Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:47 PM GMT

PDB ID	:	1CI7
Title	:	TERNARY COMPLEX OF THYMIDYLATE SYNTHASE FROM PNEUMOCYSTIS CARINII
Authors	:	Anderson, A.C.; O'Neil, R.H.; Delano, W.L.; Stroud, R.M.
Deposited on	:	1999-04-08
Resolution	:	2.60 Å(reported)

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

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

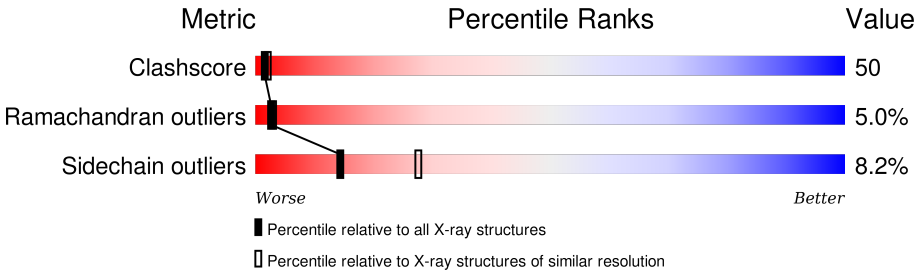
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	297	31% 57% 9%
1	B	297	36% 53% 10%

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
3	CB3	A	768	X	-	X	-

2 Entry composition

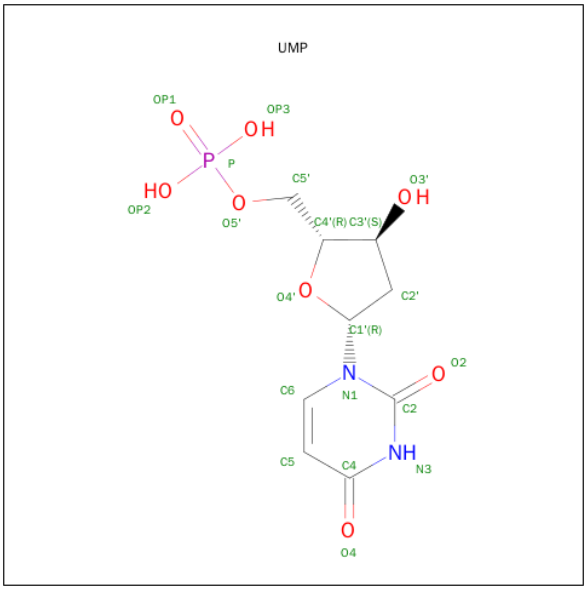
There are 4 unique types of molecules in this entry. The entry contains 5025 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (THYMIDYLATE SYNTHASE).

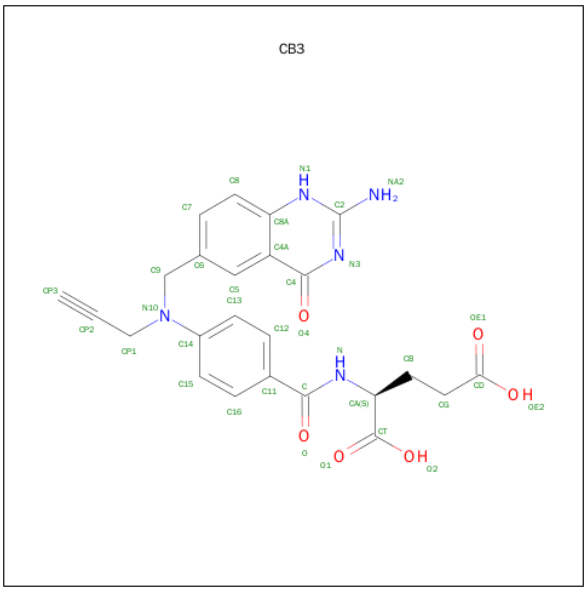
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2377	1516	410	436	15			
1	B	292	Total	C	N	O	S	0	0	0
			2377	1516	410	436	15			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 35 24 5 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	103	Total O 103 103	0	0

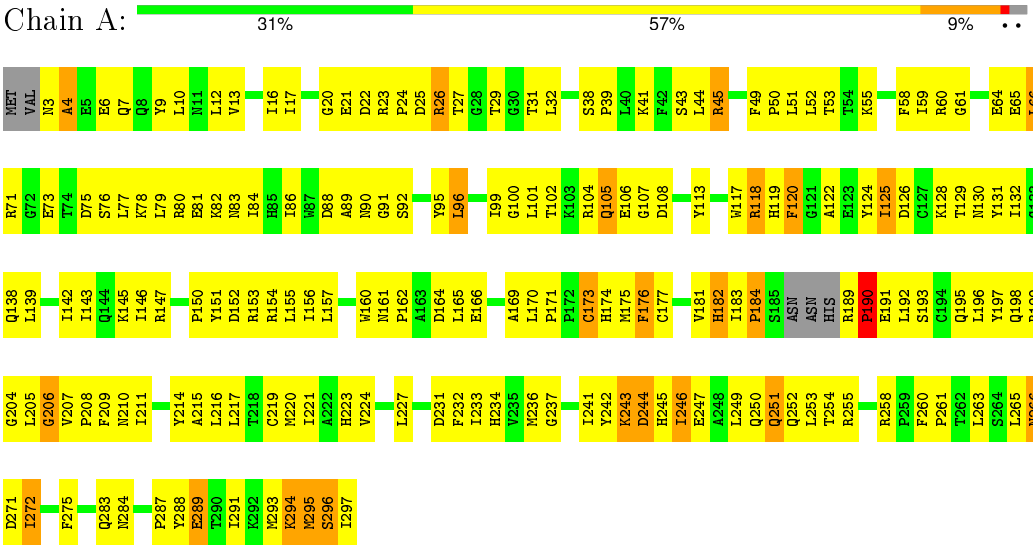
3 Residue-property plots (i)

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

Note EDS was not executed.

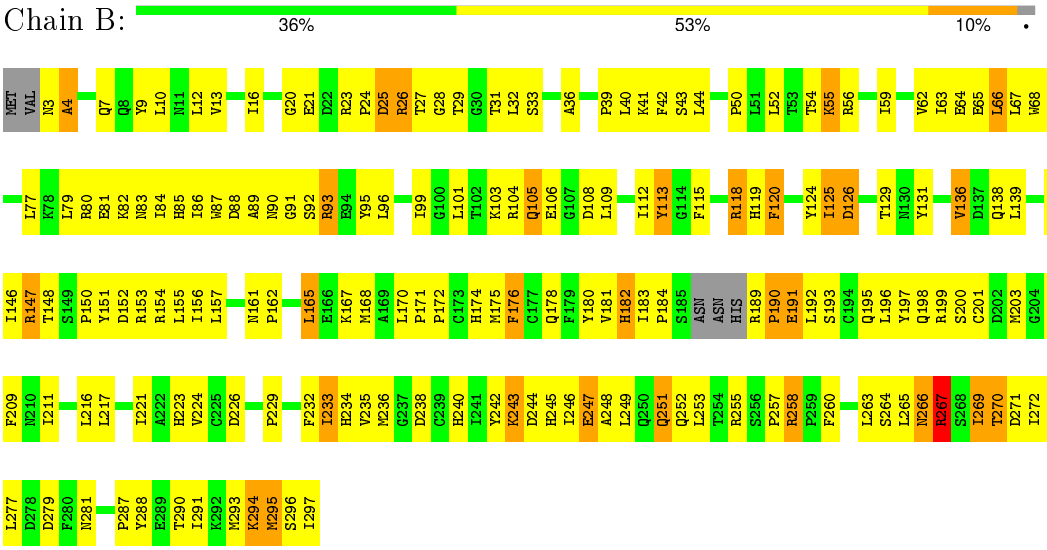
- Molecule 1: PROTEIN (THYMIDYLATE SYNTHASE)

Chain A:



- Molecule 1: PROTEIN (THYMIDYLATE SYNTHASE)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.16Å 178.76Å 54.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	75.3 (50.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	12.70	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.221 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5025	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: CB3, UMP

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	0.42	0/2437	0.77	6/3302 (0.2%)
1	B	0.43	0/2437	0.74	6/3302 (0.2%)
All	All	0.42	0/4874	0.75	12/6604 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	ASN	N-CA-C	8.50	133.94	111.00
1	A	269	ILE	N-CA-C	-7.68	90.25	111.00
1	B	267	ARG	N-CA-C	-7.55	90.60	111.00
1	A	173	CYS	CA-CB-SG	6.85	126.33	114.00
1	A	190	PRO	N-CA-C	6.54	129.10	112.10
1	A	267	ARG	N-CA-C	-6.52	93.39	111.00
1	B	266	ASN	N-CA-C	6.51	128.57	111.00
1	B	266	ASN	CB-CA-C	-6.43	97.54	110.40
1	B	269	ILE	N-CA-C	-6.39	93.76	111.00
1	B	266	ASN	CA-C-N	-6.12	103.73	117.20
1	A	266	ASN	CA-C-N	-5.90	104.22	117.20
1	B	174	HIS	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2330	270	0
1	B	2377	0	2331	232	0
2	A	20	0	10	3	0
2	B	20	0	11	3	0
3	A	35	0	21	18	0
4	A	93	0	0	4	0
4	B	103	0	0	8	0
All	All	5025	0	4703	479	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 50.

All (479) 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:223:HIS:NE2	1:B:266:ASN:ND2	1.93	1.17
1:B:223:HIS:CE1	1:B:266:ASN:HD21	1.65	1.14
1:B:183:ILE:HG23	1:B:189:ARG:HB2	1.31	1.08
1:A:294:LYS:HD2	1:A:294:LYS:H	1.25	1.01
1:A:80:ARG:HH21	1:A:88:ASP:HA	1.26	1.00
1:A:189:ARG:HB3	1:A:190:PRO:HD2	1.45	0.99
1:A:52:LEU:HD12	1:A:52:LEU:H	1.29	0.94
1:B:52:LEU:HD12	1:B:52:LEU:H	1.36	0.91
1:A:223:HIS:CE1	1:A:266:ASN:ND2	2.40	0.90
1:A:223:HIS:NE2	1:A:266:ASN:ND2	2.19	0.90
1:A:4:ALA:HA	1:A:7:GLN:HB3	1.56	0.87
1:B:126:ASP:OD1	1:B:129:THR:HG23	1.74	0.87
1:B:183:ILE:CG2	1:B:189:ARG:HB2	2.05	0.86
1:B:294:LYS:H	1:B:294:LYS:HD2	1.38	0.85
1:B:151:TYR:OH	1:B:183:ILE:HD12	1.77	0.84
1:A:120:PHE:HB3	1:A:136:VAL:HG12	1.61	0.82
1:A:151:TYR:OH	1:A:183:ILE:HD12	1.79	0.82
1:A:209:PHE:HB3	3:A:768:CB3:HP3	1.60	0.81
1:B:90:ASN:ND2	1:B:170:LEU:HD12	1.96	0.81
1:A:209:PHE:CD2	3:A:768:CB3:CP3	2.65	0.80
1:A:145:LYS:HD3	1:A:152:ASP:OD1	1.82	0.80
1:A:196:LEU:CD2	1:A:234:HIS:HA	2.12	0.80
1:B:183:ILE:HG23	1:B:189:ARG:CB	2.11	0.79
1:B:3:ASN:HD21	1:B:260:PHE:H	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:O	1:A:125:ILE:HG13	1.83	0.77
1:A:92:SER:O	1:A:96:LEU:HD23	1.85	0.76
1:B:249:LEU:O	1:B:253:LEU:HG	1.86	0.76
1:A:120:PHE:CE1	1:B:162:PRO:HD2	2.21	0.76
1:B:77:LEU:HD23	1:B:80:ARG:HH11	1.49	0.76
1:A:146:ILE:HD12	1:A:221:ILE:HD11	1.68	0.76
1:B:190:PRO:O	1:B:191:GLU:HB2	1.86	0.75
1:B:13:VAL:HB	1:B:253:LEU:HD21	1.67	0.75
1:B:271:ASP:O	1:B:272:ILE:HG22	1.87	0.74
1:B:3:ASN:N	1:B:257:PRO:HB2	2.03	0.74
1:B:217:LEU:O	1:B:221:ILE:HG22	1.88	0.74
1:B:103:LYS:HD3	1:B:103:LYS:O	1.88	0.73
1:A:223:HIS:CD2	1:A:266:ASN:HD21	2.06	0.73
1:A:198:GLN:HE21	1:A:201:CYS:HA	1.54	0.73
1:A:154:ARG:HE	2:B:765:UMP:P	2.13	0.72
1:A:266:ASN:HB3	1:A:269:ILE:HD13	1.69	0.72
1:A:223:HIS:CD2	1:A:266:ASN:ND2	2.58	0.72
1:A:209:PHE:HB3	3:A:768:CB3:CP3	2.19	0.72
1:A:271:ASP:O	1:A:272:ILE:HG22	1.89	0.71
1:B:23:ARG:HG3	1:B:33:SER:OG	1.90	0.71
1:A:13:VAL:HG11	1:A:249:LEU:HD12	1.72	0.71
1:A:160:TRP:CD2	1:A:175:MET:HE3	2.25	0.71
3:A:768:CB3:H12	3:A:768:CB3:CP2	2.20	0.71
1:B:271:ASP:HB3	1:B:274:ASP:HB2	1.73	0.70
1:A:23:ARG:NH2	1:B:181:VAL:O	2.24	0.70
1:B:25:ASP:HB3	1:B:29:THR:O	1.92	0.70
1:A:183:ILE:HG23	1:A:189:ARG:HB2	1.73	0.70
1:A:124:TYR:O	1:A:125:ILE:HG23	1.90	0.70
1:A:233:ILE:HD12	1:B:36:ALA:CB	2.21	0.70
1:A:233:ILE:HD12	1:B:36:ALA:HB3	1.72	0.69
1:B:124:TYR:O	1:B:125:ILE:HG23	1.91	0.69
1:A:205:LEU:HD21	1:A:293:MET:HB2	1.74	0.69
1:A:73:GLU:OE2	1:A:78:LYS:HG2	1.92	0.69
1:B:183:ILE:HG23	1:B:184:PRO:HD2	1.74	0.69
1:B:77:LEU:HA	1:B:80:ARG:HD2	1.75	0.68
1:B:138:GLN:O	1:B:142:ILE:HG13	1.93	0.68
1:B:68:TRP:CG	1:B:79:LEU:HD11	2.29	0.68
1:A:177:CYS:HG	1:A:214:TYR:HE1	1.42	0.68
1:A:243:LYS:HA	1:A:246:ILE:HG13	1.75	0.68
1:B:118:ARG:HE	1:B:139:LEU:HD23	1.59	0.67
1:B:44:LEU:HD23	1:B:229:PRO:HB2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:HZ3	1:A:244:ASP:N	1.92	0.67
1:B:170:LEU:HD23	1:B:171:PRO:HD2	1.76	0.67
1:A:182:HIS:HE1	1:A:193:SER:OG	1.77	0.66
1:A:170:LEU:HD23	1:A:171:PRO:HD2	1.77	0.66
1:A:192:LEU:CD2	1:A:221:ILE:HG23	2.27	0.65
1:A:55:LYS:HD2	1:A:291:ILE:HB	1.78	0.65
1:B:142:ILE:O	1:B:146:ILE:HG13	1.96	0.65
1:B:13:VAL:HG11	1:B:249:LEU:HD12	1.79	0.65
1:A:196:LEU:HD23	1:A:234:HIS:HA	1.77	0.65
1:B:144:GLN:HA	1:B:144:GLN:HE21	1.61	0.65
1:B:183:ILE:HG12	1:B:189:ARG:O	1.95	0.65
1:A:294:LYS:N	1:A:294:LYS:HD2	2.05	0.64
1:A:295:MET:HG2	1:A:296:SER:H	1.62	0.64
1:A:153:ARG:HG3	1:B:238:ASP:OD1	1.97	0.64
1:A:60:ARG:HH12	1:A:84:ILE:HD11	1.62	0.64
1:A:25:ASP:OD1	1:A:27:THR:N	2.30	0.64
1:A:295:MET:O	1:A:296:SER:HB2	1.96	0.64
1:B:93:ARG:HG2	4:B:1097:HOH:O	1.96	0.64
1:B:267:ARG:O	1:B:269:ILE:HD12	1.97	0.64
1:B:3:ASN:HD21	1:B:260:PHE:N	1.95	0.64
1:B:105:GLN:NE2	1:B:106:GLU:N	2.45	0.64
1:A:41:LYS:HE2	1:A:233:ILE:HD11	1.80	0.64
1:A:99:ILE:HD11	1:A:101:LEU:HD12	1.80	0.64
1:A:151:TYR:CE1	1:B:24:PRO:HD2	2.33	0.63
1:A:24:PRO:HD2	1:B:151:TYR:CD1	2.33	0.63
1:B:52:LEU:HA	1:B:260:PHE:HE1	1.62	0.63
1:A:196:LEU:HD21	1:A:234:HIS:CD2	2.34	0.63
1:A:96:LEU:HD12	1:A:104:ARG:HB3	1.80	0.63
1:B:196:LEU:HD21	1:B:234:HIS:CD2	2.34	0.63
1:B:125:ILE:O	1:B:126:ASP:HB3	1.99	0.63
1:A:196:LEU:HD22	1:A:232:PHE:CZ	2.34	0.63
1:A:201:CYS:SG	1:A:236:MET:HG2	2.39	0.63
1:A:160:TRP:CE3	1:A:175:MET:HE3	2.34	0.63
1:A:210:ASN:ND2	3:A:768:CB3:CP3	2.62	0.63
1:B:272:ILE:HA	1:B:275:PHE:CE1	2.34	0.63
1:A:251:GLN:HG3	1:A:252:GLN:N	2.13	0.63
1:B:201:CYS:SG	1:B:236:MET:HB3	2.39	0.62
1:B:223:HIS:CE1	1:B:266:ASN:ND2	2.49	0.62
1:B:89:ALA:HB1	1:B:297:ILE:HD13	1.81	0.62
1:B:93:ARG:HH11	1:B:93:ARG:HB2	1.65	0.62
1:B:245:HIS:O	1:B:249:LEU:HD23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:CYS:SG	1:A:236:MET:HB3	2.39	0.62
1:B:96:LEU:HB3	1:B:101:LEU:O	2.00	0.62
1:B:68:TRP:CD2	1:B:79:LEU:HD11	2.35	0.61
1:A:64:GLU:CG	1:A:82:LYS:HD3	2.29	0.61
1:B:182:HIS:HE1	1:B:193:SER:OG	1.83	0.61
1:A:270:THR:OG1	1:A:270:THR:O	2.19	0.61
1:B:64:GLU:CD	1:B:82:LYS:HD3	2.20	0.61
1:B:3:ASN:O	1:B:4:ALA:CB	2.48	0.61
1:A:146:ILE:CD1	1:A:221:ILE:HD11	2.31	0.61
1:A:184:PRO:HD2	1:A:189:ARG:HB2	1.83	0.61
1:A:207:VAL:HB	1:A:208:PRO:HD3	1.82	0.61
1:A:243:LYS:C	1:A:245:HIS:H	2.03	0.61
3:A:768:CB3:O	3:A:768:CB3:HG1	2.00	0.60
1:A:182:HIS:ND1	1:A:191:GLU:HB3	2.16	0.60
1:B:66:LEU:O	1:B:70:ILE:HG13	2.00	0.60
1:A:189:ARG:HB3	1:A:190:PRO:CD	2.28	0.60
1:A:196:LEU:HD22	1:A:232:PHE:CE1	2.37	0.60
1:B:120:PHE:HB3	1:B:136:VAL:HG13	1.83	0.60
1:B:170:LEU:HD23	1:B:171:PRO:CD	2.32	0.60
1:B:272:ILE:HA	1:B:275:PHE:CD1	2.37	0.60
1:B:99:ILE:HD11	1:B:101:LEU:HD12	1.84	0.60
1:B:243:LYS:C	1:B:245:HIS:H	2.03	0.60
1:A:162:PRO:HD2	1:B:120:PHE:CE1	2.37	0.60
1:A:195:GLN:NE2	1:B:197:TYR:HE1	2.00	0.59
1:A:58:PHE:HB2	3:A:768:CB3:HA	1.84	0.59
1:A:125:ILE:O	1:A:126:ASP:HB3	2.00	0.59
1:A:255:ARG:NH1	1:A:291:ILE:HD11	2.17	0.59
1:B:207:VAL:HB	1:B:208:PRO:HD3	1.82	0.59
1:B:182:HIS:N	1:B:182:HIS:ND1	2.50	0.59
1:A:58:PHE:O	1:A:61:GLY:N	2.36	0.59
1:A:124:TYR:O	1:A:125:ILE:CG2	2.51	0.59
1:A:183:ILE:HG23	1:A:184:PRO:HD2	1.84	0.58
1:A:52:LEU:HA	1:A:260:PHE:HE1	1.68	0.58
1:B:85:HIS:HB3	1:B:88:ASP:OD1	2.03	0.58
1:A:49:PHE:CZ	1:A:216:LEU:HG	2.39	0.58
1:A:31:THR:HG22	1:A:242:TYR:CD1	2.39	0.58
1:A:176:PHE:CE1	1:B:176:PHE:CE1	2.92	0.58
1:A:245:HIS:O	1:A:249:LEU:HD23	2.04	0.58
1:B:203:MET:SD	1:B:207:VAL:HG21	2.43	0.58
1:A:204:GLY:HA2	4:A:1116:HOH:O	2.03	0.58
1:A:52:LEU:H	1:A:52:LEU:CD1	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PRO:HG2	1:B:154:ARG:CZ	2.34	0.58
1:A:196:LEU:HD21	1:A:234:HIS:HA	1.86	0.57
1:A:223:HIS:CG	1:A:266:ASN:HD21	2.22	0.57
1:B:271:ASP:HB3	1:B:274:ASP:CB	2.34	0.57
1:B:196:LEU:HD23	1:B:196:LEU:H	1.67	0.57
1:B:12:LEU:HD21	1:B:236:MET:HE3	1.85	0.57
1:A:118:ARG:NH1	1:A:137:ASP:OD1	2.37	0.57
1:B:84:ILE:HG23	1:B:86:ILE:HG23	1.86	0.57
1:B:243:LYS:HA	1:B:246:ILE:HG13	1.85	0.57
1:B:9:TYR:O	1:B:13:VAL:HG23	2.04	0.57
1:B:183:ILE:CD1	1:B:189:ARG:N	2.67	0.57
1:A:150:PRO:HB2	1:A:181:VAL:HG11	1.87	0.57
1:A:3:ASN:O	1:A:4:ALA:HB3	2.05	0.57
1:A:195:GLN:NE2	1:B:197:TYR:CE1	2.73	0.57
1:B:77:LEU:HD23	1:B:80:ARG:NH1	2.19	0.57
1:B:189:ARG:HB3	1:B:190:PRO:HD2	1.87	0.57
1:A:104:ARG:HD3	1:A:108:ASP:O	2.04	0.57
1:B:41:LYS:HB3	1:B:41:LYS:NZ	2.19	0.57
1:A:89:ALA:C	1:A:91:GLY:H	2.09	0.56
1:B:63:ILE:O	1:B:67:LEU:HD13	2.05	0.56
1:A:210:ASN:HD21	3:A:768:CB3:CP3	2.19	0.56
1:B:86:ILE:HG13	1:B:87:TRP:CD1	2.40	0.56
1:A:151:TYR:CZ	1:A:183:ILE:HD12	2.41	0.56
1:A:64:GLU:CD	1:A:82:LYS:HD3	2.27	0.56
1:B:270:THR:OG1	1:B:270:THR:O	2.18	0.56
1:A:3:ASN:O	1:A:4:ALA:CB	2.54	0.55
1:A:243:LYS:HZ3	1:A:243:LYS:HB3	1.70	0.55
1:A:170:LEU:HD23	1:A:171:PRO:CD	2.35	0.55
1:A:267:ARG:O	1:A:269:ILE:HD12	2.06	0.55
1:A:25:ASP:OD1	1:A:27:THR:OG1	2.24	0.55
1:A:27:THR:HB	1:A:296:SER:O	2.07	0.55
1:A:243:LYS:O	1:A:245:HIS:N	2.39	0.55
1:A:105:GLN:NE2	1:A:106:GLU:N	2.54	0.55
1:A:58:PHE:HB2	3:A:768:CB3:CT	2.37	0.55
1:A:217:LEU:O	1:A:221:ILE:HG22	2.07	0.54
1:B:146:ILE:CD1	1:B:221:ILE:HD11	2.36	0.54
1:A:216:LEU:O	1:A:220:MET:HG3	2.06	0.54
1:A:181:VAL:HA	1:A:191:GLU:O	2.07	0.54
1:B:29:THR:HG21	1:B:296:SER:HB2	1.88	0.54
1:A:197:TYR:CD2	1:B:176:PHE:HZ	2.26	0.54
1:A:181:VAL:HG23	1:A:191:GLU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLN:HE21	1:A:201:CYS:CA	2.20	0.54
1:B:258:ARG:HD3	1:B:288:TYR:CE1	2.43	0.54
1:A:55:LYS:HD2	1:A:291:ILE:HD12	1.89	0.54
1:B:82:LYS:O	1:B:83:ASN:HB2	2.07	0.54
1:B:295:MET:HG2	4:B:1107:HOH:O	2.08	0.54
1:A:100:GLY:O	1:A:102:THR:N	2.39	0.53
1:A:209:PHE:HD2	3:A:768:CB3:CP3	2.19	0.53
1:B:295:MET:HG2	1:B:296:SER:H	1.73	0.53
1:A:199:ARG:NH1	1:A:200:SER:HB2	2.24	0.53
1:A:223:HIS:CE1	1:A:266:ASN:HD21	2.24	0.53
1:B:248:ALA:O	1:B:249:LEU:HD22	2.07	0.53
1:A:289:GLU:N	1:A:289:GLU:OE2	2.37	0.53
1:B:26:ARG:C	1:B:28:GLY:H	2.11	0.53
1:B:207:VAL:O	1:B:211:ILE:HG13	2.09	0.53
1:A:219:CYS:HB3	1:A:265:LEU:HD21	1.90	0.53
1:B:56:ARG:HH11	1:B:287:PRO:CG	2.22	0.53
1:A:183:ILE:CD1	1:A:189:ARG:N	2.72	0.52
1:A:96:LEU:CD1	1:A:104:ARG:HD2	2.40	0.52
1:A:66:LEU:O	1:A:70:ILE:HG13	2.09	0.52
1:B:125:ILE:O	1:B:125:ILE:HG13	2.10	0.52
1:A:16:ILE:O	1:A:20:GLY:HA3	2.09	0.52
1:A:151:TYR:CD1	1:B:24:PRO:HD2	2.44	0.52
1:B:271:ASP:OD1	1:B:273:GLU:HB2	2.10	0.52
1:B:144:GLN:HA	1:B:144:GLN:NE2	2.23	0.52
1:B:93:ARG:NH1	1:B:93:ARG:HB2	2.23	0.52
1:A:25:ASP:HB3	1:A:29:THR:O	2.10	0.52
1:B:124:TYR:O	1:B:125:ILE:CG2	2.58	0.52
1:A:13:VAL:O	1:A:17:ILE:HG13	2.10	0.52
1:A:41:LYS:HB3	1:A:41:LYS:NZ	2.24	0.52
1:A:76:SER:OG	1:A:107:GLY:HA2	2.10	0.52
1:A:77:LEU:O	1:A:81:GLU:HG3	2.10	0.52
1:A:209:PHE:CD2	3:A:768:CB3:CP2	2.92	0.52
1:B:243:LYS:O	1:B:245:HIS:N	2.43	0.52
1:A:255:ARG:HH21	1:A:288:TYR:CB	2.22	0.52
1:B:251:GLN:HG3	1:B:252:GLN:N	2.25	0.52
1:B:54:THR:O	1:B:55:LYS:HB2	2.09	0.52
1:A:4:ALA:CA	1:A:7:GLN:HB3	2.33	0.51
1:B:205:LEU:HD21	1:B:293:MET:HB2	1.92	0.51
1:B:52:LEU:H	1:B:52:LEU:CD1	2.17	0.51
1:B:247:GLU:CD	1:B:247:GLU:H	2.13	0.51
1:A:99:ILE:CD1	1:A:101:LEU:HD12	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:O	1:B:255:ARG:HB2	2.10	0.51
1:B:104:ARG:HD3	1:B:108:ASP:O	2.10	0.51
1:B:265:LEU:HD23	4:B:1143:HOH:O	2.10	0.51
3:A:768:CB3:CP2	3:A:768:CB3:C12	2.85	0.51
1:B:109:LEU:HB3	1:B:112:ILE:HD13	1.92	0.51
1:B:180:TYR:HE2	1:B:182:HIS:CD2	2.29	0.51
1:B:77:LEU:CD2	1:B:80:ARG:HH11	2.22	0.51
1:A:181:VAL:HG13	1:A:181:VAL:O	2.10	0.51
1:B:21:GLU:O	1:B:32:LEU:HA	2.11	0.51
1:B:16:ILE:O	1:B:20:GLY:HA3	2.11	0.51
1:A:261:PRO:HB3	1:A:284:ASN:O	2.11	0.51
3:A:768:CB3:H12	3:A:768:CB3:CP3	2.41	0.51
1:B:41:LYS:HG2	1:B:233:ILE:HB	1.92	0.51
1:B:183:ILE:HG21	4:B:1083:HOH:O	2.10	0.50
1:A:160:TRP:CZ2	1:B:156:ILE:HB	2.46	0.50
1:A:67:LEU:O	1:A:71:ARG:HG3	2.11	0.50
1:B:155:LEU:C	1:B:156:ILE:HD12	2.31	0.50
1:B:152:ASP:OD1	1:B:154:ARG:N	2.33	0.50
1:A:210:ASN:ND2	3:A:768:CB3:HP3	2.26	0.50
1:A:26:ARG:NH1	1:A:27:THR:HG22	2.27	0.50
1:A:139:LEU:O	1:A:143:ILE:HG12	2.11	0.50
1:B:143:ILE:HD13	1:B:221:ILE:HG13	1.94	0.50
1:B:295:MET:HG2	1:B:296:SER:N	2.27	0.50
1:B:90:ASN:HA	1:B:95:TYR:CD2	2.47	0.50
1:A:183:ILE:HD11	1:A:189:ARG:N	2.27	0.50
1:B:33:SER:HB3	1:B:240:HIS:HB3	1.93	0.50
1:B:3:ASN:O	1:B:4:ALA:HB3	2.11	0.49
1:B:181:VAL:HA	1:B:191:GLU:O	2.11	0.49
1:A:58:PHE:HB2	3:A:768:CB3:CA	2.42	0.49
1:A:261:PRO:HB3	1:A:284:ASN:C	2.32	0.49
4:A:1063:HOH:O	1:B:235:VAL:HG13	2.12	0.49
1:A:89:ALA:O	1:A:91:GLY:N	2.46	0.49
1:A:117:TRP:CG	1:A:157:LEU:HD11	2.47	0.49
1:B:276:THR:N	1:B:279:ASP:OD2	2.46	0.49
1:B:39:PRO:HA	4:B:1136:HOH:O	2.11	0.49
1:A:243:LYS:NZ	1:A:243:LYS:HB3	2.28	0.49
1:A:184:PRO:HD2	1:A:189:ARG:CB	2.42	0.49
1:A:190:PRO:O	1:A:191:GLU:HB2	2.13	0.49
1:B:216:LEU:CD2	1:B:263:LEU:HD22	2.43	0.49
1:B:59:ILE:O	1:B:59:ILE:HG13	2.12	0.49
1:B:26:ARG:C	1:B:28:GLY:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:NH1	2:B:765:UMP:OP1	2.45	0.49
1:B:263:LEU:HG	1:B:265:LEU:HD22	1.95	0.49
1:A:182:HIS:HB3	1:B:21:GLU:OE2	2.13	0.48
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.77	0.48
1:A:183:ILE:HG12	1:A:189:ARG:HB2	1.94	0.48
1:B:59:ILE:HD12	1:B:62:VAL:HB	1.95	0.48
1:A:77:LEU:HA	1:A:80:ARG:HD2	1.95	0.48
1:B:170:LEU:HD23	1:B:171:PRO:N	2.29	0.48
1:B:264:SER:HB2	1:B:281:ASN:HB3	1.94	0.48
1:B:161:ASN:O	1:B:165:LEU:HD13	2.12	0.48
1:B:139:LEU:O	1:B:143:ILE:HG12	2.13	0.48
1:A:272:ILE:HA	1:A:275:PHE:CE1	2.48	0.48
1:B:28:GLY:O	1:B:29:THR:HG23	2.14	0.48
1:A:68:TRP:CD1	1:A:73:GLU:HB2	2.48	0.48
1:B:7:GLN:O	1:B:10:LEU:N	2.47	0.48
1:A:173:CYS:SG	2:A:767:UMP:H2'	2.53	0.48
1:A:75:ASP:HB3	1:A:78:LYS:HD3	1.96	0.48
1:A:251:GLN:O	1:A:254:THR:OG1	2.31	0.48
1:A:295:MET:HG2	1:A:296:SER:N	2.28	0.48
1:A:192:LEU:HD21	1:A:221:ILE:HG23	1.96	0.48
1:B:251:GLN:NE2	1:B:291:ILE:HD11	2.29	0.48
1:B:216:LEU:HD23	1:B:263:LEU:HD22	1.95	0.48
1:B:258:ARG:HD3	1:B:288:TYR:HE1	1.78	0.48
1:A:161:ASN:O	1:A:165:LEU:HD13	2.14	0.48
1:A:125:ILE:O	1:A:125:ILE:CG1	2.58	0.48
1:B:198:GLN:HB3	1:B:201:CYS:SG	2.53	0.48
1:A:196:LEU:HD21	1:A:234:HIS:CG	2.49	0.47
1:A:118:ARG:NH1	1:A:137:ASP:OD2	2.46	0.47
1:A:224:VAL:HG12	1:A:224:VAL:O	2.13	0.47
1:A:294:LYS:O	1:A:295:MET:O	2.32	0.47
1:A:16:ILE:O	1:A:20:GLY:CA	2.62	0.47
1:A:294:LYS:H	1:A:294:LYS:CD	2.03	0.47
1:A:136:VAL:HG11	1:B:162:PRO:HB2	1.96	0.47
1:A:120:PHE:CZ	1:B:162:PRO:HD2	2.50	0.47
1:A:16:ILE:O	1:A:20:GLY:N	2.47	0.47
1:B:150:PRO:HB2	1:B:181:VAL:HG11	1.97	0.47
1:B:129:THR:OG1	1:B:131:TYR:CZ	2.67	0.47
1:A:198:GLN:HG2	1:A:201:CYS:SG	2.55	0.47
1:B:92:SER:O	1:B:96:LEU:HD23	2.15	0.47
1:A:118:ARG:NH1	1:A:137:ASP:CG	2.68	0.47
1:A:60:ARG:NH1	1:A:84:ILE:HD11	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:O	1:A:83:ASN:HB2	2.14	0.47
1:A:197:TYR:OH	1:B:195:GLN:NE2	2.48	0.47
1:A:80:ARG:NH2	1:A:88:ASP:HA	2.11	0.47
1:A:119:HIS:O	1:A:135:GLY:HA3	2.15	0.47
1:A:243:LYS:C	1:A:245:HIS:N	2.67	0.46
1:B:26:ARG:HD3	1:B:27:THR:N	2.30	0.46
1:B:272:ILE:CG2	1:B:273:GLU:N	2.78	0.46
1:A:68:TRP:CG	1:A:79:LEU:HD13	2.50	0.46
1:A:55:LYS:HZ2	1:A:291:ILE:H	1.63	0.46
1:B:294:LYS:HD2	1:B:294:LYS:N	2.20	0.46
1:A:237:GLY:HA2	1:B:195:GLN:HE22	1.80	0.46
1:B:175:MET:O	1:B:176:PHE:HB3	2.15	0.46
1:B:68:TRP:CD1	1:B:73:GLU:HB2	2.50	0.46
1:A:132:ILE:O	1:A:132:ILE:HG23	2.16	0.46
4:A:1071:HOH:O	1:B:26:ARG:HB3	2.15	0.46
1:A:171:PRO:HG2	1:B:154:ARG:HD3	1.98	0.46
1:A:155:LEU:C	1:A:156:ILE:HD12	2.37	0.46
1:A:201:CYS:SG	1:A:236:MET:CG	3.04	0.46
1:A:160:TRP:CZ2	1:A:165:LEU:HD21	2.52	0.46
1:A:153:ARG:HD2	4:B:1109:HOH:O	2.14	0.46
1:A:151:TYR:HE2	1:A:183:ILE:HG13	1.80	0.45
1:B:271:ASP:HB3	1:B:274:ASP:CG	2.36	0.45
1:B:42:PHE:CE2	1:B:211:ILE:HD13	2.51	0.45
1:A:193:SER:HA	1:A:231:ASP:O	2.17	0.45
1:B:82:LYS:O	1:B:84:ILE:HD12	2.15	0.45
1:B:183:ILE:HD13	1:B:189:ARG:N	2.31	0.45
1:A:198:GLN:NE2	1:A:201:CYS:HA	2.26	0.45
1:B:40:LEU:HG	4:B:1136:HOH:O	2.17	0.45
1:A:162:PRO:HD2	1:B:120:PHE:CZ	2.50	0.45
1:A:176:PHE:HE2	1:B:175:MET:HE1	1.80	0.45
1:B:184:PRO:HD2	1:B:189:ARG:CB	2.46	0.45
1:A:295:MET:CG	1:A:296:SER:H	2.25	0.45
1:A:126:ASP:OD1	1:A:129:THR:HG23	2.17	0.45
1:B:12:LEU:HD21	1:B:236:MET:CE	2.46	0.45
1:A:89:ALA:C	1:A:91:GLY:N	2.70	0.45
1:B:13:VAL:CG1	1:B:249:LEU:HD12	2.45	0.45
1:A:31:THR:HB	1:A:241:ILE:O	2.17	0.45
1:B:142:ILE:HD11	1:B:157:LEU:HB2	1.98	0.45
1:B:147:ARG:NH1	1:B:147:ARG:HG2	2.31	0.45
1:A:95:TYR:HE2	1:A:169:ALA:O	2.00	0.45
1:B:200:SER:OG	2:B:765:UMP:H3'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HA	1:A:24:PRO:HD3	1.80	0.45
1:B:115:PHE:CE2	1:B:124:TYR:HD1	2.35	0.45
1:B:143:ILE:O	1:B:147:ARG:HD3	2.17	0.45
1:B:192:LEU:CD2	1:B:221:ILE:HG23	2.47	0.45
1:A:41:LYS:HG2	1:A:233:ILE:HG12	1.98	0.45
1:A:130:ASN:ND2	1:A:132:ILE:HG22	2.32	0.45
1:A:131:TYR:HA	1:A:134:GLN:NE2	2.31	0.44
1:A:171:PRO:HG2	1:B:154:ARG:NE	2.32	0.44
1:A:119:HIS:O	1:A:120:PHE:C	2.55	0.44
1:B:41:LYS:CB	1:B:41:LYS:NZ	2.80	0.44
1:B:243:LYS:C	1:B:245:HIS:N	2.70	0.44
1:A:216:LEU:HD23	1:A:263:LEU:CD2	2.47	0.44
1:A:237:GLY:HA3	1:B:178:GLN:OE1	2.18	0.44
1:A:58:PHE:O	1:A:59:ILE:C	2.55	0.44
1:A:296:SER:HB3	3:A:768:CB3:NA2	2.32	0.44
1:A:156:ILE:N	1:A:156:ILE:HD12	2.32	0.44
1:B:224:VAL:HG21	1:B:272:ILE:HB	1.99	0.44
1:A:174:HIS:ND1	1:A:174:HIS:O	2.51	0.44
1:B:184:PRO:HD2	1:B:189:ARG:HB3	1.99	0.44
1:A:201:CYS:HB3	1:A:207:VAL:CG2	2.48	0.44
1:A:297:ILE:HG13	1:A:297:ILE:H	1.55	0.44
1:A:13:VAL:HG13	1:A:241:ILE:HD11	1.99	0.44
1:B:25:ASP:OD1	1:B:27:THR:N	2.51	0.44
1:B:26:ARG:NH1	1:B:27:THR:HG22	2.33	0.44
1:A:84:ILE:HD12	1:A:84:ILE:N	2.33	0.44
1:B:196:LEU:HD22	1:B:232:PHE:CE1	2.53	0.44
1:B:182:HIS:CE1	1:B:193:SER:OG	2.66	0.43
1:A:200:SER:HB3	2:A:767:UMP:H2'	2.00	0.43
1:B:168:MET:SD	1:B:172:PRO:HD3	2.58	0.43
1:B:146:ILE:HD12	1:B:221:ILE:HD11	2.00	0.43
1:A:13:VAL:HB	1:A:253:LEU:HD21	1.99	0.43
1:A:252:GLN:HA	1:A:255:ARG:HG3	2.00	0.43
1:A:211:ILE:O	1:A:215:ALA:HB2	2.18	0.43
1:B:196:LEU:CD2	1:B:234:HIS:HA	2.48	0.43
1:B:266:ASN:HB3	1:B:267:ARG:H	0.97	0.43
1:A:152:ASP:HB3	1:A:155:LEU:HD21	2.00	0.43
1:A:43:SER:OG	1:A:45:ARG:HB2	2.17	0.43
1:A:183:ILE:HG23	1:A:189:ARG:CB	2.46	0.43
1:B:247:GLU:OE1	1:B:247:GLU:N	2.52	0.43
1:B:183:ILE:HD11	1:B:189:ARG:N	2.33	0.43
1:A:27:THR:CB	1:A:296:SER:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:TYR:C	1:A:125:ILE:HG23	2.38	0.43
1:B:93:ARG:NH1	1:B:106:GLU:OE1	2.52	0.43
1:B:143:ILE:CD1	1:B:221:ILE:HG13	2.49	0.43
1:A:233:ILE:HD12	1:B:36:ALA:HB1	2.00	0.43
1:B:89:ALA:C	1:B:91:GLY:H	2.21	0.43
1:A:53:THR:O	1:A:287:PRO:HA	2.18	0.43
1:A:176:PHE:CZ	1:B:176:PHE:CE1	3.07	0.43
1:A:3:ASN:HA	4:A:1198:HOH:O	2.19	0.43
1:A:246:ILE:HG22	1:A:250:GLN:HE22	1.84	0.43
1:B:251:GLN:HG3	1:B:252:GLN:H	1.83	0.43
1:B:66:LEU:O	1:B:69:PHE:HB2	2.19	0.42
1:B:104:ARG:NH2	1:B:167:LYS:O	2.52	0.42
1:B:151:TYR:O	1:B:152:ASP:C	2.57	0.42
1:A:255:ARG:HH21	1:A:288:TYR:HB2	1.83	0.42
1:A:128:LYS:NZ	1:A:128:LYS:CB	2.82	0.42
1:A:295:MET:O	1:A:296:SER:CB	2.65	0.42
1:A:181:VAL:HG21	1:A:227:LEU:HD13	2.00	0.42
1:A:3:ASN:ND2	1:A:260:PHE:CD2	2.87	0.42
1:A:52:LEU:N	1:A:52:LEU:HD12	2.13	0.42
1:A:267:ARG:O	1:A:268:SER:C	2.56	0.42
1:A:192:LEU:HD23	1:A:221:ILE:HG23	2.02	0.42
1:B:147:ARG:HG2	1:B:147:ARG:HH11	1.84	0.42
1:B:199:ARG:HG3	1:B:200:SER:N	2.34	0.42
1:B:31:THR:HG22	1:B:242:TYR:CD1	2.55	0.42
1:A:7:GLN:OE1	1:A:10:LEU:HD12	2.19	0.42
1:B:77:LEU:O	1:B:81:GLU:HG3	2.19	0.42
1:A:160:TRP:HE1	1:A:162:PRO:HG3	1.83	0.42
1:A:49:PHE:O	1:A:51:LEU:N	2.47	0.42
1:B:65:GLU:OE1	1:B:209:PHE:HE2	2.03	0.42
1:A:143:ILE:HD13	1:A:221:ILE:HG13	2.02	0.42
1:B:43:SER:HB3	4:B:1137:HOH:O	2.18	0.42
1:A:26:ARG:HD2	2:A:767:UMP:OP3	2.19	0.42
1:A:3:ASN:HB2	1:A:6:GLU:H	1.85	0.42
1:A:60:ARG:HH12	1:A:84:ILE:CD1	2.31	0.42
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.35	0.42
1:B:3:ASN:OD1	1:B:258:ARG:O	2.37	0.42
1:A:143:ILE:CD1	1:A:221:ILE:HG13	2.49	0.42
1:B:182:HIS:O	1:B:190:PRO:O	2.37	0.42
1:B:162:PRO:HA	1:B:165:LEU:HD22	2.02	0.42
1:B:243:LYS:HZ3	1:B:243:LYS:HB3	1.85	0.42
1:A:12:LEU:HD23	1:A:203:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:HB2	1:A:134:GLN:C	2.40	0.42
1:A:189:ARG:O	1:A:227:LEU:HD22	2.19	0.42
1:A:272:ILE:HA	1:A:275:PHE:HE1	1.85	0.42
1:A:41:LYS:HE2	1:A:233:ILE:CD1	2.49	0.42
1:B:190:PRO:O	1:B:191:GLU:CB	2.60	0.41
1:A:266:ASN:OD1	1:A:269:ILE:HB	2.20	0.41
1:A:21:GLU:O	1:A:32:LEU:HA	2.20	0.41
1:A:22:ASP:HA	1:A:32:LEU:HD23	2.02	0.41
1:A:138:GLN:O	1:A:142:ILE:HG13	2.20	0.41
1:A:86:ILE:HB	3:A:768:CB3:C16	2.50	0.41
1:B:245:HIS:HB3	1:B:249:LEU:HD23	2.03	0.41
1:A:243:LYS:NZ	1:A:244:ASP:N	2.67	0.41
1:A:177:CYS:SG	1:A:214:TYR:HE1	2.41	0.41
1:A:216:LEU:HD23	1:A:263:LEU:HD21	2.02	0.41
1:B:42:PHE:HD2	1:B:232:PHE:HD2	1.67	0.41
1:B:41:LYS:HZ3	1:B:41:LYS:HB3	1.84	0.41
1:A:283:GLN:O	1:A:284:ASN:HB2	2.20	0.41
1:A:65:GLU:OE2	1:A:69:PHE:CZ	2.73	0.41
1:B:271:ASP:OD1	1:B:271:ASP:O	2.39	0.41
1:B:146:ILE:HD11	1:B:221:ILE:HD11	2.01	0.41
1:A:55:LYS:NZ	1:A:291:ILE:H	2.19	0.41
1:A:128:LYS:NZ	1:A:128:LYS:HB2	2.36	0.41
1:A:6:GLU:O	1:A:9:TYR:HB3	2.19	0.41
1:B:171:PRO:HA	1:B:172:PRO:HD3	1.95	0.41
1:A:196:LEU:O	1:A:196:LEU:HD23	2.20	0.41
1:A:206:GLY:O	1:A:207:VAL:C	2.59	0.41
1:B:119:HIS:O	1:B:120:PHE:C	2.58	0.41
1:B:42:PHE:CZ	1:B:211:ILE:HD13	2.56	0.41
1:B:39:PRO:HB2	1:B:233:ILE:HD11	2.02	0.41
1:B:112:ILE:O	1:B:113:TYR:C	2.59	0.41
1:A:38:SER:HA	1:A:39:PRO:HD2	1.91	0.41
1:B:182:HIS:O	1:B:191:GLU:HB2	2.21	0.40
1:A:91:GLY:HA2	1:A:96:LEU:HD21	2.03	0.40
1:A:160:TRP:CG	1:A:175:MET:HE3	2.56	0.40
1:A:12:LEU:O	1:A:16:ILE:HG13	2.21	0.40
1:B:243:LYS:O	1:B:246:ILE:HG13	2.21	0.40
1:B:272:ILE:HA	1:B:275:PHE:HE1	1.83	0.40
1:A:243:LYS:HZ3	1:A:243:LYS:CB	2.33	0.40
1:B:266:ASN:HB3	1:B:269:ILE:HD13	2.03	0.40
1:A:183:ILE:HD13	1:A:189:ARG:HG2	2.03	0.40
1:B:16:ILE:HD12	1:B:203:MET:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HD21	1:B:293:MET:CB	2.52	0.40
1:A:49:PHE:HZ	1:A:216:LEU:HG	1.83	0.40
1:A:209:PHE:CG	3:A:768:CB3:CP3	3.04	0.40
1:B:77:LEU:CD2	1:B:80:ARG:NH1	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/297 (97%)	235 (82%)	36 (12%)	17 (6%)	2	2
1	B	288/297 (97%)	244 (85%)	32 (11%)	12 (4%)	3	4
All	All	576/594 (97%)	479 (83%)	68 (12%)	29 (5%)	3	3

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	ILE
1	A	184	PRO
1	A	244	ASP
1	A	267	ARG
1	A	272	ILE
1	A	295	MET
1	A	296	SER
1	B	113	TYR
1	B	125	ILE
1	B	267	ARG
1	A	90	ASN
1	A	113	TYR
1	A	120	PHE
1	A	206	GLY

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Mol	Chain	Res	Type
1	B	4	ALA
1	B	55	LYS
1	B	120	PHE
1	B	190	PRO
1	B	191	GLU
1	B	244	ASP
1	B	295	MET
1	A	268	SER
1	B	148	THR
1	A	4	ALA
1	A	289	GLU
1	A	246	ILE
1	A	190	PRO
1	A	50	PRO
1	B	50	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/268 (98%)	244 (93%)	19 (7%)	18	35
1	B	263/268 (98%)	239 (91%)	24 (9%)	12	22
All	All	526/536 (98%)	483 (92%)	43 (8%)	14	27

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	44	LEU
1	A	45	ARG
1	A	66	LEU
1	A	96	LEU
1	A	105	GLN
1	A	118	ARG
1	A	147	ARG

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Mol	Chain	Res	Type
1	A	164	ASP
1	A	166	GLU
1	A	176	PHE
1	A	182	HIS
1	A	243	LYS
1	A	247	GLU
1	A	251	GLN
1	A	258	ARG
1	A	267	ARG
1	A	270	THR
1	A	294	LYS
1	B	25	ASP
1	B	26	ARG
1	B	66	LEU
1	B	93	ARG
1	B	105	GLN
1	B	118	ARG
1	B	126	ASP
1	B	136	VAL
1	B	147	ARG
1	B	153	ARG
1	B	165	LEU
1	B	176	PHE
1	B	182	HIS
1	B	226	ASP
1	B	233	ILE
1	B	243	LYS
1	B	247	GLU
1	B	251	GLN
1	B	258	ARG
1	B	267	ARG
1	B	270	THR
1	B	277	LEU
1	B	290	THR
1	B	294	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	105	GLN
1	A	130	ASN

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Mol	Chain	Res	Type
1	A	134	GLN
1	A	144	GLN
1	A	182	HIS
1	A	198	GLN
1	A	234	HIS
1	A	252	GLN
1	A	266	ASN
1	B	3	ASN
1	B	85	HIS
1	B	90	ASN
1	B	105	GLN
1	B	144	GLN
1	B	182	HIS
1	B	195	GLN
1	B	210	ASN
1	B	234	HIS
1	B	252	GLN
1	B	266	ASN
1	B	286	HIS

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	UMP	A	767	-	16,21,21	3.82	8 (50%)	23,31,31	3.83	7 (30%)
3	CB3	A	768	-	31,37,37	30.79	18 (58%)	35,51,51	12.01	12 (34%)
2	UMP	B	765	-	16,21,21	2.13	5 (31%)	23,31,31	3.39	7 (30%)

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	UMP	A	767	-	-	0/6/22/22	0/2/2/2
3	CB3	A	768	-	1/1/5/6	0/21/28/28	0/3/3/3
2	UMP	B	765	-	-	0/6/22/22	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	767	UMP	O4-C4	-2.81	1.18	1.24
2	A	767	UMP	P-O5'	-2.28	1.52	1.60
2	B	765	UMP	P-OP3	-2.15	1.47	1.54
2	A	767	UMP	P-OP3	-2.05	1.47	1.54
3	A	768	CB3	C8-C8A	2.00	1.45	1.41
3	A	768	CB3	C15-C14	2.01	1.43	1.39
2	B	765	UMP	C6-C5	2.11	1.42	1.38
3	A	768	CB3	C7-C6	2.73	1.44	1.38
3	A	768	CB3	C4-C4A	2.74	1.46	1.41
3	A	768	CB3	C16-C15	2.77	1.43	1.38
3	A	768	CB3	C4A-C8A	2.82	1.47	1.41
3	A	768	CB3	C13-C14	2.85	1.44	1.39
3	A	768	CB3	C9-N10	2.95	1.50	1.46
3	A	768	CB3	CP1-N10	3.02	1.48	1.46
2	A	767	UMP	O4'-C4'	3.15	1.52	1.45
3	A	768	CB3	C13-C12	3.16	1.44	1.38
2	B	765	UMP	O4'-C4'	3.16	1.52	1.45
3	A	768	CB3	C4-N3	3.30	1.39	1.33
3	A	768	CB3	C16-C11	3.48	1.45	1.39
3	A	768	CB3	C12-C11	3.50	1.45	1.39
3	A	768	CB3	C5-C6	3.57	1.46	1.37
2	A	767	UMP	C6-N1	3.66	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	768	CB3	C8-C7	4.04	1.45	1.36
2	A	767	UMP	O4'-C1'	4.35	1.52	1.42
2	A	767	UMP	C4-N3	4.38	1.41	1.33
2	B	765	UMP	C4-N3	4.63	1.41	1.33
2	B	765	UMP	O4'-C1'	4.84	1.53	1.42
3	A	768	CB3	O4-C4	6.23	1.39	1.24
2	A	767	UMP	C6-C5	12.19	1.64	1.38
3	A	768	CB3	C14-N10	105.93	4.28	1.38
3	A	768	CB3	C11-C	134.09	4.33	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	768	CB3	C15-C14-N10	-46.12	59.38	121.38
3	A	768	CB3	C13-C14-N10	-45.25	60.54	121.38
3	A	768	CB3	C16-C11-C	-19.74	58.01	120.60
3	A	768	CB3	C12-C11-C	-19.03	60.25	120.60
3	A	768	CB3	N1-C2-N3	-5.77	118.66	127.44
2	A	767	UMP	C5-C6-N1	-4.42	109.76	120.58
2	B	765	UMP	C5-C4-N3	-3.37	114.47	123.12
3	A	768	CB3	C4-C4A-C8A	-3.31	115.31	118.54
2	B	765	UMP	O4'-C1'-C2'	-3.13	100.04	106.27
2	A	767	UMP	C6-C5-C4	-3.12	111.44	117.28
2	A	767	UMP	O4'-C1'-C2'	-3.10	100.09	106.27
2	B	765	UMP	O4'-C4'-C3'	-3.04	98.01	105.67
2	A	767	UMP	C5-C4-N3	-2.61	116.41	123.12
2	A	767	UMP	O4'-C4'-C3'	-2.32	99.82	105.67
3	A	768	CB3	CP1-N10-C9	-2.30	111.62	117.28
3	A	768	CB3	C9-C6-C7	-2.04	116.94	120.78
2	B	765	UMP	OP2-P-O5'	2.27	113.09	106.56
2	B	765	UMP	C6-C5-C4	2.35	121.67	117.28
3	A	768	CB3	C6-C9-N10	2.50	118.67	114.51
3	A	768	CB3	C9-N10-C14	2.94	126.21	120.93
3	A	768	CB3	C5-C4A-C4	3.04	125.97	122.22
3	A	768	CB3	C4-N3-C2	4.76	122.55	115.94
2	B	765	UMP	O4'-C1'-N1	9.85	124.77	107.72
2	B	765	UMP	C4-N3-C2	10.66	124.70	114.14
2	A	767	UMP	O4'-C1'-N1	11.33	127.34	107.72
2	A	767	UMP	C4-N3-C2	11.91	125.94	114.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	768	CB3	CA

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	UMP	3	0
3	A	768	CB3	18	0
2	B	765	UMP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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