



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 06:33 PM EDT

PDB ID : 5OT0  
Title : The thermostable L-asparaginase from *Thermococcus kodakarensis*  
Authors : Guo, J.; Coker, A.R.; Wood, S.P.; Cooper, J.B.; Rashid, N.; Chohan, S.M.; Akhtar, M.  
Deposited on : 2017-08-18  
Resolution : 2.18 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](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

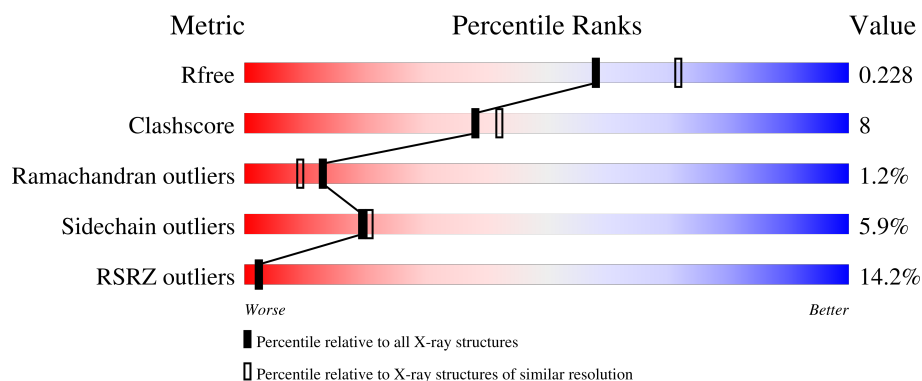
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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))
$R_{free}$	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	328	<div> <div>2%</div> <div>85% 12% ..</div> </div>
1	B	328	<div> <div>2%</div> <div>86% 11% .</div> </div>
1	C	328	<div> <div>2%</div> <div>86% 12% ..</div> </div>
1	D	328	<div> <div>5%</div> <div>87% 11% ..</div> </div>
1	E	328	<div> <div>22%</div> <div>82% 15% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	328	

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	B	401	-	X	-	-
2	PO4	C	401	-	X	-	-
2	PO4	D	401	-	X	-	-
2	PO4	E	401	-	X	-	-

## 2 Entry composition [i](#)

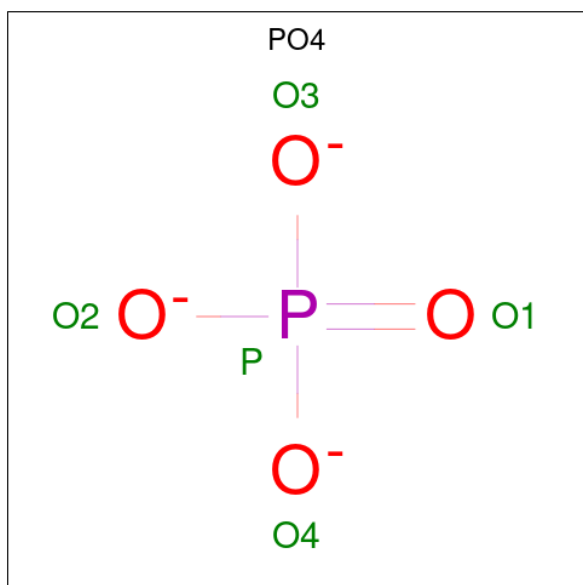
There are 5 unique types of molecules in this entry. The entry contains 15386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-asparaginase.

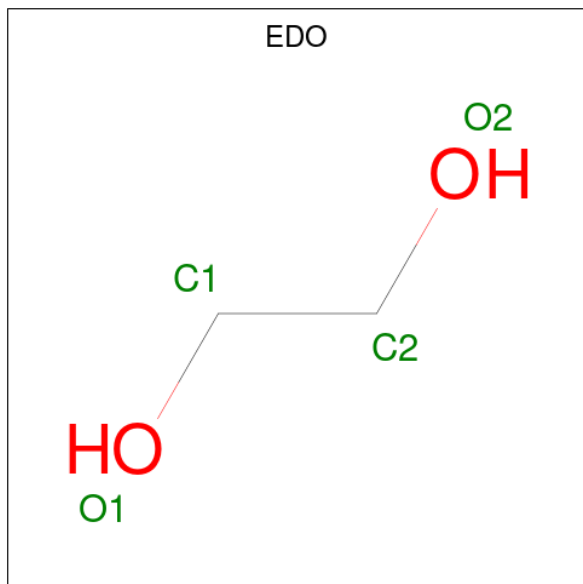
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	2	0
			2520	1595	441	474	10			
1	B	328	Total	C	N	O	S	0	3	0
			2523	1598	438	477	10			
1	C	328	Total	C	N	O	S	0	3	0
			2525	1598	442	475	10			
1	D	328	Total	C	N	O	S	0	1	0
			2510	1589	436	475	10			
1	E	328	Total	C	N	O	S	0	0	0
			2507	1587	436	474	10			
1	F	328	Total	C	N	O	S	0	1	0
			2514	1592	438	474	10			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



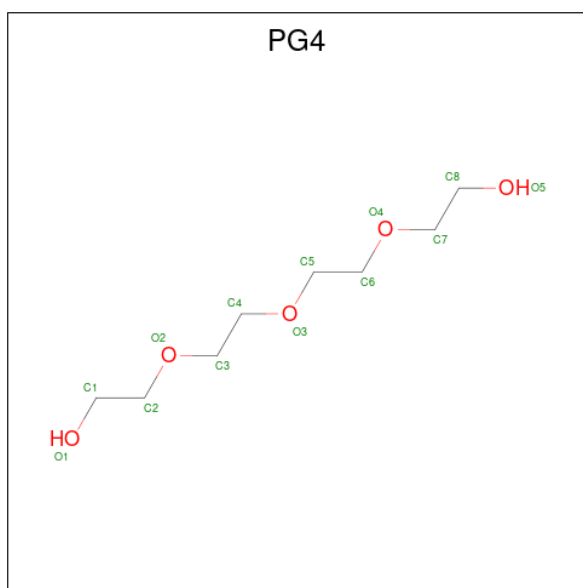
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		

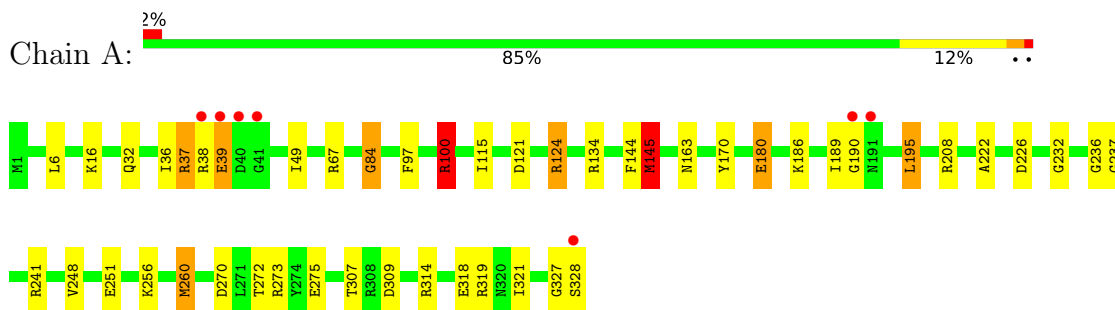
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	B	49	Total	O	0	0
			49	49		
5	C	35	Total	O	0	0
			35	35		
5	D	46	Total	O	0	0
			46	46		
5	E	25	Total	O	0	0
			25	25		
5	F	13	Total	O	0	0
			13	13		

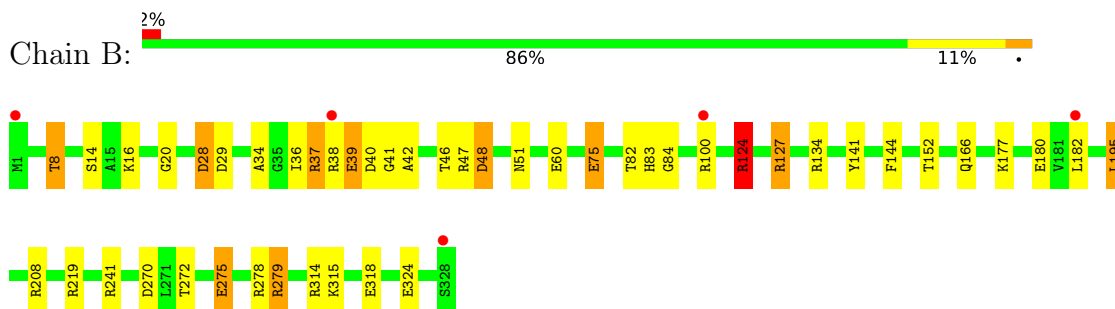
### 3 Residue-property plots [i](#)

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 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.

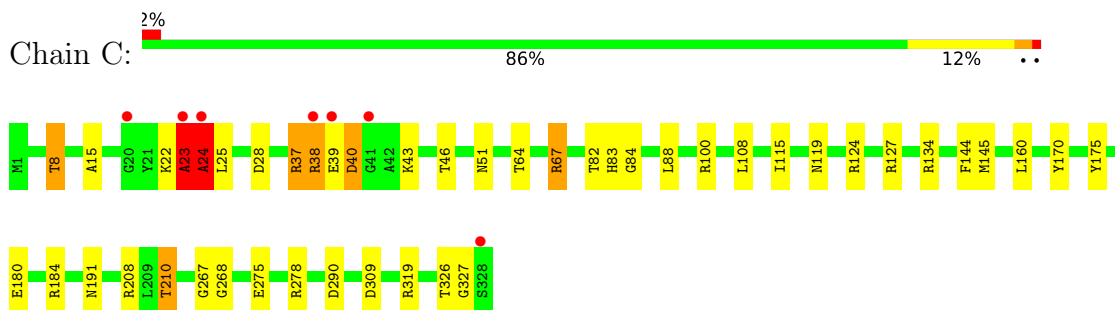
- Molecule 1: L-asparaginase



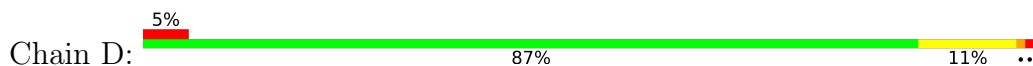
- Molecule 1: L-asparaginase

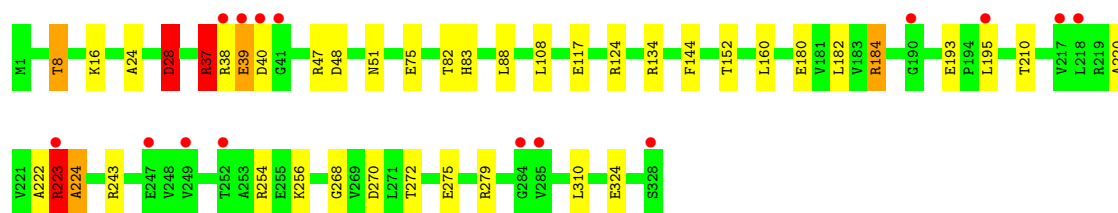


- Molecule 1: L-asparaginase

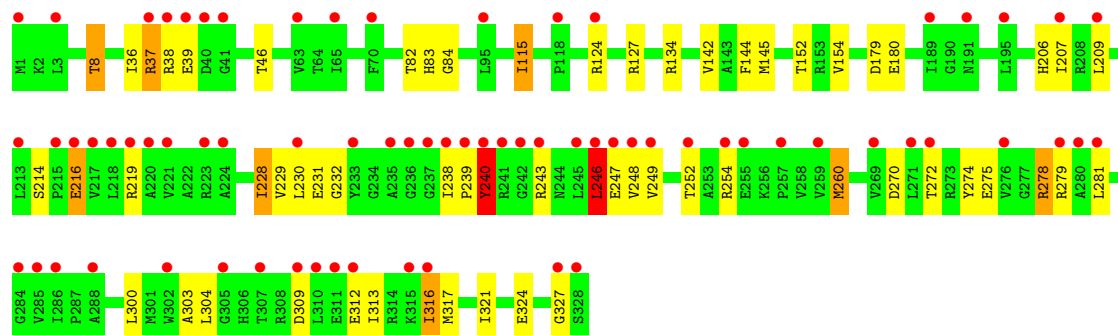
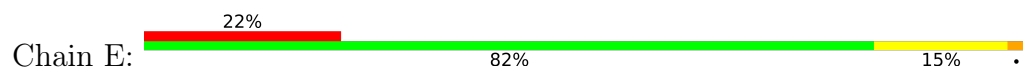


- Molecule 1: L-asparaginase

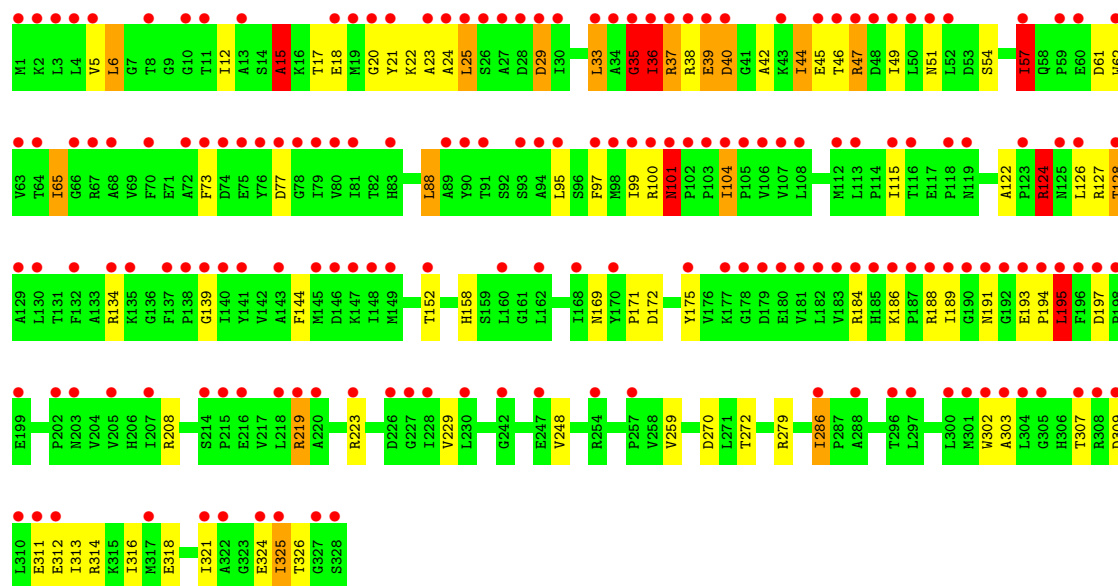
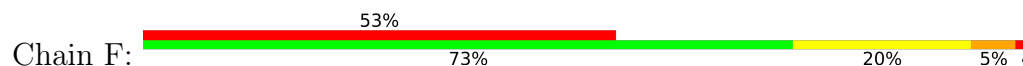




● Molecule 1: L-asparaginase



● Molecule 1: L-asparaginase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.74Å 70.96Å 107.73Å 72.13° 76.22° 87.83°	Depositor
Resolution (Å)	68.65 – 2.18 68.65 – 2.18	Depositor EDS
% Data completeness (in resolution range)	97.5 (68.65-2.18) 97.5 (68.65-2.18)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.224 0.198 , 0.228	Depositor DCC
$R_{free}$ test set	4896 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,k,k-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PG4, EDO

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	1.06	5/2573 (0.2%)	1.06	13/3491 (0.4%)
1	B	1.01	3/2581 (0.1%)	1.08	16/3503 (0.5%)
1	C	1.05	2/2582 (0.1%)	1.09	10/3503 (0.3%)
1	D	0.98	0/2557	1.09	13/3470 (0.4%)
1	E	0.87	0/2551	1.03	8/3462 (0.2%)
1	F	0.86	1/2562 (0.0%)	1.11	17/3477 (0.5%)
All	All	0.98	11/15406 (0.1%)	1.08	77/20906 (0.4%)

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	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	7

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	TYR	CE1-CZ	9.69	1.51	1.38
1	B	141	TYR	CG-CD2	6.17	1.47	1.39
1	B	241	ARG	CZ-NH1	6.16	1.41	1.33
1	A	170	TYR	CE1-CZ	5.92	1.46	1.38
1	A	180	GLU	CD-OE2	5.89	1.32	1.25

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	77	ASP	CB-CG-OD1	12.82	129.84	118.30
1	E	246	LEU	CB-CG-CD2	11.84	131.12	111.00
1	A	124	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	A	145	MET	CG-SD-CE	8.59	113.94	100.20
1	F	124	ARG	NE-CZ-NH1	7.99	124.30	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	ASP	Peptide
1	C	24	ALA	Peptide
1	C	326	THR	Peptide
1	D	37	ARG	Peptide
1	E	309	ASP	Mainchain

## 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	2520	0	2577	28	0
1	B	2523	0	2580	25	1
1	C	2525	0	2581	18	0
1	D	2510	0	2566	16	1
1	E	2507	0	2561	57	0
1	F	2514	0	2568	90	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	D	8	0	12	1	0
3	F	4	0	6	1	0
4	B	10	0	13	2	0
5	A	55	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	49	0	0	2	1
5	C	35	0	0	1	0
5	D	46	0	0	0	1
5	E	25	0	0	2	0
5	F	13	0	0	2	0
All	All	15386	0	15482	233	2

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 8.

The worst 5 of 233 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:C:15:ALA:HB2	1:C:25:LEU:HD11	1.30	1.08
1:F:101:ASN:OD1	1:F:194:PRO:HA	1.61	1.00
1:F:65:ILE:HD11	1:F:95:LEU:HD21	1.45	0.98
1:F:24:ALA:HA	1:F:51:ASN:HD21	1.30	0.97
1:F:12:ILE:HD11	1:F:126:LEU:HD21	1.47	0.94

All (2) 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)
5:B:504:HOH:O	5:D:502:HOH:O[1_445]	1.05	1.15
1:B:51:ASN:OD1	1:D:28:ASP:OD2[1_445]	2.14	0.06

## 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	328/328 (100%)	321 (98%)	5 (2%)	2 (1%)	25 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	330/328 (101%)	319 (97%)	9 (3%)	2 (1%)	25	24
1	C	329/328 (100%)	315 (96%)	9 (3%)	5 (2%)	10	7
1	D	327/328 (100%)	316 (97%)	7 (2%)	4 (1%)	13	9
1	E	326/328 (99%)	315 (97%)	8 (2%)	3 (1%)	17	15
1	F	327/328 (100%)	306 (94%)	14 (4%)	7 (2%)	7	3
All	All	1967/1968 (100%)	1892 (96%)	52 (3%)	23 (1%)	13	9

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	38	ARG
1	B	37	ARG
1	B	38	ARG
1	C	37	ARG

### 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	269/267 (101%)	259 (96%)	10 (4%)	34	40
1	B	271/267 (102%)	259 (96%)	12 (4%)	28	33
1	C	270/267 (101%)	254 (94%)	16 (6%)	19	21
1	D	268/267 (100%)	253 (94%)	15 (6%)	21	23
1	E	267/267 (100%)	247 (92%)	20 (8%)	13	12
1	F	268/267 (100%)	247 (92%)	21 (8%)	12	11
All	All	1613/1602 (101%)	1519 (94%)	94 (6%)	19	21

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	144	PHE

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Mol	Chain	Res	Type
1	E	316	ILE
1	E	179	ASP
1	E	243	ARG
1	F	36	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	51	ASN
1	E	163	ASN
1	B	166	GLN
1	B	163	ASN
1	C	119	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 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	C	401	-	4,4,4	1.67	1 (25%)	6,6,6	3.23	5 (83%)
3	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.84	0
4	PG4	B	404	-	9,9,12	0.44	0	8,8,11	1.07	1 (12%)
3	EDO	B	402	-	3,3,3	0.69	0	2,2,2	0.61	0
3	EDO	D	403	-	3,3,3	0.72	0	2,2,2	0.51	0
3	EDO	F	402	-	3,3,3	0.60	0	2,2,2	0.19	0
2	PO4	A	401	-	4,4,4	2.12	1 (25%)	6,6,6	2.41	2 (33%)
3	EDO	A	402	-	3,3,3	1.10	0	2,2,2	0.48	0
2	PO4	E	401	-	4,4,4	1.92	1 (25%)	6,6,6	1.87	3 (50%)
3	EDO	B	403	-	3,3,3	0.60	0	2,2,2	0.90	0
2	PO4	D	401	-	4,4,4	2.47	2 (50%)	6,6,6	3.93	5 (83%)
2	PO4	F	401	-	4,4,4	2.14	1 (25%)	6,6,6	1.26	1 (16%)
2	PO4	B	401	-	4,4,4	2.11	1 (25%)	6,6,6	3.15	3 (50%)

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	EDO	D	402	-	-	1/1/1/1	-
4	PG4	B	404	-	-	5/7/7/10	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	F	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PO4	P-O4	-3.89	1.42	1.54
2	F	401	PO4	P-O1	3.87	1.59	1.50
2	A	401	PO4	P-O2	-3.47	1.44	1.54
2	B	401	PO4	P-O4	-2.94	1.45	1.54
2	D	401	PO4	P-O2	-2.89	1.45	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PO4	O4-P-O1	-6.00	88.92	110.89
2	B	401	PO4	O2-P-O1	-5.71	90.00	110.89
2	C	401	PO4	O4-P-O3	5.08	124.26	107.97
2	D	401	PO4	O3-P-O2	-4.53	93.43	107.97
2	B	401	PO4	O3-P-O2	3.92	120.56	107.97

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	PG4	O2-C3-C4-O3
4	B	404	PG4	O1-C1-C2-O2
4	B	404	PG4	C6-C5-O3-C4
3	F	402	EDO	O1-C1-C2-O2
4	B	404	PG4	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	1	0
4	B	404	PG4	2	0
3	D	403	EDO	1	0
3	F	402	EDO	1	0
2	A	401	PO4	1	0
2	E	401	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	328/328 (100%)	0.45	7 (2%) 63 64	34, 56, 96, 147	0
1	B	328/328 (100%)	0.49	5 (1%) 73 74	41, 64, 107, 150	0
1	C	328/328 (100%)	0.53	7 (2%) 63 64	36, 61, 105, 145	0
1	D	328/328 (100%)	0.61	15 (4%) 32 33	41, 64, 106, 165	0
1	E	328/328 (100%)	1.23	71 (21%) 0 0	44, 78, 146, 180	0
1	F	328/328 (100%)	2.57	174 (53%) 0 0	56, 115, 167, 205	0
All	All	1968/1968 (100%)	0.98	279 (14%) 2 2	34, 69, 140, 205	0

The worst 5 of 279 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	328	SER	13.1
1	F	78	GLY	12.3
1	E	328	SER	11.9
1	E	240	TYR	11.8
1	E	242	GLY	11.7

### 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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	PO4	F	401	5/5	0.88	0.16	98,99,103,106	0
4	PG4	B	404	10/13	0.89	0.20	73,79,89,90	0
3	EDO	B	403	4/4	0.93	0.21	60,61,66,66	0
3	EDO	A	402	4/4	0.95	0.16	42,43,44,45	0
3	EDO	F	402	4/4	0.95	0.16	68,72,72,75	0
3	EDO	B	402	4/4	0.95	0.17	48,51,52,53	0
3	EDO	D	402	4/4	0.96	0.20	59,60,63,65	0
2	PO4	C	401	5/5	0.98	0.16	62,63,69,71	0
3	EDO	D	403	4/4	0.98	0.14	58,61,62,65	0
2	PO4	E	401	5/5	0.99	0.12	50,53,54,55	0
2	PO4	A	401	5/5	0.99	0.19	41,45,48,48	0
2	PO4	D	401	5/5	0.99	0.16	46,48,55,56	0
2	PO4	B	401	5/5	1.00	0.19	49,49,54,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.