



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:58 AM GMT

PDB ID : 3GR0  
Title : Periplasmic domain of the T3SS inner membrane protein PrgH from  
S.typhimurium (fragment 170-362)  
Authors : Yip, C.K.; Vockovic, M.; Yu, A.C.; Strynadka, N.C.J.  
Deposited on : 2009-03-24  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

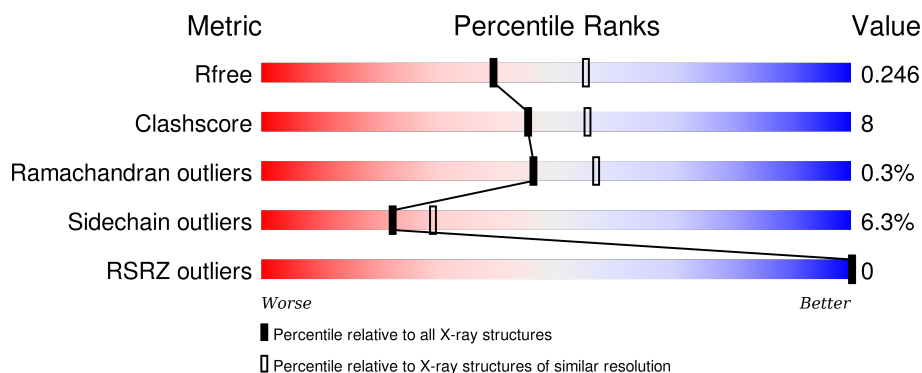
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	197	<div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div>
1	B	197	<div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	C	197	<div> <div>72%</div> <div>16%</div> <div>• 11%</div> </div>
1	D	197	<div> <div>71%</div> <div>18%</div> <div>• 9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6311 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 Protein prgH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1541	976	280	281	4			
1	B	192	Total	C	N	O	S	0	0	0
			1585	1003	286	292	4			
1	C	176	Total	C	N	O	S	0	0	0
			1461	928	268	261	4			
1	D	180	Total	C	N	O	S	0	0	0
			1493	947	272	270	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	-	EXPRESSION TAG	UNP P41783
A	167	SER	-	EXPRESSION TAG	UNP P41783
A	168	HIS	-	EXPRESSION TAG	UNP P41783
A	169	MET	-	EXPRESSION TAG	UNP P41783
B	166	GLY	-	EXPRESSION TAG	UNP P41783
B	167	SER	-	EXPRESSION TAG	UNP P41783
B	168	HIS	-	EXPRESSION TAG	UNP P41783
B	169	MET	-	EXPRESSION TAG	UNP P41783
C	166	GLY	-	EXPRESSION TAG	UNP P41783
C	167	SER	-	EXPRESSION TAG	UNP P41783
C	168	HIS	-	EXPRESSION TAG	UNP P41783
C	169	MET	-	EXPRESSION TAG	UNP P41783
D	166	GLY	-	EXPRESSION TAG	UNP P41783
D	167	SER	-	EXPRESSION TAG	UNP P41783
D	168	HIS	-	EXPRESSION TAG	UNP P41783
D	169	MET	-	EXPRESSION TAG	UNP P41783

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total 66	O 66	0	0
2	B	69	Total 69	O 69	0	0
2	C	41	Total 41	O 41	0	0
2	D	55	Total 55	O 55	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.26 Å 53.26 Å 282.53 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 2.30 94.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.00-2.30) 94.1 (94.18-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.255 0.200 , 0.246	Depositor DCC
$R_{free}$ test set	2006 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.8	EDS
Estimated twinning fraction	0.024 for -h,-k,l 0.487 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 49247 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0/1573	0.70	0/2122
1	B	0.69	1/1617 (0.1%)	0.70	1/2182 (0.0%)
1	C	0.57	0/1491	0.65	0/2011
1	D	0.58	0/1525	0.69	1/2059 (0.0%)
All	All	0.63	1/6206 (0.0%)	0.69	2/8374 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	LYS	CE-NZ	10.62	1.75	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	353	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	307	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1541	0	1530	31	0
1	B	1585	0	1572	19	0
1	C	1461	0	1462	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1493	0	1483	27	0
2	A	66	0	0	0	0
2	B	69	0	0	1	0
2	C	41	0	0	0	0
2	D	55	0	0	3	0
All	All	6311	0	6047	95	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 8.

All (95) 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:218:LYS:CE	1:B:218:LYS:NZ	1.75	1.48
1:D:263:GLN:HE22	1:D:296:ASP:H	1.25	0.81
1:C:263:GLN:HE22	1:C:296:ASP:H	1.27	0.79
1:B:263:GLN:HE21	1:B:263:GLN:H	1.30	0.78
1:A:263:GLN:H	1:A:263:GLN:HE21	1.30	0.77
1:D:263:GLN:NE2	1:D:296:ASP:H	1.83	0.76
1:A:267:MET:HE2	1:A:271:GLU:HB3	1.70	0.74
1:C:209:GLN:O	1:C:213:ARG:HG2	1.88	0.73
1:C:263:GLN:NE2	1:C:296:ASP:H	1.85	0.73
1:A:263:GLN:HE22	1:A:296:ASP:H	1.38	0.70
1:C:205:LEU:HD11	1:D:266:THR:HA	1.74	0.69
1:A:304:GLU:HG2	1:A:325:PHE:CE2	2.28	0.69
1:B:263:GLN:HE22	1:B:296:ASP:H	1.40	0.68
1:A:304:GLU:HG2	1:A:325:PHE:HE2	1.58	0.67
1:B:304:GLU:HG2	1:B:325:PHE:CE2	2.29	0.66
1:A:196:VAL:HG13	1:A:222:VAL:HG22	1.76	0.66
1:A:361:LEU:HD13	1:C:343:VAL:HG21	1.79	0.64
1:D:201:GLU:CD	1:D:201:GLU:H	2.02	0.62
1:C:263:GLN:HE21	1:C:263:GLN:H	1.47	0.62
1:A:317:ARG:HH21	1:C:356:GLN:NE2	1.98	0.62
1:C:201:GLU:OE1	1:C:202:ARG:HD3	2.00	0.61
1:B:304:GLU:HG2	1:B:325:PHE:HE2	1.65	0.61
1:D:248:ILE:HG12	1:D:258:PHE:HD1	1.66	0.61
1:B:263:GLN:NE2	1:B:296:ASP:H	1.98	0.60
1:A:180:GLU:HG3	1:A:184:PHE:CD1	2.37	0.59
1:D:353:ARG:NH2	2:D:109:HOH:O	2.35	0.59
1:B:218:LYS:CD	1:B:218:LYS:NZ	2.61	0.58
1:A:187:LEU:HD11	1:A:253:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HD3	1:B:318:ASN:OD1	2.04	0.57
1:A:196:VAL:CG1	1:A:222:VAL:HG22	2.34	0.57
1:D:304:GLU:HG2	1:D:325:PHE:CE2	2.40	0.56
1:D:304:GLU:HG2	1:D:325:PHE:HE2	1.71	0.56
1:D:263:GLN:H	1:D:263:GLN:HE21	1.53	0.55
1:A:263:GLN:NE2	1:A:296:ASP:H	2.03	0.55
1:B:225:GLU:HG3	1:B:250:PHE:CD1	2.42	0.54
1:C:248:ILE:HG12	1:C:258:PHE:HD1	1.72	0.54
1:D:263:GLN:HE22	1:D:296:ASP:N	2.03	0.53
1:B:225:GLU:HG3	1:B:250:PHE:HD1	1.73	0.53
1:D:232:ILE:HD13	1:D:248:ILE:CD1	2.39	0.53
1:D:243:LEU:HD11	1:D:260:LEU:HD11	1.91	0.53
1:D:248:ILE:HG12	1:D:258:PHE:CD1	2.44	0.52
1:A:201:GLU:O	1:A:205:LEU:HD13	2.09	0.52
1:C:304:GLU:HG3	1:C:325:PHE:CE2	2.45	0.52
1:C:306:GLY:HA3	1:C:342:PHE:CE2	2.46	0.50
1:A:317:ARG:HH21	1:C:356:GLN:HE21	1.57	0.50
1:A:201:GLU:OE2	1:A:224:ASN:ND2	2.45	0.49
1:C:234:ILE:O	1:C:237:ASP:HB2	2.12	0.49
1:D:312:LEU:HD21	1:D:339:ALA:HB2	1.94	0.49
1:B:319:HIS:ND1	2:B:366:HOH:O	2.35	0.48
1:B:235:TRP:CD2	1:B:282:LEU:HD11	2.48	0.48
1:B:187:LEU:HD11	1:B:253:PRO:HB2	1.94	0.48
1:B:177:LEU:HD21	1:B:186:VAL:HG23	1.95	0.48
1:A:306:GLY:HA3	1:A:342:PHE:CE2	2.49	0.48
1:C:202:ARG:NH2	1:C:205:LEU:HD23	2.28	0.48
1:A:361:LEU:HD21	1:C:340:ARG:HG2	1.96	0.48
1:D:240:TYR:HB3	1:D:243:LEU:HB2	1.95	0.48
1:C:339:ALA:O	1:C:343:VAL:HG23	2.13	0.47
1:C:191:ASP:C	1:C:192:LYS:HD2	2.35	0.47
1:A:313:PRO:HB3	1:D:287:ASP:HB3	1.97	0.47
1:C:228:GLU:O	1:C:232:ILE:HG12	2.16	0.47
1:A:180:GLU:HG3	1:A:184:PHE:HD1	1.80	0.46
1:D:280:ARG:HD2	1:D:288:SER:HA	1.97	0.46
1:A:263:GLN:HE21	1:A:263:GLN:N	2.05	0.46
1:C:254:ARG:HD2	1:C:254:ARG:HA	1.84	0.46
1:A:317:ARG:NH2	1:C:356:GLN:HE21	2.13	0.46
1:A:319:HIS:CE1	1:C:317:ARG:HB3	2.50	0.46
1:B:249:HIS:HE1	1:B:349:THR:HA	1.80	0.46
1:C:190:ARG:NH2	1:C:286:ALA:O	2.50	0.45
1:A:180:GLU:HG3	1:A:184:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:GLN:O	1:D:213:ARG:HG2	2.16	0.45
1:D:306:GLY:HA3	1:D:342:PHE:CE2	2.51	0.45
1:B:316:ARG:HG3	1:B:325:PHE:CE2	2.52	0.45
1:A:317:ARG:NH2	1:C:356:GLN:NE2	2.63	0.45
1:D:327:ILE:CG2	1:D:331:LEU:HD11	2.48	0.44
1:C:263:GLN:HE22	1:C:296:ASP:N	2.04	0.43
1:D:232:ILE:HD13	1:D:248:ILE:HD13	2.00	0.43
1:A:235:TRP:CD2	1:A:282:LEU:HD11	2.54	0.43
1:A:249:HIS:NE2	1:A:349:THR:O	2.50	0.43
1:B:263:GLN:NE2	1:B:263:GLN:H	2.08	0.43
1:D:262:ARG:NH2	2:D:363:HOH:O	2.50	0.43
1:D:207:ALA:HA	1:D:210:VAL:HG22	2.01	0.43
1:B:263:GLN:HE21	1:B:263:GLN:N	2.08	0.42
1:A:314:TYR:HA	1:A:326:VAL:O	2.19	0.42
1:A:263:GLN:H	1:A:263:GLN:NE2	2.09	0.42
1:C:248:ILE:HG12	1:C:258:PHE:CD1	2.53	0.42
1:A:248:ILE:HG12	1:A:258:PHE:CD1	2.55	0.41
1:D:232:ILE:HG21	1:D:248:ILE:HD11	2.02	0.41
1:A:320:LYS:HD3	1:A:320:LYS:HA	1.72	0.41
1:A:256:PRO:HD2	1:A:288:SER:O	2.21	0.41
1:D:185:GLN:HG2	1:D:187:LEU:HD11	2.02	0.41
1:B:306:GLY:HA3	1:B:342:PHE:CE2	2.56	0.40
1:D:356:GLN:HG3	2:D:368:HOH:O	2.20	0.40
1:C:240:TYR:HB3	1:C:243:LEU:HB2	2.03	0.40
1:C:263:GLN:HE22	1:C:295:ASP:HA	1.86	0.40
1:D:254:ARG:HD2	1:D:254:ARG:HA	1.99	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	184/197 (93%)	180 (98%)	4 (2%)	0	100	100
1	B	190/197 (96%)	185 (97%)	4 (2%)	1 (0%)	34	41
1	C	172/197 (87%)	170 (99%)	2 (1%)	0	100	100
1	D	178/197 (90%)	173 (97%)	4 (2%)	1 (1%)	30	36
All	All	724/788 (92%)	708 (98%)	14 (2%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	215	ASP
1	B	320	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	160/168 (95%)	150 (94%)	10 (6%)	22	29
1	B	165/168 (98%)	153 (93%)	12 (7%)	17	22
1	C	152/168 (90%)	145 (95%)	7 (5%)	33	44
1	D	155/168 (92%)	144 (93%)	11 (7%)	18	23
All	All	632/672 (94%)	592 (94%)	40 (6%)	22	29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	181	LYS
1	A	209	GLN
1	A	238	THR
1	A	263	GLN
1	A	277	GLN
1	A	307	LEU
1	A	345	SER
1	A	361	LEU

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Mol	Chain	Res	Type
1	A	362	LYS
1	B	177	LEU
1	B	181	LYS
1	B	201	GLU
1	B	226	ASN
1	B	252	GLU
1	B	263	GLN
1	B	307	LEU
1	B	309	GLN
1	B	316	ARG
1	B	336	ILE
1	B	338	ARG
1	B	361	LEU
1	C	192	LYS
1	C	194	LEU
1	C	202	ARG
1	C	263	GLN
1	C	307	LEU
1	C	338	ARG
1	C	360	GLU
1	D	192	LYS
1	D	194	LEU
1	D	211	LEU
1	D	213	ARG
1	D	255	LYS
1	D	263	GLN
1	D	264	ARG
1	D	307	LEU
1	D	309	GLN
1	D	312	LEU
1	D	320	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	263	GLN
1	A	328	GLN
1	A	341	GLN
1	B	185	GLN
1	B	199	GLN
1	B	242	GLN

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Mol	Chain	Res	Type
1	B	263	GLN
1	B	309	GLN
1	B	341	GLN
1	C	263	GLN
1	C	341	GLN
1	C	356	GLN
1	D	185	GLN
1	D	226	ASN
1	D	263	GLN

### 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](#)

There are no ligands in this entry.

## 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	186/197 (94%)	-0.29	0 100 100	10, 20, 35, 44	0
1	B	192/197 (97%)	-0.29	0 100 100	8, 22, 35, 51	0
1	C	176/197 (89%)	-0.29	0 100 100	14, 23, 34, 38	0
1	D	180/197 (91%)	-0.24	0 100 100	13, 24, 35, 40	0
All	All	734/788 (93%)	-0.28	0 100 100	8, 22, 35, 51	0

There are no RSRZ outliers to report.

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.