W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:40 PM GMT

PDB ID	:	4F92
Title	:	Brr2 Helicase Region S1087L
Authors	:	Santos, K.F.; Jovin, S.M.; Weber, G.; Pena, V.; Luehrmann, R.; Wahl, M.C.
Deposited on	:	2012-05-18
Resolution	:	2.66 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.66 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		3
Ramachandran outliers		0.6%
Sidechain outliers		12.6%
RSRZ outliers		7.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
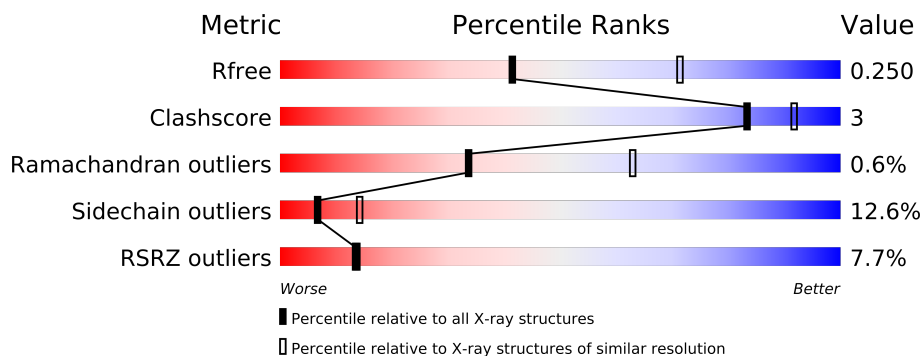
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	1724	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SAN	B	2201[A]	-	X
2	SAN	B	2201[B]	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14019 atoms, of which 0 are hydrogen and 0 are deuterium.

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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1723	Total 13866	C 8863	N 2373	O 2558	S 72	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1087	LEU	SER	ENGINEERED MUTATION	UNP O75643

- Molecule 2 is SULFANILAMIDE (three-letter code: SAN) (formula: $C_6H_8N_2O_2S$).
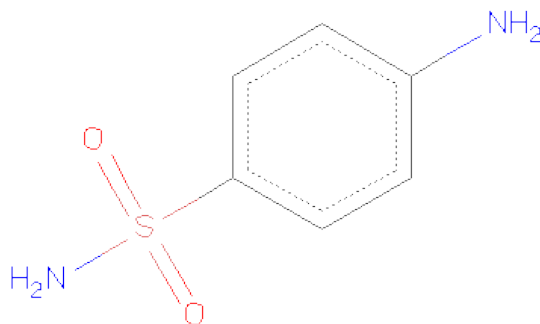
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 22	C 12	N 4	O 4	S 2	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	131	Total 131	O 131	0	0

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 errors 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: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:
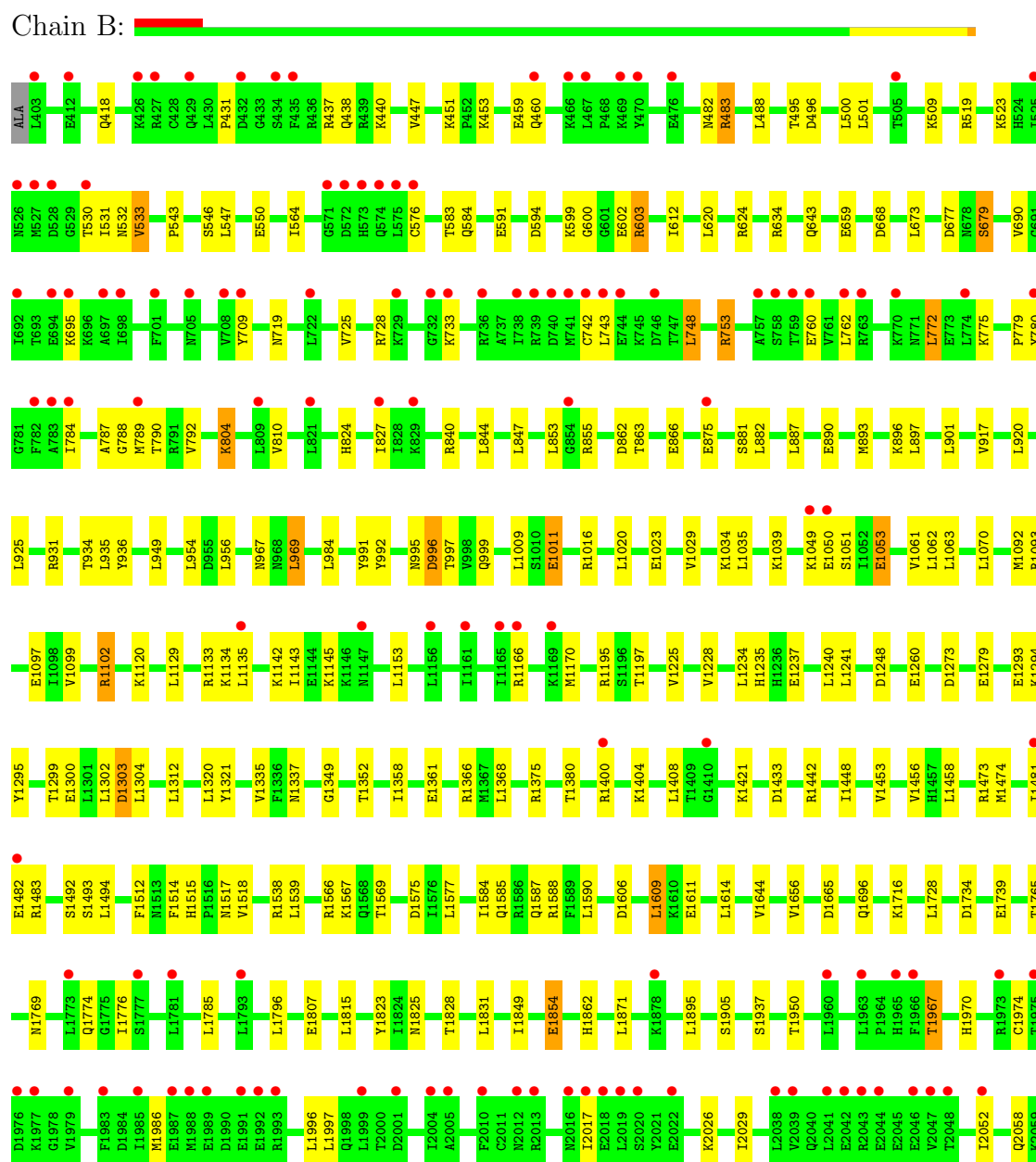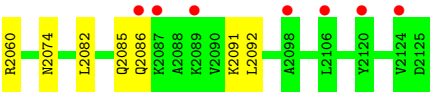
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.15Å 149.54Å 141.32Å 90.00° 120.33° 90.00°	Depositor
Resolution (Å)	35.32 – 2.66 46.36 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.32-2.66) 88.2 (46.36-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.212 , 0.259 0.203 , 0.250	Depositor DCC
R_{free} test set	3370 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.1	EDS
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.001 for h,-k,-h-l	Xtriage
L-test for twinning	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	2 of 74395 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14019	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	B	0.30	0/14161	0.51	1/19188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	969	LEU	CA-CB-CG	5.48	127.91	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13866	0	0	42	0
2	B	22	0	16	0	0
3	B	131	0	0	8	0
All	All	14019	0	16	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:600:GLY:N	3:B:2315:HOH:O	2.17	0.75
1:B:1049:LYS:O	1:B:1051:SER:N	2.24	0.71
1:B:753:ARG:NH1	1:B:779:PRO:O	2.27	0.68
1:B:997:THR:OG1	1:B:1023:GLU:OE1	2.12	0.67
1:B:668:ASP:N	3:B:2306:HOH:O	2.30	0.64
1:B:1716:LYS:NZ	3:B:2382:HOH:O	2.30	0.64
1:B:967:ASN:ND2	1:B:995:ASN:OD1	2.35	0.59
1:B:787:ALA:O	1:B:789:MET:N	2.36	0.58
1:B:543:PRO:O	1:B:624:ARG:NH2	2.37	0.57
1:B:509:LYS:NZ	3:B:2307:HOH:O	2.37	0.56
1:B:1950:THR:OG1	1:B:2060:ARG:NH2	2.38	0.56
1:B:1321:TYR:OH	1:B:1361:GLU:OE1	2.25	0.55
1:B:1606:ASP:OD1	1:B:1609:LEU:N	2.41	0.53
1:B:1433:ASP:OD1	1:B:1823:TYR:OH	2.26	0.53
1:B:1102:ARG:NH1	3:B:2392:HOH:O	2.43	0.51
1:B:1093:ARG:NH1	1:B:1273:ASP:OD2	2.43	0.51
1:B:496:ASP:OD1	1:B:519:ARG:NE	2.46	0.49
1:B:677:ASP:OD1	1:B:679:SER:OG	2.30	0.49
1:B:1493:SER:OG	1:B:1514:PHE:O	2.30	0.49
1:B:742:CYS:O	1:B:748:LEU:N	2.46	0.49
1:B:1337:ASN:N	3:B:2413:HOH:O	2.47	0.47
1:B:482:ASN:OD1	1:B:483:ARG:N	2.48	0.47
1:B:1011:GLU:OE2	3:B:2398:HOH:O	2.19	0.46
1:B:991:TYR:OH	1:B:1097:GLU:OE2	2.33	0.46
1:B:594:ASP:OD2	1:B:634:ARG:NH1	2.49	0.46
1:B:1828:THR:OG1	1:B:1854:GLU:OE2	2.35	0.45
1:B:1302:LEU:O	1:B:1304:LEU:N	2.51	0.44
1:B:1235:HIS:NE2	1:B:1237:GLU:OE1	2.51	0.44
1:B:996:ASP:OD1	1:B:996:ASP:N	2.50	0.44
1:B:824:HIS:ND1	1:B:862:ASP:OD2	2.50	0.44
1:B:1349:GLY:N	1:B:1512:PHE:O	2.51	0.44
1:B:1195:ARG:NH1	1:B:1260:GLU:OE1	2.51	0.43
1:B:603:ARG:NH2	1:B:1575:ASP:OD1	2.52	0.43
1:B:1937:SER:OG	1:B:2074:ASN:OD1	2.37	0.43
1:B:531:ILE:O	1:B:533:VAL:N	2.52	0.42
1:B:1515:HIS:ND1	1:B:1517:ASN:OD1	2.52	0.42
1:B:1769:ASN:N	3:B:2366:HOH:O	2.53	0.42
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.53	0.41
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.53	0.41
1:B:1967:THR:OG1	1:B:1970:HIS:ND1	2.54	0.41
1:B:1538:ARG:NH1	1:B:1665:ASP:OD2	2.55	0.40
1:B:890:GLU:OE1	1:B:936:TYR:OH	2.38	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	B	1722/1724 (100%)	1632 (95%)	79 (5%)	11 (1%)	33	63

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1050	GLU
1	B	1584	ILE
1	B	788	GLY
1	B	431	PRO
1	B	772	LEU
1	B	804	LYS
1	B	875	GLU
1	B	530	THR
1	B	532	ASN
1	B	1053	GLU
1	B	1303	ASP

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	B	1543/1542 (100%)	1349 (87%)	194 (13%)	7	14

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	B	437	ARG
1	B	438	GLN

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Mol	Chain	Res	Type
1	B	440	LYS
1	B	447	VAL
1	B	451	LYS
1	B	453	LYS
1	B	459	GLU
1	B	460	GLN
1	B	483	ARG
1	B	488	LEU
1	B	495	THR
1	B	500	LEU
1	B	501	LEU
1	B	523	LYS
1	B	533	VAL
1	B	546	SER
1	B	547	LEU
1	B	550	GLU
1	B	564	ILE
1	B	576	CYS
1	B	583	THR
1	B	584	GLN
1	B	591	GLU
1	B	599	LYS
1	B	602	GLU
1	B	603	ARG
1	B	612	ILE
1	B	620	LEU
1	B	643	GLN
1	B	659	GLU
1	B	673	LEU
1	B	679	SER
1	B	690	VAL
1	B	695	LYS
1	B	709	TYR
1	B	719	ASN
1	B	725	VAL
1	B	728	ARG
1	B	733	LYS
1	B	743	LEU
1	B	748	LEU
1	B	753	ARG
1	B	760	GLU
1	B	762	LEU

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Mol	Chain	Res	Type
1	B	772	LEU
1	B	775	LYS
1	B	780	TYR
1	B	784	ILE
1	B	790	THR
1	B	792	VAL
1	B	804	LYS
1	B	810	VAL
1	B	827	ILE
1	B	840	ARG
1	B	844	LEU
1	B	847	LEU
1	B	853	LEU
1	B	855	ARG
1	B	863	THR
1	B	866	GLU
1	B	881	SER
1	B	882	LEU
1	B	887	LEU
1	B	893	MET
1	B	896	LYS
1	B	897	LEU
1	B	901	LEU
1	B	917	VAL
1	B	920	LEU
1	B	925	LEU
1	B	931	ARG
1	B	934	THR
1	B	935	LEU
1	B	949	LEU
1	B	954	LEU
1	B	956	LEU
1	B	969	LEU
1	B	984	LEU
1	B	992	TYR
1	B	996	ASP
1	B	999	GLN
1	B	1009	LEU
1	B	1011	GLU
1	B	1016	ARG
1	B	1020	LEU
1	B	1029	VAL

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Mol	Chain	Res	Type
1	B	1034	LYS
1	B	1035	LEU
1	B	1039	LYS
1	B	1053	GLU
1	B	1061	VAL
1	B	1062	LEU
1	B	1063	LEU
1	B	1070	LEU
1	B	1092	MET
1	B	1099	VAL
1	B	1102	ARG
1	B	1120	LYS
1	B	1129	LEU
1	B	1133	ARG
1	B	1134	LYS
1	B	1135	LEU
1	B	1142	LYS
1	B	1143	ILE
1	B	1145	LYS
1	B	1153	LEU
1	B	1166	ARG
1	B	1170	MET
1	B	1197	THR
1	B	1225	VAL
1	B	1228	VAL
1	B	1234	LEU
1	B	1240	LEU
1	B	1241	LEU
1	B	1248	ASP
1	B	1279	GLU
1	B	1293	GLU
1	B	1294	LYS
1	B	1295	TYR
1	B	1299	THR
1	B	1300	GLU
1	B	1303	ASP
1	B	1312	LEU
1	B	1320	LEU
1	B	1335	VAL
1	B	1352	THR
1	B	1358	ILE
1	B	1366	ARG

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Mol	Chain	Res	Type
1	B	1368	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1400	ARG
1	B	1404	LYS
1	B	1408	LEU
1	B	1421	LYS
1	B	1442	ARG
1	B	1448	ILE
1	B	1453	VAL
1	B	1456	VAL
1	B	1458	LEU
1	B	1474	MET
1	B	1481	ILE
1	B	1482	GLU
1	B	1483	ARG
1	B	1492	SER
1	B	1494	LEU
1	B	1518	VAL
1	B	1539	LEU
1	B	1566	ARG
1	B	1567	LYS
1	B	1569	THR
1	B	1577	LEU
1	B	1585	GLN
1	B	1587	GLN
1	B	1588	ARG
1	B	1590	LEU
1	B	1609	LEU
1	B	1611	GLU
1	B	1614	LEU
1	B	1644	VAL
1	B	1656	VAL
1	B	1696	GLN
1	B	1728	LEU
1	B	1739	GLU
1	B	1765	THR
1	B	1774	GLN
1	B	1776	ILE
1	B	1785	LEU
1	B	1796	LEU
1	B	1807	GLU

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Mol	Chain	Res	Type
1	B	1815	LEU
1	B	1831	LEU
1	B	1849	ILE
1	B	1854	GLU
1	B	1862	HIS
1	B	1871	LEU
1	B	1895	LEU
1	B	1905	SER
1	B	1967	THR
1	B	1974	CYS
1	B	1986	MET
1	B	1996	LEU
1	B	1997	LEU
1	B	2017	ILE
1	B	2026	LYS
1	B	2029	ILE
1	B	2052	ILE
1	B	2058	GLN
1	B	2082	LEU
1	B	2085	GLN
1	B	2086	GLN
1	B	2091	LYS
1	B	2092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	SAN	B	2201[A]	-	11,11,11	2.90	1 (9%)	16,16,16	1.93	3 (18%)
2	SAN	B	2201[B]	-	11,11,11	3.14	1 (9%)	16,16,16	1.83	3 (18%)

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	SAN	B	2201[A]	-	-	0/6/6/6	0/1/1/1
2	SAN	B	2201[B]	-	-	0/6/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201[B]	SAN	C4-S	-10.35	1.60	1.77
2	B	2201[A]	SAN	C4-S	-9.57	1.61	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2201[A]	SAN	O2-S-O1	-6.11	108.16	118.78
2	B	2201[B]	SAN	O2-S-O1	-5.91	108.50	118.78
2	B	2201[B]	SAN	O2-S-C4	2.63	110.94	107.39
2	B	2201[A]	SAN	O1-S-C4	2.51	110.77	107.39
2	B	2201[B]	SAN	O1-S-N2	2.29	110.82	107.28
2	B	2201[A]	SAN	O2-S-C4	2.28	110.46	107.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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 ⓘ

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	B	1723/1724 (99%)	0.34	132 (7%)	13	14	38, 83, 156, 206	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	746	ASP	6.4
1	B	763	ARG	5.8
1	B	1977	LYS	5.6
1	B	527	MET	5.3
1	B	784	ILE	5.3
1	B	2124	VAL	5.2
1	B	571	GLY	5.0
1	B	2038	LEU	4.9
1	B	2047	VAL	4.8
1	B	1050	GLU	4.7
1	B	709	TYR	4.7
1	B	575	LEU	4.6
1	B	783	ALA	4.6
1	B	738	ILE	4.5
1	B	573	HIS	4.5
1	B	2016	ASN	4.5
1	B	2001	ASP	4.4
1	B	1979	VAL	4.3
1	B	743	LEU	4.2
1	B	528	ASP	4.2
1	B	572	ASP	4.2
1	B	2004	ILE	4.2
1	B	1135	LEU	4.2
1	B	432	ASP	4.2
1	B	2018	GLU	4.1
1	B	1985	ILE	3.9
1	B	574	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	2043	ARG	3.9
1	B	2048	THR	3.8
1	B	469	LYS	3.8
1	B	2010	PHE	3.8
1	B	1991	GLU	3.8
1	B	695	LYS	3.7
1	B	742	CYS	3.7
1	B	2044	GLU	3.7
1	B	2042	GLU	3.7
1	B	759	THR	3.7
1	B	736	ARG	3.5
1	B	740	ASP	3.5
1	B	2019	LEU	3.5
1	B	774	LEU	3.5
1	B	470	TYR	3.4
1	B	1976	ASP	3.4
1	B	1993	ARG	3.4
1	B	429	GLN	3.4
1	B	476	GLU	3.3
1	B	2022	GLU	3.3
1	B	427	ARG	3.2
1	B	2089	LYS	3.2
1	B	1987	GLU	3.2
1	B	758	SER	3.1
1	B	1983	PHE	3.1
1	B	530	THR	3.1
1	B	2013	ARG	3.1
1	B	762	LEU	3.1
1	B	2046	GLU	3.1
1	B	2086	GLN	3.1
1	B	1963	LEU	3.1
1	B	2041	LEU	3.0
1	B	1999	LEU	3.0
1	B	1161	ILE	3.0
1	B	2120	TYR	3.0
1	B	760	GLU	3.0
1	B	1966	PHE	3.0
1	B	435	PHE	2.9
1	B	526	ASN	2.9
1	B	1960	LEU	2.9
1	B	1165	ILE	2.9
1	B	1400	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	789	MET	2.9
1	B	2087	LYS	2.9
1	B	1482	GLU	2.8
1	B	1147	ASN	2.8
1	B	434	SER	2.7
1	B	739	ARG	2.7
1	B	744	GLU	2.7
1	B	770	LYS	2.7
1	B	467	LEU	2.7
1	B	1166	ARG	2.6
1	B	1156	LEU	2.6
1	B	2005	ALA	2.6
1	B	460	GLN	2.6
1	B	1992	GLU	2.6
1	B	1973	ARG	2.6
1	B	708	VAL	2.6
1	B	722	LEU	2.6
1	B	1989	GLU	2.6
1	B	1988	MET	2.6
1	B	1777	SER	2.5
1	B	698	ILE	2.5
1	B	827	ILE	2.5
1	B	694	GLU	2.5
1	B	1169	LYS	2.5
1	B	576	CYS	2.5
1	B	2012	ASN	2.5
1	B	757	ALA	2.4
1	B	426	LYS	2.4
1	B	705	ASN	2.4
1	B	741	MET	2.4
1	B	2106	LEU	2.4
1	B	733	LYS	2.3
1	B	1049	LYS	2.3
1	B	2020	SER	2.3
1	B	1965	HIS	2.2
1	B	2017	ILE	2.2
1	B	701	PHE	2.2
1	B	782	PHE	2.2
1	B	809	LEU	2.2
1	B	525	ILE	2.2
1	B	1481	ILE	2.2
1	B	1781	LEU	2.2

Mol	Chain	Res	Type	RSRZ
1	B	780	TYR	2.2
1	B	412	GLU	2.2
1	B	829	LYS	2.1
1	B	505	THR	2.1
1	B	875	GLU	2.1
1	B	692	ILE	2.1
1	B	466	LYS	2.1
1	B	2052	ILE	2.1
1	B	1773	LEU	2.1
1	B	732	GLY	2.0
1	B	1410	GLY	2.0
1	B	821	LEU	2.0
1	B	2039	VAL	2.0
1	B	854	GLY	2.0
1	B	1793	LEU	2.0
1	B	1975	THR	2.0
1	B	697	ALA	2.0
1	B	729	LYS	2.0
1	B	1878	LYS	2.0
1	B	403	LEU	2.0
1	B	2098	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	SAN	B	2201[A]	11/11	0.20	3.20	28,37,50,52	11

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
2	SAN	B	2201[B]	11/11	0.20	2.45	18,25,49,54	11

6.5 Other polymers ⓘ

There are no such residues in this entry.