



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:20 PM BST

PDB ID : 4GX7  
Title : Vibrio Cholerae Cytolysin Beta-Prism Domain With Methyl-Alpha-Mannose Bound  
Authors : Levan, S.; Olson, R.  
Deposited on : 2012-09-04  
Resolution : 2.85 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 : 2.13.1  
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) : 2.13.1

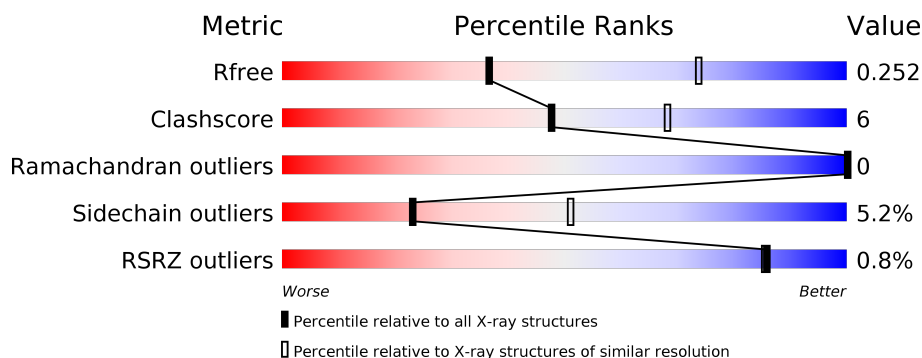
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	152	<div> <div style="width: 3%;"></div> <div style="width: 66%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 13%; background-color: grey;"></div> </div> <div>66% 20% • 13%</div>
1	B	152	<div> <div style="width: 3%;"></div> <div style="width: 67%; background-color: green;"></div> <div style="width: 18%; background-color: yellow;"></div> <div style="width: 13%; background-color: grey;"></div> </div> <div>67% 18% • 13%</div>
1	C	152	<div> <div style="width: 72%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 13%; background-color: grey;"></div> </div> <div>72% 14% • 13%</div>
1	D	152	<div> <div style="width: 73%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 13%; background-color: grey;"></div> </div> <div>73% 13% • 13%</div>
1	E	152	<div> <div style="width: 73%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 13%; background-color: grey;"></div> </div> <div>73% 13% • 13%</div>
1	F	152	<div> <div style="width: 3%;"></div> <div style="width: 76%; background-color: green;"></div> <div style="width: 11%; background-color: yellow;"></div> <div style="width: 13%; background-color: grey;"></div> </div> <div>3% 76% 11% • 13%</div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5853 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 Cytolysin and hemolysin HlyA Pore-forming toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			960	599	165	195	1			
1	B	132	Total	C	N	O	S	0	0	0
			966	602	166	196	2			
1	C	132	Total	C	N	O	S	0	0	0
			967	602	167	197	1			
1	D	132	Total	C	N	O	S	0	0	0
			962	601	164	196	1			
1	E	132	Total	C	N	O	S	0	0	0
			966	603	166	196	1			
1	F	132	Total	C	N	O	S	0	0	0
			954	596	162	195	1			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	MET	-	expression tag	UNP C2C744
A	566	GLY	-	expression tag	UNP C2C744
A	567	SER	-	expression tag	UNP C2C744
A	568	SER	-	expression tag	UNP C2C744
A	569	HIS	-	expression tag	UNP C2C744
A	570	HIS	-	expression tag	UNP C2C744
A	571	HIS	-	expression tag	UNP C2C744
A	572	HIS	-	expression tag	UNP C2C744
A	573	HIS	-	expression tag	UNP C2C744
A	574	HIS	-	expression tag	UNP C2C744
A	575	SER	-	expression tag	UNP C2C744
A	576	SER	-	expression tag	UNP C2C744
A	577	GLY	-	expression tag	UNP C2C744
A	578	LEU	-	expression tag	UNP C2C744
A	579	VAL	-	expression tag	UNP C2C744
A	580	PRO	-	expression tag	UNP C2C744
A	581	ARG	-	expression tag	UNP C2C744

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Chain	Residue	Modelled	Actual	Comment	Reference
A	582	GLY	-	expression tag	UNP C2C744
A	583	SER	-	expression tag	UNP C2C744
A	584	HIS	-	expression tag	UNP C2C744
A	585	MET	-	expression tag	UNP C2C744
A	606	ASN	HIS	conflict	UNP C2C744
B	565	MET	-	expression tag	UNP C2C744
B	566	GLY	-	expression tag	UNP C2C744
B	567	SER	-	expression tag	UNP C2C744
B	568	SER	-	expression tag	UNP C2C744
B	569	HIS	-	expression tag	UNP C2C744
B	570	HIS	-	expression tag	UNP C2C744
B	571	HIS	-	expression tag	UNP C2C744
B	572	HIS	-	expression tag	UNP C2C744
B	573	HIS	-	expression tag	UNP C2C744
B	574	HIS	-	expression tag	UNP C2C744
B	575	SER	-	expression tag	UNP C2C744
B	576	SER	-	expression tag	UNP C2C744
B	577	GLY	-	expression tag	UNP C2C744
B	578	LEU	-	expression tag	UNP C2C744
B	579	VAL	-	expression tag	UNP C2C744
B	580	PRO	-	expression tag	UNP C2C744
B	581	ARG	-	expression tag	UNP C2C744
B	582	GLY	-	expression tag	UNP C2C744
B	583	SER	-	expression tag	UNP C2C744
B	584	HIS	-	expression tag	UNP C2C744
B	585	MET	-	expression tag	UNP C2C744
B	606	ASN	HIS	conflict	UNP C2C744
C	565	MET	-	expression tag	UNP C2C744
C	566	GLY	-	expression tag	UNP C2C744
C	567	SER	-	expression tag	UNP C2C744
C	568	SER	-	expression tag	UNP C2C744
C	569	HIS	-	expression tag	UNP C2C744
C	570	HIS	-	expression tag	UNP C2C744
C	571	HIS	-	expression tag	UNP C2C744
C	572	HIS	-	expression tag	UNP C2C744
C	573	HIS	-	expression tag	UNP C2C744
C	574	HIS	-	expression tag	UNP C2C744
C	575	SER	-	expression tag	UNP C2C744
C	576	SER	-	expression tag	UNP C2C744
C	577	GLY	-	expression tag	UNP C2C744
C	578	LEU	-	expression tag	UNP C2C744
C	579	VAL	-	expression tag	UNP C2C744

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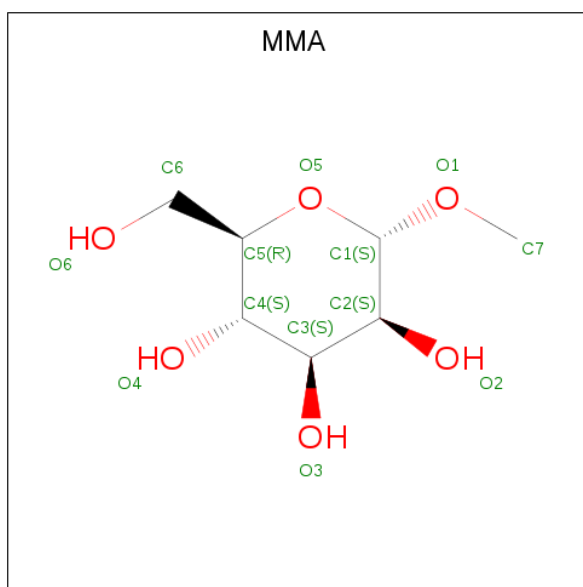
Chain	Residue	Modelled	Actual	Comment	Reference
C	580	PRO	-	expression tag	UNP C2C744
C	581	ARG	-	expression tag	UNP C2C744
C	582	GLY	-	expression tag	UNP C2C744
C	583	SER	-	expression tag	UNP C2C744
C	584	HIS	-	expression tag	UNP C2C744
C	585	MET	-	expression tag	UNP C2C744
C	606	ASN	HIS	conflict	UNP C2C744
D	565	MET	-	expression tag	UNP C2C744
D	566	GLY	-	expression tag	UNP C2C744
D	567	SER	-	expression tag	UNP C2C744
D	568	SER	-	expression tag	UNP C2C744
D	569	HIS	-	expression tag	UNP C2C744
D	570	HIS	-	expression tag	UNP C2C744
D	571	HIS	-	expression tag	UNP C2C744
D	572	HIS	-	expression tag	UNP C2C744
D	573	HIS	-	expression tag	UNP C2C744
D	574	HIS	-	expression tag	UNP C2C744
D	575	SER	-	expression tag	UNP C2C744
D	576	SER	-	expression tag	UNP C2C744
D	577	GLY	-	expression tag	UNP C2C744
D	578	LEU	-	expression tag	UNP C2C744
D	579	VAL	-	expression tag	UNP C2C744
D	580	PRO	-	expression tag	UNP C2C744
D	581	ARG	-	expression tag	UNP C2C744
D	582	GLY	-	expression tag	UNP C2C744
D	583	SER	-	expression tag	UNP C2C744
D	584	HIS	-	expression tag	UNP C2C744
D	585	MET	-	expression tag	UNP C2C744
D	606	ASN	HIS	conflict	UNP C2C744
E	565	MET	-	expression tag	UNP C2C744
E	566	GLY	-	expression tag	UNP C2C744
E	567	SER	-	expression tag	UNP C2C744
E	568	SER	-	expression tag	UNP C2C744
E	569	HIS	-	expression tag	UNP C2C744
E	570	HIS	-	expression tag	UNP C2C744
E	571	HIS	-	expression tag	UNP C2C744
E	572	HIS	-	expression tag	UNP C2C744
E	573	HIS	-	expression tag	UNP C2C744
E	574	HIS	-	expression tag	UNP C2C744
E	575	SER	-	expression tag	UNP C2C744
E	576	SER	-	expression tag	UNP C2C744
E	577	GLY	-	expression tag	UNP C2C744

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Chain	Residue	Modelled	Actual	Comment	Reference
E	578	LEU	-	expression tag	UNP C2C744
E	579	VAL	-	expression tag	UNP C2C744
E	580	PRO	-	expression tag	UNP C2C744
E	581	ARG	-	expression tag	UNP C2C744
E	582	GLY	-	expression tag	UNP C2C744
E	583	SER	-	expression tag	UNP C2C744
E	584	HIS	-	expression tag	UNP C2C744
E	585	MET	-	expression tag	UNP C2C744
E	606	ASN	HIS	conflict	UNP C2C744
F	565	MET	-	expression tag	UNP C2C744
F	566	GLY	-	expression tag	UNP C2C744
F	567	SER	-	expression tag	UNP C2C744
F	568	SER	-	expression tag	UNP C2C744
F	569	HIS	-	expression tag	UNP C2C744
F	570	HIS	-	expression tag	UNP C2C744
F	571	HIS	-	expression tag	UNP C2C744
F	572	HIS	-	expression tag	UNP C2C744
F	573	HIS	-	expression tag	UNP C2C744
F	574	HIS	-	expression tag	UNP C2C744
F	575	SER	-	expression tag	UNP C2C744
F	576	SER	-	expression tag	UNP C2C744
F	577	GLY	-	expression tag	UNP C2C744
F	578	LEU	-	expression tag	UNP C2C744
F	579	VAL	-	expression tag	UNP C2C744
F	580	PRO	-	expression tag	UNP C2C744
F	581	ARG	-	expression tag	UNP C2C744
F	582	GLY	-	expression tag	UNP C2C744
F	583	SER	-	expression tag	UNP C2C744
F	584	HIS	-	expression tag	UNP C2C744
F	585	MET	-	expression tag	UNP C2C744
F	606	ASN	HIS	conflict	UNP C2C744

- Molecule 2 is methyl alpha-D-mannopyranoside (three-letter code: MMA) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>6</sub>).

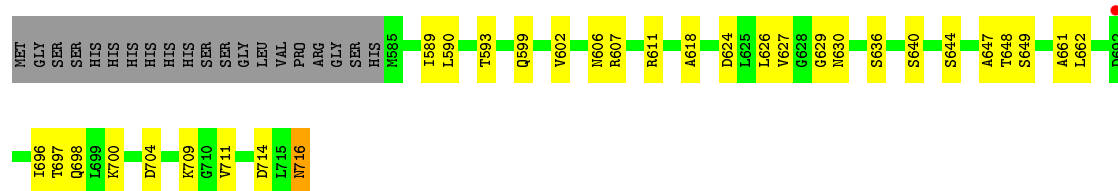


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	C	1	Total	C	O	0	0
			13	7	6		
2	D	1	Total	C	O	0	0
			13	7	6		
2	E	1	Total	C	O	0	0
			13	7	6		
2	F	1	Total	C	O	0	0
			13	7	6		

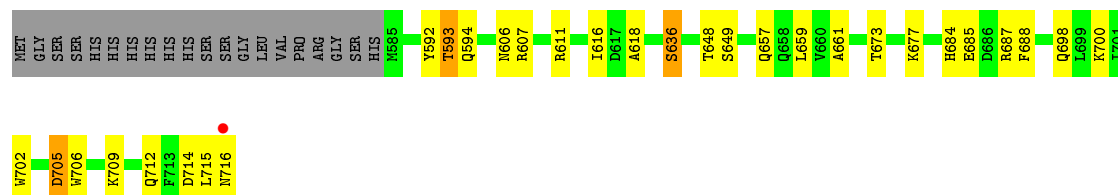
### 3 Residue-property plots [i](#)

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.

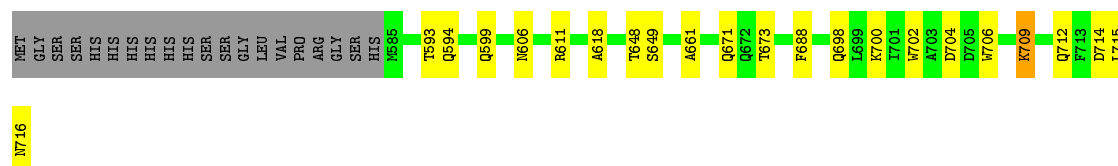
- Molecule 1: Cytolysin and hemolysin HlyA Pore-forming toxin



- Molecule 1: Cytolysin and hemolysin HlyA Pore-forming toxin



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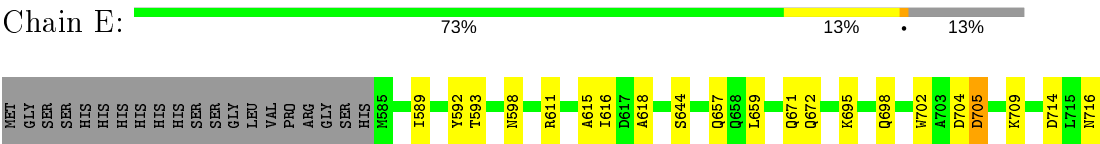


- Molecule 1: Cytolysin and hemolysin HlyA Pore-forming toxin

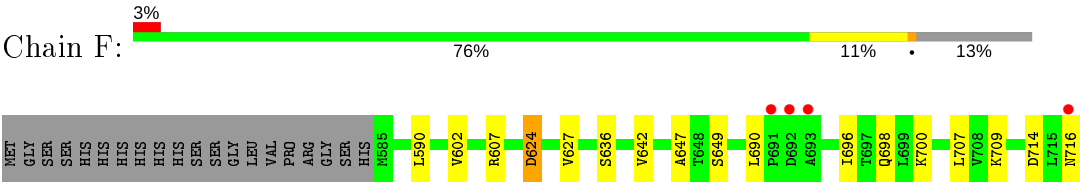


- Molecule 1: Cytolysin and hemolysin HlyA Pore-forming toxin





● Molecule 1: Cytolysin and hemolysin HlyA Pore-forming toxin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.77Å 99.77Å 172.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.89 – 2.85 24.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.89-2.85) 100.0 (24.89-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.84Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.195 , 0.248 0.197 , 0.252	Depositor DCC
$R_{free}$ test set	1182 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.29	0/975	0.55	0/1325
1	B	0.30	0/981	0.52	0/1332
1	C	0.29	0/982	0.51	0/1334
1	D	0.29	0/977	0.52	0/1327
1	E	0.31	0/980	0.53	0/1329
1	F	0.30	0/969	0.51	0/1318
All	All	0.30	0/5864	0.52	0/7965

There are no bond length outliers.

There are no bond angle outliers.

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	A	960	0	900	15	0
1	B	966	0	911	20	0
1	C	967	0	910	12	0
1	D	962	0	906	10	0
1	E	966	0	921	11	0
1	F	954	0	889	8	0
2	A	13	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	14	0	0
2	C	13	0	14	0	0
2	D	13	0	14	0	0
2	E	13	0	14	1	0
2	F	13	0	14	0	0
All	All	5853	0	5521	69	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 6.

All (69) 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:698:GLN:HB2	1:A:714:ASP:HB2	1.59	0.84
1:E:704:ASP:OD2	1:E:709:LYS:NZ	2.14	0.81
1:A:704:ASP:OD2	1:A:709:LYS:NZ	2.20	0.72
1:F:698:GLN:HB2	1:F:714:ASP:HB2	1.71	0.71
1:E:698:GLN:HB3	1:E:714:ASP:HB2	1.71	0.71
1:B:688:PHE:HZ	1:B:715:LEU:HD11	1.56	0.71
1:B:677:LYS:NZ	1:B:685:GLU:OE2	2.23	0.70
1:A:607:ARG:NE	1:A:636:SER:OG	2.26	0.67
1:E:616:ILE:HD12	1:E:659:LEU:HG	1.76	0.67
1:D:688:PHE:HZ	1:D:715:LEU:HD11	1.59	0.67
1:C:698:GLN:HB2	1:C:714:ASP:HB2	1.76	0.67
1:F:700:LYS:NZ	1:F:714:ASP:OD2	2.30	0.65
1:B:616:ILE:HD12	1:B:659:LEU:HG	1.78	0.65
1:A:611:ARG:NH2	1:A:629:GLY:O	2.31	0.64
1:C:599:GLN:NE2	1:C:698:GLN:OE1	2.24	0.63
1:A:700:LYS:NZ	1:A:714:ASP:OD2	2.30	0.63
1:E:615:ALA:N	2:E:801:MMA:O6	2.32	0.59
1:D:658:GLN:OE1	1:D:709:LYS:NZ	2.36	0.58
1:C:673:THR:HB	1:D:671:GLN:HB2	1.83	0.58
1:E:705:ASP:OD1	1:E:705:ASP:N	2.35	0.57
1:C:671:GLN:HB2	1:D:673:THR:HB	1.86	0.56
1:D:698:GLN:HB2	1:D:714:ASP:HB2	1.88	0.55
1:E:702:TRP:O	1:E:709:LYS:N	2.31	0.55
1:C:704:ASP:OD2	1:C:709:LYS:NZ	2.40	0.54
1:A:589:ILE:HG21	1:A:593:THR:HG23	1.89	0.53
1:B:700:LYS:NZ	1:B:714:ASP:OD2	2.41	0.53
1:B:705:ASP:OD1	1:B:705:ASP:N	2.42	0.52
1:B:698:GLN:HB2	1:B:714:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:THR:HG22	1:B:702:TRP:CE2	2.44	0.52
1:E:611:ARG:HB2	1:E:618:ALA:HB3	1.91	0.52
1:F:624:ASP:N	1:F:624:ASP:OD1	2.37	0.52
1:A:648:THR:HB	1:A:661:ALA:HB3	1.92	0.51
1:F:602:VAL:HG21	1:F:696:ILE:HG22	1.93	0.50
1:C:700:LYS:HB2	1:C:712:GLN:HB3	1.93	0.49
1:B:673:THR:HB	1:E:671:GLN:HB2	1.94	0.49
1:A:624:ASP:CG	1:B:687:ARG:HH22	2.16	0.48
1:F:707:LEU:O	1:F:709:LYS:NZ	2.46	0.48
1:D:607:ARG:HE	1:D:636:SER:HG	1.62	0.48
1:D:589:ILE:HG21	1:D:593:THR:HG23	1.96	0.46
1:D:611:ARG:NH1	1:D:631:GLY:O	2.49	0.46
1:A:602:VAL:HG21	1:A:696:ILE:HG22	1.97	0.46
1:B:611:ARG:HB2	1:B:618:ALA:HB3	1.97	0.46
1:F:590:LEU:HB3	1:F:647:ALA:CB	2.47	0.45
1:A:697:THR:HG21	1:A:716:ASN:HA	1.99	0.44
1:C:594:GLN:HB2	1:C:709:LYS:HG3	1.98	0.44
1:D:592:TYR:CE2	1:D:657:GLN:HB3	2.53	0.44
1:B:700:LYS:HB2	1:B:712:GLN:HB3	2.01	0.43
1:B:592:TYR:CE2	1:B:657:GLN:HB3	2.53	0.43
1:C:611:ARG:HB2	1:C:618:ALA:HB3	2.01	0.43
1:A:662:LEU:HD11	1:A:711:VAL:HG11	2.00	0.43
1:B:607:ARG:HE	1:B:636:SER:HB2	1.83	0.42
1:C:688:PHE:HZ	1:C:715:LEU:HD11	1.83	0.42
1:A:590:LEU:HB3	1:A:647:ALA:HB2	2.01	0.42
1:B:648:THR:HB	1:B:661:ALA:HB3	2.02	0.42
1:B:648:THR:HA	1:B:684:HIS:O	2.20	0.42
1:B:700:LYS:HD2	1:B:712:GLN:OE1	2.20	0.42
1:B:688:PHE:CZ	1:B:715:LEU:HD11	2.46	0.42
1:E:589:ILE:HG21	1:E:593:THR:HG23	2.03	0.41
1:A:618:ALA:HB1	1:A:626:LEU:HB3	2.02	0.41
1:C:648:THR:HB	1:C:661:ALA:HB3	2.02	0.41
1:A:611:ARG:NH2	1:A:630:ASN:HA	2.36	0.41
1:C:706:TRP:CD2	1:E:695:LYS:HD2	2.56	0.41
1:E:592:TYR:CE2	1:E:657:GLN:HB3	2.55	0.41
1:F:607:ARG:HH21	1:F:636:SER:HB3	1.86	0.41
1:C:593:THR:HG23	1:C:702:TRP:CE2	2.55	0.41
1:B:706:TRP:CD2	1:D:695:LYS:HD3	2.56	0.41
1:A:599:GLN:O	1:B:684:HIS:HA	2.22	0.40
1:B:594:GLN:HB2	1:B:709:LYS:HG2	2.02	0.40
1:F:642:VAL:HG12	1:F:690:LEU:HD13	2.04	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	130/152 (86%)	125 (96%)	5 (4%)	0	100	100
1	B	130/152 (86%)	126 (97%)	4 (3%)	0	100	100
1	C	130/152 (86%)	125 (96%)	5 (4%)	0	100	100
1	D	130/152 (86%)	126 (97%)	4 (3%)	0	100	100
1	E	130/152 (86%)	126 (97%)	4 (3%)	0	100	100
1	F	130/152 (86%)	124 (95%)	6 (5%)	0	100	100
All	All	780/912 (86%)	752 (96%)	28 (4%)	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	A	95/121 (78%)	89 (94%)	6 (6%)	18	42
1	B	97/121 (80%)	91 (94%)	6 (6%)	18	43
1	C	97/121 (80%)	93 (96%)	4 (4%)	30	61
1	D	96/121 (79%)	91 (95%)	5 (5%)	23	51
1	E	97/121 (80%)	92 (95%)	5 (5%)	23	51
1	F	94/121 (78%)	90 (96%)	4 (4%)	29	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	576/726 (79%)	546 (95%)	30 (5%)	23	51

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	606	ASN
1	A	627	VAL
1	A	640	SER
1	A	644	SER
1	A	649	SER
1	A	716	ASN
1	B	593	THR
1	B	606	ASN
1	B	636	SER
1	B	649	SER
1	B	705	ASP
1	B	716	ASN
1	C	606	ASN
1	C	649	SER
1	C	709	LYS
1	C	716	ASN
1	D	598	ASN
1	D	606	ASN
1	D	636	SER
1	D	649	SER
1	D	716	ASN
1	E	598	ASN
1	E	644	SER
1	E	672	GLN
1	E	705	ASP
1	E	716	ASN
1	F	624	ASP
1	F	627	VAL
1	F	649	SER
1	F	716	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	698	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	MMA	C	801	-	13,13,13	1.89	3 (23%)	18,18,18	1.59	4 (22%)
2	MMA	F	801	-	13,13,13	1.76	3 (23%)	18,18,18	1.87	5 (27%)
2	MMA	D	801	-	13,13,13	1.88	3 (23%)	18,18,18	1.85	5 (27%)
2	MMA	B	801	-	13,13,13	1.87	3 (23%)	18,18,18	1.48	4 (22%)
2	MMA	E	801	-	13,13,13	1.81	3 (23%)	18,18,18	1.46	1 (5%)
2	MMA	A	801	-	13,13,13	1.77	3 (23%)	18,18,18	1.65	3 (16%)

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	MMA	C	801	-	-	2/4/24/24	0/1/1/1
2	MMA	F	801	-	-	0/4/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MMA	D	801	-	-	3/4/24/24	0/1/1/1
2	MMA	B	801	-	-	2/4/24/24	0/1/1/1
2	MMA	E	801	-	-	2/4/24/24	0/1/1/1
2	MMA	A	801	-	-	2/4/24/24	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	MMA	O5-C1	4.49	1.53	1.41
2	E	801	MMA	O5-C1	4.09	1.52	1.41
2	B	801	MMA	O5-C1	4.06	1.52	1.41
2	A	801	MMA	O5-C1	4.06	1.52	1.41
2	C	801	MMA	O5-C1	3.99	1.52	1.41
2	C	801	MMA	O1-C1	-3.91	1.33	1.40
2	F	801	MMA	O5-C1	3.90	1.51	1.41
2	B	801	MMA	O1-C1	-3.89	1.33	1.40
2	F	801	MMA	O1-C1	-3.60	1.33	1.40
2	E	801	MMA	O1-C1	-3.56	1.33	1.40
2	A	801	MMA	O1-C1	-3.52	1.34	1.40
2	D	801	MMA	O1-C1	-3.44	1.34	1.40
2	D	801	MMA	C3-C2	-2.56	1.45	1.52
2	C	801	MMA	C3-C2	-2.40	1.46	1.52
2	B	801	MMA	C3-C2	-2.35	1.46	1.52
2	E	801	MMA	C3-C2	-2.31	1.46	1.52
2	F	801	MMA	C3-C2	-2.23	1.46	1.52
2	A	801	MMA	C3-C2	-2.17	1.46	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	MMA	C7-O1-C1	4.81	120.71	113.27
2	F	801	MMA	C7-O1-C1	4.25	119.83	113.27
2	A	801	MMA	C7-O1-C1	4.09	119.58	113.27
2	E	801	MMA	C7-O1-C1	4.03	119.49	113.27
2	F	801	MMA	C3-C4-C5	3.74	116.92	110.24
2	C	801	MMA	C7-O1-C1	3.67	118.94	113.27
2	C	801	MMA	O5-C5-C4	3.41	115.89	109.69
2	B	801	MMA	C7-O1-C1	3.28	118.34	113.27
2	D	801	MMA	O5-C5-C4	3.02	115.17	109.69
2	A	801	MMA	C3-C4-C5	2.99	115.58	110.24
2	F	801	MMA	C4-C3-C2	2.84	115.79	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	MMA	O5-C1-C2	2.72	116.11	110.35
2	D	801	MMA	C1-O5-C5	2.70	118.99	113.69
2	C	801	MMA	C3-C4-C5	2.63	114.94	110.24
2	A	801	MMA	O5-C5-C4	2.59	114.40	109.69
2	F	801	MMA	O5-C5-C4	2.38	114.01	109.69
2	B	801	MMA	C3-C4-C5	2.34	114.41	110.24
2	B	801	MMA	O5-C5-C4	2.23	113.74	109.69
2	C	801	MMA	C6-C5-C4	-2.18	107.90	113.00
2	D	801	MMA	C3-C4-C5	2.15	114.07	110.24
2	F	801	MMA	O6-C6-C5	2.02	118.21	111.29
2	B	801	MMA	O6-C6-C5	2.00	118.17	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	MMA	O5-C1-O1-C7
2	A	801	MMA	C4-C5-C6-O6
2	C	801	MMA	C4-C5-C6-O6
2	E	801	MMA	O5-C5-C6-O6
2	B	801	MMA	C4-C5-C6-O6
2	E	801	MMA	C4-C5-C6-O6
2	C	801	MMA	O5-C5-C6-O6
2	A	801	MMA	O5-C5-C6-O6
2	D	801	MMA	C4-C5-C6-O6
2	B	801	MMA	O5-C5-C6-O6
2	D	801	MMA	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	MMA	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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	132/152 (86%)	-0.45	1 (0%) 86 85	12, 24, 48, 74	0
1	B	132/152 (86%)	-0.56	1 (0%) 86 85	4, 21, 41, 56	0
1	C	132/152 (86%)	-0.54	0 100 100	7, 21, 43, 60	0
1	D	132/152 (86%)	-0.55	0 100 100	7, 18, 38, 56	0
1	E	132/152 (86%)	-0.59	0 100 100	7, 19, 41, 51	0
1	F	132/152 (86%)	-0.28	4 (3%) 50 45	9, 29, 68, 89	0
All	All	792/912 (86%)	-0.50	6 (0%) 86 85	4, 22, 48, 89	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	692	ASP	5.5
1	F	716	ASN	3.5
1	F	693	ALA	3.5
1	B	716	ASN	3.0
1	F	691	PRO	2.8
1	A	692	ASP	2.5

### 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( $\text{\AA}^2$ )	Q<0.9
2	MMA	C	801	13/13	0.94	0.16	8,16,24,24	0
2	MMA	F	801	13/13	0.94	0.19	11,17,29,33	0
2	MMA	B	801	13/13	0.95	0.13	8,10,20,26	0
2	MMA	A	801	13/13	0.96	0.15	5,16,28,34	0
2	MMA	E	801	13/13	0.97	0.14	10,13,25,28	0
2	MMA	D	801	13/13	0.98	0.10	4,7,18,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.