



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:05 AM GMT

PDB ID : 2PC9
Title : Crystal Structure Of ATP-Dependent Phosphoenolpyruvate Carboxykinase From *Thermus thermophilus* HB8
Authors : Sugahara, M.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-29
Resolution : 2.40 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

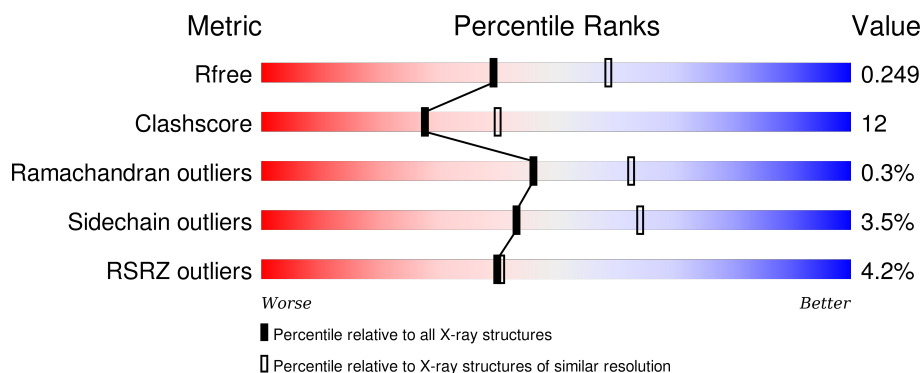
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	A	529	<div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	B	529	<div> <div>11%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	C	529	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	D	529	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>

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	PO4	B	3013	-	-	-	X
4	ATP	A	1003	-	-	-	X
4	ATP	D	1004	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17321 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 Phosphoenolpyruvate carboxykinase [ATP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4096	2637	716	733	10			
1	B	511	Total	C	N	O	S	0	0	0
			4071	2622	711	729	9			
1	C	517	Total	C	N	O	S	0	0	0
			4112	2646	717	740	9			
1	D	512	Total	C	N	O	S	0	0	0
			4071	2623	712	727	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0

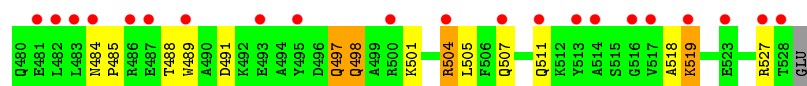
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- The diagram illustrates the chemical structure of Adenosine Triphosphate (ATP). It consists of an adenine base (labeled N1 through N7), a ribose sugar (labeled C1' through C5'), and three phosphate groups (labeled O1A through O3G). The adenine base is connected to the ribose sugar at the C1' position. The ribose sugar is connected to the first phosphate group at the C5' position. The three phosphate groups are linked sequentially by phosphoanhydride bonds. The structure is shown in a perspective view, with atoms labeled with their respective element symbols and bond orders.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	241	Total O 241 241	0	0
5	B	95	Total O 95 95	0	0
5	C	207	Total O 207 207	0	0

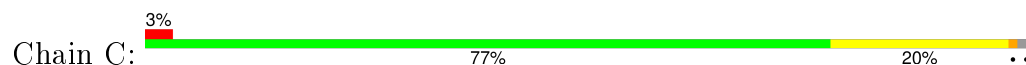
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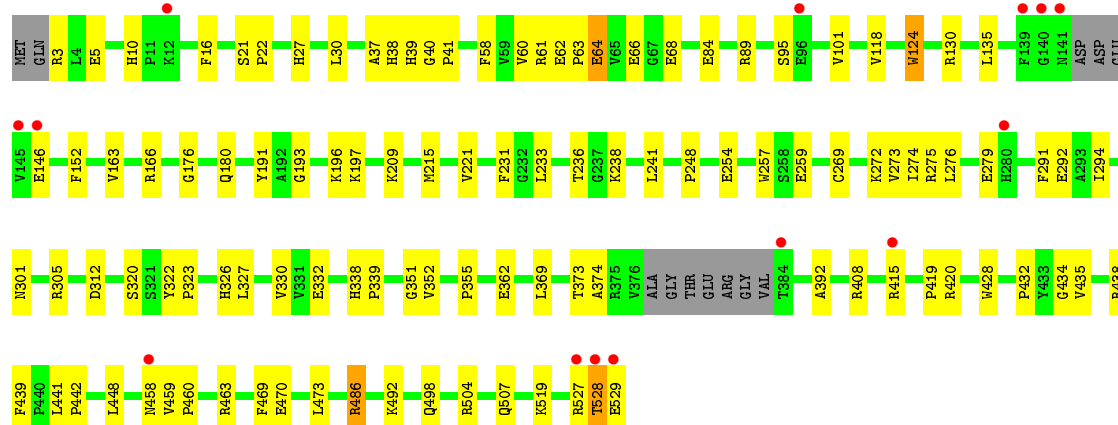
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	220	Total 220	O 220	0	0



• Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]



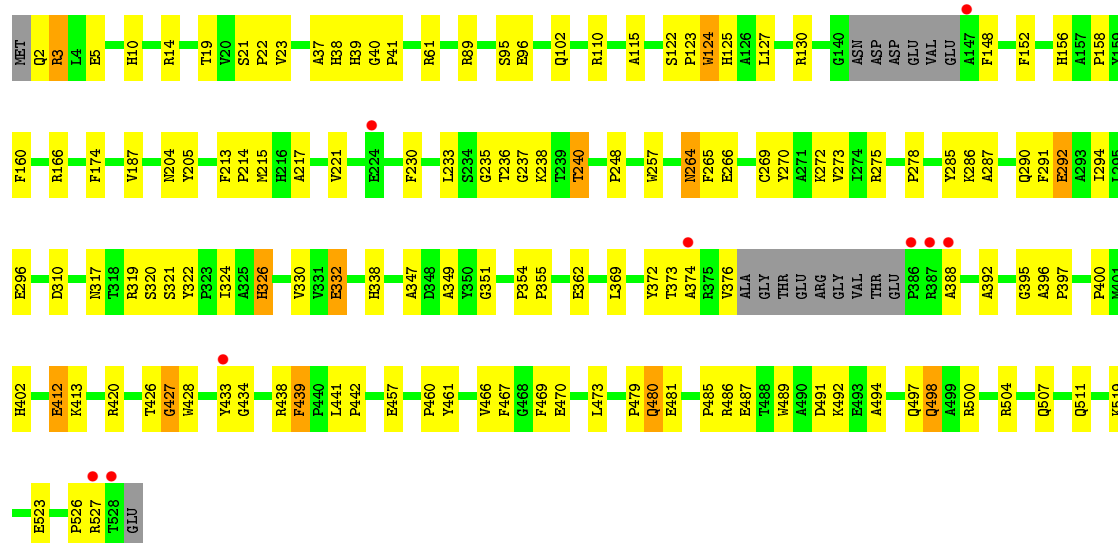
Chain C:



• Molecule 1: Phosphoenolpyruvate carboxykinase [ATP]



Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.69Å 128.55Å 178.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 2.40 39.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-2.40) 99.9 (39.91-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.250 0.212 , 0.249	Depositor DCC
R_{free} test set	4919 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 99225 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17321	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: PO4, CA, ATP

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	0.53	2/4215 (0.0%)	0.76	0/5731
1	B	0.53	3/4190 (0.1%)	0.73	0/5698
1	C	0.52	1/4231 (0.0%)	0.76	1/5753 (0.0%)
1	D	0.51	2/4190 (0.0%)	0.72	1/5697 (0.0%)
All	All	0.52	8/16826 (0.0%)	0.74	2/22879 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	TRP	NE1-CE2	8.84	1.49	1.37
1	D	489	TRP	NE1-CE2	8.79	1.49	1.37
1	B	489	TRP	NE1-CE2	8.76	1.49	1.37
1	D	124	TRP	NE1-CE2	8.76	1.49	1.37
1	A	428	TRP	NE1-CE2	8.74	1.49	1.37
1	C	124	TRP	NE1-CE2	8.73	1.49	1.37
1	B	70	TRP	NE1-CE2	8.64	1.48	1.37
1	B	124	TRP	NE1-CE2	8.61	1.48	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	LYS	O-C-N	-5.58	113.78	122.70
1	C	486	ARG	CD-NE-CZ	-5.29	116.20	123.60

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	4096	0	4026	72	0
1	B	4071	0	3998	123	0
1	C	4112	0	4034	82	0
1	D	4071	0	4003	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	0	1	0
3	B	15	0	0	0	0
3	C	30	0	0	1	0
3	D	20	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	1	0
4	C	31	0	12	3	0
4	D	31	0	12	6	0
5	A	241	0	0	2	0
5	B	95	0	0	5	0
5	C	207	0	0	6	0
5	D	220	0	0	10	0
All	All	17321	0	16109	384	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 12.

All (384) 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:2:GLN:NE2	1:B:2:GLN:HA	1.62	1.13
1:B:373:THR:HG22	1:B:374:ALA:H	1.06	1.10
1:C:291:PHE:O	1:C:292:GLU:HB2	1.50	1.10
1:B:38:HIS:O	1:B:39:HIS:HB2	1.54	1.06
1:B:10:HIS:O	1:B:95:SER:HB3	1.63	0.99
1:B:373:THR:HG22	1:B:374:ALA:N	1.86	0.89
1:D:124:TRP:HD1	5:D:3028:HOH:O	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ALA:H	1:B:373:THR:HG23	1.41	0.86
1:D:257:TRP:HE1	1:D:338:HIS:HD2	1.23	0.86
1:D:507:GLN:HA	1:D:507:GLN:HE21	1.41	0.83
1:A:415:ARG:NH1	5:A:3209:HOH:O	2.03	0.83
1:B:40:GLY:N	1:B:41:PRO:CD	2.42	0.82
1:D:40:GLY:N	1:D:41:PRO:HD2	1.95	0.81
1:B:2:GLN:CA	1:B:2:GLN:NE2	2.43	0.81
1:C:373:THR:HG23	1:C:374:ALA:N	1.96	0.81
1:D:40:GLY:N	1:D:41:PRO:CD	2.44	0.81
1:D:3:ARG:HB2	1:D:3:ARG:HH11	1.44	0.80
1:C:40:GLY:N	1:C:41:PRO:HD2	1.97	0.80
1:D:480:GLN:OE1	1:D:481:GLU:HG3	1.83	0.78
1:C:273:VAL:HG11	1:C:320:SER:HB2	1.64	0.78
1:B:460:PRO:HB2	1:B:473:LEU:HD12	1.65	0.77
1:C:163:VAL:HB	1:C:166:ARG:HB3	1.67	0.77
1:B:2:GLN:HE21	1:B:2:GLN:HA	1.50	0.77
1:D:124:TRP:CZ2	1:D:125:HIS:CE1	2.73	0.76
1:B:264:ASN:HD22	1:B:265:PHE:N	1.84	0.76
1:A:40:GLY:N	1:A:41:PRO:CD	2.48	0.76
1:B:40:GLY:N	1:B:41:PRO:HD2	2.02	0.75
1:B:332:GLU:HG2	5:B:3088:HOH:O	1.85	0.75
1:B:291:PHE:O	1:B:292:GLU:HB2	1.86	0.74
1:C:441:LEU:HB3	1:C:442:PRO:HD3	1.69	0.74
1:B:373:THR:CG2	1:B:374:ALA:H	1.87	0.74
1:A:38:HIS:O	1:A:41:PRO:HD2	1.88	0.74
1:D:96:GLU:HG2	5:D:3180:HOH:O	1.86	0.73
1:D:217:ALA:HB1	1:D:230:PHE:O	1.87	0.73
1:B:264:ASN:ND2	1:B:266:GLU:H	1.87	0.72
1:D:123:PRO:HD2	5:D:3028:HOH:O	1.90	0.71
1:D:38:HIS:O	1:D:39:HIS:HB2	1.88	0.71
1:A:276:LEU:HD21	1:A:285:TYR:HA	1.73	0.70
1:D:89:ARG:CZ	1:D:166:ARG:HD2	2.22	0.70
1:D:507:GLN:HA	1:D:507:GLN:NE2	2.07	0.70
1:D:40:GLY:H	1:D:41:PRO:HD2	1.55	0.69
1:A:291:PHE:O	1:A:292:GLU:HB2	1.93	0.69
1:D:102:GLN:HE22	1:D:130:ARG:HH11	1.41	0.69
1:D:460:PRO:HB2	1:D:473:LEU:HD12	1.74	0.68
1:C:291:PHE:O	1:C:292:GLU:CB	2.33	0.68
1:C:486:ARG:HD3	5:C:3148:HOH:O	1.93	0.68
1:B:240:THR:HG22	4:B:1001:ATP:O1A	1.93	0.67
1:A:14:ARG:CG	1:A:14:ARG:HH11	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLY:N	1:C:41:PRO:CD	2.58	0.66
1:A:276:LEU:HD12	1:A:281:GLU:HB2	1.77	0.66
1:D:461:TYR:HB3	1:D:470:GLU:HG3	1.78	0.66
1:C:338:HIS:HE1	5:C:3085:HOH:O	1.79	0.65
1:A:38:HIS:O	1:A:39:HIS:HB2	1.96	0.65
1:A:387:ARG:CG	1:A:387:ARG:O	2.44	0.65
1:A:387:ARG:HG2	1:A:387:ARG:O	1.95	0.65
1:C:415:ARG:HG2	1:C:415:ARG:HH11	1.62	0.65
1:B:40:GLY:H	1:B:41:PRO:HD2	1.60	0.64
1:D:240:THR:HG22	4:D:1004:ATP:O1A	1.97	0.64
1:B:236:THR:HG21	5:B:3018:HOH:O	1.97	0.64
1:B:375:ARG:HH11	1:B:387:ARG:HE	1.46	0.64
1:B:375:ARG:NH1	1:B:387:ARG:HE	1.96	0.64
1:C:38:HIS:O	1:C:39:HIS:HB2	1.97	0.64
1:B:65:VAL:O	1:B:69:ILE:HG12	1.99	0.63
3:C:3016:PO4:O3	4:C:1002:ATP:O1G	2.16	0.63
1:B:13:LYS:HG3	1:B:97:ARG:HA	1.81	0.63
1:A:14:ARG:HG2	1:A:14:ARG:NH1	2.13	0.63
1:C:68:GLU:OE2	1:C:209:LYS:NZ	2.33	0.62
1:A:40:GLY:N	1:A:41:PRO:HD2	2.15	0.62
1:A:14:ARG:CG	1:A:14:ARG:NH1	2.63	0.61
1:B:430:GLY:HA3	1:B:488:THR:HG22	1.81	0.61
1:B:2:GLN:CA	1:B:2:GLN:HE21	2.09	0.61
1:D:412:GLU:HG3	1:D:413:LYS:N	2.14	0.61
1:D:204:ASN:ND2	1:D:214:PRO:HB2	2.15	0.61
1:D:3:ARG:HG3	1:D:5:GLU:OE1	2.00	0.61
1:B:135:LEU:O	1:B:138:ARG:HB2	1.99	0.60
1:C:274:ILE:O	1:C:275:ARG:HB2	2.00	0.60
1:B:475:ALA:HB3	1:B:478:VAL:HB	1.83	0.60
1:A:526:PRO:O	1:A:527:ARG:C	2.39	0.60
1:D:349:ALA:H	1:D:374:ALA:HB3	1.65	0.60
1:B:498:GLN:CA	1:B:498:GLN:HE21	2.15	0.59
1:D:355:PRO:HB3	1:D:439:PHE:CZ	2.37	0.59
1:D:257:TRP:HE1	1:D:338:HIS:CD2	2.13	0.59
1:B:268:GLY:HA2	1:B:324:ILE:HG13	1.83	0.58
1:B:50:THR:HB	1:B:315:THR:HG21	1.85	0.58
1:D:264:ASN:ND2	1:D:266:GLU:H	2.01	0.58
1:D:491:ASP:OD2	1:D:494:ALA:HB2	2.04	0.58
1:D:291:PHE:O	1:D:292:GLU:HB2	2.03	0.57
1:C:273:VAL:CG1	1:C:320:SER:HB2	2.34	0.57
1:A:52:ARG:HD3	1:A:197:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:TYR:N	1:B:437:TYR:CD1	2.72	0.57
1:C:460:PRO:HB2	1:C:473:LEU:HD12	1.86	0.57
1:D:349:ALA:H	1:D:374:ALA:CB	2.17	0.57
1:B:217:ALA:HB2	1:B:231:PHE:HA	1.87	0.57
1:D:372:TYR:HE1	1:D:388:ALA:HB1	1.70	0.57
1:C:273:VAL:O	1:C:276:LEU:HB2	2.05	0.57
1:B:40:GLY:O	1:B:291:PHE:HA	2.04	0.57
1:C:89:ARG:NE	1:C:166:ARG:HD2	2.19	0.57
1:B:86:LEU:O	1:B:90:VAL:HG23	2.05	0.56
1:B:430:GLY:CA	1:B:488:THR:HG22	2.35	0.56
1:A:120:THR:HB	1:A:156:HIS:HB3	1.87	0.56
1:C:241:LEU:HD13	1:C:448:LEU:HD11	1.88	0.56
1:D:324:ILE:HG22	5:D:3164:HOH:O	2.05	0.56
1:B:3:ARG:HB2	1:B:5:GLU:HG2	1.87	0.56
1:B:204:ASN:ND2	1:B:214:PRO:HB2	2.21	0.56
1:C:408:ARG:HD3	1:D:61:ARG:HH22	1.71	0.56
1:A:276:LEU:CD1	1:A:281:GLU:HB2	2.36	0.56
1:D:102:GLN:HE22	1:D:130:ARG:NH1	2.03	0.56
1:D:491:ASP:HB3	1:D:494:ALA:HB3	1.87	0.56
1:D:347:ALA:HB3	1:D:373:THR:HG23	1.88	0.56
1:A:60:VAL:HG12	1:A:62:GLU:HG3	1.87	0.56
1:A:362:GLU:OE2	1:A:415:ARG:NH2	2.39	0.56
1:B:501:LYS:O	1:B:505:LEU:HG	2.06	0.56
1:B:273:VAL:HG11	1:B:320:SER:HB2	1.87	0.56
1:B:34:GLY:O	1:B:35:LEU:HD23	2.05	0.55
1:D:270:TYR:OH	1:D:296:GLU:OE1	2.22	0.55
1:B:39:HIS:HB3	1:B:289:ASN:O	2.06	0.55
1:B:64:GLU:CD	1:B:64:GLU:H	2.10	0.55
1:D:507:GLN:CA	1:D:507:GLN:HE21	2.14	0.55
1:A:362:GLU:CD	1:A:362:GLU:H	2.09	0.55
1:C:40:GLY:H	1:C:41:PRO:HD2	1.70	0.55
1:C:460:PRO:HG2	1:C:473:LEU:HB2	1.88	0.55
1:B:268:GLY:CA	1:B:324:ILE:HG13	2.36	0.55
1:D:38:HIS:O	1:D:41:PRO:HD2	2.07	0.55
1:D:204:ASN:HD22	1:D:214:PRO:HB2	1.73	0.54
1:D:233:LEU:HD12	1:D:373:THR:HB	1.89	0.54
1:A:469:PHE:CD1	1:A:469:PHE:C	2.81	0.54
1:B:432:PRO:HD2	1:B:435:VAL:HB	1.90	0.54
1:B:498:GLN:HA	1:B:498:GLN:HE21	1.73	0.54
1:B:339:PRO:O	1:B:419:PRO:HB3	2.07	0.54
1:C:21:SER:HB2	1:C:22:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:O	1:B:236:THR:HG23	2.08	0.54
1:B:418:ALA:N	1:B:419:PRO:HD3	2.23	0.53
1:A:191:TYR:CE2	1:A:193:GLY:HA3	2.43	0.53
1:B:276:LEU:HD12	1:B:281:GLU:OE1	2.08	0.53
1:A:16:PHE:CZ	1:A:27:HIS:HE1	2.26	0.53
1:D:37:ALA:O	1:D:38:HIS:C	2.44	0.53
1:D:233:LEU:O	1:D:236:THR:HG23	2.09	0.53
1:A:460:PRO:HD2	1:A:474:GLU:HG2	1.90	0.53
1:B:114:LEU:O	1:B:116:VAL:HG23	2.09	0.53
1:B:123:PRO:O	1:B:126:ALA:HB3	2.09	0.53
1:D:354:PRO:HA	1:D:485:PRO:HG3	1.91	0.53
1:D:264:ASN:HD22	1:D:265:PHE:N	2.07	0.53
1:B:251:GLY:HA3	1:B:255:HIS:NE2	2.23	0.53
1:A:104:LEU:CD2	1:A:135:LEU:HD23	2.39	0.53
1:D:122:SER:HB3	1:D:125:HIS:HB2	1.91	0.53
1:B:375:ARG:O	1:B:386:PRO:HA	2.09	0.53
1:C:30:LEU:HD23	1:C:30:LEU:O	2.09	0.53
1:D:21:SER:HB2	1:D:22:PRO:HD3	1.91	0.53
1:D:497:GLN:CD	1:D:500:ARG:HH12	2.12	0.52
1:B:456:LEU:HB2	5:B:3095:HOH:O	2.09	0.52
1:D:124:TRP:CD1	5:D:3028:HOH:O	2.42	0.52
1:A:46:THR:HG21	1:A:296:GLU:OE2	2.10	0.52
1:D:273:VAL:HG11	1:D:320:SER:HB2	1.91	0.52
1:D:434:GLY:HA2	5:D:3223:HOH:O	2.10	0.52
1:B:130:ARG:HG3	1:B:135:LEU:HD21	1.90	0.51
1:A:469:PHE:HD1	1:A:469:PHE:C	2.13	0.51
1:D:500:ARG:HG2	1:D:504:ARG:NH1	2.25	0.51
1:B:439:PHE:CG	1:B:440:PRO:HD2	2.46	0.51
1:B:46:THR:HG21	1:B:296:GLU:OE2	2.10	0.51
1:B:327:LEU:HD11	5:B:3044:HOH:O	2.09	0.51
1:C:30:LEU:HD23	1:C:30:LEU:C	2.30	0.51
1:A:460:PRO:HB2	1:A:473:LEU:HD12	1.92	0.51
1:A:493:GLU:HA	1:A:493:GLU:OE1	2.10	0.51
1:A:339:PRO:O	1:A:419:PRO:HB3	2.11	0.51
1:C:38:HIS:O	1:C:41:PRO:HD2	2.11	0.51
1:B:264:ASN:HD22	1:B:265:PHE:H	1.52	0.51
1:B:213:PHE:HB3	1:B:257:TRP:HB3	1.93	0.51
1:B:354:PRO:HA	1:B:485:PRO:HG3	1.93	0.51
1:C:269:CYS:HB2	1:C:322:TYR:CE1	2.46	0.51
1:D:441:LEU:HB3	1:D:442:PRO:HD3	1.92	0.51
1:D:519:LYS:O	1:D:523:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG21	1:A:433:TYR:CE2	2.46	0.51
1:C:64:GLU:HG3	1:C:180:GLN:HG3	1.93	0.51
1:C:191:TYR:CE2	1:C:193:GLY:HA3	2.46	0.50
1:D:487:GLU:O	1:D:487:GLU:HG2	2.10	0.50
1:B:462:ARG:HB3	1:B:473:LEU:HD21	1.93	0.50
1:D:237:GLY:HA2	1:D:240:THR:CG2	2.40	0.50
1:A:257:TRP:CZ2	1:A:339:PRO:HD2	2.46	0.50
1:A:375:ARG:HB2	1:A:387:ARG:HG2	1.93	0.50
1:C:274:ILE:HG23	1:C:274:ILE:O	2.10	0.50
1:D:426:THR:HB	4:D:1004:ATP:N1	2.27	0.50
1:C:339:PRO:O	1:C:419:PRO:HB3	2.12	0.50
1:D:498:GLN:HA	1:D:498:GLN:HE21	1.77	0.50
1:D:275:ARG:HA	1:D:310:ASP:OD1	2.12	0.50
1:C:215:MET:HB3	1:C:231:PHE:CE2	2.45	0.50
1:B:102:GLN:HE22	1:B:130:ARG:HH11	1.59	0.50
1:B:439:PHE:CD1	1:B:440:PRO:HD2	2.47	0.50
1:B:205:TYR:HB2	1:B:400:PRO:HG3	1.94	0.50
1:B:324:ILE:HG22	1:B:330:VAL:HG21	1.94	0.49
1:C:64:GLU:H	1:C:64:GLU:CD	2.15	0.49
1:D:351:GLY:HA2	1:D:428:TRP:O	2.12	0.49
1:A:291:PHE:O	1:A:292:GLU:CB	2.59	0.49
1:D:2:GLN:O	1:D:2:GLN:HG2	2.12	0.49
1:A:124:TRP:CE3	1:A:124:TRP:O	2.65	0.49
1:B:21:SER:HB2	1:B:22:PRO:HD3	1.94	0.49
1:D:292:GLU:OE1	1:D:326:HIS:HE1	1.96	0.49
1:C:338:HIS:CE1	5:C:3085:HOH:O	2.59	0.49
1:A:296:GLU:HG2	5:A:3195:HOH:O	2.12	0.49
1:B:154:VAL:CG2	1:B:199:ILE:HD11	2.43	0.49
1:D:287:ALA:O	1:D:326:HIS:HD2	1.94	0.49
1:D:355:PRO:HB3	1:D:439:PHE:CE2	2.48	0.48
1:C:470:GLU:OE2	5:C:3196:HOH:O	2.19	0.48
1:D:481:GLU:HA	1:D:487:GLU:OE2	2.13	0.48
1:B:191:TYR:CE2	1:B:193:GLY:HA3	2.48	0.48
1:B:174:PHE:CD1	1:B:174:PHE:C	2.86	0.48
1:C:369:LEU:O	1:C:392:ALA:HA	2.12	0.48
1:C:124:TRP:CZ3	1:C:294:ILE:HG21	2.49	0.48
1:C:415:ARG:NH1	1:C:415:ARG:HG2	2.27	0.48
1:D:127:LEU:HG	1:D:294:ILE:HD11	1.96	0.48
1:D:330:VAL:HG23	1:D:332:GLU:OE1	2.14	0.48
1:D:427:GLY:O	1:D:438:ARG:HG3	2.14	0.48
1:B:441:LEU:HB3	1:B:442:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:THR:HG23	1:C:374:ALA:H	1.75	0.48
1:A:469:PHE:HD1	1:A:469:PHE:O	1.95	0.47
1:B:354:PRO:CA	1:B:485:PRO:HG3	2.44	0.47
1:C:124:TRP:O	1:C:124:TRP:CE3	2.67	0.47
1:A:233:LEU:HD12	1:A:373:THR:HG22	1.95	0.47
1:A:495:TYR:C	1:A:495:TYR:CD1	2.87	0.47
1:B:294:ILE:HB	1:B:321:SER:HB3	1.95	0.47
1:D:110:ARG:HD2	5:D:3199:HOH:O	2.14	0.47
1:A:274:ILE:HG13	1:A:275:ARG:HG3	1.97	0.47
1:D:467:PHE:CD2	1:D:526:PRO:HB3	2.50	0.47
1:C:373:THR:CG2	1:C:374:ALA:N	2.65	0.47
1:D:89:ARG:NH2	1:D:166:ARG:HD2	2.30	0.47
1:B:104:LEU:CD2	1:B:135:LEU:HD23	2.44	0.47
1:D:486:ARG:NH1	1:D:492:LYS:HB3	2.30	0.47
1:C:458:ASN:ND2	5:C:3190:HOH:O	2.48	0.47
1:B:10:HIS:O	1:B:95:SER:CB	2.51	0.46
1:D:376:VAL:HG21	1:D:433:TYR:CE2	2.50	0.46
1:A:130:ARG:NH1	3:A:3001:PO4:O3	2.48	0.46
1:B:504:ARG:HG3	1:B:504:ARG:HH11	1.81	0.46
1:C:257:TRP:CZ2	1:C:339:PRO:HD2	2.50	0.46
1:B:189:THR:HG21	1:B:194:GLU:HG3	1.97	0.46
1:C:37:ALA:HB3	1:C:41:PRO:HG2	1.97	0.46
1:D:10:HIS:O	1:D:95:SER:HB3	2.15	0.46
1:B:157:ALA:HB3	1:B:187:VAL:HG12	1.98	0.46
1:D:369:LEU:O	1:D:392:ALA:HA	2.14	0.46
1:B:420:ARG:NH1	1:B:420:ARG:HB2	2.30	0.46
1:D:291:PHE:O	1:D:292:GLU:CB	2.63	0.46
1:D:2:GLN:HB3	5:D:3188:HOH:O	2.16	0.46
1:B:257:TRP:CZ2	1:B:339:PRO:HD2	2.51	0.46
1:C:3:ARG:HD2	1:C:3:ARG:HH11	1.60	0.46
1:D:115:ALA:HB1	1:D:148:PHE:CZ	2.51	0.46
1:C:163:VAL:HG12	1:C:166:ARG:H	1.80	0.45
1:B:498:GLN:HA	1:B:498:GLN:NE2	2.31	0.45
1:D:294:ILE:HB	1:D:321:SER:HB3	1.98	0.45
1:D:376:VAL:HG21	1:D:433:TYR:CD2	2.51	0.45
1:B:269:CYS:HB2	1:B:322:TYR:CE1	2.52	0.45
1:B:204:ASN:HD22	1:B:214:PRO:HB2	1.80	0.45
1:C:60:VAL:HG12	1:C:62:GLU:HG3	1.97	0.45
1:D:221:VAL:O	1:D:248:PRO:HD2	2.16	0.45
1:D:235:GLY:N	4:D:1004:ATP:O2B	2.49	0.45
1:D:402:HIS:HD2	5:D:3039:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ARG:NH2	5:C:3113:HOH:O	2.46	0.45
1:C:527:ARG:HG2	1:C:529:GLU:O	2.16	0.45
1:B:270:TYR:O	1:B:319:ARG:NH2	2.49	0.45
1:B:36:LEU:O	1:B:305:ARG:NH1	2.50	0.45
1:B:274:ILE:HG23	1:B:274:ILE:O	2.17	0.45
1:D:235:GLY:H	4:D:1004:ATP:PB	2.40	0.45
1:B:156:HIS:HD2	1:B:186:ILE:HB	1.81	0.45
1:C:10:HIS:O	1:C:95:SER:HB3	2.18	0.45
1:D:124:TRP:CE2	1:D:125:HIS:CE1	3.05	0.44
1:C:238:LYS:HB2	4:C:1002:ATP:O2B	2.17	0.44
1:C:408:ARG:HD3	1:D:61:ARG:NH2	2.31	0.44
1:A:65:VAL:O	1:A:69:ILE:HG12	2.17	0.44
1:C:362:GLU:CD	1:C:362:GLU:H	2.21	0.44
1:B:87:TYR:CE1	1:B:183:LEU:HD13	2.52	0.44
1:C:124:TRP:HE3	1:C:294:ILE:HD13	1.81	0.44
1:B:47:THR:HB	1:B:48:PRO:HA	2.00	0.44
1:B:462:ARG:HG3	1:B:462:ARG:O	2.16	0.44
1:B:94:LEU:O	1:B:99:LEU:HD21	2.17	0.44
1:B:19:THR:CG2	1:B:23:VAL:HB	2.48	0.44
1:D:466:VAL:O	1:D:527:ARG:HG2	2.16	0.44
1:D:290:GLN:HG3	1:D:326:HIS:CD2	2.53	0.44
1:B:217:ALA:HA	1:B:238:LYS:HD2	1.99	0.44
1:C:428:TRP:CE2	1:C:438:ARG:HD2	2.52	0.44
1:C:504:ARG:HA	1:C:507:GLN:HE21	1.81	0.44
1:A:385:GLU:HB2	1:A:386:PRO:HD2	2.00	0.44
1:D:479:PRO:CB	1:D:481:GLU:OE1	2.66	0.44
1:D:372:TYR:HE1	1:D:388:ALA:CB	2.31	0.44
1:A:372:TYR:CG	1:A:373:THR:N	2.86	0.44
1:B:497:GLN:HA	1:B:497:GLN:NE2	2.33	0.44
1:D:286:LYS:HB2	1:D:286:LYS:HE3	1.86	0.44
1:B:418:ALA:N	1:B:419:PRO:CD	2.81	0.43
1:D:420:ARG:HD3	1:D:457:GLU:OE2	2.17	0.43
1:D:14:ARG:HD2	5:D:3136:HOH:O	2.17	0.43
1:C:279:GLU:CD	1:C:279:GLU:H	2.21	0.43
1:D:174:PHE:HB3	1:D:187:VAL:HG22	2.01	0.43
1:C:274:ILE:O	1:C:274:ILE:CG2	2.66	0.43
1:A:257:TRP:HE1	1:A:338:HIS:HD2	1.65	0.43
1:B:274:ILE:O	1:B:275:ARG:HB2	2.18	0.43
1:B:420:ARG:HB2	1:B:420:ARG:HH11	1.82	0.43
1:A:301:ASN:O	1:A:305:ARG:HA	2.18	0.43
1:B:233:LEU:O	1:B:236:THR:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HG3	1:A:66:GLU:HG3	2.00	0.43
1:B:38:HIS:HB2	1:B:306:ARG:HD3	1.99	0.43
1:C:352:VAL:CG2	1:C:498:GLN:HG3	2.48	0.43
1:C:101:VAL:HA	1:C:118:VAL:O	2.19	0.43
1:B:38:HIS:O	1:B:39:HIS:CB	2.37	0.43
1:A:275:ARG:NE	1:C:434:GLY:O	2.47	0.43
1:C:130:ARG:HG3	1:C:135:LEU:HD21	2.00	0.43
1:D:374:ALA:HA	1:D:388:ALA:HA	2.00	0.43
1:B:437:TYR:N	1:B:437:TYR:HD1	2.16	0.43
1:C:527:ARG:O	1:C:528:THR:C	2.57	0.43
1:B:399:LEU:HD22	1:B:406:TYR:CE2	2.53	0.43
1:D:396:ALA:N	1:D:397:PRO:CD	2.82	0.43
1:B:244:ASP:HB3	1:B:247:ARG:HB2	2.01	0.43
1:B:257:TRP:CE2	1:B:413:LYS:HD2	2.54	0.43
1:A:355:PRO:HB2	1:A:447:LEU:CD1	2.49	0.43
1:D:238:LYS:HB3	4:D:1004:ATP:O1B	2.19	0.42
1:B:138:ARG:HD2	1:B:138:ARG:HA	1.50	0.42
1:B:205:TYR:O	1:B:209:LYS:HD3	2.19	0.42
1:D:362:GLU:CD	1:D:362:GLU:H	2.23	0.42
1:C:301:ASN:O	1:C:305:ARG:HA	2.20	0.42
1:D:317:ASN:OD1	1:D:319:ARG:HD3	2.19	0.42
1:C:196:LYS:NZ	1:C:254:GLU:OE2	2.51	0.42
1:A:199:ILE:HD13	1:A:199:ILE:HA	1.94	0.42
1:B:272:LYS:NZ	1:B:272:LYS:HB3	2.34	0.42
1:C:233:LEU:O	1:C:236:THR:HG23	2.19	0.42
1:C:351:GLY:HA2	1:C:428:TRP:O	2.20	0.42
1:C:84:GLU:HA	1:C:84:GLU:OE1	2.19	0.42
1:A:86:LEU:O	1:A:90:VAL:HG23	2.19	0.42
1:D:269:CYS:HB2	1:D:322:TYR:CE1	2.54	0.42
1:B:2:GLN:HB3	5:B:3055:HOH:O	2.20	0.42
1:A:40:GLY:H	1:A:41:PRO:HD2	1.80	0.42
1:C:257:TRP:CE2	1:C:339:PRO:HD2	2.54	0.42
1:C:5:GLU:OE1	1:C:5:GLU:N	2.51	0.42
1:B:438:ARG:HH11	1:B:438:ARG:HD3	1.61	0.42
1:A:40:GLY:N	1:A:41:PRO:HD3	2.32	0.42
1:D:240:THR:HG21	4:D:1004:ATP:H2'	2.01	0.42
1:D:278:PRO:HG3	1:D:285:TYR:CE1	2.55	0.42
1:C:221:VAL:O	1:C:248:PRO:HD2	2.19	0.42
1:D:507:GLN:CA	1:D:507:GLN:NE2	2.77	0.42
1:C:272:LYS:NZ	4:C:1002:ATP:O3G	2.41	0.42
1:B:278:PRO:HG3	1:B:285:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ASP:OD1	1:B:312:ASP:C	2.57	0.42
1:B:507:GLN:HA	1:B:507:GLN:OE1	2.20	0.42
1:C:323:PRO:O	1:C:326:HIS:HB2	2.20	0.42
1:A:270:TYR:O	1:A:319:ARG:NH1	2.53	0.42
1:C:327:LEU:HB3	1:C:330:VAL:CG1	2.49	0.42
1:A:107:GLY:HA2	1:A:265:PHE:HA	2.01	0.42
1:A:3:ARG:HB2	1:A:5:GLU:OE1	2.20	0.42
1:D:19:THR:HG22	1:D:23:VAL:HB	2.02	0.42
1:C:197:LYS:HA	1:C:197:LYS:HD3	1.75	0.42
1:B:519:LYS:H	1:B:519:LYS:HG2	1.51	0.42
1:A:124:TRP:HE3	1:A:124:TRP:O	2.03	0.41
1:A:162:ALA:O	1:A:172:GLU:HA	2.19	0.41
1:B:369:LEU:O	1:B:392:ALA:HA	2.19	0.41
1:A:432:PRO:HD3	1:A:489:TRP:CH2	2.54	0.41
1:C:63:PRO:HA	1:C:66:GLU:HG3	2.02	0.41
1:A:441:LEU:HB3	1:A:442:PRO:HD3	2.02	0.41
1:B:488:THR:HG22	1:B:488:THR:O	2.19	0.41
1:C:355:PRO:HG3	1:C:439:PHE:CE1	2.56	0.41
1:B:351:GLY:HA2	1:B:428:TRP:O	2.21	0.41
1:A:262:VAL:CG1	1:A:263:PHE:N	2.82	0.41
1:D:38:HIS:O	1:D:39:HIS:CB	2.62	0.41
1:C:312:ASP:C	1:C:312:ASP:OD1	2.59	0.41
1:D:217:ALA:HB1	1:D:230:PHE:C	2.40	0.41
1:C:432:PRO:HD2	1:C:435:VAL:HB	2.01	0.41
1:A:396:ALA:N	1:A:397:PRO:CD	2.82	0.41
1:A:227:VAL:HG12	1:A:228:ALA:N	2.35	0.41
1:A:362:GLU:CD	1:A:362:GLU:N	2.74	0.41
1:D:156:HIS:CE1	1:D:158:PRO:HD3	2.55	0.41
1:A:338:HIS:HA	1:A:339:PRO:HD3	1.94	0.41
1:B:44:VAL:HG21	1:B:124:TRP:CH2	2.55	0.41
1:D:205:TYR:HB2	1:D:400:PRO:HG3	2.03	0.41
1:B:256:GLY:O	1:B:262:VAL:HA	2.20	0.41
1:C:58:PHE:O	1:C:176:GLY:HA2	2.21	0.41
1:B:64:GLU:N	1:B:64:GLU:CD	2.72	0.41
1:B:251:GLY:HA3	1:B:255:HIS:CE1	2.56	0.41
1:A:469:PHE:CD1	1:A:469:PHE:O	2.74	0.40
1:B:300:VAL:O	1:B:300:VAL:HG13	2.21	0.40
1:D:160:PHE:C	1:D:160:PHE:CD1	2.95	0.40
1:B:65:VAL:HG11	1:B:179:PHE:HB2	2.04	0.40
1:B:338:HIS:HA	1:B:339:PRO:HD3	1.85	0.40
1:A:478:VAL:HA	1:A:479:PRO:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PHE:CE1	1:C:27:HIS:HE1	2.38	0.40
1:C:459:VAL:HB	1:C:460:PRO:HD2	2.03	0.40
1:A:296:GLU:O	1:A:297:ASN:HB2	2.21	0.40
1:A:13:LYS:HG3	1:A:97:ARG:HA	2.02	0.40
1:D:213:PHE:CE2	1:D:215:MET:HG2	2.56	0.40
1:A:124:TRP:CZ2	1:A:125:HIS:CE1	3.09	0.40
1:A:207:MET:HB2	1:A:208:PRO:HD3	2.04	0.40
1:A:290:GLN:HG3	1:A:326:HIS:CE1	2.57	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	509/529 (96%)	495 (97%)	13 (3%)	1 (0%)	52	69
1	B	505/529 (96%)	474 (94%)	29 (6%)	2 (0%)	39	56
1	C	511/529 (97%)	493 (96%)	17 (3%)	1 (0%)	52	69
1	D	506/529 (96%)	490 (97%)	13 (3%)	3 (1%)	30	43
All	All	2031/2116 (96%)	1952 (96%)	72 (4%)	7 (0%)	46	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	ALA
1	A	292	GLU
1	D	427	GLY
1	B	385	GLU
1	C	528	THR
1	D	292	GLU
1	D	395	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	427/438 (98%)	414 (97%)	13 (3%)	48	70
1	B	425/438 (97%)	401 (94%)	24 (6%)	26	41
1	C	429/438 (98%)	419 (98%)	10 (2%)	58	78
1	D	424/438 (97%)	412 (97%)	12 (3%)	51	72
All	All	1705/1752 (97%)	1646 (96%)	59 (4%)	43	64

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	14	ARG
1	A	120	THR
1	A	122	SER
1	A	152	PHE
1	A	259	GLU
1	A	332	GLU
1	A	387	ARG
1	A	416	LYS
1	A	463	ARG
1	A	469	PHE
1	A	480	GLN
1	A	527	ARG
1	B	2	GLN
1	B	5	GLU
1	B	64	GLU
1	B	132	MET
1	B	138	ARG
1	B	152	PHE
1	B	209	LYS
1	B	238	LYS
1	B	259	GLU
1	B	264	ASN
1	B	326	HIS

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Mol	Chain	Res	Type
1	B	385	GLU
1	B	408	ARG
1	B	409	MET
1	B	464	ASP
1	B	469	PHE
1	B	484	ASN
1	B	491	ASP
1	B	497	GLN
1	B	498	GLN
1	B	504	ARG
1	B	511	GLN
1	B	519	LYS
1	B	527	ARG
1	C	61	ARG
1	C	64	GLU
1	C	146	GLU
1	C	152	PHE
1	C	259	GLU
1	C	332	GLU
1	C	463	ARG
1	C	469	PHE
1	C	492	LYS
1	C	519	LYS
1	D	3	ARG
1	D	152	PHE
1	D	240	THR
1	D	264	ASN
1	D	326	HIS
1	D	332	GLU
1	D	412	GLU
1	D	439	PHE
1	D	469	PHE
1	D	480	GLN
1	D	498	GLN
1	D	511	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	458	ASN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	511	GLN
1	B	2	GLN
1	B	92	GLN
1	B	102	GLN
1	B	156	HIS
1	B	180	GLN
1	B	204	ASN
1	B	264	ASN
1	B	458	ASN
1	B	497	GLN
1	B	498	GLN
1	B	511	GLN
1	C	92	GLN
1	D	92	GLN
1	D	102	GLN
1	D	204	ASN
1	D	264	ASN
1	D	326	HIS
1	D	329	ASN
1	D	338	HIS
1	D	402	HIS
1	D	458	ASN
1	D	497	GLN
1	D	498	GLN
1	D	507	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	1003	-	24,33,33	1.20	2 (8%)	31,52,52	2.28	5 (16%)
3	PO4	A	3001	-	4,4,4	1.22	0	6,6,6	0.27	0
3	PO4	A	3005	-	4,4,4	1.10	0	6,6,6	0.27	0
3	PO4	A	3009	-	4,4,4	1.10	0	6,6,6	0.27	0
4	ATP	B	1001	-	24,33,33	1.02	1 (4%)	31,52,52	2.28	5 (16%)
3	PO4	B	3002	-	4,4,4	1.05	0	6,6,6	0.27	0
3	PO4	B	3006	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	B	3013	-	4,4,4	2.17	3 (75%)	6,6,6	0.28	0
4	ATP	C	1002	-	24,33,33	1.32	2 (8%)	31,52,52	2.38	4 (12%)
3	PO4	C	3003	-	4,4,4	1.05	0	6,6,6	0.27	0
3	PO4	C	3007	-	4,4,4	1.14	0	6,6,6	0.27	0
3	PO4	C	3010	-	4,4,4	1.07	0	6,6,6	0.27	0
3	PO4	C	3014	-	4,4,4	2.17	3 (75%)	6,6,6	0.28	0
3	PO4	C	3016	-	4,4,4	2.17	3 (75%)	6,6,6	0.28	0
3	PO4	C	3017	-	4,4,4	2.18	3 (75%)	6,6,6	0.28	0
4	ATP	D	1004	-	24,33,33	1.02	1 (4%)	31,52,52	2.31	5 (16%)
3	PO4	D	3004	-	4,4,4	1.26	0	6,6,6	0.27	0
3	PO4	D	3008	-	4,4,4	1.09	0	6,6,6	0.27	0
3	PO4	D	3011	-	4,4,4	0.99	0	6,6,6	0.27	0
3	PO4	D	3015	-	4,4,4	2.17	3 (75%)	6,6,6	0.28	0

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
4	ATP	A	1003	-	-	0/18/38/38	0/3/3/3
3	PO4	A	3001	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PO4	A	3005	-	-	0/0/0/0	0/0/0/0
3	PO4	A	3009	-	-	0/0/0/0	0/0/0/0
4	ATP	B	1001	-	-	0/18/38/38	0/3/3/3
3	PO4	B	3002	-	-	0/0/0/0	0/0/0/0
3	PO4	B	3006	-	-	0/0/0/0	0/0/0/0
3	PO4	B	3013	-	-	0/0/0/0	0/0/0/0
4	ATP	C	1002	-	-	0/18/38/38	0/3/3/3
3	PO4	C	3003	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3007	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3010	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3014	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3016	-	-	0/0/0/0	0/0/0/0
3	PO4	C	3017	-	-	0/0/0/0	0/0/0/0
4	ATP	D	1004	-	-	0/18/38/38	0/3/3/3
3	PO4	D	3004	-	-	0/0/0/0	0/0/0/0
3	PO4	D	3008	-	-	0/0/0/0	0/0/0/0
3	PO4	D	3011	-	-	0/0/0/0	0/0/0/0
3	PO4	D	3015	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3017	PO4	P-O2	-3.03	1.42	1.53
3	C	3014	PO4	P-O2	-3.02	1.42	1.53
3	D	3015	PO4	P-O2	-3.01	1.42	1.53
3	C	3016	PO4	P-O2	-3.01	1.42	1.53
3	B	3013	PO4	P-O2	-3.00	1.42	1.53
3	B	3013	PO4	P-O4	-2.23	1.45	1.53
3	C	3014	PO4	P-O4	-2.22	1.45	1.53
3	C	3017	PO4	P-O4	-2.22	1.45	1.53
3	C	3016	PO4	P-O4	-2.20	1.45	1.53
3	D	3015	PO4	P-O4	-2.19	1.45	1.53
3	D	3015	PO4	P-O1	-2.13	1.43	1.52
3	B	3013	PO4	P-O1	-2.12	1.43	1.52
3	C	3016	PO4	P-O1	-2.12	1.43	1.52
3	C	3014	PO4	P-O1	-2.11	1.43	1.52
3	C	3017	PO4	P-O1	-2.10	1.43	1.52
4	C	1002	ATP	O4'-C1'	2.05	1.43	1.41
4	D	1004	ATP	O4'-C1'	2.29	1.44	1.41
4	A	1003	ATP	O4'-C1'	2.31	1.44	1.41
4	B	1001	ATP	O4'-C1'	2.34	1.44	1.41
4	A	1003	ATP	PG-O2G	3.33	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1002	ATP	PG-O3G	4.65	1.71	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1002	ATP	N3-C2-N1	-10.64	120.75	128.89
4	B	1001	ATP	N3-C2-N1	-10.24	121.06	128.89
4	D	1004	ATP	N3-C2-N1	-10.22	121.07	128.89
4	A	1003	ATP	N3-C2-N1	-10.01	121.23	128.89
4	C	1002	ATP	PA-O3A-PB	-5.11	118.39	132.73
4	D	1004	ATP	PA-O3A-PB	-4.44	120.26	132.73
4	B	1001	ATP	PA-O3A-PB	-4.27	120.73	132.73
4	A	1003	ATP	PA-O3A-PB	-4.25	120.80	132.73
4	D	1004	ATP	PB-O3B-PG	-3.73	120.15	132.67
4	B	1001	ATP	PB-O3B-PG	-3.41	121.22	132.67
4	A	1003	ATP	PB-O3B-PG	-3.28	121.67	132.67
4	A	1003	ATP	C4'-O4'-C1'	-2.95	106.47	109.72
4	C	1002	ATP	C4'-O4'-C1'	-2.93	106.50	109.72
4	D	1004	ATP	C4'-O4'-C1'	-2.60	106.86	109.72
4	A	1003	ATP	C4-C5-N7	-2.57	107.11	109.48
4	B	1001	ATP	C4'-O4'-C1'	-2.55	106.92	109.72
4	C	1002	ATP	PB-O3B-PG	-2.54	124.14	132.67
4	D	1004	ATP	C4-C5-N7	-2.24	107.42	109.48
4	B	1001	ATP	C4-C5-N7	-2.14	107.51	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	PO4	1	0
4	B	1001	ATP	1	0
4	C	1002	ATP	3	0
3	C	3016	PO4	1	0
4	D	1004	ATP	6	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	A	515/529 (97%)	-0.29	5 (0%) 84 83	22, 35, 54, 76	0
1	B	511/529 (96%)	0.58	59 (11%) 6 6	38, 59, 97, 108	0
1	C	517/529 (97%)	-0.14	14 (2%) 58 57	27, 40, 63, 95	0
1	D	512/529 (96%)	-0.23	9 (1%) 71 71	20, 37, 66, 90	0
All	All	2055/2116 (97%)	-0.02	87 (4%) 40 41	20, 41, 79, 108	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	529	GLU	7.1
1	B	528	THR	6.9
1	B	435	VAL	5.8
1	B	527	ARG	5.6
1	B	384	THR	5.1
1	C	384	THR	4.8
1	D	387	ARG	4.7
1	B	223	LYS	4.7
1	B	2	GLN	4.5
1	C	145	VAL	4.4
1	D	147	ALA	4.4
1	B	479	PRO	4.2
1	C	528	THR	4.0
1	B	71	TRP	4.0
1	B	511	GLN	4.0
1	B	475	ALA	3.9
1	B	458	ASN	3.9
1	B	224	GLU	3.8
1	D	527	ARG	3.8
1	B	484	ASN	3.6
1	B	340	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	489	TRP	3.6
1	C	527	ARG	3.6
1	B	481	GLU	3.5
1	B	17	TRP	3.5
1	B	12	LYS	3.4
1	B	500	ARG	3.4
1	B	478	VAL	3.3
1	B	418	ALA	3.3
1	B	504	ARG	3.3
1	B	437	TYR	3.2
1	B	165	GLU	3.2
1	B	514	ALA	3.2
1	B	482	LEU	3.1
1	B	519	LYS	3.1
1	C	146	GLU	3.0
1	B	486	ARG	3.0
1	B	72	GLY	3.0
1	D	374	ALA	2.9
1	D	388	ALA	2.9
1	B	434	GLY	2.9
1	B	436	GLY	2.8
1	B	66	GLU	2.8
1	C	280	HIS	2.8
1	A	387	ARG	2.8
1	B	440	PRO	2.8
1	B	513	TYR	2.8
1	C	140	GLY	2.8
1	B	163	VAL	2.7
1	B	507	GLN	2.7
1	B	487	GLU	2.7
1	C	141	ASN	2.7
1	B	10	HIS	2.7
1	D	433	TYR	2.7
1	D	224	GLU	2.5
1	B	350	TYR	2.5
1	B	495	TYR	2.4
1	B	79	ALA	2.4
1	C	139	PHE	2.4
1	C	12	LYS	2.4
1	B	472	PRO	2.4
1	B	132	MET	2.4
1	C	458	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	328	GLU	2.4
1	A	141	ASN	2.3
1	B	168	GLY	2.3
1	B	517	VAL	2.3
1	D	386	PRO	2.3
1	B	78	PHE	2.3
1	C	96	GLU	2.2
1	B	453	SER	2.2
1	D	528	THR	2.2
1	B	3	ARG	2.2
1	B	234	SER	2.2
1	C	415	ARG	2.1
1	B	352	VAL	2.1
1	B	493	GLU	2.1
1	B	415	ARG	2.1
1	B	523	GLU	2.1
1	B	225	GLY	2.1
1	B	483	LEU	2.1
1	A	140	GLY	2.1
1	B	516	GLY	2.1
1	B	420	ARG	2.1
1	A	493	GLU	2.0
1	B	81	GLU	2.0
1	B	96	GLU	2.0

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

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
4	ATP	A	1003	31/31	0.67	0.31	5.07	91,93,103,104	0
4	ATP	D	1004	31/31	0.85	0.24	3.06	92,94,107,107	0
3	PO4	B	3013	5/5	0.94	0.31	2.10	82,82,83,83	0
3	PO4	D	3015	5/5	0.94	0.21	1.79	75,76,77,77	0
3	PO4	A	3009	5/5	0.90	0.16	0.77	59,61,62,63	0
3	PO4	C	3016	5/5	0.96	0.19	0.39	52,52,54,55	0
3	PO4	A	3001	5/5	0.98	0.14	0.14	35,36,38,40	0
4	ATP	C	1002	31/31	0.91	0.15	-0.06	32,39,65,67	0
4	ATP	B	1001	31/31	0.88	0.19	-0.13	76,78,88,89	0
3	PO4	C	3017	5/5	0.96	0.15	-0.28	53,56,56,56	0
3	PO4	C	3010	5/5	0.96	0.11	-0.28	57,58,60,61	0
2	CA	D	2004	1/1	0.94	0.14	-0.36	46,46,46,46	0
2	CA	A	2001	1/1	0.98	0.14	-0.47	43,43,43,43	0
3	PO4	D	3008	5/5	0.97	0.10	-0.75	61,62,63,63	0
3	PO4	C	3014	5/5	0.97	0.14	-0.79	46,46,47,48	0
3	PO4	B	3006	5/5	0.94	0.15	-0.81	82,83,83,83	0
3	PO4	D	3004	5/5	0.99	0.12	-0.90	31,33,33,34	0
3	PO4	C	3007	5/5	0.97	0.09	-0.96	61,62,62,64	0
3	PO4	A	3005	5/5	0.97	0.11	-1.01	57,59,60,60	0
3	PO4	B	3002	5/5	0.98	0.11	-1.33	46,49,49,51	0
3	PO4	D	3011	5/5	0.97	0.08	-1.44	48,50,52,52	0
3	PO4	C	3003	5/5	0.98	0.08	-1.47	40,43,44,44	0
2	CA	B	2002	1/1	0.95	0.05	-2.57	81,81,81,81	0
2	CA	C	2003	1/1	0.98	0.05	-2.63	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.