ASN:HB2	1.96	0.48
1:B:275:ILE:HD11	1:B:298:LEU:HD13	1.94	0.48
1:B:2:ASN:OD1	1:B:2:ASN:N	2.47	0.48
1:D:26:ARG:NH1	1:D:124:GLU:O	2.47	0.47
1:C:260:LYS:HE2	1:C:290:LEU:O	2.14	0.47
1:D:242:GLN:O	1:D:246:LYS:HG2	2.14	0.47
1:C:293:GLY:HA2	3:C:559:HOH:O	2.14	0.47
1:B:190:GLU:HG2	1:B:191:ASP:N	2.29	0.47
1:B:86:LYS:HG2	1:B:88:PHE:CZ	2.49	0.47
1:B:62:ASN:HD22	1:B:63:HIS:N	2.12	0.47
1:B:250:LYS:NZ	1:B:255:ASP:HB2	2.29	0.47
1:A:117:LEU:HB3	1:A:129:ILE:HD13	1.94	0.47
1:C:48:LYS:HG3	1:C:53:LEU:HB2	1.94	0.47
1:A:295:GLU:HG3	1:A:305:LYS:HB2	1.96	0.47
1:C:87:ILE:HG12	1:C:88:PHE:N	2.29	0.47
1:A:24:GLU:O	1:A:25:ARG:HD3	2.15	0.47
1:A:184:LYS:HB2	1:A:186:LEU:HG	1.96	0.47
1:C:150:THR:OG1	1:C:154:GLY:HA3	2.13	0.47
1:B:204:ILE:O	1:B:209:ILE:HG12	2.15	0.47
1:C:4:GLU:OE2	1:C:46:LYS:HE2	2.13	0.47
1:C:203:ARG:HD3	1:D:211:GLU:OE1	2.14	0.47
1:B:131:THR:HG23	1:B:133:HIS:H	1.80	0.47
1:A:121:LEU:HD11	1:A:164:VAL:CG2	2.40	0.47
1:B:83:ARG:NH1	1:B:83:ARG:HG3	2.29	0.47
1:D:48:LYS:O	1:D:53:LEU:HB2	2.13	0.47
1:B:285:LEU:HG	1:B:296:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:187:ARG:CG	1:C:196:GLU:HG2	2.44	0.47
1:B:134:HIS:CD2	1:B:137:ASP:H	2.33	0.47
1:C:197:VAL:CG1	1:C:197:VAL:O	2.63	0.47
1:A:229:VAL:HA	1:B:268:ARG:HH12	1.78	0.47
1:B:29:ILE:CD1	1:B:44:LEU:HD12	2.44	0.47
1:A:14:LEU:HD13	1:A:20:ILE:HG13	1.97	0.47
1:A:304:LEU:N	1:A:304:LEU:HD12	2.30	0.47
1:A:62:ASN:HD22	1:A:62:ASN:C	2.17	0.47
1:B:62:ASN:C	1:B:62:ASN:ND2	2.68	0.47
1:D:28:LEU:O	1:D:129:ILE:HA	2.14	0.46
1:C:143:LEU:HD21	1:C:212:LEU:HD11	1.97	0.46
2:A:500:ANP:H5'2	2:A:500:ANP:H8	1.97	0.46
1:C:303:VAL:O	1:C:313:PHE:HA	2.14	0.46
1:A:164:VAL:HG22	1:A:164:VAL:O	2.15	0.46
1:D:144:LEU:CD2	1:D:148:ARG:NE	2.78	0.46
1:C:289:LEU:N	1:C:289:LEU:HD22	2.30	0.46
1:B:275:ILE:HD12	1:B:286:VAL:CG2	2.42	0.46
1:D:252:ASN:O	1:D:312:CYS:SG	2.72	0.46
1:B:187:ARG:NH1	1:C:66:ARG:HD3	2.31	0.46
1:A:195:TYR:O	1:D:187:ARG:HB3	2.16	0.46
1:A:257:LYS:HE3	1:A:306:ARG:HH11	1.78	0.46
1:A:179:GLU:HG2	3:A:512:HOH:O	2.15	0.46
1:B:28:LEU:O	1:B:129:ILE:HA	2.14	0.46
1:B:133:HIS:ND1	1:B:167:ARG:NH1	2.64	0.46
1:D:150:THR:OG1	1:D:151:GLY:N	2.49	0.46
1:D:295:GLU:HG2	3:D:325:HOH:O	2.16	0.46
1:B:305:LYS:HB3	1:B:305:LYS:HZ2	1.81	0.46
1:A:263:PRO:O	1:A:267:GLN:HG3	2.16	0.46
1:A:248:VAL:O	1:A:248:VAL:HG12	2.16	0.46
1:A:68:SER:C	1:A:70:GLU:N	2.69	0.46
1:C:60:HIS:O	1:C:89:VAL:HA	2.15	0.46
1:D:202:ASN:ND2	1:D:202:ASN:N	2.55	0.46
1:A:302:LYS:HG3	1:A:302:LYS:O	2.16	0.46
1:D:190:GLU:CD	1:D:190:GLU:H	2.19	0.46
1:A:18:GLU:HG3	1:A:160:PRO:CG	2.45	0.46
1:C:36:ASP:OD2	1:C:36:ASP:N	2.48	0.46
1:C:135:LEU:HD23	1:C:220:GLU:HB3	1.98	0.46
1:D:4:GLU:HG3	1:D:184:LYS:HD2	1.97	0.46
1:C:244:LEU:HD21	1:C:262:LYS:HG3	1.97	0.46
1:D:299:GLY:O	1:D:301:GLY:N	2.48	0.46
1:D:116:PHE:CE1	1:D:120:ILE:HD11	2.51	0.46
1:A:221:ASP:HA	3:A:514:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:98:ALA:HB2	1:B:105:LEU:HD23	1.97	0.45
1:D:121:LEU:HD12	1:D:126:PHE:CB	2.45	0.45
1:B:98:ALA:CB	1:B:105:LEU:HD23	2.46	0.45
1:B:134:HIS:CD2	1:B:136:ASN:HB2	2.51	0.45
1:B:37:SER:HA	1:B:132:ALA:HB2	1.97	0.45
1:B:180:TYR:C	1:B:180:TYR:CD2	2.89	0.45
1:D:54:LYS:O	1:D:55:GLU:HB2	2.15	0.45
1:D:160:PRO:HD3	1:D:170:TYR:CE1	2.51	0.45
1:A:229:VAL:HA	1:B:268:ARG:HH11	1.81	0.45
1:D:134:HIS:CD2	1:D:136:ASN:HB2	2.51	0.45
1:D:65:LEU:HA	1:D:95:ARG:NH2	2.31	0.45
1:D:244:LEU:HD12	1:D:266:LEU:HB3	1.98	0.45
1:D:191:ASP:OD1	1:D:191:ASP:N	2.47	0.45
1:D:206:HIS:O	1:D:210:PRO:HG2	2.16	0.45
1:B:248:VAL:HG12	1:B:254:LEU:HG	1.98	0.45
1:A:299:GLY:C	3:A:546:HOH:O	2.54	0.45
1:D:35:VAL:HG22	1:D:188:TRP:CD1	2.52	0.45
1:C:252:ASN:ND2	1:C:313:PHE:H	2.15	0.45
1:C:35:VAL:HG22	1:C:188:TRP:CD1	2.51	0.45
1:D:275:ILE:O	1:D:302:LYS:HE2	2.16	0.45
1:B:134:HIS:HD2	1:B:136:ASN:N	2.12	0.45
1:C:20:ILE:HD11	1:C:160:PRO:HB2	1.99	0.45
1:A:271:ILE:O	1:A:275:ILE:HB	2.17	0.45
1:A:145:PHE:HB3	1:A:150:THR:HG21	1.98	0.45
1:A:245:TYR:CE2	1:A:273:LYS:HD2	2.52	0.45
1:C:62:ASN:C	1:C:62:ASN:ND2	2.69	0.44
1:B:26:ARG:CB	1:B:126:PHE:HA	2.48	0.44
1:D:156:ILE:HD11	1:D:234:ARG:HB2	1.99	0.44
1:D:166:ARG:O	1:D:168:PRO:HD3	2.17	0.44
1:D:144:LEU:HD21	1:D:148:ARG:HE	1.82	0.44
1:C:272:ARG:HG3	1:C:278:LYS:HA	2.00	0.44
1:A:14:LEU:HD23	1:A:171:TYR:CZ	2.53	0.44
1:D:228:LYS:HE2	3:D:327:HOH:O	2.15	0.44
1:C:165:ILE:HG21	1:C:167:ARG:NH1	2.32	0.44
1:C:296:VAL:HG23	1:C:304:LEU:O	2.17	0.44
1:C:75:PHE:CZ	1:C:188:TRP:HA	2.51	0.44
1:C:140:GLU:HB3	1:C:201:ARG:HD2	2.00	0.44
1:A:284:GLU:HG2	3:A:524:HOH:O	2.17	0.44
1:C:209:ILE:H	1:C:209:ILE:HD12	1.82	0.44
1:A:26:ARG:NH2	1:A:54:LYS:HD2	2.32	0.44
1:B:45:LEU:CD1	1:B:83:ARG:HD3	2.48	0.44
1:D:78:GLU:O	1:D:82:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:196:GLU:HG3	1:D:198:SER:OG	2.17	0.44
1:D:29:ILE:HB	1:D:58:LEU:HD23	1.99	0.44
1:B:61:PHE:CB	1:B:113:ARG:HG3	2.48	0.44
1:B:207:ARG:NH2	1:D:195:TYR:HB3	2.33	0.44
1:A:279:ASP:O	1:A:283:VAL:HG23	2.18	0.44
1:B:281:GLU:CA	1:B:281:GLU:OE2	2.65	0.44
1:C:177:ILE:O	1:C:180:TYR:HB3	2.17	0.44
1:A:149:GLY:O	1:A:150:THR:HB	2.18	0.44
1:C:245:TYR:CZ	1:C:273:LYS:HD2	2.52	0.44
1:C:172:VAL:HG12	1:C:173:LYS:O	2.18	0.44
1:A:252:ASN:ND2	1:A:252:ASN:N	2.66	0.44
1:C:207:ARG:NH2	3:C:550:HOH:O	2.51	0.43
1:B:305:LYS:HB3	1:B:305:LYS:HZ3	1.84	0.43
1:C:209:ILE:O	1:C:213:LYS:HG3	2.19	0.43
1:D:124:GLU:HB3	1:D:126:PHE:CE1	2.53	0.43
1:A:191:ASP:O	1:A:192:GLU:CB	2.66	0.43
1:C:150:THR:O	1:D:226:MET:HG3	2.18	0.43
1:D:89:VAL:CG2	1:D:90:GLY:N	2.81	0.43
1:D:285:LEU:HA	1:D:285:LEU:HD12	1.91	0.43
1:B:134:HIS:HB2	1:B:172:VAL:O	2.19	0.43
1:C:58:LEU:HB2	1:C:87:ILE:HG13	2.00	0.43
1:D:37:SER:HA	1:D:132:ALA:HB2	2.01	0.43
1:A:89:VAL:HG22	1:A:90:GLY:N	2.34	0.43
1:D:229:VAL:O	1:D:233:GLU:HG3	2.19	0.43
1:D:289:LEU:CD2	1:D:296:VAL:HG23	2.49	0.43
1:A:194:ASN:ND2	1:D:190:GLU:HG2	2.33	0.43
1:D:7:VAL:HG21	1:D:180:TYR:HB2	2.00	0.43
1:B:117:LEU:HB3	1:B:129:ILE:HD13	2.01	0.43
1:A:160:PRO:HD3	1:A:170:TYR:CE1	2.53	0.43
1:B:36:ASP:HB3	1:B:132:ALA:HB1	2.00	0.43
1:D:31:PHE:CE2	1:D:33:GLY:HA2	2.54	0.43
1:D:279:ASP:O	1:D:283:VAL:HG23	2.18	0.43
1:A:197:VAL:HG11	1:A:207:ARG:CZ	2.47	0.43
1:A:149:GLY:HA3	1:B:222:THR:HB	2.01	0.43
1:A:207:ARG:NH2	1:D:191:ASP:OD1	2.52	0.43
1:A:156:ILE:HD11	1:A:231:ARG:HA	2.01	0.43
1:B:279:ASP:OD1	1:B:282:LYS:HB2	2.18	0.43
1:D:2:ASN:O	1:D:6:ARG:HG3	2.19	0.42
1:C:68:SER:HA	1:C:71:ARG:HD3	2.00	0.42
1:D:134:HIS:CD2	1:D:136:ASN:H	2.28	0.42
1:B:288:SER:HB2	1:B:292:LYS:NZ	2.33	0.42
1:C:174:ARG:O	1:C:178:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:249:LYS:HD3	1:B:249:LYS:O	2.19	0.42
1:A:96:ALA:N	1:A:98:ALA:HB2	2.26	0.42
1:C:242:GLN:O	1:C:246:LYS:HG3	2.18	0.42
1:D:139:LEU:HA	1:D:223:PHE:CZ	2.54	0.42
1:D:294:GLY:O	1:D:305:LYS:HG3	2.19	0.42
1:C:244:LEU:O	1:C:248:VAL:HG23	2.19	0.42
1:A:211:GLU:OE1	1:B:203:ARG:HD2	2.19	0.42
1:C:197:VAL:HG12	1:C:197:VAL:O	2.19	0.42
1:D:217:GLU:HG3	1:D:218:ASN:ND2	2.34	0.42
1:B:4:GLU:O	1:B:8:ILE:HG12	2.18	0.42
1:D:204:ILE:HD13	1:D:208:VAL:HG21	2.02	0.42
1:B:14:LEU:HD11	1:B:170:TYR:CB	2.44	0.42
1:B:254:LEU:HD23	1:B:259:LEU:CD1	2.49	0.42
1:A:285:LEU:HD12	1:A:296:VAL:HG13	2.00	0.42
1:D:103:MET:SD	1:D:108:ALA:HB2	2.60	0.42
1:A:307:LYS:O	1:A:308:GLU:HB2	2.19	0.42
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.92	0.42
1:B:97:PHE:O	1:B:101:ASN:HB2	2.20	0.42
1:C:248:VAL:CG1	1:C:255:ASP:HB3	2.49	0.42
1:B:223:PHE:O	1:B:226:MET:HB3	2.19	0.42
1:B:8:ILE:HG22	1:B:12:LEU:HD22	2.02	0.42
1:B:275:ILE:HG23	1:B:277:GLU:N	2.27	0.42
1:B:131:THR:HG21	1:B:133:HIS:CE1	2.55	0.42
1:B:173:LYS:HG2	1:B:176:GLU:CG	2.46	0.42
1:D:254:LEU:HD13	1:D:274:PHE:CZ	2.55	0.42
1:D:285:LEU:O	1:D:288:SER:OG	2.34	0.42
1:D:202:ASN:HD22	1:D:202:ASN:H	1.62	0.42
1:A:140:GLU:OE2	1:A:174:ARG:NH2	2.53	0.42
1:D:255:ASP:O	1:D:256:VAL:C	2.58	0.42
1:C:143:LEU:HD21	1:C:212:LEU:CD1	2.49	0.42
1:A:63:HIS:O	1:A:64:MET:HB2	2.20	0.41
1:C:281:GLU:O	1:C:285:LEU:HB2	2.20	0.41
1:C:139:LEU:HD22	1:C:139:LEU:O	2.19	0.41
1:A:219:LEU:HD13	1:B:147:THR:HG23	2.01	0.41
1:B:59:ALA:HB3	1:B:117:LEU:CD2	2.50	0.41
1:A:47:LEU:O	1:A:48:LYS:C	2.58	0.41
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.84	0.41
1:C:277:GLU:HG2	1:C:302:LYS:HZ3	1.85	0.41
1:A:240:GLU:HB3	1:A:266:LEU:HD11	2.02	0.41
1:B:279:ASP:OD2	1:B:281:GLU:HB2	2.20	0.41
1:A:264:LEU:HD21	1:A:268:ARG:NE	2.35	0.41
1:A:99:LYS:C	1:A:101:ASN:N	2.63	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:ARG:NH1	1:A:114:TYR:HE1	2.17	0.41
1:D:275:ILE:HG22	1:D:304:LEU:HD21	2.02	0.41
1:C:121:LEU:HD13	1:C:129:ILE:HG13	2.02	0.41
1:C:209:ILE:N	1:C:210:PRO:CD	2.84	0.41
1:A:12:LEU:HA	1:A:12:LEU:HD12	1.85	0.41
1:A:239:GLU:O	1:A:243:LYS:HG3	2.20	0.41
1:C:41:THR:HG21	1:C:79:PHE:HE2	1.86	0.41
1:C:237:LEU:HD13	1:C:269:ARG:HH21	1.86	0.41
1:B:140:GLU:OE2	1:B:174:ARG:NH1	2.53	0.41
1:D:163:GLU:HB3	1:D:164:VAL:H	1.67	0.41
1:D:196:GLU:HA	1:D:196:GLU:OE1	2.21	0.41
1:D:286:VAL:O	1:D:289:LEU:HB2	2.20	0.41
1:A:83:ARG:O	1:A:84:ASN:HB2	2.20	0.41
1:C:95:ARG:HA	1:C:105:LEU:CD2	2.50	0.41
1:A:131:THR:CG2	1:A:133:HIS:CG	3.03	0.41
1:B:244:LEU:CD1	1:B:262:LYS:HG3	2.37	0.41
1:A:197:VAL:HG21	1:A:207:ARG:NE	2.35	0.41
1:C:149:GLY:HA2	1:D:222:THR:CG2	2.51	0.41
1:D:62:ASN:HB3	1:D:91:LYS:HG3	2.02	0.41
1:B:159:LEU:HD12	1:B:162:GLU:HG2	2.03	0.41
1:D:15:GLN:HA	1:D:15:GLN:OE1	2.21	0.41
1:D:34:GLY:O	1:D:38:VAL:HG23	2.21	0.41
1:B:28:LEU:HD11	1:B:59:ALA:HB2	2.02	0.41
1:B:293:GLY:HA2	1:B:306:ARG:HD3	2.03	0.41
1:B:238:GLU:O	1:B:241:ALA:HB3	2.21	0.41
1:A:96:ALA:O	1:A:98:ALA:N	2.53	0.40
1:D:121:LEU:HD21	1:D:164:VAL:CG2	2.24	0.40
1:B:26:ARG:HB3	1:B:126:PHE:HA	2.03	0.40
1:B:159:LEU:HB2	1:B:162:GLU:CG	2.50	0.40
1:C:254:LEU:HD22	1:C:274:PHE:CE1	2.57	0.40
1:A:113:ARG:HD3	2:A:500:ANP:C4	2.51	0.40
1:C:277:GLU:HG2	1:C:302:LYS:NZ	2.35	0.40
1:C:208:VAL:O	1:C:209:ILE:C	2.60	0.40
1:C:279:ASP:HB2	1:C:281:GLU:OE1	2.22	0.40
1:B:1:MET:HE1	1:B:9:ARG:HD3	2.03	0.40
1:D:95:ARG:HH11	1:D:95:ARG:HG3	1.86	0.40
1:D:2:ASN:HB2	1:D:3:PRO:HD2	2.02	0.40
1:B:27:VAL:HG23	1:B:53:LEU:HD22	2.02	0.40
1:D:156:ILE:HD12	1:D:234:ARG:HG3	2.02	0.40
1:D:27:VAL:HG23	1:D:53:LEU:HD22	2.04	0.40
1:C:24:GLU:OE1	1:C:24:GLU:N	2.40	0.40
1:A:298:LEU:HD12	1:A:302:LYS:HD2	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:LEU:HA	1:A:292:LYS:O	2.21	0.40
1:A:163:GLU:HB3	1:A:164:VAL:H	1.68	0.40
1:C:2:ASN:HB2	1:C:3:PRO:HD2	2.04	0.40
1:C:2:ASN:OD1	1:C:4:GLU:HB3	2.22	0.40
1:D:273:LYS:HB3	1:D:273:LYS:HE2	1.84	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	315/317 (99%)	284 (90%)	24 (8%)	7 (2%)	10	25
1	B	312/317 (98%)	276 (88%)	29 (9%)	7 (2%)	10	25
1	C	312/317 (98%)	291 (93%)	19 (6%)	2 (1%)	33	66
1	D	312/317 (98%)	266 (85%)	36 (12%)	10 (3%)	6	14
All	All	1251/1268 (99%)	1117 (89%)	108 (9%)	26 (2%)	11	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ALA
1	B	255	ASP
1	B	300	LYS
1	D	69	ALA
1	D	192	GLU
1	A	69	ALA
1	B	247	GLU
1	B	301	GLY
1	D	158	PHE
1	D	194	ASN
1	D	196	GLU
1	A	300	LYS
1	D	193	THR

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Mol	Chain	Res	Type
1	D	274	PHE
1	B	100	GLU
1	B	299	GLY
1	C	65	LEU
1	D	300	LYS
1	A	104	SER
1	A	260	LYS
1	A	301	GLY
1	B	245	TYR
1	C	280	TYR
1	D	102	ARG
1	D	256	VAL
1	A	149	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	285/285 (100%)	262 (92%)	23 (8%)	17	36
1	B	282/285 (99%)	259 (92%)	23 (8%)	17	36
1	C	282/285 (99%)	256 (91%)	26 (9%)	13	29
1	D	282/285 (99%)	262 (93%)	20 (7%)	21	46
All	All	1131/1140 (99%)	1039 (92%)	92 (8%)	17	36

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	12	LEU
1	A	14	LEU
1	A	35	VAL
1	A	62	ASN
1	A	71	ARG
1	A	99	LYS
1	A	100	GLU
1	A	124	GLU

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Mol	Chain	Res	Type
1	A	139	LEU
1	A	144	LEU
1	A	169	LEU
1	A	187	ARG
1	A	194	ASN
1	A	198	SER
1	A	222	THR
1	A	257	LYS
1	A	264	LEU
1	A	275	ILE
1	A	285	LEU
1	A	303	VAL
1	A	309	ARG
1	A	317	VAL
1	B	1	MET
1	B	12	LEU
1	B	14	LEU
1	B	35	VAL
1	B	62	ASN
1	B	67	GLU
1	B	92	GLU
1	B	110	ARG
1	B	119	GLU
1	B	131	THR
1	B	139	LEU
1	B	153	ASP
1	B	169	LEU
1	B	191	ASP
1	B	193	THR
1	B	197	VAL
1	B	246	LYS
1	B	252	ASN
1	B	264	LEU
1	B	279	ASP
1	B	289	LEU
1	B	292	LYS
1	B	312	CYS
1	C	12	LEU
1	C	14	LEU
1	C	36	ASP
1	C	55	GLU
1	C	62	ASN

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Mol	Chain	Res	Type
1	C	63	HIS
1	C	66	ARG
1	C	67	GLU
1	C	81	LYS
1	C	110	ARG
1	C	119	GLU
1	C	131	THR
1	C	139	LEU
1	C	144	LEU
1	C	166	ARG
1	C	175	SER
1	C	190	GLU
1	C	194	ASN
1	C	207	ARG
1	C	222	THR
1	C	239	GLU
1	C	254	LEU
1	C	259	LEU
1	C	264	LEU
1	C	281	GLU
1	C	309	ARG
1	D	14	LEU
1	D	71	ARG
1	D	87	ILE
1	D	89	VAL
1	D	124	GLU
1	D	127	ASP
1	D	139	LEU
1	D	167	ARG
1	D	191	ASP
1	D	193	THR
1	D	196	GLU
1	D	202	ASN
1	D	217	GLU
1	D	234	ARG
1	D	244	LEU
1	D	257	LYS
1	D	289	LEU
1	D	303	VAL
1	D	309	ARG
1	D	312	CYS

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	62	ASN
1	A	134	HIS
1	A	194	ASN
1	A	252	ASN
1	B	62	ASN
1	B	134	HIS
1	B	194	ASN
1	B	202	ASN
1	B	252	ASN
1	C	62	ASN
1	C	63	HIS
1	C	134	HIS
1	C	194	ASN
1	C	202	ASN
1	C	252	ASN
1	D	60	HIS
1	D	134	HIS
1	D	202	ASN
1	D	218	ASN
1	D	252	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	ANP	A	500	-	33,33,33	1.61	9 (27%)	51,52,52	3.74	12 (23%)
2	ANP	C	501	-	33,33,33	1.59	7 (21%)	51,52,52	2.64	16 (31%)

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	ANP	A	500	-	-	1/18/38/38	0/1/3/3
2	ANP	C	501	-	-	0/18/38/38	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ANP	C1'-N9	-4.94	1.33	1.48
2	A	500	ANP	C1'-N9	-4.81	1.33	1.48
2	A	500	ANP	O4'-C1'	-2.98	1.36	1.41
2	A	500	ANP	C4-N9	-2.95	1.33	1.37
2	C	501	ANP	C4-N9	-2.92	1.33	1.37
2	C	501	ANP	O4'-C1'	-2.75	1.37	1.41
2	C	501	ANP	PB-O2B	-2.37	1.48	1.55
2	C	501	ANP	PG-O2G	2.34	1.62	1.55
2	C	501	ANP	PG-O3G	2.32	1.62	1.55
2	A	500	ANP	PG-O2G	2.30	1.62	1.55
2	C	501	ANP	PG-O1G	2.24	1.48	1.46
2	A	500	ANP	PG-O3G	2.23	1.61	1.55
2	A	500	ANP	PB-O2B	-2.15	1.48	1.55
2	A	500	ANP	PB-O1B	2.12	1.48	1.46
2	A	500	ANP	PG-O1G	2.11	1.48	1.46
2	A	500	ANP	C8-N9	-2.03	1.33	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ANP	O4'-C1'-N9	20.09	127.12	108.44
2	A	500	ANP	N3-C2-N1	-10.80	119.68	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ANP	N3-C2-N1	-10.04	120.32	128.71
2	A	500	ANP	PB-N3B-PG	-7.77	117.01	130.07
2	C	501	ANP	C8-N9-C1'	-6.27	114.04	126.38
2	C	501	ANP	PB-N3B-PG	-5.96	120.04	130.07
2	C	501	ANP	O4'-C1'-N9	5.58	113.63	108.44
2	C	501	ANP	C1'-N9-C4	4.27	134.02	126.64
2	A	500	ANP	N3-C4-N9	4.11	132.85	125.43
2	A	500	ANP	O2B-PB-O1B	3.95	119.00	109.89
2	C	501	ANP	C4'-O4'-C1'	3.71	113.78	109.75
2	C	501	ANP	C2'-C1'-N9	3.69	122.75	113.27
2	A	500	ANP	PA-O3A-PB	-3.58	119.59	131.81
2	A	500	ANP	O4'-C1'-C2'	-3.47	101.45	106.77
2	C	501	ANP	C5-C4-N3	-3.43	118.24	125.70
2	A	500	ANP	O1B-PB-N3B	-3.37	106.74	111.83
2	C	501	ANP	O2B-PB-O1B	3.30	117.50	109.89
2	C	501	ANP	O3G-PG-O2G	-3.12	98.72	107.66
2	C	501	ANP	PA-O3A-PB	-3.10	121.23	131.81
2	C	501	ANP	C2-N3-C4	3.05	122.69	114.01
2	C	501	ANP	C8-N9-C4	-2.96	104.64	106.90
2	C	501	ANP	O1G-PG-N3B	2.88	116.17	111.83
2	A	500	ANP	C2-N3-C4	2.86	122.15	114.01
2	A	500	ANP	C5-C4-N3	-2.78	119.64	125.70
2	A	500	ANP	C2'-C1'-N9	2.73	120.28	113.27
2	C	501	ANP	N3-C4-N9	2.70	130.31	125.43
2	C	501	ANP	O3'-C3'-C4'	-2.44	103.90	111.08
2	A	500	ANP	C4-C5-N7	-2.40	107.46	109.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ANP	O1B-PB-N3B-PG

There are no ring outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/317 (100%)	0.04	6 (1%) 64 70	23, 48, 88, 114	0
1	B	314/317 (99%)	0.10	11 (3%) 42 47	16, 44, 90, 100	0
1	C	314/317 (99%)	0.08	7 (2%) 59 65	19, 41, 99, 112	0
1	D	314/317 (99%)	0.26	17 (5%) 25 27	27, 60, 109, 119	0
All	All	1259/1268 (99%)	0.12	41 (3%) 44 49	16, 48, 96, 119	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	LYS	4.0
1	D	105	LEU	3.8
1	B	244	LEU	3.6
1	D	251	GLY	3.4
1	D	195	TYR	3.0
1	D	66	ARG	3.0
1	B	103	MET	2.9
1	C	300	LYS	2.9
1	B	314	SER	2.8
1	D	310	TRP	2.8
1	B	300	LYS	2.8
1	B	114	TYR	2.8
1	D	300	LYS	2.7
1	A	101	ASN	2.7
1	D	121	LEU	2.7
1	D	51	PHE	2.7
1	A	97	PHE	2.6
1	B	298	LEU	2.6
1	C	298	LEU	2.6
1	D	309	ARG	2.5
1	A	112	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	296	VAL	2.4
1	C	304	LEU	2.4
1	D	94	VAL	2.3
1	D	246	LYS	2.3
1	C	309	ARG	2.3
1	B	250	LYS	2.3
1	A	96	ALA	2.3
1	D	88	PHE	2.3
1	D	250	LYS	2.3
1	D	252	ASN	2.2
1	A	102	ARG	2.2
1	D	305	LYS	2.2
1	B	97	PHE	2.2
1	C	289	LEU	2.2
1	B	275	ILE	2.1
1	A	61	PHE	2.1
1	D	102	ARG	2.1
1	C	286	VAL	2.1
1	D	308	GLU	2.0
1	B	304	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ANP	C	501	31/31	0.24	1.98	32,38,47,49	21
2	ANP	A	500	31/31	0.19	-0.20	94,100,117,118	0

6.5 Other polymers ⓘ

There are no such residues in this entry.