



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:44 PM GMT

PDB ID : 1C9K
Title : THE THREE DIMENSIONAL STRUCTURE OF ADENOSYLCOBINAMIDE KINASE/ ADENOSYLCOBINAMIDE PHOSPHATE GUALYLTRANSFERASE (COBU) COMPLEXED WITH GMP: EVIDENCE FOR A SUBSTRATE INDUCED TRANSFERASE ACTIVE SITE
Authors : Thompson, T.B.; Thomas, M.G.; Esclante-Semerena, J.C.; Rayment, I.
Deposited on : 1999-08-02
Resolution : 2.20 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

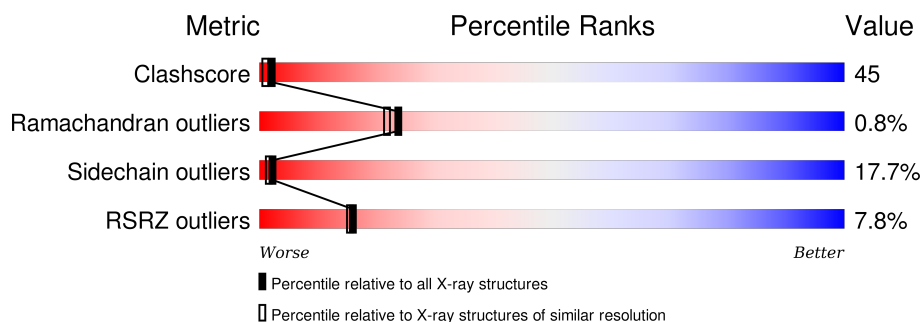
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	A	180	
1	B	180	
1	C	180	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	600	-	-	X	-
2	PO4	B	601	-	-	X	-
5	POP	C	608	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4253 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 ADENOSYLCOBINAMIDE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1287	812	232	235	8			
1	B	180	Total	C	N	O	S	0	0	0
			1328	837	240	242	9			
1	C	165	Total	C	N	O	S	0	0	0
			1214	768	215	224	7			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

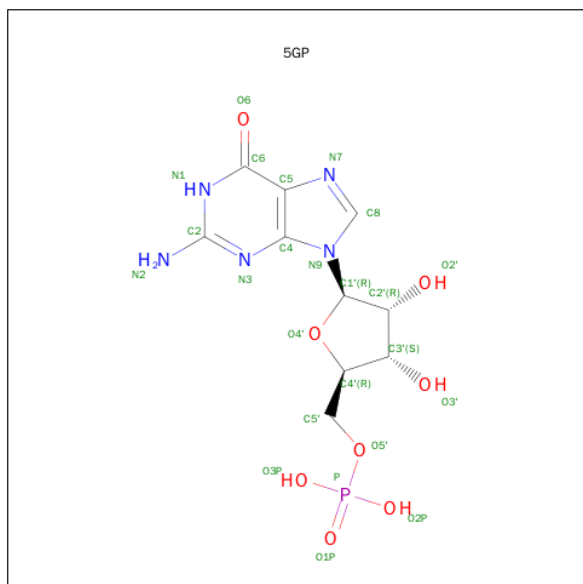


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

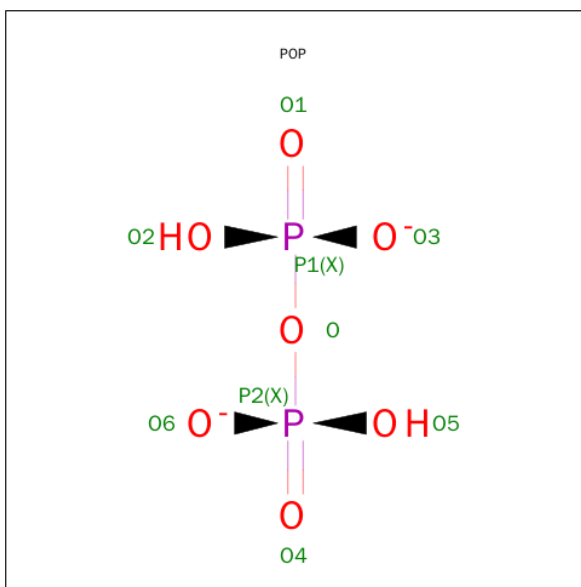
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 24 10 5 8 1	0	0
4	B	1	Total C N O P 24 10 5 8 1	0	0
4	C	1	Total C N O 20 10 5 5	0	0

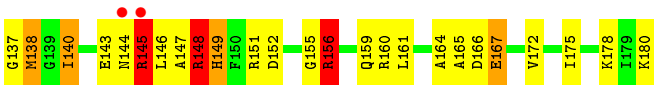
- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total	O	0	0
			134	134		
6	B	116	Total	O	0	0
			116	116		
6	C	86	Total	O	0	0
			86	86		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.38 Å 87.77 Å 101.64 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.20) 95.6 (29.30-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.53 (at 2.10 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.191 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 167.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 29766 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4253	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 5GP, MG, POP

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	0.83	8/1306 (0.6%)	1.41	26/1774 (1.5%)
1	B	0.89	6/1349 (0.4%)	1.40	23/1837 (1.3%)
1	C	0.85	7/1229 (0.6%)	1.50	30/1670 (1.8%)
All	All	0.86	21/3884 (0.5%)	1.44	79/5281 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	1
1	C	1	0
All	All	2	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	58	GLU	N-CA	-8.56	1.29	1.46
1	C	23	ALA	CA-C	-6.34	1.36	1.52
1	B	17	GLU	CD-OE2	5.81	1.32	1.25
1	A	135	GLU	CD-OE2	5.78	1.32	1.25
1	B	167	GLU	CD-OE2	5.60	1.31	1.25
1	A	100	GLU	CD-OE2	5.58	1.31	1.25
1	C	80	GLU	CD-OE2	5.48	1.31	1.25
1	B	114	GLU	CD-OE2	5.47	1.31	1.25
1	A	58	GLU	CD-OE2	5.43	1.31	1.25
1	C	17	GLU	CD-OE2	5.40	1.31	1.25
1	A	17	GLU	CD-OE2	5.38	1.31	1.25
1	A	167	GLU	CD-OE2	5.36	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	GLU	CD-OE2	5.31	1.31	1.25
1	B	58	GLU	CD-OE2	5.31	1.31	1.25
1	A	108	GLU	CD-OE2	5.30	1.31	1.25
1	C	108	GLU	CD-OE2	5.28	1.31	1.25
1	A	80	GLU	CD-OE2	5.23	1.31	1.25
1	B	135	GLU	CD-OE2	5.19	1.31	1.25
1	C	167	GLU	CD-OE2	5.10	1.31	1.25
1	C	114	GLU	CD-OE2	5.05	1.31	1.25
1	C	135	GLU	CD-OE2	5.04	1.31	1.25

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ALA	O-C-N	10.57	139.62	122.70
1	A	61	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	C	61	ARG	CA-C-N	-8.99	97.43	117.20
1	C	113	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	C	156	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	B	57	ALA	CA-C-N	-8.20	99.17	117.20
1	A	9	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	C	61	ARG	O-C-N	7.67	134.98	122.70
1	C	22	ASP	N-CA-CB	-7.53	97.04	110.60
1	A	98	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	124	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	9	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	149	HIS	CA-CB-CG	-7.29	101.21	113.60
1	C	23	ALA	O-C-N	7.24	134.86	121.10
1	B	152	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	112	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	C	61	ARG	C-N-CA	6.96	139.10	121.70
1	A	152	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	C	75	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	70	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	57	ALA	C-N-CA	6.59	138.19	121.70
1	C	113	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	112	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	22	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	70	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	113	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	22	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	C	166	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	48	ASP	CB-CG-OD1	6.21	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	22	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	166	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	62	HIS	CA-C-N	-6.13	103.72	117.20
1	A	98	ASP	CB-CG-OD1	6.13	123.81	118.30
1	C	152	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	64	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	B	152	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	48	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	169	TRP	CB-CA-C	-5.95	98.49	110.40
1	B	113	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	22	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	113	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	74	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	C	48	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	C	64	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	112	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	48	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	A	112	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	166	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	48	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	166	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	103	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	C	50	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	151	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	64	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	156	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	22	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	C	68	THR	CA-CB-CG2	5.44	120.02	112.40
1	A	32	SER	N-CA-CB	5.43	118.64	110.50
1	C	145	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	65	THR	CA-CB-CG2	5.32	119.85	112.40
1	A	172	VAL	CB-CA-C	5.32	121.51	111.40
1	B	70	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	124	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	103	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	160	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	61	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	148	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	64	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	166	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	C	75	ASP	CB-CG-OD2	-5.15	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	THR	CA-CB-OG1	5.14	119.79	109.00
1	B	64	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	14	ARG	N-CA-CB	-5.10	101.43	110.60
1	A	113	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	48	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	98	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	B	160	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	59	CYS	N-CA-CB	-5.01	101.58	110.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	172	VAL	CA
1	C	68	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	GLU	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1287	0	1297	139	0
1	B	1328	0	1317	132	0
1	C	1214	0	1215	124	0
2	A	5	0	0	2	0
2	B	5	0	0	3	0
3	C	1	0	0	0	0
4	A	24	0	12	4	0
4	B	24	0	12	1	0
4	C	20	0	12	2	0
5	C	9	0	0	0	0
6	A	134	0	0	9	0
6	B	116	0	0	6	0
6	C	86	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4253	0	3865	352	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 45.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:HG3	1:A:153:ILE:HG12	1.24	1.08
1:A:124:ARG:HH11	1:A:124:ARG:HB2	1.14	1.06
1:A:65:THR:HG22	1:A:66:LEU:HG	1.37	1.06
1:C:121:ALA:HA	1:C:124:ARG:HD3	1.38	1.05
1:B:68:THR:HG22	1:B:71:LEU:HG	1.35	1.04
1:B:1:MET:HE3	1:B:165:ALA:HB2	1.41	1.00
1:B:34:ILE:HG21	1:B:40:ALA:HB2	1.40	0.98
1:A:9:ARG:NH2	1:C:159:GLN:HE22	1.61	0.97
1:A:9:ARG:HA	1:A:9:ARG:HE	1.30	0.94
1:B:34:ILE:HG23	1:B:39:MET:HG2	1.48	0.93
1:C:145:ARG:HG3	1:C:149:HIS:CE1	2.03	0.93
1:A:156:ARG:HD3	1:B:9:ARG:HH21	1.33	0.92
1:B:179:ILE:HD12	1:C:175:ILE:HB	1.54	0.89
1:A:9:ARG:HD3	1:C:156:ARG:HD2	1.55	0.88
1:B:43:ILE:HG22	1:B:47:LYS:HE2	1.55	0.88
1:C:156:ARG:HH11	1:C:156:ARG:HG2	1.40	0.87
1:A:9:ARG:HD3	1:C:156:ARG:CD	2.05	0.86
1:A:138:MET:HB3	1:C:138:MET:HB3	1.60	0.83
1:B:141:VAL:HG22	1:B:151:ARG:NH2	1.93	0.83
1:C:121:ALA:CA	1:C:124:ARG:HD3	2.09	0.82
1:B:43:ILE:HG22	1:B:47:LYS:CE	2.09	0.82
1:B:34:ILE:HG21	1:B:40:ALA:CB	2.08	0.81
1:A:124:ARG:NH1	1:A:124:ARG:HB2	1.94	0.81
1:B:68:THR:CG2	1:B:71:LEU:HG	2.10	0.81
1:A:9:ARG:HH11	1:C:156:ARG:NH1	1.78	0.81
1:A:167:GLU:HG2	1:A:178:LYS:HE2	1.61	0.81
1:C:99:PRO:HA	1:C:102:TRP:CD2	2.15	0.81
1:A:136:VAL:HB	1:C:140:ILE:CD1	2.10	0.80
1:A:61:ARG:HG3	1:A:61:ARG:HH11	1.45	0.80
1:A:82:ILE:HD13	1:A:85:MET:CE	2.11	0.80
1:A:50:ARG:NH2	4:A:604:5GP:N7	2.30	0.80
1:B:108:GLU:HG3	1:B:153:ILE:HG12	1.64	0.80
1:B:141:VAL:HG22	1:B:151:ARG:HH22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD23	1:B:111:ILE:HD11	1.64	0.78
1:A:138:MET:HB3	1:B:138:MET:HB3	1.66	0.78
1:A:106:ALA:HA	1:A:109:ARG:NH1	1.98	0.78
1:B:138:MET:HB3	1:C:138:MET:HB3	1.63	0.77
1:C:145:ARG:HG3	1:C:149:HIS:ND1	1.99	0.77
1:A:138:MET:HB3	1:B:138:MET:CB	2.14	0.77
1:B:43:ILE:HG22	1:B:47:LYS:NZ	1.98	0.77
1:C:90:LEU:HD23	1:C:111:ILE:HD11	1.67	0.77
1:C:9:ARG:NE	1:C:9:ARG:HA	2.01	0.76
1:B:68:THR:HG22	1:B:71:LEU:CG	2.15	0.75
1:C:68:THR:HG22	1:C:71:LEU:HD13	1.69	0.75
1:A:140:ILE:HD11	1:B:151:ARG:HB2	1.68	0.74
1:C:99:PRO:HA	1:C:102:TRP:CG	2.22	0.73
1:B:138:MET:HB3	1:C:138:MET:CB	2.19	0.73
1:A:26:VAL:HG21	1:A:54:TRP:NE1	2.04	0.73
1:A:32:SER:OG	4:A:604:5GP:H1'	1.89	0.72
1:C:28:TYR:CE1	1:C:30:ALA:HB2	2.23	0.72
1:C:13:SER:O	1:C:17:GLU:HG3	1.89	0.72
1:B:152:ASP:HB3	1:B:156:ARG:NH2	2.05	0.72
1:A:68:THR:HB	1:A:71:LEU:HD22	1.71	0.71
1:A:140:ILE:O	1:A:142:PRO:HD3	1.90	0.71
1:A:53:HIS:H	1:A:53:HIS:CD2	2.09	0.71
1:A:99:PRO:HA	1:A:102:TRP:CE2	2.26	0.70
1:C:62:HIS:O	1:C:65:THR:HB	1.90	0.70
1:A:138:MET:CB	1:C:138:MET:HB3	2.21	0.70
1:A:82:ILE:HD13	1:A:85:MET:HE3	1.73	0.70
1:B:99:PRO:HA	1:B:102:TRP:CD2	2.27	0.70
1:C:144:ASN:O	1:C:147:ALA:HB3	1.91	0.70
1:A:72:ALA:HB3	1:A:75:ASP:OD1	1.91	0.69
1:B:179:ILE:HD12	1:C:175:ILE:CB	2.22	0.69
1:C:9:ARG:HA	1:C:9:ARG:HE	1.57	0.69
1:C:99:PRO:HA	1:C:102:TRP:CE2	2.27	0.69
1:C:73:PRO:HA	1:C:126:PRO:O	1.93	0.69
1:C:1:MET:HB3	1:C:129:VAL:HB	1.75	0.69
1:A:62:HIS:O	1:A:65:THR:HB	1.92	0.69
1:C:121:ALA:HA	1:C:124:ARG:CD	2.20	0.68
1:B:20:ILE:HD12	1:B:78:LEU:HG	1.75	0.68
1:A:42:ARG:N	1:A:42:ARG:HD3	2.07	0.68
1:B:47:LYS:HE3	6:B:812:HOH:O	1.92	0.68
1:B:138:MET:HG2	1:C:138:MET:HE2	1.73	0.68
1:A:99:PRO:HA	1:A:102:TRP:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:CD	1:B:9:ARG:HH21	2.07	0.68
1:A:82:ILE:HD13	1:A:85:MET:HE1	1.76	0.68
1:B:156:ARG:NH1	1:C:9:ARG:HD3	2.10	0.67
1:B:98:ASP:HB3	1:B:101:GLN:NE2	2.09	0.67
1:A:9:ARG:NH1	1:C:156:ARG:NH1	2.41	0.67
1:C:115:ILE:O	1:C:119:ILE:HG13	1.96	0.66
1:B:34:ILE:HG21	1:B:40:ALA:CA	2.26	0.66
1:A:9:ARG:HE	1:A:9:ARG:CA	2.04	0.66
1:C:61:ARG:C	1:C:63:LEU:HD23	2.16	0.66
1:B:34:ILE:HA	1:B:39:MET:HG2	1.77	0.66
1:A:61:ARG:HG3	1:A:61:ARG:NH1	2.10	0.66
1:B:11:GLY:HA2	6:B:749:HOH:O	1.96	0.66
1:B:9:ARG:HA	1:B:9:ARG:HE	1.62	0.65
1:A:9:ARG:HD3	1:C:156:ARG:NE	2.11	0.65
1:A:68:THR:H	1:A:71:LEU:CD2	2.10	0.65
1:C:119:ILE:HD13	1:C:164:ALA:HB2	1.77	0.65
1:C:68:THR:CG2	1:C:71:LEU:HD13	2.26	0.65
1:B:112:ASP:OD2	1:B:160:ARG:NH1	2.30	0.65
1:B:146:LEU:O	1:B:149:HIS:N	2.30	0.64
1:A:9:ARG:NH2	1:C:159:GLN:NE2	2.42	0.64
1:B:155:GLY:O	1:B:159:GLN:HG3	1.97	0.64
1:C:137:GLY:HA2	6:C:707:HOH:O	1.96	0.64
1:B:71:LEU:O	1:B:126:PRO:HG2	1.96	0.64
1:C:83:THR:O	1:C:86:VAL:HB	1.96	0.64
1:C:90:LEU:CD2	1:C:111:ILE:HD11	2.27	0.64
1:A:136:VAL:HB	1:C:140:ILE:HD12	1.79	0.64
1:A:82:ILE:O	1:A:86:VAL:HG23	1.98	0.64
1:C:28:TYR:HE1	1:C:30:ALA:HB2	1.62	0.64
1:A:153:ILE:HG23	6:A:862:HOH:O	1.97	0.64
1:A:27:LEU:HD11	1:A:57:ALA:HB2	1.80	0.63
1:C:68:THR:HG22	1:C:71:LEU:HD22	1.80	0.63
1:A:9:ARG:HD2	6:A:763:HOH:O	1.98	0.63
1:A:93:LEU:N	1:A:93:LEU:HD23	2.13	0.63
1:A:98:ASP:O	1:A:100:GLU:N	2.30	0.63
1:A:29:ILE:HD12	1:A:77:ILE:HG23	1.80	0.63
1:A:167:GLU:HG2	1:A:178:LYS:CE	2.28	0.62
1:A:11:GLY:N	2:A:600:PO4:O2	2.30	0.62
1:B:63:LEU:HD23	1:B:66:LEU:HD12	1.79	0.62
1:C:99:PRO:HA	1:C:102:TRP:CD1	2.34	0.62
1:C:104:TYR:HE1	1:C:145:ARG:HE	1.47	0.62
1:A:124:ARG:HH11	1:A:124:ARG:CB	2.02	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:THR:HG22	1:C:71:LEU:CD1	2.30	0.61
1:C:29:ILE:HD12	1:C:77:ILE:CG2	2.30	0.61
1:B:102:TRP:CD2	1:B:107:MET:HE3	2.36	0.61
1:C:106:ALA:HA	1:C:109:ARG:NH1	2.16	0.61
1:A:156:ARG:NH1	1:B:9:ARG:HD2	2.16	0.60
1:A:140:ILE:HD12	1:B:136:VAL:O	2.01	0.60
1:B:94:GLY:HA3	1:B:102:TRP:CZ2	2.36	0.60
1:C:145:ARG:O	1:C:149:HIS:ND1	2.34	0.60
1:B:98:ASP:HB3	1:B:101:GLN:HE21	1.65	0.60
1:A:138:MET:HE2	1:C:138:MET:HG2	1.84	0.60
1:C:155:GLY:O	1:C:159:GLN:HG3	2.01	0.60
1:B:98:ASP:O	1:B:101:GLN:HG2	2.01	0.60
1:A:61:ARG:CG	1:A:61:ARG:HH11	2.15	0.59
1:B:1:MET:CE	1:B:165:ALA:HB2	2.26	0.59
1:B:142:PRO:HG2	1:B:148:ARG:HA	1.83	0.59
1:A:60:TRP:HZ3	1:A:61:ARG:HH12	1.49	0.59
1:B:28:TYR:CE1	1:B:30:ALA:HB2	2.38	0.59
1:C:156:ARG:HH11	1:C:156:ARG:CG	2.13	0.59
1:C:145:ARG:HG3	1:C:149:HIS:HD1	1.68	0.59
1:A:156:ARG:HG3	1:B:9:ARG:HD3	1.85	0.58
1:A:32:SER:O	4:A:604:5GP:N2	2.31	0.58
1:B:20:ILE:CD1	1:B:78:LEU:HG	2.32	0.58
1:C:29:ILE:HD12	1:C:77:ILE:HG21	1.85	0.58
1:B:34:ILE:CG2	1:B:39:MET:HG2	2.28	0.58
1:A:9:ARG:NH2	2:A:600:PO4:O2	2.34	0.58
1:A:51:PRO:HB2	1:A:53:HIS:CD2	2.39	0.58
1:A:156:ARG:HD3	1:B:9:ARG:NH2	2.13	0.57
1:A:169:TRP:CZ2	1:A:178:LYS:HD2	2.39	0.57
1:B:1:MET:HE3	1:B:165:ALA:CB	2.27	0.57
1:B:34:ILE:HG12	1:B:43:ILE:HD12	1.86	0.57
1:B:102:TRP:CE3	1:B:107:MET:HE1	2.39	0.57
1:A:160:ARG:NH2	6:A:829:HOH:O	2.37	0.57
1:A:136:VAL:O	1:C:140:ILE:HD13	2.05	0.56
1:B:120:ALA:O	1:B:124:ARG:HG3	2.05	0.56
1:B:34:ILE:HG23	1:B:39:MET:CG	2.30	0.56
1:C:22:ASP:OD1	1:C:23:ALA:N	2.39	0.56
1:A:138:MET:CE	1:C:138:MET:HG2	2.36	0.56
1:B:156:ARG:HH11	1:C:9:ARG:HD3	1.69	0.56
1:C:70:ASP:HB3	6:C:963:HOH:O	2.05	0.56
1:B:44:GLN:HA	1:B:47:LYS:HE3	1.87	0.56
1:A:74:ASP:HB3	6:A:878:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:MET:HB3	1:B:138:MET:HB2	1.88	0.55
1:C:104:TYR:CD2	1:C:149:HIS:HB3	2.41	0.55
1:B:98:ASP:OD2	1:B:100:GLU:N	2.30	0.55
1:A:9:ARG:HH11	1:C:156:ARG:CZ	2.19	0.55
1:A:29:ILE:HD12	1:A:77:ILE:CG2	2.37	0.55
1:A:102:TRP:HB3	1:A:107:MET:SD	2.46	0.55
1:A:93:LEU:HD12	1:A:107:MET:HG2	1.90	0.54
1:C:105:ALA:O	1:C:109:ARG:HG3	2.07	0.54
1:B:27:LEU:HD12	1:B:55:ARG:O	2.06	0.54
1:B:170:LEU:O	1:B:177:VAL:N	2.37	0.54
1:A:87:THR:O	1:A:91:PHE:HD1	1.91	0.54
1:A:108:GLU:HG3	1:A:153:ILE:CG1	2.18	0.54
1:A:32:SER:HG	4:A:604:5GP:H1'	1.71	0.54
1:C:143:GLU:O	1:C:148:ARG:NH1	2.41	0.54
1:A:68:THR:CB	1:A:71:LEU:HD22	2.38	0.54
1:C:50:ARG:HD3	1:C:54:TRP:HE3	1.73	0.54
1:A:117:ILE:HG22	1:A:118:LEU:N	2.22	0.54
1:B:63:LEU:O	1:B:67:ILE:N	2.30	0.53
1:A:75:ASP:O	1:A:127:ALA:HB1	2.08	0.53
1:C:68:THR:HG22	1:C:71:LEU:CD2	2.39	0.53
1:A:14:ARG:HG3	1:A:15:HIS:N	2.21	0.53
1:C:144:ASN:HD22	1:C:147:ALA:HB2	1.72	0.53
1:C:120:ALA:O	1:C:123:GLN:HB2	2.08	0.53
1:B:53:HIS:HE1	6:B:881:HOH:O	1.92	0.53
1:B:34:ILE:CG2	1:B:40:ALA:HB2	2.26	0.53
1:B:159:GLN:HE22	1:C:9:ARG:HH11	1.57	0.52
1:A:28:TYR:HE1	1:A:30:ALA:HB2	1.75	0.52
1:C:28:TYR:CD1	1:C:30:ALA:HB2	2.44	0.52
1:A:9:ARG:CZ	1:C:159:GLN:HE22	2.22	0.52
1:A:27:LEU:HD11	1:A:57:ALA:CB	2.39	0.52
1:B:73:PRO:HA	1:B:126:PRO:O	2.10	0.52
1:B:47:LYS:O	1:B:50:ARG:N	2.33	0.51
1:A:71:LEU:O	1:A:126:PRO:HG2	2.11	0.51
1:B:98:ASP:OD2	1:B:99:PRO:N	2.44	0.51
1:A:117:ILE:HA	6:A:825:HOH:O	2.11	0.51
1:C:121:ALA:N	1:C:124:ARG:HH11	2.07	0.51
1:B:85:MET:O	1:B:89:LEU:HD12	2.11	0.51
1:A:34:ILE:HD13	6:A:924:HOH:O	2.11	0.51
1:C:167:GLU:HG2	1:C:178:LYS:CE	2.40	0.51
1:B:9:ARG:HA	2:B:601:PO4:O4	2.11	0.51
1:A:89:LEU:O	1:A:93:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:O	1:C:94:GLY:N	2.43	0.51
1:B:62:HIS:O	1:B:65:THR:HB	2.11	0.50
1:B:44:GLN:O	1:B:48:ASP:OD2	2.30	0.50
1:A:72:ALA:O	1:A:75:ASP:HB2	2.11	0.50
1:A:9:ARG:HA	1:A:9:ARG:NE	2.11	0.50
1:B:56:THR:HG22	1:B:57:ALA:N	2.26	0.50
1:B:141:VAL:HA	1:B:151:ARG:NH2	2.27	0.50
1:C:75:ASP:HA	6:C:758:HOH:O	2.12	0.50
1:C:98:ASP:O	1:C:101:GLN:HG2	2.12	0.49
1:B:28:TYR:HE1	1:B:30:ALA:HB2	1.77	0.49
1:B:83:THR:HG22	1:B:150:PHE:HZ	1.78	0.49
1:A:101:GLN:O	1:A:101:GLN:HG3	2.11	0.49
1:C:145:ARG:HG3	1:C:149:HIS:HE1	1.73	0.49
1:C:22:ASP:O	1:C:23:ALA:O	2.31	0.49
1:B:48:ASP:OD2	1:B:48:ASP:N	2.45	0.49
1:C:102:TRP:CZ3	1:C:146:LEU:HD12	2.48	0.49
1:A:26:VAL:HG21	1:A:54:TRP:HE1	1.77	0.48
1:A:53:HIS:HD2	1:A:53:HIS:H	1.57	0.48
1:A:67:ILE:HG22	1:A:125:CYS:HB2	1.95	0.48
1:A:60:TRP:CZ3	1:A:61:ARG:NH1	2.81	0.48
1:A:67:ILE:HG12	1:A:77:ILE:HD13	1.95	0.48
1:B:34:ILE:HG12	1:B:43:ILE:CD1	2.42	0.48
1:A:80:GLU:HA	1:A:81:CYS:HA	1.64	0.48
1:B:1:MET:HE2	1:B:165:ALA:HA	1.96	0.48
1:C:32:SER:OG	4:C:606:5GP:H1'	2.14	0.48
1:C:112:ASP:O	1:C:116:GLN:HG2	2.13	0.48
1:C:106:ALA:HA	1:C:109:ARG:CZ	2.44	0.48
1:A:108:GLU:OE2	1:A:156:ARG:NE	2.45	0.47
1:C:156:ARG:NH1	1:C:156:ARG:HG2	2.11	0.47
1:B:140:ILE:CD1	1:C:151:ARG:HB3	2.44	0.47
1:B:43:ILE:HG22	1:B:47:LYS:HZ1	1.79	0.47
1:A:60:TRP:HZ3	1:A:61:ARG:NH1	2.11	0.47
1:A:160:ARG:HD2	6:A:1056:HOH:O	2.14	0.47
1:B:124:ARG:NH2	6:B:1065:HOH:O	2.31	0.47
1:A:115:ILE:O	1:A:119:ILE:HG13	2.14	0.47
1:B:138:MET:HB3	1:C:138:MET:HB2	1.95	0.47
1:A:108:GLU:HA	1:A:111:ILE:HG13	1.96	0.47
1:C:119:ILE:HD13	1:C:164:ALA:CB	2.44	0.47
1:C:102:TRP:CE3	1:C:107:MET:HE2	2.50	0.46
1:C:71:LEU:HD12	1:C:71:LEU:HA	1.68	0.46
1:A:26:VAL:HB	1:A:54:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:ND2	1:B:145:ARG:N	2.64	0.46
1:B:53:HIS:CD2	1:B:53:HIS:H	2.32	0.46
1:C:107:MET:O	1:C:111:ILE:HD12	2.15	0.46
1:C:145:ARG:CG	1:C:149:HIS:HD1	2.28	0.46
1:C:145:ARG:HG2	1:C:146:LEU:N	2.30	0.46
1:C:93:LEU:HA	1:C:93:LEU:HD12	1.69	0.46
1:A:73:PRO:HA	1:A:126:PRO:O	2.16	0.46
1:B:79:LEU:C	1:B:79:LEU:HD23	2.36	0.46
1:C:26:VAL:HB	1:C:54:TRP:CD1	2.51	0.46
1:B:80:GLU:HG2	4:B:605:5GP:H3'	1.97	0.46
1:A:65:THR:CG2	1:A:66:LEU:HG	2.25	0.46
1:C:68:THR:HG23	1:C:70:ASP:H	1.80	0.46
1:A:68:THR:H	1:A:71:LEU:HD23	1.80	0.46
1:A:102:TRP:CE3	1:A:107:MET:HE2	2.50	0.46
1:C:110:ALA:O	1:C:113:ASP:HB2	2.16	0.46
1:B:13:SER:OG	2:B:601:PO4:O2	2.33	0.45
1:A:53:HIS:N	1:A:53:HIS:CD2	2.80	0.45
1:C:29:ILE:CD1	1:C:77:ILE:HG21	2.45	0.45
1:B:179:ILE:CD1	1:C:175:ILE:HB	2.38	0.45
1:B:99:PRO:HA	1:B:102:TRP:CG	2.51	0.45
1:A:27:LEU:HD23	1:A:29:ILE:HD11	1.98	0.45
1:B:63:LEU:CD2	1:B:66:LEU:HD12	2.46	0.45
1:C:23:ALA:HA	1:C:24:PRO:HD3	1.60	0.45
1:B:61:ARG:NH1	1:B:89:LEU:HD23	2.30	0.45
1:C:10:SER:OG	1:C:12:LYS:HG2	2.16	0.45
1:B:102:TRP:CD2	1:B:107:MET:CE	3.00	0.45
1:A:27:LEU:CD2	1:A:29:ILE:HD11	2.46	0.45
1:C:167:GLU:HA	1:C:180:LYS:OXT	2.17	0.45
1:B:9:ARG:HA	1:B:9:ARG:NE	2.30	0.45
1:A:103:ASP:OD1	1:A:106:ALA:HB2	2.16	0.45
1:A:156:ARG:CG	1:B:9:ARG:NH2	2.80	0.45
1:C:79:LEU:HD23	1:C:79:LEU:C	2.38	0.45
1:B:141:VAL:CG2	1:B:151:ARG:HH22	2.25	0.45
1:C:121:ALA:O	1:C:124:ARG:HD3	2.18	0.44
1:B:39:MET:HE2	1:B:39:MET:HB2	1.87	0.44
1:B:146:LEU:HD23	1:B:146:LEU:C	2.37	0.44
1:B:61:ARG:HH11	1:B:89:LEU:HD23	1.81	0.44
1:B:56:THR:CG2	1:B:57:ALA:N	2.80	0.44
1:C:6:GLY:O	1:C:134:ASN:HA	2.18	0.44
1:A:102:TRP:CD2	1:A:107:MET:HE1	2.51	0.44
1:A:120:ALA:O	1:A:123:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:TRP:CE3	1:B:107:MET:CE	3.00	0.44
1:B:83:THR:CG2	1:B:150:PHE:HZ	2.31	0.44
1:A:156:ARG:NH1	1:B:9:ARG:CD	2.80	0.44
1:B:94:GLY:HA3	1:B:102:TRP:CE2	2.52	0.44
1:A:156:ARG:CG	1:B:9:ARG:HH21	2.30	0.44
1:A:168:VAL:HB	1:A:180:LYS:HB3	1.99	0.44
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.84	0.44
1:A:98:ASP:O	1:A:101:GLN:HG2	2.17	0.44
1:B:31:THR:O	1:B:88:ASN:ND2	2.51	0.44
1:A:41:ALA:HB3	1:A:42:ARG:NH2	2.32	0.44
1:B:79:LEU:HD23	1:B:80:GLU:N	2.33	0.44
1:B:98:ASP:CB	1:B:101:GLN:NE2	2.80	0.44
1:B:91:PHE:CD2	1:B:102:TRP:HH2	2.36	0.44
1:B:59:CYS:SG	1:B:60:TRP:N	2.90	0.43
1:B:102:TRP:CG	1:B:107:MET:HE3	2.53	0.43
1:C:167:GLU:HG2	1:C:178:LYS:HE3	1.99	0.43
1:C:98:ASP:OD2	1:C:99:PRO:N	2.51	0.43
1:A:68:THR:HG21	1:A:70:ASP:OD1	2.18	0.43
1:A:93:LEU:H	1:A:93:LEU:HD23	1.81	0.43
1:C:144:ASN:ND2	6:C:928:HOH:O	2.51	0.43
1:C:54:TRP:N	1:C:54:TRP:CD1	2.86	0.43
1:A:99:PRO:CA	1:A:102:TRP:CE2	3.01	0.43
1:C:29:ILE:O	1:C:80:GLU:N	2.36	0.43
1:A:146:LEU:O	1:A:149:HIS:N	2.52	0.43
1:B:34:ILE:CG2	1:B:40:ALA:N	2.82	0.43
1:B:85:MET:HG2	1:B:89:LEU:HD11	1.99	0.43
1:C:12:LYS:HE3	1:C:133:THR:O	2.18	0.43
1:B:90:LEU:CD2	1:B:111:ILE:HD11	2.43	0.43
1:C:24:PRO:HD2	1:C:74:ASP:O	2.19	0.43
1:C:111:ILE:O	1:C:115:ILE:HG12	2.17	0.42
1:A:102:TRP:CG	1:A:107:MET:HE1	2.54	0.42
1:B:43:ILE:C	1:B:47:LYS:HE2	2.39	0.42
1:A:9:ARG:CD	1:C:156:ARG:HD2	2.39	0.42
1:A:68:THR:HG22	1:A:70:ASP:H	1.84	0.42
1:C:83:THR:HG23	6:C:712:HOH:O	2.19	0.42
1:C:80:GLU:HA	1:C:81:CYS:HA	1.75	0.42
1:B:1:MET:C	1:B:2:ILE:HG13	2.38	0.42
1:B:140:ILE:HG13	6:B:733:HOH:O	2.19	0.42
1:A:68:THR:HB	1:A:71:LEU:CD2	2.46	0.42
1:A:108:GLU:CG	1:A:153:ILE:HG12	2.18	0.42
1:C:17:GLU:O	1:C:20:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:THR:O	1:A:65:THR:HG23	2.20	0.42
1:A:26:VAL:CG2	1:A:54:TRP:NE1	2.80	0.42
1:C:128:LYS:HE2	1:C:128:LYS:HB2	1.93	0.42
1:A:161:LEU:O	1:A:165:ALA:N	2.40	0.42
1:B:90:LEU:HD23	1:B:111:ILE:CD1	2.40	0.42
1:A:102:TRP:CD2	1:A:107:MET:CE	3.03	0.42
1:C:121:ALA:C	1:C:124:ARG:HD3	2.39	0.41
1:A:28:TYR:CE1	1:A:30:ALA:HB2	2.55	0.41
1:A:147:ALA:O	1:A:151:ARG:HB3	2.20	0.41
1:C:161:LEU:O	1:C:165:ALA:N	2.39	0.41
1:C:16:ALA:O	1:C:19:LEU:HB2	2.20	0.41
1:B:9:ARG:NE	2:B:601:PO4:O4	2.45	0.41
1:B:168:VAL:HG23	1:B:180:LYS:HD2	2.02	0.41
1:C:140:ILE:HD12	1:C:140:ILE:HA	1.71	0.41
6:A:1095:HOH:O	1:B:14:ARG:CB	2.68	0.41
1:A:111:ILE:O	1:A:115:ILE:HG12	2.20	0.41
1:B:98:ASP:H	1:B:101:GLN:CD	2.23	0.41
1:B:145:ARG:HA	1:B:148:ARG:NH2	2.35	0.41
1:C:50:ARG:NH2	4:C:606:5GP:N7	2.67	0.41
1:A:102:TRP:CE3	1:A:107:MET:CE	3.03	0.41
1:A:33:GLN:NE2	6:A:877:HOH:O	2.53	0.41
1:B:146:LEU:O	1:B:150:PHE:N	2.49	0.41
1:A:1:MET:HG3	1:A:165:ALA:HA	2.03	0.41
1:A:156:ARG:HH11	1:B:9:ARG:HD2	1.83	0.40
1:B:44:GLN:HA	6:B:812:HOH:O	2.21	0.40
1:B:99:PRO:HA	1:B:102:TRP:CE2	2.55	0.40
1:A:169:TRP:CZ3	1:A:178:LYS:HB2	2.56	0.40
1:A:72:ALA:HA	1:A:73:PRO:HD3	1.92	0.40
1:C:29:ILE:O	1:C:79:LEU:HA	2.22	0.40
1:A:180:LYS:HB2	1:B:175:ILE:HD13	2.04	0.40
1:B:125:CYS:HA	1:B:126:PRO:HD3	1.84	0.40
1:C:82:ILE:O	1:C:86:VAL:HG23	2.21	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	164/180 (91%)	152 (93%)	11 (7%)	1 (1%)	30	29
1	B	178/180 (99%)	169 (95%)	9 (5%)	0	100	100
1	C	157/180 (87%)	149 (95%)	5 (3%)	3 (2%)	10	6
All	All	499/540 (92%)	470 (94%)	25 (5%)	4 (1%)	24	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	PRO
1	C	22	ASP
1	C	23	ALA
1	C	24	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/143 (91%)	110 (85%)	20 (15%)	3	2
1	B	129/143 (90%)	107 (83%)	22 (17%)	2	2
1	C	120/143 (84%)	95 (79%)	25 (21%)	1	1
All	All	379/429 (88%)	312 (82%)	67 (18%)	2	1

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	ARG
1	A	14	ARG
1	A	27	LEU
1	A	42	ARG

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Mol	Chain	Res	Type
1	A	51	PRO
1	A	59	CYS
1	A	61	ARG
1	A	65	THR
1	A	71	LEU
1	A	74	ASP
1	A	78	LEU
1	A	83	THR
1	A	93	LEU
1	A	123	GLN
1	A	124	ARG
1	A	140	ILE
1	A	151	ARG
1	A	172	VAL
1	A	179	ILE
1	B	1	MET
1	B	9	ARG
1	B	13	SER
1	B	19	LEU
1	B	32	SER
1	B	39	MET
1	B	42	ARG
1	B	48	ASP
1	B	61	ARG
1	B	68	THR
1	B	78	LEU
1	B	80	GLU
1	B	83	THR
1	B	101	GLN
1	B	112	ASP
1	B	116	GLN
1	B	123	GLN
1	B	124	ARG
1	B	138	MET
1	B	140	ILE
1	B	151	ARG
1	B	160	ARG
1	C	1	MET
1	C	9	ARG
1	C	22	ASP
1	C	32	SER
1	C	47	LYS

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Mol	Chain	Res	Type
1	C	50	ARG
1	C	63	LEU
1	C	70	ASP
1	C	71	LEU
1	C	78	LEU
1	C	80	GLU
1	C	83	THR
1	C	85	MET
1	C	93	LEU
1	C	107	MET
1	C	123	GLN
1	C	124	ARG
1	C	128	LYS
1	C	138	MET
1	C	140	ILE
1	C	145	ARG
1	C	148	ARG
1	C	156	ARG
1	C	160	ARG
1	C	172	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	159	GLN
1	B	53	HIS
1	B	97	ASN
1	B	101	GLN
1	B	144	ASN
1	B	159	GLN
1	C	53	HIS
1	C	134	ASN
1	C	144	ASN
1	C	159	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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
2	PO4	A	600	-	4,4,4	1.59	1 (25%)	6,6,6	0.27	0
4	5GP	A	604	-	21,26,26	1.37	3 (14%)	25,40,40	2.90	7 (28%)
2	PO4	B	601	-	4,4,4	1.52	1 (25%)	6,6,6	0.28	0
4	5GP	B	605	-	21,26,26	1.46	3 (14%)	25,40,40	4.54	8 (32%)
4	5GP	C	606	-	17,22,26	1.11	2 (11%)	19,33,40	5.75	5 (26%)
5	POP	C	608	3	8,8,8	0.89	0	13,13,13	3.56	4 (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	PO4	A	600	-	-	0/0/0/0	0/0/0/0
4	5GP	A	604	-	-	0/6/26/26	0/3/3/3
2	PO4	B	601	-	-	0/0/0/0	0/0/0/0
4	5GP	B	605	-	-	0/6/26/26	0/3/3/3
4	5GP	C	606	-	-	0/2/22/26	0/3/3/3
5	POP	C	608	3	-	0/6/6/6	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	5GP	P-O5'	-3.44	1.48	1.60
4	A	604	5GP	P-O5'	-2.98	1.50	1.60
4	C	606	5GP	C8-N7	-2.24	1.30	1.34
4	A	604	5GP	C8-N7	-2.13	1.30	1.34
4	B	605	5GP	C8-N7	-2.06	1.30	1.34
2	B	601	PO4	P-O4	2.19	1.61	1.53
2	A	600	PO4	P-O3	2.22	1.61	1.53
4	C	606	5GP	C6-N1	3.47	1.39	1.33
4	A	604	5GP	C6-N1	3.72	1.40	1.33
4	B	605	5GP	C6-N1	3.99	1.40	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	5GP	C1'-N9-C4	-21.52	94.49	126.94
4	B	605	5GP	O3P-P-O1P	-16.12	58.67	110.58
4	C	606	5GP	C5-C6-N1	-9.05	111.22	123.59
5	C	608	POP	O5-P2-O6	-8.91	74.59	110.61
4	B	605	5GP	C5-C6-N1	-8.81	111.54	123.59
4	A	604	5GP	C5-C6-N1	-8.47	112.01	123.59
4	A	604	5GP	C1'-N9-C4	-5.38	118.83	126.94
5	C	608	POP	P2-O-P1	-4.43	120.29	132.73
4	C	606	5GP	C2'-C1'-N9	-4.40	107.58	114.29
4	A	604	5GP	O3P-P-O2P	-4.27	91.11	107.38
4	A	604	5GP	C4'-O4'-C1'	-3.58	105.78	109.72
4	B	605	5GP	C2'-C1'-N9	-3.55	108.86	114.29
4	B	605	5GP	C4'-O4'-C1'	-2.60	106.86	109.72
4	A	604	5GP	N3-C2-N1	-2.35	123.87	127.44
4	C	606	5GP	N3-C2-N1	-2.09	124.26	127.44
4	B	605	5GP	C1'-N9-C4	-2.08	123.81	126.94
4	B	605	5GP	O4'-C4'-C3'	2.59	110.36	105.15
5	C	608	POP	O2-P1-O1	3.13	122.35	110.85
4	A	604	5GP	O3P-P-O1P	4.72	125.78	110.58
4	B	605	5GP	C6-N1-C2	5.73	123.90	115.94
4	A	604	5GP	C6-N1-C2	6.31	124.70	115.94
4	C	606	5GP	C6-N1-C2	6.75	125.30	115.94
5	C	608	POP	O6-P2-O4	6.79	147.35	114.72
4	B	605	5GP	O3P-P-O2P	10.00	145.45	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PO4	2	0
4	A	604	5GP	4	0
2	B	601	PO4	3	0
4	B	605	5GP	1	0
4	C	606	5GP	2	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 ⓘ

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	170/180 (94%)	0.30	10 (5%)	26 25	16, 36, 66, 97	0
1	B	180/180 (100%)	0.35	17 (9%)	11 10	13, 36, 78, 98	0
1	C	165/180 (91%)	0.28	13 (7%)	15 15	14, 38, 80, 99	0
All	All	515/540 (95%)	0.31	40 (7%)	16 15	13, 37, 78, 99	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	LEU	6.6
1	A	101	GLN	6.2
1	A	99	PRO	6.2
1	B	39	MET	6.0
1	B	98	ASP	5.9
1	C	35	LEU	5.6
1	B	99	PRO	5.5
1	C	99	PRO	5.5
1	B	41	ALA	4.4
1	C	102	TRP	4.3
1	C	144	ASN	4.0
1	B	97	ASN	3.8
1	B	101	GLN	3.6
1	B	100	GLU	3.6
1	C	21	GLY	3.6
1	C	48	ASP	3.5
1	C	101	GLN	3.5
1	B	106	ALA	3.3
1	C	45	HIS	3.2
1	A	102	TRP	3.2
1	B	36	ASP	3.1
1	A	72	ALA	3.1
1	A	98	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	PRO	3.1
1	C	61	ARG	3.0
1	B	37	ASP	3.0
1	B	43	ILE	3.0
1	C	46	HIS	2.9
1	B	38	GLU	2.8
1	A	45	HIS	2.7
1	A	52	ALA	2.7
1	A	42	ARG	2.7
1	A	106	ALA	2.6
1	B	102	TRP	2.4
1	C	72	ALA	2.4
1	B	40	ALA	2.3
1	B	95	GLY	2.3
1	B	34	ILE	2.2
1	C	98	ASP	2.1
1	C	145	ARG	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(Å ²)	Q<0.9
5	POP	C	608	9/9	0.93	0.23	4.19	6,13,51,71	9
2	PO4	B	601	5/5	0.95	0.16	0.93	29,31,63,94	0
2	PO4	A	600	5/5	0.95	0.14	0.79	43,44,57,98	0
4	5GP	C	606	20/24	0.91	0.16	-0.01	19,51,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	5GP	A	604	24/24	0.92	0.12	-0.47	23,56,98,100	0
4	5GP	B	605	24/24	0.93	0.10	-0.81	17,30,97,100	0
3	MG	C	607	1/1	0.97	0.41	-	41,41,41,41	1

6.5 Other polymers [i](#)

There are no such residues in this entry.