



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:49 PM UTC

PDB ID : 1POT / pdb_00001pot
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

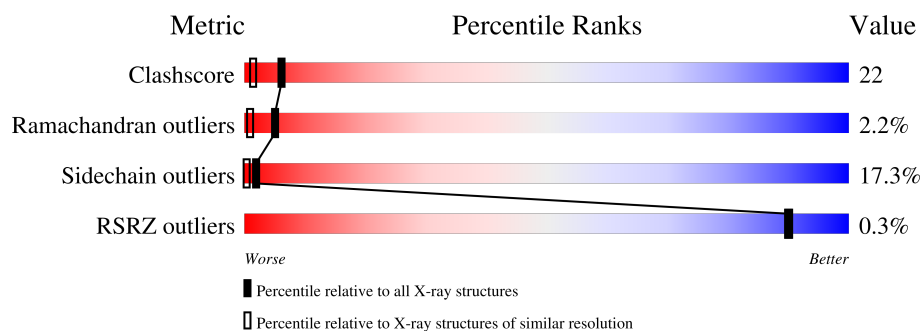
1 Overall quality at a glance

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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	325	37% 42% 18% ..

2 Entry composition [i](#)

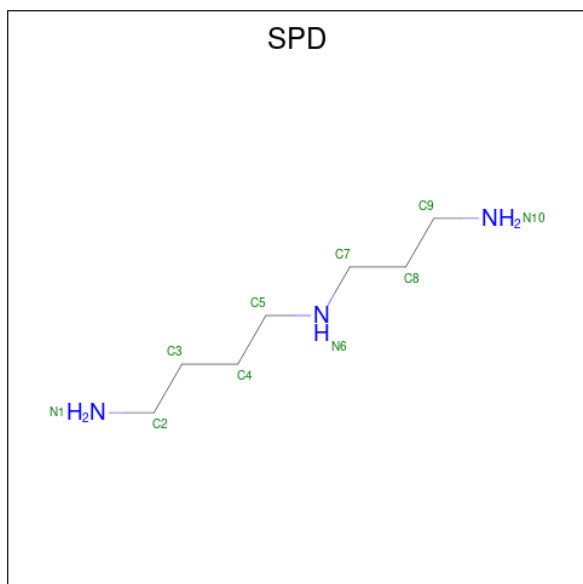
There are 3 unique types of molecules in this entry. The entry contains 2885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

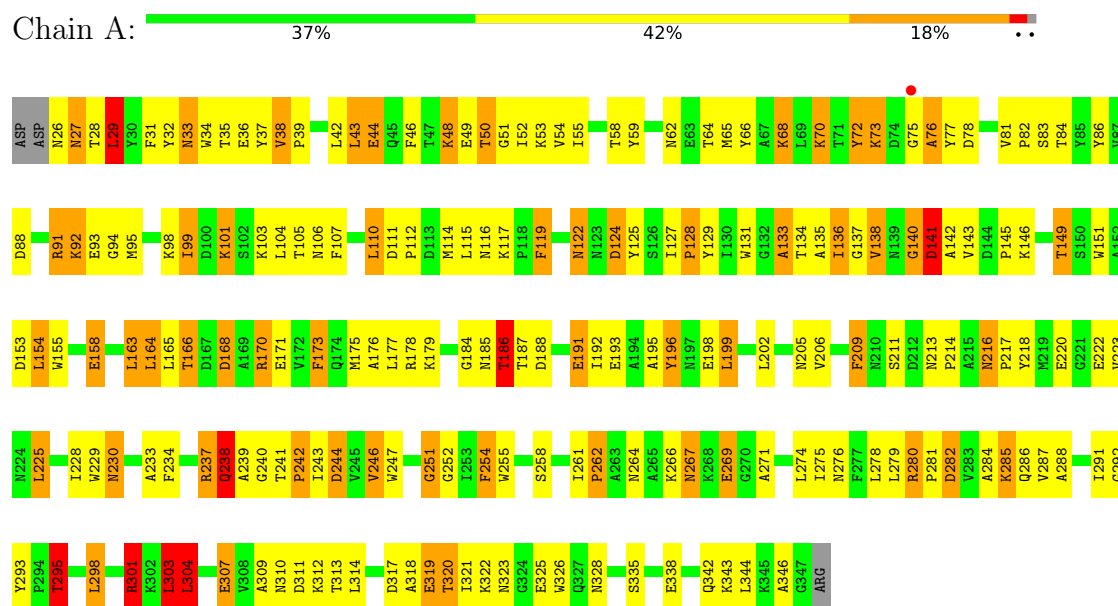
- Molecule 3 is water.

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

3 Residue-property plots [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: SPERMIDINE/PUTRESCINE-BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	130.30Å 130.30Å 38.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.80 6.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.80) 77.9 (6.00-1.80)	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.	wwPDB-VP
Wilson B-factor (Å ²)	7.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 87.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.075 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2885	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Theoretical 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: 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	1.13	4/2614 (0.2%)	2.19	120/3558 (3.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	ILE	CA-CB	6.14	1.60	1.53
1	A	135	ALA	C-O	6.06	1.29	1.24
1	A	35	THR	C-O	5.93	1.31	1.24
1	A	36	GLU	N-CA	5.13	1.52	1.46

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	CD-NE-CZ	11.61	140.65	124.40
1	A	72	TYR	N-CA-C	9.99	122.94	108.86
1	A	35	THR	N-CA-C	9.55	122.70	111.71
1	A	293	TYR	O-C-N	9.36	130.94	121.30
1	A	141	ASP	CA-CB-CG	9.17	121.77	112.60
1	A	307	GLU	CA-CB-CG	8.86	131.81	114.10
1	A	220	GLU	CA-CB-CG	8.59	131.29	114.10
1	A	31	PHE	CA-CB-CG	8.33	122.13	113.80
1	A	335	SER	O-C-N	8.04	130.35	122.07
1	A	37	TYR	CA-C-O	-7.94	111.13	120.10
1	A	62	ASN	CA-CB-CG	7.91	120.51	112.60
1	A	44	GLU	CB-CG-CD	7.78	125.83	112.60
1	A	313	THR	N-CA-C	-7.68	103.94	113.38
1	A	95	MET	N-CA-C	7.62	120.66	111.82
1	A	151	TRP	N-CA-C	-7.62	102.97	111.28
1	A	115	LEU	N-CA-C	7.60	124.69	114.12
1	A	326	TRP	CA-C-O	-7.54	112.45	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLU	CA-C-N	7.41	128.16	120.00
1	A	269	GLU	C-N-CA	7.41	128.16	120.00
1	A	247	TRP	CA-C-O	-7.34	113.22	119.76
1	A	251	GLY	N-CA-C	7.23	130.31	113.18
1	A	36	GLU	CB-CG-CD	7.17	124.78	112.60
1	A	325	GLU	CA-CB-CG	7.14	128.39	114.10
1	A	72	TYR	CA-C-N	7.07	134.74	122.09
1	A	72	TYR	C-N-CA	7.07	134.74	122.09
1	A	124	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	247	TRP	N-CA-C	-7.02	100.80	109.65
1	A	186	THR	N-CA-CB	7.00	122.32	110.49
1	A	33	ASN	CA-CB-CG	6.92	119.52	112.60
1	A	319	GLU	N-CA-CB	6.84	120.88	110.28
1	A	310	ASN	OD1-CG-ND2	6.83	129.43	122.60
1	A	295	THR	CB-CA-C	-6.79	99.23	108.68
1	A	269	GLU	CB-CG-CD	6.79	124.14	112.60
1	A	29	LEU	CB-CA-C	6.70	122.61	109.35
1	A	35	THR	CA-C-O	-6.69	112.54	120.10
1	A	173	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	76	ALA	O-C-N	6.61	130.80	123.33
1	A	218	TYR	O-C-N	6.51	129.57	122.15
1	A	335	SER	N-CA-CB	6.48	119.40	110.01
1	A	298	LEU	N-CA-CB	-6.42	100.65	110.16
1	A	170	ARG	CA-C-O	-6.40	112.61	119.97
1	A	291	ILE	CA-C-N	6.39	133.94	121.41
1	A	291	ILE	C-N-CA	6.39	133.94	121.41
1	A	343	LYS	CA-C-N	6.37	129.65	120.79
1	A	343	LYS	C-N-CA	6.37	129.65	120.79
1	A	252	GLY	N-CA-C	-6.36	96.80	111.04
1	A	36	GLU	CA-C-N	6.34	129.41	120.28
1	A	36	GLU	C-N-CA	6.34	129.41	120.28
1	A	166	THR	N-CA-C	-6.30	101.61	110.50
1	A	38	VAL	N-CA-CB	6.25	119.72	111.40
1	A	49	GLU	N-CA-C	6.24	117.74	111.07
1	A	310	ASN	O-C-N	6.23	129.66	122.25
1	A	246	VAL	CB-CA-C	6.21	120.08	110.83
1	A	99	ILE	CB-CG1-CD1	6.20	126.82	113.80
1	A	261	ILE	N-CA-C	6.13	114.16	107.60
1	A	94	GLY	CA-C-N	6.12	129.61	120.31
1	A	94	GLY	C-N-CA	6.12	129.61	120.31
1	A	319	GLU	CB-CA-C	-6.11	98.93	110.67
1	A	252	GLY	O-C-N	6.07	128.75	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	SER	N-CA-C	-6.03	102.00	110.50
1	A	206	VAL	N-CA-C	6.03	117.08	107.98
1	A	115	LEU	N-CA-CB	-6.00	102.60	110.88
1	A	175	MET	CA-C-O	-5.99	114.20	120.55
1	A	346	ALA	N-CA-C	-5.89	104.84	112.68
1	A	133	ALA	CA-C-O	5.76	127.55	121.33
1	A	33	ASN	O-C-N	5.75	129.65	122.92
1	A	186	THR	CB-CA-C	-5.74	99.00	110.42
1	A	168	ASP	N-CA-CB	-5.73	101.78	110.77
1	A	35	THR	CA-C-N	-5.71	113.64	122.49
1	A	35	THR	C-N-CA	-5.71	113.64	122.49
1	A	216	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	A	225	LEU	N-CA-CB	-5.63	101.90	111.31
1	A	311	ASP	CA-C-O	-5.61	113.94	120.62
1	A	170	ARG	CD-NE-CZ	5.60	132.24	124.40
1	A	42	LEU	CA-C-N	5.58	128.03	120.38
1	A	42	LEU	C-N-CA	5.58	128.03	120.38
1	A	137	GLY	CA-C-O	-5.56	115.86	120.92
1	A	222	GLU	N-CA-C	-5.54	104.44	113.19
1	A	149	THR	N-CA-CB	-5.54	103.64	111.00
1	A	237	ARG	N-CA-C	-5.51	104.30	111.02
1	A	129	TYR	CB-CG-CD1	5.50	129.04	120.80
1	A	37	TYR	N-CA-C	5.47	118.00	111.71
1	A	72	TYR	CA-C-O	5.47	127.47	121.40
1	A	134	THR	N-CA-C	-5.45	100.52	109.40
1	A	131	TRP	CA-CB-CG	5.45	123.95	113.60
1	A	119	PHE	N-CA-C	-5.43	106.70	113.38
1	A	320	THR	CA-C-O	-5.41	114.24	120.24
1	A	254	PHE	CB-CA-C	5.39	118.53	109.48
1	A	335	SER	CA-C-O	-5.38	115.17	120.82
1	A	304	LEU	N-CA-CB	-5.33	102.13	109.97
1	A	244	ASP	CA-C-O	-5.33	114.99	121.28
1	A	264	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	166	THR	CA-C-O	-5.30	115.79	121.56
1	A	27	ASN	CA-C-O	-5.28	115.43	121.40
1	A	158	GLU	CA-CB-CG	5.28	124.65	114.10
1	A	282	ASP	CB-CA-C	5.27	119.54	110.79
1	A	280	ARG	N-CA-C	-5.27	103.14	109.83
1	A	196	TYR	CA-C-O	5.24	126.33	120.82
1	A	303	LEU	N-CA-CB	-5.24	102.73	110.53
1	A	43	LEU	O-C-N	5.22	127.65	122.12
1	A	311	ASP	N-CA-C	-5.22	101.63	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	48	LYS	N-CA-C	-5.21	105.50	111.07
1	A	153	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	318	ALA	CA-C-O	-5.18	115.06	120.55
1	A	166	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	274	LEU	N-CA-C	-5.17	105.54	111.07
1	A	191	GLU	CG-CD-OE2	5.15	130.24	118.40
1	A	209	PHE	CA-C-O	-5.14	114.79	120.24
1	A	50	THR	N-CA-C	5.12	119.80	113.50
1	A	269	GLU	CG-CD-OE1	5.11	130.16	118.40
1	A	229	TRP	N-CA-C	-5.11	102.72	110.28
1	A	213	ASN	O-C-N	5.11	127.19	121.32
1	A	319	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	262	PRO	CA-C-N	5.09	127.10	120.28
1	A	262	PRO	C-N-CA	5.09	127.10	120.28
1	A	267	ASN	N-CA-C	5.08	116.50	109.54
1	A	137	GLY	CA-C-N	-5.07	115.41	122.71
1	A	137	GLY	C-N-CA	-5.07	115.41	122.71
1	A	220	GLU	N-CA-C	-5.01	106.43	112.54

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	114	0
2	A	10	0	19	1	0
3	A	327	0	0	15	0
All	All	2885	0	2510	114	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 (114) 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:114:MET:HE2	3:A:573:HOH:O	2.04	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:N	1:A:230:ASN:HD22	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:140:GLY:C	1:A:142:ALA:H	2.16	0.52
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
1:A:338:GLU:O	1:A:342:GLN:HG2	2.10	0.52
1:A:155:TRP:CD2	1:A:202:LEU:HD13	2.45	0.51
1:A:177:LEU:HD23	1:A:184:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:ND2	1:A:328:ASN:H	2.09	0.51
1:A:285:LYS:C	1:A:285:LYS:HD2	2.36	0.50
1:A:81:VAL:O	1:A:81:VAL:HG12	2.13	0.49
1:A:237:ARG:O	1:A:238:GLN:C	2.54	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:59:TYR:CE2	1:A:65:MET:HG3	2.49	0.47
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:73:LYS:HD3	3:A:472:HOH:O	2.15	0.47
1:A:141:ASP:CG	1:A:242:PRO:HG3	2.38	0.47
1:A:44:GLU:O	1:A:48:LYS:HG2	2.14	0.47
1:A:127:ILE:O	1:A:128:PRO:C	2.57	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: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:51:GLY:HA2	3:A:478:HOH:O	2.15	0.46
1:A:195:ALA:O	1:A:199:LEU:HB2	2.15	0.46
1:A:140:GLY:O	1:A:142:ALA:N	2.48	0.46
1:A:230:ASN:N	1:A:230:ASN:ND2	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:91:ARG:HD3	1:A:125:TYR:CE2	2.52	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:33:ASN:O	1:A:58:THR:HA	2.17	0.45
1:A:266:LYS:NZ	3:A:476:HOH:O	2.49	0.45
1:A:165:LEU:O	1:A:209:PHE:HA	2.16	0.45
1:A:66:TYR:CZ	1:A:70:LYS:HE3	2.52	0.45
1:A:140:GLY:C	1:A:142:ALA:N	2.75	0.45
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
1:A:107:PHE:O	1:A:110:LEU:HD23	2.16	0.44
1:A:301:ARG:HA	1:A:304:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:THR:HG21	3:A:509:HOH:O	2.18	0.43
1:A:287:VAL:HG13	1:A:288:ALA:N	2.33	0.43
1:A:65:MET:HE1	1:A:82:PRO:HB3	1.99	0.43
1:A:234:PHE:CD2	1:A:314:LEU:HD11	2.54	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:46:PHE:CE1	1:A:50:THR:HG21	2.55	0.42
1:A:154:LEU:N	1:A:154:LEU:CD2	2.83	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:116:ASN:O	1:A:117:LYS:C	2.63	0.40
1:A:88:ASP:OD1	1:A:91:ARG:NH2	2.54	0.40
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:237:ARG:C	1:A:239:ALA:N	2.79	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 [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	320/325 (98%)	300 (94%)	13 (4%)	7 (2%)	5 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%)	225 (83%)	47 (17%)	2 0

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	LEU
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	91	ARG
1	A	92	LYS

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Mol	Chain	Res	Type
1	A	93	GLU
1	A	99	ILE
1	A	101	LYS
1	A	110	LEU
1	A	122	ASN
1	A	128	PRO
1	A	136	ILE
1	A	138	VAL
1	A	146	LYS
1	A	149	THR
1	A	154	LEU
1	A	158	GLU
1	A	163	LEU
1	A	164	LEU
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	278	LEU
1	A	285	LYS
1	A	295	THR
1	A	301	ARG
1	A	303	LEU
1	A	304	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	33	ASN
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	123	ASN
1	A	185	ASN
1	A	205	ASN
1	A	230	ASN
1	A	238	GLN
1	A	267	ASN
1	A	276	ASN
1	A	286	GLN
1	A	310	ASN
1	A	323	ASN
1	A	342	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0	8,8,8	1.30	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	-	-	1/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	SPD	C7-N6-C5	2.81	126.70	113.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	350	SPD	N1-C2-C3-C4

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, 95th 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 ²)	Q<0.9
1	A	322/325 (99%)	-0.61	1 (0%) 90 90	9, 24, 40, 53	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	GLY	2.8

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	SPD	A	350	10/10	0.94	0.06	5,5,8,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.