



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:19 am BST

PDB ID : 6RB7  
Title : Ruminococcus gnavus sialic acid aldolase catalytic lysine mutant  
Authors : Owen, C.D.; Bell, A.; Juge, N.; Walsh, M.A.  
Deposited on : 2019-04-09  
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

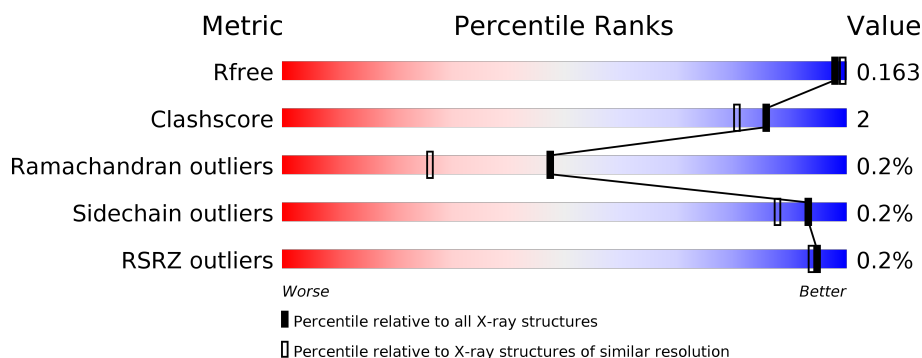
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div>86%</div> <div>5%</div> <div>9%</div> </div>
1	B	336	<div> <div>87%</div> <div>•</div> <div>9%</div> </div>
1	E	336	<div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
1	F	336	<div> <div>88%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11482 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 Putative N-acetylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	8	0
			2406	1535	397	453	21			
1	B	305	Total	C	N	O	S	0	7	0
			2402	1532	400	450	20			
1	E	305	Total	C	N	O	S	0	3	0
			2363	1510	391	441	21			
1	F	305	Total	C	N	O	S	0	5	0
			2381	1521	393	447	20			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	initiating methionine	UNP A7B555
A	-29	SER	-	expression tag	UNP A7B555
A	-28	TYR	-	expression tag	UNP A7B555
A	-27	TYR	-	expression tag	UNP A7B555
A	-26	HIS	-	expression tag	UNP A7B555
A	-25	HIS	-	expression tag	UNP A7B555
A	-24	HIS	-	expression tag	UNP A7B555
A	-23	HIS	-	expression tag	UNP A7B555
A	-22	HIS	-	expression tag	UNP A7B555
A	-21	HIS	-	expression tag	UNP A7B555
A	-20	ASP	-	expression tag	UNP A7B555
A	-19	TYR	-	expression tag	UNP A7B555
A	-18	ASP	-	expression tag	UNP A7B555
A	-17	ILE	-	expression tag	UNP A7B555
A	-16	PRO	-	expression tag	UNP A7B555
A	-15	THR	-	expression tag	UNP A7B555
A	-14	THR	-	expression tag	UNP A7B555
A	-13	GLU	-	expression tag	UNP A7B555
A	-12	ASN	-	expression tag	UNP A7B555
A	-11	LEU	-	expression tag	UNP A7B555
A	-10	TYR	-	expression tag	UNP A7B555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	PHE	-	expression tag	UNP A7B555
A	-8	GLN	-	expression tag	UNP A7B555
A	-7	GLY	-	expression tag	UNP A7B555
A	-6	ALA	-	expression tag	UNP A7B555
A	-5	MET	-	expression tag	UNP A7B555
A	-4	ALA	-	expression tag	UNP A7B555
A	-3	ASP	-	expression tag	UNP A7B555
A	-2	ILE	-	expression tag	UNP A7B555
A	-1	GLY	-	expression tag	UNP A7B555
A	0	SER	-	expression tag	UNP A7B555
A	167	ALA	LYS	conflict	UNP A7B555
B	-30	MET	-	initiating methionine	UNP A7B555
B	-29	SER	-	expression tag	UNP A7B555
B	-28	TYR	-	expression tag	UNP A7B555
B	-27	TYR	-	expression tag	UNP A7B555
B	-26	HIS	-	expression tag	UNP A7B555
B	-25	HIS	-	expression tag	UNP A7B555
B	-24	HIS	-	expression tag	UNP A7B555
B	-23	HIS	-	expression tag	UNP A7B555
B	-22	HIS	-	expression tag	UNP A7B555
B	-21	HIS	-	expression tag	UNP A7B555
B	-20	ASP	-	expression tag	UNP A7B555
B	-19	TYR	-	expression tag	UNP A7B555
B	-18	ASP	-	expression tag	UNP A7B555
B	-17	ILE	-	expression tag	UNP A7B555
B	-16	PRO	-	expression tag	UNP A7B555
B	-15	THR	-	expression tag	UNP A7B555
B	-14	THR	-	expression tag	UNP A7B555
B	-13	GLU	-	expression tag	UNP A7B555
B	-12	ASN	-	expression tag	UNP A7B555
B	-11	LEU	-	expression tag	UNP A7B555
B	-10	TYR	-	expression tag	UNP A7B555
B	-9	PHE	-	expression tag	UNP A7B555
B	-8	GLN	-	expression tag	UNP A7B555
B	-7	GLY	-	expression tag	UNP A7B555
B	-6	ALA	-	expression tag	UNP A7B555
B	-5	MET	-	expression tag	UNP A7B555
B	-4	ALA	-	expression tag	UNP A7B555
B	-3	ASP	-	expression tag	UNP A7B555
B	-2	ILE	-	expression tag	UNP A7B555
B	-1	GLY	-	expression tag	UNP A7B555
B	0	SER	-	expression tag	UNP A7B555

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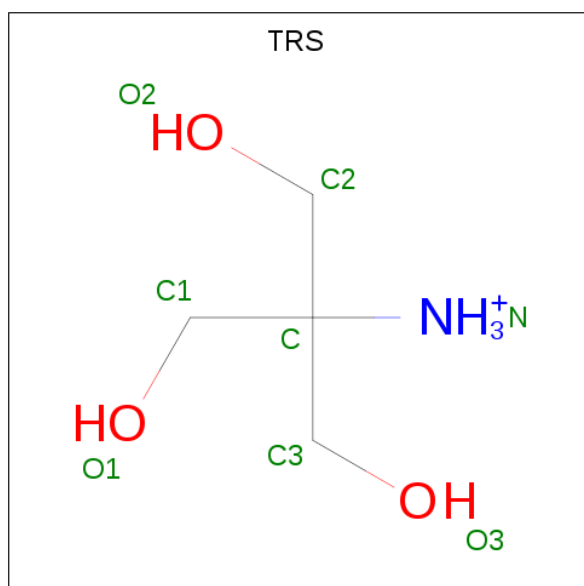
Chain	Residue	Modelled	Actual	Comment	Reference
B	167	ALA	LYS	conflict	UNP A7B555
E	-30	MET	-	initiating methionine	UNP A7B555
E	-29	SER	-	expression tag	UNP A7B555
E	-28	TYR	-	expression tag	UNP A7B555
E	-27	TYR	-	expression tag	UNP A7B555
E	-26	HIS	-	expression tag	UNP A7B555
E	-25	HIS	-	expression tag	UNP A7B555
E	-24	HIS	-	expression tag	UNP A7B555
E	-23	HIS	-	expression tag	UNP A7B555
E	-22	HIS	-	expression tag	UNP A7B555
E	-21	HIS	-	expression tag	UNP A7B555
E	-20	ASP	-	expression tag	UNP A7B555
E	-19	TYR	-	expression tag	UNP A7B555
E	-18	ASP	-	expression tag	UNP A7B555
E	-17	ILE	-	expression tag	UNP A7B555
E	-16	PRO	-	expression tag	UNP A7B555
E	-15	THR	-	expression tag	UNP A7B555
E	-14	THR	-	expression tag	UNP A7B555
E	-13	GLU	-	expression tag	UNP A7B555
E	-12	ASN	-	expression tag	UNP A7B555
E	-11	LEU	-	expression tag	UNP A7B555
E	-10	TYR	-	expression tag	UNP A7B555
E	-9	PHE	-	expression tag	UNP A7B555
E	-8	GLN	-	expression tag	UNP A7B555
E	-7	GLY	-	expression tag	UNP A7B555
E	-6	ALA	-	expression tag	UNP A7B555
E	-5	MET	-	expression tag	UNP A7B555
E	-4	ALA	-	expression tag	UNP A7B555
E	-3	ASP	-	expression tag	UNP A7B555
E	-2	ILE	-	expression tag	UNP A7B555
E	-1	GLY	-	expression tag	UNP A7B555
E	0	SER	-	expression tag	UNP A7B555
E	167	ALA	LYS	conflict	UNP A7B555
F	-30	MET	-	initiating methionine	UNP A7B555
F	-29	SER	-	expression tag	UNP A7B555
F	-28	TYR	-	expression tag	UNP A7B555
F	-27	TYR	-	expression tag	UNP A7B555
F	-26	HIS	-	expression tag	UNP A7B555
F	-25	HIS	-	expression tag	UNP A7B555
F	-24	HIS	-	expression tag	UNP A7B555
F	-23	HIS	-	expression tag	UNP A7B555
F	-22	HIS	-	expression tag	UNP A7B555

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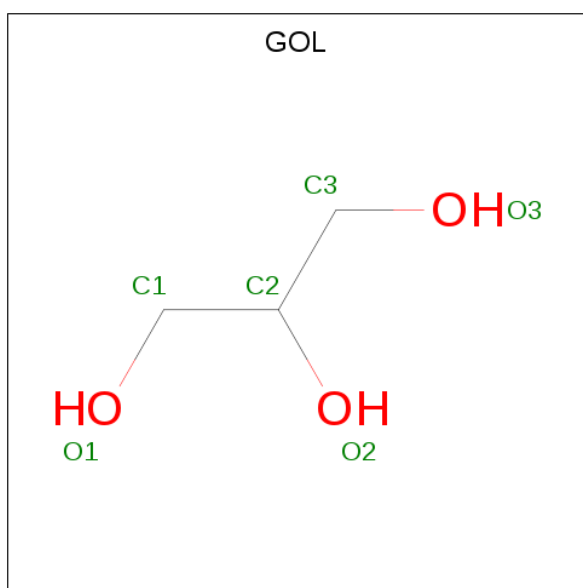
Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	HIS	-	expression tag	UNP A7B555
F	-20	ASP	-	expression tag	UNP A7B555
F	-19	TYR	-	expression tag	UNP A7B555
F	-18	ASP	-	expression tag	UNP A7B555
F	-17	ILE	-	expression tag	UNP A7B555
F	-16	PRO	-	expression tag	UNP A7B555
F	-15	THR	-	expression tag	UNP A7B555
F	-14	THR	-	expression tag	UNP A7B555
F	-13	GLU	-	expression tag	UNP A7B555
F	-12	ASN	-	expression tag	UNP A7B555
F	-11	LEU	-	expression tag	UNP A7B555
F	-10	TYR	-	expression tag	UNP A7B555
F	-9	PHE	-	expression tag	UNP A7B555
F	-8	GLN	-	expression tag	UNP A7B555
F	-7	GLY	-	expression tag	UNP A7B555
F	-6	ALA	-	expression tag	UNP A7B555
F	-5	MET	-	expression tag	UNP A7B555
F	-4	ALA	-	expression tag	UNP A7B555
F	-3	ASP	-	expression tag	UNP A7B555
F	-2	ILE	-	expression tag	UNP A7B555
F	-1	GLY	-	expression tag	UNP A7B555
F	0	SER	-	expression tag	UNP A7B555
F	167	ALA	LYS	conflict	UNP A7B555

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



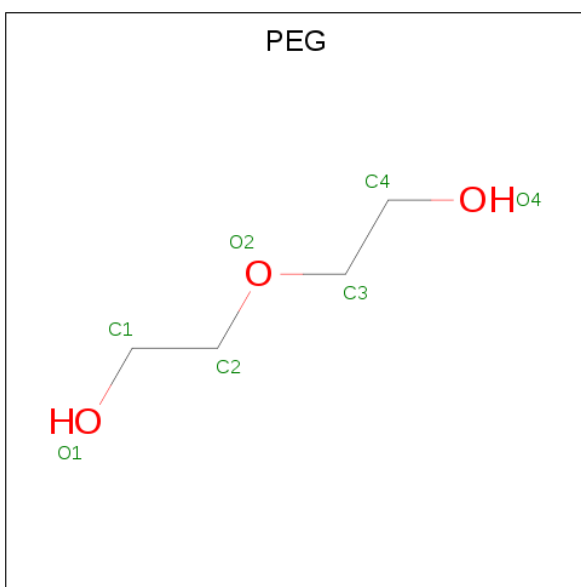
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 8 4 1 3	0	0
2	B	1	Total C N O 8 4 1 3	0	0
2	E	1	Total C N O 8 4 1 3	0	0
2	F	1	Total C N O 8 4 1 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



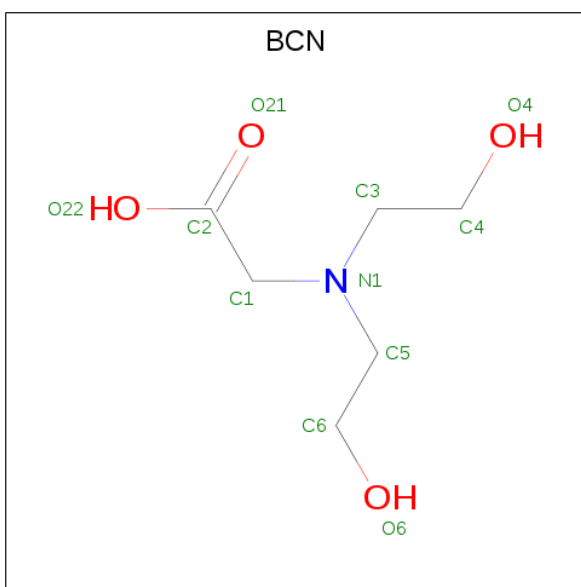
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

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



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

- Molecule 5 is BICINE (three-letter code: BCN) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		



- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Mg 1	0	0
6	A	1	Total 1	Mg 1	0	0
6	F	1	Total 1	Mg 1	0	0
6	E	1	Total 1	Mg 1	0	0

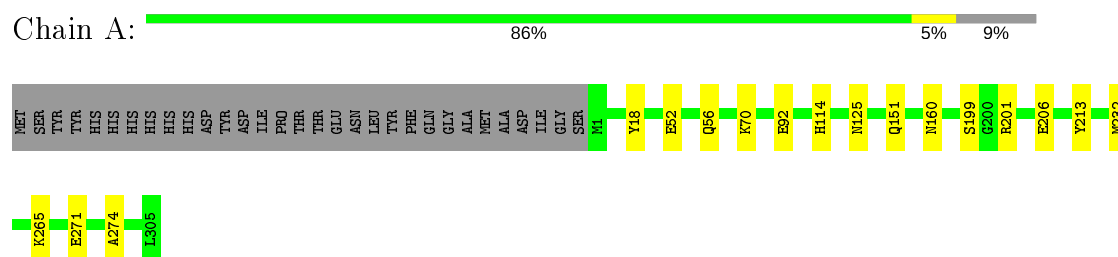
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	463	Total 463	O 463	0	0
7	B	448	Total 448	O 448	0	0
7	E	456	Total 456	O 456	0	0
7	F	459	Total 459	O 459	0	0

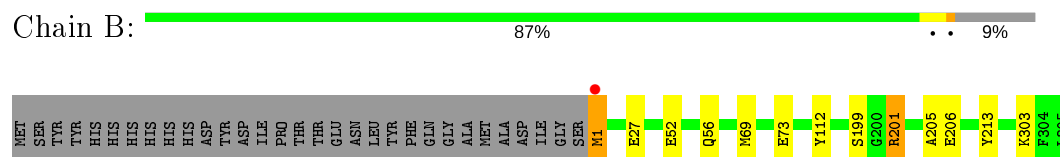
### 3 Residue-property plots [i](#)

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.

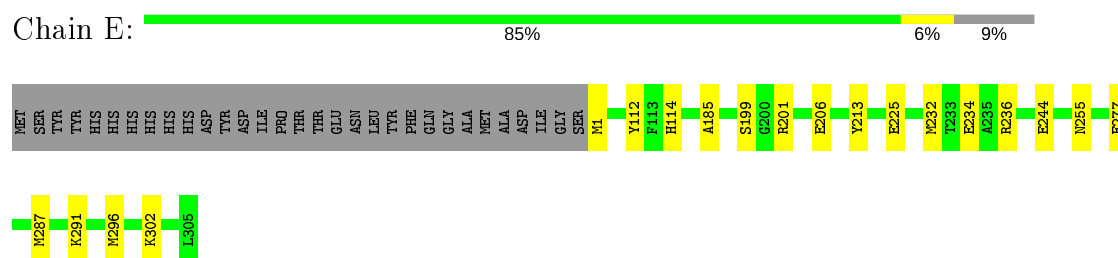
- Molecule 1: Putative N-acetylneuraminate lyase



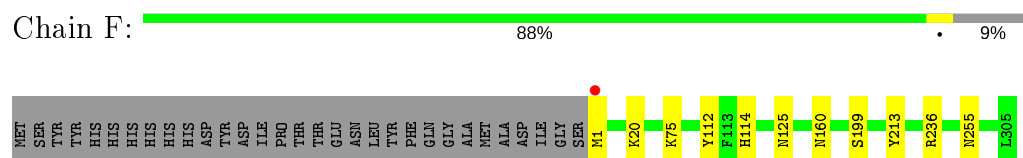
- Molecule 1: Putative N-acetylneuraminate lyase



- Molecule 1: Putative N-acetylneuraminate lyase



- Molecule 1: Putative N-acetylneuraminate lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.18 Å 121.39 Å 86.98 Å 90.00° 109.49° 90.00°	Depositor
Resolution (Å)	68.99 – 1.60 68.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.99-1.60) 99.9 (68.99-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 1.60 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.129 , 0.151 0.143 , 0.163	Depositor DCC
$R_{free}$ test set	9221 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, GOL, MG, PEG, BCN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.77	1/2449 (0.0%)	0.82	3/3310 (0.1%)
1	B	0.71	1/2444 (0.0%)	0.81	3/3299 (0.1%)
1	E	0.79	3/2406 (0.1%)	0.85	5/3251 (0.2%)
1	F	0.74	0/2423	0.81	2/3274 (0.1%)
All	All	0.75	5/9722 (0.1%)	0.82	13/13134 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	GLU	CD-OE1	11.62	1.38	1.25
1	E	277	GLU	CD-OE1	10.93	1.37	1.25
1	B	206	GLU	CD-OE1	7.20	1.33	1.25
1	E	206	GLU	CD-OE1	6.82	1.33	1.25
1	E	225	GLU	CD-OE2	-5.73	1.19	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	236	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	E	236	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	F	213	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	A	213	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	B	213	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	E	213	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	201	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	F	213	TYR	CB-CG-CD1	6.17	124.70	121.00
1	B	213	TYR	CB-CG-CD1	6.11	124.67	121.00
1	E	213	TYR	CB-CG-CD1	5.73	124.44	121.00
1	A	213	TYR	CB-CG-CD1	5.65	124.39	121.00
1	B	201	ARG	NE-CZ-NH1	5.43	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	ARG	NE-CZ-NH1	5.42	123.01	120.30

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	A	2406	0	2416	14	0
1	B	2402	0	2418	7	0
1	E	2363	0	2384	11	0
1	F	2381	0	2398	9	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	E	8	0	12	0	0
2	F	8	0	12	0	0
3	A	18	0	24	2	0
3	B	6	0	8	1	0
3	E	6	0	8	2	0
3	F	6	0	8	1	0
4	A	7	0	10	0	0
4	F	14	0	20	2	0
5	A	11	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	463	0	0	5	0
7	B	448	0	0	3	0
7	E	456	0	0	5	0
7	F	459	0	0	3	0
All	All	11482	0	9754	42	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 2.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:NZ	1:A:271[A]:GLU:OE1	1.91	1.03
1:B:69:MET:O	1:B:73[B]:GLU:HG3	1.77	0.84
3:A:402:GOL:H32	7:A:779:HOH:O	1.84	0.78
1:E:255:ASN:HD21	3:E:402:GOL:H32	1.48	0.78
1:A:232[A]:MET:HA	1:A:232[A]:MET:HE3	1.67	0.77
1:E:114:HIS:HE1	7:F:662:HOH:O	1.82	0.62
1:A:114:HIS:HE1	7:B:708:HOH:O	1.81	0.61
7:E:657:HOH:O	1:F:114:HIS:HE1	1.83	0.59
7:A:766:HOH:O	3:B:402:GOL:H32	2.03	0.58
1:E:234:GLU:HG2	7:E:897:HOH:O	2.04	0.57
1:A:52:GLU:O	1:A:56[B]:GLN:HG2	2.06	0.56
1:A:151:GLN:NE2	7:A:504:HOH:O	2.39	0.55
1:E:302:LYS:NZ	7:E:501:HOH:O	2.34	0.54
1:F:125:ASN:ND2	1:F:160:ASN:HD22	2.06	0.54
1:A:125:ASN:ND2	1:A:160:ASN:HD22	2.06	0.53
1:F:75:LYS:NZ	4:F:403:PEG:H31	2.24	0.53
1:B:52:GLU:O	1:B:56[B]:GLN:HG2	2.09	0.52
1:A:232[A]:MET:CE	1:A:232[A]:MET:HA	2.39	0.51
1:A:70:LYS:HG2	3:A:404:GOL:H12	1.93	0.51
1:E:287[B]:MET:HA	1:E:287[B]:MET:HE2	1.93	0.50
1:A:125:ASN:HD22	1:A:160:ASN:HD22	1.58	0.50
1:B:199:SER:HB3	1:F:199:SER:HB3	1.94	0.49
1:A:274:ALA:HB1	7:A:763:HOH:O	2.13	0.49
1:A:265:LYS:NZ	1:A:271[A]:GLU:CD	2.66	0.47
1:F:125:ASN:HD22	1:F:160:ASN:HD22	1.62	0.47
1:A:92:GLU:HG3	7:A:773:HOH:O	2.16	0.46
1:B:303[B]:LYS:NZ	7:B:504:HOH:O	2.49	0.46
1:B:27:GLU:HG2	7:B:780:HOH:O	2.15	0.45
1:E:1:MET:N	7:E:509:HOH:O	2.49	0.45
1:F:255:ASN:HD21	3:F:402:GOL:H12	1.82	0.45
1:B:1:MET:CE	1:B:1:MET:HA	2.47	0.45
1:E:232[A]:MET:HE3	1:E:232[A]:MET:HA	1.99	0.45
1:A:18:TYR:OH	1:A:56[B]:GLN:NE2	2.43	0.45
3:E:402:GOL:H11	7:E:718:HOH:O	2.17	0.44
1:E:244:GLU:HG2	1:E:296:MET:CE	2.50	0.42
1:E:1:MET:CE	1:E:185:ALA:HB3	2.50	0.41
1:F:20:LYS:HG2	7:F:760:HOH:O	2.20	0.41
1:F:236:ARG:HD2	4:F:404:PEG:H32	2.02	0.41
1:E:287[B]:MET:HG3	1:E:291:LYS:HE3	2.03	0.41
1:F:114:HIS:ND1	7:F:502:HOH:O	2.27	0.41
1:B:201:ARG:HD2	1:B:205:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:HB3	1:E:199:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/336 (93%)	307 (99%)	4 (1%)	0	100	100
1	B	309/336 (92%)	304 (98%)	4 (1%)	1 (0%)	41	21
1	E	306/336 (91%)	303 (99%)	2 (1%)	1 (0%)	41	21
1	F	307/336 (91%)	303 (99%)	3 (1%)	1 (0%)	41	21
All	All	1233/1344 (92%)	1217 (99%)	13 (1%)	3 (0%)	47	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	TYR
1	E	112	TYR
1	F	112	TYR

### 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	A	252/271 (93%)	252 (100%)	0	100	100
1	B	251/271 (93%)	250 (100%)	1 (0%)	91	84
1	E	247/271 (91%)	247 (100%)	0	100	100
1	F	249/271 (92%)	248 (100%)	1 (0%)	91	84
All	All	999/1084 (92%)	997 (100%)	2 (0%)	93	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	F	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	125	ASN
1	A	151	GLN
1	E	114	HIS
1	E	255	ASN
1	F	125	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	GOL	A	406	-	5,5,5	0.13	0	5,5,5	0.32	0
3	GOL	A	402	-	5,5,5	0.21	0	5,5,5	0.49	0
2	TRS	F	401	-	7,7,7	0.42	0	9,9,9	0.46	0
2	TRS	E	401	-	7,7,7	0.32	0	9,9,9	0.40	0
2	TRS	B	401	-	7,7,7	0.30	0	9,9,9	0.20	0
2	TRS	A	401	-	7,7,7	0.38	0	9,9,9	0.26	0
4	PEG	F	404	-	6,6,6	0.20	0	5,5,5	0.33	0
3	GOL	F	402	-	5,5,5	0.19	0	5,5,5	0.50	0
3	GOL	A	404	-	5,5,5	0.17	0	5,5,5	0.42	0
3	GOL	B	402	-	5,5,5	0.23	0	5,5,5	0.43	0
4	PEG	A	403	-	6,6,6	0.38	0	5,5,5	0.30	0
5	BCN	A	405	-	7,10,10	0.46	0	8,11,11	1.53	1 (12%)
3	GOL	E	402	-	5,5,5	0.24	0	5,5,5	0.67	0
4	PEG	F	403	-	6,6,6	0.28	0	5,5,5	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
2	TRS	F	401	-	-	0/9/9/9	-
2	TRS	E	401	-	-	0/9/9/9	-
2	TRS	B	401	-	-	0/9/9/9	-
2	TRS	A	401	-	-	0/9/9/9	-
4	PEG	F	404	-	-	3/4/4/4	-
3	GOL	F	402	-	-	3/4/4/4	-
3	GOL	A	404	-	-	4/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
4	PEG	A	403	-	-	0/4/4/4	-
5	BCN	A	405	-	-	2/8/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	402	-	-	2/4/4/4	-
4	PEG	F	403	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	BCN	C2-C1-N1	3.01	117.78	113.48

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	406	GOL	C1-C2-C3-O3
3	F	402	GOL	O1-C1-C2-C3
3	A	404	GOL	O1-C1-C2-C3
3	E	402	GOL	C1-C2-C3-O3
3	E	402	GOL	O2-C2-C3-O3
5	A	405	BCN	N1-C3-C4-O4
4	F	403	PEG	O2-C3-C4-O4
3	A	404	GOL	C1-C2-C3-O3
3	A	406	GOL	O2-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	A	404	GOL	O2-C2-C3-O3
4	F	403	PEG	O1-C1-C2-O2
4	F	404	PEG	C1-C2-O2-C3
4	F	404	PEG	O1-C1-C2-O2
4	F	404	PEG	O2-C3-C4-O4
3	F	402	GOL	O1-C1-C2-O2
3	F	402	GOL	O2-C2-C3-O3
5	A	405	BCN	C6-C5-N1-C1

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
4	F	404	PEG	1	0
3	F	402	GOL	1	0
3	A	404	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	1	0
3	E	402	GOL	2	0
4	F	403	PEG	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	305/336 (90%)	-0.58	0 <b>100</b> <b>100</b>	10, 15, 27, 56	0
1	B	305/336 (90%)	-0.60	1 (0%) <b>94</b> <b>93</b>	11, 15, 28, 87	0
1	E	305/336 (90%)	-0.58	0 <b>100</b> <b>100</b>	10, 14, 27, 52	0
1	F	305/336 (90%)	-0.60	1 (0%) <b>94</b> <b>93</b>	11, 15, 29, 98	0
All	All	1220/1344 (90%)	-0.59	2 (0%) <b>95</b> <b>94</b>	10, 15, 29, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	5.5
1	B	1	MET	3.4

### 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	E	402	6/6	0.68	0.17	32,51,53,56	0
5	BCN	A	405	11/11	0.69	0.15	64,75,96,101	0
3	GOL	A	404	6/6	0.69	0.16	51,56,66,76	0
3	GOL	A	406	6/6	0.81	0.19	43,60,66,71	0
3	GOL	A	402	6/6	0.87	0.19	32,40,49,49	0
3	GOL	F	402	6/6	0.89	0.20	33,48,53,62	0
4	PEG	F	404	7/7	0.90	0.10	38,42,46,46	0
3	GOL	B	402	6/6	0.91	0.14	34,40,50,51	0
4	PEG	F	403	7/7	0.91	0.12	29,34,44,47	0
2	TRS	F	401	8/8	0.93	0.12	19,25,30,34	0
4	PEG	A	403	7/7	0.95	0.09	33,33,43,43	0
2	TRS	B	401	8/8	0.95	0.09	17,24,28,33	0
2	TRS	E	401	8/8	0.96	0.08	16,25,29,37	0
2	TRS	A	401	8/8	0.96	0.07	18,25,30,32	0
6	MG	E	403	1/1	0.99	0.12	19,19,19,19	0
6	MG	B	403	1/1	0.99	0.11	18,18,18,18	0
6	MG	A	407	1/1	0.99	0.11	18,18,18,18	0
6	MG	F	405	1/1	0.99	0.06	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.