



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2016 – 07:10 PM EDT

PDB ID : 5ISX  
Title : Structure of the holo PCP-E didomain of the gramicidin S synthetase A  
Authors : Chen, W.-H.; Li, K.; Bruner, S.D.  
Deposited on : 2016-03-15  
Resolution : 2.33 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

<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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027939

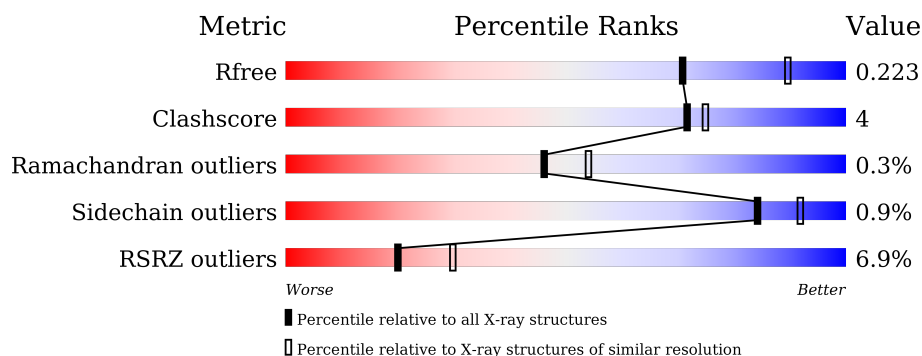
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	573	<div> <div>2%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	B	573	<div> <div>11%</div> <div>78%</div> <div>14%</div> <div>8%</div> </div>

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	PNS	B	1200	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9230 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 Gramicidin S synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4375	2808	731	823	13			
1	B	529	Total	C	N	O	S	0	0	0
			4375	2808	731	823	13			

There are 26 discrepancies between the modelled and reference sequences:

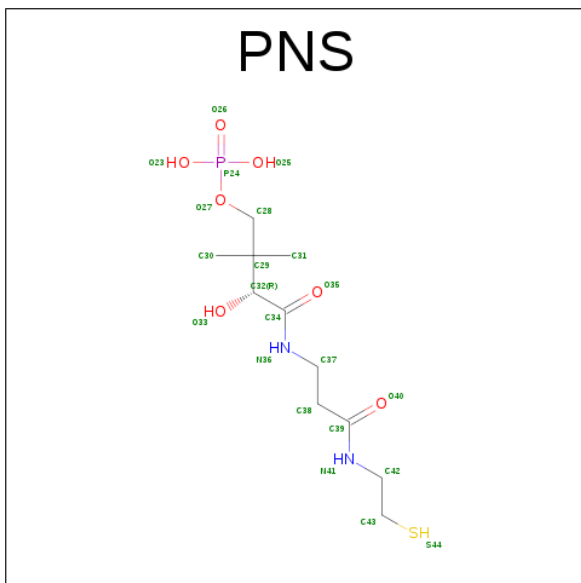
Chain	Residue	Modelled	Actual	Comment	Reference
A	537	MET	-	initiating methionine	UNP P0C062
A	1009	GLY	SER	conflict	UNP P0C062
A	1099	ASP	-	expression tag	UNP P0C062
A	1100	ASP	-	expression tag	UNP P0C062
A	1101	ASP	-	expression tag	UNP P0C062
A	1102	ASP	-	expression tag	UNP P0C062
A	1103	LYS	-	expression tag	UNP P0C062
A	1104	HIS	-	expression tag	UNP P0C062
A	1105	HIS	-	expression tag	UNP P0C062
A	1106	HIS	-	expression tag	UNP P0C062
A	1107	HIS	-	expression tag	UNP P0C062
A	1108	HIS	-	expression tag	UNP P0C062
A	1109	HIS	-	expression tag	UNP P0C062
B	537	MET	-	initiating methionine	UNP P0C062
B	1009	GLY	SER	conflict	UNP P0C062
B	1099	ASP	-	expression tag	UNP P0C062
B	1100	ASP	-	expression tag	UNP P0C062
B	1101	ASP	-	expression tag	UNP P0C062
B	1102	ASP	-	expression tag	UNP P0C062
B	1103	LYS	-	expression tag	UNP P0C062
B	1104	HIS	-	expression tag	UNP P0C062
B	1105	HIS	-	expression tag	UNP P0C062
B	1106	HIS	-	expression tag	UNP P0C062
B	1107	HIS	-	expression tag	UNP P0C062
B	1108	HIS	-	expression tag	UNP P0C062

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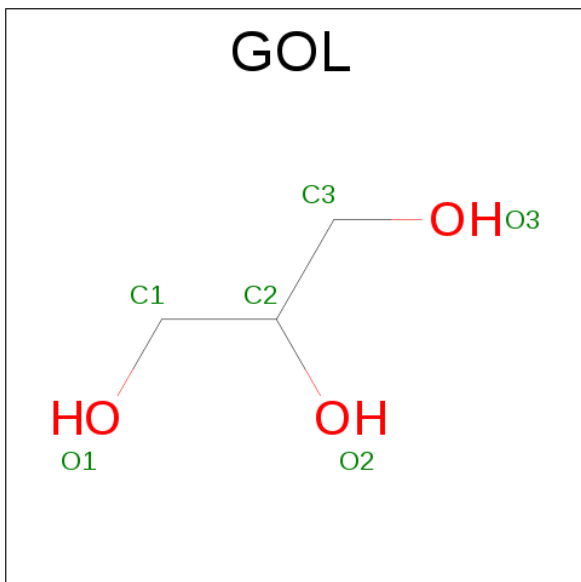
Chain	Residue	Modelled	Actual	Comment	Reference
B	1109	HIS	-	expression tag	UNP P0C062

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			22	11	2	7	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			22	11	2	7	1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

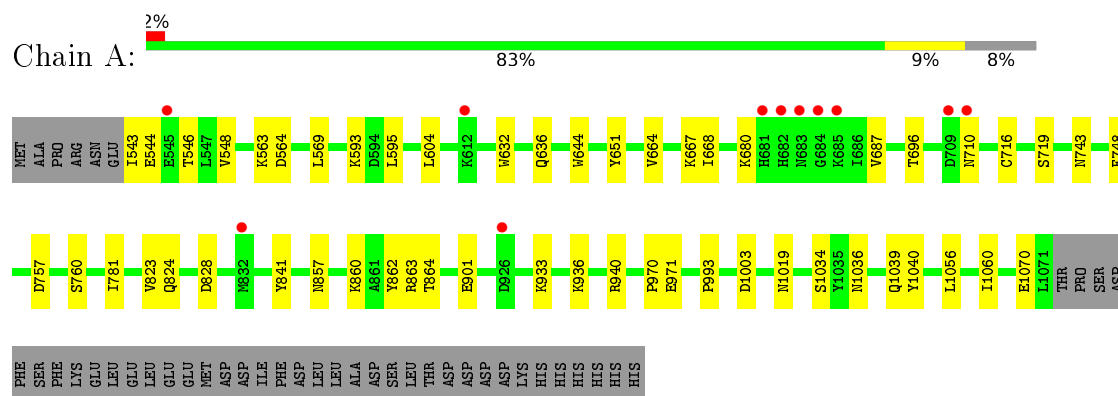
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	290	Total	O	0	0
			290	290		
4	B	140	Total	O	0	0
			140	140		

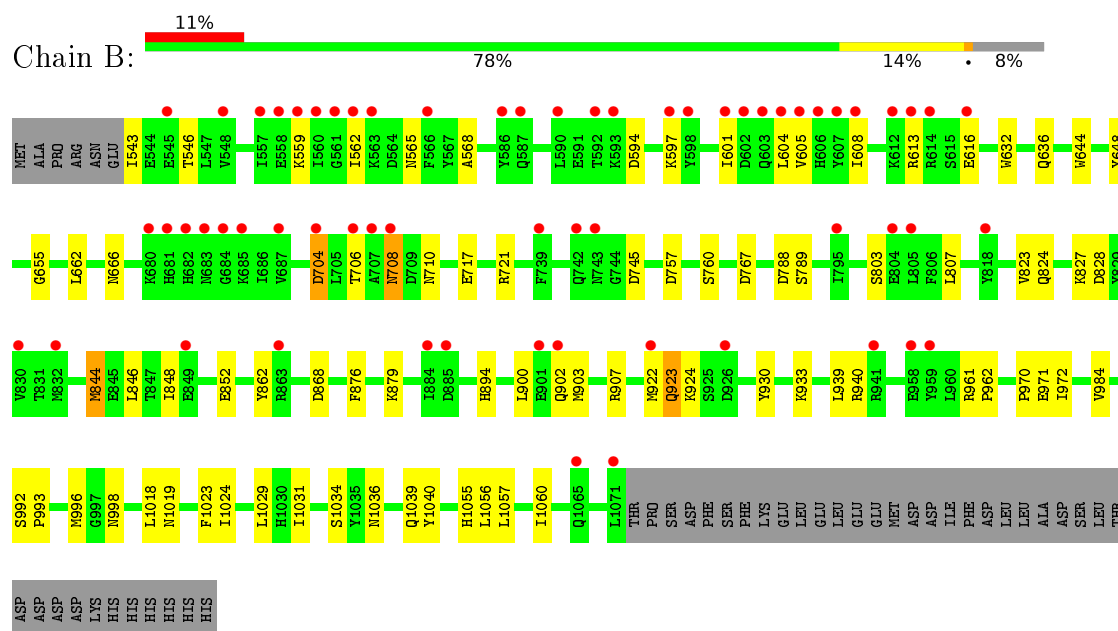
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Gramicidin S synthase 1



#### • Molecule 1: Gramicidin S synthase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.81Å 58.04Å 90.86Å 90.00° 100.64° 90.00°	Depositor
Resolution (Å)	38.97 – 2.33 38.97 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.97-2.33) 94.2 (38.97-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.187 , 0.225 0.186 , 0.223	Depositor DCC
$R_{free}$ test set	1914 reflections (4.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.8	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	0.94	EDS
Total number of atoms	9230	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 4.12% 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: GOL, PNS

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	0.28	0/4474	0.42	0/6052
1	B	0.27	0/4474	0.42	0/6052
All	All	0.27	0/8948	0.42	0/12104

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

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	4375	0	4297	30	1
1	B	4375	0	4297	46	0
2	A	22	0	21	0	0
2	B	22	0	21	1	0
3	A	6	0	8	0	0
4	A	290	0	0	1	0
4	B	140	0	0	0	0
All	All	9230	0	8644	75	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (75) 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:B:879:LYS:HD2	1:B:922:MET:HG2	1.68	0.74
1:A:841:TYR:CD2	1:A:1003:ASP:OD2	2.41	0.73
1:B:862:TYR:HD1	1:B:933:LYS:HE3	1.61	0.66
1:A:863:ARG:HD2	1:A:1070:GLU:CG	2.29	0.63
1:A:863:ARG:HD2	1:A:1070:GLU:HG2	1.82	0.62
1:B:846:LEU:HD22	1:B:1057:LEU:HD21	1.81	0.62
1:B:848:ILE:O	1:B:852:GLU:HG2	2.03	0.58
1:B:862:TYR:CD1	1:B:933:LYS:HE3	2.38	0.57
1:B:823:VAL:HG13	1:B:970:PRO:HA	1.87	0.57
1:A:543:ILE:HG23	1:A:546:THR:H	1.70	0.56
1:B:1019:ASN:HB3	1:B:1034:SER:HB2	1.89	0.55
1:A:862:TYR:HD1	1:A:933:LYS:HE3	1.71	0.55
1:A:993:PRO:O	1:B:710:ASN:ND2	2.36	0.55
1:B:704:ASP:OD2	1:B:704:ASP:N	2.37	0.55
1:B:828:ASP:HB2	1:B:1040:TYR:HA	1.88	0.54
1:A:823:VAL:HG13	1:A:970:PRO:HA	1.89	0.54
1:B:824:GLN:HG2	1:B:971:GLU:OE2	2.08	0.53
1:B:868:ASP:OD1	1:B:939:LEU:HD12	2.10	0.52
1:B:601:ILE:O	1:B:605:VAL:HG23	2.11	0.51
1:A:862:TYR:CD1	1:A:933:LYS:HE3	2.46	0.50
1:B:767:ASP:OD2	1:B:907:ARG:NH2	2.45	0.50
1:B:562:ILE:HA	1:B:601:ILE:HB	1.93	0.49
1:B:972:ILE:HG12	1:B:1018:LEU:HB2	1.94	0.49
1:A:667:LYS:HG3	1:A:781:ILE:HG21	1.95	0.49
1:B:998:ASN:HB2	1:B:1023:PHE:CE2	2.48	0.49
1:B:594:ASP:HA	1:B:597:LYS:NZ	2.28	0.49
1:B:1024:ILE:HD13	1:B:1029:LEU:HA	1.95	0.48
1:B:844:MET:HG3	1:B:1031:ILE:HB	1.95	0.48
1:A:1019:ASN:HB3	1:A:1034:SER:HB2	1.96	0.48
1:A:564:ASP:HB3	1:A:569:LEU:HD11	1.95	0.48
1:A:824:GLN:HG2	1:A:971:GLU:OE2	2.14	0.48
1:B:923:GLN:HG3	1:B:924:LYS:H	1.78	0.48
1:B:632:TRP:O	1:B:636:GLN:HG2	2.14	0.47
1:B:565:ASN:HB3	1:B:568:ALA:HB3	1.96	0.47
1:B:803:SER:O	1:B:807:LEU:HG	2.15	0.47
1:B:616:GLU:OE2	1:B:789:SER:HB3	2.15	0.47
1:A:595:LEU:HD13	1:A:604:LEU:HD22	1.95	0.47
1:A:936:LYS:O	1:A:940:ARG:HG2	2.15	0.46
1:B:613:ARG:HH22	1:B:788:ASP:CG	2.17	0.46
1:B:827:LYS:HA	1:B:1040:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:ARG:CZ	1:B:902:GLN:O	2.64	0.46
1:A:680:LYS:O	1:A:687:VAL:N	2.42	0.46
1:B:757:ASP:H	1:B:760:SER:HB2	1.80	0.46
1:B:1036:ASN:HB3	1:B:1039:GLN:HB2	1.98	0.45
1:B:924:LYS:HB2	1:B:930:TYR:CD2	2.52	0.45
1:B:662:LEU:O	1:B:666:ASN:ND2	2.47	0.45
1:B:1056:LEU:O	1:B:1060:ILE:HG13	2.17	0.45
1:B:648:TYR:OH	1:B:984:VAL:HG11	2.17	0.44
1:B:900:LEU:HB2	1:B:903:MET:HB2	1.98	0.44
1:B:961:ARG:HA	1:B:962:PRO:HD3	1.83	0.44
1:A:862:TYR:HB2	1:A:864:THR:HG23	1.99	0.44
1:A:863:ARG:HD2	1:A:1070:GLU:HB3	2.00	0.44
1:A:719:SER:HB2	1:A:748:PHE:CZ	2.53	0.43
1:A:857:ASN:OD1	1:A:860:LYS:HE3	2.17	0.43
1:B:940:ARG:HG3	1:B:940:ARG:HH11	1.83	0.43
1:B:767:ASP:CG	1:B:907:ARG:HH22	2.22	0.43
1:A:716:CYS:HB3	4:A:1553:HOH:O	2.18	0.43
1:B:876:PHE:HB3	1:B:1055:HIS:CE1	2.54	0.43
1:A:841:TYR:HD2	1:A:1003:ASP:OD2	2.00	0.43
1:B:992:SER:HA	1:B:993:PRO:HD3	1.90	0.42
1:A:828:ASP:HB2	1:A:1040:TYR:HA	2.00	0.42
1:B:559:LYS:HA	1:B:559:LYS:HD3	1.84	0.42
1:A:1056:LEU:O	1:A:1060:ILE:HG13	2.20	0.42
1:B:604:LEU:O	1:B:608:ILE:HG12	2.20	0.42
1:B:717:GLU:HB3	1:B:721:ARG:HH12	1.85	0.42
1:A:757:ASP:H	1:A:760:SER:HB2	1.84	0.42
1:A:632:TRP:O	1:A:636:GLN:HG2	2.20	0.42
1:A:544:GLU:O	1:A:548:VAL:HG23	2.19	0.42
1:B:655:GLY:HA2	1:B:745:ASP:HB2	2.01	0.41
1:A:1036:ASN:HB3	1:A:1039:GLN:HB2	2.01	0.41
1:A:664:VAL:O	1:A:668:ILE:HG12	2.21	0.41
1:B:894:HIS:N	2:B:1200:PNS:H372	2.36	0.41
1:A:710:ASN:N	1:A:710:ASN:OD1	2.54	0.40
1:B:543:ILE:HG23	1:B:546:THR:H	1.86	0.40
1:A:651:TYR:OH	1:A:743:ASN:O	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:THR:OG1	1:A:1070:GLU:OE1[1_565]	1.88	0.32

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	527/573 (92%)	516 (98%)	10 (2%)	1 (0%)	52	61
1	B	527/573 (92%)	512 (97%)	13 (2%)	2 (0%)	39	45
All	All	1054/1146 (92%)	1028 (98%)	23 (2%)	3 (0%)	46	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	901	GLU
1	B	706	THR
1	B	708	ASN

### 5.3.2 Protein sidechains

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	478/521 (92%)	475 (99%)	3 (1%)	90	96
1	B	478/521 (92%)	472 (99%)	6 (1%)	76	86
All	All	956/1042 (92%)	947 (99%)	9 (1%)	84	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	LYS
1	A	593	LYS
1	A	644	TRP

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Mol	Chain	Res	Type
1	B	644	TRP
1	B	704	ASP
1	B	708	ASN
1	B	844	MET
1	B	923	GLN
1	B	996	MET

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

### 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](#)

3 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	PNS	A	1200	1	18,21,21	1.95	2 (11%)	22,29,29	1.63	6 (27%)
3	GOL	A	1201	-	5,5,5	0.35	0	5,5,5	0.23	0
2	PNS	B	1200	1	18,21,21	1.98	2 (11%)	22,29,29	1.89	5 (22%)

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	PNS	A	1200	1	-	0/27/27/27	0/0/0/0
3	GOL	A	1201	-	-	0/4/4/4	0/0/0/0
2	PNS	B	1200	1	-	0/27/27/27	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	PNS	C39-N41	4.60	1.44	1.33
2	B	1200	PNS	C39-N41	4.72	1.44	1.33
2	B	1200	PNS	C34-N36	6.09	1.46	1.33
2	A	1200	PNS	C34-N36	6.24	1.46	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	PNS	C37-C38-C39	-3.46	106.29	112.22
2	B	1200	PNS	O40-C39-C38	-3.02	116.73	121.97
2	B	1200	PNS	C37-N36-C34	-2.73	117.14	122.62
2	B	1200	PNS	C42-N41-C39	-2.67	117.49	122.79
2	A	1200	PNS	C42-N41-C39	-2.50	117.83	122.79
2	A	1200	PNS	C37-C38-C39	-2.45	108.02	112.22
2	A	1200	PNS	O40-C39-C38	-2.44	117.73	121.97
2	A	1200	PNS	C37-N36-C34	-2.37	117.87	122.62
2	A	1200	PNS	C32-C34-N36	2.44	122.07	116.31
2	A	1200	PNS	C38-C39-N41	3.67	122.84	116.46
2	B	1200	PNS	C38-C39-N41	4.39	124.08	116.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1200	PNS	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	529/573 (92%)	0.09	11 (2%) 67 78	14, 27, 48, 77	0
1	B	529/573 (92%)	0.69	62 (11%) 6 10	18, 40, 69, 83	0
All	All	1058/1146 (92%)	0.39	73 (6%) 20 30	14, 33, 64, 83	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	832	MET	6.6
1	B	683	ASN	5.3
1	A	683	ASN	5.3
1	B	707	ALA	5.1
1	B	681	HIS	4.7
1	B	684	GLY	4.6
1	B	608	ILE	4.5
1	B	563	LYS	4.4
1	B	560	ILE	4.2
1	B	601	ILE	4.2
1	B	607	TYR	4.1
1	B	884	ILE	4.1
1	B	559	LYS	4.0
1	B	598	TYR	3.9
1	B	706	THR	3.9
1	A	682	HIS	3.9
1	B	557	ILE	3.8
1	B	605	VAL	3.8
1	B	597	LYS	3.8
1	B	602	ASP	3.7
1	B	804	GLU	3.7
1	B	959	TYR	3.7
1	B	742	GLN	3.6
1	B	612	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	681	HIS	3.6
1	B	1071	LEU	3.6
1	B	558	GLU	3.5
1	B	926	ASP	3.5
1	B	805	LEU	3.5
1	B	587	GLN	3.3
1	B	885	ASP	3.3
1	B	941	ARG	3.2
1	B	901	GLU	3.2
1	B	590	LEU	3.2
1	B	613	ARG	3.1
1	B	593	LYS	3.1
1	B	562	ILE	3.1
1	B	685	LYS	3.1
1	B	603	GLN	3.0
1	B	682	HIS	2.9
1	B	849	GLU	2.9
1	B	743	ASN	2.8
1	A	685	LYS	2.8
1	B	795	ILE	2.7
1	A	710	ASN	2.7
1	B	902	GLN	2.6
1	B	545	GLU	2.6
1	B	604	LEU	2.6
1	B	958	GLU	2.6
1	A	709	ASP	2.6
1	B	614	ARG	2.5
1	B	922	MET	2.5
1	B	606	HIS	2.4
1	B	616	GLU	2.4
1	B	586	TYR	2.4
1	A	832	MET	2.4
1	B	548	VAL	2.4
1	A	684	GLY	2.3
1	B	830	VAL	2.3
1	B	818	TYR	2.3
1	B	708	ASN	2.3
1	B	863	ARG	2.2
1	B	739	PHE	2.2
1	B	704	ASP	2.2
1	B	561	GLY	2.2
1	B	592	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1065	GLN	2.1
1	B	687	VAL	2.1
1	A	926	ASP	2.0
1	B	566	PHE	2.0
1	B	680	LYS	2.0
1	A	545	GLU	2.0
1	A	612	LYS	2.0

## 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. 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( $\text{\AA}^2$ )	Q<0.9
2	PNS	B	1200	22/22	0.92	0.25	2.76	24,32,42,58	0
2	PNS	A	1200	22/22	0.96	0.21	1.31	15,22,31,55	0
3	GOL	A	1201	6/6	0.80	0.24	-	21,41,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.