



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 8, 2025 – 01:34 pm BST

PDB ID : 9HNC / pdb\_00009hnc  
Title : Crystal structure of potassium-independent L-asparaginase from Phaseolus vulgaris (PvAIII, PvAspG2)  
Authors : Loch, J.I.; Pierog, I.; Imiolczyk, B.; Barciszewski, J.; Marsolais, F.; Gilski, M.; Jaskolski, M.  
Deposited on : 2024-12-10  
Resolution : 1.88 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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>.

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
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) : 2.43.1

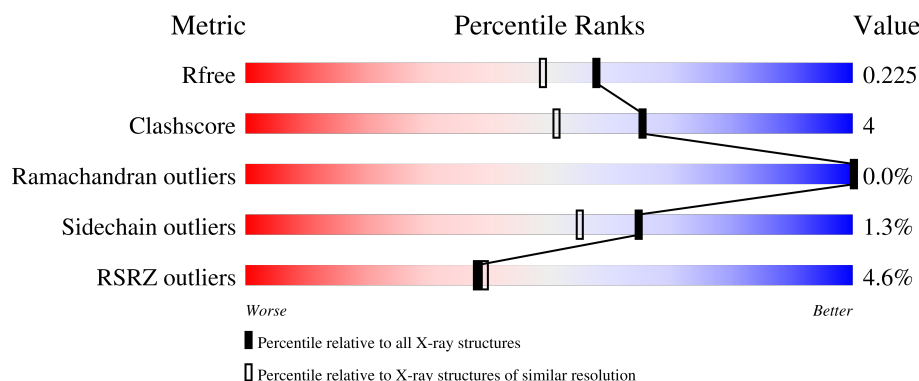
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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	AAA	322	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>
1	BBB	322	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	CCC	322	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	DDD	322	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	EEE	322	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	FFF	322	
1	GGG	322	
1	HHH	322	
1	III	322	
1	JJJ	322	
1	KKK	322	
1	LLL	322	
1	MMM	322	
1	NNN	322	
1	OOO	322	
1	PPP	322	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36793 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 beta-aspartyl-peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	288	Total	C	N	O	S	0	1	0
			2114	1314	372	414	14			
1	BBB	290	Total	C	N	O	S	0	0	0
			2127	1321	375	416	15			
1	CCC	298	Total	C	N	O	S	0	4	0
			2216	1380	389	433	14			
1	DDD	289	Total	C	N	O	S	0	1	0
			2124	1319	374	417	14			
1	EEE	289	Total	C	N	O	S	0	1	0
			2123	1320	374	415	14			
1	FFF	290	Total	C	N	O	S	0	0	0
			2127	1321	375	416	15			
1	GGG	292	Total	C	N	O	S	0	0	0
			2146	1332	381	419	14			
1	HHH	289	Total	C	N	O	S	0	0	0
			2119	1316	374	415	14			
1	III	289	Total	C	N	O	S	0	0	0
			2119	1316	374	415	14			
1	JJJ	288	Total	C	N	O	S	0	0	0
			2113	1313	373	413	14			
1	KKK	288	Total	C	N	O	S	0	0	0
			2113	1313	373	413	14			
1	LLL	291	Total	C	N	O	S	0	1	0
			2145	1332	382	417	14			
1	MMM	289	Total	C	N	O	S	0	0	0
			2119	1316	374	415	14			
1	NNN	288	Total	C	N	O	S	0	3	0
			2130	1325	375	416	14			
1	OOO	289	Total	C	N	O	S	0	2	0
			2131	1325	377	415	14			
1	PPP	288	Total	C	N	O	S	0	0	0
			2113	1313	373	413	14			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total 2	Na 2	0	0
2	BBB	2	Total 2	Na 2	0	0
2	CCC	2	Total 2	Na 2	0	0
2	DDD	2	Total 2	Na 2	0	0
2	EEE	2	Total 2	Na 2	0	0
2	FFF	2	Total 2	Na 2	0	0
2	GGG	2	Total 2	Na 2	0	0
2	HHH	2	Total 2	Na 2	0	0
2	III	2	Total 2	Na 2	0	0
2	JJJ	2	Total 2	Na 2	0	0
2	KKK	3	Total 3	Na 3	0	0
2	LLL	2	Total 2	Na 2	0	0
2	MMM	2	Total 2	Na 2	0	0
2	NNN	2	Total 2	Na 2	0	0
2	OOO	2	Total 2	Na 2	0	0
2	PPP	2	Total 2	Na 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	DDD	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	FFF	1	Total	O	S	0	0
			5	4	1		
3	GGG	1	Total	O	S	0	0
			5	4	1		
3	HHH	1	Total	O	S	0	0
			5	4	1		
3	III	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	JJJ	1	Total	O	S	0	0
			5	4	1		
3	LLL	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	MMM	1	Total	O	S	0	0
			5	4	1		
3	NNN	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	OOO	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		
3	PPP	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

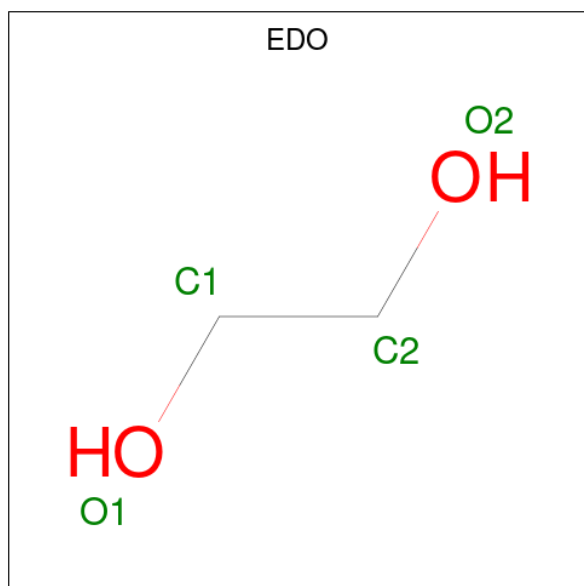
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Cl	0	0
			1	1		
4	BBB	4	Total	Cl	0	0
			4	4		
4	CCC	3	Total	Cl	0	0
			3	3		
4	DDD	2	Total	Cl	0	0
			2	2		
4	EEE	2	Total	Cl	0	0
			2	2		
4	FFF	1	Total	Cl	0	0
			1	1		
4	GGG	3	Total	Cl	0	0
			3	3		
4	HHH	1	Total	Cl	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	III	1	Total 1	Cl 1	0	0
4	JJJ	1	Total 1	Cl 1	0	0
4	KKK	2	Total 2	Cl 2	0	0
4	LLL	1	Total 1	Cl 1	0	0
4	MMM	1	Total 1	Cl 1	0	0
4	NNN	2	Total 2	Cl 2	0	0
4	OOO	2	Total 2	Cl 2	0	0
4	PPP	2	Total 2	Cl 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

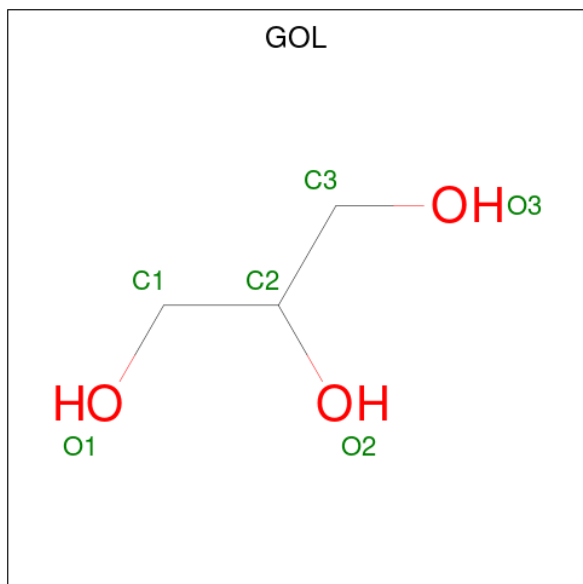
*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	EEE	1	Total	C	O	0	0
			4	2	2		
5	GGG	1	Total	C	O	0	0
			4	2	2		
5	HHH	1	Total	C	O	0	0
			4	2	2		
5	III	1	Total	C	O	0	0
			4	2	2		
5	MMM	1	Total	C	O	0	0
			4	2	2		
5	OOO	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	161	Total	O	0	2
			163	163		
7	BBB	158	Total	O	0	2
			160	160		

*Continued on next page...*

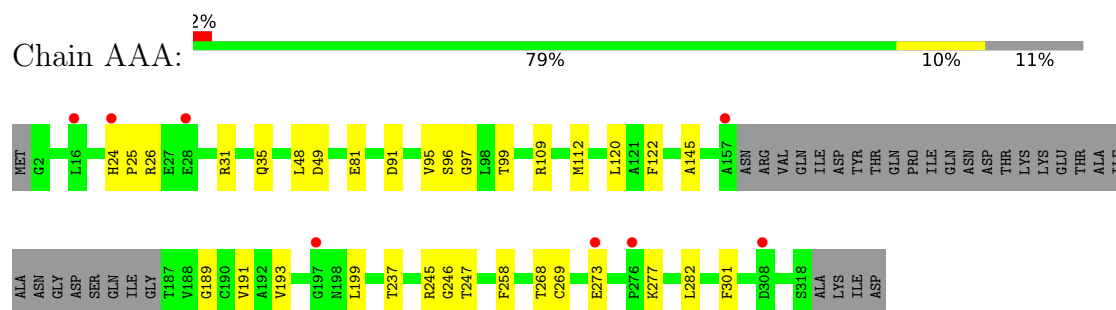
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	152	Total 156	O 156	0	4
7	DDD	159	Total 159	O 159	0	0
7	EEE	155	Total 157	O 157	0	2
7	FFF	163	Total 164	O 164	0	1
7	GGG	152	Total 153	O 153	0	1
7	HHH	145	Total 146	O 146	0	1
7	III	165	Total 166	O 166	0	1
7	JJJ	138	Total 138	O 138	0	0
7	KKK	133	Total 133	O 133	0	0
7	LLL	150	Total 150	O 150	0	0
7	MMM	159	Total 160	O 160	0	1
7	NNN	157	Total 157	O 157	0	0
7	OOO	160	Total 164	O 164	0	4
7	PPP	159	Total 159	O 159	0	0

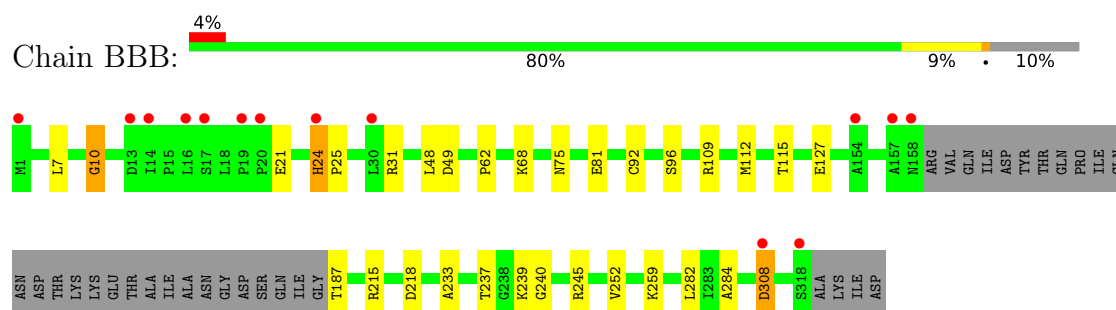
### 3 Residue-property plots [i](#)

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.

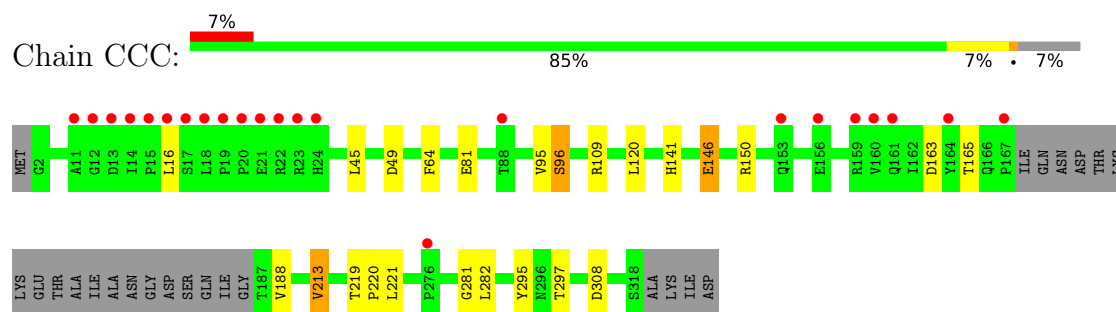
- Molecule 1: beta-aspartyl-peptidase



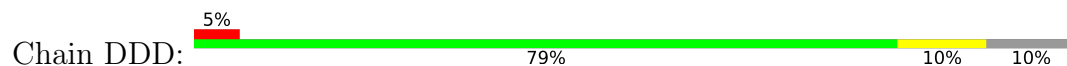
- Molecule 1: beta-aspartyl-peptidase

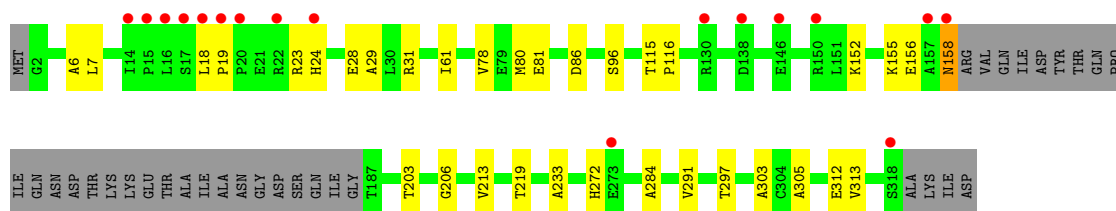


- Molecule 1: beta-aspartyl-peptidase

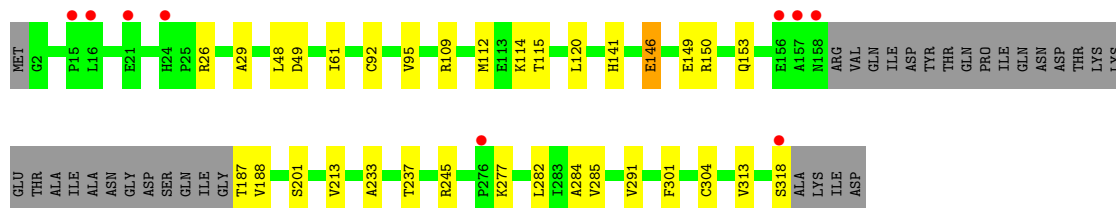
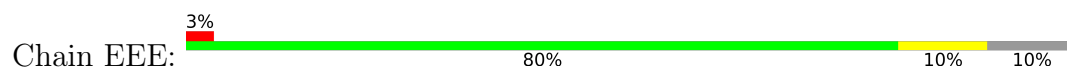


- Molecule 1: beta-aspartyl-peptidase

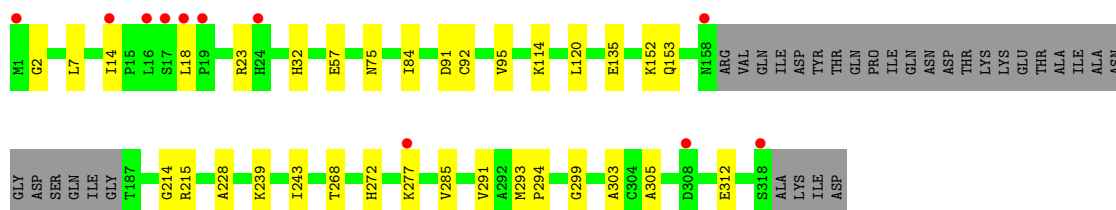
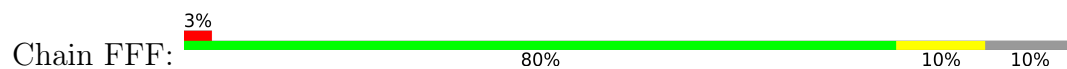




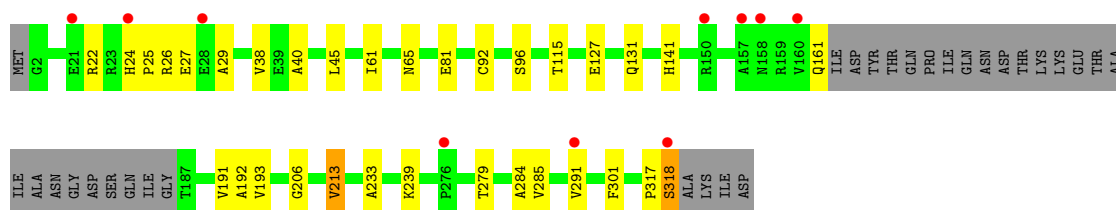
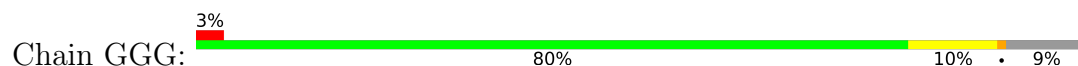
- Molecule 1: beta-aspartyl-peptidase



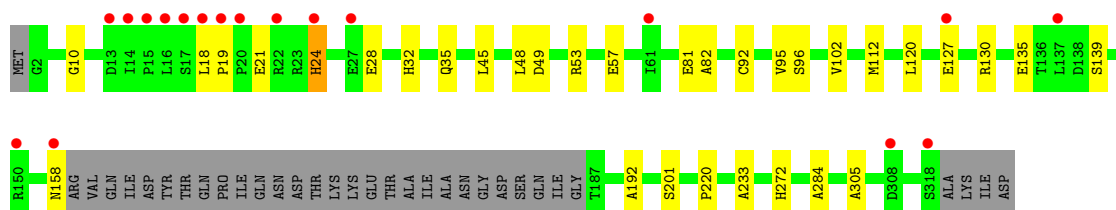
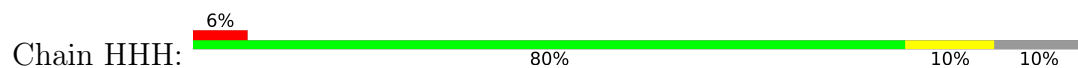
- Molecule 1: beta-aspartyl-peptidase



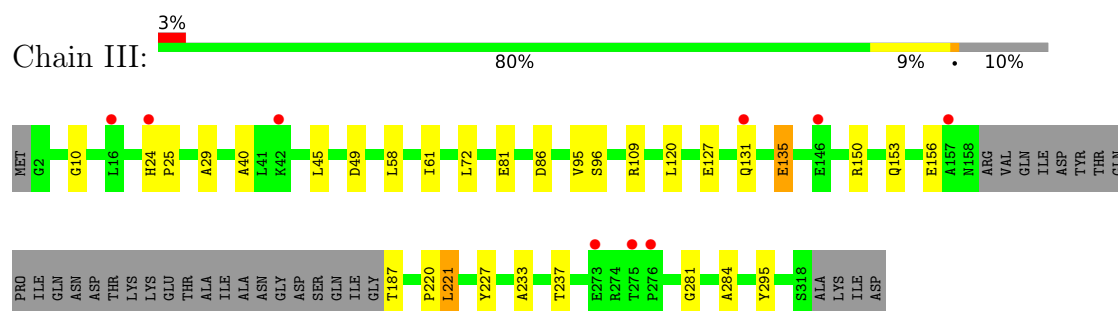
- Molecule 1: beta-aspartyl-peptidase



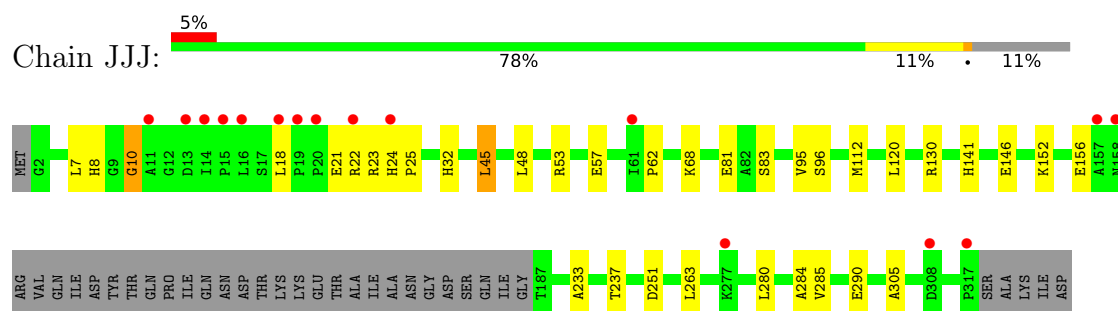
- Molecule 1: beta-aspartyl-peptidase



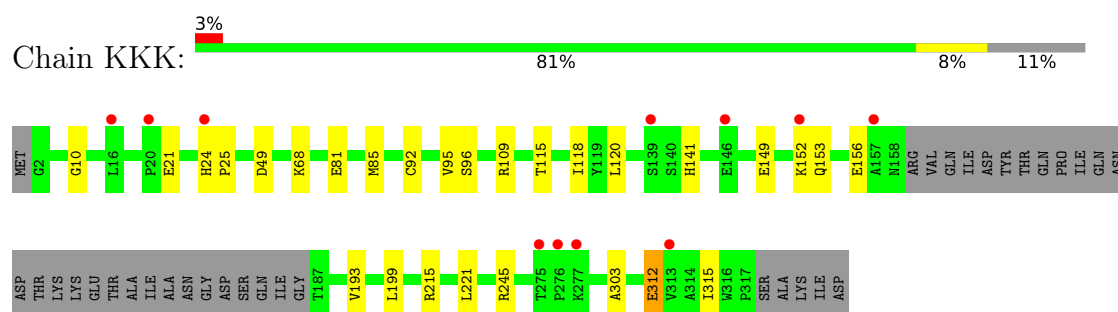
- Molecule 1: beta-aspartyl-peptidase



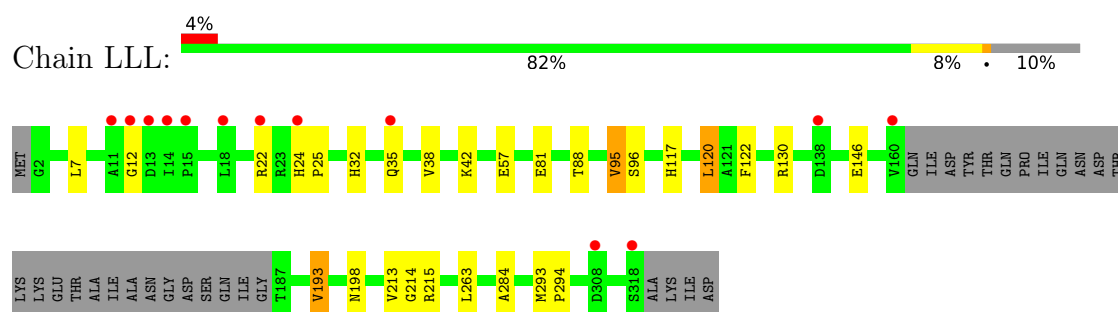
- Molecule 1: beta-aspartyl-peptidase



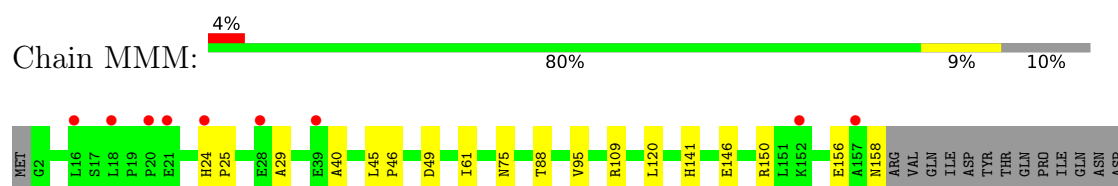
- Molecule 1: beta-aspartyl-peptidase



- Molecule 1: beta-aspartyl-peptidase

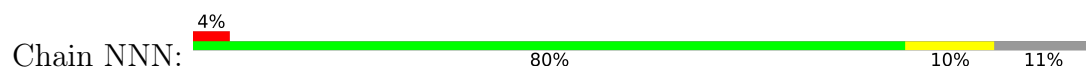


- Molecule 1: beta-aspartyl-peptidase

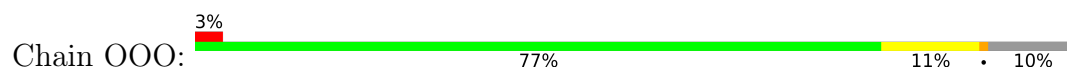




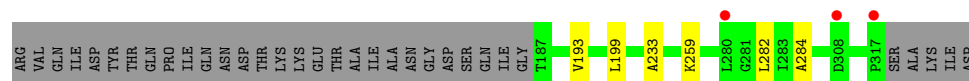
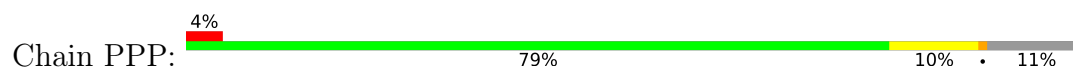
- Molecule 1: beta-aspartyl-peptidase



- Molecule 1: beta-aspartyl-peptidase



- Molecule 1: beta-aspartyl-peptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.76Å 123.64Å 187.68Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	47.69 – 1.88 47.69 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.69-1.88) 99.6 (47.69-1.88)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.182 , 0.211 0.193 , 0.225	Depositor DCC
$R_{free}$ test set	7949 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l 0.015 for -k,-h,-l 0.028 for h,-k,-l	Xtriage
Reported twinning fraction	0.825 for H, K, L 0.060 for -h,-k,l 0.056 for K, H, -L 0.059 for -K, -H, -L	Depositor
Outliers	4 of 456774 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	36793	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7869e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NA, CL, SO4, EDO, GOL

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	1.21	3/2147 (0.1%)	1.38	4/2910 (0.1%)
1	BBB	1.22	4/2157 (0.2%)	1.37	4/2923 (0.1%)
1	CCC	1.20	6/2257 (0.3%)	1.40	4/3062 (0.1%)
1	DDD	1.21	3/2157 (0.1%)	1.37	5/2924 (0.2%)
1	EEE	1.23	5/2156 (0.2%)	1.38	1/2923 (0.0%)
1	FFF	1.28	8/2157 (0.4%)	1.37	4/2923 (0.1%)
1	GGG	1.23	8/2176 (0.4%)	1.39	4/2949 (0.1%)
1	HHH	1.22	7/2149 (0.3%)	1.37	2/2913 (0.1%)
1	III	1.21	6/2149 (0.3%)	1.39	1/2913 (0.0%)
1	JJJ	1.19	3/2143 (0.1%)	1.38	1/2905 (0.0%)
1	KKK	1.21	4/2143 (0.2%)	1.38	2/2905 (0.1%)
1	LLL	1.24	4/2178 (0.2%)	1.37	1/2951 (0.0%)
1	MMM	1.21	3/2149 (0.1%)	1.34	0/2913
1	NNN	1.20	1/2169 (0.0%)	1.35	2/2939 (0.1%)
1	OOO	1.20	5/2167 (0.2%)	1.39	4/2937 (0.1%)
1	PPP	1.20	2/2143 (0.1%)	1.39	2/2905 (0.1%)
All	All	1.22	72/34597 (0.2%)	1.38	41/46895 (0.1%)

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	JJJ	83	SER	C-O	7.14	1.32	1.23
1	KKK	10	GLY	C-O	6.89	1.32	1.24
1	III	220	PRO	C-O	-6.66	1.15	1.24
1	CCC	188	VAL	C-O	6.63	1.30	1.23
1	AAA	191	VAL	C-O	6.61	1.30	1.24

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	308	ASP	CA-CB-CG	6.49	119.09	112.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	146	GLU	CB-CG-CD	6.26	123.24	112.60
1	BBB	239	LYS	CA-C-N	6.19	126.98	119.99
1	BBB	239	LYS	C-N-CA	6.19	126.98	119.99
1	DDD	206	GLY	CA-C-N	6.08	127.03	121.31

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	2114	0	2122	13	0
1	BBB	2127	0	2135	17	0
1	CCC	2216	0	2227	12	0
1	DDD	2124	0	2127	16	0
1	EEE	2123	0	2132	16	0
1	FFF	2127	0	2135	15	0
1	GGG	2146	0	2153	13	0
1	HHH	2119	0	2123	13	0
1	III	2119	0	2123	13	0
1	JJJ	2113	0	2118	25	0
1	KKK	2113	0	2118	14	0
1	LLL	2145	0	2158	16	0
1	MMM	2119	0	2123	19	0
1	NNN	2130	0	2143	17	0
1	OOO	2131	0	2145	21	0
1	PPP	2113	0	2118	20	0
2	AAA	2	0	0	0	0
2	BBB	2	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	2	0	0	0	0
2	EEE	2	0	0	0	0
2	FFF	2	0	0	0	0
2	GGG	2	0	0	0	0
2	HHH	2	0	0	0	0
2	III	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	JJJ	2	0	0	0	0
2	KKK	3	0	0	0	0
2	LLL	2	0	0	0	0
2	MMM	2	0	0	0	0
2	NNN	2	0	0	0	0
2	OOO	2	0	0	0	0
2	PPP	2	0	0	0	0
3	AAA	15	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	15	0	0	0	0
3	DDD	5	0	0	0	0
3	EEE	10	0	0	0	0
3	FFF	5	0	0	0	0
3	GGG	5	0	0	0	0
3	HHH	5	0	0	0	0
3	III	5	0	0	0	0
3	JJJ	15	0	0	0	0
3	LLL	5	0	0	1	0
3	MMM	10	0	0	0	0
3	NNN	5	0	0	0	0
3	OOO	10	0	0	0	0
3	PPP	10	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	4	0	0	0	0
4	CCC	3	0	0	0	0
4	DDD	2	0	0	0	0
4	EEE	2	0	0	0	0
4	FFF	1	0	0	0	0
4	GGG	3	0	0	1	0
4	HHH	1	0	0	1	0
4	III	1	0	0	0	0
4	JJJ	1	0	0	0	0
4	KKK	2	0	0	0	0
4	LLL	1	0	0	0	0
4	MMM	1	0	0	0	0
4	NNN	2	0	0	0	0
4	OOO	2	0	0	0	0
4	PPP	2	0	0	0	0
5	AAA	4	0	6	0	0
5	BBB	4	0	6	0	0
5	CCC	4	0	6	0	0
5	EEE	4	0	6	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	GGG	4	0	6	0	0
5	HHH	4	0	6	0	0
5	III	4	0	6	1	0
5	MMM	4	0	6	0	0
5	OOO	4	0	6	2	0
6	DDD	6	0	8	1	0
7	AAA	163	0	0	0	0
7	BBB	160	0	0	2	0
7	CCC	156	0	0	1	0
7	DDD	159	0	0	2	0
7	EEE	157	0	0	3	0
7	FFF	164	0	0	8	0
7	GGG	153	0	0	1	0
7	HHH	146	0	0	3	0
7	III	166	0	0	1	0
7	JJJ	138	0	0	2	0
7	KKK	133	0	0	3	0
7	LLL	150	0	0	2	0
7	MMM	160	0	0	8	0
7	NNN	157	0	0	2	0
7	OOO	164	0	0	3	0
7	PPP	159	0	0	3	0
All	All	36793	0	34262	254	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 4.

The worst 5 of 254 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:DDD:155:LYS:HG2	6:DDD:404:GOL:H2	1.53	0.91
1:GGG:29:ALA:HB1	1:GGG:61:ILE:HD13	1.73	0.71
1:EEE:29:ALA:HB1	1:EEE:61:ILE:HD13	1.74	0.69
1:EEE:146:GLU:OE1	1:EEE:150:ARG:NH1	2.27	0.67
1:PPP:24:HIS:HB2	1:PPP:25:PRO:HD3	1.76	0.67

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	285/322 (88%)	277 (97%)	8 (3%)	0	100	100
1	BBB	286/322 (89%)	274 (96%)	11 (4%)	1 (0%)	37	26
1	CCC	298/322 (92%)	292 (98%)	6 (2%)	0	100	100
1	DDD	286/322 (89%)	274 (96%)	12 (4%)	0	100	100
1	EEE	286/322 (89%)	279 (98%)	7 (2%)	0	100	100
1	FFF	286/322 (89%)	278 (97%)	8 (3%)	0	100	100
1	GGG	288/322 (89%)	277 (96%)	11 (4%)	0	100	100
1	HHH	285/322 (88%)	277 (97%)	8 (3%)	0	100	100
1	III	285/322 (88%)	279 (98%)	6 (2%)	0	100	100
1	JJJ	284/322 (88%)	272 (96%)	12 (4%)	0	100	100
1	KKK	284/322 (88%)	275 (97%)	9 (3%)	0	100	100
1	LLL	288/322 (89%)	280 (97%)	8 (3%)	0	100	100
1	MMM	285/322 (88%)	276 (97%)	9 (3%)	0	100	100
1	NNN	287/322 (89%)	274 (96%)	13 (4%)	0	100	100
1	OOO	287/322 (89%)	278 (97%)	9 (3%)	0	100	100
1	PPP	284/322 (88%)	277 (98%)	7 (2%)	0	100	100
All	All	4584/5152 (89%)	4439 (97%)	144 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	24	HIS

### 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	221/249 (89%)	218 (99%)	3 (1%)	62	52
1	BBB	222/249 (89%)	218 (98%)	4 (2%)	54	40
1	CCC	233/249 (94%)	232 (100%)	1 (0%)	89	86
1	DDD	222/249 (89%)	220 (99%)	2 (1%)	75	69
1	EEE	222/249 (89%)	217 (98%)	5 (2%)	45	30
1	FFF	222/249 (89%)	221 (100%)	1 (0%)	86	84
1	GGG	224/249 (90%)	222 (99%)	2 (1%)	75	69
1	HHH	221/249 (89%)	217 (98%)	4 (2%)	54	40
1	III	221/249 (89%)	218 (99%)	3 (1%)	62	52
1	JJJ	220/249 (88%)	216 (98%)	4 (2%)	54	40
1	KKK	220/249 (88%)	217 (99%)	3 (1%)	62	52
1	LLL	224/249 (90%)	222 (99%)	2 (1%)	75	69
1	MMM	221/249 (89%)	218 (99%)	3 (1%)	62	52
1	NNN	223/249 (90%)	221 (99%)	2 (1%)	75	69
1	OOO	223/249 (90%)	218 (98%)	5 (2%)	47	32
1	PPP	220/249 (88%)	218 (99%)	2 (1%)	75	69
All	All	3559/3984 (89%)	3513 (99%)	46 (1%)	65	55

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	JJJ	251	ASP
1	MMM	221	LEU
1	KKK	92	CYS
1	LLL	22	ARG
1	NNN	31	ARG

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

### 5.3.3 RNA ⓘ

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 97 ligands modelled in this entry, 62 are monoatomic - leaving 35 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	SO4	FFF	402	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	PPP	403	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	JJJ	403	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	CCC	403	-	4,4,4	0.46	0	6,6,6	0.10	0
3	SO4	LLL	402	-	4,4,4	0.45	0	6,6,6	0.09	0
3	SO4	PPP	402	-	4,4,4	0.39	0	6,6,6	0.08	0
3	SO4	CCC	406	-	4,4,4	0.47	0	6,6,6	0.12	0
3	SO4	JJJ	402	-	4,4,4	0.46	0	6,6,6	0.13	0
3	SO4	NNN	402	-	4,4,4	0.43	0	6,6,6	0.19	0
3	SO4	EEE	403	-	4,4,4	0.40	0	6,6,6	0.10	0
3	SO4	III	404	-	4,4,4	0.47	0	6,6,6	0.15	0
3	SO4	OOO	403	-	4,4,4	0.40	0	6,6,6	0.12	0
3	SO4	AAA	404	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	MMM	404	-	4,4,4	0.45	0	6,6,6	0.09	0
6	GOL	DDD	404	-	5,5,5	0.11	0	5,5,5	0.38	0
3	SO4	OOO	406	-	4,4,4	0.36	0	6,6,6	0.04	0
3	SO4	HHH	402	-	4,4,4	0.36	0	6,6,6	0.09	0
5	EDO	CCC	402	-	3,3,3	0.38	0	2,2,2	0.42	0
5	EDO	III	402	-	3,3,3	0.07	0	2,2,2	0.21	0
3	SO4	BBB	403	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	EEE	404	-	4,4,4	0.40	0	6,6,6	0.11	0
5	EDO	HHH	403	-	3,3,3	0.12	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	MMM	402	-	3,3,3	0.32	0	2,2,2	0.34	0
5	EDO	EEE	402	-	3,3,3	0.22	0	2,2,2	0.06	0
3	SO4	AAA	403	-	4,4,4	0.38	0	6,6,6	0.08	0
3	SO4	CCC	404	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	MMM	403	-	4,4,4	0.41	0	6,6,6	0.09	0
3	SO4	GGG	403	-	4,4,4	0.43	0	6,6,6	0.09	0
5	EDO	AAA	406	-	3,3,3	0.16	0	2,2,2	0.33	0
3	SO4	AAA	402	-	4,4,4	0.42	0	6,6,6	0.17	0
5	EDO	OOO	402	-	3,3,3	0.15	0	2,2,2	0.07	0
5	EDO	GGG	401	-	3,3,3	0.20	0	2,2,2	0.14	0
3	SO4	JJJ	405	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	DDD	402	-	4,4,4	0.28	0	6,6,6	0.06	0
5	EDO	BBB	402	-	3,3,3	0.21	0	2,2,2	0.23	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
5	EDO	III	402	-	-	1/1/1/1	-
5	EDO	AAA	406	-	-	1/1/1/1	-
5	EDO	HHH	403	-	-	1/1/1/1	-
5	EDO	MMM	402	-	-	1/1/1/1	-
5	EDO	OOO	402	-	-	1/1/1/1	-
5	EDO	EEE	402	-	-	0/1/1/1	-
6	GOL	DDD	404	-	-	0/4/4/4	-
5	EDO	GGG	401	-	-	1/1/1/1	-
5	EDO	CCC	402	-	-	1/1/1/1	-
5	EDO	BBB	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	406	EDO	O1-C1-C2-O2
5	GGG	401	EDO	O1-C1-C2-O2
5	MMM	402	EDO	O1-C1-C2-O2
5	III	402	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	HHH	403	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	LLL	402	SO4	1	0
6	DDD	404	GOL	1	0
5	III	402	EDO	1	0
5	EEE	402	EDO	1	0
5	OOO	402	EDO	2	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	AAA	288/322 (89%)	0.36	8 (2%) 55 59	21, 31, 49, 66	1 (0%)
1	BBB	290/322 (90%)	0.39	14 (4%) 36 37	22, 31, 48, 65	0
1	CCC	298/322 (92%)	0.42	23 (7%) 21 23	15, 29, 53, 73	4 (1%)
1	DDD	289/322 (89%)	0.40	17 (5%) 29 30	21, 30, 48, 67	1 (0%)
1	EEE	289/322 (89%)	0.32	9 (3%) 51 55	20, 29, 48, 67	1 (0%)
1	FFF	290/322 (90%)	0.37	11 (3%) 44 47	20, 30, 47, 64	0
1	GGG	292/322 (90%)	0.44	10 (3%) 48 51	22, 31, 50, 71	0
1	HHH	289/322 (89%)	0.53	18 (6%) 28 29	23, 31, 50, 74	0
1	III	289/322 (89%)	0.42	9 (3%) 51 55	20, 30, 49, 66	0
1	JJJ	288/322 (89%)	0.48	16 (5%) 31 32	22, 32, 49, 67	0
1	KKK	288/322 (89%)	0.46	11 (3%) 44 47	21, 31, 50, 68	0
1	LLL	291/322 (90%)	0.44	13 (4%) 39 40	20, 31, 47, 59	1 (0%)
1	MMM	289/322 (89%)	0.42	13 (4%) 39 40	21, 31, 50, 64	0
1	NNN	288/322 (89%)	0.42	14 (4%) 36 37	21, 31, 49, 65	3 (1%)
1	OOO	289/322 (89%)	0.29	11 (3%) 44 47	19, 29, 49, 67	2 (0%)
1	PPP	288/322 (89%)	0.38	14 (4%) 36 37	20, 31, 47, 69	0
All	All	4635/5152 (89%)	0.41	211 (4%) 38 39	15, 31, 50, 74	13 (0%)

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	16	LEU	5.5
1	KKK	24	HIS	5.3
1	CCC	18	LEU	5.2
1	DDD	18	LEU	5.0
1	MMM	318	SER	4.4

## 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
5	EDO	CCC	402	4/4	0.70	0.27	55,56,57,58	0
3	SO4	EEE	403	5/5	0.72	0.15	79,82,86,87	0
5	EDO	BBB	402	4/4	0.74	0.20	48,48,49,50	0
5	EDO	GGG	401	4/4	0.75	0.28	49,50,51,53	0
5	EDO	EEE	402	4/4	0.80	0.18	44,44,49,51	0
3	SO4	EEE	404	5/5	0.81	0.15	66,71,72,73	0
3	SO4	III	404	5/5	0.81	0.18	37,41,44,46	5
3	SO4	AAA	404	5/5	0.81	0.14	62,65,68,69	0
5	EDO	III	402	4/4	0.81	0.20	42,42,43,44	0
5	EDO	MMM	402	4/4	0.81	0.20	47,48,49,50	0
3	SO4	AAA	403	5/5	0.82	0.11	79,79,83,83	0
4	CL	GGG	406	1/1	0.82	0.21	87,87,87,87	0
4	CL	KKK	404	1/1	0.82	0.18	58,58,58,58	0
6	GOL	DDD	404	6/6	0.82	0.16	52,55,56,57	0
4	CL	BBB	405	1/1	0.83	0.19	71,71,71,71	0
5	EDO	AAA	406	4/4	0.84	0.21	54,55,57,60	0
3	SO4	JJJ	405	5/5	0.84	0.12	45,47,51,55	5
3	SO4	OOO	403	5/5	0.85	0.15	56,63,68,69	0
2	NA	HHH	405	1/1	0.85	0.29	48,48,48,48	0
5	EDO	OOO	402	4/4	0.86	0.17	43,46,47,49	0
4	CL	CCC	405	1/1	0.86	0.15	64,64,64,64	0
4	CL	NNN	403	1/1	0.87	0.19	74,74,74,74	0
3	SO4	FFF	402	5/5	0.87	0.12	58,58,64,65	0
4	CL	BBB	404	1/1	0.88	0.20	74,74,74,74	0
3	SO4	HHH	402	5/5	0.88	0.12	60,60,62,63	0
3	SO4	CCC	403	5/5	0.88	0.14	68,70,76,78	0
3	SO4	MMM	404	5/5	0.89	0.19	42,45,46,48	5

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	GGG	403	5/5	0.89	0.13	62,64,69,69	0
4	CL	OOO	405	1/1	0.89	0.21	66,66,66,66	0
3	SO4	DDD	402	5/5	0.89	0.11	53,53,58,59	0
5	EDO	HHH	403	4/4	0.90	0.14	51,57,58,59	0
3	SO4	CCC	406	5/5	0.90	0.11	61,63,65,72	0
3	SO4	BBB	403	5/5	0.90	0.10	51,54,57,57	0
3	SO4	JJJ	403	5/5	0.90	0.13	57,63,71,72	0
3	SO4	PPP	403	5/5	0.90	0.16	74,76,78,81	0
3	SO4	AAA	402	5/5	0.91	0.11	54,58,62,65	0
4	CL	GGG	405	1/1	0.91	0.15	68,68,68,68	0
3	SO4	LLL	402	5/5	0.91	0.09	60,60,63,63	0
3	SO4	PPP	402	5/5	0.91	0.11	53,54,55,57	0
2	NA	FFF	404	1/1	0.92	0.14	45,45,45,45	0
3	SO4	MMM	403	5/5	0.92	0.10	55,63,65,68	0
3	SO4	CCC	404	5/5	0.92	0.10	47,48,51,56	0
2	NA	AAA	407	1/1	0.92	0.18	44,44,44,44	0
4	CL	NNN	404	1/1	0.92	0.11	45,45,45,45	0
3	SO4	OOO	406	5/5	0.92	0.12	71,73,76,78	0
4	CL	EEE	406	1/1	0.92	0.17	59,59,59,59	0
4	CL	FFF	403	1/1	0.92	0.13	40,40,40,40	0
3	SO4	NNN	402	5/5	0.93	0.09	53,55,57,57	0
4	CL	BBB	407	1/1	0.93	0.28	70,70,70,70	0
3	SO4	JJJ	402	5/5	0.93	0.08	54,55,57,59	0
4	CL	PPP	404	1/1	0.93	0.26	73,73,73,73	0
4	CL	JJJ	404	1/1	0.93	0.10	50,50,50,50	0
2	NA	BBB	408	1/1	0.93	0.17	44,44,44,44	0
4	CL	MMM	405	1/1	0.93	0.10	41,41,41,41	0
4	CL	CCC	408	1/1	0.94	0.09	39,39,39,39	0
4	CL	DDD	405	1/1	0.94	0.24	75,75,75,75	0
2	NA	NNN	405	1/1	0.94	0.15	40,40,40,40	0
2	NA	PPP	406	1/1	0.94	0.20	49,49,49,49	0
4	CL	BBB	406	1/1	0.94	0.11	44,44,44,44	0
2	NA	CCC	409	1/1	0.94	0.10	41,41,41,41	0
4	CL	HHH	404	1/1	0.94	0.08	46,46,46,46	0
4	CL	AAA	405	1/1	0.94	0.11	48,48,48,48	0
2	NA	MMM	406	1/1	0.95	0.15	47,47,47,47	0
4	CL	CCC	407	1/1	0.95	0.10	57,57,57,57	0
4	CL	GGG	404	1/1	0.95	0.08	45,45,45,45	0
2	NA	III	405	1/1	0.95	0.10	39,39,39,39	0
4	CL	DDD	403	1/1	0.95	0.08	45,45,45,45	0
2	NA	JJJ	406	1/1	0.95	0.23	39,39,39,39	0
4	CL	EEE	405	1/1	0.95	0.09	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	KKK	403	1/1	0.95	0.09	47,47,47,47	0
4	CL	III	403	1/1	0.96	0.12	46,46,46,46	0
2	NA	GGG	407	1/1	0.96	0.13	46,46,46,46	0
4	CL	OOO	404	1/1	0.96	0.08	40,40,40,40	0
2	NA	HHH	401	1/1	0.96	0.09	27,27,27,27	0
2	NA	LLL	404	1/1	0.96	0.20	38,38,38,38	0
4	CL	PPP	405	1/1	0.96	0.09	45,45,45,45	0
4	CL	LLL	403	1/1	0.96	0.08	42,42,42,42	0
2	NA	DDD	406	1/1	0.96	0.24	39,39,39,39	0
2	NA	EEE	401	1/1	0.97	0.07	27,27,27,27	0
2	NA	FFF	401	1/1	0.97	0.05	29,29,29,29	0
2	NA	NNN	401	1/1	0.97	0.10	28,28,28,28	0
2	NA	III	401	1/1	0.97	0.09	26,26,26,26	0
2	NA	PPP	401	1/1	0.97	0.07	29,29,29,29	0
2	NA	AAA	401	1/1	0.97	0.10	29,29,29,29	0
2	NA	CCC	401	1/1	0.97	0.10	27,27,27,27	0
2	NA	KKK	402	1/1	0.97	0.07	38,38,38,38	0
2	NA	KKK	405	1/1	0.97	0.12	41,41,41,41	0
2	NA	LLL	401	1/1	0.97	0.06	29,29,29,29	0
2	NA	BBB	401	1/1	0.98	0.06	28,28,28,28	0
2	NA	JJJ	401	1/1	0.98	0.05	30,30,30,30	0
2	NA	OOO	401	1/1	0.98	0.08	29,29,29,29	0
2	NA	OOO	407	1/1	0.98	0.07	37,37,37,37	0
2	NA	DDD	401	1/1	0.98	0.04	30,30,30,30	0
2	NA	MMM	401	1/1	0.98	0.06	31,31,31,31	0
2	NA	EEE	407	1/1	0.98	0.07	38,38,38,38	0
2	NA	GGG	402	1/1	0.99	0.07	31,31,31,31	0
2	NA	KKK	401	1/1	0.99	0.07	28,28,28,28	0

## 6.5 Other polymers

There are no such residues in this entry.