



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 AM GMT

PDB ID : 2DU3
Title : Crystal structure of Archaeoglobus fulgidus O-phosphoseryl-tRNA synthetase complexed with tRNACys and O-phosphoserine
Authors : Fukunaga, R.
Deposited on : 2006-07-20
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 ⓘ 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

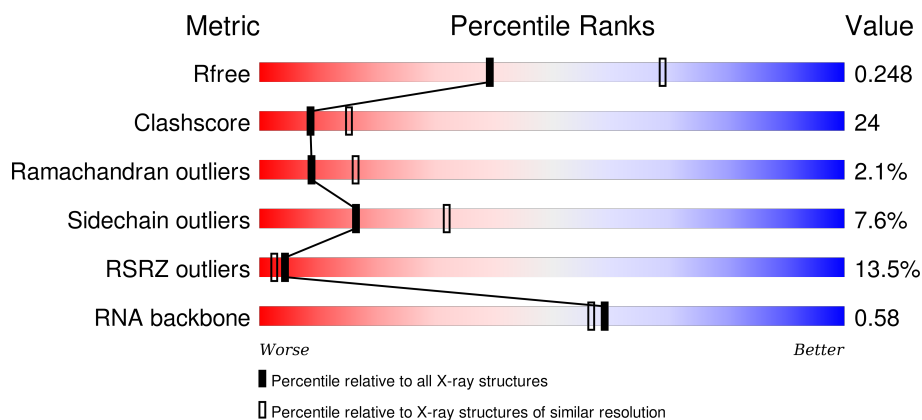
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

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.

Mol	Chain	Length	Quality of chain
1	D	71	<div> <div>54%</div> <div> <div></div> <div>49%</div> <div>30%</div> <div>20%</div> <div>.</div> </div> </div>
2	A	534	<div> <div>14%</div> <div> <div></div> <div>57%</div> <div>38%</div> <div>5%</div> <div>.</div> </div> </div>
2	B	534	<div> <div>6%</div> <div> <div></div> <div>53%</div> <div>30%</div> <div>.</div> <div>13%</div> </div> </div>

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.

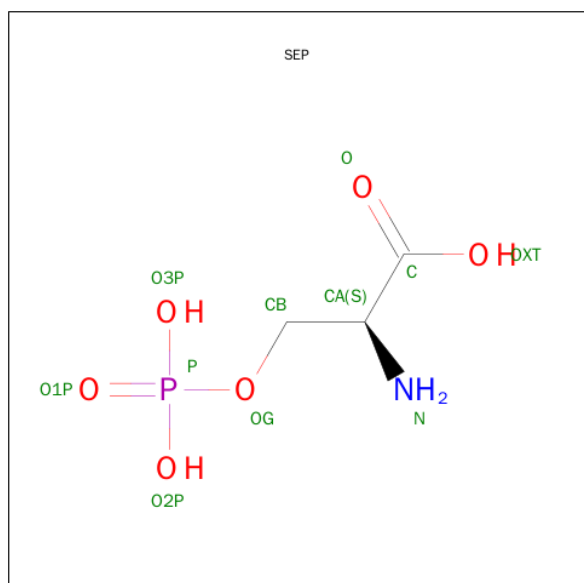
- Molecule 1 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	71	Total	C	N	O	P	0	0	0
			1520	675	272	502	71			

- Molecule 2 is a protein called O-phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	534	Total 4321	C 2786	N 719	O 803	S 13	0	0	0
2	B	465	Total 3763	C 2429	N 630	O 691	S 13	0	0	0

- Molecule 3 is PHOSPHOSERINE (three-letter code: SEP) (formula: $\text{C}_3\text{H}_8\text{NO}_6\text{P}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	2	Total	C	N	O	P	0	0
			22	6	2	12	2		

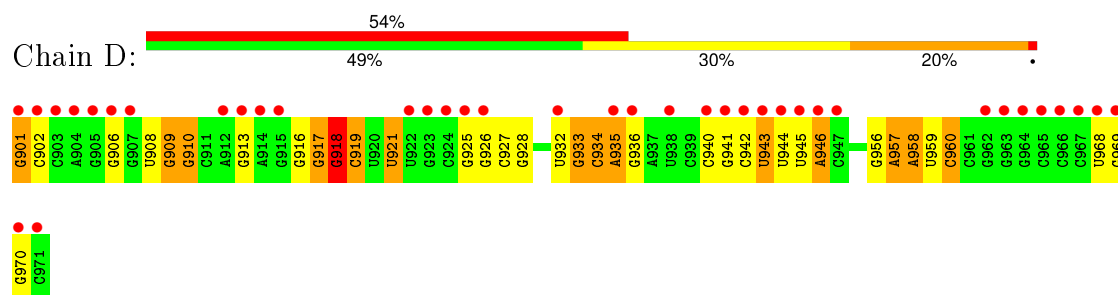
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total 62	O 62	0	0
4	B	60	Total 60	O 60	0	0

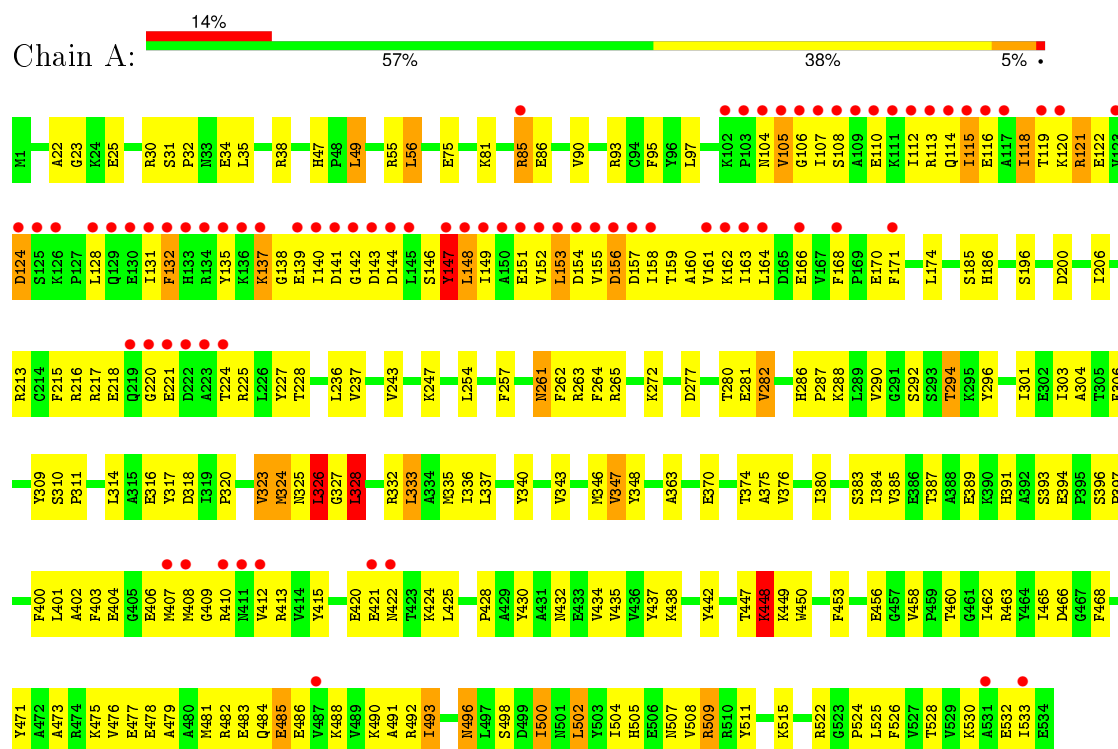
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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



• Molecule 2: O-phosphoseryl-tRNA synthetase



• Molecule 2: O-phosphoseryl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.12Å 149.12Å 153.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.46 – 2.60 49.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.46-2.60) 99.6 (49.46-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.249 0.203 , 0.248	Depositor DCC
R_{free} test set	3077 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.7	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60911 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9748	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	D	0.35	1/1697 (0.1%)	0.72	2/2644 (0.1%)
2	A	0.42	0/4418	0.64	2/5968 (0.0%)
2	B	0.43	0/3851	0.67	1/5202 (0.0%)
All	All	0.41	1/9966 (0.0%)	0.67	5/13814 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	901	G	OP3-P	-6.84	1.52	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	918	G	N9-C1'-C2'	8.25	124.72	114.00
2	B	328	LEU	CA-CB-CG	6.32	129.83	115.30
2	A	328	LEU	CA-CB-CG	5.99	129.07	115.30
2	A	326	LEU	CA-CB-CG	5.45	127.83	115.30
1	D	901	G	OP1-P-OP2	-5.15	111.88	119.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	918	G	Sidechain

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	D	1520	0	769	40	0
2	A	4321	0	4339	246	0
2	B	3763	0	3774	166	0
3	A	22	0	10	1	0
4	A	62	0	0	6	0
4	B	60	0	0	3	0
All	All	9748	0	8892	437	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 24.

All (437) 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)
2:B:464:TYR:HA	2:B:500:ILE:HD11	1.16	1.13
2:B:55:ARG:HH21	2:B:55:ARG:HG2	1.12	1.10
2:A:85:ARG:HD2	2:A:85:ARG:H	1.19	1.07
2:B:376:VAL:HA	2:B:379:LYS:HE2	1.43	1.00
1:D:933:G:H22	2:A:492:ARG:HD3	1.28	0.98
2:B:448:LYS:HD3	2:B:448:LYS:H	1.26	0.97
2:B:216:ARG:HG2	2:B:218:GLU:HG2	1.49	0.94
2:B:504:ILE:HB	2:B:508:VAL:HG21	1.49	0.92
2:B:47:HIS:HD2	2:B:49:LEU:H	1.16	0.92
2:B:376:VAL:HG11	2:B:407:MET:HB3	1.55	0.89
2:B:397:PRO:HD3	2:B:421:GLU:HA	1.55	0.88
2:A:478:GLU:HB3	2:A:482:ARG:HH22	1.36	0.88
2:A:504:ILE:HB	2:A:508:VAL:HG21	1.56	0.88
2:A:22:ALA:O	2:A:25:GLU:HG2	1.73	0.88
2:B:75:GLU:OE2	2:B:180:THR:HG23	1.74	0.87
2:A:106:GLY:HA2	2:A:110:GLU:HB2	1.56	0.87
2:B:47:HIS:CD2	2:B:49:LEU:H	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:294:THR:HG23	2:A:296:TYR:H	1.39	0.86
2:B:267:ASP:HB3	2:B:279:GLN:HG2	1.59	0.85
1:D:942:C:O2'	1:D:943:U:H5'	1.77	0.85
2:B:85:ARG:N	2:B:85:ARG:HD2	1.91	0.85
2:A:144:ASP:HA	2:A:147:TYR:CE1	2.12	0.84
2:A:496:ASN:ND2	2:A:498:SER:HB3	1.92	0.84
2:B:407:MET:HE1	2:B:477:GLU:HG3	1.61	0.83
2:B:55:ARG:NH2	2:B:55:ARG:HG2	1.91	0.82
1:D:933:G:N2	2:A:492:ARG:HD3	1.95	0.81
2:A:110:GLU:HA	2:A:113:ARG:HB3	1.61	0.81
2:A:394:GLU:HG3	2:A:400:PHE:HZ	1.45	0.81
2:A:413:ARG:NH1	2:A:532:GLU:HG3	1.96	0.81
2:A:131:ILE:H	2:A:131:ILE:HD12	1.46	0.80
2:A:394:GLU:HG3	2:A:400:PHE:CZ	2.17	0.79
2:A:387:THR:HG21	2:A:402:ALA:HA	1.65	0.78
2:A:47:HIS:CD2	2:A:49:LEU:H	2.01	0.78
2:B:474:ARG:HH11	2:B:474:ARG:HG3	1.48	0.78
2:A:460:THR:HG23	2:A:462:ILE:H	1.47	0.78
1:D:933:G:H1	2:A:492:ARG:HE	1.31	0.77
2:A:157:ASP:HB3	2:A:161:VAL:HG13	1.65	0.77
2:A:47:HIS:HD2	2:A:49:LEU:H	1.33	0.77
2:B:504:ILE:HD12	2:B:508:VAL:HG23	1.67	0.76
2:B:397:PRO:HG3	2:B:419:GLU:O	1.84	0.76
2:B:55:ARG:HH21	2:B:55:ARG:CG	1.95	0.76
2:A:500:ILE:HG22	2:A:502:LEU:HB2	1.67	0.76
2:A:505:HIS:O	2:A:508:VAL:HG22	1.86	0.75
2:B:85:ARG:H	2:B:85:ARG:HD2	1.51	0.75
2:A:475:LYS:HE2	2:A:475:LYS:HA	1.68	0.75
2:B:447:THR:HG23	2:B:448:LYS:HE2	1.68	0.75
2:B:464:TYR:HA	2:B:500:ILE:CD1	2.09	0.75
2:B:448:LYS:CD	2:B:448:LYS:H	1.93	0.74
2:B:504:ILE:HB	2:B:508:VAL:CG2	2.17	0.74
2:A:31:SER:HB2	2:A:32:PRO:HD2	1.70	0.74
2:A:118:ILE:HD12	2:A:118:ILE:H	1.52	0.74
2:A:90:VAL:O	2:A:93:ARG:HG2	1.88	0.74
2:B:448:LYS:N	2:B:448:LYS:HD3	2.04	0.73
2:A:85:ARG:H	2:A:85:ARG:CD	1.99	0.73
1:D:957:A:H4'	1:D:958:A:OP1	1.85	0.73
2:A:504:ILE:HB	2:A:508:VAL:CG2	2.18	0.72
2:B:175:LYS:N	2:B:175:LYS:HD2	2.04	0.72
2:B:347:VAL:HG22	2:B:348:TYR:CD2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:HIS:O	2:B:508:VAL:HG22	1.90	0.72
2:A:500:ILE:CG2	2:A:502:LEU:HD22	2.19	0.72
2:A:218:GLU:HG3	2:A:225:ARG:HG2	1.71	0.72
2:A:488:LYS:HD3	2:A:530:LYS:HE2	1.70	0.72
2:A:324:MET:HE1	2:A:325:ASN:C	2.10	0.71
2:A:148:LEU:HG	2:A:160:ALA:HB2	1.71	0.71
2:A:110:GLU:HG2	2:A:114:GLN:HE21	1.55	0.71
2:B:447:THR:HG22	2:B:449:LYS:H	1.56	0.70
2:A:374:THR:HG22	2:A:376:VAL:H	1.55	0.69
2:A:404:GLU:OE2	2:A:413:ARG:HB3	1.92	0.69
1:D:933:G:H1	2:A:492:ARG:NE	1.90	0.69
1:D:941:G:H2'	1:D:942:C:H5'	1.74	0.69
2:A:347:VAL:HG22	2:A:348:TYR:CD2	2.28	0.68
1:D:916:G:H2'	1:D:959:U:O2'	1.93	0.68
2:A:306:PHE:HB2	2:A:324:MET:CE	2.23	0.68
2:A:465:ILE:HD12	2:A:466:ASP:H	1.59	0.68
2:A:434:VAL:HB	2:A:460:THR:HG21	1.75	0.68
2:A:287:PRO:O	2:A:290:VAL:HG22	1.93	0.68
2:A:149:ILE:HG13	2:A:155:VAL:HA	1.74	0.68
2:A:153:LEU:O	2:A:154:ASP:HB2	1.94	0.68
2:B:372:PRO:HB2	2:B:378:LEU:HD23	1.76	0.68
2:B:409:GLY:C	2:B:410:ARG:HD3	2.14	0.68
2:A:496:ASN:HD21	2:A:498:SER:HB3	1.59	0.67
2:B:47:HIS:HD2	2:B:49:LEU:N	1.90	0.67
2:B:490:LYS:HB3	2:B:528:THR:HG23	1.75	0.67
2:A:157:ASP:HA	2:A:160:ALA:HB3	1.76	0.67
2:A:500:ILE:HG21	2:A:502:LEU:HD22	1.75	0.67
2:A:306:PHE:HB2	2:A:324:MET:HE3	1.76	0.66
2:A:85:ARG:N	2:A:85:ARG:HH21	1.94	0.66
1:D:942:C:C2'	1:D:943:U:H5'	2.25	0.66
2:A:493:ILE:HD12	2:A:493:ILE:H	1.61	0.65
2:B:286:HIS:HD2	2:B:288:LYS:H	1.43	0.65
1:D:959:U:H5'	1:D:960:C:OP2	1.97	0.65
2:B:287:PRO:O	2:B:290:VAL:HG22	1.96	0.65
2:B:192:PHE:HE2	2:B:314:LEU:HD13	1.62	0.65
2:A:85:ARG:HD2	2:A:85:ARG:N	2.02	0.65
2:B:37:PRO:O	2:B:364:ARG:HG3	1.97	0.64
1:D:934:C:H4'	1:D:935:A:OP2	1.97	0.64
2:A:430:TYR:O	2:A:465:ILE:HG13	1.98	0.64
2:A:56:LEU:HD13	2:A:257:PHE:CZ	2.33	0.63
1:D:957:A:O2'	1:D:958:A:O5'	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:478:GLU:HA	2:A:481:MET:HE2	1.80	0.63
2:A:448:LYS:CD	2:A:448:LYS:H	2.12	0.63
2:A:428:PRO:HG2	2:A:524:PRO:HG2	1.80	0.63
2:A:396:SER:HB3	2:A:420:GLU:O	1.99	0.62
2:A:47:HIS:HD2	2:A:49:LEU:N	1.97	0.62
2:A:131:ILE:HD12	2:A:131:ILE:N	2.12	0.62
2:A:465:ILE:HD12	2:A:466:ASP:N	2.14	0.62
2:B:4:ASP:HB3	2:B:7:LYS:HD3	1.81	0.62
2:B:451:ARG:HH21	2:B:451:ARG:HG3	1.64	0.62
2:A:448:LYS:H	2:A:448:LYS:CE	2.12	0.62
2:B:376:VAL:HA	2:B:379:LYS:CE	2.27	0.61
2:A:406:GLU:OE1	2:A:409:GLY:HA2	1.99	0.61
2:A:55:ARG:HD2	4:A:1062:HOH:O	1.99	0.61
1:D:941:G:C2'	1:D:942:C:H5'	2.30	0.61
2:A:243:VAL:HG12	2:A:247:LYS:HE3	1.81	0.61
2:A:220:GLY:HA2	2:A:227:TYR:OH	2.00	0.61
2:B:11:LEU:O	2:B:11:LEU:HD23	2.01	0.60
2:A:311:PRO:HA	2:A:314:LEU:HD23	1.82	0.60
2:B:479:ALA:HB2	2:B:487:VAL:HG11	1.84	0.60
2:B:485:GLU:HA	2:B:533:ILE:HG12	1.84	0.60
2:A:118:ILE:HD12	2:A:118:ILE:N	2.16	0.60
2:B:496:ASN:HD22	2:B:496:ASN:C	2.04	0.60
2:A:434:VAL:O	2:A:460:THR:HG22	2.02	0.60
2:B:343:VAL:HG23	4:B:569:HOH:O	2.02	0.60
2:B:328:LEU:HD12	2:B:328:LEU:C	2.22	0.60
2:A:393:SER:O	2:A:424:LYS:HD3	2.02	0.59
2:A:335:MET:HE2	2:A:343:VAL:HG13	1.84	0.59
2:A:257:PHE:O	2:A:286:HIS:HE1	1.85	0.59
2:B:496:ASN:ND2	2:B:499:ASP:H	1.99	0.59
2:A:335:MET:HE1	2:A:343:VAL:HG22	1.83	0.59
2:A:303:ILE:O	2:A:328:LEU:HD22	2.03	0.59
2:A:460:THR:HG23	2:A:462:ILE:N	2.16	0.59
2:B:277:ASP:HB2	4:B:576:HOH:O	2.03	0.59
2:A:504:ILE:HD12	2:A:508:VAL:HG23	1.83	0.58
1:D:909:G:H4'	1:D:910:G:OP2	2.02	0.58
2:A:148:LEU:HG	2:A:160:ALA:CB	2.32	0.58
2:B:32:PRO:O	2:B:38:ARG:NH1	2.36	0.58
2:B:408:MET:CE	2:B:481:MET:HB3	2.33	0.58
1:D:909:G:H1'	1:D:946:A:H1'	1.85	0.58
2:A:185:SER:HA	2:A:215:PHE:O	2.04	0.58
2:B:433:GLU:OE2	2:B:459:PRO:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:137:LYS:HE3	2:A:137:LYS:HA	1.86	0.58
2:B:192:PHE:CE2	2:B:314:LEU:HD13	2.39	0.57
2:A:412:VAL:HG22	2:A:533:ILE:HG22	1.86	0.57
1:D:917:G:H4'	1:D:918:G:OP1	2.05	0.57
2:B:226:LEU:HD21	2:B:344:ARG:HG2	1.86	0.57
2:B:391:HIS:O	2:B:425:LEU:HD23	2.03	0.57
2:A:383:SER:O	2:A:387:THR:HG23	2.05	0.57
2:A:471:TYR:O	2:A:475:LYS:HG2	2.04	0.57
2:B:485:GLU:HA	2:B:533:ILE:CG1	2.35	0.57
2:B:174:LEU:C	2:B:175:LYS:HD2	2.26	0.56
2:B:396:SER:HA	2:B:397:PRO:C	2.24	0.56
2:A:200:ASP:HB2	2:B:510:ARG:HE	1.69	0.56
1:D:913:G:H21	1:D:921:U:H5	1.52	0.56
2:A:81:LYS:NZ	2:A:316:GLU:HB3	2.21	0.56
2:A:335:MET:CE	2:A:343:VAL:HG22	2.36	0.56
2:A:407:MET:HG2	2:A:408:MET:SD	2.46	0.56
1:D:918:G:O2'	1:D:919:C:OP1	2.23	0.56
2:A:200:ASP:HA	2:B:507:ASN:ND2	2.21	0.56
2:B:401:LEU:HD13	2:B:415:TYR:CE1	2.41	0.56
2:A:30:ARG:HB2	2:A:35:LEU:CD1	2.35	0.56
2:A:500:ILE:HG23	2:A:500:ILE:O	2.05	0.56
2:A:448:LYS:HE2	2:A:448:LYS:H	1.69	0.56
2:A:118:ILE:H	2:A:118:ILE:CD1	2.19	0.55
2:A:324:MET:HE1	2:A:326:LEU:N	2.22	0.55
2:A:491:ALA:O	2:A:526:PHE:HA	2.06	0.55
2:A:139:GLU:HB3	2:A:143:ASP:OD1	2.05	0.55
1:D:968:U:H2'	1:D:969:G:C8	2.42	0.55
2:A:343:VAL:HG23	4:A:1022:HOH:O	2.06	0.55
2:A:115:ILE:O	2:A:115:ILE:HD13	2.05	0.55
2:A:485:GLU:HA	2:A:533:ILE:HG13	1.89	0.55
2:B:222:ASP:OD2	2:B:344:ARG:HD3	2.06	0.54
2:A:478:GLU:HA	2:A:481:MET:CE	2.38	0.54
2:B:222:ASP:HA	2:B:225:ARG:O	2.07	0.54
2:B:93:ARG:HD2	2:B:216:ARG:HD2	1.89	0.53
2:A:448:LYS:H	2:A:448:LYS:HD3	1.73	0.53
2:A:412:VAL:HG13	2:A:533:ILE:HG22	1.91	0.53
2:B:292:SER:OG	2:B:294:THR:HG22	2.08	0.53
2:A:148:LEU:HG	2:A:160:ALA:CA	2.39	0.53
2:A:407:MET:O	2:A:408:MET:HB2	2.07	0.53
2:A:264:PHE:HB3	2:A:280:THR:CG2	2.39	0.53
2:B:4:ASP:OD1	2:B:7:LYS:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:LYS:N	2:B:7:LYS:HD2	2.23	0.53
2:A:490:LYS:HB3	2:A:528:THR:HG23	1.90	0.53
2:A:478:GLU:HB3	2:A:482:ARG:NH2	2.14	0.53
2:A:347:VAL:HG22	2:A:348:TYR:CE2	2.44	0.53
2:B:372:PRO:HG3	2:B:473:ALA:HB3	1.91	0.53
2:A:131:ILE:H	2:A:131:ILE:CD1	2.17	0.52
2:B:4:ASP:CG	2:B:7:LYS:HD3	2.29	0.52
2:B:482:ARG:HG3	2:B:482:ARG:HH21	1.73	0.52
2:B:482:ARG:O	2:B:483:GLU:HB2	2.09	0.52
1:D:926:G:H2'	1:D:927:C:C6	2.45	0.52
2:A:301:ILE:HD11	2:A:332:ARG:HD3	1.91	0.52
2:A:437:TYR:OH	2:A:438:LYS:HE2	2.09	0.52
2:B:395:PRO:O	2:B:398:CYS:HB3	2.10	0.52
2:B:465:ILE:HG13	2:B:466:ASP:N	2.24	0.52
1:D:970:G:N3	1:D:970:G:H2'	2.24	0.52
2:A:488:LYS:HG2	2:A:530:LYS:HG2	1.91	0.52
1:D:917:G:O2'	1:D:918:G:H5'	2.10	0.52
2:B:5:PRO:O	2:B:9:ARG:HB2	2.10	0.52
2:A:47:HIS:CD2	2:A:49:LEU:HB2	2.45	0.51
2:A:488:LYS:HE2	2:A:530:LYS:HD3	1.92	0.51
2:B:4:ASP:CB	2:B:7:LYS:HD3	2.41	0.51
2:A:135:TYR:HA	2:A:139:GLU:HG3	1.92	0.51
2:A:158:ILE:HG13	2:A:159:THR:N	2.26	0.51
2:B:335:MET:SD	2:B:343:VAL:HG22	2.50	0.51
2:A:118:ILE:HG22	2:A:119:THR:N	2.25	0.51
2:B:32:PRO:HG3	2:B:470:TYR:CZ	2.44	0.51
1:D:918:G:HO2'	1:D:919:C:P	2.33	0.51
2:A:144:ASP:C	2:A:146:SER:H	2.13	0.51
2:A:128:LEU:HA	2:A:131:ILE:HD13	1.92	0.51
1:D:925:G:H2'	1:D:926:G:O4'	2.10	0.51
2:A:401:LEU:HA	2:A:415:TYR:CD1	2.46	0.51
2:B:396:SER:HB2	2:B:423:THR:HG23	1.92	0.51
1:D:917:G:H2'	1:D:956:G:H22	1.76	0.51
1:D:917:G:H2'	1:D:956:G:N2	2.26	0.51
2:B:47:HIS:CD2	2:B:49:LEU:HB2	2.46	0.50
2:A:447:THR:O	2:A:449:LYS:N	2.44	0.50
2:A:481:MET:C	2:A:483:GLU:H	2.15	0.50
2:A:32:PRO:O	2:A:38:ARG:NH1	2.44	0.50
1:D:927:C:H2'	1:D:928:G:H8	1.76	0.50
2:B:468:PHE:CE2	2:B:491:ALA:HB2	2.47	0.50
2:A:292:SER:OG	2:A:294:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:294:THR:HG23	2:A:296:TYR:N	2.17	0.50
2:A:380:ILE:O	2:A:384:ILE:HG13	2.12	0.50
2:A:261:ASN:HD22	2:A:262:PHE:H	1.60	0.50
2:A:160:ALA:O	2:A:164:LEU:HG	2.12	0.50
2:B:465:ILE:HG13	2:B:466:ASP:H	1.77	0.49
2:B:183:LEU:HD13	2:B:215:PHE:CG	2.47	0.49
2:A:224:THR:O	2:A:225:ARG:HB2	2.11	0.49
2:B:380:ILE:HG12	2:B:403:PHE:CD1	2.47	0.49
2:A:509:ARG:HD2	4:A:1024:HOH:O	2.13	0.49
2:A:448:LYS:N	2:A:448:LYS:HD3	2.27	0.49
2:A:243:VAL:CG1	2:A:247:LYS:HE3	2.43	0.49
2:A:81:LYS:HZ2	2:A:316:GLU:HB3	1.77	0.49
2:B:392:ALA:HB1	2:B:426:CYS:HB2	1.94	0.49
2:B:368:VAL:HA	2:B:502:LEU:HD12	1.95	0.49
2:A:324:MET:CE	2:A:325:ASN:C	2.80	0.49
2:B:480:ALA:HA	2:B:533:ILE:CD1	2.43	0.49
2:A:385:VAL:O	2:A:389:GLU:HG3	2.13	0.48
2:B:83:PHE:CD2	2:B:90:VAL:HG21	2.48	0.48
2:A:264:PHE:HB3	2:A:280:THR:HG21	1.95	0.48
2:B:480:ALA:HA	2:B:533:ILE:HD13	1.96	0.48
2:B:484:GLN:O	2:B:533:ILE:HD11	2.12	0.48
2:A:458:VAL:HG23	2:A:458:VAL:O	2.14	0.48
2:A:156:ASP:OD1	2:A:158:ILE:HG23	2.14	0.48
2:A:447:THR:HG22	2:A:449:LYS:H	1.78	0.48
2:A:112:ILE:HD12	2:A:115:ILE:HG21	1.95	0.48
2:B:474:ARG:NH1	2:B:474:ARG:HG3	2.22	0.48
2:A:370:GLU:HG3	2:A:471:TYR:CD2	2.48	0.48
2:A:428:PRO:HG2	2:A:524:PRO:CG	2.43	0.48
2:A:363:ALA:HB2	2:A:458:VAL:CG2	2.43	0.48
2:B:328:LEU:C	2:B:328:LEU:CD1	2.82	0.48
2:A:196:SER:HB3	2:A:317:TYR:HB3	1.95	0.48
2:A:75:GLU:HB3	4:A:1012:HOH:O	2.12	0.48
2:B:497:LEU:O	2:B:500:ILE:HG22	2.14	0.48
2:B:396:SER:HB2	2:B:423:THR:CG2	2.44	0.48
2:A:490:LYS:HD2	2:A:492:ARG:HH12	1.80	0.47
2:A:509:ARG:NH1	4:A:1003:HOH:O	2.42	0.47
2:B:83:PHE:CE2	2:B:90:VAL:HG21	2.49	0.47
2:A:155:VAL:O	2:A:158:ILE:HG12	2.15	0.47
2:A:106:GLY:CA	2:A:110:GLU:HB2	2.38	0.47
2:B:85:ARG:H	2:B:85:ARG:CD	2.26	0.47
2:A:162:LYS:O	2:A:166:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:LEU:HD13	2:A:327:GLY:N	2.30	0.47
1:D:934:C:H5''	1:D:935:A:O5'	2.14	0.47
2:A:135:TYR:HA	2:A:139:GLU:CG	2.45	0.47
2:A:31:SER:CB	2:A:32:PRO:HD2	2.44	0.47
1:D:935:A:H1'	2:A:524:PRO:HD3	1.95	0.47
2:A:447:THR:C	2:A:449:LYS:N	2.68	0.47
2:A:301:ILE:HD13	2:A:336:ILE:HD11	1.97	0.47
2:B:197:HIS:HE1	4:B:577:HOH:O	1.98	0.47
2:B:493:ILE:HD12	2:B:493:ILE:H	1.80	0.47
2:A:460:THR:CG2	2:A:462:ILE:H	2.23	0.47
2:A:154:ASP:CB	2:A:158:ILE:HD11	2.45	0.47
2:B:294:THR:HG23	2:B:296:TYR:HB2	1.97	0.47
2:A:168:PHE:C	2:A:170:GLU:H	2.17	0.47
2:B:251:GLU:HG3	2:B:262:PHE:CE2	2.49	0.46
2:B:218:GLU:C	2:B:220:GLY:H	2.19	0.46
2:A:121:ARG:HH11	2:A:121:ARG:HG3	1.80	0.46
2:B:6:GLN:O	2:B:10:GLU:HG2	2.15	0.46
2:A:110:GLU:CG	2:A:114:GLN:HE21	2.24	0.46
2:A:139:GLU:HA	2:A:139:GLU:OE1	2.15	0.46
2:A:327:GLY:HA3	3:A:1001:SEP:CB	2.44	0.46
1:D:946:A:N3	1:D:946:A:H2'	2.29	0.46
2:A:432:ASN:O	2:A:463:ARG:HA	2.15	0.46
2:A:160:ALA:O	2:A:163:ILE:HG22	2.15	0.46
2:A:376:VAL:O	2:A:380:ILE:HG13	2.16	0.46
2:A:493:ILE:CD1	2:A:493:ILE:H	2.23	0.46
2:A:410:ARG:O	2:A:412:VAL:HG23	2.15	0.46
2:B:75:GLU:HB3	2:B:77:VAL:HG12	1.98	0.46
2:B:290:VAL:HA	2:B:297:SER:O	2.16	0.46
2:B:31:SER:HB2	2:B:32:PRO:HD2	1.97	0.46
2:B:390:LYS:HG3	2:B:391:HIS:CD2	2.50	0.46
2:A:128:LEU:HD23	2:A:128:LEU:H	1.80	0.46
2:B:394:GLU:HG3	2:B:400:PHE:HZ	1.81	0.46
1:D:935:A:OP2	2:A:428:PRO:HG3	2.16	0.46
2:B:404:GLU:HG3	2:B:413:ARG:HG2	1.98	0.46
2:B:175:LYS:N	2:B:175:LYS:CD	2.78	0.46
2:A:448:LYS:CD	2:A:448:LYS:N	2.79	0.46
2:B:225:ARG:HH21	2:B:225:ARG:HG3	1.80	0.46
2:A:30:ARG:HB3	2:A:34:GLU:HB2	1.97	0.46
2:A:447:THR:O	2:A:450:TRP:N	2.39	0.46
2:A:484:GLN:NE2	2:A:486:GLU:O	2.46	0.45
2:A:479:ALA:C	2:A:481:MET:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:146:SER:C	2:A:148:LEU:H	2.20	0.45
2:A:161:VAL:HG23	2:A:162:LYS:N	2.31	0.45
2:B:364:ARG:O	2:B:367:LYS:NZ	2.48	0.45
2:B:72:LEU:HD23	2:B:72:LEU:O	2.17	0.45
2:B:394:GLU:HG3	2:B:400:PHE:CZ	2.51	0.45
2:A:105:VAL:HG11	2:A:132:PHE:CE1	2.51	0.45
2:B:410:ARG:N	2:B:410:ARG:HD3	2.31	0.45
2:A:38:ARG:CZ	2:A:462:ILE:HD11	2.47	0.45
2:A:475:LYS:CA	2:A:475:LYS:HE2	2.44	0.45
2:A:507:ASN:ND2	2:B:204:LEU:HD13	2.32	0.45
2:A:442:TYR:CE2	2:A:453:PHE:HE2	2.34	0.45
2:B:85:ARG:C	2:B:87:ALA:H	2.20	0.45
2:A:434:VAL:HB	2:A:460:THR:CG2	2.44	0.44
2:B:7:LYS:CD	2:B:7:LYS:H	2.30	0.44
2:B:385:VAL:HG13	2:B:465:ILE:HD12	1.98	0.44
1:D:936:G:O2'	2:A:522:ARG:CZ	2.65	0.44
2:B:496:ASN:HD21	2:B:498:SER:HB3	1.82	0.44
2:B:412:VAL:CG2	2:B:533:ILE:HG22	2.47	0.44
2:A:137:LYS:HG3	2:A:138:GLY:N	2.33	0.44
2:A:106:GLY:O	2:A:108:SER:N	2.50	0.44
1:D:940:C:H2'	1:D:941:G:H8	1.82	0.44
2:A:93:ARG:O	2:A:217:ARG:HG2	2.18	0.44
1:D:909:G:C4'	1:D:910:G:OP2	2.66	0.44
2:A:286:HIS:HD2	2:A:288:LYS:H	1.65	0.44
2:B:496:ASN:ND2	2:B:498:SER:HB3	2.33	0.44
2:B:344:ARG:HG3	2:B:344:ARG:HH21	1.82	0.44
2:B:380:ILE:O	2:B:384:ILE:HG13	2.17	0.44
2:A:363:ALA:HB2	2:A:458:VAL:HG23	1.99	0.44
2:B:447:THR:HG22	2:B:448:LYS:N	2.33	0.44
2:A:120:LYS:O	2:A:121:ARG:C	2.54	0.44
2:A:485:GLU:OE1	2:A:486:GLU:N	2.49	0.44
2:A:122:GLU:OE1	2:A:124:ASP:HB2	2.17	0.44
2:B:347:VAL:CG2	2:B:348:TYR:CE2	3.01	0.44
1:D:917:G:O2'	1:D:918:G:C5'	2.65	0.44
2:B:326:LEU:HD13	2:B:326:LEU:C	2.38	0.44
2:B:479:ALA:HB2	2:B:487:VAL:CG1	2.48	0.44
2:A:511:TYR:CZ	2:A:515:LYS:HG3	2.52	0.44
2:A:310:SER:O	2:A:314:LEU:HD22	2.17	0.43
2:A:437:TYR:CZ	2:A:438:LYS:HE2	2.53	0.43
2:A:397:PRO:CG	2:A:421:GLU:HG2	2.48	0.43
2:A:477:GLU:O	2:A:481:MET:HE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:340:TYR:CG	2:A:346:MET:HG2	2.53	0.43
2:B:204:LEU:HD23	2:B:239:GLU:HG3	2.01	0.43
2:A:306:PHE:HB3	2:A:326:LEU:HD22	2.01	0.43
2:A:484:GLN:HG2	2:A:485:GLU:H	1.83	0.43
2:B:257:PHE:O	2:B:286:HIS:HE1	2.00	0.43
2:A:485:GLU:HA	2:A:533:ILE:O	2.17	0.43
2:B:478:GLU:O	2:B:482:ARG:HB2	2.18	0.43
2:A:23:GLY:HA3	4:A:1016:HOH:O	2.18	0.43
2:A:113:ARG:C	2:A:115:ILE:H	2.20	0.43
2:B:6:GLN:HE21	2:B:9:ARG:HH11	1.67	0.43
2:A:282:VAL:HG13	2:A:304:ALA:C	2.39	0.43
2:A:121:ARG:NH1	2:A:122:GLU:O	2.51	0.43
2:A:306:PHE:CD1	2:A:306:PHE:C	2.91	0.43
2:B:491:ALA:O	2:B:526:PHE:HA	2.18	0.43
2:B:295:LYS:C	2:B:297:SER:H	2.21	0.43
2:A:333:LEU:HD22	2:A:337:LEU:HG	2.01	0.43
1:D:935:A:C4	2:A:524:PRO:HD2	2.53	0.43
2:B:326:LEU:HD13	2:B:327:GLY:N	2.33	0.43
2:B:405:GLY:O	2:B:411:ASN:HA	2.19	0.43
2:A:141:ASP:CG	2:A:142:GLY:N	2.72	0.42
2:A:148:LEU:HG	2:A:160:ALA:HA	2.01	0.42
2:A:171:PHE:CD2	2:A:171:PHE:N	2.87	0.42
2:A:370:GLU:HG3	2:A:471:TYR:HD2	1.82	0.42
2:A:442:TYR:CD2	2:A:453:PHE:HE2	2.36	0.42
2:B:56:LEU:HB3	2:B:211:ILE:CD1	2.50	0.42
2:A:397:PRO:HG3	2:A:421:GLU:HG2	2.01	0.42
2:B:408:MET:HE3	2:B:481:MET:HB3	2.01	0.42
2:B:294:THR:CG2	2:B:296:TYR:HB2	2.50	0.42
2:A:507:ASN:HD22	2:B:204:LEU:HD13	1.84	0.42
2:A:200:ASP:HA	2:B:507:ASN:HD21	1.85	0.42
2:A:437:TYR:HE2	2:A:456:GLU:HB2	1.84	0.42
2:A:215:PHE:CD1	2:A:215:PHE:N	2.87	0.42
2:B:292:SER:O	2:B:294:THR:N	2.46	0.42
2:B:385:VAL:O	2:B:389:GLU:HG3	2.19	0.42
2:A:146:SER:O	2:A:148:LEU:N	2.46	0.42
2:B:7:LYS:CD	2:B:7:LYS:N	2.82	0.42
2:B:451:ARG:NH2	2:B:451:ARG:HG3	2.31	0.42
2:B:467:GLY:O	2:B:501:ASN:HB3	2.19	0.42
2:B:310:SER:HA	2:B:311:PRO:HD3	1.97	0.42
1:D:901:G:H2'	1:D:902:C:C6	2.55	0.42
2:B:412:VAL:HG12	2:B:413:ARG:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:185:SER:HB2	2:A:216:ARG:HD3	2.01	0.42
1:D:917:G:O2'	1:D:918:G:P	2.77	0.42
2:B:475:LYS:HA	2:B:475:LYS:HD2	1.74	0.42
2:A:143:ASP:O	2:A:146:SER:HB3	2.20	0.41
2:B:474:ARG:NH1	2:B:474:ARG:CG	2.81	0.41
2:A:309:TYR:HB2	2:A:323:VAL:HG13	2.02	0.41
2:B:56:LEU:HB3	2:B:211:ILE:HD13	2.01	0.41
2:A:206:ILE:HB	2:A:237:VAL:HB	2.02	0.41
2:B:218:GLU:O	2:B:219:GLN:HB3	2.20	0.41
2:A:122:GLU:OE2	2:A:122:GLU:HA	2.21	0.41
2:B:494:VAL:O	2:B:522:ARG:HA	2.20	0.41
2:B:421:GLU:CD	2:B:421:GLU:H	2.22	0.41
2:B:6:GLN:HG2	2:B:9:ARG:NH1	2.36	0.41
2:A:340:TYR:CD1	2:A:346:MET:HG2	2.53	0.41
2:A:115:ILE:O	2:A:115:ILE:HG23	2.20	0.41
2:A:144:ASP:HA	2:A:147:TYR:CZ	2.54	0.41
2:A:261:ASN:HD21	2:A:263:ARG:HH22	1.68	0.41
2:A:282:VAL:HG13	2:A:304:ALA:O	2.21	0.41
2:B:500:ILE:HG23	2:B:502:LEU:HD22	2.01	0.41
2:B:90:VAL:O	2:B:93:ARG:HG2	2.20	0.41
2:A:403:PHE:O	2:A:413:ARG:HA	2.20	0.41
2:A:86:GLU:OE1	2:A:272:LYS:HG2	2.19	0.41
2:B:301:ILE:HD13	2:B:336:ILE:HD11	2.02	0.41
2:A:265:ARG:NE	2:A:281:GLU:OE1	2.49	0.41
2:A:468:PHE:O	2:A:471:TYR:HB3	2.20	0.41
2:B:399:SER:HA	2:B:417:VAL:HG12	2.02	0.41
2:B:364:ARG:HG3	2:B:364:ARG:HH21	1.86	0.41
2:B:385:VAL:HG23	2:B:469:ALA:CB	2.51	0.41
1:D:933:G:H1	2:A:492:ARG:CD	2.33	0.41
2:A:116:GLU:O	2:A:118:ILE:HD12	2.20	0.41
2:A:95:PHE:CE2	2:B:97:LEU:HD23	2.55	0.41
2:A:220:GLY:C	2:A:221:GLU:HG3	2.40	0.41
2:A:314:LEU:HD11	2:A:323:VAL:CG1	2.50	0.41
2:B:215:PHE:N	2:B:215:PHE:CD1	2.89	0.41
2:A:213:ARG:HH21	2:A:228:THR:CG2	2.34	0.41
2:B:377:GLY:O	2:B:380:ILE:HB	2.21	0.40
2:B:285:PHE:HB2	2:B:300:TRP:CE2	2.57	0.40
2:B:102:LYS:O	2:B:104:ASN:N	2.54	0.40
2:A:490:LYS:CD	2:A:492:ARG:HH12	2.34	0.40
2:A:141:ASP:C	2:A:143:ASP:H	2.23	0.40
2:A:121:ARG:NH1	2:A:121:ARG:HG3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:A:H1'	1:D:959:U:C5	2.56	0.40
2:B:103:PRO:HG3	2:B:174:LEU:HD12	2.03	0.40
2:A:473:ALA:O	2:A:476:VAL:HG22	2.21	0.40
2:A:391:HIS:O	2:A:425:LEU:HD23	2.22	0.40
2:A:292:SER:CB	2:A:294:THR:HG22	2.52	0.40
2:A:374:THR:HG22	2:A:375:ALA:N	2.37	0.40
2:B:406:GLU:HB3	2:B:411:ASN:OD1	2.22	0.40
2:A:479:ALA:C	2:A:481:MET:N	2.75	0.40
2:A:119:THR:HG22	2:A:120:LYS:N	2.36	0.40
2:B:440:ASP:HB2	2:B:442:TYR:CE2	2.57	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	
2	A	532/534 (100%)	467 (88%)	51 (10%)	14 (3%)	7	11
2	B	461/534 (86%)	423 (92%)	31 (7%)	7 (2%)	13	26
All	All	993/1068 (93%)	890 (90%)	82 (8%)	21 (2%)	9	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	118	ILE
2	A	156	ASP
2	A	107	ILE
2	A	124	ASP
2	A	140	ILE
2	A	174	LEU
2	A	448	LYS
2	B	484	GLN

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Mol	Chain	Res	Type
2	A	147	TYR
2	A	294	THR
2	B	32	PRO
2	B	103	PRO
2	B	422	ASN
2	A	151	GLU
2	A	153	LEU
2	A	121	ARG
2	B	526	PHE
2	B	353	GLY
2	A	152	VAL
2	A	105	VAL
2	B	394	GLU

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	
2	A	464/464 (100%)	430 (93%)	34 (7%)	17	35
2	B	402/464 (87%)	370 (92%)	32 (8%)	15	29
All	All	866/928 (93%)	800 (92%)	66 (8%)	16	32

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	49	LEU
2	A	56	LEU
2	A	85	ARG
2	A	97	LEU
2	A	104	ASN
2	A	115	ILE
2	A	132	PHE
2	A	137	LYS
2	A	147	TYR
2	A	148	LEU

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Mol	Chain	Res	Type
2	A	186	HIS
2	A	236	LEU
2	A	254	LEU
2	A	261	ASN
2	A	277	ASP
2	A	282	VAL
2	A	318	ASP
2	A	320	PRO
2	A	323	VAL
2	A	324	MET
2	A	326	LEU
2	A	328	LEU
2	A	333	LEU
2	A	347	VAL
2	A	422	ASN
2	A	435	VAL
2	A	448	LYS
2	A	485	GLU
2	A	493	ILE
2	A	496	ASN
2	A	500	ILE
2	A	502	LEU
2	A	509	ARG
2	A	525	LEU
2	B	7	LYS
2	B	32	PRO
2	B	37	PRO
2	B	42	SER
2	B	49	LEU
2	B	55	ARG
2	B	56	LEU
2	B	68	VAL
2	B	85	ARG
2	B	99	THR
2	B	102	LYS
2	B	186	HIS
2	B	204	LEU
2	B	228	THR
2	B	236	LEU
2	B	243	VAL
2	B	254	LEU
2	B	255	ARG

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Mol	Chain	Res	Type
2	B	261	ASN
2	B	282	VAL
2	B	314	LEU
2	B	328	LEU
2	B	333	LEU
2	B	373	GLN
2	B	410	ARG
2	B	448	LYS
2	B	476	VAL
2	B	485	GLU
2	B	493	ILE
2	B	496	ASN
2	B	502	LEU
2	B	525	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	47	HIS
2	A	104	ASN
2	A	114	GLN
2	A	129	GLN
2	A	133	HIS
2	A	261	ASN
2	A	286	HIS
2	A	382	GLN
2	A	422	ASN
2	A	496	ASN
2	B	6	GLN
2	B	47	HIS
2	B	219	GLN
2	B	261	ASN
2	B	286	HIS
2	B	382	GLN
2	B	496	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	70/71 (98%)	17 (24%)	5 (7%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	906	G
1	D	908	U
1	D	909	G
1	D	910	G
1	D	917	G
1	D	918	G
1	D	919	C
1	D	921	U
1	D	932	U
1	D	933	G
1	D	935	A
1	D	943	U
1	D	944	U
1	D	945	U
1	D	946	A
1	D	958	A
1	D	960	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	909	G
1	D	917	G
1	D	918	G
1	D	934	C
1	D	957	A

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](#)

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$
3	SEP	A	1001	-	7,10,10	1.54	1 (14%)	7,14,14	2.05	1 (14%)
3	SEP	A	1002	-	7,10,10	1.54	1 (14%)	7,14,14	2.25	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	A	1001	-	-	0/6/10/10	0/0/0/0
3	SEP	A	1002	-	-	0/6/10/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	SEP	P-O1P	3.08	1.61	1.51
3	A	1002	SEP	P-O1P	3.09	1.61	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	SEP	O3P-P-OG	2.01	112.36	106.56
3	A	1001	SEP	OG-CB-CA	4.64	111.57	108.18
3	A	1002	SEP	OG-CB-CA	5.27	112.02	108.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	SEP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	D	71/71 (100%)	2.97	38 (53%) 0 0	91, 166, 199, 200	0
2	A	534/534 (100%)	0.83	75 (14%) 4 2	32, 65, 182, 200	0
2	B	465/534 (87%)	0.39	31 (6%) 21 15	34, 60, 139, 189	0
All	All	1070/1139 (93%)	0.78	144 (13%) 4 2	32, 65, 180, 200	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	109	ALA	13.3
2	A	223	ALA	12.5
2	A	149	ILE	12.4
2	A	132	PHE	9.7
2	A	116	GLU	9.1
1	D	904	A	9.0
2	B	223	ALA	8.2
1	D	944	U	8.0
1	D	902	C	7.9
2	A	114	GLN	7.7
1	D	901	G	7.6
1	D	969	G	7.6
1	D	970	G	7.5
1	D	903	C	7.3
1	D	968	U	7.2
2	A	115	ILE	6.7
2	A	150	ALA	6.7
2	A	106	GLY	6.6
1	D	971	C	6.6
2	A	220	GLY	6.6
1	D	905	G	6.4
1	D	906	G	6.4
2	A	110	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	D	945	U	6.3
2	A	155	VAL	6.0
2	B	222	ASP	6.0
2	A	108	SER	5.9
2	A	219	GLN	5.8
2	A	113	ARG	5.7
2	A	123	VAL	5.7
1	D	966	C	5.7
2	A	222	ASP	5.4
2	B	224	THR	5.4
2	A	135	TYR	5.2
2	A	126	LYS	5.2
2	A	125	SER	5.2
2	A	162	LYS	5.0
2	B	534	GLU	4.9
2	A	221	GLU	4.8
2	A	156	ASP	4.8
1	D	925	G	4.8
2	A	161	VAL	4.8
2	A	103	PRO	4.8
2	A	133	HIS	4.7
1	D	967	C	4.6
2	A	152	VAL	4.6
2	B	401	LEU	4.5
2	B	221	GLU	4.5
2	A	111	LYS	4.5
2	A	117	ALA	4.5
2	A	142	GLY	4.4
1	D	943	U	4.3
1	D	965	C	4.3
1	D	964	G	4.3
2	B	407	MET	4.2
1	D	913	G	4.2
2	A	130	GLU	4.2
2	A	131	ILE	4.2
1	D	907	G	4.2
2	B	414	VAL	4.0
2	A	85	ARG	3.9
2	A	154	ASP	3.9
2	A	147	TYR	3.9
2	A	107	ILE	3.8
1	D	924	C	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	402	ALA	3.8
2	B	412	VAL	3.8
2	B	529	VAL	3.8
2	A	145	LEU	3.8
2	A	148	LEU	3.8
2	A	137	LYS	3.8
2	A	158	ILE	3.8
2	A	140	ILE	3.7
2	B	403	PHE	3.7
2	B	295	LYS	3.7
2	B	531	ALA	3.7
2	A	129	GLN	3.7
2	A	533	ILE	3.7
2	A	224	THR	3.6
1	D	932	U	3.6
2	A	166	GLU	3.6
2	A	104	ASN	3.5
2	A	141	ASP	3.5
2	A	119	THR	3.5
2	A	157	ASP	3.5
2	A	168	PHE	3.5
2	A	120	LYS	3.5
2	A	408	MET	3.4
2	B	487	VAL	3.3
2	A	134	ARG	3.2
2	A	163	ILE	3.2
2	A	128	LEU	3.2
2	A	112	ILE	3.2
2	B	103	PRO	3.1
2	A	143	ASP	3.0
1	D	935	A	3.0
1	D	923	G	3.0
2	A	411	ASN	3.0
2	A	410	ARG	2.8
2	A	421	GLU	2.8
1	D	963	G	2.8
2	A	164	LEU	2.7
2	B	219	GLN	2.7
2	B	410	ARG	2.7
1	D	912	A	2.7
2	B	416	VAL	2.7
1	D	922	U	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	926	G	2.7
2	B	174	LEU	2.7
2	A	171	PHE	2.7
2	B	390	LYS	2.6
2	A	139	GLU	2.6
1	D	947	C	2.6
2	B	413	ARG	2.6
2	B	533	ILE	2.6
2	A	153	LEU	2.6
2	B	408	MET	2.6
2	A	124	ASP	2.6
2	B	481	MET	2.5
1	D	940	C	2.5
2	B	409	GLY	2.5
2	A	412	VAL	2.4
1	D	941	G	2.4
1	D	942	C	2.4
2	B	404	GLU	2.4
2	B	486	GLU	2.4
2	A	105	VAL	2.4
2	A	531	ALA	2.4
1	D	946	A	2.4
2	A	144	ASP	2.3
1	D	936	G	2.3
2	B	468	PHE	2.3
2	A	407	MET	2.3
2	A	136	LYS	2.3
2	B	220	GLY	2.3
1	D	915	G	2.3
2	A	422	ASN	2.3
2	B	532	GLU	2.2
1	D	938	U	2.2
1	D	962	G	2.1
2	A	487	VAL	2.1
1	D	914	A	2.1
2	A	102	LYS	2.0
2	A	151	GLU	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SEP	A	1002	11/11	0.95	0.21	1.17	43,47,68,111	0
3	SEP	A	1001	11/11	0.96	0.23	0.74	43,55,81,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.