Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1U9Z
Title	:	Crystal Structure of Phosphoribosyl Diphosphate Synthase Complexed with AMP and Ribose 5-Phosphate
Authors	:	Kadziola, A.; Johansson, E.; Jepsen, C.H.; McGuire, J.; Larsen, S.; Hove-Jensen, B.
Deposited on	:	2004-08-11
Resolution	:	2.80 Å(reported)

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 (i)

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		18
Ramachandran outliers		1.1%
Sidechain outliers		1.7%
RSRZ outliers		3.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
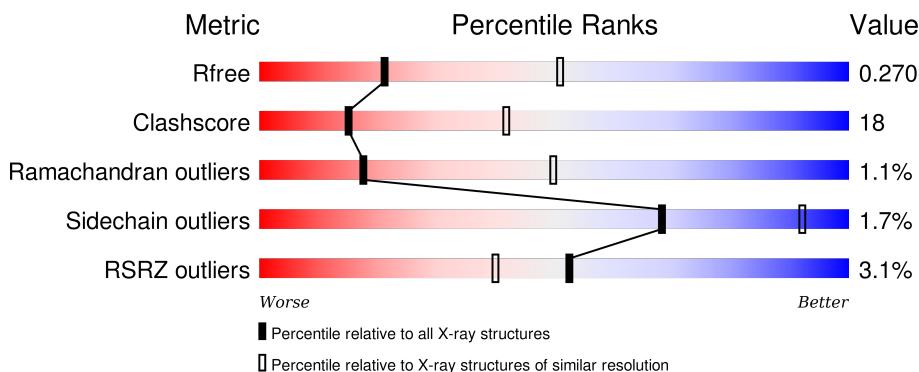
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

| Mol	Chain	Length	Quality of chain
1	A	284	3% 62% 33% ·· ·
1	B	284	3% 62% 33% ··
1	C	284	3% 62% 33% ·· ·
1	D	284	3% 62% 33% ··

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8878 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 Ribose-phosphate pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2131	1370	346	411	4			
1	B	274	Total	C	N	O	S	0	0	0
			2131	1370	346	411	4			
1	C	274	Total	C	N	O	S	0	0	0
			2131	1370	346	411	4			
1	D	274	Total	C	N	O	S	0	0	0
			2131	1370	346	411	4			

- Molecule 2 is OPEN FORM OF RIBOFURANOSE-5'-PHOSPHATE (three-letter code: R5P) (formula: $C_5H_{11}O_8P$).
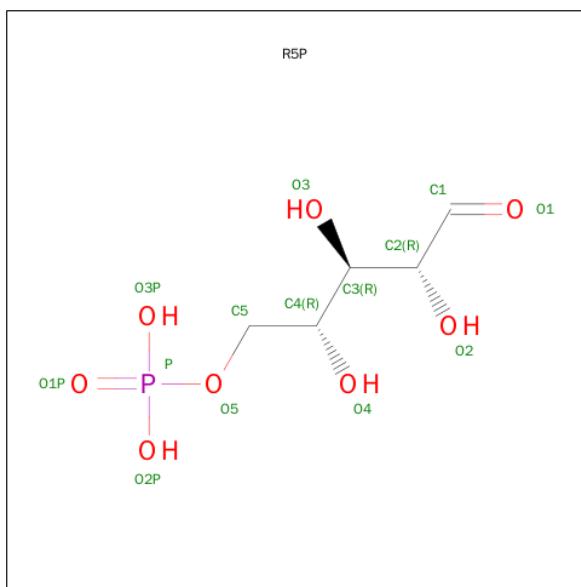
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			14	5	8	1		
2	B	1	Total	C	O	P	0	0
			14	5	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			14	5	8	1		
2	D	1	Total	C	O	P	0	0
			14	5	8	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
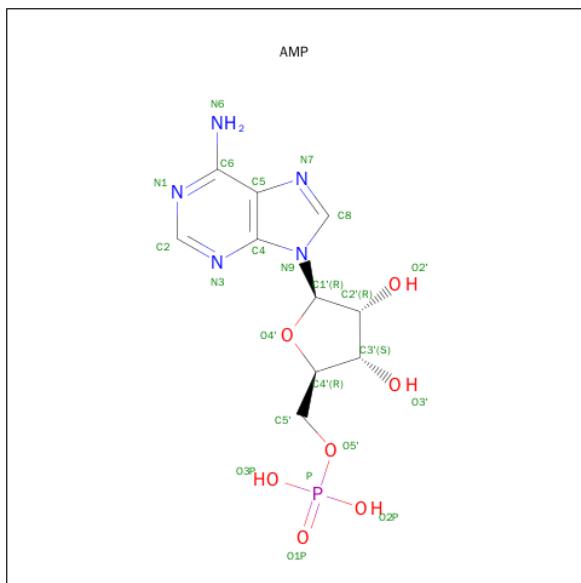
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	52	Total	O	0	0
			52	52		
4	C	52	Total	O	0	0
			52	52		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	52	Total O 52 52		0	0

3 Residue-property plots (i)

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

- Molecule 1: Ribose-phosphate pyrophosphokinase
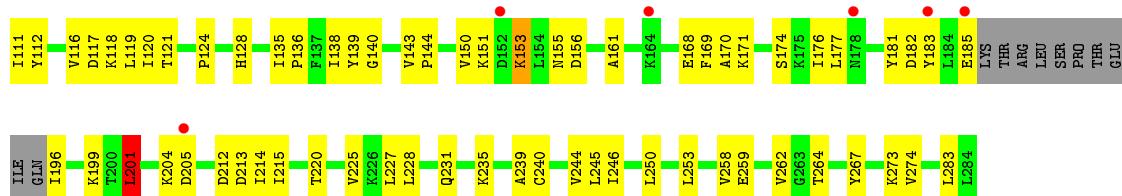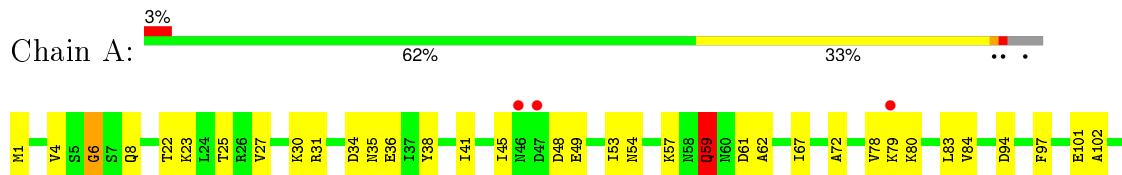
- Molecule 1: Ribose-phosphate pyrophosphokinase

- Molecule 1: Ribose-phosphate pyrophosphokinase

• Molecule 1: Ribose-phosphate pyrophosphokinase

Chain D:
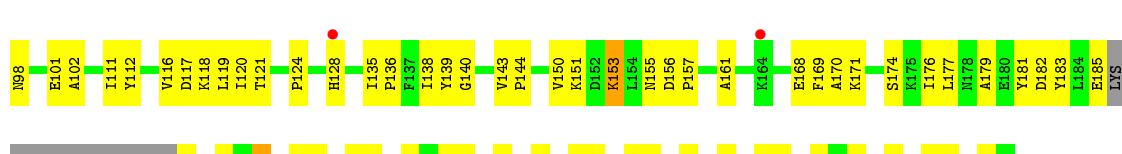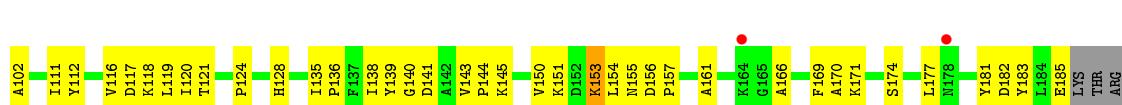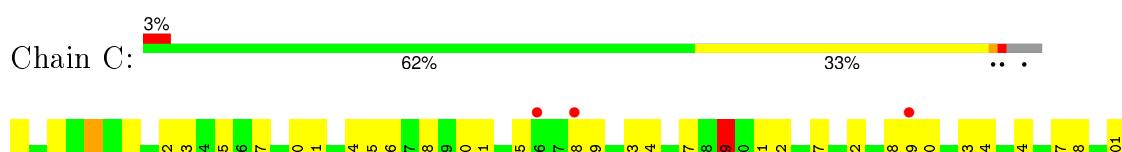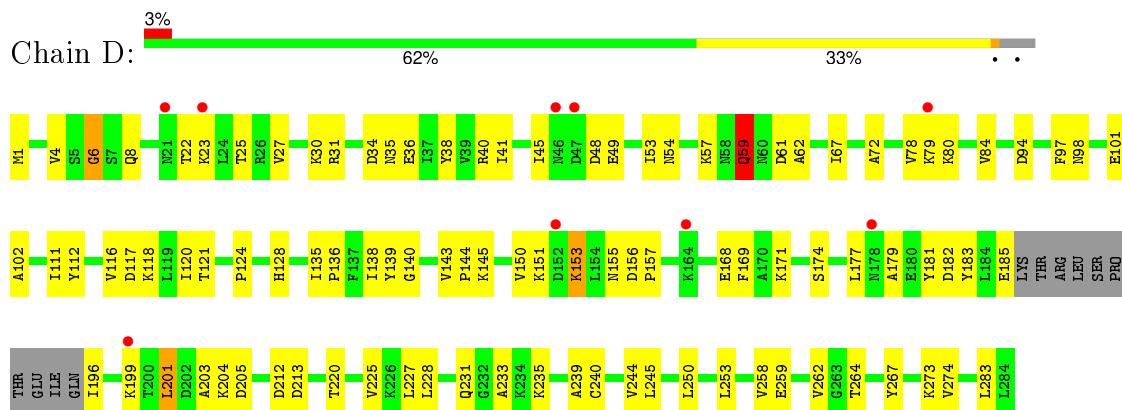
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.26Å 138.25Å 138.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 24.82 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.00-2.80) 96.4 (24.82-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.80Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.238 , 0.272 0.235 , 0.270	Depositor DCC
R_{free} test set	1676 reflections (5.06%)	DCC
Wilson B-factor (Å²)	53.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.35 , 41.1	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 33097 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8878	wwPDB-VP
Average B, all atoms (Å²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.2492e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AMP, R5P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.42	0/2161	0.63	1/2930 (0.0%)
1	B	0.43	0/2161	0.63	1/2930 (0.0%)
1	C	0.43	0/2161	0.62	1/2930 (0.0%)
1	D	0.42	0/2161	0.63	1/2930 (0.0%)
All	All	0.43	0/8644	0.62	4/11720 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	6	GLY	N-CA-C	-5.20	100.10	113.10
1	A	6	GLY	N-CA-C	-5.18	100.14	113.10
1	B	6	GLY	N-CA-C	-5.16	100.21	113.10
1	C	6	GLY	N-CA-C	-5.06	100.44	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2131	0	2210	83	0
1	B	2131	0	2210	78	0
1	C	2131	0	2210	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2131	0	2210	82	0
2	A	14	0	9	0	0
2	B	14	0	9	0	0
2	C	14	0	9	0	0
2	D	14	0	9	0	0
3	B	46	0	24	4	0
3	C	23	0	12	2	0
3	D	23	0	12	2	0
4	A	50	0	0	1	0
4	B	52	0	0	0	0
4	C	52	0	0	0	0
4	D	52	0	0	1	0
All	All	8878	0	8924	308	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 18.

All (308) 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:227:LEU:HD21	1:A:231:GLN:NE2	1.87	0.90
1:C:227:LEU:HD21	1:C:231:GLN:NE2	1.87	0.89
1:D:262:VAL:HG23	1:D:273:LYS:HD2	1.55	0.88
1:D:227:LEU:HD21	1:D:231:GLN:NE2	1.88	0.88
1:B:227:LEU:HD21	1:B:231:GLN:NE2	1.89	0.86
1:A:262:VAL:HG23	1:A:273:LYS:HD2	1.56	0.86
1:B:262:VAL:HG23	1:B:273:LYS:HD2	1.58	0.84
1:C:262:VAL:HG23	1:C:273:LYS:HD2	1.59	0.84
1:B:235:LYS:HE3	1:B:259:GLU:HG2	1.73	0.70
1:C:227:LEU:HD23	1:C:228:LEU:N	2.07	0.69
1:A:235:LYS:HE3	1:A:259:GLU:HG2	1.74	0.69
1:B:227:LEU:HD23	1:B:228:LEU:N	2.08	0.69
1:D:235:LYS:HE3	1:D:259:GLU:HG2	1.74	0.68
1:D:4:VAL:HG13	1:D:27:VAL:HG21	1.75	0.68
1:C:235:LYS:HE3	1:C:259:GLU:HG2	1.77	0.67
1:D:227:LEU:HD23	1:D:228:LEU:N	2.09	0.67
1:A:227:LEU:HD23	1:A:228:LEU:N	2.10	0.67
1:A:59:GLN:HG2	1:B:36:GLU:HG2	1.76	0.65
1:C:140:GLY:HA3	1:C:283:LEU:HD11	1.78	0.65
1:A:140:GLY:HA3	1:A:283:LEU:HD11	1.79	0.65
1:C:4:VAL:HG13	1:C:27:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ALA:HB2	1:D:72:ALA:HB2	1.79	0.65
1:C:72:ALA:HB2	1:D:102:ALA:HB2	1.78	0.64
1:B:4:VAL:HG13	1:B:27:VAL:HG21	1.78	0.64
1:A:183:TYR:CZ	1:A:199:LYS:HG3	2.33	0.63
1:D:57:LYS:HG3	1:D:267:TYR:CZ	2.33	0.63
1:D:140:GLY:HA3	1:D:283:LEU:HD11	1.81	0.63
1:D:143:VAL:HB	1:D:144:PRO:HD3	1.80	0.63
1:A:4:VAL:HG13	1:A:27:VAL:HG21	1.79	0.63
1:A:59:GLN:NE2	1:A:59:GLN:H	1.97	0.62
1:B:143:VAL:HB	1:B:144:PRO:HD3	1.82	0.62
1:A:57:LYS:HG3	1:A:267:TYR:CZ	2.35	0.62
1:A:227:LEU:C	1:A:227:LEU:HD23	2.20	0.61
1:C:227:LEU:HD23	1:C:227:LEU:C	2.20	0.61
1:B:140:GLY:HA3	1:B:283:LEU:HD11	1.80	0.61
1:C:57:LYS:HG3	1:C:267:TYR:CZ	2.35	0.61
1:D:227:LEU:C	1:D:227:LEU:HD23	2.22	0.61
1:B:183:TYR:CZ	1:B:199:LYS:HG3	2.36	0.60
1:A:111:ILE:CD1	1:B:67:ILE:HD13	2.30	0.60
1:A:143:VAL:HB	1:A:144:PRO:HD3	1.81	0.60
1:A:253:LEU:O	1:A:258:VAL:HG22	2.01	0.60
1:A:101:GLU:HG2	1:B:40:ARG:HD2	1.83	0.60
1:B:227:LEU:HD23	1:B:227:LEU:C	2.22	0.60
1:A:36:GLU:HG2	1:B:59:GLN:HG2	1.82	0.60
1:C:36:GLU:HG2	1:D:59:GLN:HG2	1.84	0.60
1:C:143:VAL:HB	1:C:144:PRO:HD3	1.83	0.60
1:D:183:TYR:CZ	1:D:199:LYS:HG3	2.36	0.59
1:C:59:GLN:H	1:C:59:GLN:NE2	2.00	0.59
1:A:102:ALA:HB2	1:B:72:ALA:HB2	1.82	0.59
1:B:57:LYS:HG3	1:B:267:TYR:CZ	2.38	0.59
1:C:59:GLN:HG2	1:D:36:GLU:HG2	1.85	0.59
1:A:94:ASP:HB3	1:A:128:HIS:HE1	1.67	0.59
1:A:48:ASP:HB2	1:A:79:LYS:CD	2.33	0.59
1:A:72:ALA:HB2	1:B:102:ALA:HB2	1.85	0.59
1:D:59:GLN:H	1:D:59:GLN:NE2	2.01	0.58
1:C:183:TYR:CZ	1:C:199:LYS:HG3	2.38	0.58
1:B:150:VAL:HA	1:B:153:LYS:HD3	1.85	0.58
1:B:59:GLN:NE2	1:B:59:GLN:H	2.01	0.58
1:C:94:ASP:HB3	1:C:128:HIS:HE1	1.68	0.58
1:D:48:ASP:HB2	1:D:79:LYS:CD	2.34	0.58
1:B:48:ASP:HB2	1:B:79:LYS:CD	2.34	0.58
1:D:253:LEU:O	1:D:258:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:SER:HB2	1:C:181:TYR:HB3	1.85	0.58
1:D:94:ASP:HB3	1:D:128:HIS:HE1	1.69	0.57
1:A:171:LYS:O	1:A:174:SER:HB3	2.03	0.57
1:B:48:ASP:HB2	1:B:79:LYS:HD2	1.86	0.57
1:B:174:SER:HB2	1:B:181:TYR:HB3	1.85	0.57
1:B:94:ASP:HB3	1:B:128:HIS:HE1	1.70	0.57
1:C:185:GLU:O	1:C:196:ILE:HA	2.05	0.57
1:C:1:MET:HG2	1:C:49:GLU:OE1	2.05	0.57
1:B:253:LEU:O	1:B:258:VAL:HG22	2.05	0.56
1:A:174:SER:HB2	1:A:181:TYR:HB3	1.86	0.56
1:C:48:ASP:HB2	1:C:79:LYS:CD	2.35	0.56
1:D:171:LYS:O	1:D:174:SER:HB3	2.06	0.56
1:A:121:THR:HG23	1:A:124:PRO:HG3	1.87	0.56
1:C:67:ILE:HD13	1:D:111:ILE:CD1	2.36	0.56
1:A:150:VAL:HA	1:A:153:LYS:HD3	1.88	0.56
1:C:121:THR:HG23	1:C:124:PRO:HG3	1.88	0.56
1:D:48:ASP:HB2	1:D:79:LYS:HD2	1.88	0.56
1:B:171:LYS:O	1:B:174:SER:HB3	2.06	0.56
1:A:185:GLU:O	1:A:196:ILE:HA	2.06	0.55
1:C:150:VAL:HA	1:C:153:LYS:HD3	1.88	0.55
1:B:140:GLY:CA	1:B:283:LEU:HD11	2.37	0.55
1:C:171:LYS:O	1:C:174:SER:HB3	2.05	0.55
1:D:117:ASP:O	1:D:136:PRO:HD2	2.07	0.55
1:A:48:ASP:HB2	1:A:79:LYS:HD2	1.88	0.55
1:D:150:VAL:HA	1:D:153:LYS:HD3	1.89	0.55
1:C:48:ASP:HB2	1:C:79:LYS:HD2	1.89	0.55
1:D:174:SER:HB2	1:D:181:TYR:HB3	1.88	0.55
1:B:80:LYS:HA	1:B:117:ASP:OD2	2.07	0.54
1:D:80:LYS:HA	1:D:117:ASP:OD2	2.07	0.54
1:A:140:GLY:CA	1:A:283:LEU:HD11	2.38	0.54
1:D:121:THR:HG23	1:D:124:PRO:HG3	1.90	0.54
1:B:121:THR:HG23	1:B:124:PRO:HG3	1.90	0.54
1:C:140:GLY:CA	1:C:283:LEU:HD11	2.38	0.54
1:B:135:ILE:HB	1:B:136:PRO:CD	2.37	0.54
1:A:80:LYS:HA	1:A:117:ASP:OD2	2.07	0.54
1:C:80:LYS:HA	1:C:117:ASP:OD2	2.07	0.54
1:B:185:GLU:O	1:B:196:ILE:HA	2.08	0.54
1:C:111:ILE:CD1	1:D:67:ILE:HD13	2.38	0.54
1:A:117:ASP:O	1:A:136:PRO:HD2	2.08	0.53
1:B:112:TYR:O	1:B:116:VAL:HG22	2.08	0.53
1:C:253:LEU:O	1:C:258:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:HG22	1:C:23:LYS:N	2.23	0.53
1:A:112:TYR:O	1:A:116:VAL:HG22	2.08	0.53
1:D:22:THR:HG22	1:D:23:LYS:N	2.23	0.53
1:D:181:TYR:O	1:D:182:ASP:HB2	2.09	0.53
1:B:117:ASP:O	1:B:136:PRO:HD2	2.09	0.53
1:D:140:GLY:CA	1:D:283:LEU:HD11	2.40	0.52
1:D:112:TYR:O	1:D:116:VAL:HG22	2.09	0.52
1:B:22:THR:HG22	1:B:23:LYS:N	2.25	0.52
1:D:264:THR:HA	1:D:274:VAL:O	2.10	0.52
1:D:135:ILE:HB	1:D:136:PRO:CD	2.39	0.52
1:A:1:MET:HG2	1:A:49:GLU:OE1	2.10	0.52
1:A:22:THR:HG22	1:A:23:LYS:N	2.24	0.52
1:C:112:TYR:O	1:C:116:VAL:HG22	2.10	0.52
1:C:40:ARG:HD2	1:D:101:GLU:HG2	1.93	0.51
1:B:1:MET:HG2	1:B:49:GLU:OE1	2.10	0.51
1:B:181:TYR:O	1:B:182:ASP:HB2	2.11	0.51
1:D:185:GLU:O	1:D:196:ILE:HA	2.11	0.51
1:B:30:LYS:HG2	1:B:38:TYR:CD2	2.45	0.51
1:C:169:PHE:CE1	1:C:213:ASP:HB3	2.46	0.51
1:B:135:ILE:HB	1:B:136:PRO:HD2	1.93	0.50
1:C:264:THR:HA	1:C:274:VAL:O	2.11	0.50
1:A:183:TYR:OH	1:A:199:LYS:HG3	2.11	0.50
1:B:264:THR:HA	1:B:274:VAL:O	2.11	0.50
1:A:101:GLU:CG	1:B:40:ARG:HD2	2.41	0.50
1:C:135:ILE:HB	1:C:136:PRO:CD	2.41	0.50
1:B:225:VAL:HG21	1:B:258:VAL:CG1	2.42	0.50
1:A:169:PHE:CE1	1:A:213:ASP:HB3	2.47	0.50
1:B:1:MET:HA	1:B:49:GLU:O	2.12	0.50
1:A:135:ILE:HB	1:A:136:PRO:CD	2.41	0.50
1:A:225:VAL:HG21	1:A:258:VAL:CG1	2.42	0.50
1:C:41:ILE:HG21	1:C:45:ILE:HD11	1.93	0.49
1:C:121:THR:CG2	1:C:124:PRO:HG3	2.41	0.49
1:D:169:PHE:CE1	1:D:213:ASP:HB3	2.48	0.49
1:A:181:TYR:O	1:A:182:ASP:HB2	2.11	0.49
1:C:101:GLU:HG2	1:D:40:ARG:HD2	1.95	0.49
1:C:117:ASP:O	1:C:136:PRO:HD2	2.11	0.49
1:A:264:THR:HA	1:A:274:VAL:O	2.12	0.49
1:B:183:TYR:OH	1:B:199:LYS:HG3	2.11	0.49
1:C:225:VAL:HG21	1:C:258:VAL:CG1	2.42	0.49
1:C:30:LYS:HG2	1:C:38:TYR:CD2	2.48	0.48
1:D:1:MET:HA	1:D:49:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:NE2	1:A:59:GLN:N	2.61	0.48
1:D:227:LEU:CD2	1:D:231:GLN:NE2	2.71	0.48
1:A:25:THR:O	1:A:27:VAL:HG23	2.13	0.48
1:A:212:ASP:O	1:A:240:CYS:HA	2.14	0.48
1:C:181:TYR:O	1:C:182:ASP:HB2	2.13	0.48
1:D:135:ILE:HB	1:D:136:PRO:HD2	1.96	0.48
1:A:121:THR:CG2	1:A:124:PRO:HG3	2.43	0.48
1:D:225:VAL:HG21	1:D:258:VAL:CG1	2.44	0.47
1:A:30:LYS:HG2	1:A:38:TYR:CD2	2.48	0.47
1:B:169:PHE:CE1	1:B:213:ASP:HB3	2.50	0.47
1:B:34:ASP:O	1:B:35:ASN:CB	2.62	0.47
1:C:212:ASP:O	1:C:240:CYS:HA	2.14	0.47
1:D:121:THR:CG2	1:D:124:PRO:HG3	2.44	0.47
1:C:25:THR:O	1:C:27:VAL:HG23	2.15	0.47
1:B:8:GLN:NE2	1:B:62:ALA:HB2	2.29	0.47
1:B:204:LYS:HE3	1:B:205:ASP:OD1	2.15	0.47
1:A:244:VAL:HA	1:A:267:TYR:CE2	2.50	0.47
1:C:1:MET:HA	1:C:49:GLU:O	2.14	0.47
1:B:30:LYS:HG2	1:B:38:TYR:HD2	1.80	0.47
1:B:41:ILE:HG21	1:B:45:ILE:HD11	1.97	0.47
1:D:34:ASP:O	1:D:35:ASN:CB	2.63	0.47
3:C:8302:AMP:H3'	1:D:97:PHE:CD2	2.49	0.47
1:A:227:LEU:CD2	1:A:231:GLN:NE2	2.70	0.47
1:D:1:MET:HG2	1:D:49:GLU:OE1	2.14	0.47
1:C:34:ASP:O	1:C:35:ASN:CB	2.62	0.47
1:C:59:GLN:N	1:C:59:GLN:NE2	2.64	0.46
1:D:244:VAL:HA	1:D:267:TYR:CE2	2.51	0.46
1:C:121:THR:O	1:C:139:TYR:HA	2.16	0.46
1:D:53:ILE:HG12	1:D:84:VAL:HB	1.98	0.46
1:D:30:LYS:HG2	1:D:38:TYR:CD2	2.50	0.46
1:A:48:ASP:HB2	1:A:79:LYS:HD3	1.97	0.46
1:B:121:THR:CG2	1:B:124:PRO:HG3	2.45	0.46
1:A:8:GLN:NE2	1:A:62:ALA:HB2	2.30	0.46
1:B:53:ILE:HG12	1:B:84:VAL:HB	1.98	0.46
1:D:212:ASP:O	1:D:240:CYS:HA	2.16	0.46
1:C:53:ILE:HG12	1:C:84:VAL:HB	1.98	0.46
1:C:97:PHE:CD2	3:D:7302:AMP:H3'	2.50	0.46
1:B:97:PHE:CD2	3:B:6302:AMP:H3'	2.51	0.46
1:B:227:LEU:CD2	1:B:231:GLN:NE2	2.72	0.46
1:D:183:TYR:OH	1:D:199:LYS:HG3	2.15	0.46
1:B:25:THR:O	1:B:27:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:HG3	1:A:136:PRO:HB2	1.98	0.46
1:B:212:ASP:O	1:B:240:CYS:HA	2.16	0.46
3:C:8302:AMP:H3'	1:D:97:PHE:CE2	2.51	0.45
1:D:25:THR:O	1:D:27:VAL:HG23	2.16	0.45
1:B:244:VAL:HA	1:B:267:TYR:CE2	2.51	0.45
1:A:135:ILE:HB	1:A:136:PRO:HD2	1.97	0.45
1:C:244:VAL:HA	1:C:267:TYR:CE2	2.52	0.45
1:B:121:THR:O	1:B:139:TYR:HA	2.17	0.45
1:A:53:ILE:HG12	1:A:84:VAL:HB	1.99	0.45
1:C:151:LYS:HE3	1:C:151:LYS:HB2	1.71	0.45
1:C:227:LEU:CD2	1:C:231:GLN:NE2	2.71	0.45
1:C:97:PHE:CE2	3:D:7302:AMP:H3'	2.52	0.45
1:D:245:LEU:HD13	1:D:250:LEU:HG	1.98	0.45
1:D:48:ASP:HB2	1:D:79:LYS:HD3	1.99	0.45
1:A:1:MET:HA	1:A:49:GLU:O	2.16	0.45
1:A:41:ILE:HG21	1:A:45:ILE:HD11	1.98	0.45
1:D:8:GLN:NE2	1:D:62:ALA:HB2	2.31	0.45
1:A:121:THR:O	1:A:139:TYR:HA	2.18	0.44
1:A:34:ASP:O	1:A:35:ASN:CB	2.64	0.44
1:C:135:ILE:HB	1:C:136:PRO:HD2	1.98	0.44
1:B:245:LEU:HD13	1:B:250:LEU:HG	1.98	0.44
1:D:6:GLY:HA3	1:D:54:ASN:HB2	1.99	0.44
1:D:120:ILE:HG12	1:D:138:ILE:HB	1.99	0.44
1:A:6:GLY:HA3	1:A:54:ASN:HB2	2.00	0.44
1:A:59:GLN:CD	1:A:59:GLN:H	2.20	0.44
1:D:41:ILE:HG21	1:D:45:ILE:HD11	2.00	0.44
1:C:235:LYS:HG3	1:C:259:GLU:HG2	2.00	0.44
1:A:97:PHE:CD2	3:B:5302:AMP:H3'	2.52	0.44
1:B:120:ILE:HG12	1:B:138:ILE:HB	1.98	0.44
1:B:59:GLN:NE2	1:B:59:GLN:N	2.64	0.44
1:B:118:LYS:HG3	1:B:136:PRO:HB2	2.00	0.44
1:B:6:GLY:HA3	1:B:54:ASN:HB2	1.99	0.44
1:D:155:ASN:O	1:D:156:ASP:C	2.56	0.44
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.72	0.44
1:C:6:GLY:HA3	1:C:54:ASN:HB2	2.00	0.43
1:C:183:TYR:OH	1:C:199:LYS:HG3	2.18	0.43
1:A:120:ILE:HG12	1:A:138:ILE:HB	2.00	0.43
1:C:203:ALA:HB1	1:C:233:ALA:HB2	2.00	0.43
1:A:196:ILE:O	1:A:227:LEU:HD11	2.18	0.43
1:C:8:GLN:NE2	1:C:62:ALA:HB2	2.33	0.43
1:C:120:ILE:HG12	1:C:138:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:THR:CG2	1:D:23:LYS:N	2.82	0.43
1:B:97:PHE:CE2	3:B:6302:AMP:H3'	2.54	0.43
1:A:67:ILE:HD13	1:B:111:ILE:CD1	2.49	0.43
1:A:83:LEU:O	1:A:119:LEU:HD12	2.19	0.43
1:C:118:LYS:HG3	1:C:136:PRO:HB2	2.01	0.43
1:D:239:ALA:HA	1:D:262:VAL:O	2.18	0.42
1:B:48:ASP:OD1	1:B:79:LYS:HD3	2.19	0.42
1:D:121:THR:O	1:D:139:TYR:HA	2.19	0.42
1:A:262:VAL:O	1:A:262:VAL:HG13	2.20	0.42
1:D:59:GLN:N	1:D:59:GLN:NE2	2.65	0.42
1:D:118:LYS:HG3	1:D:136:PRO:HB2	2.01	0.42
1:B:49:GLU:HG3	1:B:80:LYS:HB3	2.00	0.42
1:A:155:ASN:O	1:A:156:ASP:C	2.57	0.42
1:D:151:LYS:HE3	1:D:151:LYS:HB2	1.73	0.42
1:C:48:ASP:OD1	1:C:79:LYS:HD3	2.20	0.42
1:D:204:LYS:HE3	1:D:205:ASP:OD1	2.19	0.42
1:D:59:GLN:H	1:D:59:GLN:CD	2.22	0.42
1:C:59:GLN:H	1:C:59:GLN:CD	2.21	0.42
1:D:30:LYS:HG2	1:D:38:TYR:HD2	1.85	0.42
1:A:245:LEU:HD13	1:A:250:LEU:HG	2.01	0.42
1:C:48:ASP:HB2	1:C:79:LYS:HD3	2.00	0.42
1:D:22:THR:HG22	1:D:23:LYS:O	2.20	0.42
1:C:154:LEU:HD22	1:C:207:ASP:HB3	2.01	0.42
1:C:155:ASN:O	1:C:156:ASP:C	2.58	0.42
1:B:48:ASP:HB2	1:B:79:LYS:HD3	2.02	0.42
1:C:161:ALA:HB2	1:C:170:ALA:HB2	2.02	0.42
1:C:201:LEU:N	1:C:201:LEU:HD23	2.34	0.42
1:A:220:THR:HB	4:A:5445:HOH:O	2.20	0.42
1:D:157:PRO:O	1:D:179:ALA:HB1	2.20	0.42
1:B:83:LEU:O	1:B:119:LEU:HD12	2.19	0.42
1:A:22:THR:HG22	1:A:23:LYS:O	2.20	0.42
1:A:151:LYS:HB2	1:A:177:LEU:HD23	2.01	0.42
1:A:59:GLN:HG2	1:B:36:GLU:CG	2.45	0.41
1:C:22:THR:CG2	1:C:23:LYS:N	2.83	0.41
1:B:22:THR:CG2	1:B:23:LYS:N	2.83	0.41
1:A:97:PHE:CE2	3:B:5302:AMP:H3'	2.55	0.41
1:A:204:LYS:HE3	1:A:205:ASP:OD1	2.20	0.41
1:D:48:ASP:OD1	1:D:79:LYS:HD3	2.20	0.41
1:B:151:LYS:HB2	1:B:151:LYS:HE3	1.69	0.41
1:B:59:GLN:H	1:B:59:GLN:CD	2.23	0.41
1:C:31:ARG:HH22	1:C:61:ASP:CG	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:OD1	1:A:79:LYS:HD3	2.20	0.41
1:C:49:GLU:HG3	1:C:80:LYS:HB3	2.01	0.41
1:D:196:ILE:O	1:D:227:LEU:HD11	2.19	0.41
1:B:239:ALA:HA	1:B:262:VAL:O	2.20	0.41
1:D:235:LYS:HG3	1:D:259:GLU:HG2	2.03	0.41
1:D:57:LYS:HG3	1:D:267:TYR:CE1	2.55	0.41
1:A:49:GLU:HG3	1:A:80:LYS:HB3	2.01	0.41
1:C:225:VAL:HG21	1:C:258:VAL:HG13	2.03	0.41
1:A:22:THR:CG2	1:A:23:LYS:N	2.84	0.41
1:A:30:LYS:HG2	1:A:38:TYR:HD2	1.84	0.41
1:B:31:ARG:HH22	1:B:61:ASP:CG	2.23	0.41
1:B:176:ILE:HG22	1:B:176:ILE:O	2.21	0.41
1:D:203:ALA:HB1	1:D:233:ALA:HB2	2.02	0.41
1:C:244:VAL:HG12	1:C:246:ILE:HG13	2.03	0.41
1:B:161:ALA:HB2	1:B:170:ALA:HB2	2.02	0.41
1:A:201:LEU:N	1:A:201:LEU:HD23	2.36	0.41
1:D:262:VAL:HG13	1:D:262:VAL:O	2.21	0.40
1:A:239:ALA:HA	1:A:262:VAL:O	2.22	0.40
1:C:161:ALA:HB1	1:C:166:ALA:HB3	2.03	0.40
1:A:214:ILE:HG22	1:A:215:ILE:N	2.37	0.40
1:A:176:ILE:HG22	1:A:176:ILE:O	2.20	0.40
1:D:145:LYS:HD2	1:D:145:LYS:N	2.36	0.40
1:B:98:ASN:HB2	1:B:101:GLU:HG3	2.04	0.40
1:B:155:ASN:O	1:B:156:ASP:C	2.58	0.40
1:C:262:VAL:O	1:C:262:VAL:HG13	2.22	0.40
1:D:98:ASN:HB2	1:D:101:GLU:HG3	2.04	0.40
1:C:151:LYS:HB2	1:C:177:LEU:HD23	2.02	0.40
1:B:151:LYS:HB2	1:B:177:LEU:HD23	2.02	0.40
1:A:161:ALA:HB2	1:A:170:ALA:HB2	2.04	0.40
1:D:235:LYS:CE	1:D:259:GLU:HG2	2.49	0.40
1:C:141:ASP:OD1	1:C:143:VAL:HG23	2.22	0.40
1:C:98:ASN:HB2	1:C:101:GLU:HG3	2.03	0.40
1:B:157:PRO:O	1:B:179:ALA:HB1	2.22	0.40
1:A:244:VAL:HG12	1:A:246:ILE:HG13	2.04	0.40
1:C:30:LYS:HG2	1:C:38:TYR:HD2	1.85	0.40
1:C:145:LYS:HD2	1:C:145:LYS:N	2.36	0.40
1:D:151:LYS:HB2	1:D:177:LEU:HD23	2.02	0.40
1:D:220:THR:HB	4:D:8445:HOH:O	2.21	0.40
1:A:31:ARG:HH22	1:A:61:ASP:CG	2.24	0.40
1:D:31:ARG:HH22	1:D:61:ASP:CG	2.24	0.40
1:C:83:LEU:O	1:C:119:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/284 (95%)	251 (93%)	16 (6%)	3 (1%)	17	50
1	B	270/284 (95%)	248 (92%)	19 (7%)	3 (1%)	17	50
1	C	270/284 (95%)	249 (92%)	18 (7%)	3 (1%)	17	50
1	D	270/284 (95%)	249 (92%)	18 (7%)	3 (1%)	17	50
All	All	1080/1136 (95%)	997 (92%)	71 (7%)	12 (1%)	17	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	VAL
1	B	78	VAL
1	C	78	VAL
1	D	78	VAL
1	A	201	LEU
1	B	201	LEU
1	C	201	LEU
1	D	201	LEU
1	A	59	GLN
1	B	59	GLN
1	C	59	GLN
1	D	59	GLN

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/245 (96%)	231 (98%)	4 (2%)	68	92
1	B	235/245 (96%)	231 (98%)	4 (2%)	68	92
1	C	235/245 (96%)	231 (98%)	4 (2%)	68	92
1	D	235/245 (96%)	231 (98%)	4 (2%)	68	92
All	All	940/980 (96%)	924 (98%)	16 (2%)	68	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	153	LYS
1	A	168	GLU
1	A	201	LEU
1	B	59	GLN
1	B	153	LYS
1	B	168	GLU
1	B	201	LEU
1	C	59	GLN
1	C	153	LYS
1	C	157	PRO
1	C	201	LEU
1	D	59	GLN
1	D	153	LYS
1	D	168	GLU
1	D	201	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	128	HIS
1	A	231	GLN
1	B	59	GLN
1	B	128	HIS
1	B	231	GLN
1	C	59	GLN
1	C	128	HIS
1	C	231	GLN
1	D	59	GLN

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Mol	Chain	Res	Type
1	D	128	HIS
1	D	231	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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	R5P	A	5301	-	13,13,13	1.74	3 (23%)	15,18,18	1.06	1 (6%)
3	AMP	B	5302	-	20,25,25	2.08	4 (20%)	22,38,38	2.80	7 (31%)
2	R5P	B	6301	-	13,13,13	1.67	3 (23%)	15,18,18	1.10	3 (20%)
3	AMP	B	6302	-	20,25,25	1.98	4 (20%)	22,38,38	2.82	7 (31%)
2	R5P	C	7301	-	13,13,13	1.71	3 (23%)	15,18,18	1.08	2 (13%)
3	AMP	C	8302	-	20,25,25	1.94	4 (20%)	22,38,38	2.89	8 (36%)
3	AMP	D	7302	-	20,25,25	2.03	4 (20%)	22,38,38	2.81	7 (31%)
2	R5P	D	8301	-	13,13,13	1.73	4 (30%)	15,18,18	1.16	3 (20%)

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	R5P	A	5301	-	-	0/14/16/16	0/0/0/0
3	AMP	B	5302	-	-	0/6/26/26	0/3/3/3
2	R5P	B	6301	-	-	0/14/16/16	0/0/0/0
3	AMP	B	6302	-	-	0/6/26/26	0/3/3/3
2	R5P	C	7301	-	-	0/14/16/16	0/0/0/0
3	AMP	C	8302	-	-	0/6/26/26	0/3/3/3
3	AMP	D	7302	-	-	0/6/26/26	0/3/3/3
2	R5P	D	8301	-	-	0/14/16/16	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8301	R5P	P-O3P	-2.12	1.47	1.54
3	D	7302	AMP	C2'-C3'	2.06	1.59	1.53
3	B	6302	AMP	C2'-C3'	2.11	1.59	1.53
3	C	8302	AMP	C2'-C3'	2.25	1.59	1.53
3	B	5302	AMP	C2'-C3'	2.33	1.59	1.53
2	D	8301	R5P	C3-C2	2.36	1.57	1.53
2	B	6301	R5P	C3-C2	2.44	1.57	1.53
3	B	6302	AMP	C2-N3	2.46	1.36	1.32
2	D	8301	R5P	P-O1P	2.47	1.59	1.51
2	A	5301	R5P	P-O1P	2.58	1.59	1.51
2	C	7301	R5P	C3-C2	2.59	1.57	1.53
3	C	8302	AMP	C2-N3	2.62	1.36	1.32
2	A	5301	R5P	C3-C2	2.70	1.57	1.53
3	B	5302	AMP	C2-N3	2.83	1.37	1.32
2	B	6301	R5P	P-O1P	2.88	1.60	1.51
3	D	7302	AMP	C2-N3	2.92	1.37	1.32
2	C	7301	R5P	P-O1P	3.01	1.61	1.51
2	B	6301	R5P	C5-C4	3.30	1.56	1.51
3	B	6302	AMP	O3'-C3'	3.32	1.50	1.43
3	B	5302	AMP	O3'-C3'	3.42	1.51	1.43
2	D	8301	R5P	C5-C4	3.45	1.56	1.51
3	D	7302	AMP	O3'-C3'	3.47	1.51	1.43
3	C	8302	AMP	O3'-C3'	3.48	1.51	1.43
2	C	7301	R5P	C5-C4	3.48	1.57	1.51
2	A	5301	R5P	C5-C4	3.56	1.57	1.51
3	C	8302	AMP	C3'-C4'	6.22	1.69	1.53
3	B	6302	AMP	C3'-C4'	6.40	1.70	1.53
3	B	5302	AMP	C3'-C4'	6.51	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7302	AMP	C3'-C4'	6.61	1.70	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8302	AMP	N3-C2-N1	-9.91	121.31	128.89
3	B	5302	AMP	N3-C2-N1	-9.66	121.50	128.89
3	D	7302	AMP	N3-C2-N1	-9.60	121.55	128.89
3	B	6302	AMP	N3-C2-N1	-9.53	121.60	128.89
3	C	8302	AMP	O4'-C4'-C5'	-3.27	97.61	109.32
3	D	7302	AMP	O4'-C4'-C5'	-3.18	97.94	109.32
3	B	6302	AMP	O4'-C4'-C5'	-3.12	98.16	109.32
3	B	5302	AMP	O4'-C4'-C5'	-2.99	98.64	109.32
3	D	7302	AMP	O5'-P-O1P	-2.62	100.47	107.14
3	C	8302	AMP	O5'-P-O1P	-2.54	100.67	107.14
3	B	5302	AMP	O5'-P-O1P	-2.45	100.89	107.14
2	D	8301	R5P	O3-C3-C2	-2.36	104.76	108.93
2	B	6301	R5P	O3-C3-C2	-2.26	104.93	108.93
3	B	6302	AMP	O5'-P-O1P	-2.24	101.43	107.14
2	D	8301	R5P	O1-C1-C2	-2.24	119.08	125.60
2	C	7301	R5P	O1-C1-C2	-2.20	119.18	125.60
2	C	7301	R5P	O3-C3-C2	-2.13	105.17	108.93
2	B	6301	R5P	O1-C1-C2	-2.12	119.41	125.60
2	A	5301	R5P	O1-C1-C2	-2.05	119.61	125.60
2	D	8301	R5P	O3P-P-O5	2.16	112.80	106.56
2	B	6301	R5P	O3P-P-O5	2.23	112.98	106.56
3	C	8302	AMP	C2'-C1'-N9	2.33	117.84	114.29
3	B	5302	AMP	N6-C6-N1	2.47	124.51	119.20
3	D	7302	AMP	N6-C6-N1	2.49	124.54	119.20
3	D	7302	AMP	C2-N1-C6	2.50	123.24	118.77
3	C	8302	AMP	N6-C6-N1	2.50	124.58	119.20
3	B	5302	AMP	C2-N1-C6	2.59	123.39	118.77
3	C	8302	AMP	C2-N1-C6	2.62	123.44	118.77
3	B	6302	AMP	C2-N1-C6	2.65	123.50	118.77
3	B	6302	AMP	N6-C6-N1	2.67	124.93	119.20
3	B	5302	AMP	C4'-O4'-C1'	3.23	113.27	109.72
3	B	6302	AMP	C4'-O4'-C1'	3.31	113.36	109.72
3	D	7302	AMP	C4'-O4'-C1'	3.37	113.42	109.72
3	C	8302	AMP	C4'-O4'-C1'	3.40	113.45	109.72
3	D	7302	AMP	C4-C5-N7	4.94	114.02	109.48
3	B	5302	AMP	C4-C5-N7	5.04	114.12	109.48
3	C	8302	AMP	C4-C5-N7	5.18	114.24	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	6302	AMP	C4-C5-N7	5.40	114.44	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5302	AMP	2	0
3	B	6302	AMP	2	0
3	C	8302	AMP	2	0
3	D	7302	AMP	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	274/284 (96%)	-0.11	9 (3%)	50	38	26, 44, 60, 70	0
1	B	274/284 (96%)	-0.02	8 (2%)	55	43	26, 44, 60, 74	0
1	C	274/284 (96%)	-0.02	8 (2%)	55	43	25, 45, 63, 69	0
1	D	274/284 (96%)	-0.10	9 (3%)	50	38	27, 43, 61, 70	0
All	All	1096/1136 (96%)	-0.06	34 (3%)	52	40	25, 44, 62, 74	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ASN	4.4
1	B	46	ASN	3.8
1	C	205	ASP	3.6
1	D	46	ASN	3.6
1	A	164	LYS	3.5
1	C	178	ASN	3.4
1	D	178	ASN	3.3
1	C	79	LYS	3.1
1	B	21	ASN	3.0
1	C	230	GLU	2.7
1	C	204	LYS	2.4
1	B	95	LYS	2.4
1	A	79	LYS	2.4
1	C	164	LYS	2.4
1	B	44	GLU	2.4
1	B	94	ASP	2.4
1	A	185	GLU	2.4
1	A	183	TYR	2.4
1	D	47	ASP	2.3
1	A	47	ASP	2.3
1	A	152	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	164	LYS	2.3
1	B	79	LYS	2.2
1	B	128	HIS	2.2
1	C	48	ASP	2.2
1	A	46	ASN	2.1
1	D	152	ASP	2.1
1	A	205	ASP	2.1
1	D	21	ASN	2.1
1	D	79	LYS	2.1
1	D	23	LYS	2.0
1	B	164	LYS	2.0
1	D	199	LYS	2.0
1	C	46	ASN	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
2	R5P	B	6301	14/14	0.90	0.19	0.74	49,51,54,56	0
3	AMP	C	8302	23/23	0.90	0.17	-0.13	45,47,53,55	0
3	AMP	D	7302	23/23	0.89	0.17	-0.25	46,49,54,57	0
2	R5P	D	8301	14/14	0.90	0.18	-0.44	46,48,52,53	0
3	AMP	B	6302	23/23	0.91	0.17	-0.49	52,54,57,60	0
2	R5P	A	5301	14/14	0.93	0.16	-0.75	45,49,54,56	0
3	AMP	B	5302	23/23	0.89	0.17	-0.76	44,48,54,57	0
2	R5P	C	7301	14/14	0.93	0.15	-1.05	48,50,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.