



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:03 PM UTC

PDB ID : 5YWL / pdb_00005ywl
Title : SsCR_L211H
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Deposited on : 2017-11-29
Resolution : 2.10 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

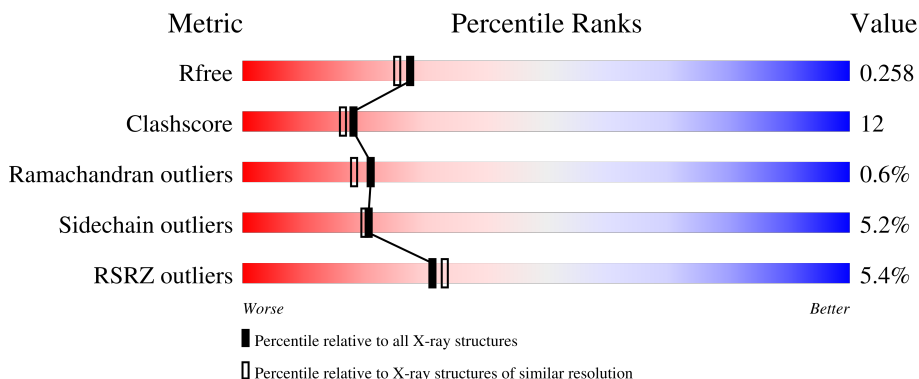
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	334	5% 45% 46% 7% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2835 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 induced by osmotic stress.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2593	1663	422	505	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	HIS	LEU	engineered mutation	UNP A3LWG4

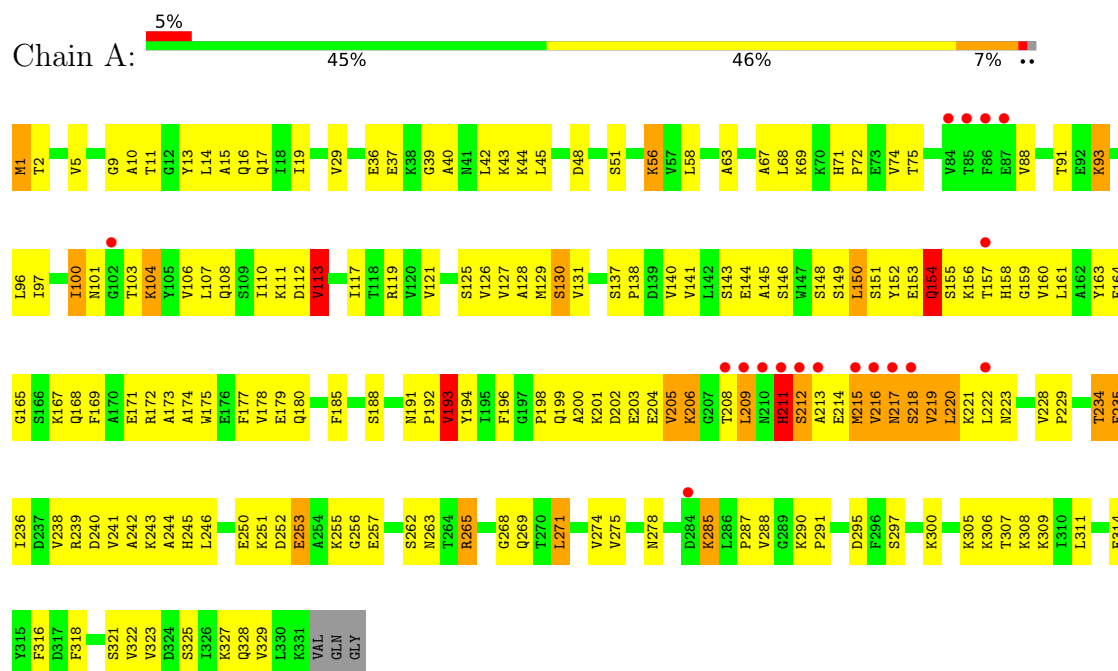
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	242	Total	O	0	0
			242	242		

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: Protein induced by osmotic stress



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.76Å 53.15Å 140.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.43 – 2.10 34.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (34.43-2.10) 97.6 (34.43-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.32 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.206 , 0.265 (Not available) , 0.258	Depositor DCC
R_{free} test set	1090 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2835	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

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	2.34	149/2646 (5.6%)	1.28	13/3583 (0.4%)

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	LYS	C-O	-8.95	1.13	1.24
1	A	163	TYR	C-O	-8.93	1.13	1.24
1	A	126	VAL	C-O	-8.82	1.13	1.24
1	A	242	ALA	C-O	-8.65	1.14	1.24
1	A	128	ALA	C-O	-8.41	1.13	1.24
1	A	311	LEU	C-O	-8.30	1.14	1.24
1	A	323	VAL	C-O	-8.20	1.14	1.24
1	A	255	LYS	C-O	-7.75	1.14	1.23
1	A	14	LEU	C-O	-7.72	1.15	1.24
1	A	144	GLU	C-O	-7.72	1.14	1.24
1	A	288	VAL	C-O	-7.72	1.15	1.23
1	A	143	SER	C-O	-7.63	1.14	1.24
1	A	141	VAL	C-O	-7.60	1.16	1.24
1	A	110	ILE	C-O	-7.55	1.15	1.24
1	A	171	GLU	C-O	-7.51	1.15	1.24
1	A	215	MET	C-O	-7.45	1.14	1.24
1	A	58	LEU	C-O	-7.41	1.14	1.24
1	A	238	VAL	C-O	-7.32	1.15	1.24
1	A	111	LYS	C-O	-7.31	1.15	1.24
1	A	263	ASN	C-O	-7.31	1.14	1.24
1	A	117	ILE	C-O	-7.29	1.16	1.24
1	A	309	LYS	C-O	-7.26	1.15	1.24
1	A	236	ILE	C-O	-7.25	1.15	1.23
1	A	127	VAL	C-O	-7.24	1.14	1.24
1	A	168	GLN	C-O	-7.21	1.15	1.24
1	A	140	VAL	C-O	-7.19	1.15	1.24
1	A	10	ALA	C-O	-7.18	1.14	1.24
1	A	19	ILE	C-O	-7.18	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	GLN	C-O	-7.14	1.15	1.24
1	A	169	PHE	C-O	-7.08	1.15	1.24
1	A	275	VAL	C-O	-7.06	1.16	1.24
1	A	256	GLY	C-O	-7.04	1.13	1.23
1	A	193	VAL	C-O	-7.03	1.15	1.24
1	A	148	SER	C-O	-7.01	1.15	1.23
1	A	308	LYS	C-O	-6.97	1.16	1.24
1	A	173	ALA	C-O	-6.95	1.16	1.24
1	A	278	ASN	C-O	-6.94	1.15	1.24
1	A	180	GLN	C-O	-6.92	1.16	1.24
1	A	322	VAL	C-O	-6.91	1.16	1.24
1	A	16	GLN	C-O	-6.90	1.16	1.24
1	A	253	GLU	C-O	-6.87	1.15	1.24
1	A	325	SER	C-O	-6.84	1.16	1.24
1	A	63	ALA	C-O	-6.80	1.16	1.24
1	A	167	LYS	C-O	-6.78	1.16	1.24
1	A	101	ASN	C-O	-6.76	1.16	1.24
1	A	321	SER	C-O	-6.75	1.16	1.24
1	A	245	HIS	C-O	-6.74	1.16	1.24
1	A	11	THR	C-O	-6.73	1.15	1.24
1	A	145	ALA	C-O	-6.73	1.15	1.24
1	A	69	LYS	C-O	-6.70	1.16	1.24
1	A	96	LEU	C-O	-6.69	1.16	1.24
1	A	252	ASP	C-O	-6.66	1.16	1.24
1	A	156	LYS	C-O	-6.63	1.15	1.24
1	A	150	LEU	C-O	-6.62	1.16	1.23
1	A	250	GLU	C-O	-6.59	1.16	1.24
1	A	328	GLN	C-O	-6.57	1.16	1.24
1	A	239	ARG	C-O	-6.51	1.16	1.24
1	A	72	PRO	C-O	-6.47	1.15	1.24
1	A	106	VAL	C-O	-6.42	1.16	1.24
1	A	246	LEU	C-O	-6.40	1.16	1.24
1	A	108	GLN	C-O	-6.39	1.16	1.24
1	A	251	LYS	C-O	-6.37	1.16	1.23
1	A	37	GLU	C-O	-6.36	1.16	1.24
1	A	327	LYS	C-O	-6.36	1.16	1.24
1	A	297	SER	C-O	-6.35	1.16	1.24
1	A	172	ARG	C-O	-6.33	1.16	1.24
1	A	318	PHE	C-O	-6.27	1.16	1.24
1	A	205	VAL	C-O	-6.26	1.16	1.24
1	A	240	ASP	C-O	-6.23	1.16	1.24
1	A	271	LEU	C-O	-6.21	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	ALA	C-O	-6.20	1.16	1.24
1	A	40	ALA	C-O	-6.20	1.16	1.24
1	A	93	LYS	C-O	-6.19	1.16	1.24
1	A	274	VAL	C-O	-6.16	1.17	1.24
1	A	155	SER	C-O	-6.14	1.16	1.24
1	A	191	ASN	C-O	-6.12	1.17	1.24
1	A	146	SER	C-O	-6.10	1.16	1.24
1	A	121	VAL	C-O	-6.08	1.17	1.24
1	A	125	SER	C-O	-6.07	1.16	1.23
1	A	67	ALA	C-O	-6.03	1.17	1.24
1	A	138	PRO	C-O	-6.00	1.16	1.24
1	A	36	GLU	C-O	-5.99	1.17	1.24
1	A	174	ALA	C-O	-5.99	1.17	1.24
1	A	234	THR	C-O	-5.98	1.16	1.23
1	A	192	PRO	C-O	-5.92	1.17	1.23
1	A	307	THR	C-O	-5.91	1.17	1.24
1	A	152	TYR	C-O	-5.91	1.17	1.24
1	A	290	LYS	C-O	-5.90	1.17	1.24
1	A	13	TYR	C-O	-5.89	1.17	1.24
1	A	9	GLY	C-O	-5.88	1.16	1.23
1	A	306	LYS	C-O	-5.86	1.17	1.24
1	A	314	GLU	C-O	-5.81	1.17	1.23
1	A	287	PRO	C-O	-5.80	1.17	1.23
1	A	104	LYS	C-O	-5.77	1.17	1.24
1	A	153	GLU	C-O	-5.77	1.17	1.24
1	A	45	LEU	C-O	-5.76	1.17	1.24
1	A	157	THR	C-O	-5.76	1.16	1.24
1	A	103	THR	C-O	-5.76	1.17	1.24
1	A	48	ASP	C-O	-5.71	1.17	1.24
1	A	300	LYS	C-O	-5.71	1.17	1.23
1	A	119	ARG	C-O	-5.67	1.17	1.24
1	A	262	SER	C-O	-5.65	1.17	1.23
1	A	131	VAL	C-O	-5.62	1.18	1.24
1	A	257	GLU	C-O	-5.57	1.17	1.23
1	A	268	GLY	C-O	-5.57	1.17	1.23
1	A	269	GLN	C-O	-5.57	1.17	1.24
1	A	185	PHE	C-O	-5.57	1.17	1.23
1	A	201	LYS	C-O	-5.55	1.17	1.23
1	A	97	ILE	C-O	-5.54	1.17	1.24
1	A	42	LEU	C-O	-5.54	1.17	1.24
1	A	159	GLY	C-O	-5.53	1.17	1.23
1	A	5	VAL	C-O	-5.52	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ILE	N-CA	-5.52	1.40	1.46
1	A	15	ALA	C-O	-5.50	1.17	1.24
1	A	44	LYS	C-O	-5.48	1.17	1.24
1	A	129	MET	N-CA	-5.48	1.38	1.46
1	A	91	THR	C-O	-5.47	1.17	1.24
1	A	175	TRP	C-O	-5.45	1.17	1.24
1	A	149	SER	C-O	-5.43	1.17	1.24
1	A	161	LEU	C-O	-5.41	1.17	1.24
1	A	75	THR	C-O	-5.40	1.17	1.24
1	A	316	PHE	C-O	-5.40	1.17	1.23
1	A	295	ASP	C-O	-5.39	1.18	1.24
1	A	100	ILE	C-O	-5.36	1.18	1.24
1	A	228	VAL	C-O	-5.26	1.18	1.25
1	A	137	SER	C-O	-5.26	1.17	1.24
1	A	178	VAL	C-O	-5.26	1.18	1.24
1	A	265	ARG	CZ-NH2	-5.23	1.26	1.33
1	A	130	SER	C-O	-5.21	1.18	1.23
1	A	305	LYS	C-O	-5.21	1.18	1.24
1	A	107	LEU	C-O	-5.20	1.18	1.24
1	A	217	ASN	CA-C	-5.17	1.46	1.52
1	A	29	VAL	C-O	-5.16	1.18	1.24
1	A	43	LYS	C-O	-5.13	1.18	1.24
1	A	179	GLU	C-O	-5.13	1.18	1.24
1	A	39	GLY	C-O	-5.11	1.17	1.23
1	A	112	ASP	C-O	-5.08	1.18	1.24
1	A	244	ALA	C-O	-5.08	1.18	1.24
1	A	198	PRO	C-O	-5.07	1.17	1.23
1	A	194	TYR	C-O	-5.07	1.17	1.24
1	A	229	PRO	CA-C	-5.06	1.46	1.52
1	A	241	VAL	C-O	-5.06	1.18	1.24
1	A	165	GLY	C-O	-5.05	1.17	1.23
1	A	177	PHE	C-O	-5.05	1.18	1.24
1	A	17	GLN	C-O	-5.04	1.18	1.24
1	A	202	ASP	C-O	-5.04	1.18	1.24
1	A	188	SER	CA-C	5.04	1.58	1.52
1	A	164	PHE	C-O	-5.02	1.18	1.24
1	A	291	PRO	C-O	-5.00	1.17	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	VAL	N-CA-C	8.73	118.80	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLU	N-CA-C	7.91	119.98	111.36
1	A	211	HIS	N-CA-C	7.39	120.21	107.28
1	A	56	LYS	N-CA-C	7.32	119.34	111.36
1	A	180	GLN	N-CA-C	6.86	118.55	111.14
1	A	45	LEU	N-CA-C	6.41	118.35	111.36
1	A	130	SER	N-CA-C	6.38	117.00	108.38
1	A	58	LEU	N-CA-C	6.07	118.69	111.71
1	A	88	VAL	CB-CA-C	-5.65	102.41	110.83
1	A	113	VAL	CB-CA-C	5.48	115.78	110.63
1	A	278	ASN	N-CA-C	5.36	118.04	111.82
1	A	218	SER	N-CA-C	-5.18	105.53	111.07
1	A	2	THR	N-CA-C	-5.12	101.93	110.17

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	2593	0	2596	63	0
2	A	242	0	0	2	0
All	All	2835	0	2596	63	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 12.

All (63) 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:211:HIS:CB	1:A:217:ASN:HB2	1.65	1.24
1:A:211:HIS:HB3	1:A:217:ASN:CB	1.84	1.06
1:A:211:HIS:HB3	1:A:217:ASN:HB2	1.06	1.02
1:A:209:LEU:HA	1:A:329:VAL:HG13	1.44	0.98
1:A:211:HIS:HB2	1:A:214:GLU:HA	1.48	0.95
1:A:211:HIS:CB	1:A:214:GLU:HA	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:OG	1:A:154:GLN:HG2	1.74	0.88
1:A:213:ALA:O	1:A:216:VAL:CG2	2.24	0.85
1:A:211:HIS:O	1:A:211:HIS:ND1	2.10	0.85
1:A:208:THR:O	1:A:209:LEU:HB2	1.78	0.83
1:A:213:ALA:O	1:A:216:VAL:HG22	1.79	0.82
1:A:203:GLU:OE1	1:A:203:GLU:N	2.11	0.80
1:A:211:HIS:O	1:A:214:GLU:CA	2.39	0.71
1:A:211:HIS:O	1:A:214:GLU:HB3	1.92	0.69
1:A:211:HIS:CG	1:A:217:ASN:HB2	2.26	0.69
1:A:211:HIS:CG	1:A:214:GLU:HA	2.28	0.68
1:A:211:HIS:O	1:A:214:GLU:HA	1.95	0.67
1:A:211:HIS:O	1:A:214:GLU:CB	2.43	0.66
1:A:211:HIS:CE1	1:A:214:GLU:HB2	2.30	0.66
1:A:100:ILE:HG22	1:A:104:LYS:HE3	1.79	0.64
1:A:158:HIS:CE1	1:A:160:VAL:HG23	2.33	0.63
1:A:211:HIS:C	1:A:214:GLU:HA	2.24	0.62
1:A:219:VAL:HG21	1:A:271:LEU:CD2	2.32	0.60
1:A:209:LEU:HA	1:A:329:VAL:CG1	2.27	0.58
1:A:214:GLU:O	1:A:217:ASN:N	2.31	0.57
1:A:151:SER:HG	1:A:154:GLN:HG2	1.72	0.54
1:A:211:HIS:HD2	1:A:217:ASN:C	2.16	0.54
1:A:219:VAL:HG21	1:A:271:LEU:HD23	1.89	0.54
1:A:211:HIS:HB2	1:A:214:GLU:CA	2.32	0.53
1:A:100:ILE:CG2	1:A:104:LYS:HE3	2.38	0.53
1:A:158:HIS:HE1	1:A:160:VAL:HG23	1.70	0.53
1:A:219:VAL:HA	1:A:222:LEU:HG	1.92	0.52
1:A:218:SER:O	1:A:221:LYS:HG2	2.11	0.51
1:A:211:HIS:ND1	1:A:214:GLU:HB2	2.26	0.50
1:A:212:SER:HA	1:A:214:GLU:N	2.28	0.49
1:A:212:SER:HA	1:A:213:ALA:C	2.36	0.49
1:A:212:SER:CA	1:A:213:ALA:C	2.85	0.48
1:A:196:PHE:CD2	1:A:216:VAL:HG13	2.50	0.47
1:A:211:HIS:C	1:A:211:HIS:HD1	2.21	0.47
1:A:213:ALA:O	1:A:216:VAL:HG23	2.13	0.46
1:A:206:LYS:HD3	1:A:206:LYS:C	2.41	0.46
1:A:211:HIS:HB2	1:A:217:ASN:HB2	1.79	0.46
1:A:219:VAL:CG2	1:A:271:LEU:HD23	2.46	0.46
1:A:150:LEU:HD12	1:A:154:GLN:HG3	1.98	0.45
1:A:205:VAL:O	1:A:205:VAL:HG12	2.16	0.45
1:A:196:PHE:CD1	1:A:235:PHE:HB2	2.52	0.45
1:A:217:ASN:HD22	1:A:220:LEU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:HIS:CD2	1:A:217:ASN:CB	2.99	0.44
1:A:211:HIS:CG	1:A:214:GLU:CA	2.99	0.44
1:A:204:GLU:O	1:A:206:LYS:N	2.51	0.44
1:A:211:HIS:ND1	1:A:214:GLU:CB	2.82	0.43
1:A:71:HIS:HB3	1:A:74:VAL:HG23	2.00	0.43
1:A:211:HIS:HB3	1:A:217:ASN:CG	2.37	0.43
1:A:56:LYS:HE2	1:A:56:LYS:HB3	1.88	0.43
1:A:211:HIS:O	1:A:211:HIS:CG	2.69	0.43
1:A:193:VAL:HG11	1:A:234:THR:OG1	2.19	0.42
1:A:206:LYS:C	1:A:206:LYS:CD	2.92	0.42
1:A:211:HIS:CG	1:A:214:GLU:HB2	2.55	0.41
1:A:68:LEU:HB3	1:A:113:VAL:HG12	2.02	0.41
1:A:1:MET:HG2	2:A:607:HOH:O	2.20	0.41
1:A:223:ASN:HA	1:A:285:LYS:O	2.20	0.41
1:A:253:GLU:CD	1:A:253:GLU:H	2.29	0.40
1:A:265:ARG:HG3	2:A:609:HOH:O	2.20	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	329/334 (98%)	322 (98%)	5 (2%)	2 (1%)	21 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	LEU
1	A	193	VAL

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	287/289 (99%)	272 (95%)	15 (5%)	21	20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	51	SER
1	A	93	LYS
1	A	113	VAL
1	A	130	SER
1	A	154	GLN
1	A	199	GLN
1	A	206	LYS
1	A	211	HIS
1	A	212	SER
1	A	215	MET
1	A	216	VAL
1	A	220	LEU
1	A	235	PHE
1	A	285	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	180	GLN
1	A	217	ASN

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 oligosaccharides 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, 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	331/334 (99%)	0.21	18 (5%) 31 33	5, 19, 50, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	SER	5.2
1	A	209	LEU	5.0
1	A	86	PHE	4.5
1	A	216	VAL	4.4
1	A	85	THR	4.3
1	A	208	THR	4.1
1	A	212	SER	3.6
1	A	222	LEU	3.5
1	A	102	GLY	3.3
1	A	213	ALA	3.3
1	A	210	ASN	3.1
1	A	284	ASP	2.5
1	A	157	THR	2.5
1	A	215	MET	2.3
1	A	84	VAL	2.3
1	A	217	ASN	2.3
1	A	87	GLU	2.1
1	A	211	HIS	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.