



wwPDB X-ray Structure Validation Summary Report

Oct 15, 2014 – 05:06 PM EDT

PDB ID : 4MLB
Title : Reverse polarity of binding pocket suggests different function of a MOP superfamily transporter from *Pyrococcus furiosus* Vc1 (DSM3638)
Authors : Malviya, V.N.; Nonaka, T.; Muenke, C.; Koepke, J.; Michel, H.
Deposited on : 2013-09-06
Resolution : 2.35 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

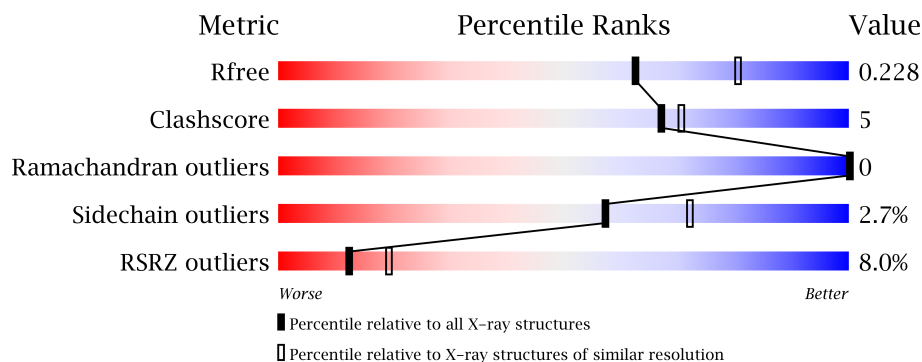
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23828
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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}	66092	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	492	
1	B	492	
1	C	492	
1	D	492	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CXE	A	502	-	X
2	CXE	A	503	-	X
2	CXE	A	505	-	X
2	CXE	A	506	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	CXE	A	507	-	X
2	CXE	A	508	-	X
2	CXE	A	509	-	X
2	CXE	A	510	-	X
2	CXE	A	511	-	X
2	CXE	A	512	-	X
2	CXE	A	513	-	X
2	CXE	A	514	-	X
2	CXE	A	517	-	X
2	CXE	B	502	-	X
2	CXE	B	504	-	X
2	CXE	B	505	-	X
2	CXE	B	506	-	X
2	CXE	B	507	-	X
2	CXE	B	508	-	X
2	CXE	B	509	-	X
2	CXE	B	511	-	X
2	CXE	B	512	-	X
2	CXE	C	501	-	X
2	CXE	C	502	-	X
2	CXE	C	503	-	X
2	CXE	C	504	-	X
2	CXE	C	505	-	X
2	CXE	C	506	-	X
2	CXE	C	507	-	X
2	CXE	C	508	-	X
2	CXE	C	509	-	X
2	CXE	C	510	-	X
2	CXE	C	511	-	X
2	CXE	C	512	-	X
2	CXE	C	514	-	X
2	CXE	C	515	-	X
2	CXE	C	516	-	X
2	CXE	D	502	-	X
2	CXE	D	505	-	X
2	CXE	D	507	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14749 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PF0708.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	1	0
			3412	2237	557	597	21			
1	B	454	Total	C	N	O	S	0	0	0
			3413	2237	555	600	21			
1	C	452	Total	C	N	O	S	0	2	0
			3418	2241	559	597	21			
1	D	452	Total	C	N	O	S	0	2	0
			3418	2241	559	597	21			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q8U2X0
A	-5	GLY	-	EXPRESSION TAG	UNP Q8U2X0
A	-4	GLY	-	EXPRESSION TAG	UNP Q8U2X0
A	-3	SER	-	EXPRESSION TAG	UNP Q8U2X0
A	-2	GLU	-	EXPRESSION TAG	UNP Q8U2X0
A	-1	ILE	-	EXPRESSION TAG	UNP Q8U2X0
A	0	PRO	-	EXPRESSION TAG	UNP Q8U2X0
A	298	THR	ALA	CONFLICT	UNP Q8U2X0
A	462	ARG	-	EXPRESSION TAG	UNP Q8U2X0
A	463	ASN	-	EXPRESSION TAG	UNP Q8U2X0
A	464	SER	-	EXPRESSION TAG	UNP Q8U2X0
A	465	GLU	-	EXPRESSION TAG	UNP Q8U2X0
A	466	ASN	-	EXPRESSION TAG	UNP Q8U2X0
A	467	LEU	-	EXPRESSION TAG	UNP Q8U2X0
A	468	TYR	-	EXPRESSION TAG	UNP Q8U2X0
A	469	PHE	-	EXPRESSION TAG	UNP Q8U2X0
A	470	GLN	-	EXPRESSION TAG	UNP Q8U2X0
A	471	GLY	-	EXPRESSION TAG	UNP Q8U2X0
A	472	GLY	-	EXPRESSION TAG	UNP Q8U2X0
A	473	ARG	-	EXPRESSION TAG	UNP Q8U2X0
A	474	GLY	-	EXPRESSION TAG	UNP Q8U2X0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	EXPRESSION TAG	UNP Q8U2X0
A	476	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	477	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	478	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	479	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	480	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	481	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	482	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	483	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	484	HIS	-	EXPRESSION TAG	UNP Q8U2X0
A	485	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	-6	MET	-	EXPRESSION TAG	UNP Q8U2X0
B	-5	GLY	-	EXPRESSION TAG	UNP Q8U2X0
B	-4	GLY	-	EXPRESSION TAG	UNP Q8U2X0
B	-3	SER	-	EXPRESSION TAG	UNP Q8U2X0
B	-2	GLU	-	EXPRESSION TAG	UNP Q8U2X0
B	-1	ILE	-	EXPRESSION TAG	UNP Q8U2X0
B	0	PRO	-	EXPRESSION TAG	UNP Q8U2X0
B	298	THR	ALA	CONFLICT	UNP Q8U2X0
B	462	ARG	-	EXPRESSION TAG	UNP Q8U2X0
B	463	ASN	-	EXPRESSION TAG	UNP Q8U2X0
B	464	SER	-	EXPRESSION TAG	UNP Q8U2X0
B	465	GLU	-	EXPRESSION TAG	UNP Q8U2X0
B	466	ASN	-	EXPRESSION TAG	UNP Q8U2X0
B	467	LEU	-	EXPRESSION TAG	UNP Q8U2X0
B	468	TYR	-	EXPRESSION TAG	UNP Q8U2X0
B	469	PHE	-	EXPRESSION TAG	UNP Q8U2X0
B	470	GLN	-	EXPRESSION TAG	UNP Q8U2X0
B	471	GLY	-	EXPRESSION TAG	UNP Q8U2X0
B	472	GLY	-	EXPRESSION TAG	UNP Q8U2X0
B	473	ARG	-	EXPRESSION TAG	UNP Q8U2X0
B	474	GLY	-	EXPRESSION TAG	UNP Q8U2X0
B	475	SER	-	EXPRESSION TAG	UNP Q8U2X0
B	476	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	477	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	478	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	479	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	480	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	481	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	482	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	483	HIS	-	EXPRESSION TAG	UNP Q8U2X0
B	484	HIS	-	EXPRESSION TAG	UNP Q8U2X0

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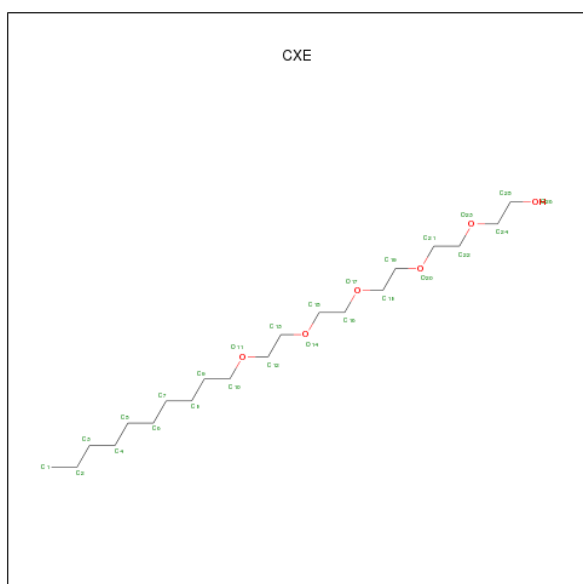
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	-6	MET	-	EXPRESSION TAG	UNP Q8U2X0
C	-5	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	-4	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	-3	SER	-	EXPRESSION TAG	UNP Q8U2X0
C	-2	GLU	-	EXPRESSION TAG	UNP Q8U2X0
C	-1	ILE	-	EXPRESSION TAG	UNP Q8U2X0
C	0	PRO	-	EXPRESSION TAG	UNP Q8U2X0
C	298	THR	ALA	CONFLICT	UNP Q8U2X0
C	462	ARG	-	EXPRESSION TAG	UNP Q8U2X0
C	463	ASN	-	EXPRESSION TAG	UNP Q8U2X0
C	464	SER	-	EXPRESSION TAG	UNP Q8U2X0
C	465	GLU	-	EXPRESSION TAG	UNP Q8U2X0
C	466	ASN	-	EXPRESSION TAG	UNP Q8U2X0
C	467	LEU	-	EXPRESSION TAG	UNP Q8U2X0
C	468	TYR	-	EXPRESSION TAG	UNP Q8U2X0
C	469	PHE	-	EXPRESSION TAG	UNP Q8U2X0
C	470	GLN	-	EXPRESSION TAG	UNP Q8U2X0
C	471	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	472	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	473	ARG	-	EXPRESSION TAG	UNP Q8U2X0
C	474	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	475	SER	-	EXPRESSION TAG	UNP Q8U2X0
C	476	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	477	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	478	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	479	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	480	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	481	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	482	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	483	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	484	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	485	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	-6	MET	-	EXPRESSION TAG	UNP Q8U2X0
D	-5	GLY	-	EXPRESSION TAG	UNP Q8U2X0
D	-4	GLY	-	EXPRESSION TAG	UNP Q8U2X0
D	-3	SER	-	EXPRESSION TAG	UNP Q8U2X0
D	-2	GLU	-	EXPRESSION TAG	UNP Q8U2X0
D	-1	ILE	-	EXPRESSION TAG	UNP Q8U2X0
D	0	PRO	-	EXPRESSION TAG	UNP Q8U2X0
D	298	THR	ALA	CONFLICT	UNP Q8U2X0
D	462	ARG	-	EXPRESSION TAG	UNP Q8U2X0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	463	ASN	-	EXPRESSION TAG	UNP Q8U2X0
D	464	SER	-	EXPRESSION TAG	UNP Q8U2X0
D	465	GLU	-	EXPRESSION TAG	UNP Q8U2X0
D	466	ASN	-	EXPRESSION TAG	UNP Q8U2X0
D	467	LEU	-	EXPRESSION TAG	UNP Q8U2X0
D	468	TYR	-	EXPRESSION TAG	UNP Q8U2X0
D	469	PHE	-	EXPRESSION TAG	UNP Q8U2X0
D	470	GLN	-	EXPRESSION TAG	UNP Q8U2X0
D	471	GLY	-	EXPRESSION TAG	UNP Q8U2X0
D	472	GLY	-	EXPRESSION TAG	UNP Q8U2X0
D	473	ARG	-	EXPRESSION TAG	UNP Q8U2X0
D	474	GLY	-	EXPRESSION TAG	UNP Q8U2X0
D	475	SER	-	EXPRESSION TAG	UNP Q8U2X0
D	476	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	477	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	478	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	479	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	480	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	481	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	482	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	483	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	484	HIS	-	EXPRESSION TAG	UNP Q8U2X0
D	485	HIS	-	EXPRESSION TAG	UNP Q8U2X0

- Molecule 2 is PENTAETHYLENE GLYCOL MONODECYL ETHER (three-letter code: CXE) (formula: $C_{20}H_{42}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 26 20 6	0	0
2	A	1	Total C O 26 20 6	0	0
2	A	1	Total C O 26 20 6	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C O 14 12 2	0	0
2	A	1	Total C O 23 18 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 5 5	0	0
2	B	1	Total C O 26 20 6	0	0
2	B	1	Total C O 20 16 4	0	0
2	B	1	Total C O 17 14 3	0	0
2	B	1	Total C O 11 10 1	0	0
2	B	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 17 14 3	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 9 9	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 15 13 2	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C O 17 14 3	0	0
2	C	1	Total C O 23 18 5	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C O 16 10 6	0	0
2	C	1	Total C O 23 18 5	0	0
2	C	1	Total C O 17 14 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 4 4	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 20 16 4	0	0
2	D	1	Total C O 14 12 2	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C O 14 12 2	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C 5 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

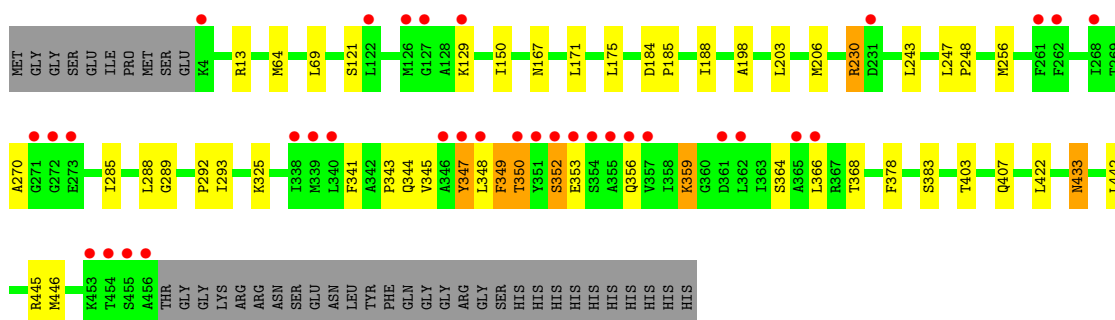
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	74	Total O 74 74	0	0
4	C	112	Total O 112 112	0	0
4	D	30	Total O 30 30	0	0

3 Residue-property plots

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

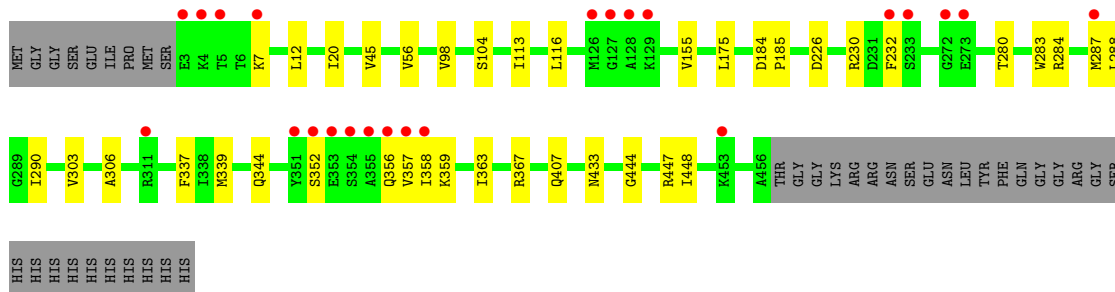
• Molecule 1: PF0708

Chain A: 



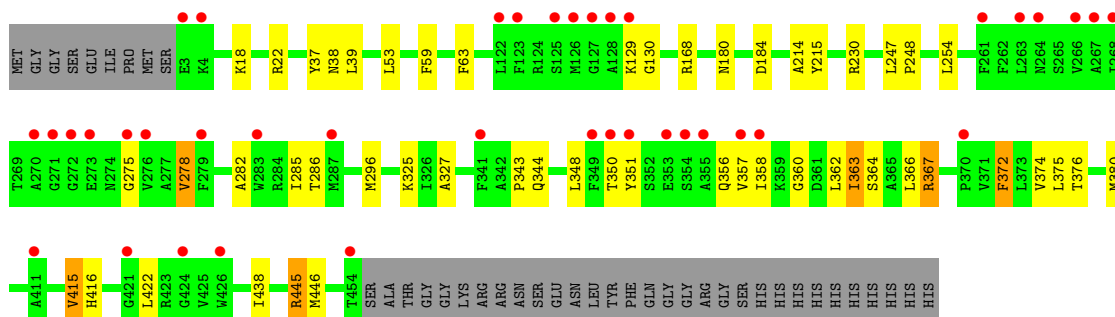
• Molecule 1: PF0708

Chain B: 



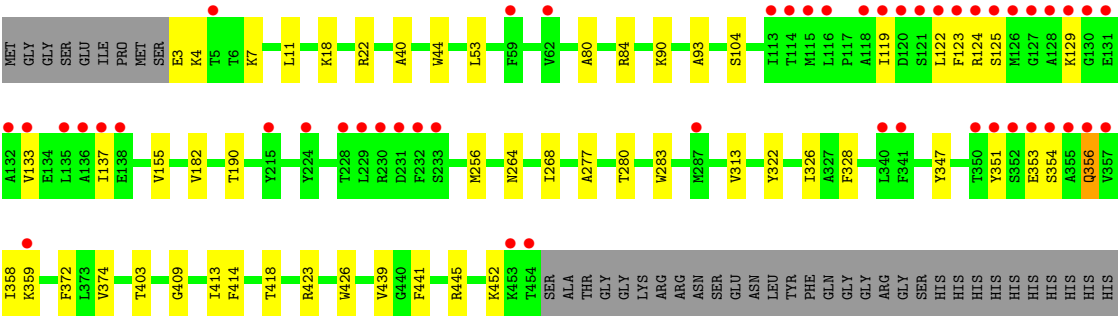
• Molecule 1: PF0708

Chain C: 



● Molecule 1: PF0708

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.56Å 94.55Å 138.82Å 90.00° 126.47° 90.00°	Depositor
Resolution (Å)	45.24 – 2.35 45.24 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.24-2.35) 99.7 (45.24-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.231 0.197 , 0.228	Depositor DCC
R_{free} test set	4735 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 95102 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14749	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.25	0/3476	0.43	0/4714
1	B	0.23	0/3474	0.40	0/4712
1	C	0.25	0/3485	0.43	0/4725
1	D	0.24	0/3485	0.43	0/4725
All	All	0.24	0/13920	0.42	0/18876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3412	0	3601	33	0
1	B	3413	0	3594	26	0
1	C	3418	0	3610	40	0
1	D	3418	0	3610	33	0
2	A	246	0	420	21	0
2	B	144	0	253	11	0
2	C	273	0	450	23	0
2	D	96	0	174	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	1	0
4	A	111	0	0	4	0
4	B	74	0	0	1	0
4	C	112	0	0	0	0
4	D	30	0	0	1	0
All	All	14749	0	15712	152	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 152 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:344:GLN:HG2	2:B:506:CXE:H091	1.59	0.82
1:C:445:ARG:HG2	1:C:445:ARG:HH11	1.51	0.76
1:A:349:PHE:H	1:A:349:PHE:HD2	1.37	0.72
2:B:501:CXE:H222	1:C:39:LEU:HD11	1.72	0.72
2:A:501:CXE:H062	2:A:515:CXE:H022	1.74	0.70

There are no symmetry-related clashes.

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	452/492 (92%)	444 (98%)	8 (2%)	0	100	100
1	B	452/492 (92%)	446 (99%)	6 (1%)	0	100	100
1	C	452/492 (92%)	444 (98%)	8 (2%)	0	100	100
1	D	452/492 (92%)	445 (98%)	7 (2%)	0	100	100
All	All	1808/1968 (92%)	1779 (98%)	29 (2%)	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	358/389 (92%)	343 (96%)	15 (4%)	40	52
1	B	358/389 (92%)	356 (99%)	2 (1%)	92	97
1	C	359/389 (92%)	347 (97%)	12 (3%)	50	64
1	D	359/389 (92%)	350 (98%)	9 (2%)	60	75
All	All	1434/1556 (92%)	1396 (97%)	38 (3%)	57	73

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	53	LEU
1	C	350	THR
1	D	353	GLU
1	C	278	VAL
1	C	351	TYR

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

Mol	Chain	Res	Type
1	B	167	ASN
1	D	356	GLN
1	B	433	ASN
1	A	433	ASN
1	B	407	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 55 ligands modelled in this entry, 2 are monoatomic - leaving 53 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
2	CXE	A	501	-	25,25,25	0.41	0	24,24,24	0.51	0
2	CXE	A	502	-	25,25,25	0.41	0	24,24,24	0.43	0
2	CXE	A	503	-	25,25,25	0.35	0	24,24,24	0.69	0
2	CXE	A	504	-	19,19,25	0.38	0	18,18,24	0.71	0
2	CXE	A	505	-	9,9,25	1.68	1 (11%)	8,8,24	0.89	0
2	CXE	A	506	-	19,19,25	0.37	0	18,18,24	0.68	0
2	CXE	A	507	-	6,6,25	2.33	1 (16%)	5,5,24	0.53	0
2	CXE	A	508	-	13,13,25	0.39	0	12,12,24	0.73	0
2	CXE	A	509	-	22,22,25	0.44	0	21,21,24	0.52	0
2	CXE	A	510	-	9,9,25	1.89	1 (11%)	8,8,24	0.61	0
2	CXE	A	511	-	9,9,25	1.97	1 (11%)	8,8,24	0.63	0
2	CXE	A	512	-	5,5,25	2.68	1 (20%)	4,4,24	0.56	0
2	CXE	A	513	-	19,19,25	0.39	0	18,18,24	0.65	0
2	CXE	A	514	-	8,8,25	1.89	1 (12%)	7,7,24	0.57	0
2	CXE	A	515	-	6,6,25	2.41	1 (16%)	5,5,24	0.56	0
2	CXE	A	516	-	6,6,25	2.45	1 (16%)	5,5,24	0.70	0
2	CXE	A	517	-	4,4,25	3.13	1 (25%)	3,3,24	0.77	0
2	CXE	B	501	-	25,25,25	0.40	0	24,24,24	0.45	0
2	CXE	B	502	-	19,19,25	0.47	0	18,18,24	0.57	0
2	CXE	B	503	-	16,16,25	0.42	0	15,15,24	0.67	0
2	CXE	B	504	-	10,10,25	0.43	0	9,9,24	0.69	0
2	CXE	B	505	-	9,9,25	1.98	1 (11%)	8,8,24	0.61	0
2	CXE	B	506	-	16,16,25	0.44	0	15,15,24	0.65	0
2	CXE	B	507	-	8,8,25	2.08	1 (12%)	7,7,24	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CXE	B	508	-	6,6,25	2.28	1 (16%)	5,5,24	0.46	0
2	CXE	B	509	-	5,5,25	2.52	1 (20%)	4,4,24	0.40	0
2	CXE	B	510	-	5,5,25	2.61	1 (20%)	4,4,24	0.57	0
2	CXE	B	511	-	5,5,25	2.62	1 (20%)	4,4,24	0.56	0
2	CXE	B	512	-	8,8,25	2.21	1 (12%)	7,7,24	0.54	0
2	CXE	C	501	-	25,25,25	0.42	0	24,24,24	0.44	0
2	CXE	C	502	-	25,25,25	0.39	0	24,24,24	0.59	0
2	CXE	C	503	-	25,25,25	0.40	0	24,24,24	0.61	0
2	CXE	C	504	-	25,25,25	0.41	0	24,24,24	0.49	0
2	CXE	C	505	-	19,19,25	0.45	0	18,18,24	0.77	0
2	CXE	C	506	-	13,14,25	0.44	0	12,13,24	0.55	0
2	CXE	C	507	-	9,9,25	2.02	1 (11%)	8,8,24	0.56	0
2	CXE	C	508	-	6,6,25	2.40	1 (16%)	5,5,24	0.63	0
2	CXE	C	509	-	16,16,25	0.44	0	15,15,24	0.74	0
2	CXE	C	510	-	22,22,25	0.43	0	21,21,24	0.59	0
2	CXE	C	511	-	9,9,25	2.00	1 (11%)	8,8,24	0.63	0
2	CXE	C	512	-	15,15,25	0.52	0	14,14,24	0.59	0
2	CXE	C	513	-	22,22,25	0.43	0	21,21,24	0.81	1 (4%)
2	CXE	C	514	-	16,16,25	0.42	0	15,15,24	0.59	0
2	CXE	C	515	-	3,3,25	3.25	1 (33%)	2,2,24	0.29	0
2	CXE	C	516	-	6,6,25	1.96	1 (16%)	5,5,24	0.52	0
2	CXE	D	501	-	10,10,25	0.38	0	9,9,24	0.75	0
2	CXE	D	502	-	19,19,25	0.37	0	18,18,24	0.68	0
2	CXE	D	503	-	13,13,25	0.41	0	12,12,24	0.60	0
2	CXE	D	504	-	9,9,25	2.08	1 (11%)	8,8,24	0.69	0
2	CXE	D	505	-	13,13,25	0.37	0	12,12,24	0.64	0
2	CXE	D	506	-	10,10,25	0.44	0	9,9,24	0.67	0
2	CXE	D	507	-	10,10,25	0.41	0	9,9,24	0.72	0
2	CXE	D	508	-	4,4,25	3.07	1 (25%)	3,3,24	0.53	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
2	CXE	A	501	-	-	0/23/23/23	0/0/0/0
2	CXE	A	502	-	-	0/23/23/23	0/0/0/0
2	CXE	A	503	-	-	0/23/23/23	0/0/0/0
2	CXE	A	504	-	-	0/17/17/23	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CXE	A	505	-	-	0/7/7/23	0/0/0/0
2	CXE	A	506	-	-	0/17/17/23	0/0/0/0
2	CXE	A	507	-	-	0/4/4/23	0/0/0/0
2	CXE	A	508	-	-	0/11/11/23	0/0/0/0
2	CXE	A	509	-	-	0/20/20/23	0/0/0/0
2	CXE	A	510	-	-	0/7/7/23	0/0/0/0
2	CXE	A	511	-	-	0/7/7/23	0/0/0/0
2	CXE	A	512	-	-	0/3/3/23	0/0/0/0
2	CXE	A	513	-	-	0/17/17/23	0/0/0/0
2	CXE	A	514	-	-	0/6/6/23	0/0/0/0
2	CXE	A	515	-	-	0/4/4/23	0/0/0/0
2	CXE	A	516	-	-	0/4/4/23	0/0/0/0
2	CXE	A	517	-	-	0/2/2/23	0/0/0/0
2	CXE	B	501	-	-	0/23/23/23	0/0/0/0
2	CXE	B	502	-	-	0/17/17/23	0/0/0/0
2	CXE	B	503	-	-	0/14/14/23	0/0/0/0
2	CXE	B	504	-	-	0/8/8/23	0/0/0/0
2	CXE	B	505	-	-	0/7/7/23	0/0/0/0
2	CXE	B	506	-	-	0/14/14/23	0/0/0/0
2	CXE	B	507	-	-	0/6/6/23	0/0/0/0
2	CXE	B	508	-	-	0/4/4/23	0/0/0/0
2	CXE	B	509	-	-	0/3/3/23	0/0/0/0
2	CXE	B	510	-	-	0/3/3/23	0/0/0/0
2	CXE	B	511	-	-	0/3/3/23	0/0/0/0
2	CXE	B	512	-	-	0/6/6/23	0/0/0/0
2	CXE	C	501	-	-	0/23/23/23	0/0/0/0
2	CXE	C	502	-	-	0/23/23/23	0/0/0/0
2	CXE	C	503	-	-	0/23/23/23	0/0/0/0
2	CXE	C	504	-	-	0/23/23/23	0/0/0/0
2	CXE	C	505	-	-	0/17/17/23	0/0/0/0
2	CXE	C	506	-	-	0/12/12/23	0/0/0/0
2	CXE	C	507	-	-	0/7/7/23	0/0/0/0
2	CXE	C	508	-	-	0/4/4/23	0/0/0/0
2	CXE	C	509	-	-	0/14/14/23	0/0/0/0
2	CXE	C	510	-	-	0/20/20/23	0/0/0/0
2	CXE	C	511	-	-	0/7/7/23	0/0/0/0
2	CXE	C	512	-	-	0/13/13/23	0/0/0/0
2	CXE	C	513	-	-	0/20/20/23	0/0/0/0
2	CXE	C	514	-	-	0/14/14/23	0/0/0/0
2	CXE	C	515	-	-	0/1/1/23	0/0/0/0
2	CXE	C	516	-	-	0/4/4/23	0/0/0/0
2	CXE	D	501	-	-	0/8/8/23	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CXE	D	502	-	-	0/17/17/23	0/0/0/0
2	CXE	D	503	-	-	0/11/11/23	0/0/0/0
2	CXE	D	504	-	-	0/7/7/23	0/0/0/0
2	CXE	D	505	-	-	0/11/11/23	0/0/0/0
2	CXE	D	506	-	-	0/8/8/23	0/0/0/0
2	CXE	D	507	-	-	0/8/8/23	0/0/0/0
2	CXE	D	508	-	-	0/2/2/23	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	517	CXE	C5-C4	-6.26	1.52	1.55
2	B	512	CXE	C9-C8	-6.22	1.52	1.55
2	D	504	CXE	C10-C9	-6.22	1.52	1.55
2	D	508	CXE	C5-C4	-6.13	1.52	1.55
2	C	507	CXE	C10-C9	-6.02	1.52	1.55

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	513	CXE	O23-C22-C21	-2.09	107.40	114.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	453/492 (92%)	0.14	34 (7%) 14 21	19, 37, 89, 146	0
1	B	454/492 (92%)	0.16	23 (5%) 27 38	21, 42, 76, 113	0
1	C	452/492 (91%)	0.29	39 (8%) 11 17	19, 35, 105, 142	0
1	D	452/492 (91%)	0.54	49 (10%) 6 10	33, 53, 97, 129	0
All	All	1811/1968 (92%)	0.28	145 (8%) 12 19	19, 44, 91, 146	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	SER	9.2
1	A	456	ALA	7.9
1	C	353	GLU	7.5
1	A	351	TYR	7.0
1	B	357	VAL	7.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CXE	A	510	10/26	0.40	19.40	36,63,68,69	0
2	CXE	C	516	7/26	0.27	16.78	51,65,67,68	0
2	CXE	C	504	26/26	0.32	12.02	50,72,102,105	0
2	CXE	B	511	6/26	0.78	11.88	34,38,39,42	6
2	CXE	B	508	7/26	0.27	11.79	44,52,67,68	0
2	CXE	C	509	17/26	0.19	11.24	54,76,85,95	0
2	CXE	B	505	10/26	0.24	11.13	46,60,72,77	0
2	CXE	A	503	26/26	0.41	8.27	65,77,83,85	0
2	CXE	C	511	10/26	0.26	7.82	48,56,65,67	0
2	CXE	A	507	7/26	0.16	7.46	42,52,59,62	0
2	CXE	B	502	20/26	0.26	7.24	36,50,62,65	0
2	CXE	C	501	26/26	0.25	7.06	26,43,88,95	0
2	CXE	A	509	23/26	0.38	6.80	56,83,102,104	0
2	CXE	B	507	9/26	0.25	6.71	36,61,73,84	0
2	CXE	C	506	15/26	0.19	6.69	37,47,71,75	0
2	CXE	C	512	16/26	0.24	6.54	38,57,82,89	0
2	CXE	B	504	11/26	0.22	6.19	36,74,78,81	0
2	CXE	C	503	26/26	0.22	6.04	47,57,74,78	0
2	CXE	B	506	17/26	0.22	5.79	56,70,84,84	0
2	CXE	B	512	9/26	0.21	5.27	44,53,62,65	0
2	CXE	C	514	17/26	0.35	4.93	50,70,93,93	0
2	CXE	B	509	6/26	0.79	4.91	32,36,42,45	6
2	CXE	A	514	9/26	0.26	4.77	55,62,69,73	0
2	CXE	C	510	23/26	0.27	4.67	49,73,80,88	0
2	CXE	C	507	10/26	0.30	4.64	60,68,79,80	0
2	CXE	C	505	20/26	0.28	4.64	46,62,82,83	0
2	CXE	A	517	5/26	0.29	4.55	56,60,63,68	0
2	CXE	C	515	4/26	0.19	4.42	48,50,54,66	0
2	CXE	A	513	20/26	0.25	3.98	42,74,102,106	0
2	CXE	A	511	10/26	0.30	3.98	58,66,74,74	0
2	CXE	A	505	10/26	0.62	3.89	38,42,47,63	10
2	CXE	A	512	6/26	0.20	3.70	34,49,53,65	0
2	CXE	C	502	26/26	0.33	3.44	40,76,83,87	0
2	CXE	D	507	11/26	0.24	3.29	48,58,67,70	0
2	CXE	A	506	20/26	0.21	2.98	24,39,57,58	0
2	CXE	A	502	26/26	0.23	2.78	29,48,74,81	0
2	CXE	D	502	20/26	0.20	2.54	38,48,56,58	10
2	CXE	C	508	7/26	0.22	2.31	52,59,64,66	0
2	CXE	A	508	14/26	0.34	2.20	63,78,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CXE	D	505	14/26	0.24	2.16	49,66,77,78	0
2	CXE	A	504	20/26	0.18	1.87	43,61,77,81	0
2	CXE	D	504	10/26	0.26	1.83	55,59,73,74	0
2	CXE	C	513	23/26	0.24	1.72	57,67,81,85	0
2	CXE	D	506	11/26	0.25	1.25	64,68,87,91	0
2	CXE	A	515	7/26	0.20	1.00	38,53,65,65	0
2	CXE	B	503	17/26	0.22	1.00	46,53,66,68	3
2	CXE	D	508	5/26	0.22	0.95	56,57,57,58	0
2	CXE	A	516	7/26	0.19	0.69	52,57,70,73	0
2	CXE	A	501	26/26	0.17	0.47	35,49,60,64	0
2	CXE	B	501	26/26	0.17	0.42	35,50,77,86	0
2	CXE	D	501	11/26	0.14	0.04	41,46,65,65	0
2	CXE	D	503	14/26	0.15	-0.24	53,61,65,76	0
2	CXE	B	510	6/26	0.15	-0.84	62,69,71,72	0
3	CL	A	519	1/1	0.09	-2.68	37,37,37,37	0
3	CL	A	518	1/1	0.06	-2.78	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.