



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 23, 2019 – 03:22 PM EST

PDB ID : 6T5O
Title : Bacteroides salyersiae GH164 beta-mannosidase
Authors : Armstrong, Z.; Davies, G.
Deposited on : 2019-10-16
Resolution : 1.91 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

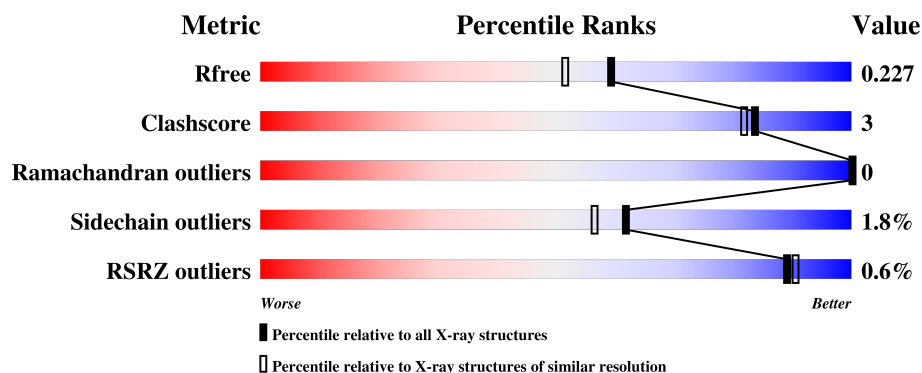
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	111664	6904 (1.94-1.90)
Clashscore	122126	7577 (1.94-1.90)
Ramachandran outliers	120053	7491 (1.94-1.90)
Sidechain outliers	120020	7491 (1.94-1.90)
RSRZ outliers	108989	6759 (1.94-1.90)

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. 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	674	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>
1	BBB	674	<div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	CCC	674	<div> <div></div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	DDD	674	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>..</div> </div> </div>
1	EEE	674	<div> <div></div> <div>89%</div> <div>7%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	674	<div><div></div><div>89%</div><div>7% . .</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 64651 atoms, of which 31065 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 Glyco_hydro_42M domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	658	Total	C	H	N	O	S	285	0	0
			10476	3418	5184	875	980	19			
1	DDD	654	Total	C	H	N	O	S	283	0	0
			10413	3399	5155	869	971	19			
1	CCC	650	Total	C	H	N	O	S	283	0	0
			10358	3378	5126	866	969	19			
1	BBB	651	Total	C	H	N	O	S	283	0	0
			10368	3381	5131	867	970	19			
1	FFF	652	Total	C	H	N	O	S	284	1	0
			10393	3389	5143	869	973	19			
1	EEE	651	Total	C	H	N	O	S	283	0	0
			10368	3381	5131	867	970	19			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	MET	-	initiating methionine	UNP I9SUA3
AAA	11	GLY	-	expression tag	UNP I9SUA3
AAA	12	SER	-	expression tag	UNP I9SUA3
AAA	13	SER	-	expression tag	UNP I9SUA3
AAA	14	HIS	-	expression tag	UNP I9SUA3
AAA	15	HIS	-	expression tag	UNP I9SUA3
AAA	16	HIS	-	expression tag	UNP I9SUA3
AAA	17	HIS	-	expression tag	UNP I9SUA3
AAA	18	HIS	-	expression tag	UNP I9SUA3
AAA	19	HIS	-	expression tag	UNP I9SUA3
AAA	20	SER	-	expression tag	UNP I9SUA3
AAA	21	SER	-	expression tag	UNP I9SUA3
AAA	22	GLY	-	expression tag	UNP I9SUA3
AAA	23	LEU	-	expression tag	UNP I9SUA3
AAA	24	GLU	-	expression tag	UNP I9SUA3
AAA	25	VAL	-	expression tag	UNP I9SUA3
AAA	26	LEU	-	expression tag	UNP I9SUA3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	27	PHE	-	expression tag	UNP I9SUA3
AAA	28	GLN	-	expression tag	UNP I9SUA3
AAA	29	GLY	-	expression tag	UNP I9SUA3
AAA	30	PRO	-	expression tag	UNP I9SUA3
AAA	31	ALA	-	expression tag	UNP I9SUA3
DDD	10	MET	-	initiating methionine	UNP I9SUA3
DDD	11	GLY	-	expression tag	UNP I9SUA3
DDD	12	SER	-	expression tag	UNP I9SUA3
DDD	13	SER	-	expression tag	UNP I9SUA3
DDD	14	HIS	-	expression tag	UNP I9SUA3
DDD	15	HIS	-	expression tag	UNP I9SUA3
DDD	16	HIS	-	expression tag	UNP I9SUA3
DDD	17	HIS	-	expression tag	UNP I9SUA3
DDD	18	HIS	-	expression tag	UNP I9SUA3
DDD	19	HIS	-	expression tag	UNP I9SUA3
DDD	20	SER	-	expression tag	UNP I9SUA3
DDD	21	SER	-	expression tag	UNP I9SUA3
DDD	22	GLY	-	expression tag	UNP I9SUA3
DDD	23	LEU	-	expression tag	UNP I9SUA3
DDD	24	GLU	-	expression tag	UNP I9SUA3
DDD	25	VAL	-	expression tag	UNP I9SUA3
DDD	26	LEU	-	expression tag	UNP I9SUA3
DDD	27	PHE	-	expression tag	UNP I9SUA3
DDD	28	GLN	-	expression tag	UNP I9SUA3
DDD	29	GLY	-	expression tag	UNP I9SUA3
DDD	30	PRO	-	expression tag	UNP I9SUA3
DDD	31	ALA	-	expression tag	UNP I9SUA3
CCC	10	MET	-	initiating methionine	UNP I9SUA3
CCC	11	GLY	-	expression tag	UNP I9SUA3
CCC	12	SER	-	expression tag	UNP I9SUA3
CCC	13	SER	-	expression tag	UNP I9SUA3
CCC	14	HIS	-	expression tag	UNP I9SUA3
CCC	15	HIS	-	expression tag	UNP I9SUA3
CCC	16	HIS	-	expression tag	UNP I9SUA3
CCC	17	HIS	-	expression tag	UNP I9SUA3
CCC	18	HIS	-	expression tag	UNP I9SUA3
CCC	19	HIS	-	expression tag	UNP I9SUA3
CCC	20	SER	-	expression tag	UNP I9SUA3
CCC	21	SER	-	expression tag	UNP I9SUA3
CCC	22	GLY	-	expression tag	UNP I9SUA3
CCC	23	LEU	-	expression tag	UNP I9SUA3
CCC	24	GLU	-	expression tag	UNP I9SUA3

Continued on next page...

Continued from previous page...

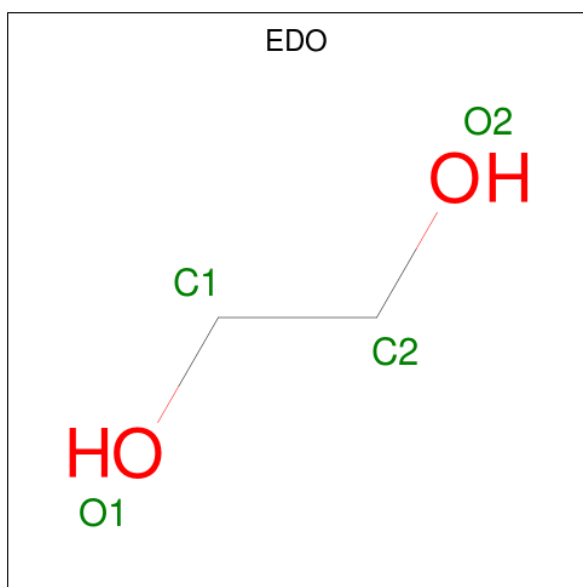
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	25	VAL	-	expression tag	UNP I9SUA3
CCC	26	LEU	-	expression tag	UNP I9SUA3
CCC	27	PHE	-	expression tag	UNP I9SUA3
CCC	28	GLN	-	expression tag	UNP I9SUA3
CCC	29	GLY	-	expression tag	UNP I9SUA3
CCC	30	PRO	-	expression tag	UNP I9SUA3
CCC	31	ALA	-	expression tag	UNP I9SUA3
BBB	10	MET	-	initiating methionine	UNP I9SUA3
BBB	11	GLY	-	expression tag	UNP I9SUA3
BBB	12	SER	-	expression tag	UNP I9SUA3
BBB	13	SER	-	expression tag	UNP I9SUA3
BBB	14	HIS	-	expression tag	UNP I9SUA3
BBB	15	HIS	-	expression tag	UNP I9SUA3
BBB	16	HIS	-	expression tag	UNP I9SUA3
BBB	17	HIS	-	expression tag	UNP I9SUA3
BBB	18	HIS	-	expression tag	UNP I9SUA3
BBB	19	HIS	-	expression tag	UNP I9SUA3
BBB	20	SER	-	expression tag	UNP I9SUA3
BBB	21	SER	-	expression tag	UNP I9SUA3
BBB	22	GLY	-	expression tag	UNP I9SUA3
BBB	23	LEU	-	expression tag	UNP I9SUA3
BBB	24	GLU	-	expression tag	UNP I9SUA3
BBB	25	VAL	-	expression tag	UNP I9SUA3
BBB	26	LEU	-	expression tag	UNP I9SUA3
BBB	27	PHE	-	expression tag	UNP I9SUA3
BBB	28	GLN	-	expression tag	UNP I9SUA3
BBB	29	GLY	-	expression tag	UNP I9SUA3
BBB	30	PRO	-	expression tag	UNP I9SUA3
BBB	31	ALA	-	expression tag	UNP I9SUA3
FFF	10	MET	-	initiating methionine	UNP I9SUA3
FFF	11	GLY	-	expression tag	UNP I9SUA3
FFF	12	SER	-	expression tag	UNP I9SUA3
FFF	13	SER	-	expression tag	UNP I9SUA3
FFF	14	HIS	-	expression tag	UNP I9SUA3
FFF	15	HIS	-	expression tag	UNP I9SUA3
FFF	16	HIS	-	expression tag	UNP I9SUA3
FFF	17	HIS	-	expression tag	UNP I9SUA3
FFF	18	HIS	-	expression tag	UNP I9SUA3
FFF	19	HIS	-	expression tag	UNP I9SUA3
FFF	20	SER	-	expression tag	UNP I9SUA3
FFF	21	SER	-	expression tag	UNP I9SUA3
FFF	22	GLY	-	expression tag	UNP I9SUA3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	23	LEU	-	expression tag	UNP I9SUA3
FFF	24	GLU	-	expression tag	UNP I9SUA3
FFF	25	VAL	-	expression tag	UNP I9SUA3
FFF	26	LEU	-	expression tag	UNP I9SUA3
FFF	27	PHE	-	expression tag	UNP I9SUA3
FFF	28	GLN	-	expression tag	UNP I9SUA3
FFF	29	GLY	-	expression tag	UNP I9SUA3
FFF	30	PRO	-	expression tag	UNP I9SUA3
FFF	31	ALA	-	expression tag	UNP I9SUA3
EEE	10	MET	-	initiating methionine	UNP I9SUA3
EEE	11	GLY	-	expression tag	UNP I9SUA3
EEE	12	SER	-	expression tag	UNP I9SUA3
EEE	13	SER	-	expression tag	UNP I9SUA3
EEE	14	HIS	-	expression tag	UNP I9SUA3
EEE	15	HIS	-	expression tag	UNP I9SUA3
EEE	16	HIS	-	expression tag	UNP I9SUA3
EEE	17	HIS	-	expression tag	UNP I9SUA3
EEE	18	HIS	-	expression tag	UNP I9SUA3
EEE	19	HIS	-	expression tag	UNP I9SUA3
EEE	20	SER	-	expression tag	UNP I9SUA3
EEE	21	SER	-	expression tag	UNP I9SUA3
EEE	22	GLY	-	expression tag	UNP I9SUA3
EEE	23	LEU	-	expression tag	UNP I9SUA3
EEE	24	GLU	-	expression tag	UNP I9SUA3
EEE	25	VAL	-	expression tag	UNP I9SUA3
EEE	26	LEU	-	expression tag	UNP I9SUA3
EEE	27	PHE	-	expression tag	UNP I9SUA3
EEE	28	GLN	-	expression tag	UNP I9SUA3
EEE	29	GLY	-	expression tag	UNP I9SUA3
EEE	30	PRO	-	expression tag	UNP I9SUA3
EEE	31	ALA	-	expression tag	UNP I9SUA3

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



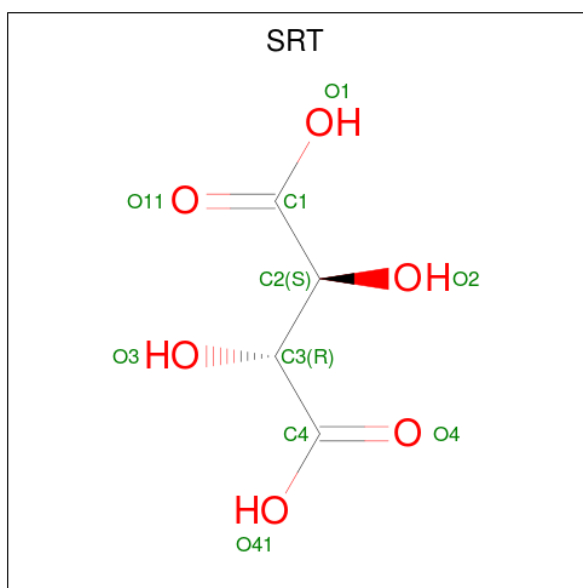
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	CCC	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
2	EEE	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 3 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C₄H₆O₆).

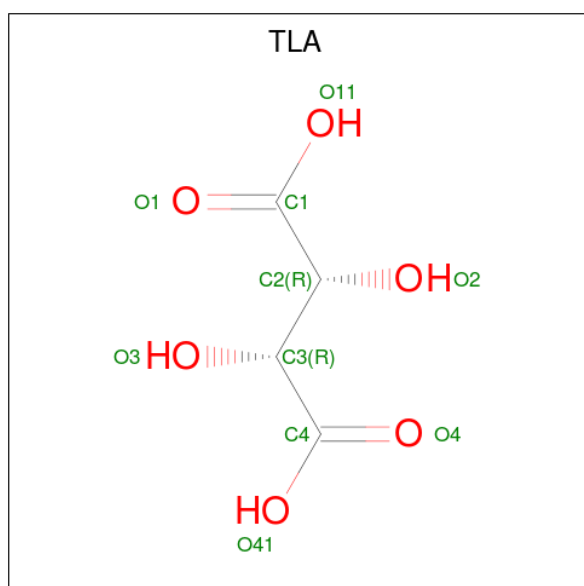


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	2	0
			14	4	4	6		
3	CCC	1	Total	C	H	O	2	0
			14	4	4	6		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

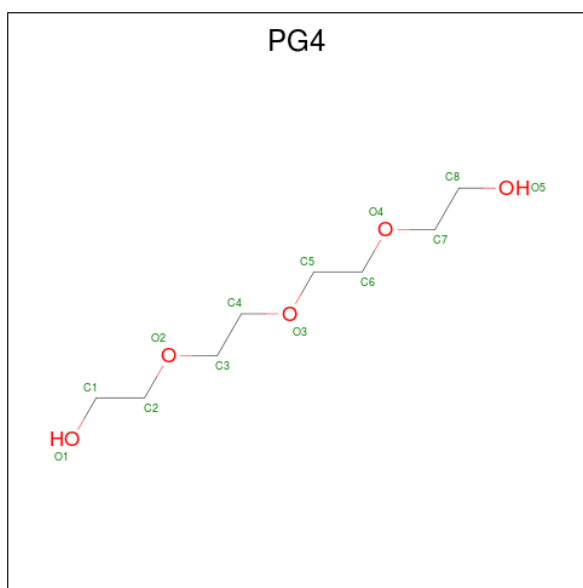
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	DDD	1	Total	Cl	0	0
			1	1		
4	AAA	1	Total	Cl	0	0
			1	1		
4	CCC	1	Total	Cl	0	0
			1	1		
4	FFF	1	Total	Cl	0	0
			1	1		
4	EEE	1	Total	Cl	0	0
			1	1		
4	BBB	1	Total	Cl	0	0
			1	1		

- Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



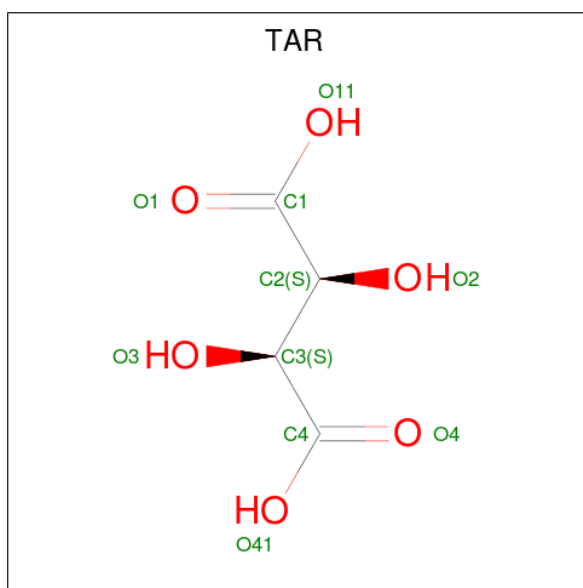
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	DDD	1	Total	C	H	O	2	0
			14	4	4	6		
5	FFF	1	Total	C	H	O	2	0
			14	4	4	6		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	CCC	1	Total	C	H	O	1	0
			26	7	15	4		

- Molecule 7 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	BBB	1	Total	C	H	O	2	0
			14	4	4	6		
7	EEE	1	Total	C	H	O	2	0
			14	4	4	6		

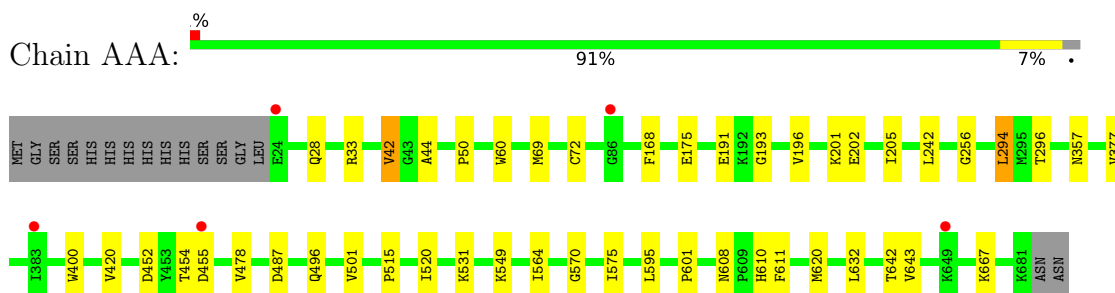
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	292	Total 292	O 292	0	0
8	DDD	299	Total 299	O 299	0	0
8	CCC	348	Total 348	O 348	0	0
8	BBB	359	Total 359	O 359	0	0
8	FFF	324	Total 324	O 324	0	0
8	EEE	277	Total 277	O 277	0	0

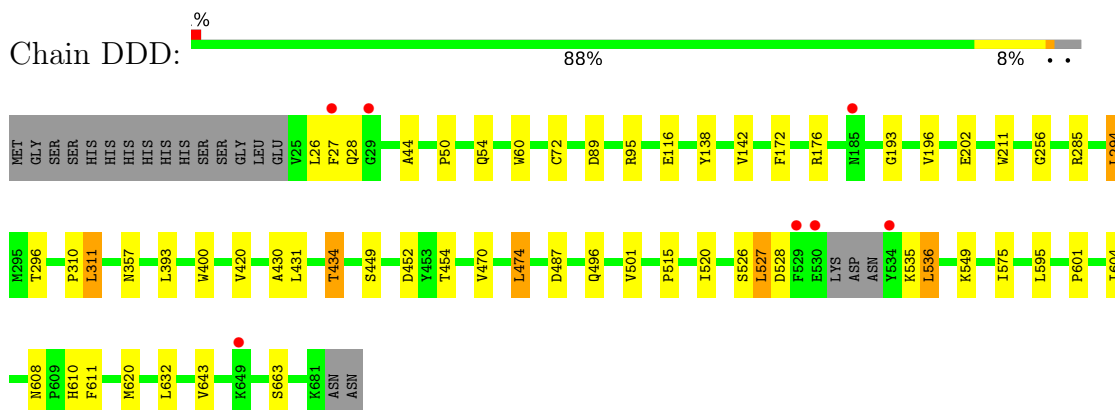
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

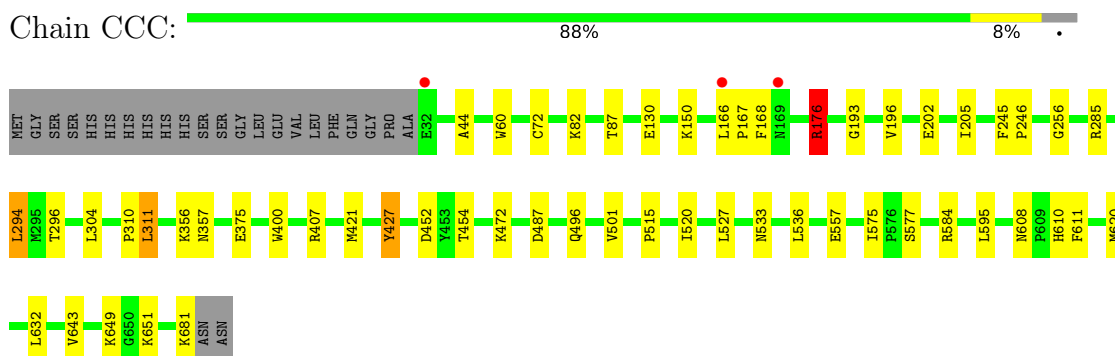
- Molecule 1: Glyco_hydro_42M domain-containing protein



- Molecule 1: Glyco_hydro_42M domain-containing protein

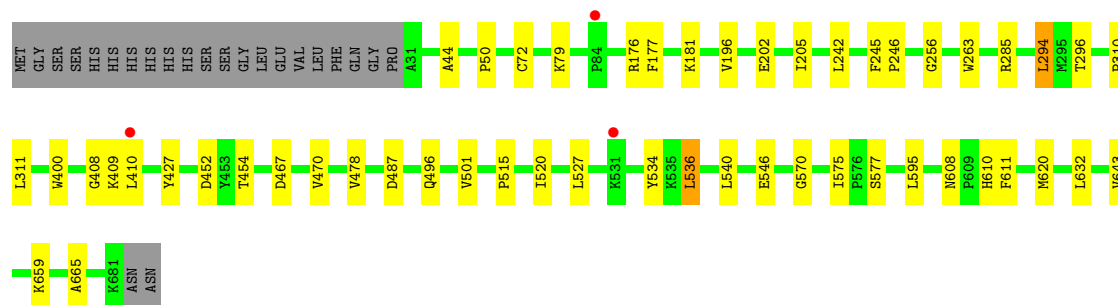


- Molecule 1: Glyco_hydro_42M domain-containing protein



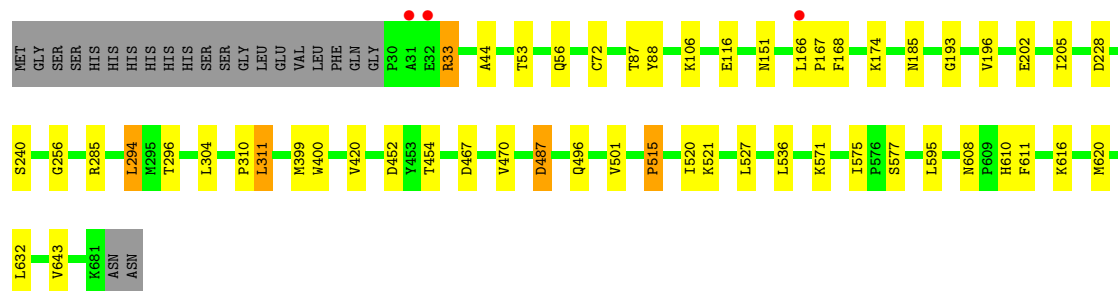
- Molecule 1: Glyco_hydro_42M domain-containing protein

Chain BBB:  89% 7% .



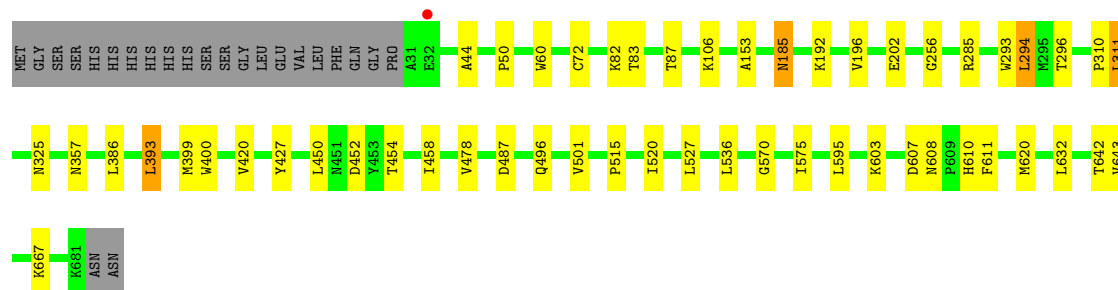
- Molecule 1: Glyco_hydro_42M domain-containing protein

Chain FFF:  89% 7% ..



- Molecule 1: Glyco_hydro_42M domain-containing protein

Chain EEE:  89% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.15Å 103.91Å 169.16Å 92.48° 97.34° 106.43°	Depositor
Resolution (Å)	66.85 – 1.91 66.76 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.0 (66.85-1.91) 96.0 (66.76-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.190 , 0.221 0.197 , 0.227	Depositor DCC
R_{free} test set	16536 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	64651	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: TAR, CL, PG4, EDO, TLA, SRT

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	0.66	0/5438	0.76	0/7362
1	BBB	0.67	0/5381	0.77	2/7284 (0.0%)
1	CCC	0.66	0/5376	0.79	6/7277 (0.1%)
1	DDD	0.65	0/5403	0.77	2/7314 (0.0%)
1	EEE	0.65	0/5381	0.77	2/7284 (0.0%)
1	FFF	0.66	0/5395	0.78	2/7303 (0.0%)
All	All	0.66	0/32374	0.77	14/43824 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	285	ARG	NE-CZ-NH1	-8.77	115.91	120.30
1	FFF	285	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	DDD	285	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	CCC	285	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	EEE	285	ARG	NE-CZ-NH1	7.19	123.89	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	5292	5184	5165	26	0
1	BBB	5237	5131	5112	33	0
1	CCC	5232	5126	5107	27	0
1	DDD	5258	5155	5135	35	0
1	EEE	5237	5131	5112	27	0
1	FFF	5250	5143	5124	34	0
2	AAA	12	18	18	0	0
2	BBB	20	30	30	2	0
2	CCC	20	30	30	1	0
2	DDD	12	18	18	0	0
2	EEE	24	36	36	0	0
2	FFF	16	24	24	0	0
3	AAA	10	4	4	1	0
3	CCC	10	4	4	1	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	1	0	0	0	0
5	DDD	10	4	4	0	0
5	FFF	10	4	4	0	0
6	CCC	11	15	13	1	0
7	BBB	10	4	4	0	0
7	EEE	10	4	4	0	0
8	AAA	292	0	0	0	0
8	BBB	359	0	0	1	0
8	CCC	348	0	0	2	0
8	DDD	299	0	0	1	0
8	EEE	277	0	0	0	0
8	FFF	324	0	0	4	0
All	All	33586	31065	30948	165	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 3.

The worst 5 of 165 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:FFF:53:THR:H	1:FFF:56:GLN:HE21	1.19	0.86
1:CCC:166:LEU:HD23	1:CCC:168:PHE:CE2	2.19	0.77
1:BBB:408:GLY:O	1:BBB:410:LEU:CD1	2.33	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:166:LEU:HD23	1:FFF:168:PHE:CE2	2.25	0.72
1:FFF:166:LEU:HD22	1:FFF:205:ILE:HG12	1.73	0.71

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	656/674 (97%)	636 (97%)	20 (3%)	0	100	100
1	BBB	649/674 (96%)	630 (97%)	19 (3%)	0	100	100
1	CCC	648/674 (96%)	629 (97%)	19 (3%)	0	100	100
1	DDD	650/674 (96%)	630 (97%)	20 (3%)	0	100	100
1	EEE	649/674 (96%)	629 (97%)	20 (3%)	0	100	100
1	FFF	651/674 (97%)	632 (97%)	19 (3%)	0	100	100
All	All	3903/4044 (96%)	3786 (97%)	117 (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	568/582 (98%)	561 (99%)	7 (1%)	74	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BBB	562/582 (97%)	557 (99%)	5 (1%)	81	80
1	CCC	562/582 (97%)	546 (97%)	16 (3%)	47	37
1	DDD	564/582 (97%)	550 (98%)	14 (2%)	50	42
1	EEE	562/582 (97%)	552 (98%)	10 (2%)	62	56
1	FFF	564/582 (97%)	553 (98%)	11 (2%)	58	52
All	All	3382/3492 (97%)	3319 (98%)	63 (2%)	62	54

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	311	LEU
1	CCC	649	LYS
1	EEE	386	LEU
1	CCC	407	ARG
1	CCC	427	TYR

Some 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 ⓘ

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 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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	EDO	AAA	701	-	3,3,3	0.18	0	2,2,2	0.57	0
2	EDO	AAA	702	-	3,3,3	0.43	0	2,2,2	0.17	0
2	EDO	AAA	703	-	3,3,3	0.33	0	2,2,2	0.13	0
3	SRT	AAA	704	-	3,9,9	0.50	0	6,12,12	0.73	0
2	EDO	BBB	701	-	3,3,3	0.32	0	2,2,2	0.55	0
2	EDO	BBB	702	-	3,3,3	0.38	0	2,2,2	0.25	0
2	EDO	BBB	703	-	3,3,3	0.19	0	2,2,2	0.12	0
2	EDO	BBB	704	-	3,3,3	0.39	0	2,2,2	0.12	0
2	EDO	BBB	705	-	3,3,3	0.24	0	2,2,2	0.18	0
7	TAR	BBB	706	-	3,9,9	0.41	0	6,12,12	0.41	0
2	EDO	CCC	701	-	3,3,3	0.43	0	2,2,2	0.47	0
2	EDO	CCC	702	-	3,3,3	0.34	0	2,2,2	0.10	0
2	EDO	CCC	703	-	3,3,3	0.41	0	2,2,2	0.23	0
2	EDO	CCC	704	-	3,3,3	0.31	0	2,2,2	0.39	0
6	PG4	CCC	705	-	10,10,12	0.47	0	9,9,11	0.36	0
2	EDO	CCC	706	-	3,3,3	0.41	0	2,2,2	0.29	0
3	SRT	CCC	707	-	3,9,9	0.61	0	6,12,12	0.76	0
2	EDO	DDD	701	-	3,3,3	0.11	0	2,2,2	0.37	0
2	EDO	DDD	702	-	3,3,3	0.20	0	2,2,2	0.34	0
2	EDO	DDD	703	-	3,3,3	0.14	0	2,2,2	0.06	0
5	TLA	DDD	704	-	3,9,9	0.31	0	6,12,12	0.80	0
2	EDO	EEE	701	-	3,3,3	0.51	0	2,2,2	0.56	0
2	EDO	EEE	702	-	3,3,3	0.35	0	2,2,2	0.20	0
2	EDO	EEE	703	-	3,3,3	0.32	0	2,2,2	0.14	0
2	EDO	EEE	704	-	3,3,3	0.15	0	2,2,2	0.37	0
2	EDO	EEE	705	-	3,3,3	0.21	0	2,2,2	0.16	0
2	EDO	EEE	706	-	3,3,3	0.27	0	2,2,2	1.23	0
7	TAR	EEE	707	-	3,9,9	0.13	0	6,12,12	1.44	1 (16%)
2	EDO	FFF	701	-	3,3,3	0.16	0	2,2,2	0.41	0
2	EDO	FFF	702	-	3,3,3	0.20	0	2,2,2	0.02	0
2	EDO	FFF	703	-	3,3,3	0.12	0	2,2,2	0.11	0
2	EDO	FFF	704	-	3,3,3	0.16	0	2,2,2	0.10	0
5	TLA	FFF	705	-	3,9,9	0.34	0	6,12,12	0.73	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	AAA	701	-	-	0/1/1/1	-
2	EDO	AAA	702	-	-	0/1/1/1	-
2	EDO	AAA	703	-	-	0/1/1/1	-
3	SRT	AAA	704	-	-	2/4/12/12	-
2	EDO	BBB	701	-	-	0/1/1/1	-
2	EDO	BBB	702	-	-	1/1/1/1	-
2	EDO	BBB	703	-	-	0/1/1/1	-
2	EDO	BBB	704	-	-	1/1/1/1	-
2	EDO	BBB	705	-	-	1/1/1/1	-
7	TAR	BBB	706	-	-	0/4/12/12	-
2	EDO	CCC	701	-	-	0/1/1/1	-
2	EDO	CCC	702	-	-	0/1/1/1	-
2	EDO	CCC	703	-	-	0/1/1/1	-
2	EDO	CCC	704	-	-	1/1/1/1	-
6	PG4	CCC	705	-	-	6/8/8/10	-
2	EDO	CCC	706	-	-	0/1/1/1	-
3	SRT	CCC	707	-	-	4/4/12/12	-
2	EDO	DDD	701	-	-	0/1/1/1	-
2	EDO	DDD	702	-	-	0/1/1/1	-
2	EDO	DDD	703	-	-	0/1/1/1	-
5	TLA	DDD	704	-	-	0/4/12/12	-
2	EDO	EEE	701	-	-	0/1/1/1	-
2	EDO	EEE	702	-	-	0/1/1/1	-
2	EDO	EEE	703	-	-	0/1/1/1	-
2	EDO	EEE	704	-	-	0/1/1/1	-
2	EDO	EEE	705	-	-	0/1/1/1	-
2	EDO	EEE	706	-	-	1/1/1/1	-
7	TAR	EEE	707	-	-	0/4/12/12	-
2	EDO	FFF	701	-	-	0/1/1/1	-
2	EDO	FFF	702	-	-	0/1/1/1	-
2	EDO	FFF	703	-	-	1/1/1/1	-
2	EDO	FFF	704	-	-	0/1/1/1	-
5	TLA	FFF	705	-	-	0/4/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	EEE	707	TAR	C4-C3-C2	-2.01	108.78	113.11

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CCC	707	SRT	C1-C2-C3-C4
3	CCC	707	SRT	O2-C2-C3-O3
3	CCC	707	SRT	O2-C2-C3-C4
6	CCC	705	PG4	O3-C5-C6-O4
2	EEE	706	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	704	SRT	1	0
2	BBB	701	EDO	1	0
2	BBB	704	EDO	1	0
2	CCC	704	EDO	1	0
6	CCC	705	PG4	1	0
3	CCC	707	SRT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	658/674 (97%)	-0.03	5 (0%) 86 87	21, 32, 54, 86	0
1	BBB	651/674 (96%)	-0.10	3 (0%) 90 92	18, 27, 47, 87	0
1	CCC	650/674 (96%)	-0.08	3 (0%) 90 92	19, 28, 52, 84	0
1	DDD	654/674 (97%)	-0.05	7 (1%) 80 83	22, 32, 55, 81	0
1	EEE	651/674 (96%)	-0.12	1 (0%) 94 95	23, 33, 55, 88	0
1	FFF	652/674 (96%)	-0.07	3 (0%) 90 92	20, 30, 51, 80	0
All	All	3916/4044 (96%)	-0.07	22 (0%) 89 90	18, 30, 53, 88	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	529	PHE	5.1
1	FFF	166	LEU	4.0
1	CCC	166	LEU	3.6
1	DDD	29	GLY	3.4
1	BBB	84	PRO	3.3

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 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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TAR	BBB	706	10/10	0.81	0.14	36,60,74,81	2
2	EDO	EEE	704	4/4	0.83	0.16	50,57,62,62	1
6	PG4	CCC	705	11/13	0.85	0.15	39,53,64,65	1
7	TAR	EEE	707	10/10	0.86	0.12	36,47,52,53	2
2	EDO	BBB	705	4/4	0.87	0.24	50,54,56,56	1
2	EDO	CCC	704	4/4	0.89	0.18	49,49,55,55	1
2	EDO	EEE	706	4/4	0.89	0.10	25,35,41,41	1
3	SRT	AAA	704	10/10	0.91	0.14	44,57,61,67	2
5	TLA	DDD	704	10/10	0.92	0.09	42,47,50,59	2
2	EDO	EEE	705	4/4	0.92	0.07	40,43,44,44	1
3	SRT	CCC	707	10/10	0.92	0.14	35,41,44,45	2
5	TLA	FFF	705	10/10	0.94	0.09	36,41,50,51	2
2	EDO	DDD	703	4/4	0.94	0.16	38,38,41,41	1
2	EDO	FFF	702	4/4	0.95	0.12	33,35,38,38	1
2	EDO	EEE	703	4/4	0.95	0.11	35,37,39,39	1
2	EDO	AAA	703	4/4	0.95	0.10	30,32,37,37	1
2	EDO	EEE	701	4/4	0.95	0.12	30,35,36,36	1
2	EDO	BBB	704	4/4	0.96	0.09	38,39,43,43	1
2	EDO	CCC	706	4/4	0.96	0.11	23,29,37,37	1
2	EDO	CCC	701	4/4	0.96	0.10	23,27,31,31	1
2	EDO	CCC	703	4/4	0.96	0.09	28,30,34,34	1
2	EDO	AAA	702	4/4	0.96	0.14	34,37,43,43	1
2	EDO	BBB	701	4/4	0.96	0.12	27,33,33,33	1
2	EDO	FFF	704	4/4	0.96	0.12	31,35,37,37	1
2	EDO	FFF	701	4/4	0.96	0.09	25,27,30,30	1
2	EDO	AAA	701	4/4	0.97	0.10	25,26,29,29	1
2	EDO	BBB	702	4/4	0.97	0.13	28,33,34,34	1
2	EDO	CCC	702	4/4	0.97	0.13	30,30,33,33	1
2	EDO	BBB	703	4/4	0.97	0.10	23,29,36,36	1
2	EDO	DDD	702	4/4	0.97	0.08	28,32,37,37	1
2	EDO	FFF	703	4/4	0.98	0.10	27,31,34,34	1
2	EDO	DDD	701	4/4	0.98	0.09	25,30,30,30	1
2	EDO	EEE	702	4/4	0.98	0.10	33,34,35,35	1
4	CL	AAA	705	1/1	0.98	0.08	28,28,28,28	0
4	CL	DDD	705	1/1	0.99	0.09	26,26,26,26	0
4	CL	EEE	708	1/1	0.99	0.09	30,30,30,30	0
4	CL	BBB	707	1/1	0.99	0.07	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	CCC	708	1/1	0.99	0.10	25,25,25,25	0
4	CL	FFF	706	1/1	1.00	0.08	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.