



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 18, 2018 – 08:26 AM EST

PDB ID : 5MDR  
Title : Crystal structure of in vitro folded Chitoporin VhChip from *Vibrio harveyi* in complex with chitohexaose  
Authors : Zahn, M.; van den Berg, B.  
Deposited on : 2016-11-13  
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

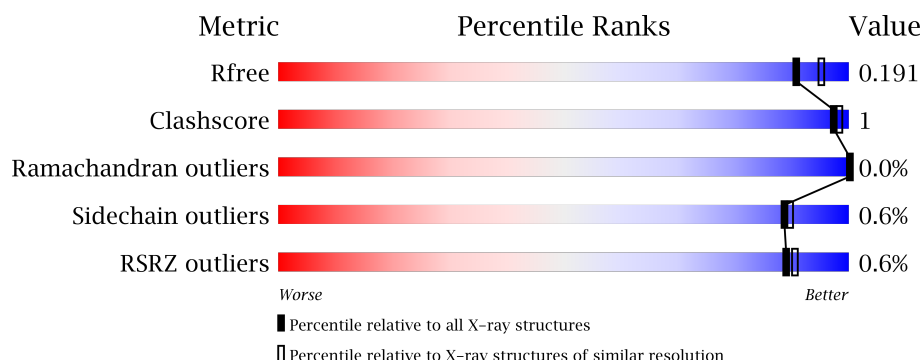
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.



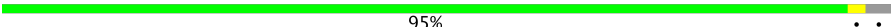
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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  $\geq 3$ , 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	A	352	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 94%; text-align: center;">94%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="width: 94%; text-align: center;">94%</div> </div>
1	B	352	<div> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 94%; text-align: center;">94%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="width: 94%; text-align: center;">94%</div> </div>
1	C	352	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 94%; text-align: center;">94%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="width: 94%; text-align: center;">94%</div> </div>
1	D	352	<div> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 94%; text-align: center;">94%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="width: 94%; text-align: center;">94%</div> </div>
1	E	352	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 95%; height: 10px; background-color: green;"></div> <div style="width: 95%; text-align: center;">95%</div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="width: 95%; text-align: center;">95%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	352	 95%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	A	401	-	-	-	X
2	C8E	A	403	-	-	-	X
2	C8E	A	404	-	-	-	X
2	C8E	A	406	-	-	-	X
2	C8E	B	401	-	-	-	X
2	C8E	C	401	-	-	-	X
2	C8E	D	401	-	-	-	X
2	C8E	D	402	-	-	-	X
2	C8E	D	403	-	-	-	X
2	C8E	E	401	-	-	-	X
2	C8E	F	401	-	-	-	X
3	NAG	A	410	-	-	-	X
3	NAG	A	412	-	-	-	X
3	NAG	B	404	-	-	-	X
3	NAG	B	405	-	-	-	X
3	NAG	B	406	-	-	-	X
3	NAG	B	408	-	-	-	X
3	NAG	C	403	-	-	-	X
3	NAG	C	404	-	-	-	X
3	NAG	C	405	-	-	-	X
3	NAG	D	405	-	-	-	X
3	NAG	D	406	-	-	-	X
3	NAG	D	407	-	-	-	X
3	NAG	E	404	-	-	-	X
3	NAG	E	405	-	-	-	X
3	NAG	E	406	-	-	-	X
3	NAG	E	408	-	-	-	X
3	NAG	F	405	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18479 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.

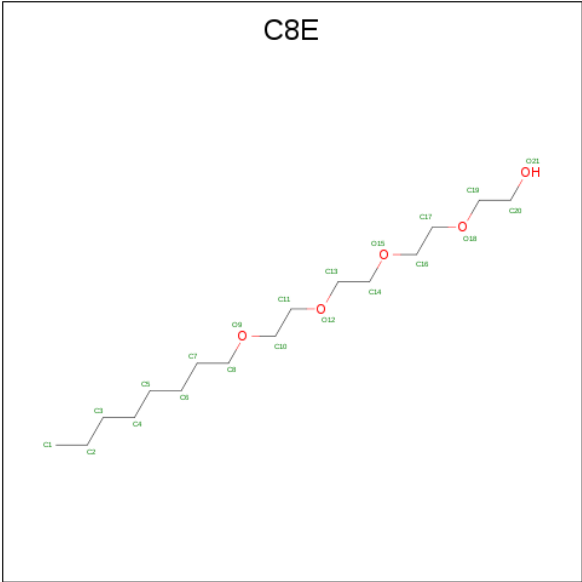
- Molecule 1 is a protein called Chitoporin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	Se	0	1	0
			2677	1689	439	540	9			
1	B	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	C	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	D	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	E	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			
1	F	341	Total	C	N	O	Se	0	0	0
			2665	1680	438	538	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	initiating methionine	UNP L0RVU0
A	0	GLY	-	expression tag	UNP L0RVU0
B	-1	MSE	-	initiating methionine	UNP L0RVU0
B	0	GLY	-	expression tag	UNP L0RVU0
C	-1	MSE	-	initiating methionine	UNP L0RVU0
C	0	GLY	-	expression tag	UNP L0RVU0
D	-1	MSE	-	initiating methionine	UNP L0RVU0
D	0	GLY	-	expression tag	UNP L0RVU0
E	-1	MSE	-	initiating methionine	UNP L0RVU0
E	0	GLY	-	expression tag	UNP L0RVU0
F	-1	MSE	-	initiating methionine	UNP L0RVU0
F	0	GLY	-	expression tag	UNP L0RVU0

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



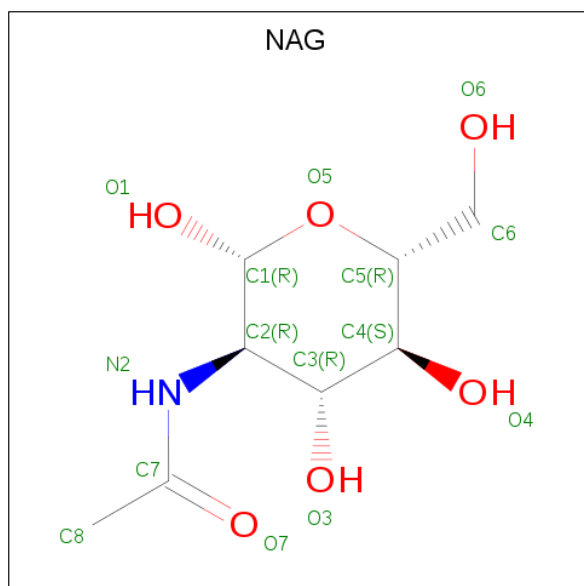
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	8	4		
2	A	1	Total	C	O	0	0
			9	6	3		
2	A	1	Total	C	O	0	0
			14	9	5		
2	A	1	Total	C	O	0	0
			9	8	1		
2	A	1	Total	C		0	0
			8	8			
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			13	11	2		
2	B	1	Total	C	O	0	0
			12	10	2		
2	C	1	Total	C	O	0	0
			21	16	5		
2	D	1	Total	C	O	0	0
			14	12	2		
2	D	1	Total	C	O	0	0
			13	11	2		
2	D	1	Total	C	O	0	0
			11	10	1		
2	E	1	Total	C	O	0	0
			12	10	2		
2	E	1	Total	C	O	0	0
			15	12	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	C	O	0	0
			17	14	3		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	8	1	6		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			15	8	1	6		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			15	8	1	6		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			15	8	1	6		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			15	8	1	6		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total	Na	0	0
			4	4		
4	E	3	Total	Na	0	0
			3	3		
4	B	3	Total	Na	0	0
			3	3		
4	C	2	Total	Na	0	0
			2	2		
4	A	4	Total	Na	0	0
			4	4		
4	F	2	Total	Na	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	314	Total	O	0	0
			314	314		
5	B	275	Total	O	0	0
			275	275		
5	C	288	Total	O	0	0
			288	288		
5	D	280	Total	O	0	0
			280	280		
5	E	279	Total	O	0	0
			279	279		
5	F	312	Total	O	0	0
			312	312		



### 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: Chitoporin

Chain A:  94%



#### • Molecule 1: Chitoporin

Chain B:  94%



#### • Molecule 1: Chitoporin

Chain C:  94%



#### • Molecule 1: Chitoporin

Chain D:  94%



#### • Molecule 1: Chitoporin

Chain E:  95%



#### • Molecule 1: Chitoporin

Chain F: 

95%

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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.55Å 121.94Å 147.16Å 90.00° 117.92° 90.00°	Depositor
Resolution (Å)	130.02 – 1.90 64.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (130.02-1.90) 99.6 (64.75-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.172 , 0.183 0.182 , 0.191	Depositor DCC
$R_{free}$ test set	3476 reflections (0.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h-l,k,h 0.010 for l,k,-h-l 0.015 for h,-k,-h-l 0.017 for -h-l,-k,l 0.125 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18479	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

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

<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, NAG, C8E

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	0.66	0/2738	0.82	5/3695 (0.1%)
1	B	0.65	0/2725	0.81	5/3677 (0.1%)
1	C	0.61	0/2725	0.80	5/3677 (0.1%)
1	D	0.66	0/2725	0.82	6/3677 (0.2%)
1	E	0.62	0/2725	0.81	3/3677 (0.1%)
1	F	0.66	0/2725	0.81	5/3677 (0.1%)
All	All	0.64	0/16363	0.81	29/22080 (0.1%)

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MSE	CG-SE-CE	-8.72	79.71	98.90
1	E	257	MSE	CG-SE-CE	6.58	113.37	98.90
1	E	38	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	257	MSE	CG-SE-CE	-6.34	84.95	98.90
1	F	38	ASP	CB-CG-OD1	6.26	123.93	118.30

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	A	2677	0	2428	2	0
1	B	2665	0	2420	2	0
1	C	2665	0	2420	3	0
1	D	2665	0	2420	2	0
1	E	2665	0	2420	3	0
1	F	2665	0	2420	1	0
2	A	73	0	109	1	0
2	B	25	0	42	0	0
2	C	21	0	34	0	0
2	D	38	0	63	0	0
2	E	27	0	46	0	0
2	F	17	0	27	0	0
3	A	85	0	75	3	0
3	B	85	0	75	4	0
3	C	85	0	75	5	0
3	D	85	0	75	4	0
3	E	85	0	75	1	0
3	F	85	0	75	3	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
5	A	314	0	0	0	0
5	B	275	0	0	3	0
5	C	288	0	0	0	0
5	D	280	0	0	1	0
5	E	279	0	0	1	0
5	F	312	0	0	1	0
All	All	18479	0	15299	31	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 1.

The worst 5 of 31 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)
3:A:410:NAG:O3	3:A:411:NAG:O5	1.96	0.83
3:C:405:NAG:O3	3:C:406:NAG:O5	2.06	0.72
3:E:406:NAG:O3	3:E:407:NAG:O5	2.07	0.71
1:A:291:SER:OG	2:A:403:C8E:H171	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:406:NAG:O3	3:B:407:NAG:O5	2.11	0.66

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	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
1	B	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
1	C	339/352 (96%)	331 (98%)	7 (2%)	1 (0%)	44	34
1	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
1	E	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
1	F	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
All	All	2035/2112 (96%)	1990 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	PRO

### 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	263/258 (102%)	261 (99%)	2 (1%)	85	85
1	B	262/258 (102%)	261 (100%)	1 (0%)	93	93
1	C	262/258 (102%)	260 (99%)	2 (1%)	85	85
1	D	262/258 (102%)	261 (100%)	1 (0%)	93	93
1	E	262/258 (102%)	260 (99%)	2 (1%)	85	85
1	F	262/258 (102%)	261 (100%)	1 (0%)	93	93
All	All	1573/1548 (102%)	1564 (99%)	9 (1%)	89	90

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	257	MSE
1	F	55	ARG
1	E	55	ARG
1	B	55	ARG
1	D	55	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	336	ASN
1	F	336	ASN
1	D	336	ASN
1	B	336	ASN
1	E	336	ASN

### 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 69 ligands modelled in this entry, 18 are monoatomic - leaving 51 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	C8E	A	401	-	11,11,20	0.42	0	10,10,19	0.25	0
2	C8E	A	402	-	8,8,20	0.56	0	7,7,19	0.25	0
2	C8E	A	403	-	13,13,20	0.45	0	12,12,19	0.55	0
2	C8E	A	404	-	8,8,20	0.26	0	7,7,19	0.37	0
2	C8E	A	405	-	7,7,20	0.27	0	6,6,19	0.38	0
2	C8E	A	406	-	20,20,20	0.49	0	19,19,19	0.66	0
3	NAG	A	407	3	15,15,15	0.87	0	21,21,21	1.56	3 (14%)
3	NAG	A	408	3	14,14,15	0.40	0	15,19,21	1.27	2 (13%)
3	NAG	A	409	3	14,14,15	0.41	0	15,19,21	1.00	1 (6%)
3	NAG	A	410	3	14,14,15	0.72	0	15,19,21	2.23	6 (40%)
3	NAG	A	411	3	14,14,15	0.78	0	15,19,21	3.11	9 (60%)
3	NAG	A	412	3	14,14,15	0.84	0	15,19,21	2.95	4 (26%)
2	C8E	B	401	-	12,12,20	0.43	0	11,11,19	0.52	0
2	C8E	B	402	-	11,11,20	0.30	0	10,10,19	0.47	0
3	NAG	B	403	3	15,15,15	0.82	0	21,21,21	1.76	4 (19%)
3	NAG	B	404	3	14,14,15	0.54	0	15,19,21	1.15	0
3	NAG	B	405	3	14,14,15	0.42	0	15,19,21	0.97	0
3	NAG	B	406	3	14,14,15	0.61	0	15,19,21	2.20	7 (46%)
3	NAG	B	407	3	14,14,15	0.79	0	15,19,21	2.30	6 (40%)
3	NAG	B	408	3	14,14,15	0.83	0	15,19,21	2.49	3 (20%)
2	C8E	C	401	-	20,20,20	0.43	0	19,19,19	0.46	0
3	NAG	C	402	3	15,15,15	0.94	0	21,21,21	1.82	5 (23%)
3	NAG	C	403	3	14,14,15	0.48	0	15,19,21	1.47	3 (20%)
3	NAG	C	404	3	14,14,15	0.34	0	15,19,21	1.23	1 (6%)
3	NAG	C	405	3	14,14,15	0.57	0	15,19,21	2.08	5 (33%)
3	NAG	C	406	3	14,14,15	0.76	0	15,19,21	1.91	4 (26%)
3	NAG	C	407	3	14,14,15	0.85	1 (7%)	15,19,21	2.93	5 (33%)
2	C8E	D	401	-	13,13,20	0.52	0	12,12,19	0.69	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	C8E	D	402	-	12,12,20	0.46	0	11,11,19	0.48	0
2	C8E	D	403	-	10,10,20	0.44	0	9,9,19	0.40	0
3	NAG	D	404	3	15,15,15	0.88	0	21,21,21	1.80	5 (23%)
3	NAG	D	405	3	14,14,15	0.55	0	15,19,21	1.34	2 (13%)
3	NAG	D	406	3	14,14,15	0.45	0	15,19,21	1.10	1 (6%)
3	NAG	D	407	3	14,14,15	0.59	0	15,19,21	1.77	4 (26%)
3	NAG	D	408	3	14,14,15	0.66	0	15,19,21	1.87	4 (26%)
3	NAG	D	409	3	14,14,15	0.80	0	15,19,21	2.79	3 (20%)
2	C8E	E	401	-	11,11,20	0.24	0	10,10,19	0.48	0
2	C8E	E	402	-	14,14,20	0.37	0	13,13,19	0.76	0
3	NAG	E	403	3	15,15,15	0.91	0	21,21,21	1.62	5 (23%)
3	NAG	E	404	3	14,14,15	0.37	0	15,19,21	1.12	0
3	NAG	E	405	3	14,14,15	0.31	0	15,19,21	1.28	0
3	NAG	E	406	3	14,14,15	0.60	0	15,19,21	1.82	6 (40%)
3	NAG	E	407	3	14,14,15	0.59	0	15,19,21	1.45	2 (13%)
3	NAG	E	408	3	14,14,15	0.71	0	15,19,21	2.43	3 (20%)
2	C8E	F	401	-	16,16,20	0.38	0	15,15,19	0.33	0
3	NAG	F	402	3	15,15,15	0.84	0	21,21,21	1.80	4 (19%)
3	NAG	F	403	3	14,14,15	0.41	0	15,19,21	1.12	1 (6%)
3	NAG	F	404	3	14,14,15	0.29	0	15,19,21	0.85	1 (6%)
3	NAG	F	405	3	14,14,15	0.62	0	15,19,21	1.44	2 (13%)
3	NAG	F	406	3	14,14,15	0.78	0	15,19,21	3.06	8 (53%)
3	NAG	F	407	3	14,14,15	0.65	0	15,19,21	2.84	4 (26%)

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	C8E	A	401	-	-	0/9/9/18	0/0/0/0
2	C8E	A	402	-	-	0/6/6/18	0/0/0/0
2	C8E	A	403	-	-	0/11/11/18	0/0/0/0
2	C8E	A	404	-	-	0/6/6/18	0/0/0/0
2	C8E	A	405	-	-	0/5/5/18	0/0/0/0
2	C8E	A	406	-	-	0/18/18/18	0/0/0/0
3	NAG	A	407	3	-	0/6/26/26	0/1/1/1
3	NAG	A	408	3	-	0/6/23/26	0/1/1/1
3	NAG	A	409	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	410	3	-	0/6/23/26	0/1/1/1
3	NAG	A	411	3	-	0/6/23/26	0/1/1/1
3	NAG	A	412	3	-	0/6/23/26	0/1/1/1
2	C8E	B	401	-	-	0/10/10/18	0/0/0/0
2	C8E	B	402	-	-	0/9/9/18	0/0/0/0
3	NAG	B	403	3	-	0/6/26/26	0/1/1/1
3	NAG	B	404	3	-	0/6/23/26	0/1/1/1
3	NAG	B	405	3	-	0/6/23/26	0/1/1/1
3	NAG	B	406	3	-	0/6/23/26	0/1/1/1
3	NAG	B	407	3	-	0/6/23/26	0/1/1/1
3	NAG	B	408	3	-	0/6/23/26	0/1/1/1
2	C8E	C	401	-	-	0/18/18/18	0/0/0/0
3	NAG	C	402	3	-	0/6/26/26	0/1/1/1
3	NAG	C	403	3	-	0/6/23/26	0/1/1/1
3	NAG	C	404	3	-	0/6/23/26	0/1/1/1
3	NAG	C	405	3	-	0/6/23/26	0/1/1/1
3	NAG	C	406	3	-	0/6/23/26	0/1/1/1
3	NAG	C	407	3	-	0/6/23/26	0/1/1/1
2	C8E	D	401	-	-	0/11/11/18	0/0/0/0
2	C8E	D	402	-	-	0/10/10/18	0/0/0/0
2	C8E	D	403	-	-	0/8/8/18	0/0/0/0
3	NAG	D	404	3	-	0/6/26/26	0/1/1/1
3	NAG	D	405	3	-	0/6/23/26	0/1/1/1
3	NAG	D	406	3	-	0/6/23/26	0/1/1/1
3	NAG	D	407	3	-	0/6/23/26	0/1/1/1
3	NAG	D	408	3	-	0/6/23/26	0/1/1/1
3	NAG	D	409	3	-	0/6/23/26	0/1/1/1
2	C8E	E	401	-	-	0/9/9/18	0/0/0/0
2	C8E	E	402	-	-	0/12/12/18	0/0/0/0
3	NAG	E	403	3	-	0/6/26/26	0/1/1/1
3	NAG	E	404	3	-	0/6/23/26	0/1/1/1
3	NAG	E	405	3	-	0/6/23/26	0/1/1/1
3	NAG	E	406	3	-	0/6/23/26	0/1/1/1
3	NAG	E	407	3	-	0/6/23/26	0/1/1/1
3	NAG	E	408	3	-	0/6/23/26	0/1/1/1
2	C8E	F	401	-	-	0/14/14/18	0/0/0/0
3	NAG	F	402	3	-	0/6/26/26	0/1/1/1
3	NAG	F	403	3	-	0/6/23/26	0/1/1/1
3	NAG	F	404	3	-	0/6/23/26	0/1/1/1
3	NAG	F	405	3	-	0/6/23/26	0/1/1/1
3	NAG	F	406	3	-	0/6/23/26	0/1/1/1
3	NAG	F	407	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	407	NAG	C1-C2	2.22	1.55	1.52

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	406	NAG	C3-C4-C5	-4.25	102.73	110.22
3	D	408	NAG	O5-C1-C2	-3.81	106.17	111.47
3	A	410	NAG	C3-C4-C5	-3.47	104.10	110.22
3	C	406	NAG	C1-C2-N2	-3.38	104.71	110.49
3	B	403	NAG	C1-C2-C3	-3.36	105.96	110.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	C8E	1	0
3	A	410	NAG	3	0
3	A	411	NAG	3	0
3	B	406	NAG	3	0
3	B	407	NAG	2	0
3	C	402	NAG	1	0
3	C	403	NAG	1	0
3	C	405	NAG	4	0
3	C	406	NAG	2	0
3	D	404	NAG	1	0
3	D	405	NAG	1	0
3	D	406	NAG	1	0
3	D	407	NAG	3	0
3	D	408	NAG	2	0
3	E	406	NAG	1	0
3	E	407	NAG	1	0
3	F	405	NAG	2	0
3	F	406	NAG	3	0
3	F	407	NAG	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	332/352 (94%)	-0.46	2 (0%) 89 90	21, 30, 46, 82	0
1	B	332/352 (94%)	-0.53	1 (0%) 93 94	21, 30, 48, 85	0
1	C	332/352 (94%)	-0.52	2 (0%) 89 90	21, 32, 49, 75	0
1	D	332/352 (94%)	-0.59	1 (0%) 93 94	21, 30, 46, 81	0
1	E	332/352 (94%)	-0.51	4 (1%) 79 82	21, 32, 49, 84	0
1	F	332/352 (94%)	-0.46	1 (0%) 93 94	20, 29, 46, 86	0
All	All	1992/2112 (94%)	-0.52	11 (0%) 89 90	20, 31, 48, 86	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	TYR	2.5
1	E	11	TYR	2.4
1	E	162	ASP	2.4
1	A	10	GLU	2.4
1	C	194	LEU	2.3

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	B	408	14/15	0.63	0.28	37.13	67,87,89,91	0
3	NAG	E	408	14/15	0.57	0.33	32.10	75,91,93,94	0
3	NAG	A	412	14/15	0.50	0.29	19.78	67,80,85,86	0
2	C8E	D	403	11/21	0.84	0.23	11.74	49,55,65,66	0
3	NAG	C	405	14/15	0.85	0.16	10.00	62,67,75,77	0
2	C8E	A	403	14/21	0.91	0.16	8.18	35,44,65,69	0
3	NAG	B	406	14/15	0.91	0.18	7.48	69,75,83,89	0
2	C8E	A	404	9/21	0.92	0.17	6.88	57,59,66,69	0
3	NAG	D	407	14/15	0.84	0.14	6.58	65,70,79,80	0
3	NAG	F	405	14/15	0.86	0.14	5.56	68,72,77,83	0
3	NAG	E	406	14/15	0.87	0.15	5.02	70,75,81,83	0
2	C8E	A	401	12/21	0.92	0.11	4.35	42,50,55,56	0
3	NAG	E	404	14/15	0.91	0.16	3.79	46,54,69,71	0
2	C8E	D	402	13/21	0.83	0.13	3.48	56,59,66,66	0
2	C8E	A	406	21/21	0.88	0.18	3.41	45,56,62,62	0
2	C8E	C	401	21/21	0.74	0.21	3.39	51,59,64,66	0
3	NAG	C	403	14/15	0.87	0.13	3.31	45,51,62,62	0
3	NAG	A	410	14/15	0.86	0.14	2.95	60,64,72,74	0
2	C8E	D	401	14/21	0.87	0.12	2.85	40,44,52,53	0
3	NAG	D	406	14/15	0.85	0.10	2.57	41,48,59,61	0
3	NAG	E	405	14/15	0.90	0.12	2.46	43,51,63,65	0
2	C8E	F	401	17/21	0.90	0.14	2.26	40,46,50,53	0
3	NAG	C	404	14/15	0.90	0.10	2.22	42,52,58,60	0
3	NAG	B	405	14/15	0.91	0.11	2.18	40,50,59,63	0
2	C8E	E	401	12/21	0.93	0.11	2.16	38,43,60,65	0
3	NAG	D	405	14/15	0.89	0.11	2.10	42,48,60,61	0
2	C8E	B	401	13/21	0.90	0.14	2.10	53,56,74,75	0
3	NAG	B	404	14/15	0.91	0.11	2.09	43,50,61,63	0
2	C8E	E	402	15/21	0.86	0.12	1.98	43,47,57,60	0
2	C8E	B	402	12/21	0.84	0.14	1.69	61,64,69,73	0
3	NAG	A	409	14/15	0.92	0.11	1.42	38,47,55,60	0
3	NAG	F	404	14/15	0.92	0.10	1.37	35,47,55,62	0
3	NAG	F	403	14/15	0.92	0.10	1.04	42,48,58,58	0
4	NA	E	410	1/1	0.99	0.08	0.78	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	408	14/15	0.91	0.10	0.68	42,49,59,59	0
4	NA	D	413	1/1	0.99	0.08	0.32	29,29,29,29	0
4	NA	E	411	1/1	0.99	0.08	-0.53	27,27,27,27	0
4	NA	A	414	1/1	0.99	0.07	-0.79	28,28,28,28	0
4	NA	A	416	1/1	0.99	0.06	-1.39	24,24,24,24	0
4	NA	F	409	1/1	0.99	0.07	-1.82	29,29,29,29	0
4	NA	A	415	1/1	0.99	0.06	-1.84	30,30,30,30	0
4	NA	D	411	1/1	1.00	0.06	-2.08	29,29,29,29	0
4	NA	D	410	1/1	0.99	0.06	-2.87	25,25,25,25	0
4	NA	C	409	1/1	1.00	0.05	-3.52	31,31,31,31	0
4	NA	B	411	1/1	0.99	0.05	-3.61	27,27,27,27	0
4	NA	B	409	1/1	0.99	0.04	-3.67	29,29,29,29	0
4	NA	E	409	1/1	0.98	0.07	-	31,31,31,31	0
4	NA	A	413	1/1	0.98	0.07	-	26,26,26,26	0
3	NAG	D	409	14/15	0.55	0.28	-	77,83,87,87	0
2	C8E	A	402	9/21	0.79	0.15	-	56,61,64,66	0
3	NAG	A	407	15/15	0.74	0.24	-	59,73,79,81	0
3	NAG	F	407	14/15	0.67	0.24	-	66,80,83,84	0
3	NAG	B	407	14/15	0.84	0.22	-	78,84,90,91	0
4	NA	F	408	1/1	0.98	0.07	-	26,26,26,26	0
3	NAG	D	408	14/15	0.82	0.14	-	78,82,85,86	0
3	NAG	F	402	15/15	0.82	0.23	-	59,77,85,87	0
3	NAG	C	407	14/15	0.54	0.32	-	81,95,97,97	0
4	NA	B	410	1/1	0.96	0.06	-	31,31,31,31	0
4	NA	C	408	1/1	0.99	0.06	-	31,31,31,31	0
3	NAG	A	411	14/15	0.76	0.19	-	76,82,85,87	0
3	NAG	E	407	14/15	0.83	0.19	-	84,86,89,89	0
4	NA	D	412	1/1	0.99	0.06	-	30,30,30,30	0
2	C8E	A	405	8/21	0.92	0.14	-	52,53,61,64	0
3	NAG	B	403	15/15	0.73	0.26	-	58,77,79,80	0
3	NAG	D	404	15/15	0.70	0.20	-	54,74,78,79	0
3	NAG	F	406	14/15	0.69	0.22	-	82,86,89,95	0
3	NAG	E	403	15/15	0.61	0.32	-	65,78,82,85	0
3	NAG	C	402	15/15	0.69	0.27	-	60,79,84,84	0
3	NAG	C	406	14/15	0.80	0.17	-	82,85,92,94	0

## 6.5 Other polymers

There are no such residues in this entry.