



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:15 AM UTC

PDB ID : 8U1G / pdb_00008u1g
Title : Prefusion-stabilized SARS-CoV-2 S2 subunit
Authors : Hsieh, C.-L.; McLellan, J.S.
Deposited on : 2023-08-31
Resolution : 3.20 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

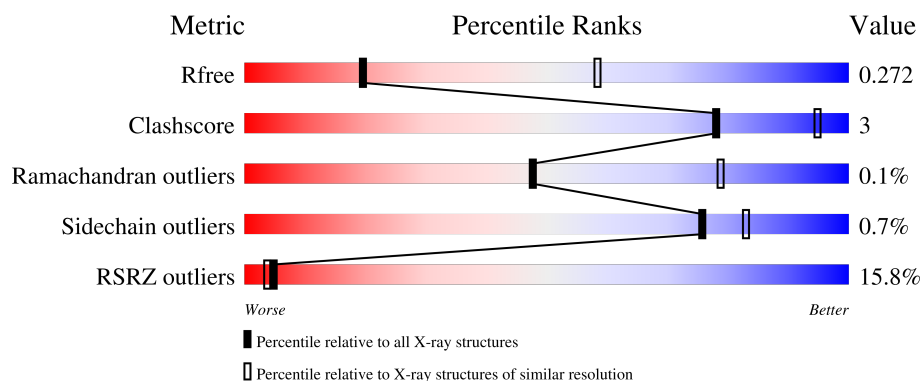
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	530	13% 69% 7% 23%
1	B	530	11% 71% 5% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6244 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 Spike protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3124	1988	525	594	17			
1	B	403	Total	C	N	O	S	0	0	0
			3106	1973	521	595	17			

There are 188 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	671	MET	-	initiating methionine	UNP P0DTC2
A	672	ARG	-	expression tag	UNP P0DTC2
A	673	PRO	-	expression tag	UNP P0DTC2
A	674	THR	-	expression tag	UNP P0DTC2
A	675	TRP	-	expression tag	UNP P0DTC2
A	676	ALA	-	expression tag	UNP P0DTC2
A	677	TRP	-	expression tag	UNP P0DTC2
A	678	TRP	-	expression tag	UNP P0DTC2
A	679	LEU	-	expression tag	UNP P0DTC2
A	680	PHE	-	expression tag	UNP P0DTC2
A	681	LEU	-	expression tag	UNP P0DTC2
A	682	VAL	-	expression tag	UNP P0DTC2
A	683	LEU	-	expression tag	UNP P0DTC2
A	684	LEU	-	expression tag	UNP P0DTC2
A	685	LEU	-	expression tag	UNP P0DTC2
A	686	ALA	-	expression tag	UNP P0DTC2
A	687	LEU	-	expression tag	UNP P0DTC2
A	688	TRP	-	expression tag	UNP P0DTC2
A	689	ALA	-	expression tag	UNP P0DTC2
A	690	PRO	-	expression tag	UNP P0DTC2
A	691	ALA	-	expression tag	UNP P0DTC2
A	692	ARG	-	expression tag	UNP P0DTC2
A	693	GLY	-	expression tag	UNP P0DTC2
A	694	ALA	-	expression tag	UNP P0DTC2
A	695	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	696	GLN	-	expression tag	UNP P0DTC2
A	704	CYS	SER	engineered mutation	UNP P0DTC2
A	790	CYS	LYS	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	957	GLU	GLN	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1142	GLY	-	expression tag	UNP P0DTC2
A	1143	SER	-	expression tag	UNP P0DTC2
A	1144	GLY	-	expression tag	UNP P0DTC2
A	1145	TYR	-	expression tag	UNP P0DTC2
A	1146	ILE	-	expression tag	UNP P0DTC2
A	1147	PRO	-	expression tag	UNP P0DTC2
A	1148	GLU	-	expression tag	UNP P0DTC2
A	1149	ALA	-	expression tag	UNP P0DTC2
A	1150	PRO	-	expression tag	UNP P0DTC2
A	1151	ARG	-	expression tag	UNP P0DTC2
A	1152	ASP	-	expression tag	UNP P0DTC2
A	1153	GLY	-	expression tag	UNP P0DTC2
A	1154	GLN	-	expression tag	UNP P0DTC2
A	1155	ALA	-	expression tag	UNP P0DTC2
A	1156	TYR	-	expression tag	UNP P0DTC2
A	1157	VAL	-	expression tag	UNP P0DTC2
A	1158	ARG	-	expression tag	UNP P0DTC2
A	1159	LYS	-	expression tag	UNP P0DTC2
A	1160	ASP	-	expression tag	UNP P0DTC2
A	1161	GLY	-	expression tag	UNP P0DTC2
A	1162	GLU	-	expression tag	UNP P0DTC2
A	1163	TRP	-	expression tag	UNP P0DTC2
A	1164	VAL	-	expression tag	UNP P0DTC2
A	1165	LEU	-	expression tag	UNP P0DTC2
A	1166	LEU	-	expression tag	UNP P0DTC2
A	1167	SER	-	expression tag	UNP P0DTC2
A	1168	THR	-	expression tag	UNP P0DTC2
A	1169	PHE	-	expression tag	UNP P0DTC2
A	1170	LEU	-	expression tag	UNP P0DTC2
A	1171	GLY	-	expression tag	UNP P0DTC2
A	1172	ARG	-	expression tag	UNP P0DTC2
A	1173	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	LEU	-	expression tag	UNP P0DTC2
A	1175	GLU	-	expression tag	UNP P0DTC2
A	1176	VAL	-	expression tag	UNP P0DTC2
A	1177	LEU	-	expression tag	UNP P0DTC2
A	1178	PHE	-	expression tag	UNP P0DTC2
A	1179	GLN	-	expression tag	UNP P0DTC2
A	1180	GLY	-	expression tag	UNP P0DTC2
A	1181	PRO	-	expression tag	UNP P0DTC2
A	1182	GLY	-	expression tag	UNP P0DTC2
A	1183	HIS	-	expression tag	UNP P0DTC2
A	1184	HIS	-	expression tag	UNP P0DTC2
A	1185	HIS	-	expression tag	UNP P0DTC2
A	1186	HIS	-	expression tag	UNP P0DTC2
A	1187	HIS	-	expression tag	UNP P0DTC2
A	1188	HIS	-	expression tag	UNP P0DTC2
A	1189	HIS	-	expression tag	UNP P0DTC2
A	1190	HIS	-	expression tag	UNP P0DTC2
A	1191	SER	-	expression tag	UNP P0DTC2
A	1192	ALA	-	expression tag	UNP P0DTC2
A	1193	TRP	-	expression tag	UNP P0DTC2
A	1194	SER	-	expression tag	UNP P0DTC2
A	1195	HIS	-	expression tag	UNP P0DTC2
A	1196	PRO	-	expression tag	UNP P0DTC2
A	1197	GLN	-	expression tag	UNP P0DTC2
A	1198	PHE	-	expression tag	UNP P0DTC2
A	1199	GLU	-	expression tag	UNP P0DTC2
A	1200	LYS	-	expression tag	UNP P0DTC2
B	671	MET	-	initiating methionine	UNP P0DTC2
B	672	ARG	-	expression tag	UNP P0DTC2
B	673	PRO	-	expression tag	UNP P0DTC2
B	674	THR	-	expression tag	UNP P0DTC2
B	675	TRP	-	expression tag	UNP P0DTC2
B	676	ALA	-	expression tag	UNP P0DTC2
B	677	TRP	-	expression tag	UNP P0DTC2
B	678	TRP	-	expression tag	UNP P0DTC2
B	679	LEU	-	expression tag	UNP P0DTC2
B	680	PHE	-	expression tag	UNP P0DTC2
B	681	LEU	-	expression tag	UNP P0DTC2
B	682	VAL	-	expression tag	UNP P0DTC2
B	683	LEU	-	expression tag	UNP P0DTC2
B	684	LEU	-	expression tag	UNP P0DTC2
B	685	LEU	-	expression tag	UNP P0DTC2

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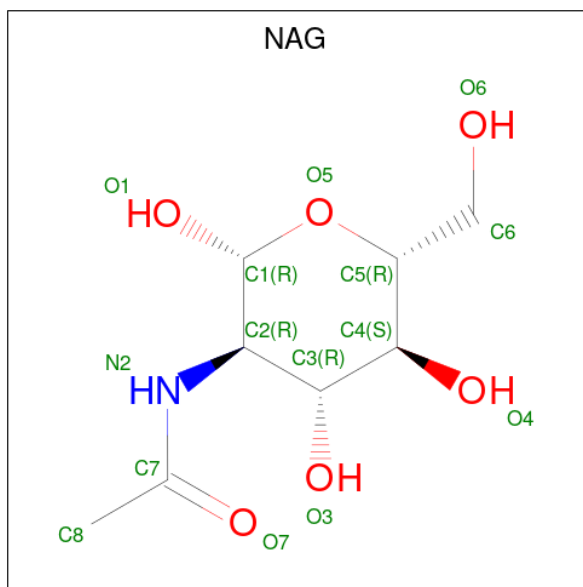
Chain	Residue	Modelled	Actual	Comment	Reference
B	686	ALA	-	expression tag	UNP P0DTC2
B	687	LEU	-	expression tag	UNP P0DTC2
B	688	TRP	-	expression tag	UNP P0DTC2
B	689	ALA	-	expression tag	UNP P0DTC2
B	690	PRO	-	expression tag	UNP P0DTC2
B	691	ALA	-	expression tag	UNP P0DTC2
B	692	ARG	-	expression tag	UNP P0DTC2
B	693	GLY	-	expression tag	UNP P0DTC2
B	694	ALA	-	expression tag	UNP P0DTC2
B	695	SER	-	expression tag	UNP P0DTC2
B	696	GLN	-	expression tag	UNP P0DTC2
B	704	CYS	SER	engineered mutation	UNP P0DTC2
B	790	CYS	LYS	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	957	GLU	GLN	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1142	GLY	-	expression tag	UNP P0DTC2
B	1143	SER	-	expression tag	UNP P0DTC2
B	1144	GLY	-	expression tag	UNP P0DTC2
B	1145	TYR	-	expression tag	UNP P0DTC2
B	1146	ILE	-	expression tag	UNP P0DTC2
B	1147	PRO	-	expression tag	UNP P0DTC2
B	1148	GLU	-	expression tag	UNP P0DTC2
B	1149	ALA	-	expression tag	UNP P0DTC2
B	1150	PRO	-	expression tag	UNP P0DTC2
B	1151	ARG	-	expression tag	UNP P0DTC2
B	1152	ASP	-	expression tag	UNP P0DTC2
B	1153	GLY	-	expression tag	UNP P0DTC2
B	1154	GLN	-	expression tag	UNP P0DTC2
B	1155	ALA	-	expression tag	UNP P0DTC2
B	1156	TYR	-	expression tag	UNP P0DTC2
B	1157	VAL	-	expression tag	UNP P0DTC2
B	1158	ARG	-	expression tag	UNP P0DTC2
B	1159	LYS	-	expression tag	UNP P0DTC2
B	1160	ASP	-	expression tag	UNP P0DTC2
B	1161	GLY	-	expression tag	UNP P0DTC2
B	1162	GLU	-	expression tag	UNP P0DTC2
B	1163	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1164	VAL	-	expression tag	UNP P0DTC2
B	1165	LEU	-	expression tag	UNP P0DTC2
B	1166	LEU	-	expression tag	UNP P0DTC2
B	1167	SER	-	expression tag	UNP P0DTC2
B	1168	THR	-	expression tag	UNP P0DTC2
B	1169	PHE	-	expression tag	UNP P0DTC2
B	1170	LEU	-	expression tag	UNP P0DTC2
B	1171	GLY	-	expression tag	UNP P0DTC2
B	1172	ARG	-	expression tag	UNP P0DTC2
B	1173	SER	-	expression tag	UNP P0DTC2
B	1174	LEU	-	expression tag	UNP P0DTC2
B	1175	GLU	-	expression tag	UNP P0DTC2
B	1176	VAL	-	expression tag	UNP P0DTC2
B	1177	LEU	-	expression tag	UNP P0DTC2
B	1178	PHE	-	expression tag	UNP P0DTC2
B	1179	GLN	-	expression tag	UNP P0DTC2
B	1180	GLY	-	expression tag	UNP P0DTC2
B	1181	PRO	-	expression tag	UNP P0DTC2
B	1182	GLY	-	expression tag	UNP P0DTC2
B	1183	HIS	-	expression tag	UNP P0DTC2
B	1184	HIS	-	expression tag	UNP P0DTC2
B	1185	HIS	-	expression tag	UNP P0DTC2
B	1186	HIS	-	expression tag	UNP P0DTC2
B	1187	HIS	-	expression tag	UNP P0DTC2
B	1188	HIS	-	expression tag	UNP P0DTC2
B	1189	HIS	-	expression tag	UNP P0DTC2
B	1190	HIS	-	expression tag	UNP P0DTC2
B	1191	SER	-	expression tag	UNP P0DTC2
B	1192	ALA	-	expression tag	UNP P0DTC2
B	1193	TRP	-	expression tag	UNP P0DTC2
B	1194	SER	-	expression tag	UNP P0DTC2
B	1195	HIS	-	expression tag	UNP P0DTC2
B	1196	PRO	-	expression tag	UNP P0DTC2
B	1197	GLN	-	expression tag	UNP P0DTC2
B	1198	PHE	-	expression tag	UNP P0DTC2
B	1199	GLU	-	expression tag	UNP P0DTC2
B	1200	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

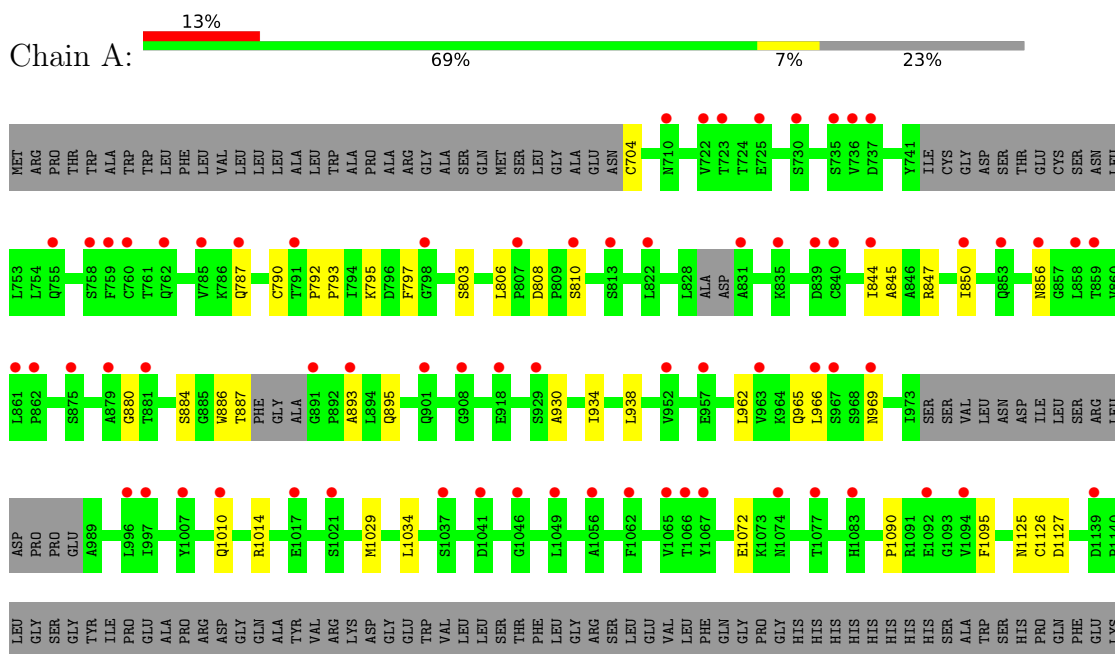


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	14	8	1	5	0	0

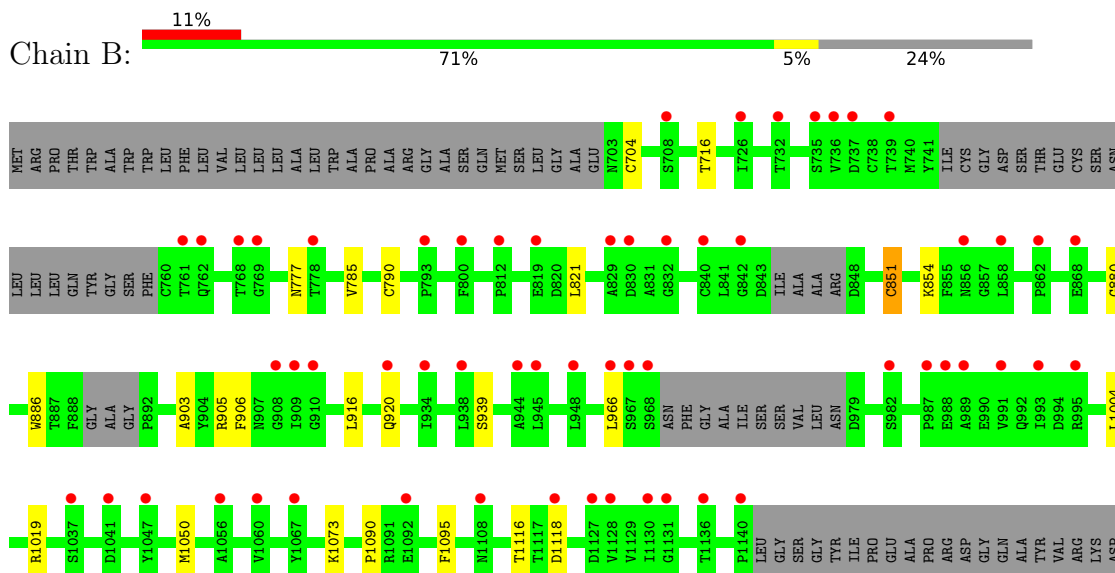
3 Residue-property plots

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: Spike protein S2



• Molecule 1: Spike protein S2



GLY	GLU	TRP	VAL	LEU	SER	THR	PHE	LEU	GLY	ARG	SER	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	GLY	HIS	HIS	HIS	HIS	HIS	HIS	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	78.99Å 78.99Å 479.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.72 – 3.20 67.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (67.72-3.20) 99.6 (67.72-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1913.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.226 , 0.262 0.228 , 0.272	Depositor DCC
R_{free} test set	958 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 252.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.329 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	6244	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.12	0/3185	0.35	0/4330
1	B	0.12	0/3167	0.33	0/4308
All	All	0.12	0/6352	0.34	0/8638

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3124	0	3103	20	1
1	B	3106	0	3077	15	2
2	B	14	0	13	0	0
All	All	6244	0	6193	35	3

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 3.

All (35) 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:808:ASP:OD2	1:A:810:SER:OG	1.99	0.81
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.21	0.74
1:A:795:LYS:HG2	1:A:806:LEU:HD12	1.76	0.68
1:B:903:ALA:HA	1:B:916:LEU:HD13	1.81	0.63
1:A:887:THR:H	1:A:893:ALA:HB2	1.65	0.62
1:B:906:PHE:HB2	1:B:916:LEU:HD11	1.87	0.56
1:B:821:LEU:HD21	1:B:939:SER:HB2	1.87	0.56
1:B:851:CYS:HA	1:B:854:LYS:HD3	1.91	0.53
1:B:906:PHE:CG	1:B:916:LEU:HD11	2.46	0.51
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.47	0.50
1:B:880:GLY:HA3	1:B:886:TRP:CZ2	2.46	0.50
1:A:844:ILE:HG13	1:A:845:ALA:H	1.76	0.50
1:B:905:ARG:HD2	1:B:1050:MET:HE2	1.94	0.49
1:B:716:THR:HG21	1:B:1073:LYS:HE2	1.97	0.47
1:A:847:ARG:H	1:A:850:ILE:HG22	1.79	0.47
1:A:880:GLY:HA3	1:A:886:TRP:CZ2	2.49	0.46
1:B:906:PHE:CB	1:B:916:LEU:HD11	2.46	0.46
1:A:792:PRO:HB2	1:A:793:PRO:HA	1.98	0.46
1:A:930:ALA:O	1:A:934:ILE:HG12	2.16	0.46
1:A:795:LYS:HD2	1:A:803:SER:HA	1.97	0.45
1:A:792:PRO:HB3	1:A:797:PHE:HZ	1.81	0.45
1:B:785:VAL:HG21	1:B:886:TRP:CZ3	2.52	0.45
1:A:962:LEU:O	1:A:966:LEU:HG	2.17	0.44
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.17	0.44
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.53	0.43
1:A:1029:MET:HG3	1:A:1034:LEU:HD23	1.99	0.43
1:A:1125:ASN:OD1	1:A:1126:CYS:N	2.52	0.43
1:B:906:PHE:CD1	1:B:916:LEU:HD21	2.53	0.43
1:A:1125:ASN:ND2	1:A:1127:ASP:OD2	2.45	0.42
1:B:916:LEU:O	1:B:920:GLN:N	2.52	0.42
1:A:795:LYS:HB2	1:A:795:LYS:HE3	1.84	0.42
1:A:884:SER:HB2	1:A:895:GLN:HA	2.01	0.42
1:A:934:ILE:O	1:A:938:LEU:HG	2.21	0.41
1:A:965:GLN:O	1:A:969:ASN:HB2	2.20	0.41
1:A:1010:GLN:O	1:A:1014:ARG:HG2	2.20	0.41

All (3) 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)
1:A:704:CYS:CB	1:A:790:CYS:SG[2_545]	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:CYS:SG	1:B:790:CYS:CB[3_655]	1.78	0.42
1:B:704:CYS:CB	1:B:790:CYS:SG[3_655]	1.98	0.22

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	396/530 (75%)	379 (96%)	16 (4%)	1 (0%)	36	68
1	B	393/530 (74%)	376 (96%)	17 (4%)	0	100	100
All	All	789/1060 (74%)	755 (96%)	33 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	856	ASN

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	348/450 (77%)	346 (99%)	2 (1%)	78	84
1	B	349/450 (78%)	346 (99%)	3 (1%)	70	81
All	All	697/900 (77%)	692 (99%)	5 (1%)	76	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	787	GLN
1	A	1072	GLU
1	B	851	CYS
1	B	966	LEU
1	B	1004	LEU

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	856	ASN
1	A	1071	GLN
1	A	1074	ASN
1	A	1088	HIS
1	B	764	ASN
1	B	774	GLN
1	B	824	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](#)

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	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.35	0

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	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	NAG	C4-C5-C6-O6
2	B	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	406/530 (76%)	1.21	69 (16%) 4 3	34, 51, 101, 155	0
1	B	403/530 (76%)	1.11	59 (14%) 6 4	29, 50, 90, 149	0
All	All	809/1060 (76%)	1.16	128 (15%) 5 4	29, 50, 93, 155	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	908	GLY	5.2
1	A	862	PRO	4.7
1	A	859	THR	4.6
1	B	840	CYS	4.2
1	B	968	SER	3.6
1	A	996	LEU	3.6
1	A	1092	GLU	3.6
1	B	868	GLU	3.5
1	A	759	PHE	3.5
1	A	879	ALA	3.4
1	A	1046	GLY	3.4
1	A	831	ALA	3.4
1	B	737	ASP	3.3
1	B	829	ALA	3.2
1	B	735	SER	3.2
1	B	991	VAL	3.2
1	A	730	SER	3.1
1	A	1066	THR	3.1
1	A	853	GLN	3.1
1	B	793	PRO	3.1
1	A	807	PRO	3.0
1	A	755	GLN	3.0
1	A	737	ASP	3.0
1	A	1065	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	769	GLY	3.0
1	A	822	LEU	2.9
1	A	963	VAL	2.9
1	B	856	ASN	2.9
1	B	1136	THR	2.9
1	A	1049	LEU	2.9
1	A	918	GLU	2.9
1	B	1140	PRO	2.9
1	B	1108	ASN	2.8
1	B	966	LEU	2.8
1	B	967	SER	2.8
1	A	952	VAL	2.8
1	B	1047	TYR	2.8
1	A	875	SER	2.8
1	B	982	SER	2.8
1	B	858	LEU	2.8
1	B	988	GLU	2.8
1	B	830	ASP	2.8
1	A	723	THR	2.8
1	B	842	GLY	2.7
1	B	910	GLY	2.7
1	A	1083	HIS	2.7
1	A	760	CYS	2.7
1	B	1131	GLY	2.7
1	A	967	SER	2.7
1	B	761	THR	2.7
1	B	944	ALA	2.7
1	A	1021	SER	2.6
1	B	995	ARG	2.6
1	B	812	PRO	2.6
1	B	920	GLN	2.6
1	A	835	LYS	2.6
1	B	832	GLY	2.6
1	B	800	PHE	2.5
1	B	1118	ASP	2.5
1	B	1037	SER	2.5
1	B	1067	TYR	2.5
1	A	1017	GLU	2.5
1	A	1077	THR	2.5
1	A	810	SER	2.5
1	A	839	ASP	2.5
1	A	785	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	929	SER	2.4
1	A	997	ILE	2.4
1	A	969	ASN	2.4
1	A	791	THR	2.4
1	B	862	PRO	2.4
1	A	908	GLY	2.4
1	A	710	ASN	2.4
1	A	736	VAL	2.4
1	A	850	ILE	2.4
1	B	993	ILE	2.4
1	B	708	SER	2.4
1	A	1139	ASP	2.4
1	A	891	GLY	2.4
1	A	1010	GLN	2.4
1	A	813	SER	2.4
1	A	858	LEU	2.3
1	B	736	VAL	2.3
1	A	844	ILE	2.3
1	B	726	ILE	2.3
1	B	1130	ILE	2.3
1	A	856	ASN	2.3
1	A	861	LEU	2.3
1	B	739	THR	2.3
1	B	768	THR	2.3
1	B	1128	VAL	2.3
1	A	725	GLU	2.2
1	B	778	THR	2.2
1	A	1067	TYR	2.2
1	A	722	VAL	2.2
1	A	1094	VAL	2.2
1	B	945	LEU	2.2
1	B	948	LEU	2.2
1	A	798	GLY	2.2
1	A	787	GLN	2.2
1	B	987	PRO	2.2
1	B	732	THR	2.1
1	A	762	GLN	2.1
1	A	966	LEU	2.1
1	A	957	GLU	2.1
1	A	893	ALA	2.1
1	B	909	ILE	2.1
1	A	735	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	758	SER	2.1
1	A	1037	SER	2.1
1	A	840	CYS	2.1
1	A	1041	ASP	2.1
1	B	934	ILE	2.1
1	A	1056	ALA	2.1
1	A	1062	PHE	2.1
1	B	1092	GLU	2.1
1	B	1041	ASP	2.1
1	B	1127	ASP	2.1
1	B	989	ALA	2.1
1	A	1074	ASN	2.0
1	A	1007	TYR	2.0
1	A	901	GLN	2.0
1	B	762	GLN	2.0
1	B	1060	VAL	2.0
1	A	881	THR	2.0
1	B	1056	ALA	2.0
1	B	819	GLU	2.0
1	B	938	LEU	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 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($\text{\AA}^2$)	Q<0.9
2	NAG	B	1301	14/15	0.94	0.16	47,60,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.