wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 11:20 am BST

PDB ID	:	8AXG
Title	:	Crystal structure of Fusobacterium nucleatum fusolisin protease
Authors	:	Isupov, M.N.; Wiener, R.; Rouvinski, A.; Fahoum, J.; Kumar, M.; Read, R.J.
Deposited on	:	2022-08-31
Resolution	:	2.04 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 (1)) were used in the production of this report:

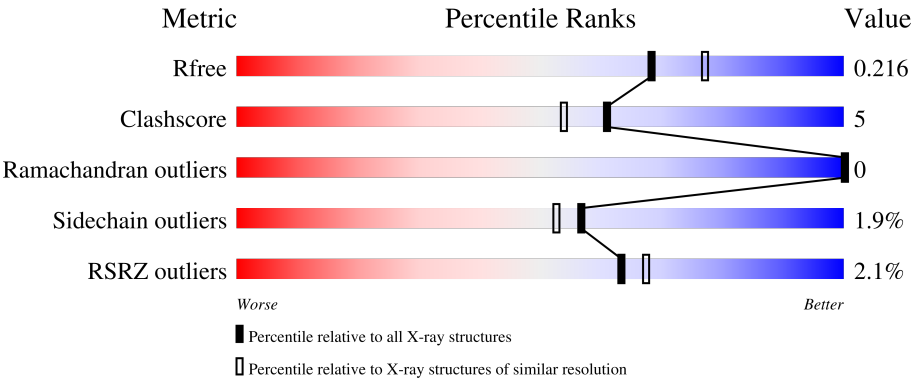
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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% 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	AAA	585	2% 90% 6%
1	BBB	585	89% 6% 5%
1	CCC	585	3% 90% 6%
1	DDD	585	2% 88% 8%

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	EDO	BBB	614	-	-	X	-
2	EDO	CCC	606	-	-	X	-
2	EDO	CCC	609	-	-	-	X
2	EDO	CCC	610	-	-	X	-
4	PEG	AAA	611	-	-	X	-
4	PEG	BBB	603	-	-	X	-
4	PEG	DDD	602	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19583 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 Fusolisin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	563	Total	C	N	O	S	0	10	0
			4335	2717	755	856	7			
1	BBB	554	Total	C	N	O	S	0	13	0
			4286	2687	751	841	7			
1	CCC	561	Total	C	N	O	S	0	9	0
			4321	2706	759	849	7			
1	DDD	562	Total	C	N	O	S	0	14	0
			4352	2729	756	860	7			

There are 24 discrepancies between the modelled and reference sequences:

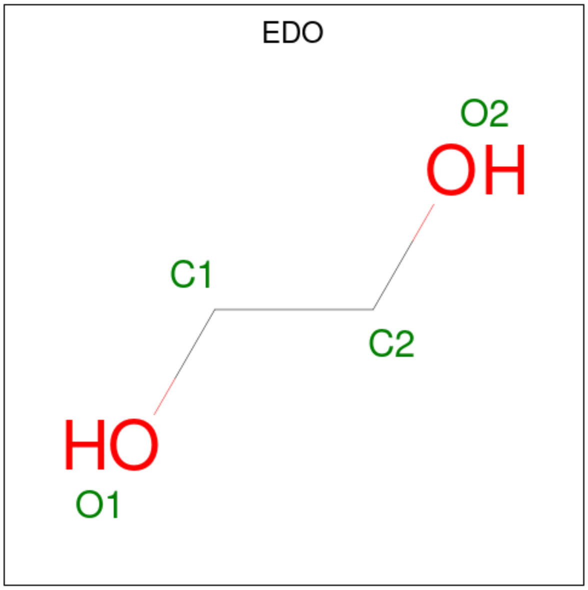
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	HIS	-	expression tag	UNP A0A068B7P9
AAA	2	HIS	-	expression tag	UNP A0A068B7P9
AAA	3	HIS	-	expression tag	UNP A0A068B7P9
AAA	4	HIS	-	expression tag	UNP A0A068B7P9
AAA	5	HIS	-	expression tag	UNP A0A068B7P9
AAA	6	HIS	-	expression tag	UNP A0A068B7P9
BBB	1	HIS	-	expression tag	UNP A0A068B7P9
BBB	2	HIS	-	expression tag	UNP A0A068B7P9
BBB	3	HIS	-	expression tag	UNP A0A068B7P9
BBB	4	HIS	-	expression tag	UNP A0A068B7P9
BBB	5	HIS	-	expression tag	UNP A0A068B7P9
BBB	6	HIS	-	expression tag	UNP A0A068B7P9
CCC	1	HIS	-	expression tag	UNP A0A068B7P9
CCC	2	HIS	-	expression tag	UNP A0A068B7P9
CCC	3	HIS	-	expression tag	UNP A0A068B7P9
CCC	4	HIS	-	expression tag	UNP A0A068B7P9
CCC	5	HIS	-	expression tag	UNP A0A068B7P9
CCC	6	HIS	-	expression tag	UNP A0A068B7P9
DDD	1	HIS	-	expression tag	UNP A0A068B7P9
DDD	2	HIS	-	expression tag	UNP A0A068B7P9
DDD	3	HIS	-	expression tag	UNP A0A068B7P9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	4	HIS	-	expression tag	UNP A0A068B7P9
DDD	5	HIS	-	expression tag	UNP A0A068B7P9
DDD	6	HIS	-	expression tag	UNP A0A068B7P9

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	AAA	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	BBB	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

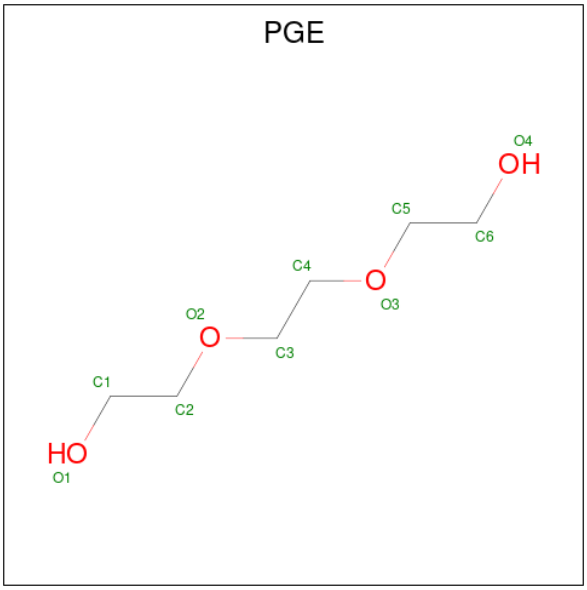
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4	2	2		
2	DDD	1	Total	C	O	0	0
			4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

Continued on next page...

Continued from previous page...

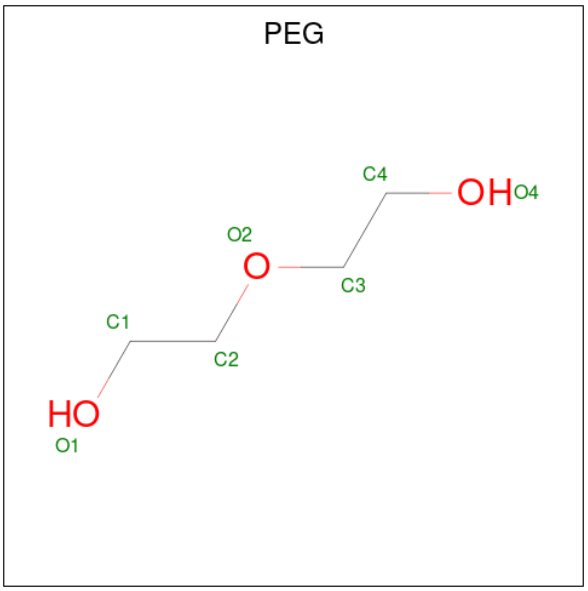
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0
2	DDD	1	Total C O 4 2 2	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



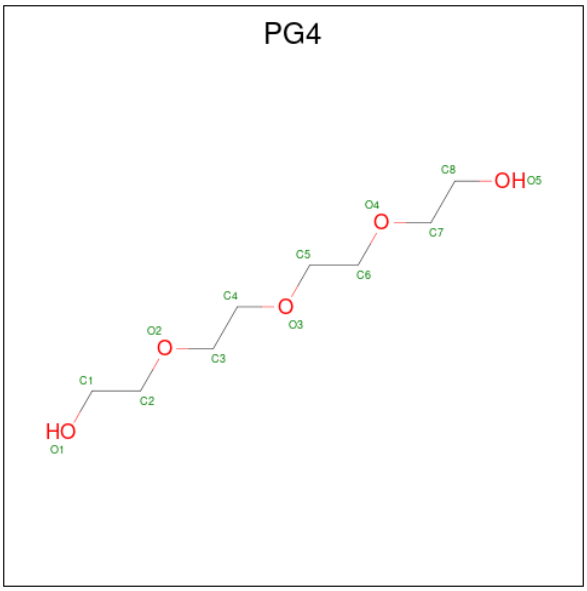
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 10 6 4	0	0
3	DDD	1	Total C O 10 6 4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 7 4 3	0	0
4	BBB	1	Total C O 7 4 3	0	0
4	BBB	1	Total C O 7 4 3	0	0
4	CCC	1	Total C O 7 4 3	0	0
4	CCC	1	Total C O 7 4 3	0	0
4	CCC	1	Total C O 7 4 3	0	0
4	DDD	1	Total C O 7 4 3	0	0
4	DDD	1	Total C O 7 4 3	0	0
4	DDD	1	Total C O 7 4 3	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total C O 13 8 5	0	0

- Molecule 6 is water.

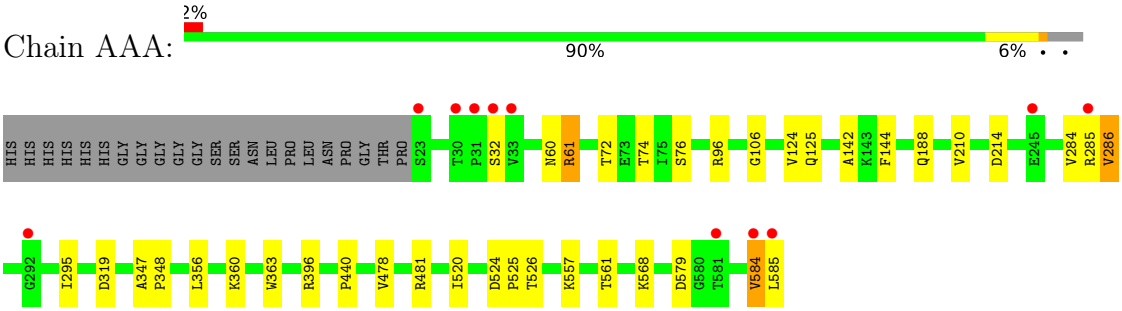
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	422	Total O 422 422	0	0
6	BBB	424	Total O 424 424	0	0
6	CCC	411	Total O 411 411	0	0
6	DDD	448	Total O 448 448	0	0

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 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.

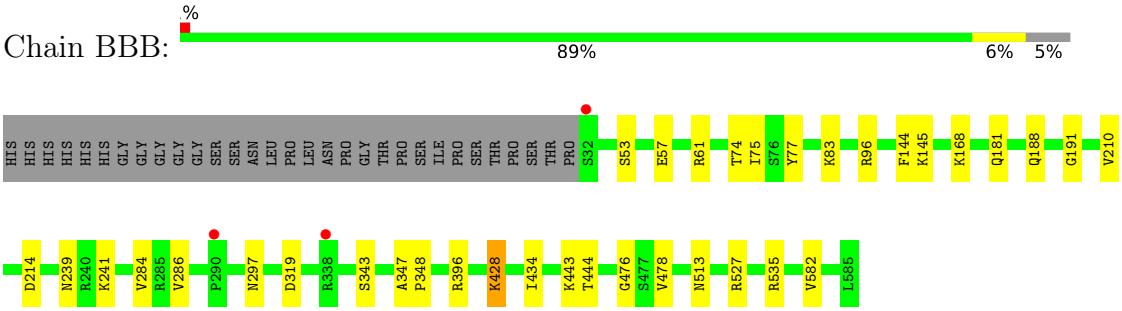
• Molecule 1: Fusolisin

Chain AAA:



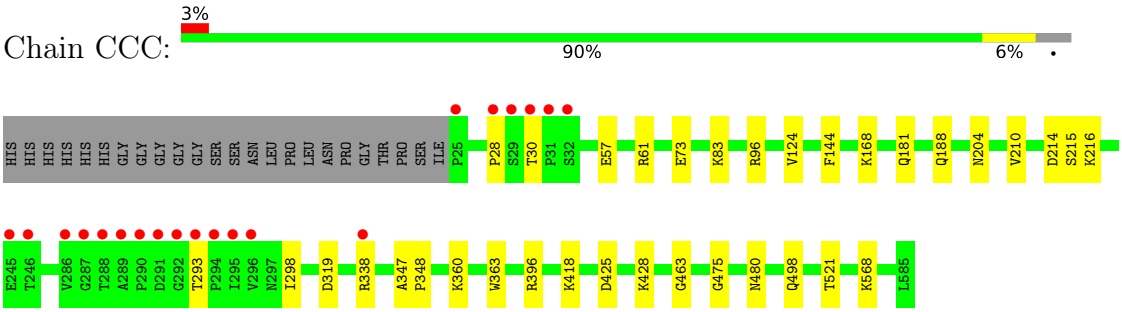
• Molecule 1: Fusolisin

Chain BBB:



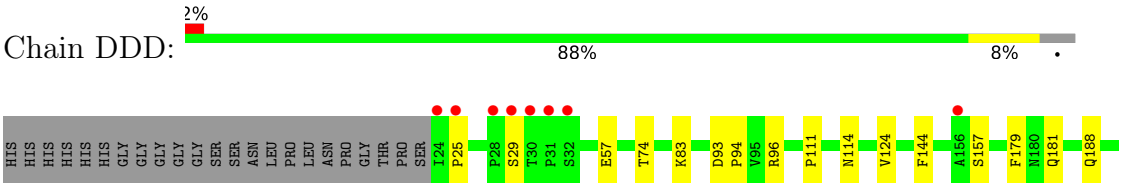
• Molecule 1: Fusolisin

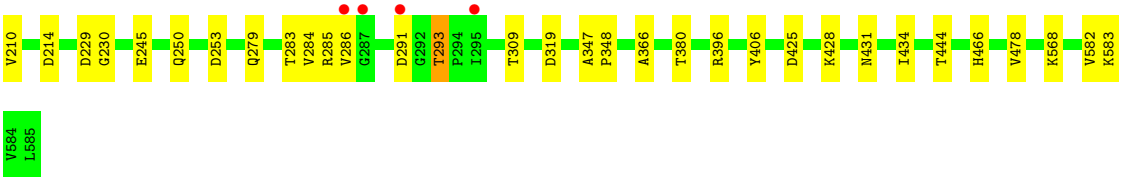
Chain CCC:



• Molecule 1: Fusolisin

Chain DDD:




V210
D214
D229
G230
E245
Q250
D253
Q279
T283
V284
R285
V286
G287
D291
G292
T293
P294
I295
T309
D319
A347
P348
A366
T380
R396
Y406
D425
K428
M431
I434
T444
H466
V478
K568
V582
K583
V584
L585

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	115.47Å 115.47Å 196.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.89 – 2.04 75.42 – 2.04	Depositor EDS
% Data completeness (in resolution range)	91.3 (74.89-2.04) 91.3 (75.42-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.216 0.177 , 0.216	Depositor DCC
R_{free} test set	7308 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19583	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, EDO, PG4, PEG

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	AAA	0.40	0/4447	0.69	2/6035 (0.0%)
1	BBB	0.40	0/4404	0.68	0/5970
1	CCC	0.39	0/4427	0.68	0/6004
1	DDD	0.41	0/4473	0.68	0/6069
All	All	0.40	0/17751	0.68	2/24078 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	61[A]	ARG	CB-CG-CD	-5.03	98.53	111.60
1	AAA	61[B]	ARG	CB-CG-CD	-5.03	98.53	111.60

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	AAA	4335	0	4311	38	0
1	BBB	4286	0	4278	35	0
1	CCC	4321	0	4300	36	0
1	DDD	4352	0	4334	48	0
2	AAA	140	0	210	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	136	0	204	16	0
2	CCC	92	0	138	14	0
2	DDD	120	0	180	10	0
3	AAA	10	0	14	5	0
3	DDD	10	0	14	2	0
4	AAA	7	0	10	8	0
4	BBB	14	0	20	11	0
4	CCC	21	0	30	4	0
4	DDD	21	0	30	11	0
5	CCC	13	0	18	4	0
6	AAA	422	0	0	7	0
6	BBB	424	0	0	3	0
6	CCC	411	0	0	9	0
6	DDD	448	0	0	7	0
All	All	19583	0	18091	163	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 5.

The worst 5 of 163 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)
4:AAA:611:PEG:H42	6:AAA:896:HOH:O	1.68	0.94
1:CCC:215:SER:H	2:CCC:610:EDO:H12	1.38	0.87
1:BBB:96:ARG:HE	2:BBB:621:EDO:H21	1.40	0.85
1:CCC:96:ARG:HG3	2:CCC:606:EDO:H11	1.59	0.85
1:CCC:498:GLN:HG3	6:CCC:948:HOH:O	1.79	0.81

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	AAA	571/585 (98%)	557 (98%)	14 (2%)	0	100	100
1	BBB	565/585 (97%)	551 (98%)	14 (2%)	0	100	100
1	CCC	568/585 (97%)	554 (98%)	14 (2%)	0	100	100
1	DDD	574/585 (98%)	557 (97%)	17 (3%)	0	100	100
All	All	2278/2340 (97%)	2219 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	470/476 (99%)	460 (98%)	10 (2%)	53	48
1	BBB	464/476 (98%)	454 (98%)	10 (2%)	52	46
1	CCC	467/476 (98%)	460 (98%)	7 (2%)	65	62
1	DDD	473/476 (99%)	461 (98%)	12 (2%)	47	40
All	All	1874/1904 (98%)	1835 (98%)	39 (2%)	57	48

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	57	GLU
1	DDD	293	THR
1	DDD	144	PHE
1	DDD	250[A]	GLN
1	DDD	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

134 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	EDO	CCC	616	-	3,3,3	0.20	0	2,2,2	0.28	0
2	EDO	AAA	624	-	3,3,3	0.50	0	2,2,2	0.81	0
2	EDO	BBB	622	-	3,3,3	0.08	0	2,2,2	0.58	0
2	EDO	DDD	607	-	3,3,3	0.10	0	2,2,2	0.26	0
2	EDO	AAA	619	-	3,3,3	0.08	0	2,2,2	0.09	0
2	EDO	AAA	602	-	3,3,3	0.08	0	2,2,2	0.25	0
2	EDO	AAA	607	-	3,3,3	0.05	0	2,2,2	0.33	0
2	EDO	BBB	609	-	3,3,3	0.22	0	2,2,2	0.66	0
2	EDO	AAA	637	-	3,3,3	0.23	0	2,2,2	0.46	0
2	EDO	AAA	615	-	3,3,3	0.08	0	2,2,2	0.08	0
2	EDO	AAA	626	-	3,3,3	0.09	0	2,2,2	0.36	0
2	EDO	AAA	609	-	3,3,3	0.12	0	2,2,2	0.11	0
2	EDO	BBB	615	-	3,3,3	0.13	0	2,2,2	0.27	0
2	EDO	AAA	620	-	3,3,3	0.18	0	2,2,2	0.27	0
2	EDO	AAA	632	-	3,3,3	0.11	0	2,2,2	0.20	0
2	EDO	CCC	608	-	3,3,3	0.10	0	2,2,2	0.37	0
2	EDO	BBB	617	-	3,3,3	0.15	0	2,2,2	0.46	0
2	EDO	DDD	613	-	3,3,3	0.54	0	2,2,2	0.98	0
2	EDO	DDD	614	-	3,3,3	0.14	0	2,2,2	0.53	0
2	EDO	CCC	606	-	3,3,3	0.09	0	2,2,2	0.44	0
2	EDO	BBB	612	-	3,3,3	0.09	0	2,2,2	0.10	0
2	EDO	CCC	603	-	3,3,3	0.09	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	AAA	621	-	3,3,3	0.29	0	2,2,2	0.76	0
2	EDO	AAA	633	-	3,3,3	0.17	0	2,2,2	0.12	0
2	EDO	CCC	612	-	3,3,3	0.09	0	2,2,2	0.12	0
2	EDO	BBB	610	-	3,3,3	0.05	0	2,2,2	0.37	0
2	EDO	DDD	627	-	3,3,3	0.56	0	2,2,2	0.73	0
2	EDO	BBB	608	-	3,3,3	0.13	0	2,2,2	0.33	0
2	EDO	BBB	614	-	3,3,3	0.18	0	2,2,2	0.16	0
2	EDO	DDD	606	-	3,3,3	0.08	0	2,2,2	0.35	0
2	EDO	BBB	625	-	3,3,3	0.09	0	2,2,2	0.27	0
2	EDO	CCC	622	-	3,3,3	0.13	0	2,2,2	0.22	0
2	EDO	BBB	605	-	3,3,3	0.22	0	2,2,2	0.42	0
2	EDO	BBB	621	-	3,3,3	0.26	0	2,2,2	0.21	0
2	EDO	AAA	603	-	3,3,3	0.29	0	2,2,2	0.78	0
2	EDO	DDD	628	-	3,3,3	0.11	0	2,2,2	0.33	0
2	EDO	CCC	625	-	3,3,3	0.07	0	2,2,2	0.17	0
2	EDO	DDD	622	-	3,3,3	0.05	0	2,2,2	0.16	0
2	EDO	CCC	615	-	3,3,3	0.30	0	2,2,2	0.58	0
2	EDO	BBB	611	-	3,3,3	0.18	0	2,2,2	0.38	0
2	EDO	DDD	631	-	3,3,3	0.17	0	2,2,2	0.61	0
2	EDO	DDD	619	-	3,3,3	0.26	0	2,2,2	0.53	0
2	EDO	BBB	601	-	3,3,3	0.12	0	2,2,2	0.36	0
4	PEG	AAA	611	-	6,6,6	0.27	0	5,5,5	0.28	0
2	EDO	BBB	626	-	3,3,3	0.15	0	2,2,2	0.55	0
2	EDO	CCC	602	-	3,3,3	0.16	0	2,2,2	0.76	0
2	EDO	AAA	617	-	3,3,3	0.05	0	2,2,2	0.27	0
2	EDO	DDD	618	-	3,3,3	0.18	0	2,2,2	0.31	0
2	EDO	BBB	604	-	3,3,3	0.12	0	2,2,2	0.17	0
2	EDO	BBB	627	-	3,3,3	0.17	0	2,2,2	0.38	0
2	EDO	DDD	603	-	3,3,3	0.20	0	2,2,2	0.45	0
2	EDO	BBB	635	-	3,3,3	0.17	0	2,2,2	0.27	0
2	EDO	CCC	613	-	3,3,3	0.40	0	2,2,2	0.34	0
2	EDO	DDD	630	-	3,3,3	0.11	0	2,2,2	0.69	0
2	EDO	BBB	619	-	3,3,3	0.08	0	2,2,2	0.62	0
2	EDO	DDD	625	-	3,3,3	0.16	0	2,2,2	0.39	0
2	EDO	CCC	627	-	3,3,3	0.36	0	2,2,2	0.68	0
2	EDO	AAA	636	-	3,3,3	0.29	0	2,2,2	0.43	0
4	PEG	DDD	602	-	6,6,6	0.17	0	5,5,5	0.40	0
4	PEG	BBB	634	-	6,6,6	0.35	0	5,5,5	0.35	0
2	EDO	DDD	634	-	3,3,3	0.15	0	2,2,2	0.20	0
2	EDO	AAA	605	-	3,3,3	0.19	0	2,2,2	0.12	0
2	EDO	AAA	622	-	3,3,3	0.08	0	2,2,2	0.49	0
2	EDO	DDD	610	-	3,3,3	0.25	0	2,2,2	0.45	0
2	EDO	BBB	616	-	3,3,3	0.14	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PGE	DDD	624	-	9,9,9	0.53	0	8,8,8	0.46	0
2	EDO	CCC	620	-	3,3,3	0.05	0	2,2,2	0.22	0
4	PEG	DDD	621	-	6,6,6	0.22	0	5,5,5	0.19	0
2	EDO	DDD	623	-	3,3,3	0.10	0	2,2,2	0.44	0
4	PEG	CCC	617	-	6,6,6	0.22	0	5,5,5	0.23	0
2	EDO	CCC	618	-	3,3,3	0.27	0	2,2,2	0.09	0
2	EDO	AAA	614	-	3,3,3	0.21	0	2,2,2	0.57	0
2	EDO	DDD	605	-	3,3,3	0.17	0	2,2,2	0.18	0
2	EDO	BBB	607	-	3,3,3	0.07	0	2,2,2	0.03	0
4	PEG	CCC	604	-	6,6,6	0.17	0	5,5,5	0.14	0
2	EDO	DDD	629	-	3,3,3	0.27	0	2,2,2	0.58	0
2	EDO	DDD	633	-	3,3,3	0.26	0	2,2,2	0.50	0
2	EDO	AAA	634	-	3,3,3	0.13	0	2,2,2	0.28	0
2	EDO	BBB	624	-	3,3,3	0.05	0	2,2,2	0.13	0
2	EDO	DDD	601	-	3,3,3	0.08	0	2,2,2	0.10	0
2	EDO	AAA	610	-	3,3,3	0.36	0	2,2,2	0.06	0
2	EDO	BBB	632	-	3,3,3	0.17	0	2,2,2	0.82	0
2	EDO	BBB	623	-	3,3,3	0.04	0	2,2,2	0.19	0
2	EDO	BBB	631	-	3,3,3	0.14	0	2,2,2	0.57	0
2	EDO	BBB	630	-	3,3,3	0.19	0	2,2,2	0.47	0
2	EDO	AAA	618	-	3,3,3	0.36	0	2,2,2	0.77	0
2	EDO	CCC	610	-	3,3,3	0.17	0	2,2,2	0.19	0
4	PEG	BBB	603	-	6,6,6	0.21	0	5,5,5	0.15	0
2	EDO	BBB	620	-	3,3,3	0.10	0	2,2,2	0.40	0
2	EDO	CCC	611	-	3,3,3	0.19	0	2,2,2	0.30	0
2	EDO	BBB	628	-	3,3,3	0.29	0	2,2,2	0.57	0
2	EDO	AAA	613	-	3,3,3	0.31	0	2,2,2	0.78	0
2	EDO	CCC	605	-	3,3,3	0.15	0	2,2,2	0.51	0
2	EDO	BBB	613	-	3,3,3	0.11	0	2,2,2	0.13	0
2	EDO	DDD	616	-	3,3,3	0.09	0	2,2,2	0.58	0
2	EDO	DDD	611	-	3,3,3	0.36	0	2,2,2	0.18	0
4	PEG	DDD	604	-	6,6,6	0.29	0	5,5,5	0.18	0
2	EDO	DDD	612	-	3,3,3	0.03	0	2,2,2	0.10	0
2	EDO	CCC	601	-	3,3,3	0.13	0	2,2,2	0.19	0
2	EDO	DDD	608	-	3,3,3	0.21	0	2,2,2	0.18	0
3	PGE	AAA	608	-	9,9,9	0.30	0	8,8,8	0.15	0
2	EDO	AAA	635	-	3,3,3	0.17	0	2,2,2	0.31	0
2	EDO	AAA	606	-	3,3,3	0.19	0	2,2,2	0.31	0
2	EDO	CCC	609	-	3,3,3	0.13	0	2,2,2	0.20	0
2	EDO	AAA	604	-	3,3,3	0.11	0	2,2,2	0.41	0
2	EDO	AAA	612	-	3,3,3	0.12	0	2,2,2	0.66	0
2	EDO	AAA	629	-	3,3,3	0.21	0	2,2,2	0.52	0
2	EDO	DDD	617	-	3,3,3	0.11	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	BBB	629	-	3,3,3	0.18	0	2,2,2	0.11	0
2	EDO	DDD	620	-	3,3,3	0.06	0	2,2,2	0.19	0
2	EDO	AAA	631	-	3,3,3	0.23	0	2,2,2	0.35	0
2	EDO	CCC	614	-	3,3,3	0.12	0	2,2,2	0.65	0
2	EDO	DDD	609	-	3,3,3	0.06	0	2,2,2	0.23	0
2	EDO	BBB	606	-	3,3,3	0.30	0	2,2,2	0.30	0
2	EDO	CCC	607	-	3,3,3	0.21	0	2,2,2	0.27	0
2	EDO	AAA	628	-	3,3,3	0.26	0	2,2,2	0.80	0
2	EDO	AAA	627	-	3,3,3	0.05	0	2,2,2	0.41	0
2	EDO	BBB	602	-	3,3,3	0.25	0	2,2,2	0.18	0
2	EDO	AAA	616	-	3,3,3	0.14	0	2,2,2	0.09	0
2	EDO	AAA	625	-	3,3,3	0.22	0	2,2,2	0.41	0
2	EDO	CCC	626	-	3,3,3	0.08	0	2,2,2	0.53	0
2	EDO	AAA	623	-	3,3,3	0.29	0	2,2,2	0.54	0
2	EDO	AAA	630	-	3,3,3	0.10	0	2,2,2	0.21	0
5	PG4	CCC	623	-	12,12,12	0.44	0	11,11,11	0.37	0
2	EDO	AAA	601	-	3,3,3	0.14	0	2,2,2	0.51	0
2	EDO	CCC	621	-	3,3,3	0.08	0	2,2,2	0.56	0
2	EDO	DDD	615	-	3,3,3	0.39	0	2,2,2	0.91	0
4	PEG	CCC	619	-	6,6,6	0.19	0	5,5,5	0.29	0
2	EDO	CCC	624	-	3,3,3	0.14	0	2,2,2	0.48	0
2	EDO	DDD	632	-	3,3,3	0.09	0	2,2,2	0.05	0
2	EDO	BBB	618	-	3,3,3	0.21	0	2,2,2	0.32	0
2	EDO	BBB	636	-	3,3,3	0.15	0	2,2,2	0.22	0
2	EDO	BBB	633	-	3,3,3	0.17	0	2,2,2	0.30	0
2	EDO	DDD	626	-	3,3,3	0.24	0	2,2,2	0.55	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	EDO	CCC	616	-	-	1/1/1/1	-
2	EDO	AAA	624	-	-	1/1/1/1	-
2	EDO	BBB	622	-	-	1/1/1/1	-
2	EDO	DDD	607	-	-	0/1/1/1	-
2	EDO	AAA	619	-	-	1/1/1/1	-
2	EDO	AAA	602	-	-	1/1/1/1	-
2	EDO	AAA	607	-	-	0/1/1/1	-
2	EDO	BBB	609	-	-	0/1/1/1	-
2	EDO	AAA	637	-	-	1/1/1/1	-
2	EDO	AAA	615	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	AAA	626	-	-	0/1/1/1	-
2	EDO	AAA	609	-	-	0/1/1/1	-
2	EDO	BBB	615	-	-	1/1/1/1	-
2	EDO	AAA	620	-	-	0/1/1/1	-
2	EDO	AAA	632	-	-	1/1/1/1	-
2	EDO	CCC	608	-	-	1/1/1/1	-
2	EDO	BBB	617	-	-	1/1/1/1	-
2	EDO	DDD	613	-	-	1/1/1/1	-
2	EDO	DDD	614	-	-	0/1/1/1	-
2	EDO	CCC	606	-	-	0/1/1/1	-
2	EDO	BBB	612	-	-	1/1/1/1	-
2	EDO	CCC	603	-	-	1/1/1/1	-
2	EDO	AAA	621	-	-	0/1/1/1	-
2	EDO	AAA	633	-	-	0/1/1/1	-
2	EDO	CCC	612	-	-	0/1/1/1	-
2	EDO	BBB	610	-	-	1/1/1/1	-
2	EDO	DDD	627	-	-	1/1/1/1	-
2	EDO	BBB	608	-	-	0/1/1/1	-
2	EDO	BBB	614	-	-	0/1/1/1	-
2	EDO	DDD	606	-	-	0/1/1/1	-
2	EDO	BBB	625	-	-	0/1/1/1	-
2	EDO	CCC	622	-	-	0/1/1/1	-
2	EDO	BBB	605	-	-	1/1/1/1	-
2	EDO	BBB	621	-	-	0/1/1/1	-
2	EDO	AAA	603	-	-	1/1/1/1	-
2	EDO	DDD	628	-	-	1/1/1/1	-
2	EDO	CCC	625	-	-	0/1/1/1	-
2	EDO	DDD	622	-	-	1/1/1/1	-
2	EDO	CCC	615	-	-	0/1/1/1	-
2	EDO	BBB	611	-	-	0/1/1/1	-
2	EDO	DDD	631	-	-	0/1/1/1	-
2	EDO	DDD	619	-	-	0/1/1/1	-
2	EDO	BBB	601	-	-	1/1/1/1	-
4	PEG	AAA	611	-	-	2/4/4/4	-
2	EDO	BBB	626	-	-	0/1/1/1	-
2	EDO	CCC	602	-	-	1/1/1/1	-
2	EDO	AAA	617	-	-	1/1/1/1	-
2	EDO	DDD	618	-	-	1/1/1/1	-
2	EDO	BBB	604	-	-	1/1/1/1	-
2	EDO	BBB	627	-	-	1/1/1/1	-
2	EDO	DDD	603	-	-	1/1/1/1	-
2	EDO	BBB	635	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	CCC	613	-	-	1/1/1/1	-
2	EDO	DDD	630	-	-	1/1/1/1	-
2	EDO	BBB	619	-	-	1/1/1/1	-
2	EDO	DDD	625	-	-	0/1/1/1	-
2	EDO	CCC	627	-	-	0/1/1/1	-
2	EDO	AAA	636	-	-	0/1/1/1	-
4	PEG	DDD	602	-	-	3/4/4/4	-
4	PEG	BBB	634	-	-	0/4/4/4	-
2	EDO	DDD	634	-	-	1/1/1/1	-
2	EDO	AAA	605	-	-	1/1/1/1	-
2	EDO	AAA	622	-	-	0/1/1/1	-
2	EDO	DDD	610	-	-	1/1/1/1	-
2	EDO	BBB	616	-	-	0/1/1/1	-
3	PGE	DDD	624	-	-	3/7/7/7	-
2	EDO	CCC	620	-	-	1/1/1/1	-
4	PEG	DDD	621	-	-	0/4/4/4	-
2	EDO	DDD	623	-	-	0/1/1/1	-
4	PEG	CCC	617	-	-	4/4/4/4	-
2	EDO	CCC	618	-	-	1/1/1/1	-
2	EDO	AAA	614	-	-	0/1/1/1	-
2	EDO	DDD	605	-	-	0/1/1/1	-
2	EDO	BBB	607	-	-	1/1/1/1	-
4	PEG	CCC	604	-	-	3/4/4/4	-
2	EDO	DDD	629	-	-	0/1/1/1	-
2	EDO	DDD	633	-	-	1/1/1/1	-
2	EDO	AAA	634	-	-	1/1/1/1	-
2	EDO	BBB	624	-	-	1/1/1/1	-
2	EDO	DDD	601	-	-	1/1/1/1	-
2	EDO	AAA	610	-	-	0/1/1/1	-
2	EDO	BBB	632	-	-	1/1/1/1	-
2	EDO	BBB	623	-	-	1/1/1/1	-
2	EDO	BBB	631	-	-	0/1/1/1	-
2	EDO	BBB	630	-	-	0/1/1/1	-
2	EDO	AAA	618	-	-	0/1/1/1	-
2	EDO	CCC	610	-	-	0/1/1/1	-
4	PEG	BBB	603	-	-	3/4/4/4	-
2	EDO	BBB	620	-	-	1/1/1/1	-
2	EDO	CCC	611	-	-	1/1/1/1	-
2	EDO	BBB	628	-	-	1/1/1/1	-
2	EDO	AAA	613	-	-	1/1/1/1	-
2	EDO	CCC	605	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	BBB	613	-	-	0/1/1/1	-
2	EDO	DDD	616	-	-	0/1/1/1	-
2	EDO	DDD	611	-	-	0/1/1/1	-
4	PEG	DDD	604	-	-	1/4/4/4	-
2	EDO	DDD	612	-	-	0/1/1/1	-
2	EDO	CCC	601	-	-	0/1/1/1	-
2	EDO	DDD	608	-	-	1/1/1/1	-
3	PGE	AAA	608	-	-	4/7/7/7	-
2	EDO	AAA	635	-	-	1/1/1/1	-
2	EDO	AAA	606	-	-	1/1/1/1	-
2	EDO	CCC	609	-	-	0/1/1/1	-
2	EDO	AAA	604	-	-	0/1/1/1	-
2	EDO	AAA	612	-	-	1/1/1/1	-
2	EDO	AAA	629	-	-	1/1/1/1	-
2	EDO	DDD	617	-	-	1/1/1/1	-
2	EDO	BBB	629	-	-	0/1/1/1	-
2	EDO	DDD	620	-	-	1/1/1/1	-
2	EDO	AAA	631	-	-	0/1/1/1	-
2	EDO	CCC	614	-	-	1/1/1/1	-
2	EDO	DDD	609	-	-	0/1/1/1	-
2	EDO	BBB	606	-	-	1/1/1/1	-
2	EDO	CCC	607	-	-	1/1/1/1	-
2	EDO	AAA	628	-	-	1/1/1/1	-
2	EDO	AAA	627	-	-	1/1/1/1	-
2	EDO	BBB	602	-	-	0/1/1/1	-
2	EDO	AAA	616	-	-	0/1/1/1	-
2	EDO	AAA	625	-	-	1/1/1/1	-
2	EDO	CCC	626	-	-	1/1/1/1	-
2	EDO	AAA	623	-	-	1/1/1/1	-
2	EDO	AAA	630	-	-	0/1/1/1	-
5	PG4	CCC	623	-	-	3/10/10/10	-
2	EDO	AAA	601	-	-	1/1/1/1	-
2	EDO	CCC	621	-	-	1/1/1/1	-
2	EDO	DDD	615	-	-	0/1/1/1	-
4	PEG	CCC	619	-	-	2/4/4/4	-
2	EDO	CCC	624	-	-	1/1/1/1	-
2	EDO	DDD	632	-	-	1/1/1/1	-
2	EDO	BBB	618	-	-	1/1/1/1	-
2	EDO	BBB	636	-	-	0/1/1/1	-
2	EDO	BBB	633	-	-	1/1/1/1	-
2	EDO	DDD	626	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	608	PGE	O2-C3-C4-O3
3	DDD	624	PGE	O2-C3-C4-O3
5	CCC	623	PG4	O3-C5-C6-O4
4	CCC	604	PEG	C4-C3-O2-C2
4	CCC	604	PEG	O2-C3-C4-O4

There are no ring outliers.

47 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	616	EDO	1	0
2	BBB	622	EDO	1	0
2	DDD	607	EDO	1	0
2	AAA	632	EDO	1	0
2	BBB	617	EDO	3	0
2	DDD	613	EDO	2	0
2	CCC	606	EDO	4	0
2	BBB	614	EDO	4	0
2	BBB	621	EDO	2	0
4	AAA	611	PEG	8	0
2	BBB	626	EDO	1	0
2	AAA	617	EDO	1	0
2	BBB	604	EDO	1	0
2	DDD	603	EDO	2	0
4	DDD	602	PEG	6	0
2	DDD	610	EDO	1	0
3	DDD	624	PGE	2	0
2	CCC	620	EDO	1	0
4	DDD	621	PEG	2	0
4	CCC	617	PEG	2	0
4	CCC	604	PEG	1	0
2	BBB	632	EDO	1	0
2	AAA	618	EDO	1	0
2	CCC	610	EDO	5	0
4	BBB	603	PEG	11	0
2	BBB	628	EDO	2	0
2	AAA	613	EDO	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	613	EDO	2	0
2	DDD	616	EDO	1	0
4	DDD	604	PEG	3	0
2	CCC	601	EDO	1	0
3	AAA	608	PGE	5	0
2	AAA	606	EDO	3	0
2	AAA	612	EDO	1	0
2	DDD	617	EDO	1	0
2	AAA	631	EDO	1	0
2	CCC	614	EDO	1	0
2	DDD	609	EDO	1	0
2	AAA	628	EDO	2	0
2	AAA	616	EDO	1	0
2	AAA	623	EDO	3	0
5	CCC	623	PG4	4	0
2	DDD	615	EDO	1	0
4	CCC	619	PEG	1	0
2	CCC	624	EDO	1	0
2	BBB	636	EDO	1	0
2	DDD	626	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^{th} 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	AAA	563/585 (96%)	-0.30	11 (1%) 65 69	23, 37, 71, 118	0
1	BBB	554/585 (94%)	-0.35	3 (0%) 91 92	21, 35, 65, 116	0
1	CCC	561/585 (95%)	-0.21	20 (3%) 42 46	23, 37, 71, 128	0
1	DDD	562/585 (96%)	-0.31	12 (2%) 63 67	23, 34, 64, 125	0
All	All	2240/2340 (95%)	-0.29	46 (2%) 63 67	21, 36, 70, 128	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	31	PRO	10.0
1	CCC	30	THR	7.9
1	DDD	24	ILE	7.7
1	DDD	31	PRO	6.5
1	CCC	32	SER	6.0

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
2	EDO	DDD	634	4/4	0.66	0.34	68,77,81,82	0
2	EDO	AAA	627	4/4	0.67	0.18	54,56,57,64	4
2	EDO	DDD	601	4/4	0.69	0.17	60,62,68,68	0
3	PGE	DDD	624	10/10	0.71	0.22	36,42,51,51	10
2	EDO	AAA	637	4/4	0.72	0.12	72,72,74,88	0
2	EDO	AAA	626	4/4	0.75	0.16	58,64,64,66	0
2	EDO	CCC	616	4/4	0.77	0.19	64,66,68,71	4
2	EDO	CCC	603	4/4	0.77	0.15	63,64,66,72	0
5	PG4	CCC	623	13/13	0.77	0.20	48,63,69,75	0
2	EDO	AAA	628	4/4	0.78	0.22	41,42,45,50	0
2	EDO	DDD	603	4/4	0.78	0.20	50,51,52,53	0
2	EDO	DDD	613	4/4	0.78	0.13	49,50,54,54	0
2	EDO	CCC	609	4/4	0.78	0.41	67,69,74,75	0
2	EDO	BBB	621	4/4	0.78	0.20	50,53,60,64	0
2	EDO	CCC	624	4/4	0.78	0.31	65,69,71,74	0
2	EDO	BBB	610	4/4	0.79	0.14	53,56,56,57	0
2	EDO	DDD	620	4/4	0.79	0.22	54,54,56,56	4
2	EDO	BBB	626	4/4	0.79	0.16	52,56,56,62	0
2	EDO	BBB	618	4/4	0.79	0.17	56,63,64,68	0
2	EDO	BBB	619	4/4	0.79	0.21	75,77,79,88	0
4	PEG	DDD	621	7/7	0.80	0.19	43,48,60,64	0
2	EDO	BBB	630	4/4	0.81	0.20	66,68,69,74	0
2	EDO	AAA	602	4/4	0.81	0.25	72,73,73,78	0
2	EDO	DDD	616	4/4	0.81	0.13	68,69,71,78	0
2	EDO	BBB	627	4/4	0.81	0.16	50,55,57,60	0
4	PEG	CCC	604	7/7	0.82	0.21	59,68,72,77	0
2	EDO	BBB	615	4/4	0.82	0.15	65,71,72,75	0
2	EDO	DDD	631	4/4	0.82	0.15	43,47,53,55	0
2	EDO	BBB	611	4/4	0.83	0.21	68,76,78,80	0
2	EDO	BBB	612	4/4	0.83	0.21	53,56,58,60	0
2	EDO	AAA	620	4/4	0.83	0.19	64,66,67,73	0
2	EDO	AAA	612	4/4	0.83	0.21	53,60,64,73	0
2	EDO	BBB	631	4/4	0.83	0.12	53,56,57,73	0
4	PEG	CCC	617	7/7	0.83	0.27	60,77,81,81	0
2	EDO	AAA	619	4/4	0.83	0.18	53,55,56,76	0
2	EDO	CCC	608	4/4	0.83	0.11	60,65,72,74	0
2	EDO	DDD	607	4/4	0.84	0.21	53,63,64,65	0
4	PEG	CCC	619	7/7	0.84	0.18	44,52,70,78	0
2	EDO	DDD	609	4/4	0.85	0.12	54,57,60,67	0
2	EDO	BBB	635	4/4	0.85	0.16	83,86,88,96	0
2	EDO	CCC	602	4/4	0.85	0.16	51,54,56,59	0
2	EDO	AAA	603	4/4	0.85	0.18	54,61,62,73	0
2	EDO	BBB	625	4/4	0.85	0.19	63,67,69,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	BBB	617	4/4	0.85	0.17	63,63,63,79	0
2	EDO	DDD	625	4/4	0.86	0.13	59,60,64,68	0
2	EDO	DDD	628	4/4	0.86	0.20	50,51,54,60	4
2	EDO	AAA	621	4/4	0.86	0.15	51,52,56,56	0
2	EDO	DDD	605	4/4	0.86	0.14	56,59,62,72	0
2	EDO	AAA	633	4/4	0.86	0.17	58,64,65,74	0
2	EDO	AAA	635	4/4	0.86	0.18	49,51,54,54	4
2	EDO	DDD	612	4/4	0.86	0.18	44,49,50,53	0
2	EDO	AAA	636	4/4	0.86	0.18	53,56,60,66	4
2	EDO	BBB	636	4/4	0.86	0.18	74,78,78,79	0
2	EDO	AAA	624	4/4	0.86	0.20	42,44,46,48	0
2	EDO	AAA	606	4/4	0.87	0.15	61,63,64,66	0
2	EDO	CCC	610	4/4	0.87	0.13	66,68,71,71	0
4	PEG	DDD	602	7/7	0.87	0.19	46,51,66,69	0
2	EDO	CCC	625	4/4	0.87	0.25	40,49,51,56	4
2	EDO	DDD	606	4/4	0.87	0.13	56,57,57,70	0
2	EDO	AAA	617	4/4	0.88	0.14	59,61,63,63	0
2	EDO	DDD	617	4/4	0.88	0.09	56,58,61,63	0
4	PEG	AAA	611	7/7	0.88	0.21	44,53,58,61	0
4	PEG	BBB	603	7/7	0.88	0.18	44,56,63,63	0
4	PEG	BBB	634	7/7	0.88	0.20	47,52,59,65	0
2	EDO	AAA	625	4/4	0.88	0.22	39,46,47,54	4
2	EDO	CCC	611	4/4	0.88	0.15	55,67,68,75	0
2	EDO	CCC	612	4/4	0.88	0.13	52,52,54,54	0
2	EDO	DDD	630	4/4	0.88	0.14	67,70,72,77	0
2	EDO	AAA	613	4/4	0.88	0.25	55,56,57,59	0
2	EDO	DDD	632	4/4	0.88	0.22	38,43,47,49	4
2	EDO	BBB	628	4/4	0.89	0.20	56,57,67,72	0
2	EDO	CCC	621	4/4	0.89	0.14	61,62,65,66	0
2	EDO	DDD	627	4/4	0.89	0.25	32,37,38,46	0
2	EDO	BBB	624	4/4	0.89	0.25	61,62,63,67	0
4	PEG	DDD	604	7/7	0.89	0.17	44,56,69,69	0
2	EDO	AAA	623	4/4	0.89	0.17	60,63,64,66	0
2	EDO	CCC	626	4/4	0.89	0.21	50,58,59,61	0
2	EDO	BBB	620	4/4	0.90	0.21	69,70,71,75	0
2	EDO	CCC	614	4/4	0.90	0.14	43,43,47,52	0
2	EDO	CCC	627	4/4	0.90	0.13	59,60,64,65	0
2	EDO	BBB	629	4/4	0.90	0.23	58,59,62,68	0
2	EDO	AAA	630	4/4	0.90	0.11	59,59,60,61	0
2	EDO	DDD	629	4/4	0.90	0.13	49,58,59,59	0
2	EDO	AAA	604	4/4	0.90	0.19	45,52,56,63	0
2	EDO	DDD	626	4/4	0.91	0.20	52,53,54,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	DDD	633	4/4	0.91	0.17	41,46,50,60	4
2	EDO	CCC	601	4/4	0.91	0.13	54,60,63,69	0
2	EDO	AAA	634	4/4	0.91	0.15	52,58,58,67	0
2	EDO	BBB	633	4/4	0.91	0.21	48,56,60,60	0
2	EDO	DDD	623	4/4	0.91	0.14	39,54,56,58	0
2	EDO	CCC	606	4/4	0.91	0.20	60,61,66,70	0
2	EDO	AAA	614	4/4	0.92	0.15	42,45,48,52	0
2	EDO	BBB	606	4/4	0.92	0.22	54,55,58,59	0
2	EDO	AAA	609	4/4	0.92	0.18	42,45,52,54	0
2	EDO	AAA	605	4/4	0.92	0.10	67,69,73,81	0
2	EDO	AAA	607	4/4	0.92	0.14	42,45,45,50	0
2	EDO	BBB	613	4/4	0.92	0.21	50,53,54,57	0
2	EDO	DDD	608	4/4	0.92	0.16	47,52,56,64	0
2	EDO	CCC	622	4/4	0.92	0.26	70,72,74,76	0
2	EDO	CCC	607	4/4	0.92	0.11	66,69,72,75	0
2	EDO	BBB	622	4/4	0.92	0.16	50,53,57,61	0
2	EDO	DDD	614	4/4	0.92	0.11	42,48,48,60	0
2	EDO	BBB	614	4/4	0.92	0.10	42,42,42,43	0
2	EDO	DDD	610	4/4	0.93	0.14	40,43,44,47	0
2	EDO	AAA	616	4/4	0.93	0.12	39,44,46,49	0
2	EDO	AAA	622	4/4	0.93	0.18	51,54,58,60	0
2	EDO	AAA	610	4/4	0.93	0.13	32,32,32,35	0
2	EDO	DDD	615	4/4	0.93	0.12	51,56,60,62	0
3	PGE	AAA	608	10/10	0.94	0.17	33,45,53,54	0
2	EDO	AAA	632	4/4	0.94	0.15	51,61,67,74	0
2	EDO	CCC	620	4/4	0.94	0.23	62,70,71,72	0
2	EDO	DDD	618	4/4	0.94	0.11	32,34,39,43	0
2	EDO	BBB	623	4/4	0.94	0.10	50,50,54,61	0
2	EDO	AAA	601	4/4	0.94	0.08	46,47,51,52	0
2	EDO	CCC	618	4/4	0.95	0.10	42,44,46,49	0
2	EDO	BBB	607	4/4	0.95	0.09	38,45,48,55	0
2	EDO	BBB	609	4/4	0.95	0.09	30,32,33,35	0
2	EDO	AAA	631	4/4	0.95	0.14	40,50,51,58	0
2	EDO	BBB	604	4/4	0.95	0.16	61,69,70,76	0
2	EDO	DDD	619	4/4	0.95	0.15	45,46,47,54	0
2	EDO	BBB	605	4/4	0.95	0.10	31,36,40,41	0
2	EDO	CCC	613	4/4	0.95	0.20	37,44,45,48	0
2	EDO	BBB	632	4/4	0.95	0.13	35,44,44,49	0
2	EDO	AAA	629	4/4	0.95	0.15	44,48,53,61	0
2	EDO	DDD	622	4/4	0.96	0.11	55,57,57,62	0
2	EDO	AAA	615	4/4	0.96	0.11	41,43,44,46	0
2	EDO	BBB	608	4/4	0.96	0.10	41,43,43,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	AAA	618	4/4	0.96	0.16	42,54,59,63	0
2	EDO	BBB	616	4/4	0.97	0.11	43,52,54,59	0
2	EDO	DDD	611	4/4	0.97	0.07	28,32,32,34	0
2	EDO	BBB	601	4/4	0.97	0.13	45,46,49,51	0
2	EDO	CCC	605	4/4	0.97	0.12	36,39,39,39	0
2	EDO	BBB	602	4/4	0.97	0.10	32,33,34,36	0
2	EDO	CCC	615	4/4	0.98	0.10	29,31,32,38	0

6.5 Other polymers (i)

There are no such residues in this entry.