



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1SVN / pdb_00001svn
Title : SAVINASE
Authors : Betzel, C.; Klupsch, S.; Papendorf, G.; Hastrup, S.; Branner, S.; Wilson, K.S.
Deposited on : 1995-09-01
Resolution : 1.40 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
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

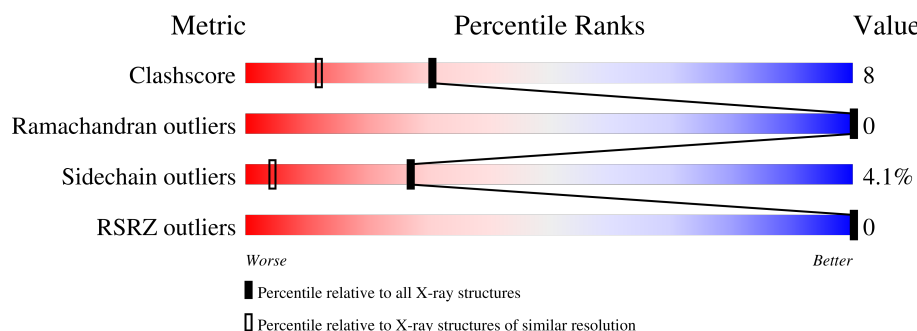
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	269	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2042 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 SAVINASE (TM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	1	0	0
			1880	1150	347	380	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

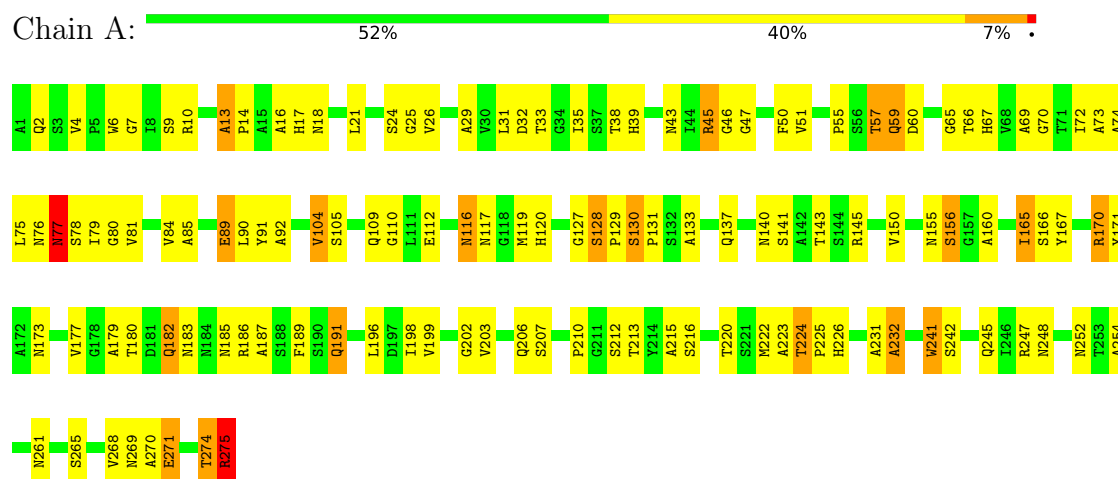
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		

3 Residue-property plots

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: SAVINASE (TM)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.47Å 64.24Å 42.89Å 90.00° 118.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.40 10.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	77.0 (10.00-1.40) 76.7 (10.00-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.79 (at 1.40Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.152 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.5	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2042	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA

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	1.67	13/1914 (0.7%)	2.71	167/2614 (6.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ARG	C-OXT	12.55	1.48	1.23
1	A	9	SER	C-N	6.83	1.42	1.33
1	A	75	LEU	C-O	-6.70	1.15	1.23
1	A	74	ALA	CA-C	6.56	1.61	1.52
1	A	32	ASP	CA-CB	6.20	1.60	1.54
1	A	222	MET	C-O	5.83	1.31	1.24
1	A	224	THR	CA-CB	5.75	1.60	1.53
1	A	199	VAL	C-O	5.70	1.29	1.23
1	A	196	LEU	N-CA	5.59	1.52	1.46
1	A	13	ALA	CA-C	5.47	1.59	1.52
1	A	81	VAL	CA-CB	5.33	1.61	1.54
1	A	31	LEU	N-CA	5.20	1.53	1.46
1	A	78	SER	CA-CB	5.14	1.60	1.53

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ARG	NE-CZ-NH1	16.60	138.10	121.50
1	A	165	ILE	CA-CB-CG2	15.86	137.46	110.50
1	A	116	ASN	OD1-CG-ND2	15.50	138.10	122.60
1	A	170	ARG	NE-CZ-NH2	-12.57	107.89	119.20
1	A	170	ARG	CD-NE-CZ	12.30	141.62	124.40
1	A	252	ASN	CA-CB-CG	-11.42	101.18	112.60
1	A	18	ASN	OD1-CG-ND2	11.21	133.81	122.60
1	A	145	ARG	CD-NE-CZ	11.11	139.95	124.40
1	A	165	ILE	CA-CB-CG1	-10.57	92.43	110.40
1	A	145	ARG	CG-CD-NE	10.39	134.86	112.00
1	A	206	GLN	OE1-CD-NE2	10.06	132.66	122.60
1	A	252	ASN	OD1-CG-ND2	-9.86	112.74	122.60
1	A	224	THR	O-C-N	9.84	129.90	120.55
1	A	155	ASN	O-C-N	9.73	134.65	122.20
1	A	271	GLU	O-C-N	-9.57	111.75	122.09
1	A	39	HIS	O-C-N	9.55	129.28	121.83
1	A	183	ASN	OD1-CG-ND2	9.39	131.99	122.60
1	A	25	GLY	CA-C-N	-9.37	111.58	123.19
1	A	25	GLY	C-N-CA	-9.37	111.58	123.19
1	A	89	GLU	CB-CG-CD	-9.08	97.16	112.60
1	A	32	ASP	CA-C-O	-8.84	113.82	120.19
1	A	170	ARG	CG-CD-NE	-8.67	92.93	112.00
1	A	17	HIS	CG-CD2-NE2	-8.54	98.66	107.20
1	A	247	ARG	NH1-CZ-NH2	8.30	130.09	119.30
1	A	70	GLY	O-C-N	-8.29	113.45	122.24
1	A	186	ARG	O-C-N	-8.24	112.79	122.93
1	A	17	HIS	ND1-CG-CD2	8.20	114.30	106.10
1	A	131	PRO	N-CA-CB	8.20	110.48	103.35
1	A	166	SER	CA-CB-OG	-8.20	94.71	111.10
1	A	105	SER	CA-CB-OG	-8.17	94.76	111.10
1	A	10	ARG	NE-CZ-NH1	8.14	129.65	121.50
1	A	145	ARG	NE-CZ-NH1	8.11	129.61	121.50
1	A	73	ALA	N-CA-CB	-8.09	102.08	111.79
1	A	130	SER	N-CA-C	7.90	121.11	109.42
1	A	155	ASN	OD1-CG-ND2	7.89	130.49	122.60
1	A	105	SER	O-C-N	7.87	130.18	122.07
1	A	185	ASN	CA-CB-CG	-7.81	104.79	112.60
1	A	274	THR	O-C-N	7.81	131.54	122.25
1	A	85	ALA	CA-C-N	7.78	127.45	119.82
1	A	85	ALA	C-N-CA	7.78	127.45	119.82
1	A	4	VAL	O-C-N	7.31	127.65	120.92
1	A	220	THR	N-CA-C	-7.31	103.62	112.54
1	A	254	ALA	O-C-N	7.27	131.08	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	SER	CB-CA-C	7.19	121.99	110.19
1	A	50	PHE	CA-CB-CG	-7.12	106.68	113.80
1	A	128	SER	CA-C-N	7.00	126.63	119.56
1	A	128	SER	C-N-CA	7.00	126.63	119.56
1	A	16	ALA	CA-C-O	-6.97	113.03	120.42
1	A	43	ASN	CA-C-N	-6.97	114.06	123.12
1	A	43	ASN	C-N-CA	-6.97	114.06	123.12
1	A	25	GLY	O-C-N	6.93	131.07	122.41
1	A	270	ALA	O-C-N	6.92	130.78	122.27
1	A	226	HIS	N-CA-C	-6.87	103.87	111.36
1	A	137	GLN	O-C-N	6.87	129.40	122.12
1	A	13	ALA	O-C-N	6.80	127.11	120.71
1	A	91	TYR	O-C-N	6.77	131.28	123.29
1	A	241	TRP	O-C-N	6.70	130.53	122.96
1	A	165	ILE	CA-C-O	-6.67	113.10	120.84
1	A	137	GLN	CA-C-O	-6.64	113.51	120.55
1	A	78	SER	CA-CB-OG	-6.63	97.84	111.10
1	A	127	GLY	O-C-N	6.61	131.29	122.70
1	A	73	ALA	CA-C-O	-6.57	115.11	121.02
1	A	155	ASN	CA-C-O	-6.55	112.62	120.55
1	A	60	ASP	CA-C-O	6.51	127.72	120.43
1	A	261	ASN	OD1-CG-ND2	6.50	129.10	122.60
1	A	133	ALA	CA-C-O	6.48	127.43	119.97
1	A	67	HIS	O-C-N	-6.44	115.43	122.07
1	A	268	VAL	O-C-N	6.44	129.46	122.63
1	A	69	ALA	CA-C-O	-6.44	113.72	120.55
1	A	183	ASN	O-C-N	6.39	130.01	122.34
1	A	78	SER	CA-C-O	6.39	128.51	120.65
1	A	231	ALA	O-C-N	6.38	129.42	122.15
1	A	18	ASN	O-C-N	-6.37	114.77	122.22
1	A	160	ALA	CA-C-O	-6.27	114.41	121.81
1	A	57	THR	O-C-N	-6.25	114.83	122.34
1	A	171	TYR	CA-C-O	-6.25	114.16	121.16
1	A	72	ILE	CB-CA-C	-6.25	103.87	112.24
1	A	35	ILE	N-CA-C	-6.20	99.12	108.17
1	A	105	SER	CB-CA-C	-6.17	101.20	110.88
1	A	116	ASN	CB-CG-ND2	-6.14	107.19	116.40
1	A	247	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	186	ARG	NE-CZ-NH2	-6.04	113.77	119.20
1	A	59	GLN	OE1-CD-NE2	6.03	128.63	122.60
1	A	110	GLY	O-C-N	-5.99	115.75	122.28
1	A	210	PRO	CA-C-O	5.99	128.14	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ALA	N-CA-C	5.96	118.60	110.55
1	A	130	SER	CA-C-O	5.94	124.03	119.46
1	A	72	ILE	CA-C-O	-5.94	114.35	120.71
1	A	213	THR	CA-CB-OG1	-5.92	100.73	109.60
1	A	187	ALA	N-CA-C	-5.89	102.33	110.35
1	A	90	LEU	CB-CA-C	-5.89	100.14	109.80
1	A	191	GLN	CA-CB-CG	-5.88	102.34	114.10
1	A	80	GLY	N-CA-C	5.86	121.91	111.02
1	A	271	GLU	CA-C-O	5.84	126.71	120.70
1	A	140	ASN	CA-CB-CG	-5.83	106.77	112.60
1	A	46	GLY	O-C-N	5.81	129.40	123.88
1	A	45	ARG	CB-CG-CD	-5.79	97.99	111.30
1	A	223	ALA	CA-C-O	5.76	126.53	120.42
1	A	17	HIS	CE1-NE2-CD2	5.74	114.74	109.00
1	A	109	GLN	CB-CG-CD	-5.72	102.87	112.60
1	A	215	ALA	CA-C-O	5.72	127.39	120.99
1	A	165	ILE	N-CA-C	5.68	117.18	108.71
1	A	216	SER	O-C-N	-5.68	116.57	123.27
1	A	89	GLU	O-C-N	5.67	129.74	122.93
1	A	155	ASN	CB-CG-ND2	-5.64	107.95	116.40
1	A	77	ASN	OD1-CG-ND2	5.63	128.23	122.60
1	A	112	GLU	O-C-N	5.60	128.53	122.15
1	A	4	VAL	CA-C-O	-5.60	113.79	119.89
1	A	156	SER	CA-C-O	-5.57	111.98	119.11
1	A	242	SER	N-CA-CB	-5.54	102.01	110.49
1	A	198	ILE	N-CA-CB	-5.51	102.13	111.23
1	A	212	SER	CB-CA-C	-5.50	103.76	111.80
1	A	171	TYR	CA-C-N	5.49	127.90	120.38
1	A	171	TYR	C-N-CA	5.49	127.90	120.38
1	A	79	ILE	CB-CA-C	-5.47	101.93	110.52
1	A	110	GLY	CA-C-N	5.46	127.59	120.28
1	A	110	GLY	C-N-CA	5.46	127.59	120.28
1	A	183	ASN	CB-CA-C	-5.46	101.34	110.56
1	A	104	VAL	CA-CB-CG2	-5.45	101.14	110.40
1	A	275	ARG	CG-CD-NE	5.44	123.97	112.00
1	A	269	ASN	O-C-N	5.44	130.10	123.14
1	A	185	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	A	31	LEU	O-C-N	5.42	129.56	122.68
1	A	67	HIS	ND1-CG-CD2	5.41	111.51	106.10
1	A	84	VAL	N-CA-C	-5.41	105.26	110.72
1	A	275	ARG	CB-CA-C	5.41	120.37	110.10
1	A	145	ARG	CA-CB-CG	-5.38	103.35	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	HIS	CA-C-O	5.36	126.45	120.82
1	A	65	GLY	O-C-N	5.35	127.38	122.19
1	A	213	THR	OG1-CB-CG2	5.34	119.99	109.30
1	A	241	TRP	CA-C-N	-5.32	111.96	122.02
1	A	241	TRP	C-N-CA	-5.32	111.96	122.02
1	A	128	SER	CA-C-O	5.32	125.34	119.91
1	A	247	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	A	39	HIS	N-CA-CB	-5.32	103.38	110.77
1	A	224	THR	CA-C-O	-5.30	113.75	118.63
1	A	183	ASN	CA-C-N	-5.29	115.12	122.74
1	A	183	ASN	C-N-CA	-5.29	115.12	122.74
1	A	120	HIS	ND1-CG-CD2	5.28	111.38	106.10
1	A	38	THR	N-CA-C	-5.24	103.23	110.35
1	A	33	THR	O-C-N	5.22	130.82	122.42
1	A	16	ALA	N-CA-C	-5.20	105.69	111.36
1	A	232	ALA	CA-C-O	-5.20	114.91	120.42
1	A	55	PRO	N-CA-C	5.20	120.38	113.57
1	A	143	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	180	THR	CA-CB-CG2	5.17	119.29	110.50
1	A	85	ALA	O-C-N	-5.16	116.79	121.17
1	A	207	SER	CA-C-O	5.16	126.83	121.31
1	A	51	VAL	CA-C-O	5.15	124.56	119.62
1	A	265	SER	CA-CB-OG	-5.14	100.83	111.10
1	A	117	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	182	GLN	O-C-N	-5.13	115.72	122.39
1	A	167	TYR	CA-CB-CG	-5.12	104.68	113.90
1	A	109	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	66	THR	CA-C-N	5.10	127.08	120.44
1	A	66	THR	C-N-CA	5.10	127.08	120.44
1	A	248	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	A	182	GLN	CB-CG-CD	5.09	121.25	112.60
1	A	17	HIS	CA-CB-CG	-5.08	108.72	113.80
1	A	141	SER	N-CA-CB	-5.08	102.71	110.07
1	A	177	VAL	N-CA-C	5.07	115.15	107.75
1	A	7	GLY	CA-C-O	5.06	125.86	120.40
1	A	203	VAL	CA-C-O	-5.03	115.11	120.39
1	A	170	ARG	N-CA-CB	-5.02	102.06	110.39
1	A	77	ASN	CA-C-N	-5.00	114.63	122.79
1	A	77	ASN	C-N-CA	-5.00	114.63	122.79
1	A	9	SER	CA-CB-OG	-5.00	101.09	111.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	THR	Mainchain

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	1880	0	1838	31	0
2	A	2	0	0	0	0
3	A	160	0	0	6	1
All	All	2042	0	1838	31	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 8.

All (31) 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:89:GLU:CD	3:A:332:HOH:O	1.84	1.19
1:A:45:ARG:HH11	1:A:45:ARG:HB3	1.20	1.06
1:A:45:ARG:CZ	3:A:373:HOH:O	2.19	0.90
1:A:45:ARG:HB3	1:A:45:ARG:NH1	1.90	0.86
1:A:156:SER:H	1:A:191:GLN:HE21	1.28	0.82
1:A:89:GLU:CG	3:A:332:HOH:O	2.24	0.78
1:A:45:ARG:HD2	1:A:89:GLU:HG2	1.70	0.73
1:A:59:GLN:HG3	3:A:317:HOH:O	1.90	0.72
1:A:45:ARG:HD2	1:A:89:GLU:CG	2.26	0.66
1:A:173:ASN:O	3:A:414:HOH:O	2.14	0.64
1:A:128:SER:HB2	1:A:129:PRO:HD2	1.84	0.58
1:A:45:ARG:HD2	1:A:89:GLU:CB	2.37	0.55
1:A:156:SER:H	1:A:191:GLN:NE2	1.99	0.55
1:A:2:GLN:HE22	1:A:76:ASN:HD22	1.54	0.55
1:A:241:TRP:HA	1:A:245:GLN:OE1	2.08	0.54
1:A:45:ARG:CD	1:A:89:GLU:HB3	2.40	0.52
1:A:47:GLY:HA3	1:A:92:ALA:O	2.12	0.50
1:A:45:ARG:NH2	3:A:373:HOH:O	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:HD22	1:A:77:ASN:C	2.21	0.48
1:A:2:GLN:HE22	1:A:76:ASN:ND2	2.12	0.47
1:A:45:ARG:HD2	1:A:89:GLU:HB3	1.98	0.44
1:A:6:TRP:CZ2	1:A:182:GLN:HG3	2.52	0.44
1:A:13:ALA:N	1:A:14:PRO:CD	2.81	0.43
1:A:29:ALA:HB2	1:A:119:MET:HG3	1.99	0.43
1:A:21:LEU:CD1	1:A:274:THR:HB	2.49	0.42
1:A:224:THR:N	1:A:225:PRO:HD2	2.33	0.42
1:A:179:ALA:HB1	1:A:202:GLY:HA3	2.02	0.41
1:A:271:GLU:OE1	1:A:275:ARG:NH2	2.48	0.41
1:A:26:VAL:HG11	1:A:232:ALA:HA	2.03	0.40
1:A:150:VAL:HG12	1:A:224:THR:HG23	2.04	0.40
1:A:189:PHE:CD1	1:A:189:PHE:C	2.99	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)
3:A:372:HOH:O	3:A:396:HOH:O[2_646]	2.15	0.05

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	267/269 (99%)	261 (98%)	6 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	194/194 (100%)	186 (96%)	8 (4%)	27 4

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	77	ASN
1	A	104	VAL
1	A	116	ASN
1	A	130	SER
1	A	165	ILE
1	A	170	ARG
1	A	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	77	ASN
1	A	173	ASN
1	A	182	GLN
1	A	191	GLN
1	A	204	ASN
1	A	261	ASN

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	269/269 (100%)	-0.66	0 100 100	4, 9, 19, 28	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 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	CA	A	277	1/1	0.98	0.10	14,14,14,14	1
2	CA	A	276	1/1	1.00	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.