



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 01:55 AM EST

PDB ID : 3PEI  
Title : Crystal Structure of Cytosol Aminopeptidase from *Francisella tularensis*  
Authors : Maltseva, N.; Kim, Y.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2010-10-26  
Resolution : 2.70 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](mailto: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 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

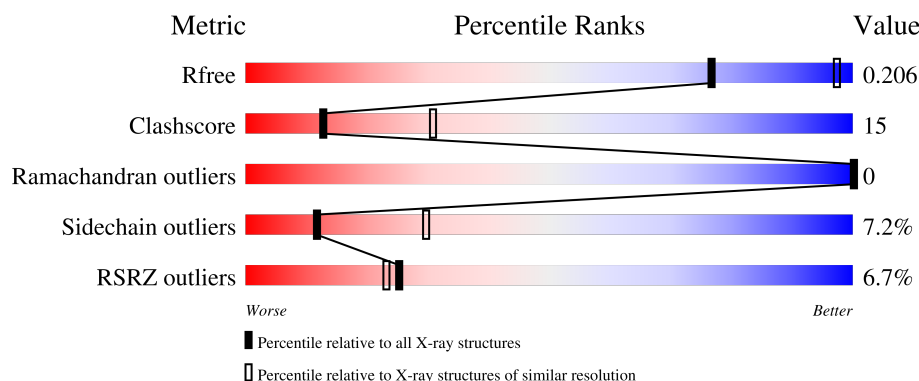
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	486	

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
3	EDO	A	506	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	510	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4014 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 Cytosol aminopeptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	Se	8	11	0
			3572	2252	589	703	7	21			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	expression tag	UNP Q5NFC1
A	480	GLU	-	expression tag	UNP Q5NFC1
A	481	ASN	-	expression tag	UNP Q5NFC1
A	482	LEU	-	expression tag	UNP Q5NFC1
A	483	TYR	-	expression tag	UNP Q5NFC1
A	484	PHE	-	expression tag	UNP Q5NFC1
A	485	GLN	-	expression tag	UNP Q5NFC1

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	K	0	0
			3	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

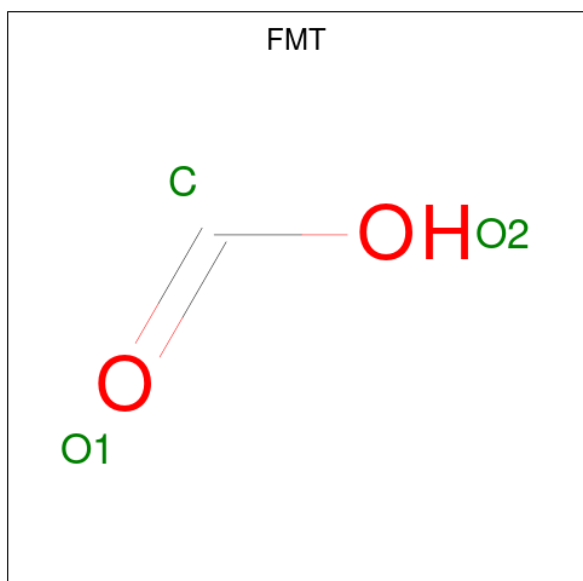


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

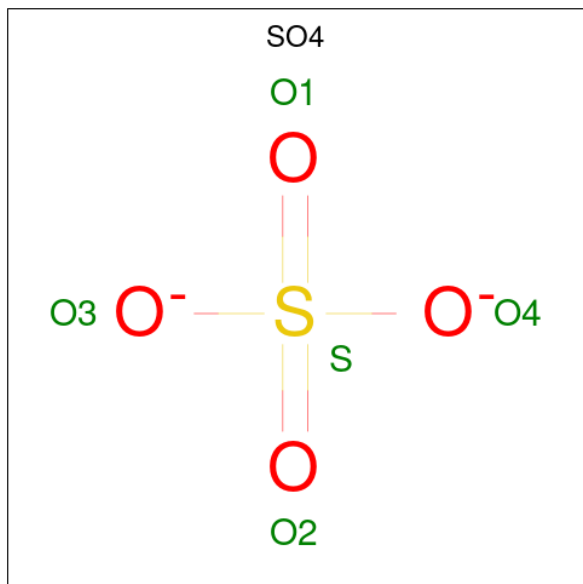
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Cl	0	0
			5	5		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		

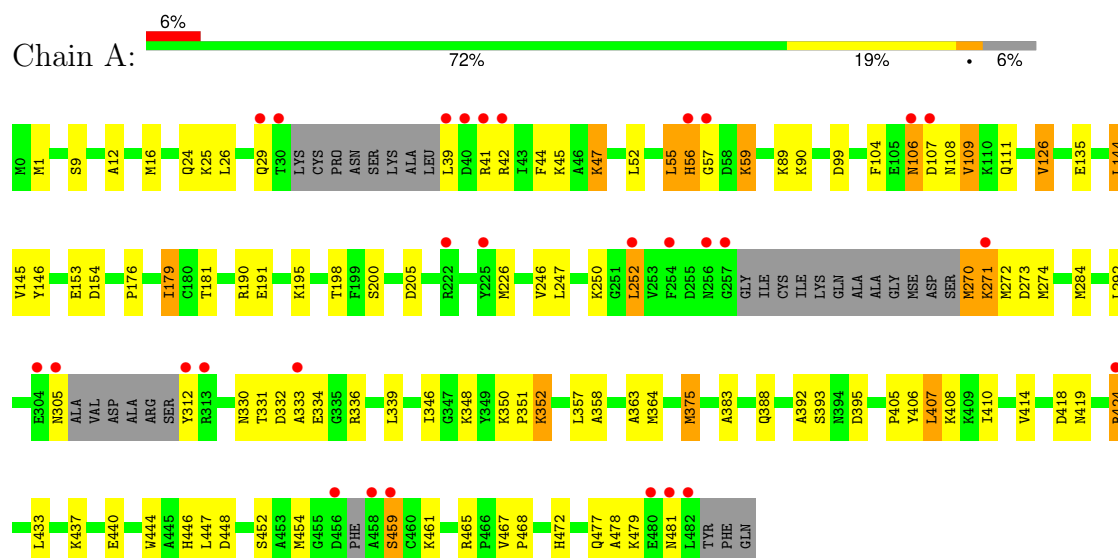
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	366	Total	O	0	0
			366	366		

### 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: Cytosol aminopeptidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.48Å 161.48Å 105.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.70) 99.7 (50.00-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.02 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.165 , 0.210 0.161 , 0.206	Depositor DCC
$R_{free}$ test set	1159 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: PEG, CL, EDO, K, FMT, SO4

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	0.53	0/3596	0.65	1/4815 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	144	LEU	CA-CB-CG	-5.05	103.69	115.30

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	3572	0	3586	105	0
2	A	3	0	0	0	0
3	A	40	0	60	12	0
4	A	14	0	20	3	0
5	A	5	0	0	1	0
6	A	9	0	3	1	0
7	A	5	0	0	0	0
8	A	366	0	0	30	0
All	All	4014	0	3669	109	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 15.

All (109) 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:25:LYS:HZ2	4:A:492:PEG:H22	1.40	0.86
1:A:252:LEU:HD22	1:A:305:ASN:OD1	1.80	0.82
1:A:424[A]:ARG:HH11	1:A:424[A]:ARG:HG3	1.45	0.81
1:A:24:GLN:HG3	1:A:41:ARG:HH22	1.43	0.81
1:A:191[B]:GLU:HG2	8:A:813:HOH:O	1.83	0.78
1:A:55:LEU:H	1:A:55:LEU:HD12	1.48	0.77
1:A:181:THR:HG22	1:A:226:MSE:HE2	1.67	0.77
1:A:25:LYS:NZ	4:A:492:PEG:H22	2.03	0.74
1:A:408:LYS:HE2	3:A:506:EDO:H11	1.70	0.73
1:A:25:LYS:HE2	1:A:29:GLN:NE2	2.02	0.73
1:A:42:ARG:O	1:A:42:ARG:HD2	1.89	0.73
1:A:176:PRO:HG2	1:A:179:ILE:HG13	1.70	0.72
1:A:16:MSE:HE3	1:A:26:LEU:HD11	1.72	0.72
1:A:252:LEU:CD2	1:A:305:ASN:OD1	2.37	0.72
1:A:408:LYS:HE2	3:A:506:EDO:C1	2.19	0.72
1:A:395:ASP:OD1	1:A:465:ARG:HD2	1.91	0.71
1:A:352:LYS:HZ3	1:A:477:GLN:HE21	1.39	0.71
1:A:205:ASP:HB2	8:A:722:HOH:O	1.93	0.69
1:A:352:LYS:NZ	1:A:477:GLN:NE2	2.40	0.69
1:A:312:TYR:CD2	8:A:728:HOH:O	2.45	0.69
1:A:250:LYS:HA	8:A:853:HOH:O	1.95	0.67
1:A:25:LYS:HE2	1:A:29:GLN:HE21	1.59	0.66
1:A:352:LYS:HZ3	1:A:477:GLN:NE2	1.93	0.65
1:A:24:GLN:HG3	1:A:41:ARG:NH2	2.12	0.65
1:A:106:ASN:OD1	1:A:107:ASP:N	2.30	0.65
5:A:505:CL:CL	8:A:770:HOH:O	2.51	0.65
1:A:111:GLN:HE22	1:A:472:HIS:HE1	1.48	0.62
3:A:493:EDO:H22	8:A:710:HOH:O	1.99	0.61
1:A:405:PRO:O	1:A:408:LYS:HD2	2.01	0.60
1:A:364:MSE:HE3	1:A:448:ASP:HB3	1.83	0.60
1:A:44:PHE:HB2	1:A:52:LEU:HD22	1.84	0.59
1:A:90:LYS:HE3	8:A:867:HOH:O	2.02	0.59
1:A:59:LYS:HE2	8:A:852:HOH:O	2.02	0.59
1:A:57:GLY:HA3	8:A:669:HOH:O	2.02	0.58
1:A:388:GLN:NE2	8:A:752:HOH:O	2.35	0.58
1:A:393:SER:HB3	1:A:472:HIS:CD2	2.38	0.58
1:A:467:VAL:N	1:A:468:PRO:CD	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HD12	1:A:284:MSE:HE3	1.86	0.58
1:A:106:ASN:OD1	1:A:106:ASN:C	2.43	0.57
1:A:352:LYS:NZ	1:A:477:GLN:HE21	1.98	0.57
1:A:89:LYS:HE2	1:A:135:GLU:OE2	2.04	0.56
1:A:56:HIS:ND1	1:A:57:GLY:N	2.52	0.56
1:A:424[A]:ARG:HG3	1:A:424[A]:ARG:NH1	2.17	0.56
1:A:109:VAL:HG11	1:A:146:TYR:CE1	2.41	0.55
1:A:363:ALA:HB1	8:A:821:HOH:O	2.06	0.55
1:A:392:ALA:CB	3:A:510:EDO:H22	2.37	0.54
1:A:246:VAL:HG23	1:A:351:PRO:HB3	1.89	0.54
1:A:468:PRO:O	1:A:472:HIS:HD2	1.89	0.54
1:A:270:MSE:SE	1:A:272:MSE:HE3	2.57	0.54
1:A:357:LEU:HG	8:A:762:HOH:O	2.07	0.53
1:A:55:LEU:HD12	1:A:55:LEU:N	2.22	0.53
1:A:25:LYS:O	1:A:29:GLN:HG2	2.08	0.53
1:A:1:MSE:HE1	3:A:507:EDO:H21	1.91	0.53
1:A:408:LYS:CE	3:A:506:EDO:H11	2.39	0.53
1:A:273:ASP:HB2	8:A:711:HOH:O	2.08	0.52
1:A:333:ALA:O	1:A:336:ARG:HG2	2.09	0.52
1:A:424[B]:ARG:NE	8:A:851:HOH:O	2.41	0.52
1:A:479:LYS:HE3	8:A:730:HOH:O	2.10	0.52
1:A:108:ASN:HA	8:A:747:HOH:O	2.09	0.52
1:A:407:LEU:HD13	1:A:433:LEU:HB3	1.91	0.52
1:A:90:LYS:CE	8:A:867:HOH:O	2.57	0.52
3:A:511:EDO:H22	8:A:866:HOH:O	2.08	0.52
1:A:478:ALA:O	1:A:481:ASN:HB2	2.10	0.51
1:A:273:ASP:OD1	3:A:503:EDO:H11	2.11	0.51
1:A:392:ALA:HB2	3:A:510:EDO:H22	1.93	0.51
1:A:39:LEU:HD23	1:A:42:ARG:CB	2.41	0.51
1:A:270:MSE:SE	1:A:272:MSE:CE	3.09	0.50
1:A:444:TRP:CZ2	1:A:446:HIS:HB2	2.47	0.49
1:A:111:GLN:HE22	1:A:472:HIS:CE1	2.28	0.48
1:A:191[A]:GLU:O	1:A:195:LYS:HG3	2.13	0.48
1:A:461:LYS:NZ	8:A:673:HOH:O	2.46	0.48
1:A:271:LYS:O	1:A:454[A]:MSE:HE1	2.14	0.47
1:A:42:ARG:HD2	1:A:42:ARG:C	2.34	0.47
1:A:39:LEU:HB3	1:A:42:ARG:HB3	1.96	0.47
1:A:271:LYS:HG2	8:A:839:HOH:O	2.13	0.47
1:A:331:THR:O	1:A:334:GLU:HG3	2.15	0.47
1:A:339:LEU:HD11	1:A:358:ALA:HB2	1.98	0.46
1:A:89:LYS:HE3	8:A:861:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLU:HG2	8:A:835:HOH:O	2.16	0.46
1:A:272:MSE:HE2	1:A:454[B]:MSE:HE1	1.97	0.46
1:A:1:MSE:HE2	1:A:1:MSE:HB2	1.95	0.45
1:A:59:LYS:CE	8:A:852:HOH:O	2.63	0.45
1:A:104:PHE:HA	6:A:500:FMT:H	1.98	0.45
1:A:350:LYS:N	1:A:351:PRO:CD	2.80	0.45
1:A:437:LYS:HA	1:A:437:LYS:HD2	1.79	0.45
1:A:99:ASP:HA	1:A:145:VAL:HB	1.98	0.45
1:A:350:LYS:N	1:A:351:PRO:HD3	2.32	0.44
1:A:375:MSE:HB3	1:A:447:LEU:HD23	1.99	0.44
1:A:408:LYS:CE	3:A:506:EDO:C1	2.91	0.44
1:A:459:SER:O	8:A:668:HOH:O	2.21	0.44
1:A:274:MSE:HB3	8:A:831:HOH:O	2.17	0.44
1:A:126:VAL:HG22	8:A:803:HOH:O	2.19	0.43
1:A:375:MSE:HE1	1:A:383:ALA:HA	2.01	0.43
1:A:333:ALA:HB3	1:A:419:ASN:ND2	2.34	0.42
1:A:375:MSE:CB	1:A:447:LEU:HD23	2.49	0.42
1:A:12:ALA:O	1:A:59:LYS:HB2	2.19	0.42
1:A:330:ASN:OD1	1:A:332:ASP:HB2	2.20	0.42
1:A:39:LEU:C	1:A:41:ARG:N	2.70	0.42
1:A:406:TYR:HD1	3:A:493:EDO:H11	1.85	0.41
1:A:247:LEU:HD12	1:A:284:MSE:CE	2.49	0.41
1:A:246:VAL:CG2	1:A:351:PRO:HB3	2.50	0.41
1:A:39:LEU:HD12	1:A:39:LEU:N	2.35	0.41
1:A:126:VAL:HG13	8:A:582:HOH:O	2.20	0.41
1:A:190:ARG:NH2	8:A:761:HOH:O	2.33	0.41
1:A:424[A]:ARG:NE	8:A:827:HOH:O	2.41	0.41
4:A:508:PEG:H32	8:A:715:HOH:O	2.20	0.41
1:A:45:LYS:HB2	1:A:47:LYS:HD3	2.01	0.40
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.86	0.40
1:A:452:SER:O	3:A:504:EDO:H22	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	457/486 (94%)	444 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	385/376 (102%)	356 (92%)	29 (8%)	11	28

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	47	LYS
1	A	55	LEU
1	A	56	HIS
1	A	59	LYS
1	A	106	ASN
1	A	109	VAL
1	A	126	VAL
1	A	144	LEU
1	A	153	GLU
1	A	154	ASP
1	A	179	ILE
1	A	198	THR
1	A	200	SER
1	A	252	LEU
1	A	270	MSE
1	A	271	LYS
1	A	346	ILE
1	A	348	LYS
1	A	352	LYS
1	A	375	MSE

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Mol	Chain	Res	Type
1	A	407	LEU
1	A	410[A]	ILE
1	A	410[B]	ILE
1	A	414	VAL
1	A	418	ASP
1	A	424[A]	ARG
1	A	424[B]	ARG
1	A	459	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	388	GLN
1	A	472	HIS
1	A	477	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](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	EDO	A	511	-	3,3,3	0.50	0	2,2,2	0.28	0
3	EDO	A	512	-	3,3,3	0.42	0	2,2,2	0.38	0
6	FMT	A	500	-	2,2,2	0.67	0	1,1,1	0.03	0
3	EDO	A	507	-	3,3,3	0.39	0	2,2,2	0.46	0
3	EDO	A	493	-	3,3,3	0.46	0	2,2,2	0.08	0
3	EDO	A	491	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	506	-	3,3,3	0.33	0	2,2,2	0.80	0
3	EDO	A	504	-	3,3,3	0.50	0	2,2,2	0.16	0
3	EDO	A	510	-	3,3,3	0.13	0	2,2,2	2.42	2 (100%)
4	PEG	A	492	-	6,6,6	0.44	0	5,5,5	0.53	0
4	PEG	A	508	-	6,6,6	0.49	0	5,5,5	0.46	0
6	FMT	A	501	-	2,2,2	0.64	0	1,1,1	0.03	0
6	FMT	A	509	-	2,2,2	0.66	0	1,1,1	0.09	0
7	SO4	A	513	-	4,4,4	0.30	0	6,6,6	0.32	0
3	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.22	0
3	EDO	A	502	-	3,3,3	0.50	0	2,2,2	0.63	0

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	A	511	-	-	1/1/1/1	-
3	EDO	A	512	-	-	1/1/1/1	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	A	493	-	-	0/1/1/1	-
3	EDO	A	491	-	-	0/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
4	PEG	A	492	-	-	1/4/4/4	-
4	PEG	A	508	-	-	3/4/4/4	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	EDO	O1-C1-C2	-2.46	93.67	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	EDO	O2-C2-C1	-2.39	94.19	112.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	508	PEG	O2-C3-C4-O4
4	A	508	PEG	O1-C1-C2-O2
3	A	510	EDO	O1-C1-C2-O2
3	A	506	EDO	O1-C1-C2-O2
3	A	512	EDO	O1-C1-C2-O2
4	A	508	PEG	C1-C2-O2-C3
4	A	492	PEG	C4-C3-O2-C2
3	A	511	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	511	EDO	1	0
6	A	500	FMT	1	0
3	A	507	EDO	1	0
3	A	493	EDO	2	0
3	A	506	EDO	4	0
3	A	504	EDO	1	0
3	A	510	EDO	2	0
4	A	492	PEG	2	0
4	A	508	PEG	1	0
3	A	503	EDO	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 ⓘ

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	435/486 (89%)	-0.41	29 (6%) 25 23	20, 43, 99, 169	9 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	TYR	7.6
1	A	225[A]	TYR	6.4
1	A	106	ASN	4.9
1	A	254	PHE	4.8
1	A	458	ALA	4.7
1	A	56	HIS	4.5
1	A	40	ASP	4.2
1	A	41	ARG	4.2
1	A	459	SER	4.1
1	A	482	LEU	4.1
1	A	39	LEU	3.7
1	A	305	ASN	3.6
1	A	257	GLY	3.6
1	A	481	ASN	3.3
1	A	30	THR	3.3
1	A	107	ASP	3.2
1	A	222	ARG	3.2
1	A	456	ASP	3.1
1	A	424[A]	ARG	2.9
1	A	271	LYS	2.9
1	A	313	ARG	2.6
1	A	304	GLU	2.5
1	A	480[A]	GLU	2.4
1	A	42	ARG	2.4
1	A	57	GLY	2.3
1	A	29	GLN	2.1
1	A	256	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	2.1
1	A	252	LEU	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 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
3	EDO	A	502	4/4	0.79	0.28	67,71,73,74	0
4	PEG	A	508	7/7	0.83	0.22	86,92,99,101	0
5	CL	A	514	1/1	0.86	0.14	37,37,37,37	0
3	EDO	A	512	4/4	0.88	0.13	69,70,70,70	4
3	EDO	A	506	4/4	0.89	0.15	54,55,62,74	0
3	EDO	A	503	4/4	0.91	0.17	68,69,70,72	0
4	PEG	A	492	7/7	0.91	0.15	80,86,92,94	0
6	FMT	A	500	3/3	0.92	0.15	67,67,68,68	0
3	EDO	A	511	4/4	0.94	0.17	46,48,56,62	0
6	FMT	A	501	3/3	0.94	0.18	72,72,72,74	0
6	FMT	A	509	3/3	0.94	0.15	67,67,71,73	0
7	SO4	A	513	5/5	0.94	0.25	39,40,40,40	0
5	CL	A	498	1/1	0.96	0.10	85,85,85,85	0
3	EDO	A	504	4/4	0.96	0.19	68,71,71,72	0
3	EDO	A	493	4/4	0.96	0.08	51,53,56,63	0
2	K	A	497	1/1	0.97	0.06	83,83,83,83	0
3	EDO	A	507	4/4	0.97	0.11	71,72,74,75	0
3	EDO	A	491	4/4	0.97	0.10	65,66,70,75	0
5	CL	A	496	1/1	0.98	0.05	52,52,52,52	0
2	K	A	490	1/1	0.98	0.06	48,48,48,48	0
5	CL	A	505	1/1	0.98	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	A	495	1/1	0.98	0.07	48,48,48,48	0
3	EDO	A	510	4/4	0.99	0.05	29,34,37,38	0
5	CL	A	494	1/1	0.99	0.08	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.