



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:21 am GMT

PDB ID : 3HW5
Title : crystal structure of avian influenza virus PA_N in complex with AMP
Authors : Zhao, C.; Lou, Z.; Guo, Y.; Ma, M.; Chen, Y.; Liang, S.; Rao, Z.
Deposited on : 2009-06-17
Resolution : 1.81 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

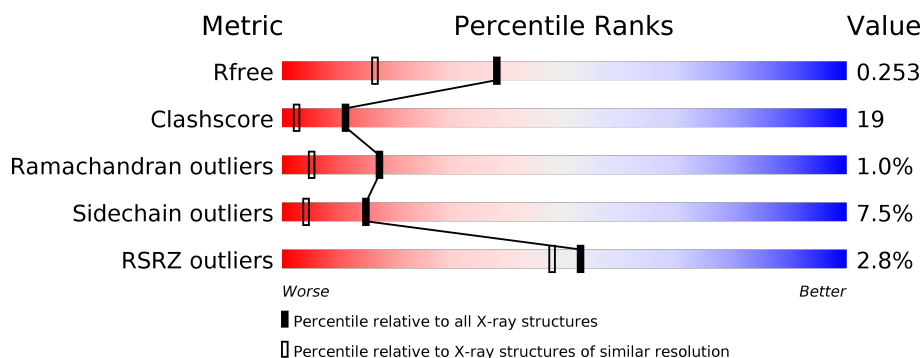
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	111664	6455 (1.84-1.80)
Clashscore	122126	7349 (1.84-1.80)
Ramachandran outliers	120053	7272 (1.84-1.80)
Sidechain outliers	120020	7272 (1.84-1.80)
RSRZ outliers	108989	6347 (1.84-1.80)

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 $\leq 5\%$. 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	261	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 48%, yellow 16%, orange 2%, grey 32%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 48% 16% • • 32% </div> </div>
1	B	261	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 49%, yellow 15%, orange 5%, grey 31%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 49% 15% 5% 31% </div> </div>
1	C	261	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 48%, yellow 13%, orange 5%, grey 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 48% 13% 5% • 33% </div> </div>
1	D	261	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 46%, yellow 17%, orange 2%, grey 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 46% 17% • • 33% </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	A	257	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6523 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1462	924	251	276	11			
1	B	180	Total	C	N	O	S	0	0	0
			1496	948	258	279	11			
1	C	176	Total	C	N	O	S	0	0	0
			1453	919	250	273	11			
1	D	176	Total	C	N	O	S	0	0	0
			1453	919	250	273	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
A	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
A	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
B	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
B	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
B	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
B	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
C	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
C	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
C	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
C	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
D	-4	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	-3	PRO	-	EXPRESSION TAG	UNP Q9Q0U9
D	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9

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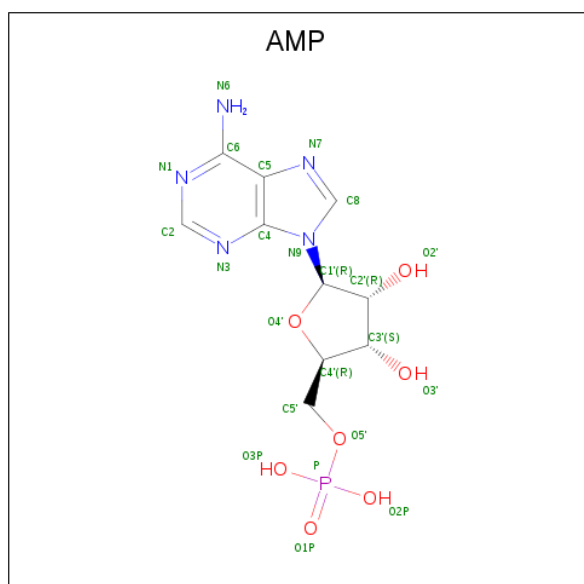
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
D	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 23 10 5 7 1	0	0

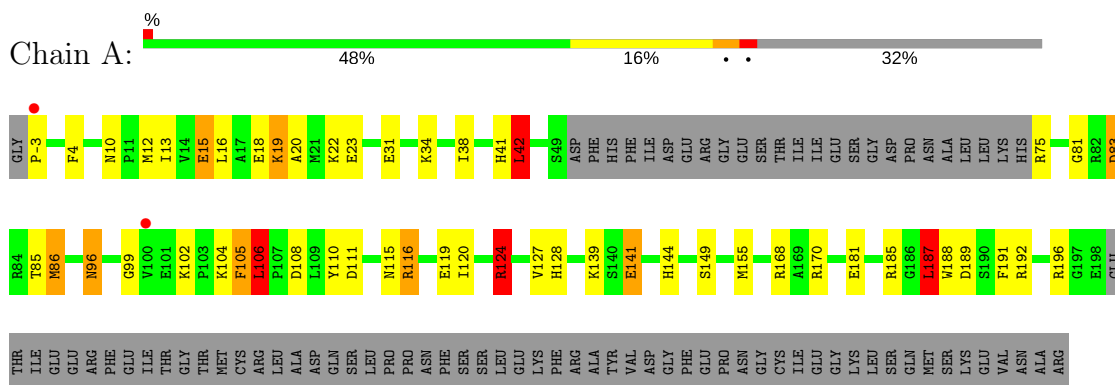
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total 180	O 180	0	0
4	B	150	Total 150	O 150	0	0
4	C	141	Total 141	O 141	0	0
4	D	161	Total 161	O 161	0	0

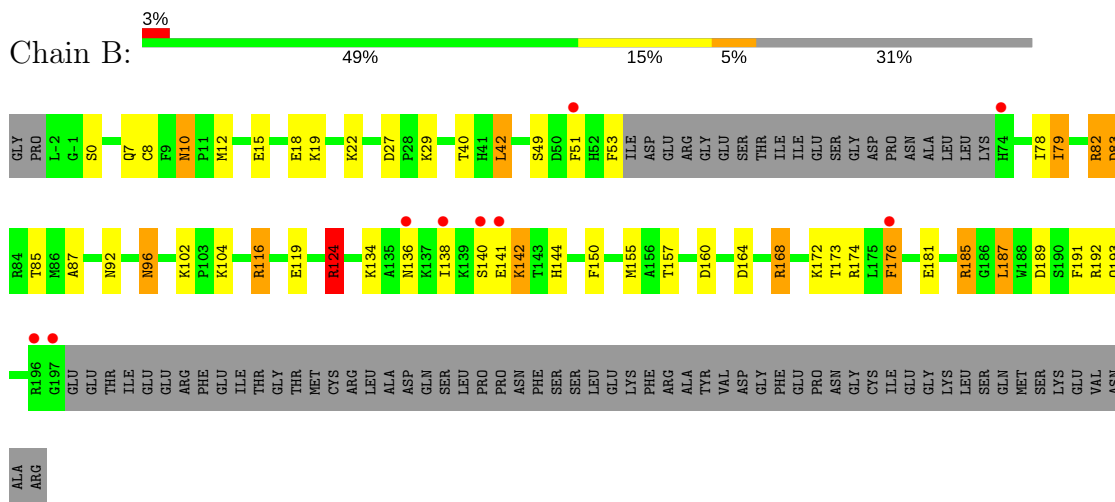
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

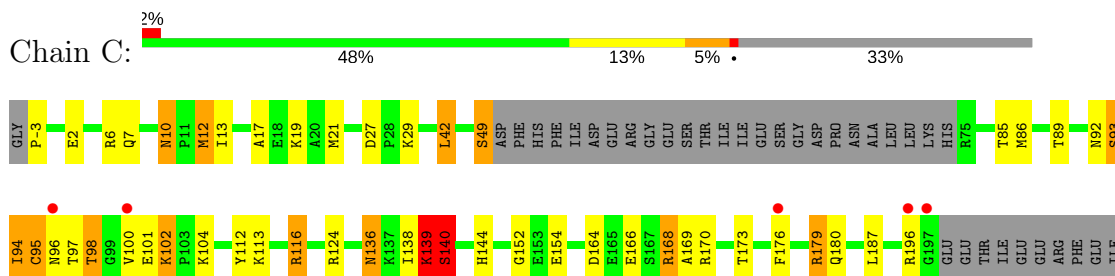
• Molecule 1: Polymerase acidic protein



• Molecule 1: Polymerase acidic protein

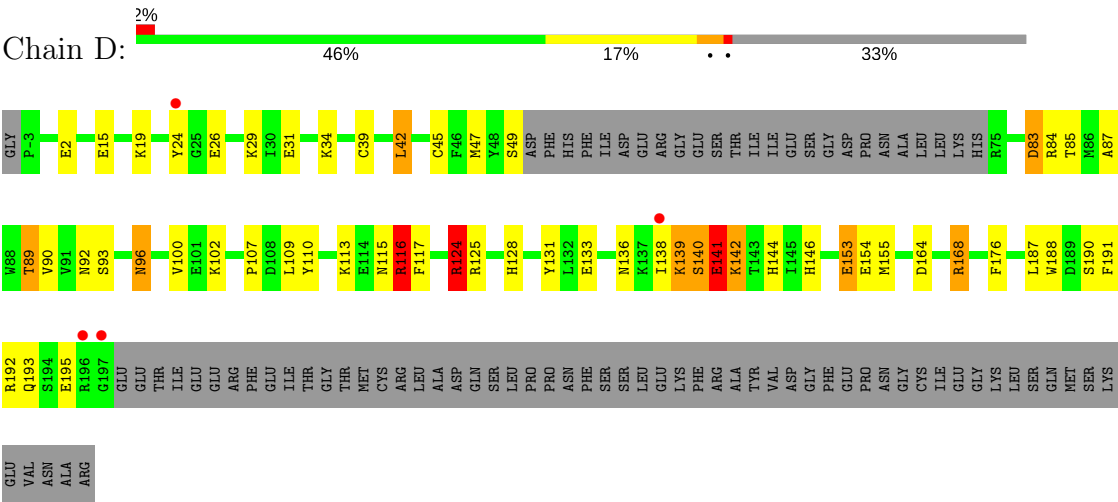


• Molecule 1: Polymerase acidic protein



THR	GLY	THR	MET	CYS	ARG	LEU	ALA	ASP	GLN	SER	LEU	PRO	PRO	ASN	PHE	SER	SER	LEU	GLU	LYS	PHE	ARG	ALA	TYR	VAL	ASP	GLY	PHE	GLU	PRO	ASN	GLY	CYS	ILE	GLY	LYS	LEU	SER	GLN	MET	SER	LYS	GLU	VAL	ASN	ALA	ARG
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● Molecule 1: Polymerase acidic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.62Å 60.03Å 67.18Å 96.02° 96.22° 109.35°	Depositor
Resolution (Å)	50.00 – 1.81 48.13 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (50.00-1.81) 91.8 (48.13-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.206 , 0.263 0.201 , 0.253	Depositor DCC
R_{free} test set	3187 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6523	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: AMP, MG

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	1.23	4/1491 (0.3%)	1.46	16/2000 (0.8%)
1	B	1.15	2/1528 (0.1%)	1.36	15/2050 (0.7%)
1	C	1.10	3/1482 (0.2%)	1.23	12/1988 (0.6%)
1	D	1.13	5/1482 (0.3%)	1.33	12/1988 (0.6%)
All	All	1.15	14/5983 (0.2%)	1.35	55/8026 (0.7%)

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	0	1
1	C	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	GLU	CG-CD	9.20	1.65	1.51
1	A	106	LEU	N-CA	8.66	1.63	1.46
1	D	153	GLU	CG-CD	7.49	1.63	1.51
1	A	116	ARG	CZ-NH1	6.42	1.41	1.33
1	B	15	GLU	CG-CD	6.29	1.61	1.51
1	B	116	ARG	CZ-NH1	6.21	1.41	1.33
1	C	116	ARG	CG-CD	-5.85	1.37	1.51
1	A	18	GLU	CD-OE2	-5.68	1.19	1.25
1	A	168	ARG	CD-NE	-5.47	1.37	1.46
1	C	166	GLU	CB-CG	5.37	1.62	1.52
1	D	153	GLU	CB-CG	5.16	1.61	1.52
1	D	39	CYS	CB-SG	5.15	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	45	CYS	CB-SG	-5.13	1.73	1.81
1	D	110	TYR	CD2-CE2	5.07	1.47	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH2	-21.18	109.71	120.30
1	A	116	ARG	NE-CZ-NH2	-19.53	110.54	120.30
1	A	116	ARG	NE-CZ-NH1	19.31	129.95	120.30
1	C	168	ARG	NE-CZ-NH1	18.48	129.54	120.30
1	C	168	ARG	NE-CZ-NH2	-17.91	111.34	120.30
1	B	168	ARG	NE-CZ-NH2	-17.46	111.57	120.30
1	D	168	ARG	NE-CZ-NH2	-17.08	111.76	120.30
1	B	116	ARG	NE-CZ-NH2	-16.84	111.88	120.30
1	B	116	ARG	NE-CZ-NH1	16.23	128.41	120.30
1	D	116	ARG	NE-CZ-NH1	16.13	128.37	120.30
1	A	168	ARG	NE-CZ-NH1	15.33	127.97	120.30
1	D	168	ARG	NE-CZ-NH1	14.96	127.78	120.30
1	D	116	ARG	NE-CZ-NH2	-14.87	112.86	120.30
1	D	47	MET	CG-SD-CE	-13.35	78.84	100.20
1	B	168	ARG	NE-CZ-NH1	13.09	126.85	120.30
1	B	124	ARG	NE-CZ-NH1	12.65	126.62	120.30
1	A	116	ARG	CD-NE-CZ	10.15	137.81	123.60
1	A	105	PHE	C-N-CA	-9.81	97.18	121.70
1	A	106	LEU	N-CA-CB	9.77	129.94	110.40
1	B	124	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	D	164	ASP	CB-CG-OD2	8.60	126.04	118.30
1	B	160	ASP	CB-CG-OD1	8.55	125.99	118.30
1	A	105	PHE	O-C-N	-8.30	109.43	122.70
1	A	196	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	D	124	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	42	LEU	CB-CG-CD1	7.69	124.08	111.00
1	B	116	ARG	CD-NE-CZ	7.69	134.37	123.60
1	B	185	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	164	ASP	CB-CG-OD2	7.40	124.96	118.30
1	C	124	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	D	42	LEU	CA-CB-CG	6.78	130.89	115.30
1	A	106	LEU	CA-CB-CG	6.70	130.70	115.30
1	C	164	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	A	42	LEU	CA-CB-CG	6.40	130.02	115.30
1	C	168	ARG	CD-NE-CZ	6.32	132.44	123.60
1	B	164	ASP	CB-CG-OD2	6.27	123.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	LEU	CB-CG-CD1	-6.27	100.35	111.00
1	A	42	LEU	CB-CG-CD1	5.86	120.96	111.00
1	A	124	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	174	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	164	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	C	98	THR	N-CA-C	-5.74	95.51	111.00
1	B	187	LEU	CA-CB-CG	5.73	128.47	115.30
1	D	116	ARG	CB-CG-CD	5.72	126.47	111.60
1	C	140	SER	N-CA-CB	-5.61	102.09	110.50
1	B	42	LEU	CB-CG-CD2	5.56	120.45	111.00
1	C	27	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	168	ARG	CD-NE-CZ	5.54	131.36	123.60
1	B	83	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	187	LEU	CB-CG-CD2	5.45	120.26	111.00
1	D	124	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	124	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	176	PHE	CB-CA-C	-5.31	99.77	110.40
1	C	168	ARG	CG-CD-NE	-5.17	100.95	111.80
1	A	111	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	GLY	Peptide
1	C	139	LYS	Peptide

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	1462	0	1435	58	0
1	B	1496	0	1458	58	1
1	C	1453	0	1429	47	1
1	D	1453	0	1429	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	12	17	0
4	A	180	0	0	17	0
4	B	150	0	0	20	0
4	C	141	0	0	17	0
4	D	161	0	0	22	0
All	All	6523	0	5763	223	1

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 19.

All (223) 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:-3:PRO:HA	4:A:478:HOH:O	1.16	1.33
1:A:115:ASN:HB2	4:A:351:HOH:O	1.30	1.28
1:D:100:VAL:HB	4:D:446:HOH:O	1.14	1.26
1:B:7:GLN:NE2	4:B:398:HOH:O	1.67	1.23
1:B:155:MET:HG2	4:B:487:HOH:O	1.00	1.18
1:A:105:PHE:O	1:A:106:LEU:HB2	1.29	1.10
1:A:42:LEU:CD1	3:A:257:AMP:HN61	1.69	1.05
1:A:105:PHE:O	1:A:106:LEU:CB	1.88	1.05
1:D:141:GLU:OE2	4:D:449:HOH:O	1.73	1.04
1:C:138:ILE:HG13	1:C:140:SER:HB3	1.35	1.03
1:A:38:ILE:HG12	3:A:257:AMP:H1'	1.40	1.03
3:A:257:AMP:H2	4:A:585:HOH:O	1.41	1.02
1:D:49:SER:C	4:D:466:HOH:O	2.02	0.97
1:B:7:GLN:CD	4:B:398:HOH:O	1.95	0.96
1:B:51:PHE:HE1	4:C:493:HOH:O	1.50	0.95
1:D:128:HIS:HA	1:D:155:MET:HE1	1.49	0.94
1:B:19:LYS:HZ2	1:B:22:LYS:HE2	1.34	0.92
1:D:138:ILE:O	4:D:1055:HOH:O	1.86	0.92
1:D:83:ASP:OD1	4:D:1065:HOH:O	1.86	0.92
1:A:124:ARG:HD2	1:A:191:PHE:O	1.71	0.91
1:A:42:LEU:HD11	3:A:257:AMP:HN61	1.35	0.89
1:D:84:ARG:NH1	4:D:1005:HOH:O	2.06	0.89
1:B:176:PHE:HD1	4:B:377:HOH:O	1.55	0.89
1:A:-3:PRO:CA	4:A:478:HOH:O	1.88	0.88
1:D:116:ARG:HD2	4:D:1027:HOH:O	1.76	0.85
1:D:49:SER:O	4:D:531:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLN:HG3	4:C:605:HOH:O	1.75	0.84
1:B:124:ARG:HD2	1:B:191:PHE:O	1.76	0.84
1:A:10:ASN:HD21	1:A:12:MET:HB3	1.43	0.83
1:D:34:LYS:HB3	1:D:34:LYS:HZ3	1.42	0.83
1:C:49:SER:O	4:C:541:HOH:O	1.98	0.81
1:C:94:ILE:HG22	1:C:95:CYS:H	1.43	0.81
1:A:108:ASP:OD2	4:A:1004:HOH:O	1.99	0.80
1:A:42:LEU:HD13	3:A:257:AMP:HN61	1.46	0.80
1:B:8:CYS:HB2	4:B:398:HOH:O	1.82	0.80
1:D:31:GLU:CD	1:D:34:LYS:HZ1	1.83	0.79
1:B:119:GLU:CG	4:B:564:HOH:O	2.31	0.79
1:A:42:LEU:HD11	3:A:257:AMP:N6	1.98	0.78
1:D:141:GLU:HA	4:D:610:HOH:O	1.83	0.77
1:C:93:SER:O	1:C:94:ILE:O	2.02	0.77
1:C:94:ILE:O	1:C:96:ASN:N	2.18	0.77
1:B:7:GLN:NE2	1:B:185:ARG:NH2	2.33	0.77
1:A:170:ARG:HG3	4:A:603:HOH:O	1.83	0.77
1:D:49:SER:CA	4:D:466:HOH:O	2.32	0.76
3:A:257:AMP:N6	4:A:347:HOH:O	2.15	0.75
1:A:4:PHE:HE1	1:A:181:GLU:HG3	1.50	0.74
1:B:82:ARG:HG3	1:B:87:ALA:HB2	1.71	0.73
1:A:120:ILE:O	4:A:1004:HOH:O	2.06	0.73
1:B:79:ILE:O	1:B:82:ARG:HG2	1.90	0.72
1:C:138:ILE:CG1	1:C:140:SER:HB3	2.16	0.71
1:D:124:ARG:HG2	1:D:195:GLU:OE1	1.91	0.71
3:A:257:AMP:C2	4:A:585:HOH:O	2.27	0.71
1:C:85:THR:O	1:C:89:THR:HG23	1.90	0.71
1:D:49:SER:C	4:D:502:HOH:O	2.28	0.71
1:A:10:ASN:ND2	1:A:12:MET:HB3	2.05	0.70
1:B:140:SER:HB3	4:B:598:HOH:O	1.92	0.70
1:A:75:ARG:N	4:A:1046:HOH:O	2.24	0.69
1:B:92:ASN:ND2	1:B:102:LYS:NZ	2.40	0.69
1:C:86:MET:HG2	4:C:331:HOH:O	1.93	0.69
1:D:31:GLU:CD	1:D:34:LYS:NZ	2.45	0.69
1:A:115:ASN:CB	4:A:351:HOH:O	2.07	0.69
1:B:19:LYS:HE2	4:B:583:HOH:O	1.92	0.68
1:D:87:ALA:O	1:D:90:VAL:HG12	1.93	0.68
1:C:152:GLY:O	4:C:395:HOH:O	2.12	0.68
1:C:154:GLU:OE2	1:C:168:ARG:HD2	1.94	0.68
1:C:93:SER:C	1:C:94:ILE:O	2.30	0.67
1:B:141:GLU:O	1:B:142:LYS:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:HB3	3:A:257:AMP:H8	1.61	0.66
1:C:112:TYR:O	4:C:332:HOH:O	2.12	0.66
1:B:181:GLU:OE2	4:B:1062:HOH:O	2.14	0.66
1:C:94:ILE:HG22	1:C:95:CYS:N	2.11	0.65
1:D:34:LYS:HB3	1:D:34:LYS:NZ	2.11	0.65
1:A:85:THR:HB	1:B:83:ASP:OD1	1.97	0.65
1:B:176:PHE:CD1	4:B:377:HOH:O	2.40	0.65
1:A:20:ALA:HB1	3:A:257:AMP:C2	2.32	0.65
1:D:188:TRP:HE1	1:D:192:ARG:CZ	2.09	0.65
1:B:10:ASN:HD22	1:B:12:MET:H	1.44	0.64
1:B:119:GLU:OE2	4:B:1005:HOH:O	2.14	0.64
1:D:141:GLU:CA	4:D:610:HOH:O	2.43	0.63
1:D:85:THR:O	1:D:89:THR:HG23	1.98	0.63
1:B:19:LYS:NZ	1:B:22:LYS:HE2	2.12	0.63
1:B:92:ASN:ND2	1:B:102:LYS:HZ2	1.96	0.63
1:C:169:ALA:O	1:C:173:THR:HG22	2.00	0.61
1:A:4:PHE:CE1	1:A:181:GLU:HG3	2.35	0.61
1:D:128:HIS:HA	1:D:155:MET:CE	2.25	0.61
1:D:26:GLU:OE2	1:D:34:LYS:HE3	2.00	0.61
1:C:29:LYS:HD2	4:C:1044:HOH:O	2.00	0.61
1:D:31:GLU:HB3	1:D:34:LYS:NZ	2.15	0.61
1:B:96:ASN:ND2	4:B:357:HOH:O	2.34	0.60
1:A:119:GLU:OE2	4:A:294:HOH:O	2.16	0.60
1:A:38:ILE:HG23	3:A:257:AMP:C4	2.37	0.60
1:D:34:LYS:CB	1:D:34:LYS:NZ	2.64	0.60
1:B:192:ARG:HD2	4:B:1031:HOH:O	2.02	0.59
1:D:124:ARG:HD2	1:D:191:PHE:O	2.02	0.59
1:A:185:ARG:HB2	1:A:187:LEU:HD22	1.84	0.59
1:C:-3:PRO:CD	4:C:1043:HOH:O	2.51	0.59
1:D:142:LYS:HE2	4:D:392:HOH:O	2.02	0.58
1:D:176:PHE:CD1	4:D:354:HOH:O	2.52	0.58
1:C:96:ASN:O	4:C:1029:HOH:O	2.17	0.58
1:A:128:HIS:CE1	1:A:155:MET:HE1	2.39	0.58
1:A:141:GLU:CD	1:A:141:GLU:H	2.06	0.58
1:C:116:ARG:HD3	1:C:144:HIS:HB2	1.85	0.58
1:D:136:ASN:O	1:D:139:LYS:HD2	2.04	0.58
1:B:173:THR:O	1:B:176:PHE:HB2	2.04	0.57
1:C:170:ARG:HA	1:C:173:THR:HG22	1.87	0.57
1:A:41:HIS:CE1	3:A:257:AMP:H5'2	2.40	0.56
1:D:31:GLU:OE2	1:D:34:LYS:NZ	2.38	0.56
1:B:27:ASP:OD1	1:B:29:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HB	4:B:598:HOH:O	2.06	0.55
1:D:93:SER:HA	1:D:96:ASN:ND2	2.22	0.55
1:B:7:GLN:NE2	1:B:185:ARG:HH22	2.04	0.55
1:B:51:PHE:CE1	4:C:493:HOH:O	2.37	0.55
1:C:140:SER:HA	4:C:1039:HOH:O	2.05	0.55
1:A:115:ASN:CG	4:A:351:HOH:O	2.38	0.55
3:A:257:AMP:P	4:A:1004:HOH:O	2.64	0.54
1:B:192:ARG:CD	4:B:1031:HOH:O	2.55	0.54
1:D:140:SER:O	1:D:141:GLU:HB3	2.08	0.54
1:C:-3:PRO:HD2	4:C:1043:HOH:O	2.07	0.54
1:D:15:GLU:HG3	4:D:594:HOH:O	2.07	0.53
1:D:188:TRP:HE1	1:D:192:ARG:NH1	2.06	0.53
1:D:31:GLU:HB3	1:D:34:LYS:HZ3	1.71	0.53
1:A:41:HIS:ND1	3:A:257:AMP:C8	2.76	0.53
1:B:124:ARG:HG3	1:B:192:ARG:HA	1.89	0.53
1:D:190:SER:HA	1:D:193:GLN:HG2	1.90	0.53
1:B:119:GLU:CD	4:B:564:HOH:O	2.44	0.53
1:B:119:GLU:OE1	4:B:1003:HOH:O	2.19	0.53
1:B:141:GLU:O	1:B:141:GLU:HG3	2.09	0.53
1:A:4:PHE:HE1	1:A:181:GLU:CG	2.19	0.53
1:A:85:THR:HB	1:B:83:ASP:CG	2.29	0.53
1:A:128:HIS:CE1	1:A:155:MET:CE	2.92	0.52
3:A:257:AMP:N9	3:A:257:AMP:H5'1	2.25	0.52
1:D:125:ARG:NH1	1:D:195:GLU:OE2	2.44	0.51
1:A:127:VAL:CG1	1:A:149:SER:HB3	2.40	0.51
1:A:19:LYS:NZ	1:A:22:LYS:HE2	2.26	0.51
1:B:92:ASN:ND2	1:B:102:LYS:HZ1	2.09	0.51
1:B:19:LYS:HZ2	1:B:22:LYS:CE	2.15	0.51
1:B:92:ASN:HD21	1:B:102:LYS:NZ	2.09	0.50
1:C:138:ILE:HG13	1:C:140:SER:CB	2.24	0.50
1:A:23:GLU:OE1	1:B:85:THR:HG23	2.11	0.50
1:C:154:GLU:OE2	1:C:168:ARG:CD	2.60	0.49
1:D:154:GLU:OE2	1:D:168:ARG:HD2	2.12	0.49
1:B:49:SER:OG	1:B:78:ILE:HD11	2.13	0.49
1:C:173:THR:HG23	4:C:1021:HOH:O	2.12	0.49
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.13	0.49
1:D:87:ALA:O	1:D:90:VAL:CG1	2.61	0.49
1:D:115:ASN:HB2	4:D:380:HOH:O	2.13	0.49
1:D:176:PHE:HD1	4:D:354:HOH:O	1.95	0.48
1:C:136:ASN:HB3	4:C:298:HOH:O	2.14	0.48
1:D:142:LYS:CE	4:D:392:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD2	1:B:85:THR:HB	2.14	0.48
1:D:92:ASN:HD21	1:D:102:LYS:HE2	1.77	0.48
1:A:115:ASN:ND2	4:A:351:HOH:O	2.47	0.48
1:C:98:THR:OG1	1:C:100:VAL:HG23	2.14	0.48
1:D:34:LYS:CB	1:D:34:LYS:HZ3	2.18	0.48
1:A:110:TYR:OH	1:A:115:ASN:ND2	2.46	0.48
1:A:10:ASN:HB3	1:A:13:ILE:HD12	1.96	0.48
1:A:34:LYS:HB2	1:A:34:LYS:HE2	1.35	0.48
1:B:144:HIS:CE1	1:B:157:THR:HB	2.49	0.47
1:D:142:LYS:HG3	4:D:522:HOH:O	2.13	0.47
1:D:2:GLU:OE2	1:D:29:LYS:HG2	2.14	0.47
1:D:49:SER:HB2	4:D:466:HOH:O	2.14	0.47
1:C:17:ALA:O	1:C:21:MET:HG3	2.14	0.47
1:A:42:LEU:CD1	3:A:257:AMP:N6	2.52	0.47
1:A:188:TRP:NE1	1:A:192:ARG:HD3	2.30	0.47
1:B:10:ASN:ND2	1:B:12:MET:H	2.11	0.47
1:B:119:GLU:HG2	4:B:564:HOH:O	2.05	0.46
1:D:141:GLU:HG2	1:D:142:LYS:N	2.30	0.46
1:B:116:ARG:HD2	1:B:144:HIS:HB2	1.97	0.46
1:B:18:GLU:O	1:B:22:LYS:HG3	2.15	0.46
1:D:155:MET:HE3	1:D:155:MET:HB3	1.30	0.46
1:D:85:THR:O	1:D:89:THR:CG2	2.62	0.46
1:C:96:ASN:HB3	4:C:418:HOH:O	2.16	0.46
1:D:146:HIS:HE1	1:D:168:ARG:HD3	1.80	0.46
1:A:10:ASN:HD22	1:A:13:ILE:H	1.64	0.46
1:C:10:ASN:HD22	1:C:13:ILE:H	1.63	0.46
1:C:104:LYS:HZ1	1:C:139:LYS:HB3	1.81	0.45
1:D:125:ARG:NH2	1:D:133:GLU:OE1	2.45	0.45
1:C:179:ARG:C	1:C:179:ARG:HD2	2.37	0.45
1:D:19:LYS:HE3	4:D:442:HOH:O	2.16	0.45
1:D:93:SER:HA	1:D:96:ASN:HD21	1.82	0.44
1:B:19:LYS:NZ	1:B:22:LYS:CE	2.79	0.44
1:B:168:ARG:O	1:B:172:LYS:HG3	2.17	0.44
1:B:82:ARG:HE	1:B:82:ARG:HB3	1.34	0.44
1:C:97:THR:O	1:C:97:THR:HG22	2.18	0.44
1:A:86:MET:HG2	4:A:391:HOH:O	2.18	0.44
1:A:16:LEU:HD22	1:A:81:GLY:O	2.18	0.43
1:B:7:GLN:HE21	1:B:185:ARG:NH2	2.14	0.43
1:B:92:ASN:HD22	1:B:102:LYS:NZ	2.14	0.43
1:C:196:ARG:NH2	4:C:440:HOH:O	2.51	0.43
1:C:179:ARG:HD2	1:C:180:GLN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HZ1	1:A:139:LYS:HB2	1.83	0.43
1:C:10:ASN:ND2	1:C:12:MET:H	2.16	0.43
1:C:170:ARG:HA	1:C:173:THR:CG2	2.47	0.43
1:C:12:MET:HE3	1:C:12:MET:HB3	1.97	0.43
1:B:116:ARG:NE	4:B:1059:HOH:O	2.00	0.43
1:C:104:LYS:NZ	1:C:139:LYS:HB2	2.34	0.43
1:C:-3:PRO:N	4:C:1043:HOH:O	2.52	0.43
1:C:2:GLU:O	1:C:6:ARG:HG3	2.18	0.43
1:A:185:ARG:CB	1:A:187:LEU:HD22	2.48	0.42
1:A:96:ASN:HD22	1:A:96:ASN:C	2.21	0.42
1:C:97:THR:CG2	1:C:97:THR:O	2.66	0.42
1:D:83:ASP:CB	4:D:1065:HOH:O	2.67	0.42
1:A:15:GLU:OE2	1:A:19:LYS:HE2	2.19	0.42
1:B:119:GLU:OE2	1:B:134:LYS:HE3	2.19	0.42
1:B:181:GLU:HG3	4:B:1062:HOH:O	2.18	0.42
1:B:40:THR:HG21	1:B:150:PHE:CZ	2.54	0.42
1:D:116:ARG:HD3	1:D:144:HIS:HB2	2.02	0.42
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.42	0.42
1:C:19:LYS:HD3	1:C:19:LYS:HA	1.85	0.42
1:C:104:LYS:NZ	1:C:139:LYS:CB	2.82	0.42
1:D:138:ILE:O	1:D:139:LYS:C	2.57	0.42
1:D:138:ILE:HG13	1:D:140:SER:HB3	2.01	0.42
1:A:38:ILE:HG23	3:A:257:AMP:C5	2.54	0.41
1:A:116:ARG:HD2	1:A:144:HIS:HB2	2.01	0.41
1:B:53:PHE:HD1	1:C:12:MET:HE1	1.86	0.41
1:C:92:ASN:HD21	1:C:102:LYS:HD3	1.85	0.41
1:C:116:ARG:CD	1:C:144:HIS:HB2	2.49	0.41
1:D:131:TYR:HB3	1:D:155:MET:HE1	2.03	0.41
1:A:83:ASP:HB3	1:B:83:ASP:OD1	2.21	0.40
1:D:141:GLU:HG2	1:D:142:LYS:HB2	2.03	0.40
1:A:115:ASN:O	4:A:1060:HOH:O	2.22	0.40
1:A:128:HIS:NE2	1:A:155:MET:HE1	2.36	0.40
1:D:107:PRO:HG3	1:D:117:PHE:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASN:ND2	1:C:136:ASN:OD1[1_445]	2.18	0.02

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	173/261 (66%)	169 (98%)	3 (2%)	1 (1%)	27	13
1	B	176/261 (67%)	169 (96%)	6 (3%)	1 (1%)	27	13
1	C	172/261 (66%)	166 (96%)	3 (2%)	3 (2%)	10	2
1	D	172/261 (66%)	163 (95%)	7 (4%)	2 (1%)	14	4
All	All	693/1044 (66%)	667 (96%)	19 (3%)	7 (1%)	17	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	B	142	LYS
1	C	94	ILE
1	C	95	CYS
1	D	140	SER
1	D	141	GLU
1	C	139	LYS

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	159/232 (68%)	148 (93%)	11 (7%)	17	5
1	B	162/232 (70%)	151 (93%)	11 (7%)	17	5
1	C	158/232 (68%)	145 (92%)	13 (8%)	12	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	158/232 (68%)	145 (92%)	13 (8%)	12	3
All	All	637/928 (69%)	589 (92%)	48 (8%)	15	4

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	19	LYS
1	A	42	LEU
1	A	83	ASP
1	A	86	MET
1	A	96	ASN
1	A	102	LYS
1	A	124	ARG
1	A	141	GLU
1	A	187	LEU
1	A	189	ASP
1	B	0	SER
1	B	10	ASN
1	B	42	LEU
1	B	79	ILE
1	B	82	ARG
1	B	96	ASN
1	B	104	LYS
1	B	124	ARG
1	B	187	LEU
1	B	189	ASP
1	B	193	GLN
1	C	10	ASN
1	C	12	MET
1	C	42	LEU
1	C	49	SER
1	C	93	SER
1	C	101	GLU
1	C	102	LYS
1	C	113	LYS
1	C	136	ASN
1	C	140	SER
1	C	176	PHE
1	C	179	ARG
1	C	187	LEU
1	D	24	TYR

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Mol	Chain	Res	Type
1	D	42	LEU
1	D	83	ASP
1	D	89	THR
1	D	96	ASN
1	D	113	LYS
1	D	116	ARG
1	D	124	ARG
1	D	139	LYS
1	D	141	GLU
1	D	142	LYS
1	D	153	GLU
1	D	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	92	ASN
1	A	96	ASN
1	A	115	ASN
1	A	180	GLN
1	B	7	GLN
1	B	10	ASN
1	B	92	ASN
1	B	136	ASN
1	C	10	ASN
1	C	92	ASN
1	D	7	GLN
1	D	92	ASN
1	D	96	ASN
1	D	193	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
3	AMP	A	257	2	22,25,25	1.12	1 (4%)	23,38,38	2.01	9 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	257	2	-	0/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	257	AMP	C5-C4	3.76	1.49	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	257	AMP	N3-C2-N1	-4.85	124.71	128.86
3	A	257	AMP	C4'-O4'-C1'	-3.68	105.99	109.83
3	A	257	AMP	C2'-C3'-C4'	-3.02	96.82	102.62
3	A	257	AMP	O5'-P-O1P	-2.77	98.69	106.47
3	A	257	AMP	O3'-C3'-C4'	-2.21	104.66	111.06
3	A	257	AMP	O2P-P-O5'	-2.19	100.89	106.73
3	A	257	AMP	O4'-C4'-C5'	-2.11	102.36	109.39
3	A	257	AMP	O2P-P-O1P	2.11	118.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	257	AMP	O3P-P-O2P	2.16	116.15	107.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	257	AMP	17	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	177/261 (67%)	-0.21	2 (1%) 80 78	14, 24, 38, 45	0
1	B	180/261 (68%)	0.01	9 (5%) 29 23	15, 25, 44, 56	0
1	C	176/261 (67%)	-0.02	5 (2%) 53 48	17, 29, 45, 61	0
1	D	176/261 (67%)	-0.06	4 (2%) 60 56	16, 27, 44, 64	0
All	All	709/1044 (67%)	-0.07	20 (2%) 53 48	14, 26, 44, 64	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	5.9
1	B	196	ARG	5.7
1	C	100	VAL	4.9
1	C	197	GLY	4.9
1	B	176	PHE	4.7
1	C	196	ARG	4.3
1	B	141	GLU	4.2
1	B	51	PHE	3.9
1	D	196	ARG	3.8
1	B	140	SER	3.7
1	D	24	TYR	3.5
1	B	197	GLY	3.4
1	C	176	PHE	3.4
1	B	74	HIS	3.3
1	C	96	ASN	2.7
1	D	138	ILE	2.4
1	B	138	ILE	2.3
1	A	100	VAL	2.1
1	B	136	ASN	2.1
1	A	-3	PRO	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. 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	B-factors(\AA^2)	Q<0.9
3	AMP	A	257	23/23	0.83	0.34	20,54,60,61	0
2	MG	B	999	1/1	0.96	0.05	28,28,28,28	0
2	MG	C	999	1/1	0.97	0.07	25,25,25,25	0
2	MG	D	999	1/1	0.98	0.05	27,27,27,27	0
2	MG	A	999	1/1	0.99	0.06	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.