



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 08:08 AM GMT

PDB ID : 6YRO  
Title : Streptococcus suis SadP mutant - N285D  
Authors : Papageorgiou, A.C.; Haataja, S.  
Deposited on : 2020-04-20  
Resolution : 2.05 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 : 2.17.1.dev1  
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) : 2.17.1.dev1

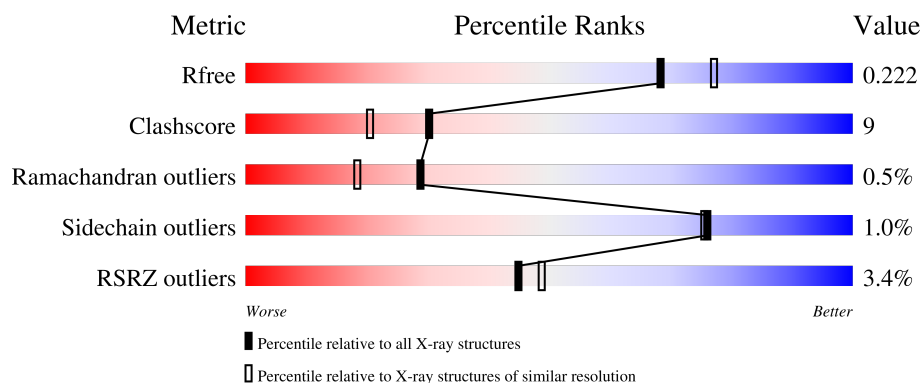
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 of 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	223	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	223	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div></div> <div>9%</div> </div> </div>
1	C	223	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	223	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	223	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div></div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9198 atoms, of which 56 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 SadP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	204	Total	C	N	O	S	0	1	0
			1643	1030	278	334	1			
1	A	204	Total	C	N	O	S	0	0	0
			1635	1025	275	334	1			
1	B	204	Total	C	N	O	S	0	0	0
			1635	1025	275	334	1			
1	C	204	Total	C	N	O	S	0	1	0
			1643	1030	278	334	1			
1	E	204	Total	C	N	O	S	0	0	0
			1635	1025	275	334	1			

There are 95 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	121	MET	-	initiating methionine	UNP G5DSS1
D	122	HIS	-	expression tag	UNP G5DSS1
D	123	HIS	-	expression tag	UNP G5DSS1
D	124	HIS	-	expression tag	UNP G5DSS1
D	125	HIS	-	expression tag	UNP G5DSS1
D	126	HIS	-	expression tag	UNP G5DSS1
D	127	HIS	-	expression tag	UNP G5DSS1
D	128	SER	-	expression tag	UNP G5DSS1
D	129	SER	-	expression tag	UNP G5DSS1
D	130	GLY	-	expression tag	UNP G5DSS1
D	131	LEU	-	expression tag	UNP G5DSS1
D	132	VAL	-	expression tag	UNP G5DSS1
D	133	PRO	-	expression tag	UNP G5DSS1
D	134	ARG	-	expression tag	UNP G5DSS1
D	135	GLY	-	expression tag	UNP G5DSS1
D	136	SER	-	expression tag	UNP G5DSS1
D	137	HIS	-	expression tag	UNP G5DSS1
D	138	MET	-	expression tag	UNP G5DSS1
D	285	ASP	ASN	conflict	UNP G5DSS1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	initiating methionine	UNP G5DSS1
A	122	HIS	-	expression tag	UNP G5DSS1
A	123	HIS	-	expression tag	UNP G5DSS1
A	124	HIS	-	expression tag	UNP G5DSS1
A	125	HIS	-	expression tag	UNP G5DSS1
A	126	HIS	-	expression tag	UNP G5DSS1
A	127	HIS	-	expression tag	UNP G5DSS1
A	128	SER	-	expression tag	UNP G5DSS1
A	129	SER	-	expression tag	UNP G5DSS1
A	130	GLY	-	expression tag	UNP G5DSS1
A	131	LEU	-	expression tag	UNP G5DSS1
A	132	VAL	-	expression tag	UNP G5DSS1
A	133	PRO	-	expression tag	UNP G5DSS1
A	134	ARG	-	expression tag	UNP G5DSS1
A	135	GLY	-	expression tag	UNP G5DSS1
A	136	SER	-	expression tag	UNP G5DSS1
A	137	HIS	-	expression tag	UNP G5DSS1
A	138	MET	-	expression tag	UNP G5DSS1
A	285	ASP	ASN	conflict	UNP G5DSS1
B	121	MET	-	initiating methionine	UNP G5DSS1
B	122	HIS	-	expression tag	UNP G5DSS1
B	123	HIS	-	expression tag	UNP G5DSS1
B	124	HIS	-	expression tag	UNP G5DSS1
B	125	HIS	-	expression tag	UNP G5DSS1
B	126	HIS	-	expression tag	UNP G5DSS1
B	127	HIS	-	expression tag	UNP G5DSS1
B	128	SER	-	expression tag	UNP G5DSS1
B	129	SER	-	expression tag	UNP G5DSS1
B	130	GLY	-	expression tag	UNP G5DSS1
B	131	LEU	-	expression tag	UNP G5DSS1
B	132	VAL	-	expression tag	UNP G5DSS1
B	133	PRO	-	expression tag	UNP G5DSS1
B	134	ARG	-	expression tag	UNP G5DSS1
B	135	GLY	-	expression tag	UNP G5DSS1
B	136	SER	-	expression tag	UNP G5DSS1
B	137	HIS	-	expression tag	UNP G5DSS1
B	138	MET	-	expression tag	UNP G5DSS1
B	285	ASP	ASN	conflict	UNP G5DSS1
C	121	MET	-	initiating methionine	UNP G5DSS1
C	122	HIS	-	expression tag	UNP G5DSS1
C	123	HIS	-	expression tag	UNP G5DSS1
C	124	HIS	-	expression tag	UNP G5DSS1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	125	HIS	-	expression tag	UNP G5DSS1
C	126	HIS	-	expression tag	UNP G5DSS1
C	127	HIS	-	expression tag	UNP G5DSS1
C	128	SER	-	expression tag	UNP G5DSS1
C	129	SER	-	expression tag	UNP G5DSS1
C	130	GLY	-	expression tag	UNP G5DSS1
C	131	LEU	-	expression tag	UNP G5DSS1
C	132	VAL	-	expression tag	UNP G5DSS1
C	133	PRO	-	expression tag	UNP G5DSS1
C	134	ARG	-	expression tag	UNP G5DSS1
C	135	GLY	-	expression tag	UNP G5DSS1
C	136	SER	-	expression tag	UNP G5DSS1
C	137	HIS	-	expression tag	UNP G5DSS1
C	138	MET	-	expression tag	UNP G5DSS1
C	285	ASP	ASN	conflict	UNP G5DSS1
E	121	MET	-	initiating methionine	UNP G5DSS1
E	122	HIS	-	expression tag	UNP G5DSS1
E	123	HIS	-	expression tag	UNP G5DSS1
E	124	HIS	-	expression tag	UNP G5DSS1
E	125	HIS	-	expression tag	UNP G5DSS1
E	126	HIS	-	expression tag	UNP G5DSS1
E	127	HIS	-	expression tag	UNP G5DSS1
E	128	SER	-	expression tag	UNP G5DSS1
E	129	SER	-	expression tag	UNP G5DSS1
E	130	GLY	-	expression tag	UNP G5DSS1
E	131	LEU	-	expression tag	UNP G5DSS1
E	132	VAL	-	expression tag	UNP G5DSS1
E	133	PRO	-	expression tag	UNP G5DSS1
E	134	ARG	-	expression tag	UNP G5DSS1
E	135	GLY	-	expression tag	UNP G5DSS1
E	136	SER	-	expression tag	UNP G5DSS1
E	137	HIS	-	expression tag	UNP G5DSS1
E	138	MET	-	expression tag	UNP G5DSS1
E	285	ASP	ASN	conflict	UNP G5DSS1

- Molecule 2 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
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

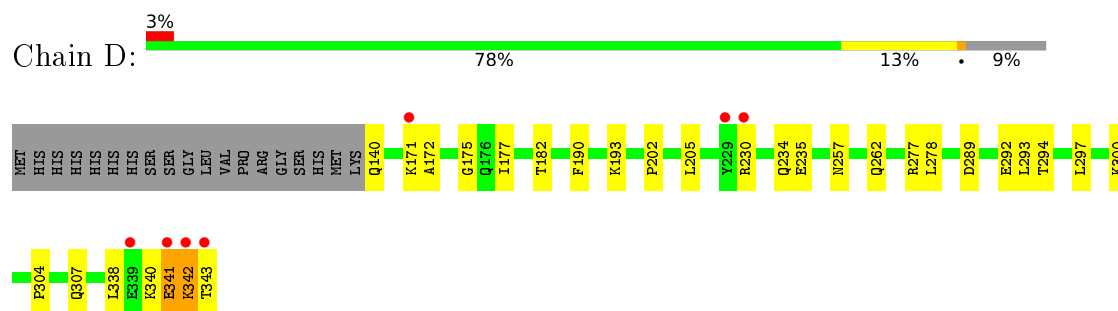
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	181	Total 181	O 181	0	0
4	A	197	Total 197	O 197	0	0
4	B	195	Total 195	O 195	0	0
4	C	185	Total 185	O 185	0	0
4	E	148	Total 148	O 148	0	0

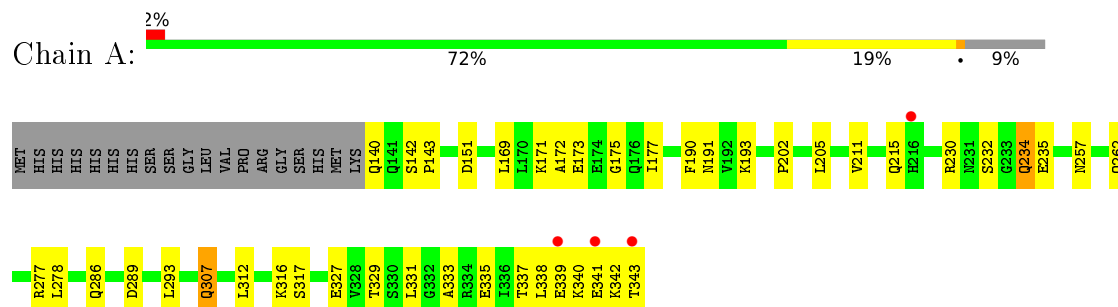
### 3 Residue-property plots [i](#)

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.

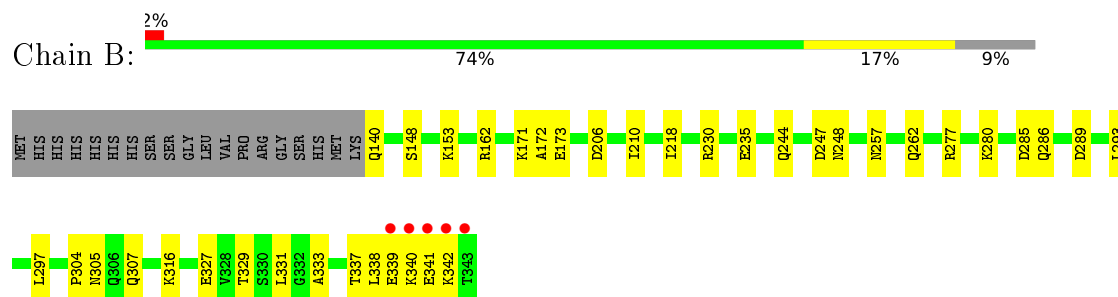
- Molecule 1: SadP



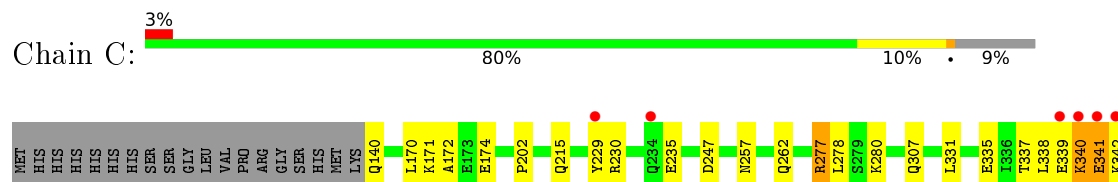
- Molecule 1: SadP



- Molecule 1: SadP



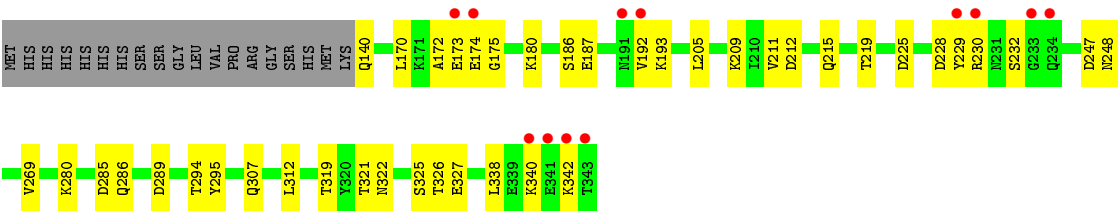
- Molecule 1: SadP





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● Molecule 1: SadP



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.13Å 80.80Å 130.74Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	45.68 – 2.05 45.68 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.8 (45.68-2.05) 86.5 (45.68-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.174 , 0.222 0.174 , 0.222	Depositor DCC
$R_{free}$ test set	1712 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9198	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 4.88% 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, GOL

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	0.41	0/1669	0.57	0/2261
1	B	0.42	0/1669	0.58	0/2261
1	C	0.42	0/1680	0.59	1/2275 (0.0%)
1	D	0.48	1/1680 (0.1%)	0.67	3/2275 (0.1%)
1	E	0.36	0/1669	0.53	0/2261
All	All	0.42	1/8367 (0.0%)	0.59	4/11333 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	171	LYS	CD-CE	-5.11	1.38	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	LYS	CD-CE-NZ	-10.96	86.50	111.70
1	D	171	LYS	CG-CD-CE	-6.85	91.34	111.90
1	C	215	GLN	CB-CA-C	5.30	121.00	110.40
1	D	171	LYS	CB-CA-C	-5.16	100.09	110.40

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	1635	0	1573	29	0
1	B	1635	0	1573	28	1
1	C	1643	0	1586	38	0
1	D	1643	0	1586	25	1
1	E	1635	0	1573	34	0
2	A	12	16	15	0	0
2	B	12	16	16	1	0
2	C	6	8	8	0	0
2	D	12	16	15	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	197	0	0	3	0
4	B	195	0	0	5	0
4	C	185	0	0	8	1
4	D	181	0	0	3	0
4	E	148	0	0	7	1
All	All	9142	56	7945	151	2

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 9.

All (151) 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:140:GLN:N	4:A:801:HOH:O	1.73	1.20
1:E:340:LYS:HE2	4:E:503:HOH:O	1.44	1.11
1:E:280:LYS:HD3	4:E:583:HOH:O	1.55	1.05
1:E:289:ASP:OD2	4:E:501:HOH:O	1.75	1.03
1:C:343:THR:OXT	4:C:901:HOH:O	1.78	1.00
1:D:342:LYS:O	1:D:343:THR:HG23	1.64	0.96
1:D:304:PRO:O	1:D:340:LYS:HE2	1.67	0.94
1:C:277[A]:ARG:HH11	1:C:277[A]:ARG:HG2	1.29	0.92
1:D:172:ALA:HB1	1:D:338:LEU:HD11	1.50	0.89
1:C:140:GLN:N	4:C:903:HOH:O	2.05	0.88
1:E:321:THR:HG21	1:E:325:SER:HA	1.54	0.88
1:E:186:SER:O	4:E:502:HOH:O	1.91	0.88
1:D:292:GLU:OE1	1:D:294:THR:OG1	1.94	0.85
1:B:172:ALA:HB1	1:B:338:LEU:HD13	1.61	0.81
1:A:341:GLU:O	1:A:343:THR:N	2.15	0.79
1:B:277:ARG:HG2	1:B:277:ARG:HH11	1.48	0.79
1:C:335:GLU:OE1	4:C:902:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HE3	1:A:173:GLU:CD	2.05	0.77
1:E:140:GLN:N	4:E:504:HOH:O	2.17	0.77
1:C:174:GLU:H	1:C:340:LYS:HZ1	1.31	0.76
1:A:230:ARG:O	1:A:235:GLU:HG3	1.87	0.75
1:C:174:GLU:HG2	1:C:340:LYS:HE3	1.70	0.73
1:C:257:ASN:ND2	4:C:904:HOH:O	2.18	0.72
1:D:304:PRO:O	1:D:340:LYS:CE	2.37	0.71
1:C:277[A]:ARG:HG2	1:C:277[A]:ARG:NH1	2.05	0.71
1:E:321:THR:CG2	1:E:325:SER:HA	2.20	0.70
1:A:175:GLY:H	1:A:340:LYS:NZ	1.90	0.69
1:D:230:ARG:O	1:D:235:GLU:HG3	1.94	0.68
1:D:235:GLU:OE2	4:D:801:HOH:O	2.12	0.68
1:A:175:GLY:H	1:A:340:LYS:HZ2	1.43	0.66
1:A:338:LEU:O	1:A:340:LYS:N	2.28	0.66
1:D:172:ALA:CB	1:D:338:LEU:HD11	2.24	0.65
1:C:174:GLU:H	1:C:340:LYS:NZ	1.95	0.64
1:D:289:ASP:CG	1:D:293:LEU:HD21	2.19	0.63
1:C:174:GLU:OE2	1:C:343:THR:HB	1.99	0.63
1:A:338:LEU:HD23	1:A:340:LYS:NZ	2.14	0.62
1:E:173:GLU:O	1:E:174:GLU:HG2	2.00	0.62
1:C:340:LYS:O	1:C:341:GLU:HB2	1.99	0.62
1:E:205:LEU:O	1:E:280:LYS:NZ	2.34	0.60
1:A:277:ARG:NH2	1:A:335:GLU:OE2	2.34	0.60
1:B:304:PRO:O	1:B:340:LYS:HE2	2.01	0.59
1:C:229:TYR:CD2	1:E:230:ARG:HD2	2.37	0.59
1:C:230:ARG:O	1:C:235:GLU:HG3	2.02	0.59
1:A:289:ASP:CG	1:A:293:LEU:HD21	2.23	0.59
1:C:339:GLU:O	1:C:340:LYS:HG3	2.03	0.59
1:C:172:ALA:HB1	1:C:338:LEU:HD23	1.85	0.59
1:C:174:GLU:H	1:C:340:LYS:CE	2.16	0.58
1:E:211:VAL:CG1	1:E:215:GLN:HA	2.33	0.58
1:C:174:GLU:CD	1:C:343:THR:HB	2.24	0.58
1:E:228:ASP:OD2	1:E:229:TYR:N	2.37	0.57
1:C:340:LYS:HB2	1:C:340:LYS:HZ3	1.70	0.57
1:E:342:LYS:O	1:E:342:LYS:HG2	2.05	0.57
1:C:257:ASN:O	1:C:262:GLN:HG3	2.05	0.57
1:E:193:LYS:HG3	1:E:319:THR:HG21	1.85	0.57
1:B:230:ARG:O	1:B:235:GLU:HG3	2.05	0.56
1:E:321:THR:HG22	1:E:322:ASN:O	2.05	0.56
1:D:341:GLU:CD	1:D:342:LYS:H	2.09	0.56
1:D:342:LYS:O	1:D:343:THR:CG2	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLN:NE2	4:A:804:HOH:O	2.35	0.56
1:C:342:LYS:O	1:C:342:LYS:HG3	2.06	0.56
1:C:202:PRO:HA	1:C:278:LEU:HA	1.88	0.56
1:D:175:GLY:O	1:D:300:LYS:HD2	2.06	0.55
1:E:269:VAL:HG13	1:E:312:LEU:HD21	1.88	0.55
1:B:257:ASN:O	1:B:262:GLN:HG3	2.07	0.55
1:A:171:LYS:HE3	1:A:173:GLU:CG	2.37	0.55
1:E:192:VAL:O	1:E:193:LYS:HD3	2.06	0.55
1:E:247:ASP:O	1:E:248:ASN:HB2	2.07	0.54
1:C:171:LYS:HD3	4:C:968:HOH:O	2.07	0.54
1:D:257:ASN:O	1:D:262:GLN:HG3	2.07	0.53
1:E:187:GLU:HG2	4:E:569:HOH:O	2.08	0.53
1:D:277[A]:ARG:HH11	1:D:277[A]:ARG:HG2	1.75	0.52
1:E:170:LEU:HD21	1:E:180:LYS:HE3	1.92	0.52
1:D:177:ILE:HD12	1:D:205:LEU:HD21	1.91	0.51
1:A:232:SER:OG	1:A:234:GLN:HG3	2.11	0.51
1:C:174:GLU:H	1:C:340:LYS:HE3	1.77	0.50
1:D:307:GLN:OE1	1:D:340:LYS:HD2	2.12	0.50
1:A:331:LEU:HD12	1:A:331:LEU:C	2.32	0.50
1:E:175:GLY:N	4:E:503:HOH:O	2.11	0.50
1:D:202:PRO:HA	1:D:278:LEU:HA	1.95	0.49
1:C:340:LYS:HE2	1:C:343:THR:HG22	1.94	0.49
1:C:170:LEU:O	1:C:171:LYS:HE3	2.13	0.49
1:A:177:ILE:HD12	1:A:205:LEU:HD21	1.96	0.48
1:B:327:GLU:OE2	2:B:702:GOL:O2	2.32	0.48
1:C:170:LEU:O	1:C:171:LYS:CE	2.61	0.48
1:C:247:ASP:OD1	4:C:905:HOH:O	2.20	0.47
1:C:229:TYR:CE2	1:E:230:ARG:HD2	2.50	0.47
1:D:177:ILE:HD11	1:D:338:LEU:HD21	1.97	0.47
1:E:180:LYS:HG3	1:E:294:THR:HG23	1.96	0.47
1:A:316:LYS:HB3	1:A:329:THR:HG23	1.95	0.47
1:C:307:GLN:O	1:C:337:THR:HA	2.15	0.47
1:E:321:THR:CG2	1:E:325:SER:CA	2.91	0.47
1:B:277:ARG:CD	4:B:902:HOH:O	2.63	0.47
1:C:174:GLU:N	1:C:340:LYS:HE3	2.30	0.47
1:E:172:ALA:O	1:E:173:GLU:HB3	2.14	0.47
1:A:257:ASN:O	1:A:262:GLN:HG3	2.15	0.47
1:B:140:GLN:N	4:B:805:HOH:O	2.47	0.47
1:C:280:LYS:HD3	4:C:920:HOH:O	2.14	0.46
1:D:297:LEU:HD12	1:D:297:LEU:N	2.30	0.46
1:C:331:LEU:C	1:C:331:LEU:HD12	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:THR:HG23	1:E:326:THR:N	2.30	0.46
1:B:148:SER:HB3	1:B:162:ARG:HA	1.97	0.46
1:E:285:ASP:OD1	1:E:286:GLN:N	2.46	0.46
1:B:297:LEU:HD12	1:B:297:LEU:N	2.30	0.46
1:A:307:GLN:O	1:A:337:THR:HA	2.16	0.45
1:B:277:ARG:HG2	1:B:277:ARG:NH1	2.22	0.45
1:B:339:GLU:O	1:B:340:LYS:HG3	2.17	0.45
1:D:342:LYS:O	1:D:342:LYS:HG2	2.16	0.45
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.82	0.45
1:B:341:GLU:O	1:B:342:LYS:HG3	2.16	0.45
1:E:327:GLU:H	1:E:327:GLU:HG3	1.56	0.45
1:D:341:GLU:CG	1:D:342:LYS:H	2.29	0.45
1:B:172:ALA:O	1:B:173:GLU:HB3	2.17	0.45
1:C:277[A]:ARG:NH1	1:C:277[A]:ARG:CG	2.75	0.45
1:B:340:LYS:NZ	1:B:340:LYS:HB2	2.32	0.44
1:B:210:ILE:HG23	1:B:218:ILE:HG13	1.98	0.44
1:C:343:THR:HG21	4:C:1026:HOH:O	2.16	0.43
1:A:338:LEU:HD23	1:A:340:LYS:HZ3	1.82	0.43
1:D:341:GLU:CG	1:D:342:LYS:N	2.81	0.43
1:C:174:GLU:N	1:C:340:LYS:HZ1	2.08	0.43
1:A:202:PRO:HA	1:A:278:LEU:HA	2.00	0.43
1:B:305:ASN:O	1:B:307:GLN:NE2	2.51	0.43
1:E:225:ASP:C	1:E:225:ASP:OD1	2.57	0.43
1:A:190:PHE:HA	1:A:193:LYS:O	2.19	0.43
1:C:229:TYR:CG	1:E:230:ARG:HD2	2.54	0.43
1:A:177:ILE:HG12	1:A:338:LEU:HD11	2.01	0.42
1:B:247:ASP:O	1:B:248:ASN:HB2	2.19	0.42
4:D:935:HOH:O	1:A:191:ASN:HB2	2.18	0.42
1:A:169:LEU:HD11	1:A:172:ALA:HB2	2.01	0.42
1:A:211:VAL:CG1	1:A:215:GLN:HA	2.50	0.42
1:E:321:THR:HG21	1:E:325:SER:CA	2.39	0.42
1:D:190:PHE:HA	1:D:193:LYS:O	2.20	0.42
1:B:280:LYS:HE2	1:B:280:LYS:HB2	1.81	0.41
1:E:174:GLU:O	1:E:174:GLU:CG	2.68	0.41
1:E:212:ASP:HA	1:E:295:TYR:CD2	2.55	0.41
1:B:289:ASP:CG	1:B:293:LEU:HD21	2.40	0.41
1:E:209:LYS:HA	1:E:219:THR:OG1	2.20	0.41
1:B:247:ASP:HB3	4:B:847:HOH:O	2.20	0.41
1:C:171:LYS:HE2	1:C:171:LYS:HA	2.03	0.41
1:D:140:GLN:N	4:D:808:HOH:O	2.53	0.41
1:A:151:ASP:HB2	4:A:873:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:THR:HG23	4:B:859:HOH:O	2.20	0.41
1:B:277:ARG:NH1	1:B:277:ARG:CG	2.82	0.41
1:B:153:LYS:NZ	4:B:812:HOH:O	2.53	0.41
1:B:316:LYS:HB3	1:B:329:THR:HG23	2.02	0.41
1:B:331:LEU:HD21	1:B:333:ALA:HB2	2.03	0.41
1:A:312:LEU:HD13	1:A:333:ALA:HB2	2.03	0.40
1:C:342:LYS:O	1:C:343:THR:C	2.60	0.40
1:A:142:SER:HB2	1:A:143:PRO:CD	2.51	0.40
1:B:285:ASP:OD1	1:B:286:GLN:N	2.52	0.40
1:D:182:THR:HG23	1:D:292:GLU:HG2	2.04	0.40
1:A:317:SER:O	1:A:327:GLU:HB3	2.21	0.40

All (2) 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:D:342:LYS:NZ	1:B:244:GLN:O[2_555]	1.08	1.12
4:C:1008:HOH:O	4:E:553:HOH:O[3_455]	1.66	0.54

## 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	202/223 (91%)	190 (94%)	10 (5%)	2 (1%)	15	6
1	B	202/223 (91%)	192 (95%)	10 (5%)	0	100	100
1	C	203/223 (91%)	192 (95%)	9 (4%)	2 (1%)	15	6
1	D	203/223 (91%)	194 (96%)	8 (4%)	1 (0%)	29	18
1	E	202/223 (91%)	186 (92%)	16 (8%)	0	100	100
All	All	1012/1115 (91%)	954 (94%)	53 (5%)	5 (0%)	29	18



All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	LYS
1	A	339	GLU
1	C	341	GLU
1	D	341	GLU
1	C	340	LYS

### 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	185/202 (92%)	183 (99%)	2 (1%)	73	73
1	B	185/202 (92%)	183 (99%)	2 (1%)	73	73
1	C	186/202 (92%)	184 (99%)	2 (1%)	73	73
1	D	186/202 (92%)	185 (100%)	1 (0%)	88	89
1	E	185/202 (92%)	182 (98%)	3 (2%)	62	59
All	All	927/1010 (92%)	917 (99%)	10 (1%)	76	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	234	GLN
1	A	234	GLN
1	A	307	GLN
1	B	171	LYS
1	B	206	ASP
1	C	277[A]	ARG
1	C	277[B]	ARG
1	E	232	SER
1	E	307	GLN
1	E	338	LEU

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

Mol	Chain	Res	Type
1	B	255	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 ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	GOL	B	701	-	5,5,5	0.95	0	5,5,5	0.89	0
2	GOL	D	701	-	5,5,5	1.16	1 (20%)	5,5,5	1.10	0
2	GOL	A	701	-	5,5,5	1.27	1 (20%)	5,5,5	1.36	1 (20%)
2	GOL	D	702	-	5,5,5	0.83	0	5,5,5	1.00	0
2	GOL	C	801	-	5,5,5	0.86	0	5,5,5	1.18	1 (20%)
2	GOL	A	702	-	5,5,5	0.94	0	5,5,5	1.13	0
2	GOL	B	702	-	5,5,5	0.92	0	5,5,5	1.25	1 (20%)

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	GOL	B	701	-	-	1/4/4/4	-
2	GOL	D	701	-	-	2/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	D	702	-	-	2/4/4/4	-
2	GOL	C	801	-	-	1/4/4/4	-
2	GOL	A	702	-	-	2/4/4/4	-
2	GOL	B	702	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GOL	O2-C2	-2.44	1.36	1.43
2	D	701	GOL	O2-C2	-2.31	1.36	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	GOL	C3-C2-C1	-2.38	102.44	111.70
2	A	701	GOL	C3-C2-C1	-2.28	102.84	111.70
2	C	801	GOL	C3-C2-C1	-2.15	103.33	111.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	GOL	O1-C1-C2-O2
2	D	701	GOL	O1-C1-C2-C3
2	D	702	GOL	O1-C1-C2-C3
2	A	701	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-C3
2	A	702	GOL	O1-C1-C2-C3
2	B	702	GOL	C1-C2-C3-O3
2	D	702	GOL	O1-C1-C2-O2
2	B	702	GOL	O2-C2-C3-O3
2	A	702	GOL	O1-C1-C2-O2
2	C	801	GOL	C1-C2-C3-O3
2	B	701	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	GOL	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

### 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	204/223 (91%)	-0.15	4 (1%) 65 69	22, 29, 48, 103	0
1	B	204/223 (91%)	-0.10	5 (2%) 57 61	23, 31, 47, 104	0
1	C	204/223 (91%)	0.09	7 (3%) 45 49	21, 30, 48, 111	0
1	D	204/223 (91%)	-0.08	7 (3%) 45 49	20, 30, 51, 84	0
1	E	204/223 (91%)	0.27	12 (5%) 22 24	25, 37, 60, 110	0
All	All	1020/1115 (91%)	0.00	35 (3%) 45 49	20, 31, 53, 111	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	THR	11.0
1	A	343	THR	11.0
1	B	342	LYS	7.0
1	C	342	LYS	6.9
1	C	341	GLU	6.9
1	E	343	THR	6.4
1	B	343	THR	6.4
1	B	340	LYS	6.3
1	D	343	THR	6.0
1	E	341	GLU	6.0
1	C	340	LYS	5.8
1	E	340	LYS	5.3
1	E	342	LYS	5.1
1	E	229	TYR	5.1
1	E	234	GLN	5.0
1	B	341	GLU	4.9
1	C	229	TYR	4.1
1	B	339	GLU	3.7
1	E	233	GLY	3.5
1	D	229	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	173	GLU	3.1
1	A	216	HIS	2.8
1	C	339	GLU	2.8
1	A	339	GLU	2.8
1	E	230	ARG	2.7
1	D	230	ARG	2.6
1	D	341	GLU	2.6
1	D	171	LYS	2.5
1	E	191	ASN	2.4
1	D	339	GLU	2.4
1	E	174	GLU	2.3
1	A	341	GLU	2.3
1	C	234	GLN	2.1
1	E	192	VAL	2.1
1	D	342	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 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(Å <sup>2</sup> )	Q<0.9
2	GOL	D	702	6/6	0.83	0.14	41,50,66,70	0
2	GOL	A	702	6/6	0.90	0.13	29,40,45,50	0
3	NA	A	703	1/1	0.91	0.12	44,44,44,44	0
3	NA	C	802	1/1	0.91	0.15	52,52,52,52	0
3	NA	E	401	1/1	0.92	0.17	57,57,57,57	0
2	GOL	A	701	6/6	0.93	0.11	27,33,40,40	0
2	GOL	B	702	6/6	0.94	0.12	33,40,48,50	0
2	GOL	D	701	6/6	0.94	0.11	27,37,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	801	6/6	0.97	0.09	29,34,40,40	0
2	GOL	B	701	6/6	0.97	0.11	27,33,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.