wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2024 – 04:13 AM EDT

PDB ID	:	1T8Y
Title	:	Crystal Structure of E.coli AMP Nucleosidase complexed with phosphate
Authors	:	Zhang, Y.; Cottet, S.E.; Ealick, S.E.
Deposited on	:	2004-05-13
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

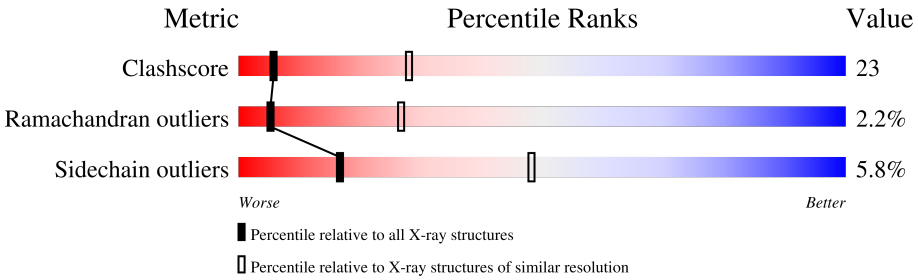
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.00 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	484	61% 31% • 5%
1	B	484	60% 31% • 5%
1	C	484	61% 31% • 5%
1	D	484	58% 33% • 5%
1	E	484	57% 35% • 5%
1	F	484	57% 34% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22005 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	B	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	C	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	D	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	E	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	F	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MSE	MET	modified residue	UNP P15272
A	260	MSE	MET	modified residue	UNP P15272
A	302	MSE	MET	modified residue	UNP P15272
A	404	MSE	MET	modified residue	UNP P15272
B	138	MSE	MET	modified residue	UNP P15272
B	260	MSE	MET	modified residue	UNP P15272
B	302	MSE	MET	modified residue	UNP P15272
B	404	MSE	MET	modified residue	UNP P15272
C	138	MSE	MET	modified residue	UNP P15272
C	260	MSE	MET	modified residue	UNP P15272
C	302	MSE	MET	modified residue	UNP P15272
C	404	MSE	MET	modified residue	UNP P15272
D	138	MSE	MET	modified residue	UNP P15272
D	260	MSE	MET	modified residue	UNP P15272
D	302	MSE	MET	modified residue	UNP P15272
D	404	MSE	MET	modified residue	UNP P15272
E	138	MSE	MET	modified residue	UNP P15272

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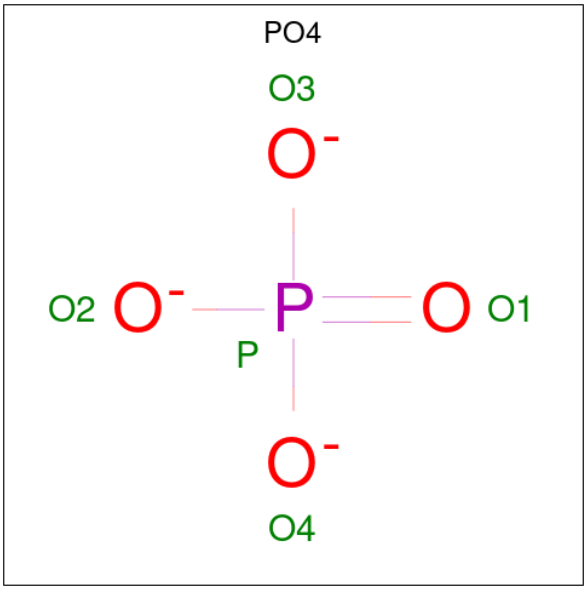
Chain	Residue	Modelled	Actual	Comment	Reference
E	260	MSE	MET	modified residue	UNP P15272
E	302	MSE	MET	modified residue	UNP P15272
E	404	MSE	MET	modified residue	UNP P15272
F	138	MSE	MET	modified residue	UNP P15272
F	260	MSE	MET	modified residue	UNP P15272
F	302	MSE	MET	modified residue	UNP P15272
F	404	MSE	MET	modified residue	UNP P15272

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	B	21	Total O 21 21	0	0
3	C	12	Total O 12 12	0	0
3	D	13	Total O 13 13	0	0
3	E	14	Total O 14 14	0	0
3	F	12	Total O 12 12	0	0

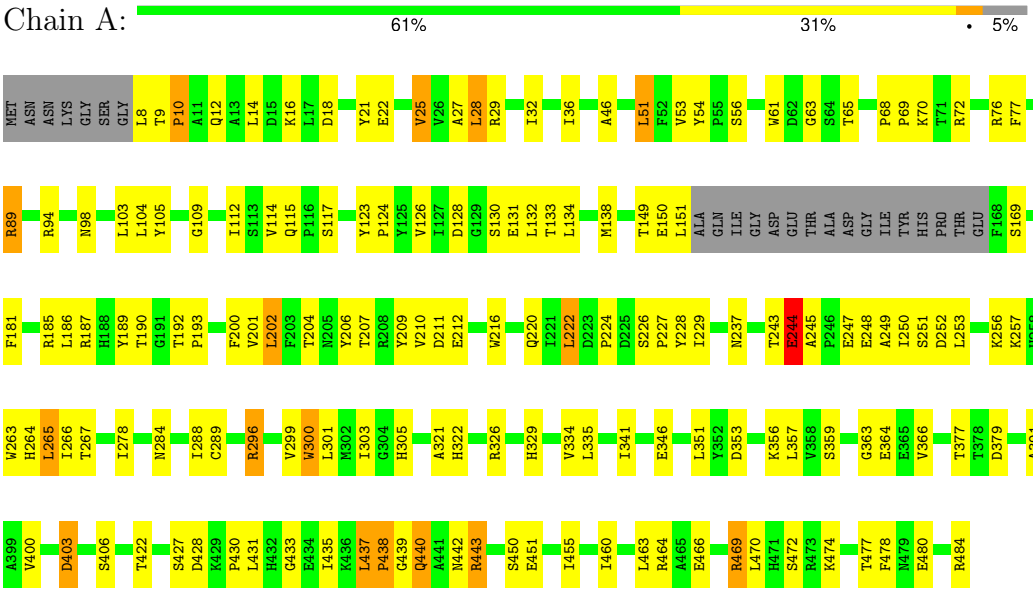
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

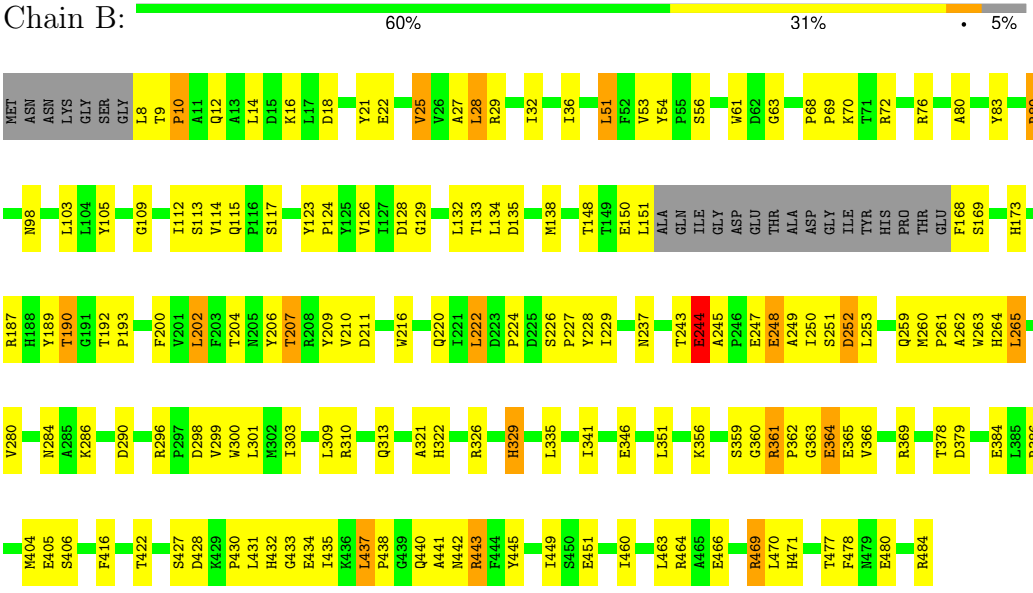
• Molecule 1: AMP nucleosidase

Chain A:



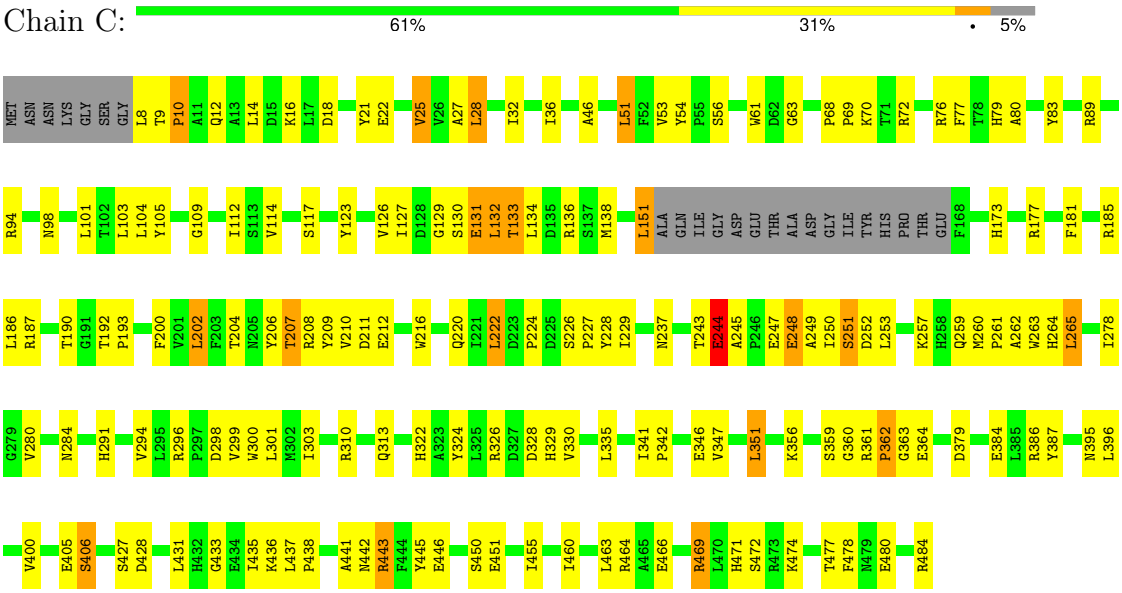
• Molecule 1: AMP nucleosidase

Chain B:



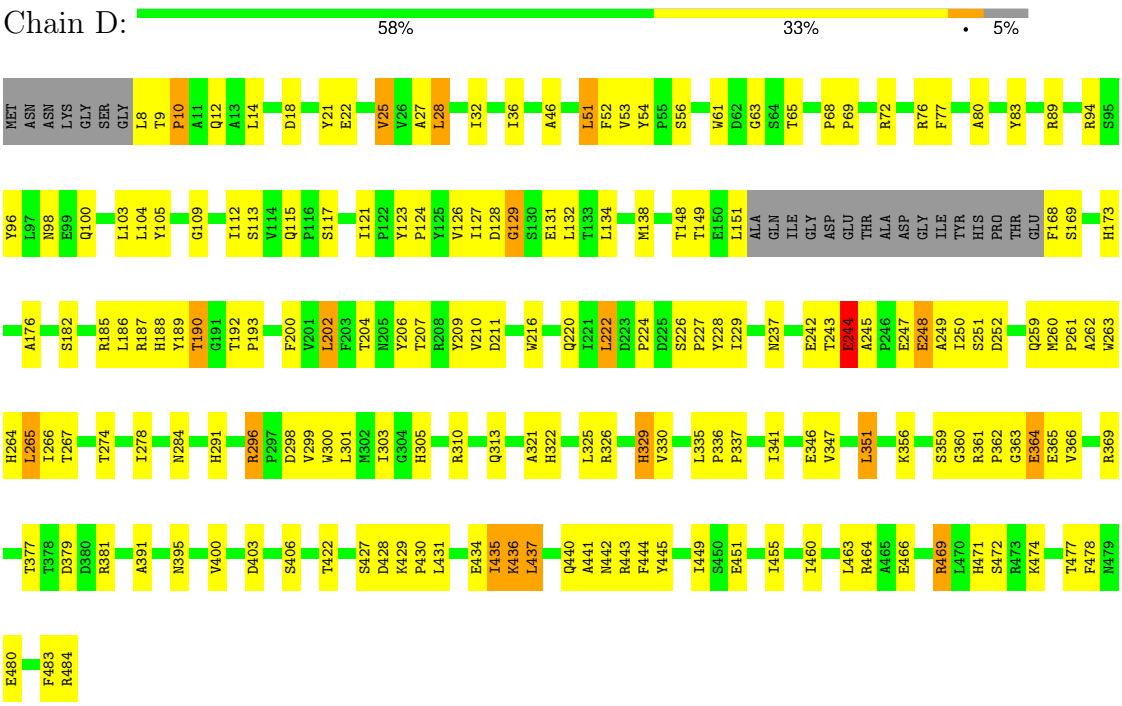
• Molecule 1: AMP nucleosidase

Chain C:



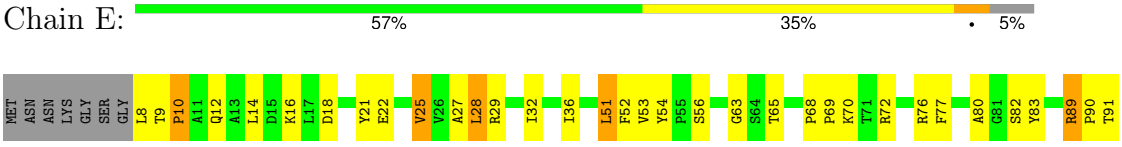
• Molecule 1: AMP nucleosidase

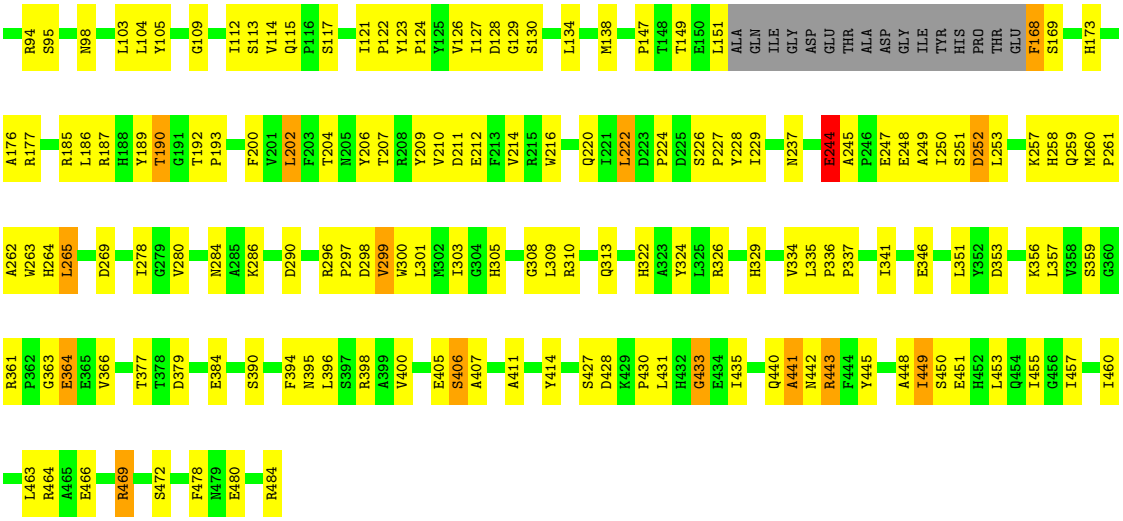
Chain D:



• Molecule 1: AMP nucleosidase

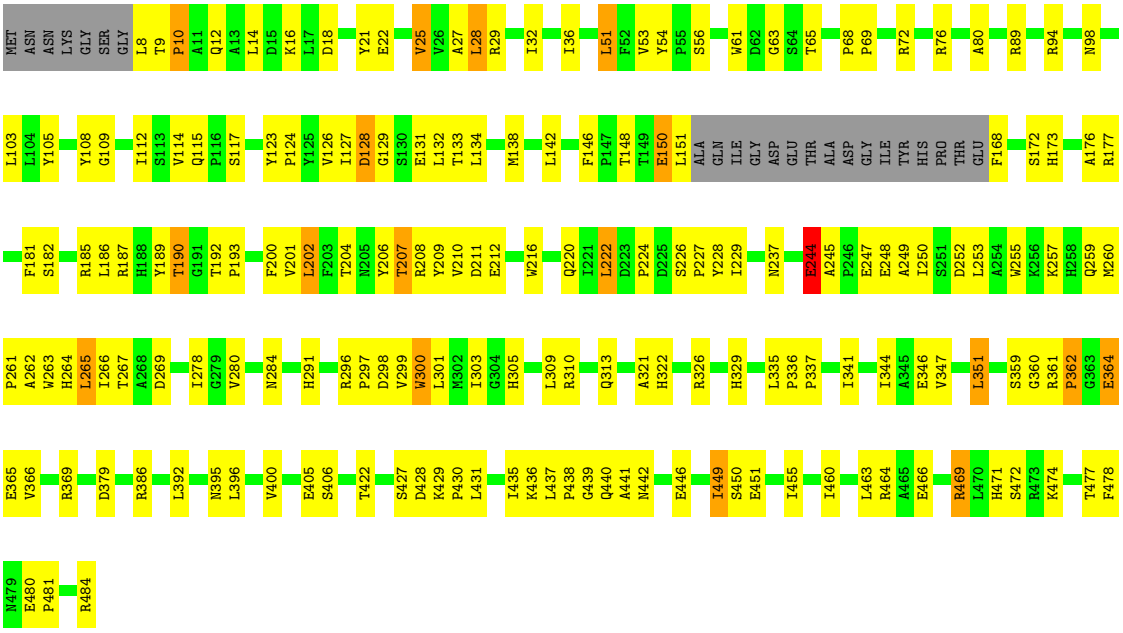
Chain E:





- Molecule 1: AMP nucleosidase

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	268.50Å 268.50Å 114.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.07 – 3.00	Depositor
% Data completeness (in resolution range)	96.0 (34.07-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22005	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.43	0/3738	0.64	0/5088
1	B	0.44	0/3738	0.64	0/5088
1	C	0.44	0/3738	0.66	0/5088
1	D	0.44	0/3738	0.64	0/5088
1	E	0.46	0/3738	0.64	0/5088
1	F	0.44	0/3738	0.65	0/5088
All	All	0.44	0/22428	0.64	0/30528

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3648	0	3576	171	0
1	B	3648	0	3576	177	0
1	C	3648	0	3576	176	0
1	D	3648	0	3576	176	0
1	E	3648	0	3576	178	0
1	F	3648	0	3576	199	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	15	0	0	1	0
3	B	21	0	0	1	0
3	C	12	0	0	2	0
3	D	13	0	0	1	0
3	E	14	0	0	1	0
3	F	12	0	0	1	0
All	All	22005	0	21456	987	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 23.

The worst 5 of 987 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:HH11	1:B:443:ARG:HB3	1.20	1.05
1:E:192:THR:HG21	1:E:264:HIS:NE2	1.72	1.05
1:C:192:THR:HG21	1:C:264:HIS:NE2	1.75	1.02
1:A:131:GLU:HB2	1:B:441:ALA:HB3	1.41	1.02
1:C:151:LEU:H	1:C:151:LEU:HD22	1.22	1.02

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	457/484 (94%)	408 (89%)	39 (8%)	10 (2%)	5 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	457/484 (94%)	409 (90%)	38 (8%)	10 (2%)	5	27
1	C	457/484 (94%)	407 (89%)	41 (9%)	9 (2%)	6	29
1	D	457/484 (94%)	403 (88%)	42 (9%)	12 (3%)	4	23
1	E	457/484 (94%)	410 (90%)	37 (8%)	10 (2%)	5	27
1	F	457/484 (94%)	399 (87%)	50 (11%)	8 (2%)	7	32
All	All	2742/2904 (94%)	2436 (89%)	247 (9%)	59 (2%)	5	27

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	B	244	GLU
1	C	244	GLU
1	D	244	GLU
1	D	436	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	390/403 (97%)	369 (95%)	21 (5%)	18	50
1	B	390/403 (97%)	364 (93%)	26 (7%)	13	43
1	C	390/403 (97%)	368 (94%)	22 (6%)	17	49
1	D	390/403 (97%)	369 (95%)	21 (5%)	18	50
1	E	390/403 (97%)	367 (94%)	23 (6%)	16	47
1	F	390/403 (97%)	367 (94%)	23 (6%)	16	47
All	All	2340/2418 (97%)	2204 (94%)	136 (6%)	17	48

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	51	LEU

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Mol	Chain	Res	Type
1	F	168	PHE
1	F	351	LEU
1	C	28	LEU
1	C	25	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	220	GLN
1	F	284	ASN
1	C	237	ASN
1	C	220	GLN
1	F	313	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	PO4	A	506	-	4,4,4	1.62	0	6,6,6	0.47	0
2	PO4	B	503	-	4,4,4	1.77	2 (50%)	6,6,6	0.50	0
2	PO4	C	502	-	4,4,4	1.66	1 (25%)	6,6,6	0.50	0
2	PO4	E	504	-	4,4,4	1.64	1 (25%)	6,6,6	0.51	0
2	PO4	D	505	-	4,4,4	1.85	2 (50%)	6,6,6	0.47	0
2	PO4	F	501	-	4,4,4	1.70	1 (25%)	6,6,6	0.47	0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	505	PO4	P-O4	-2.42	1.47	1.54
2	F	501	PO4	P-O4	-2.27	1.48	1.54
2	C	502	PO4	P-O4	-2.24	1.48	1.54
2	B	503	PO4	P-O4	-2.15	1.48	1.54
2	E	504	PO4	P-O4	-2.15	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	504	PO4	1	0
2	F	501	PO4	1	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.