



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:03 am GMT

PDB ID : 1POT  
Title : SPERMIDINE/PUTRESCINE-BINDING PROTEIN COMPLEXED WITH SPERMIDINE (MONOMER FORM)  
Authors : Sugiyama, S.; Maenaka, K.; Matsushima, M.; Morikawa, K.  
Deposited on : 1996-02-02  
Resolution : 1.80 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

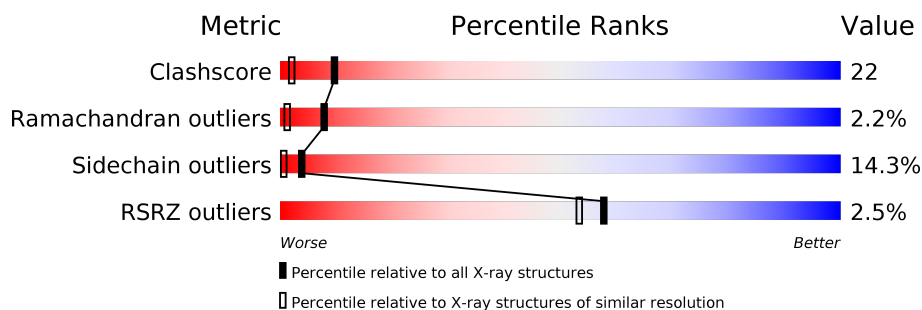
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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	325	

## 2 Entry composition [i](#)

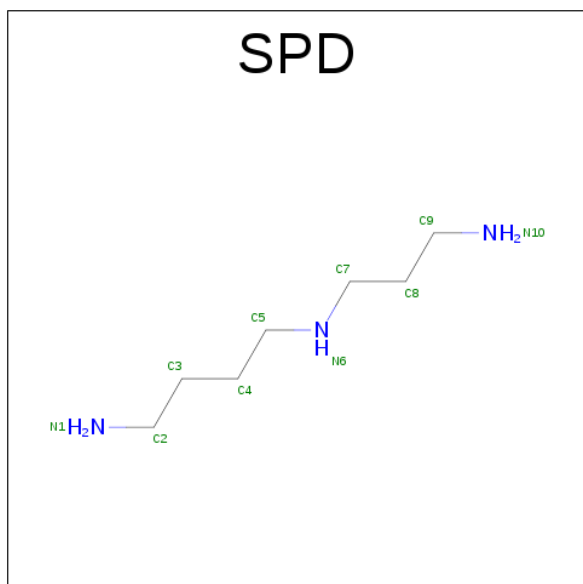
There are 3 unique types of molecules in this entry. The entry contains 2885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SPERMIDINE/PUTRESCINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2548	1637	408	494	9			

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	7	3		

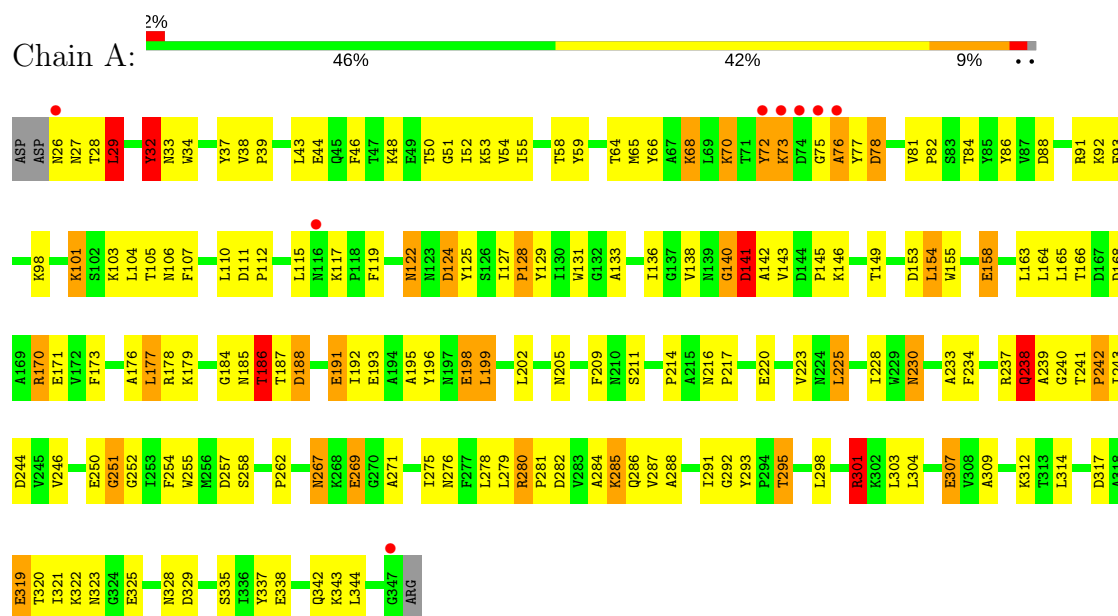
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	327	Total	O	0	0
			327	327		

### 3 Residue-property plots

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: SPERMIDINE/PUTRESCINE-BINDING PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.30Å 130.30Å 38.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80 29.14 – 1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.80) 61.2 (29.14-1.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.198 , (Not available) 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	7.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 131.9	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.075 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</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: SPD

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	0.90	0/2614	1.77	48/3558 (1.3%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	TYR	CB-CG-CD1	13.40	129.04	121.00
1	A	170	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	A	301	ARG	CD-NE-CZ	12.18	140.65	123.60
1	A	129	TYR	CB-CG-CD2	-10.88	114.47	121.00
1	A	301	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	124	ASP	CB-CG-OD1	10.60	127.84	118.30
1	A	37	TYR	CB-CG-CD2	-9.67	115.20	121.00
1	A	170	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	37	TYR	CB-CG-CD1	8.89	126.33	121.00
1	A	307	GLU	CA-CB-CG	8.37	131.81	113.40
1	A	220	GLU	CA-CB-CG	8.13	131.29	113.40
1	A	141	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	257	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	280	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	329	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	337	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	A	251	GLY	N-CA-C	6.88	130.31	113.10
1	A	325	GLU	CA-CB-CG	6.81	128.39	113.40
1	A	301	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	250	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	A	29	LEU	CB-CA-C	6.53	122.61	110.20
1	A	252	GLY	N-CA-C	-6.52	96.80	113.10
1	A	153	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	186	THR	N-CA-CB	6.33	122.32	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	170	ARG	CD-NE-CZ	6.17	132.24	123.60
1	A	191	GLU	CG-CD-OE2	5.97	130.24	118.30
1	A	78	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	A	335	SER	N-CA-CB	5.93	119.40	110.50
1	A	269	GLU	CG-CD-OE1	5.93	130.16	118.30
1	A	32	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	A	319	GLU	CB-CA-C	-5.73	98.93	110.40
1	A	319	GLU	N-CA-CB	5.71	120.88	110.60
1	A	250	GLU	CG-CD-OE2	5.68	129.66	118.30
1	A	225	LEU	CB-CA-C	5.58	120.79	110.20
1	A	291	ILE	C-N-CA	5.54	133.94	122.30
1	A	76	ALA	N-CA-CB	5.43	117.70	110.10
1	A	188	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	131	TRP	CA-CB-CG	5.39	123.95	113.70
1	A	78	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	72	TYR	C-N-CA	5.22	134.74	121.70
1	A	293	TYR	O-C-N	5.18	130.94	121.10
1	A	29	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	198	GLU	CG-CD-OE1	5.12	128.54	118.30
1	A	158	GLU	CA-CB-CG	5.11	124.65	113.40
1	A	177	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	115	LEU	N-CA-C	5.07	124.69	111.00
1	A	76	ALA	O-C-N	5.06	130.80	122.70

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	2548	0	2491	109	0
2	A	10	0	19	1	0
3	A	327	0	0	14	0
All	All	2885	0	2510	109	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 22.

All (109) 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:32:TYR:HB2	1:A:76:ALA:HB3	1.27	1.16
1:A:136:ILE:HB	1:A:246:VAL:HG13	1.58	0.85
1:A:32:TYR:HB2	1:A:76:ALA:CB	2.07	0.83
1:A:164:LEU:HB2	1:A:223:VAL:HG21	1.61	0.81
1:A:284:ALA:HB1	1:A:295:THR:HG21	1.68	0.76
1:A:285:LYS:HG3	1:A:303:LEU:HB3	1.68	0.76
1:A:110:LEU:HD21	1:A:279:LEU:HD22	1.68	0.73
1:A:216:ASN:HB3	1:A:217:PRO:HD3	1.71	0.72
1:A:280:ARG:HD2	1:A:282:ASP:OD1	1.90	0.72
1:A:106:ASN:N	1:A:276:ASN:HD21	1.89	0.71
1:A:82:PRO:HD2	1:A:258:SER:O	1.91	0.71
1:A:287:VAL:HG11	3:A:645:HOH:O	1.91	0.69
1:A:199:LEU:HG	1:A:344:LEU:HD21	1.76	0.68
1:A:228:ILE:HD13	1:A:233:ALA:HB2	1.75	0.68
1:A:173:PHE:O	1:A:177:LEU:HB2	1.95	0.67
1:A:271:ALA:O	1:A:275:ILE:HG13	1.96	0.65
1:A:106:ASN:H	1:A:276:ASN:HD21	1.44	0.63
1:A:154:LEU:HB3	1:A:163:LEU:HD21	1.83	0.60
1:A:106:ASN:H	1:A:276:ASN:ND2	1.99	0.60
1:A:286:GLN:NE2	3:A:511:HOH:O	2.37	0.57
1:A:136:ILE:HB	1:A:246:VAL:CG1	2.33	0.57
1:A:185:ASN:HD21	1:A:328:ASN:H	1.51	0.56
1:A:177:LEU:HD13	1:A:195:ALA:HB2	1.86	0.56
1:A:143:VAL:O	1:A:145:PRO:HD3	2.06	0.56
1:A:111:ASP:HB2	1:A:298:LEU:HD13	1.86	0.55
1:A:163:LEU:HB2	1:A:205:ASN:O	2.07	0.55
1:A:237:ARG:O	1:A:240:GLY:N	2.22	0.55
1:A:84:THR:HB	1:A:119:PHE:CZ	2.41	0.54
1:A:103:LYS:HE2	3:A:730:HOH:O	2.08	0.54
1:A:179:LYS:NZ	1:A:198:GLU:OE1	2.39	0.54
1:A:27:ASN:HB3	1:A:52:ILE:HG12	1.88	0.54
1:A:145:PRO:HG2	1:A:244:ASP:OD2	2.07	0.54
1:A:230:ASN:HD22	1:A:230:ASN:N	2.04	0.54
1:A:176:ALA:HB2	1:A:199:LEU:HD13	1.90	0.53
1:A:59:TYR:OH	1:A:81:VAL:O	2.26	0.53
1:A:29:LEU:HD13	1:A:78:ASP:HB2	1.92	0.52
1:A:237:ARG:O	1:A:239:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:O	1:A:342:GLN:HG2	2.10	0.52
1:A:177:LEU:HD23	1:A:184:GLY:HA2	1.93	0.51
1:A:155:TRP:CD2	1:A:202:LEU:HD13	2.45	0.51
1:A:185:ASN:ND2	1:A:328:ASN:H	2.09	0.51
1:A:81:VAL:HG12	1:A:81:VAL:O	2.13	0.49
1:A:237:ARG:NH2	3:A:659:HOH:O	2.46	0.49
1:A:214:PRO:O	1:A:217:PRO:HD2	2.13	0.49
1:A:170:ARG:NH2	1:A:185:ASN:HD22	2.09	0.49
1:A:68:LYS:HB2	1:A:68:LYS:NZ	2.27	0.48
1:A:140:GLY:C	1:A:142:ALA:H	2.16	0.48
1:A:154:LEU:HD13	1:A:163:LEU:HD11	1.95	0.47
1:A:193:GLU:O	1:A:196:TYR:HB3	2.14	0.47
1:A:59:TYR:CE2	1:A:65:MET:HG3	2.49	0.47
1:A:73:LYS:HD3	3:A:472:HOH:O	2.15	0.47
1:A:44:GLU:O	1:A:48:LYS:HG2	2.14	0.47
1:A:122:ASN:OD1	1:A:124:ASP:OD2	2.32	0.47
1:A:77:TYR:O	1:A:262:PRO:HG2	2.15	0.47
1:A:33:ASN:ND2	1:A:34:TRP:H	2.13	0.46
1:A:110:LEU:HD21	1:A:279:LEU:CD2	2.43	0.46
1:A:186:THR:HG21	1:A:191:GLU:OE1	2.15	0.46
1:A:216:ASN:CB	1:A:217:PRO:HD3	2.43	0.46
1:A:343:LYS:NZ	3:A:647:HOH:O	2.45	0.46
1:A:255:TRP:CH2	2:A:350:SPD:H52	2.50	0.46
1:A:28:THR:HA	1:A:53:LYS:O	2.16	0.46
1:A:195:ALA:O	1:A:199:LEU:HB2	2.15	0.46
1:A:51:GLY:HA2	3:A:478:HOH:O	2.15	0.46
1:A:140:GLY:O	1:A:142:ALA:N	2.48	0.46
1:A:230:ASN:ND2	1:A:230:ASN:N	2.64	0.46
1:A:133:ALA:HB2	1:A:254:PHE:CE1	2.50	0.45
1:A:312:LYS:NZ	3:A:581:HOH:O	2.48	0.45
1:A:101:LYS:HA	1:A:104:LEU:HB2	1.99	0.45
1:A:166:THR:HG21	1:A:171:GLU:OE1	2.16	0.45
1:A:91:ARG:HD3	1:A:125:TYR:CE2	2.52	0.45
1:A:285:LYS:HD2	1:A:285:LYS:C	2.36	0.45
1:A:33:ASN:O	1:A:58:THR:HA	2.17	0.45
1:A:165:LEU:O	1:A:209:PHE:HA	2.16	0.45
1:A:237:ARG:O	1:A:238:GLN:C	2.54	0.45
1:A:66:TYR:CZ	1:A:70:LYS:HE3	2.52	0.45
1:A:107:PHE:O	1:A:110:LEU:HD23	2.16	0.44
1:A:39:PRO:HB3	3:A:720:HOH:O	2.17	0.44
1:A:73:LYS:HA	3:A:627:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ARG:HA	1:A:304:LEU:HD22	1.98	0.44
1:A:73:LYS:HB3	1:A:77:TYR:OH	2.18	0.44
1:A:111:ASP:CB	1:A:298:LEU:HD13	2.48	0.43
1:A:138:VAL:HG13	1:A:244:ASP:HB2	2.00	0.43
1:A:287:VAL:HG13	1:A:288:ALA:N	2.33	0.43
1:A:64:THR:HG21	3:A:509:HOH:O	2.18	0.43
1:A:234:PHE:CD2	1:A:314:LEU:HD11	2.54	0.43
1:A:141:ASP:CG	1:A:242:PRO:HG3	2.38	0.43
1:A:112:PRO:HG3	3:A:671:HOH:O	2.19	0.43
1:A:170:ARG:NH2	1:A:185:ASN:ND2	2.67	0.43
1:A:188:ASP:O	1:A:192:ILE:HG13	2.19	0.42
1:A:127:ILE:O	1:A:128:PRO:C	2.57	0.42
1:A:154:LEU:N	1:A:154:LEU:CD2	2.83	0.42
1:A:46:PHE:CE1	1:A:50:THR:HG21	2.55	0.42
1:A:55:ILE:HD13	3:A:610:HOH:O	2.19	0.42
1:A:98:LYS:HG3	1:A:125:TYR:CE1	2.55	0.42
1:A:267:ASN:ND2	1:A:269:GLU:HG2	2.35	0.42
1:A:228:ILE:HD12	1:A:243:ILE:HD11	2.02	0.42
1:A:304:LEU:HB3	1:A:309:ALA:HB2	2.02	0.42
1:A:170:ARG:HH22	1:A:185:ASN:HD22	1.68	0.41
1:A:91:ARG:HD3	1:A:125:TYR:CZ	2.56	0.41
1:A:105:THR:HG23	3:A:436:HOH:O	2.21	0.41
1:A:122:ASN:ND2	1:A:124:ASP:OD1	2.53	0.41
1:A:241:THR:O	1:A:243:ILE:N	2.40	0.41
1:A:92:LYS:NZ	1:A:92:LYS:CB	2.84	0.41
1:A:117:LYS:HB3	1:A:119:PHE:CE2	2.55	0.41
1:A:168:ASP:HB3	1:A:171:GLU:HB2	2.02	0.41
1:A:98:LYS:HG2	1:A:124:ASP:HB3	2.04	0.40
1:A:280:ARG:HA	1:A:281:PRO:HD3	1.85	0.40
1:A:88:ASP:OD1	1:A:91:ARG:NH2	2.54	0.40
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

## 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	320/325 (98%)	300 (94%)	13 (4%)	7 (2%)	8 1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	238	GLN
1	A	75	GLY
1	A	292	GLY
1	A	251	GLY
1	A	140	GLY
1	A	242	PRO

### 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	272/275 (99%)	233 (86%)	39 (14%)	4 0

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	LEU
1	A	32	TYR
1	A	38	VAL
1	A	43	LEU
1	A	54	VAL
1	A	68	LYS
1	A	70	LYS
1	A	72	TYR
1	A	73	LYS
1	A	86	TYR
1	A	93	GLU

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Mol	Chain	Res	Type
1	A	101	LYS
1	A	122	ASN
1	A	128	PRO
1	A	146	LYS
1	A	149	THR
1	A	154	LEU
1	A	158	GLU
1	A	178	ARG
1	A	186	THR
1	A	187	THR
1	A	199	LEU
1	A	211	SER
1	A	225	LEU
1	A	230	ASN
1	A	238	GLN
1	A	267	ASN
1	A	278	LEU
1	A	285	LYS
1	A	295	THR
1	A	301	ARG
1	A	307	GLU
1	A	317	ASP
1	A	319	GLU
1	A	320	THR
1	A	321	ILE
1	A	322	LYS
1	A	323	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	33	ASN
1	A	123	ASN
1	A	185	ASN
1	A	205	ASN
1	A	216	ASN
1	A	230	ASN
1	A	238	GLN
1	A	267	ASN
1	A	276	ASN
1	A	323	ASN

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Mol	Chain	Res	Type
1	A	342	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](#)

1 ligand is 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	SPD	A	350	-	9,9,9	0.95	1 (11%)	8,8,8	1.57	1 (12%)

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	SPD	A	350	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	SPD	C7-N6	-2.04	1.40	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	SPD	C7-N6-C5	3.68	126.70	113.33

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	A	350	SPD	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	322/325 (99%)	-0.29	8 (2%) 58 53	9, 24, 40, 53	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ASN	5.3
1	A	74	ASP	5.0
1	A	73	LYS	4.4
1	A	75	GLY	3.8
1	A	347	GLY	3.6
1	A	72	TYR	2.6
1	A	76	ALA	2.3
1	A	116	ASN	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	SPD	A	350	10/10	0.96	0.08	-0.34	5,5,8,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.