



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:59 PM UTC

PDB ID : 4F92 / pdb_00004f92
Title : Brr2 Helicase Region S1087L
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Deposited on : 2012-05-18
Resolution : 2.66 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

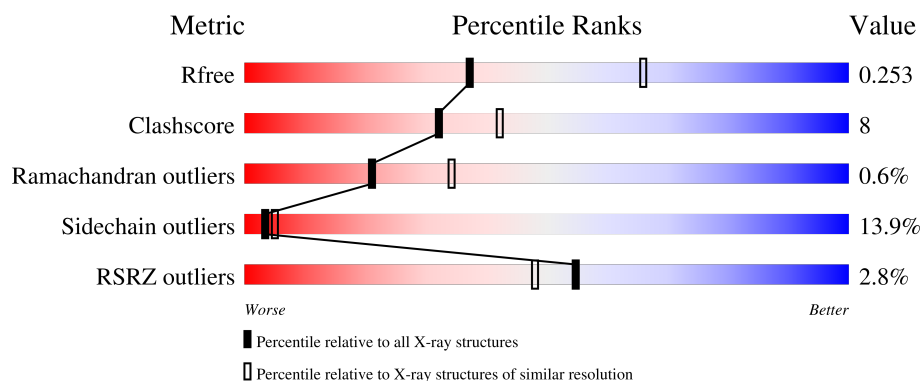
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

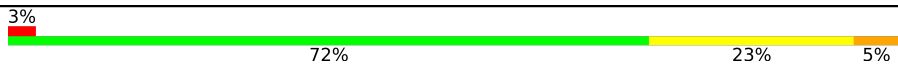
The reported resolution of this entry is 2.66 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	B	1724	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14019 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.

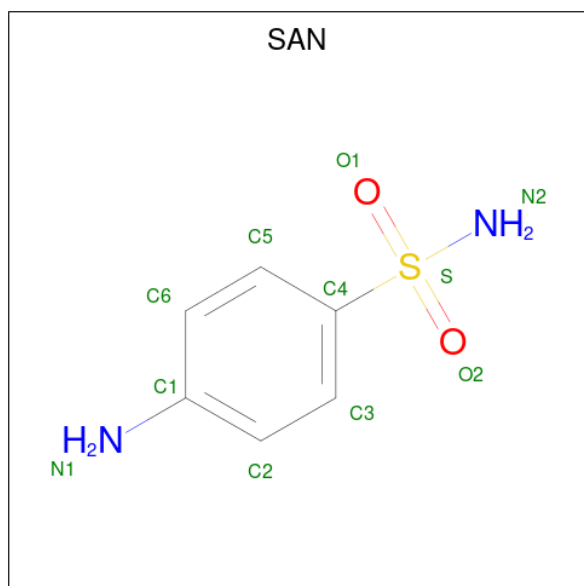
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1723	13866	8863	2373	2558	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 (CCD ID: SAN) (formula: $C_6H_8N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	22	12	4	4	2	0	1

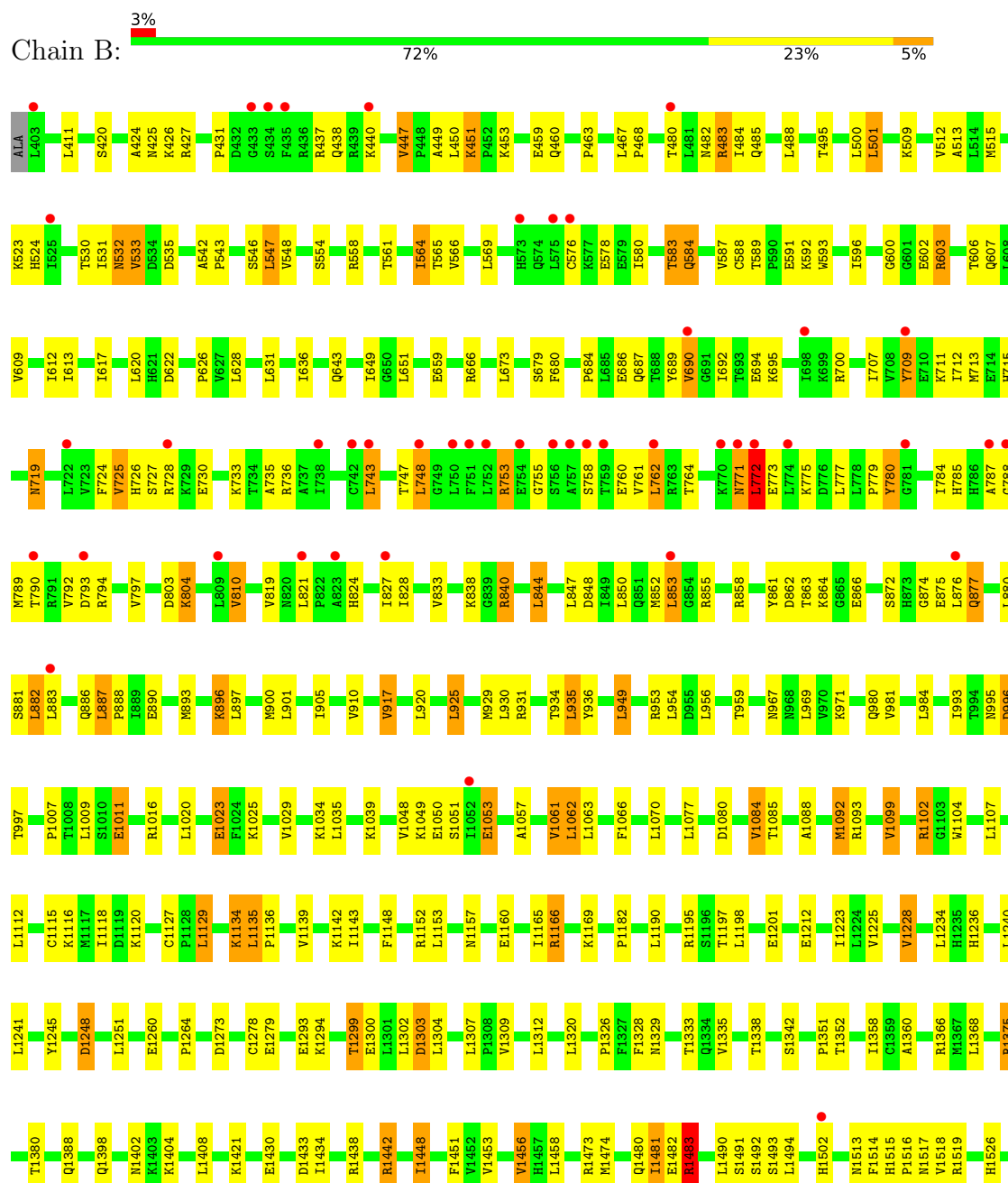
- Molecule 3 is water.

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, 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: U5 small nuclear ribonucleoprotein 200 kDa helicase



L1539	M1692	T1840	M1994	Y2113
L1540	R1693	K1841	A1995	M2114
V1559	Q1696	L1845	L1996	D2125
I1560	C1702	I1849	L1997	
S1565	V1703	E1854	Q1998	
R1566	K1716	Y1855	L1999	
K1567	L1728	H1862	C2011	
Q1568	D1729	L1871	R2012	
T1569	M1732	V1875	Y2014	
D1575	E1739	K1883	P2015	
I1576	I1740	D1886	R2016	
L1577	V1741	P1887	I2017	
I1584	T1744	T1891	K2026	
Q1585	L1755	L1895	I2029	
R1586	L1760	S1905	V2035	
Q1587	Y1761	A1906	V2039	
R1588	R1762	E1907	Q2040	
F1589	M1764	L1908	L2041	
L1590	T1765	Q1909	E2042	
K1595	P1768	T1923	R2043	
I1598	Q1774	A1939	V2046	
L1604	G1775	M1943	V2047	
D1606	I1776	E1944	V2051	
L1614	L1781	L1945	I2052	
H1621	L1785	A1946	A2053	
S1625	L1796	Q1947	P2054	
E1628	K1800	M1948	F2056	
L1631	G1801	T1950	L2055	
F1636	I1802	M1953	P2057	
Q1642	E1807	W1954	Q2058	
V1643	L1815	T1967	R2059	
V1644	A1819	S1968	R2060	
S1649	Y1823	E1969	V2066	
V1656	I1829	R1973	V2067	
A1658	E1830	C1974	I2068	
H1659	L1831	V1982	I2077	
L1660	K1839	T1985	S2078	
V1661		M1986	I2079	
		E1987	L2084	
		M1988	Q2085	
			Q2086	
			K2087	
			K2091	
			L2092	
			A2096	
			P2097	

4 Data and refinement statistics

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 35.32 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.32-2.66) 88.2 (35.32-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.212 , 0.259 0.208 , 0.253	Depositor DCC
R_{free} test set	3747 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.010 for h,-k,-h-l	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 3.90% 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: 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	0.39	0/14161	0.81	14/19188 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	771	ASN	N-CA-C	9.55	122.16	110.41
1	B	877	GLN	N-CA-C	-7.95	102.65	113.30
1	B	1565	SER	N-CA-C	6.03	117.06	108.74
1	B	1483	ARG	CA-C-N	5.82	127.11	119.84
1	B	1483	ARG	C-N-CA	5.82	127.11	119.84
1	B	1659	HIS	N-CA-C	-5.76	106.38	113.41
1	B	588	CYS	N-CA-C	5.39	116.18	108.74
1	B	2084	LEU	N-CA-C	5.30	120.01	113.50
1	B	1875	VAL	CA-C-N	5.25	124.87	119.05
1	B	1875	VAL	C-N-CA	5.25	124.87	119.05
1	B	2053	ALA	CA-C-N	5.08	124.86	119.28
1	B	2053	ALA	C-N-CA	5.08	124.86	119.28
1	B	876	LEU	N-CA-C	5.02	116.77	107.73
1	B	2085	GLN	CB-CA-C	-5.02	110.41	117.23

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	B	13866	0	14008	222	0
2	B	22	0	16	0	0
3	B	131	0	0	8	0
All	All	14019	0	14024	222	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 8.

All (222) 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:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.64	0.80
1:B:600:GLY:N	3:B:2315:HOH:O	2.17	0.72
1:B:1049:LYS:O	1:B:1051:SER:N	2.24	0.71
1:B:501:LEU:HD13	1:B:509:LYS:HG2	1.74	0.68
1:B:564:ILE:HG12	1:B:584:GLN:HG3	1.75	0.68
1:B:753:ARG:NH1	1:B:779:PRO:O	2.27	0.68
1:B:1051:SER:HB3	1:B:1057:ALA:HB2	1.76	0.67
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.76	0.67
1:B:997:THR:OG1	1:B:1023:GLU:OE1	2.12	0.65
1:B:771:ASN:HB3	1:B:772:LEU:HD13	1.79	0.64
1:B:1716:LYS:NZ	3:B:2382:HOH:O	2.30	0.64
1:B:447:VAL:HG13	1:B:687:GLN:HG3	1.81	0.62
1:B:1973:ARG:HB2	1:B:1997:LEU:HD11	1.82	0.62
1:B:626:PRO:HG2	1:B:896:LYS:HG3	1.80	0.61
1:B:1049:LYS:C	1:B:1051:SER:H	2.09	0.61
1:B:1768:PRO:HG3	1:B:1776:ILE:HG22	1.82	0.61
1:B:882:LEU:HG	1:B:887:LEU:HD12	1.83	0.60
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.81	0.60
1:B:1604:LEU:HD21	1:B:1631:LEU:HD22	1.83	0.60
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.84	0.59
1:B:967:ASN:ND2	1:B:995:ASN:OD1	2.35	0.59
1:B:524:HIS:HB3	1:B:532:ASN:HB2	1.84	0.58
1:B:1456:VAL:HG23	1:B:1491:SER:HB2	1.85	0.58
1:B:758:SER:HB2	1:B:762:LEU:HB2	1.85	0.58
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.86	0.57
1:B:761:VAL:HA	1:B:764:THR:HG22	1.86	0.57
1:B:971:LYS:HB2	1:B:980:GLN:HB2	1.85	0.57
1:B:743:LEU:HA	1:B:747:THR:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:HIS:HB3	1:B:719:ASN:HB3	1.86	0.57
1:B:828:ILE:HD13	1:B:852:MET:HE3	1.87	0.57
1:B:949:LEU:O	1:B:953:ARG:HG3	2.05	0.56
1:B:690:VAL:HG21	1:B:707:ILE:HD13	1.87	0.56
1:B:713:MET:HE2	1:B:748:LEU:HD23	1.86	0.56
1:B:603:ARG:O	1:B:607:GLN:HB2	2.05	0.56
1:B:603:ARG:HB3	1:B:1540:LEU:HD13	1.88	0.56
1:B:1945:LEU:HA	1:B:1948:MET:HG2	1.87	0.56
1:B:736:ARG:HH21	1:B:773:GLU:HG2	1.71	0.55
1:B:1157:ASN:HB3	1:B:1160:GLU:OE1	2.07	0.55
1:B:787:ALA:O	1:B:789:MET:N	2.36	0.54
1:B:1228:VAL:HG11	1:B:1264:PRO:HD2	1.89	0.54
1:B:543:PRO:HD2	1:B:547:LEU:HD12	1.89	0.54
1:B:1329:ASN:O	1:B:1333:THR:HG23	2.07	0.54
1:B:858:ARG:HD2	1:B:861:TYR:HB2	1.90	0.53
1:B:617:ILE:HD12	1:B:628:LEU:HD13	1.90	0.53
1:B:692:ILE:HG13	1:B:872:SER:HA	1.90	0.53
1:B:1307:LEU:HB2	1:B:1333:THR:HB	1.90	0.53
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.91	0.53
1:B:606:THR:HA	1:B:609:VAL:HG23	1.91	0.53
1:B:1604:LEU:HD13	1:B:1609:LEU:HD13	1.91	0.53
1:B:725:VAL:HG11	1:B:730:GLU:HG2	1.91	0.53
1:B:1606:ASP:OD1	1:B:1609:LEU:N	2.41	0.53
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	1.90	0.53
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.90	0.53
1:B:1729:ASP:HA	1:B:1732:MET:HE2	1.91	0.53
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.92	0.52
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.91	0.52
1:B:1307:LEU:H	1:B:1333:THR:HG21	1.74	0.52
1:B:1430:GLU:H	1:B:1430:GLU:CD	2.18	0.52
1:B:2059:LYS:H	1:B:2059:LYS:HD2	1.74	0.52
1:B:617:ILE:HG22	1:B:651:LEU:O	2.10	0.52
1:B:853:LEU:HD22	1:B:883:LEU:HD22	1.92	0.52
1:B:1909:GLN:HG3	3:B:2396:HOH:O	2.10	0.51
1:B:425:ASN:HB2	1:B:888:PRO:HD3	1.92	0.51
1:B:512:VAL:HA	1:B:515:MET:HE2	1.92	0.51
1:B:1093:ARG:NH1	1:B:1273:ASP:OD2	2.43	0.51
1:B:753:ARG:C	1:B:755:GLY:H	2.19	0.51
1:B:565:THR:HB	1:B:583:THR:HA	1.94	0.50
1:B:709:TYR:O	1:B:713:MET:HG2	2.10	0.50
1:B:692:ILE:HD11	1:B:700:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:LYS:O	1:B:900:MET:HG2	2.12	0.50
1:B:1988:MET:HE1	1:B:1996:LEU:HD23	1.94	0.49
1:B:753:ARG:HD3	1:B:780:TYR:HA	1.94	0.49
1:B:735:ALA:HB2	1:B:810:VAL:HG11	1.94	0.49
1:B:684:PRO:HB2	1:B:864:LYS:HD2	1.94	0.49
1:B:1845:LEU:O	1:B:1849:ILE:HG22	2.13	0.49
1:B:1438:ARG:O	1:B:1442:ARG:HG2	2.13	0.49
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.95	0.49
1:B:1099:VAL:HG21	1:B:1107:LEU:HD23	1.95	0.49
1:B:1481:ILE:HD13	1:B:1483:ARG:HD2	1.94	0.49
1:B:1502[B]:HIS:CE1	1:B:1762:ARG:HE	2.31	0.49
1:B:758:SER:HA	1:B:761:VAL:HB	1.95	0.48
1:B:1566:ARG:O	1:B:1569:THR:HG22	2.13	0.48
1:B:709:TYR:HE1	1:B:748:LEU:HD22	1.78	0.48
1:B:692:ILE:HD13	1:B:700:ARG:HG3	1.95	0.48
1:B:1986:MET:SD	1:B:2011:CYS:HB3	2.53	0.48
1:B:1994:ASN:HB2	1:B:1999:LEU:HD13	1.95	0.48
1:B:1526:HIS:HB2	1:B:1703:VAL:HG22	1.95	0.48
1:B:1099:VAL:HG22	1:B:1104:TRP:HB2	1.94	0.48
1:B:1169:LYS:H	1:B:1169:LYS:HD2	1.78	0.48
1:B:1519:ARG:NH2	1:B:1692:ASN:HB2	2.29	0.48
1:B:484:ILE:HD11	1:B:680:PHE:HB3	1.96	0.48
1:B:709:TYR:CE1	1:B:748:LEU:HD22	2.49	0.47
1:B:736:ARG:HH21	1:B:773:GLU:CG	2.27	0.47
1:B:1796:LEU:HB3	1:B:1802:ILE:HG12	1.94	0.47
1:B:793:ASP:O	1:B:797:VAL:HG23	2.14	0.47
1:B:930:LEU:HD23	1:B:949:LEU:HD22	1.95	0.47
1:B:509:LYS:NZ	3:B:2307:HOH:O	2.37	0.47
1:B:542:ALA:O	1:B:589:THR:HA	2.14	0.47
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.49	0.47
1:B:482:ASN:HB3	1:B:485:GLN:CD	2.40	0.47
1:B:1080:ASP:O	1:B:1084:VAL:HG13	2.15	0.47
1:B:1148:PHE:CZ	1:B:1152:ARG:HD2	2.50	0.47
1:B:1636:PHE:CE1	1:B:1644:VAL:HG22	2.49	0.47
1:B:877:GLN:HB2	1:B:880:LEU:HD12	1.97	0.47
1:B:1112:LEU:HG	1:B:1116:LYS:HE2	1.96	0.47
1:B:1939:ALA:O	1:B:1943:MET:HG3	2.15	0.47
1:B:694:GLU:HB3	3:B:2428:HOH:O	2.14	0.47
1:B:1245:TYR:O	1:B:1248:ASP:HB2	2.14	0.47
1:B:2029:ILE:HG12	1:B:2035:VAL:HG22	1.96	0.47
1:B:1011:GLU:OE2	3:B:2398:HOH:O	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:ASN:OD1	1:B:483:ARG:N	2.48	0.46
1:B:420:SER:HB2	1:B:622:ASP:HA	1.97	0.46
1:B:569:LEU:O	1:B:592:LYS:HG2	2.15	0.46
1:B:593:TRP:HD1	1:B:631:LEU:HD22	1.79	0.46
1:B:1567:LYS:H	1:B:1567:LYS:HZ2	1.63	0.46
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.96	0.46
1:B:1839:LYS:O	1:B:1841:LYS:HE3	2.16	0.46
1:B:2039:VAL:HG21	1:B:2066:VAL:HG11	1.98	0.46
1:B:1328:PHE:HB2	1:B:1333:THR:HG22	1.97	0.46
1:B:1338:THR:O	1:B:1342:SER:HB2	2.15	0.46
1:B:1102:ARG:NH1	3:B:2392:HOH:O	2.43	0.45
1:B:1182:PRO:HB2	1:B:1278:CYS:SG	2.56	0.45
1:B:411:LEU:HD13	1:B:959:THR:HG21	1.98	0.45
1:B:1585:GLN:O	1:B:1588:ARG:HB3	2.16	0.45
1:B:424:ALA:HB1	1:B:935:LEU:HD11	1.97	0.45
1:B:1165:ILE:O	1:B:1166:ARG:HG3	2.17	0.45
1:B:1135:LEU:HD13	1:B:1136:PRO:HD2	1.98	0.45
1:B:449:ALA:H	1:B:686:GLU:HG2	1.81	0.45
1:B:450:LEU:HD22	1:B:450:LEU:H	1.82	0.45
1:B:687:GLN:HG3	1:B:689:TYR:HE1	1.81	0.44
1:B:1062:LEU:HD12	1:B:1062:LEU:HA	1.73	0.44
1:B:1595:LYS:HA	1:B:1598:ILE:HD12	1.98	0.44
1:B:1190:LEU:HD11	1:B:1198:LEU:HD13	1.99	0.44
1:B:1049:LYS:C	1:B:1051:SER:N	2.75	0.44
1:B:1302:LEU:O	1:B:1304:LEU:N	2.51	0.44
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.18	0.44
1:B:996:ASP:OD1	1:B:996:ASP:N	2.50	0.44
1:B:463:PRO:HA	1:B:480:THR:HA	1.99	0.44
1:B:1375:ARG:HH11	1:B:1375:ARG:HB2	1.82	0.44
1:B:531:ILE:HD12	1:B:533:VAL:HG23	1.99	0.44
1:B:2067:VAL:HG22	1:B:2079:ILE:HG13	1.99	0.44
1:B:467:LEU:HB2	1:B:468:PRO:HD2	2.00	0.44
1:B:2017:ILE:HG23	1:B:2043:ARG:HB3	1.98	0.44
1:B:542:ALA:HB1	1:B:547:LEU:HD13	2.00	0.43
1:B:848:ASP:O	1:B:852:MET:HG2	2.18	0.43
1:B:719:ASN:HD22	1:B:719:ASN:HA	1.51	0.43
1:B:1048:VAL:HG12	1:B:1051:SER:HB2	2.00	0.43
1:B:1165:ILE:HD13	1:B:1165:ILE:HA	1.84	0.43
1:B:1195:ARG:NH1	1:B:1260:GLU:OE1	2.51	0.43
1:B:1299:THR:CG2	1:B:1513:ASN:H	2.31	0.43
1:B:2042:GLU:HG3	1:B:2087:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ASN:HB3	1:B:535:ASP:OD2	2.19	0.43
1:B:753:ARG:HD2	1:B:761:VAL:HG22	2.00	0.43
1:B:1127:CYS:SG	1:B:1129:LEU:HB2	2.58	0.43
1:B:785:HIS:CD2	1:B:794:ARG:HB2	2.54	0.43
1:B:874:GLY:HA2	3:B:2323:HOH:O	2.18	0.43
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.18	0.43
1:B:1442:ARG:HG2	1:B:1442:ARG:H	1.72	0.43
1:B:425:ASN:HD21	1:B:886:GLN:HB3	1.83	0.43
1:B:603:ARG:NH2	1:B:1575:ASP:OD1	2.52	0.43
1:B:917:VAL:HG23	1:B:953:ARG:NH2	2.34	0.43
1:B:1212:GLU:H	1:B:1212:GLU:CD	2.26	0.43
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	2.01	0.43
1:B:2013:ARG:HD3	1:B:2052:ILE:HD13	2.01	0.43
1:B:2043:ARG:HD3	1:B:2085:GLN:O	2.19	0.43
1:B:727:SER:HB2	1:B:730:GLU:HB2	2.01	0.43
1:B:2096:ALA:HA	1:B:2097:PRO:HD3	1.85	0.43
1:B:1448:ILE:HD11	1:B:1451:PHE:HB2	2.00	0.43
1:B:580:ILE:HA	1:B:583:THR:HG23	2.01	0.43
1:B:426:LYS:HG2	1:B:427:ARG:HG3	2.00	0.42
1:B:548:VAL:HG13	1:B:587:VAL:HG12	2.00	0.42
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.19	0.42
1:B:666:ARG:HA	1:B:666:ARG:HD2	1.89	0.42
1:B:707:ILE:O	1:B:711:LYS:HD3	2.19	0.42
1:B:1589:PHE:HD2	1:B:1642:GLN:OE1	2.02	0.42
1:B:1515:HIS:ND1	1:B:1517:ASN:OD1	2.52	0.42
1:B:1883:LYS:HD3	1:B:1883:LYS:HA	1.78	0.42
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.60	0.42
1:B:1997:LEU:HB3	1:B:1998:GLN:H	1.71	0.42
1:B:724:PHE:CE2	1:B:852:MET:HB2	2.54	0.42
1:B:1398:GLN:O	1:B:1402:ASN:HA	2.20	0.42
1:B:1577:LEU:HD12	1:B:1577:LEU:HA	1.84	0.42
1:B:1950:THR:OG1	1:B:2060:ARG:NH2	2.38	0.42
1:B:1800:LYS:HB3	1:B:1815:LEU:HD23	2.00	0.42
1:B:554:SER:O	1:B:558:ARG:HG2	2.20	0.42
1:B:1309:VAL:HG23	1:B:1326:PRO:O	2.20	0.42
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.53	0.41
1:B:1567:LYS:HB3	1:B:1567:LYS:HE3	1.81	0.41
1:B:726:HIS:CD2	1:B:844:LEU:HD13	2.56	0.41
1:B:1088:ALA:HB1	1:B:1118:ILE:HD13	2.02	0.41
1:B:821:LEU:HD12	1:B:821:LEU:O	2.19	0.41
1:B:1760:LEU:HD11	1:B:1764:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1886:ASP:HA	1:B:1887:PRO:HD2	1.90	0.41
1:B:2014:TYR:HA	1:B:2015:PRO:HD3	1.85	0.41
1:B:1502[B]:HIS:CE1	1:B:1762:ARG:HH11	2.39	0.41
1:B:1493:SER:OG	1:B:1514:PHE:O	2.30	0.41
1:B:1923:ILE:HG21	1:B:1946:ALA:HB2	2.02	0.41
1:B:631:LEU:HA	1:B:631:LEU:HD23	1.76	0.41
1:B:824:HIS:ND1	1:B:862:ASP:OD2	2.50	0.41
1:B:838:LYS:O	1:B:840:ARG:HG2	2.20	0.41
1:B:1092:MET:HB3	1:B:1115:CYS:SG	2.60	0.41
1:B:1982:VAL:O	1:B:1985:ILE:HG13	2.20	0.41
1:B:1134:LYS:HD3	1:B:1134:LYS:HA	1.84	0.41
1:B:1693:ARG:CZ	1:B:1696:GLN:HG3	2.51	0.41
1:B:1895:LEU:HD12	1:B:1895:LEU:HA	1.89	0.41
1:B:451:LYS:H	1:B:451:LYS:HG3	1.40	0.40
1:B:531:ILE:O	1:B:533:VAL:N	2.52	0.40
1:B:925:LEU:HD13	1:B:929:MET:HE2	2.03	0.40
1:B:1953:MET:HE2	1:B:2114:MET:HE2	2.04	0.40
1:B:2047:VAL:HG21	1:B:2085:GLN:HA	2.04	0.40
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.56	0.40
1:B:2056:PHE:HA	1:B:2057:PRO:HD3	1.84	0.40
1:B:1057:ALA:O	1:B:1061:VAL:HG13	2.22	0.40
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.57	0.40
1:B:1569:THR:HG21	1:B:1621:HIS:HB3	2.02	0.40
1:B:1755:LEU:HD13	1:B:1785:LEU:HD12	2.02	0.40
1:B:1136:PRO:HB2	1:B:1139:VAL:HG23	2.03	0.40
1:B:1307:LEU:H	1:B:1333:THR:CG2	2.35	0.40
1:B:1456:VAL:CG2	1:B:1491:SER:HB2	2.49	0.40
1:B:2053:ALA:HA	1:B:2054:PRO:HD2	1.90	0.40
1:B:890:GLU:OE1	1:B:936:TYR:OH	2.38	0.40
1:B:1948:MET:HE3	1:B:1954:TRP:HA	2.04	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%)	21	34

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 [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	B	1543/1542 (100%)	1329 (86%)	214 (14%)	3	5

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	437	ARG
1	B	438	GLN
1	B	440	LYS
1	B	447	VAL
1	B	451	LYS
1	B	453	LYS
1	B	459	GLU
1	B	460	GLN

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Mol	Chain	Res	Type
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	561	THR
1	B	564	ILE
1	B	566	VAL
1	B	576	CYS
1	B	578	GLU
1	B	583	THR
1	B	584	GLN
1	B	591	GLU
1	B	596	ILE
1	B	602	GLU
1	B	603	ARG
1	B	612	ILE
1	B	620	LEU
1	B	636	ILE
1	B	643	GLN
1	B	649	ILE
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	712	ILE
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
1	B	772	LEU

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Mol	Chain	Res	Type
1	B	775	LYS
1	B	777	LEU
1	B	780	TYR
1	B	784	ILE
1	B	790	THR
1	B	792	VAL
1	B	803	ASP
1	B	804	LYS
1	B	810	VAL
1	B	819	VAL
1	B	827	ILE
1	B	833	VAL
1	B	840	ARG
1	B	844	LEU
1	B	847	LEU
1	B	850	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	910	VAL
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	993	ILE
1	B	996	ASP
1	B	1009	LEU

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Mol	Chain	Res	Type
1	B	1011	GLU
1	B	1016	ARG
1	B	1020	LEU
1	B	1023	GLU
1	B	1025	LYS
1	B	1029	VAL
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	1077	LEU
1	B	1084	VAL
1	B	1092	MET
1	B	1099	VAL
1	B	1102	ARG
1	B	1120	LYS
1	B	1129	LEU
1	B	1134	LYS
1	B	1135	LEU
1	B	1142	LYS
1	B	1143	ILE
1	B	1153	LEU
1	B	1166	ARG
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	1299	THR
1	B	1300	GLU
1	B	1303	ASP
1	B	1312	LEU
1	B	1320	LEU

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Mol	Chain	Res	Type
1	B	1335	VAL
1	B	1352	THR
1	B	1358	ILE
1	B	1366	ARG
1	B	1368	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1388	GLN
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	1480	GLN
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	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	1649	SER
1	B	1656	VAL
1	B	1696	GLN
1	B	1728	LEU
1	B	1739	GLU
1	B	1741	VAL

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Mol	Chain	Res	Type
1	B	1765	THR
1	B	1774	GLN
1	B	1776	ILE
1	B	1781	LEU
1	B	1785	LEU
1	B	1796	LEU
1	B	1807	GLU
1	B	1815	LEU
1	B	1829	ILE
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	1907	GLU
1	B	1967	THR
1	B	1969	GLU
1	B	1974	CYS
1	B	1985	ILE
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	2039	VAL
1	B	2041	LEU
1	B	2046	GLU
1	B	2047	VAL
1	B	2052	ILE
1	B	2058	GLN
1	B	2077	ILE
1	B	2085	GLN
1	B	2086	GLN
1	B	2091	LYS
1	B	2092	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	ASN
1	B	702	GLN
1	B	719	ASN
1	B	720	GLN
1	B	990	HIS
1	B	999	GLN
1	B	1003	GLN
1	B	1175	HIS
1	B	1281	GLN
1	B	1341	ASN
1	B	1388	GLN
1	B	1568	GLN
1	B	1667	GLN
1	B	1674	HIS
1	B	1696	GLN
1	B	1707	GLN
1	B	1766	GLN
1	B	1870	GLN
1	B	1909	GLN
1	B	1962	GLN
1	B	2086	GLN
1	B	2118	GLN

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](#)

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[B]	-	11,11,11	3.35	1 (9%)	16,16,16	2.08	3 (18%)
2	SAN	B	2201[A]	-	11,11,11	3.10	1 (9%)	16,16,16	2.23	4 (25%)

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[B]	-	-	4/6/6/6	0/1/1/1
2	SAN	B	2201[A]	-	-	4/6/6/6	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	-11.05	1.60	1.77
2	B	2201[A]	SAN	C4-S	-10.21	1.61	1.77

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2201[A]	SAN	O2-S-O1	-6.92	108.16	118.80
2	B	2201[B]	SAN	O2-S-O1	-6.69	108.50	118.80
2	B	2201[B]	SAN	O2-S-C4	3.17	110.94	107.35
2	B	2201[A]	SAN	O1-S-C4	3.02	110.77	107.35
2	B	2201[A]	SAN	O2-S-C4	2.75	110.46	107.35
2	B	2201[B]	SAN	O1-S-N2	2.41	110.82	107.35
2	B	2201[A]	SAN	C6-C5-C4	2.00	121.39	119.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2201[B]	SAN	C5-C4-S-N2
2	B	2201[A]	SAN	C5-C4-S-O1

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Mol	Chain	Res	Type	Atoms
2	B	2201[B]	SAN	C3-C4-S-N2
2	B	2201[A]	SAN	C3-C4-S-O1
2	B	2201[A]	SAN	C5-C4-S-N2
2	B	2201[A]	SAN	C3-C4-S-N2
2	B	2201[B]	SAN	C5-C4-S-O2
2	B	2201[B]	SAN	C3-C4-S-O2

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	B	1723/1724 (99%)	0.17	49 (2%) 55 48	38, 83, 156, 206	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	752	LEU	4.2
1	B	1502[A]	HIS	4.1
1	B	403	LEU	4.0
1	B	743	LEU	3.8
1	B	757	ALA	3.7
1	B	433	GLY	3.7
1	B	821	LEU	3.5
1	B	759	THR	3.3
1	B	762	LEU	3.3
1	B	1999	LEU	3.2
1	B	748	LEU	3.1
1	B	774	LEU	3.1
1	B	575	LEU	2.9
1	B	525	ILE	2.8
1	B	827	ILE	2.7
1	B	809	LEU	2.7
1	B	883	LEU	2.7
1	B	435	PHE	2.7
1	B	709	TYR	2.6
1	B	772	LEU	2.5
1	B	742	CYS	2.5
1	B	440	LYS	2.5
1	B	722	LEU	2.4
1	B	751	PHE	2.4
1	B	750	LEU	2.4
1	B	756	SER	2.4
1	B	576	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	781	GLY	2.4
1	B	876	LEU	2.3
1	B	573	HIS	2.3
1	B	758	SER	2.3
1	B	787	ALA	2.3
1	B	690	VAL	2.3
1	B	1052	ILE	2.3
1	B	434	SER	2.2
1	B	1996	LEU	2.2
1	B	770	LYS	2.2
1	B	754	GLU	2.2
1	B	728	ARG	2.2
1	B	853	LEU	2.2
1	B	790	THR	2.2
1	B	793	ASP	2.2
1	B	1997	LEU	2.1
1	B	738	ILE	2.1
1	B	823	ALA	2.1
1	B	771	ASN	2.1
1	B	698	ILE	2.0
1	B	788	GLY	2.0
1	B	480	THR	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(Å ²)	Q<0.9
2	SAN	B	2201[A]	11/11	0.92	0.13	28,37,50,52	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAN	B	2201[B]	11/11	0.92	0.13	18,25,49,54	11

6.5 Other polymers [i](#)

There are no such residues in this entry.