

Full wwPDB X-ray Structure Validation Report (i)

Jun 2, 2021 - 04:07 am BST

PDB ID	:	7BDJ
Title	:	Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and mant-
		ATPgammaS
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Deposited on	:	2020-12-21
Resolution	:	2.59 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	•	4.02b-467
Mogul		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		1.13
EDŚ	:	2.19
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.19

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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 $(\#Entries, resolution, range(Å))$
\mathbf{R}_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	$3455\ (2.60-2.60)$
Sidechain outliers	138945	3455(2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	В	1747	77%	20%	•••	i
2	J	263	<mark>6%</mark> 88%	1	.1% •	1



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16197 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		
1	В	1722	Total 13847	C 8850	N 2369	O 2557	S 71	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	390	GLY	-	expression tag	UNP 075643
В	391	ALA	-	expression tag	UNP 075643
В	392	GLU	-	expression tag	UNP 075643
В	393	PHE	-	expression tag	UNP 075643

• Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	J	262	Total 2118	$\begin{array}{c} \mathrm{C} \\ 1356 \end{array}$	N 364	O 386	S 12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2058	GLY	-	expression tag	UNP Q6P2Q9
J	2059	PRO	-	expression tag	UNP Q6P2Q9
J	2060	LEU	-	expression tag	UNP Q6P2Q9
J	2061	GLY	-	expression tag	UNP Q6P2Q9
J	2062	SER	-	expression tag	UNP Q6P2Q9
J	2063	MET	-	expression tag	UNP Q6P2Q9

• Molecule 3 is [[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3-[2-(methylamino)phenyl] carbonyloxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl] oxy-sulfanyl-phosphinic acid (three-letter code: TGB) (formula: C₁₈H₂₃N₆O₁₃P₃S) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		A	ton	ıs			ZeroOcc	AltConf	
3	В	1	Total	С	Ν	Ο	Р	S	0	Ο	
	D	L	41	18	6	13	3	1	0	0	
2	р	1	Total	С	Ν	Ο	Р	S	0	0	
J J	D	L	41	18	6	13	3	1	0	0	

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	2	Total Mg 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	123	Total O 123 123	0	0
5	J	25	TotalO2525	0	0



3 Residue-property plots (i)

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





• Molecule 2: Pre-mRNA-processing-splicing factor 8





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	99.61Å 118.91Å 187.35Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
\mathbf{B} as a solution (\mathbf{A})	48.34 - 2.59	Depositor
Resolution (A)	48.34 - 2.59	EDS
$\% { m Data \ completeness}$	99.3 (48.34-2.59)	Depositor
(in resolution range $)$	99.3(48.34-2.59)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.32 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
B B.	0.230 , 0.289	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.230 , 0.289	DCC
R_{free} test set	2100 reflections $(3.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.7	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.28 , 33.9	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16197	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: TGB, MG

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).

Mal	Chain	Bond lengths		Bond angles	
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.26	0/14140	0.46	1/19158~(0.0%)
2	J	0.25	0/2185	0.45	0/2975
All	All	0.26	0/16325	0.46	1/22133~(0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	В	0	3
2	J	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	752	LEU	CA-CB-CG	6.37	129.95	115.30

There are no chirality outliers.

All (5) planarity outliers are listed belo	ow:
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Mol	Chain	Res	Type	Group
1	В	1260	GLU	Peptide
1	В	1858	ILE	Peptide
1	В	1993	ARG	Peptide
2	J	2097	ILE	Peptide
2	J	2099	GLU	Peptide



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	В	13847	0	13988	257	0
2	J	2118	0	2061	19	0
3	В	82	0	0	1	0
4	В	2	0	0	0	0
5	В	123	0	0	3	0
5	J	25	0	0	0	0
All	All	16197	0	16049	273	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 9.

All (273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:B:580:ILE:HD13	1:B:605:TYR:HB3	1.47	0.95
1:B:1988:MET:H	1:B:1993:ARG:HH22	1.00	0.94
1:B:1988:MET:N	1:B:1993:ARG:HH22	1.71	0.88
1:B:1990:ASP:HA	1:B:1993:ARG:HG2	1.54	0.87
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.58	0.85
1:B:1994:ASN:HB2	1:B:1998:GLN:HG3	1.59	0.84
1:B:1600:TYR:HB3	1:B:1631:LEU:HD21	1.58	0.83
1:B:1988:MET:O	1:B:1993:ARG:NH2	2.12	0.83
1:B:1970:HIS:HA	1:B:1973:ARG:HB2	1.61	0.82
1:B:1413:SER:HA	1:B:1416:LEU:HD12	1.63	0.81
1:B:601:GLY:HA2	1:B:1536:GLN:HG3	1.63	0.80
1:B:1988:MET:H	1:B:1993:ARG:NH2	1.80	0.78
1:B:1879:LEU:HD21	1:B:1893:LEU:HD21	1.66	0.77
1:B:1945:LEU:HA	1:B:1948:MET:HB2	1.66	0.75
1:B:571:GLY:HA3	1:B:579:GLU:HB3	1.65	0.75
1:B:2013:ARG:HH12	1:B:2062:GLU:HG3	1.52	0.75
1:B:760:GLU:O	1:B:764:THR:N	2.17	0.74
1:B:1963:LEU:HD22	1:B:2007:VAL:HG13	1.69	0.73
1:B:739:ARG:NH1	1:B:776:ASP:OD1	2.21	0.72
2:J:2096:ASP:HB3	2:J:2098:LYS:HG2	1.70	0.72
1:B:1044:VAL:O	2:J:2074:ARG:NH1	2.21	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:1157:ASN:ND2	1:B:1159:ASN:OD1	2.24	0.70
1:B:752:LEU:HD11	1:B:780:TYR:HA	1.74	0.69
1:B:1556:LYS:H	1:B:1556:LYS:HD3	1.57	0.69
1:B:2046:GLU:HA	1:B:2086:GLN:HE22	1.58	0.69
1:B:1302:LEU:N	1:B:1334:GLN:OE1	2.25	0.68
1:B:1970:HIS:HA	1:B:1973:ARG:CB	2.24	0.68
1:B:1967:THR:OG1	1:B:1970:HIS:CE1	2.47	0.68
1:B:1430:GLU:HG2	1:B:1466:VAL:HG11	1.74	0.68
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.77	0.67
1:B:1871:LEU:HD22	1:B:1893:LEU:HB3	1.76	0.67
1:B:2043:ARG:HB2	1:B:2084:LEU:HD11	1.78	0.66
1:B:1672:LYS:HE3	1:B:1859:PRO:HA	1.78	0.65
1:B:1456:VAL:HG12	1:B:1491:SER:HB2	1.78	0.65
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.79	0.65
1:B:1667:GLN:NE2	5:B:2302:HOH:O	2.31	0.64
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.79	0.64
1:B:1316:ALA:HB1	1:B:1401:LEU:HD22	1.81	0.63
1:B:1156:LEU:HD23	1:B:1160:GLU:HB3	1.80	0.63
1:B:1979:VAL:HG13	1:B:1984:ASP:OD2	1.98	0.63
1:B:603:ARG:HD3	1:B:605:TYR:H	1.63	0.63
2:J:2167:GLU:HA	2:J:2170:LYS:HE2	1.81	0.63
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.80	0.63
1:B:1864:GLU:HG3	1:B:1867:LEU:HB3	1.81	0.62
2:J:2099:GLU:HB2	2:J:2100:THR:HG23	1.81	0.62
1:B:1871:LEU:O	1:B:1874:LYS:N	2.31	0.62
1:B:1777:SER:HB3	1:B:1780:HIS:CG	2.36	0.61
1:B:1867:LEU:O	1:B:1871:LEU:N	2.33	0.61
1:B:1138:GLU:N	1:B:1138:GLU:OE1	2.32	0.61
1:B:726:HIS:NE2	1:B:830:GLY:O	2.31	0.60
1:B:749:GLY:HA2	1:B:753:ARG:CB	2.30	0.60
1:B:1940:LEU:HD11	1:B:2067:VAL:HG11	1.81	0.60
1:B:1967:THR:HG1	1:B:1970:HIS:CG	2.19	0.60
1:B:1259:PHE:HD2	1:B:1261:PRO:HD2	1.67	0.60
1:B:1967:THR:OG1	1:B:1970:HIS:ND1	2.35	0.60
1:B:2043:ARG:NE	1:B:2084:LEU:HD12	2.16	0.59
1:B:1593:THR:HG21	1:B:1596:ASP:H	1.68	0.59
1:B:607:GLN:O	1:B:610:ARG:NH1	2.33	0.59
1:B:1994:ASN:CB	1:B:1998:GLN:HG3	2.30	0.59
1:B:1851:ASN:HA	1:B:1888:HIS:CG	2.38	0.59
1:B:1967:THR:OG1	1:B:1970:HIS:CG	2.56	0.59
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.84	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:761:VAL:HA	1:B:764:THR:HG22	1.86	0.58
1:B:1139:VAL:HG21	1:B:1174:ILE:HD11	1.85	0.58
1:B:753:ARG:NE	1:B:753:ARG:HA	2.18	0.58
1:B:1993:ARG:NH2	1:B:1993:ARG:HB2	2.17	0.58
2:J:2277:SER:OG	2:J:2278:SER:N	2.36	0.58
1:B:2040:GLN:HG3	1:B:2089:LYS:HG2	1.85	0.57
2:J:2236:GLU:OE2	2:J:2239:ARG:NH1	2.37	0.57
1:B:1592:CYS:SG	1:B:1593:THR:HG22	2.45	0.57
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.87	0.57
1:B:654:THR:HG21	1:B:676:PHE:O	2.06	0.56
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.87	0.56
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.40	0.56
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.39	0.56
1:B:525:ILE:HA	1:B:531:ILE:HG22	1.88	0.55
1:B:703:ILE:O	1:B:707:ILE:HG13	2.07	0.55
1:B:2066:VAL:HG21	1:B:2090:VAL:HG11	1.89	0.55
1:B:749:GLY:HA2	1:B:753:ARG:HB3	1.88	0.55
1:B:438:GLN:NE2	1:B:439:ARG:O	2.39	0.55
1:B:1011:GLU:HG3	1:B:1110:LYS:HD3	1.89	0.55
1:B:1195:ARG:NH1	1:B:1260:GLU:OE2	2.40	0.55
1:B:2046:GLU:HA	1:B:2086:GLN:NE2	2.20	0.55
1:B:569:LEU:HD22	1:B:592:LYS:HE2	1.89	0.55
1:B:1967:THR:HG1	1:B:1970:HIS:CE1	2.26	0.54
1:B:1973:ARG:NE	1:B:1996:LEU:HB3	2.22	0.54
1:B:1993:ARG:HB2	1:B:1993:ARG:CZ	2.37	0.54
1:B:1974:CYS:O	1:B:1978:GLY:N	2.40	0.54
1:B:414:LEU:HB2	1:B:894:VAL:HG11	1.89	0.54
1:B:545:ARG:NH1	1:B:568:GLU:OE2	2.40	0.54
1:B:1157:ASN:HD22	1:B:1159:ASN:H	1.54	0.54
1:B:1997:LEU:HD12	1:B:1998:GLN:H	1.71	0.54
1:B:1159:ASN:OD1	1:B:1159:ASN:N	2.41	0.54
1:B:1434:ILE:HG23	1:B:1435:LEU:HD23	1.90	0.53
1:B:1499:ASP:OD1	1:B:1762:ARG:NH2	2.42	0.53
1:B:1603:LYS:N	1:B:1603:LYS:HD2	2.24	0.53
1:B:1879:LEU:HB2	1:B:1882:PRO:HG3	1.89	0.53
1:B:1851:ASN:OD1	1:B:1851:ASN:N	2.42	0.53
1:B:1865:ASP:OD2	1:B:1866:ASN:N	2.41	0.53
1:B:1871:LEU:HA	1:B:1874:LYS:HB2	1.92	0.52
1:B:2010:PHE:HA	1:B:2052:ILE:HD12	1.91	0.52
1:B:526:ASN:ND2	1:B:527:MET:H	2.07	0.52
1:B:1904:LEU:HB2	1:B:1908:LEU:HD22	1.92	0.52



	h i n	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1368:LEU:HD22	1:B:1403:LYS:HE2	1.92	0.52
1:B:1271:VAL:HG12	1:B:1279:GLU:HB2	1.91	0.51
1:B:1135:LEU:HD12	1:B:1136:PRO:HD2	1.91	0.51
1:B:1593:THR:HG21	1:B:1596:ASP:HB2	1.92	0.51
1:B:766:ALA:HA	1:B:769:CYS:HB2	1.91	0.51
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	1.91	0.51
1:B:1997:LEU:HG	1:B:1999:LEU:HG	1.92	0.51
1:B:753:ARG:HA	1:B:753:ARG:HE	1.76	0.51
1:B:1736:PHE:O	1:B:1740:ILE:HG12	2.11	0.51
1:B:834:TYR:OH	1:B:1030:ARG:NH1	2.44	0.50
1:B:2091:LYS:NZ	1:B:2093:ASP:HB3	2.27	0.50
1:B:566:VAL:HG22	1:B:585:ILE:HB	1.93	0.50
1:B:743:LEU:HD12	1:B:748:LEU:HD11	1.93	0.50
1:B:1042:GLU:O	2:J:2074:ARG:NH2	2.45	0.50
1:B:1601:LEU:HD21	1:B:1613:LEU:HB2	1.93	0.50
1:B:721:VAL:HG22	1:B:825:THR:HB	1.93	0.50
1:B:1739:GLU:HA	1:B:1742:THR:HG22	1.94	0.50
1:B:528:ASP:OD2	1:B:530:THR:OG1	2.31	0.49
1:B:1599:PRO:O	1:B:1603:LYS:NZ	2.45	0.49
1:B:771:ASN:HB3	1:B:774:LEU:HB3	1.94	0.49
1:B:1593:THR:HG21	1:B:1596:ASP:CB	2.41	0.49
1:B:639:ILE:O	1:B:643:GLN:N	2.43	0.49
1:B:1024:PHE:HB3	1:B:1027:ILE:HD12	1.95	0.49
1:B:812:THR:OG1	1:B:813:ALA:N	2.46	0.49
1:B:436:ARG:O	1:B:437:ARG:HD3	2.12	0.48
1:B:525:ILE:HG12	1:B:531:ILE:HG22	1.95	0.48
1:B:571:GLY:HA2	1:B:574:GLN:NE2	2.28	0.48
1:B:1142:LYS:HA	1:B:1145:LYS:HG2	1.95	0.48
1:B:2045:GLU:HG2	1:B:2046:GLU:H	1.78	0.48
1:B:791:ARG:HD2	1:B:794:ARG:HH21	1.78	0.48
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.49	0.48
1:B:1905:SER:OG	1:B:1906:ALA:N	2.47	0.48
1:B:1732:MET:HE3	1:B:1788:LEU:HD21	1.96	0.48
1:B:1601:LEU:O	1:B:1602:GLU:HB2	2.14	0.48
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.22	0.48
1:B:2051:VAL:HG11	1:B:2112:ALA:HB1	1.96	0.47
1:B:1981:SER:O	1:B:1983:PHE:N	2.45	0.47
1:B:1630:ARG:HH22	1:B:1634:GLN:HG3	1.79	0.47
1:B:1846:ILE:O	1:B:1850:SER:OG	2.30	0.47
1:B:1593:THR:HG21	1:B:1596:ASP:OD2	2.14	0.47
1:B:2026:LYS:HA	1:B:2029:ILE:HD11	1.96	0.47



	h h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:2037:VAL:CG1	1:B:2092:LEU:HB2	2.43	0.47
1:B:1406:VAL:HG23	1:B:1425:ILE:HA	1.94	0.47
1:B:2018:GLU:HB3	1:B:2042:GLU:HB3	1.97	0.47
2:J:2098:LYS:O	2:J:2099:GLU:HB2	2.14	0.47
1:B:626:PRO:HB3	1:B:893:MET:HG2	1.96	0.47
1:B:1350:ALA:O	1:B:1492:SER:HA	2.15	0.47
1:B:406:ARG:NH2	1:B:954:LEU:HG	2.30	0.47
1:B:1442:ARG:O	1:B:1446:GLN:NE2	2.47	0.47
1:B:1989:GLU:O	1:B:1993:ARG:N	2.44	0.47
1:B:1672:LYS:HE2	1:B:1857:ASN:HA	1.97	0.47
1:B:459:GLU:OE1	1:B:483:ARG:HD3	2.15	0.46
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.96	0.46
1:B:2078:SER:OG	1:B:2092:LEU:HB3	2.15	0.46
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.97	0.46
1:B:2027:ASP:OD1	1:B:2027:ASP:N	2.48	0.46
1:B:2036:VAL:HG22	1:B:2091:LYS:HZ2	1.80	0.46
1:B:1995:ALA:O	1:B:1997:LEU:N	2.42	0.46
1:B:1416:LEU:HA	1:B:1419:LEU:HD13	1.98	0.46
1:B:1593:THR:OG1	1:B:1594:GLU:N	2.48	0.46
1:B:1259:PHE:CD2	1:B:1261:PRO:HD2	2.49	0.46
1:B:1088:ALA:HB1	1:B:1118:ILE:HD13	1.98	0.46
1:B:1970:HIS:NE2	1:B:1997:LEU:HD23	2.31	0.46
1:B:1973:ARG:HE	1:B:1996:LEU:HB3	1.80	0.46
1:B:1009:LEU:HD11	1:B:1013:GLU:HG2	1.98	0.45
1:B:1467:LEU:HD12	1:B:1470:ILE:HD11	1.97	0.45
1:B:1594:GLU:HG2	1:B:1595:LYS:N	2.31	0.45
1:B:542:ALA:HB3	1:B:548:VAL:HG22	1.98	0.45
1:B:1406:VAL:HG11	1:B:1418:LEU:HB3	1.98	0.45
1:B:1597:LEU:HA	1:B:1600:TYR:HD1	1.81	0.45
1:B:1438:ARG:NH2	1:B:1821:TYR:O	2.49	0.45
1:B:1866:ASN:HA	1:B:1869:ARG:HB2	1.97	0.45
1:B:726:HIS:CE1	1:B:844:LEU:HD11	2.50	0.45
1:B:2015:PRO:HG2	1:B:2116:CYS:SG	2.57	0.45
1:B:719:ASN:ND2	5:B:2307:HOH:O	2.42	0.45
1:B:1162:GLY:O	1:B:1167:MET:N	2.42	0.45
1:B:1375:ARG:HH12	1:B:1420:GLY:HA2	1.81	0.45
1:B:1417:LYS:HB3	1:B:1417:LYS:HE3	1.71	0.45
1:B:2035:VAL:HG21	1:B:2094:PHE:CD2	2.52	0.45
1:B:578:GLU:OE2	1:B:578:GLU:N	2.50	0.45
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.98	0.45
1:B:1439:TRP:CD2	1:B:1477:ILE:HG12	2.51	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:406:ARG:CZ	1:B:406:ARG:HB2	2.47	0.45
1:B:420:SER:HB2	1:B:622:ASP:HA	1.99	0.44
1:B:1973:ARG:HD2	1:B:1996:LEU:HD13	2.00	0.44
1:B:1988:MET:C	1:B:1993:ARG:NH2	2.69	0.44
1:B:2036:VAL:HG22	1:B:2091:LYS:NZ	2.33	0.44
1:B:944:LYS:C	1:B:946:ASP:H	2.20	0.44
1:B:1707:GLN:HB2	5:B:2302:HOH:O	2.17	0.44
2:J:2125:ALA:HB2	2:J:2157:VAL:HG21	2.00	0.44
1:B:565:THR:HG23	1:B:583:THR:HA	2.00	0.44
1:B:1043:ARG:HG3	2:J:2317:PHE:CE1	2.52	0.44
1:B:1165:ILE:HG13	1:B:1167:MET:HB2	1.99	0.44
1:B:1765:THR:HG22	1:B:1781:LEU:HD11	2.00	0.44
1:B:1972:LYS:O	1:B:1975:THR:OG1	2.24	0.44
2:J:2099:GLU:CB	2:J:2100:THR:HG23	2.46	0.44
1:B:1654:MET:HG2	1:B:1656:VAL:HG22	1.98	0.44
1:B:1988:MET:CA	1:B:1993:ARG:HH22	2.29	0.44
1:B:785:HIS:CE1	1:B:794:ARG:HD2	2.52	0.44
2:J:2149:PRO:HD3	2:J:2274:PRO:HG3	1.99	0.44
1:B:603:ARG:HD3	1:B:605:TYR:N	2.30	0.44
1:B:1378:TYR:HA	1:B:1452:VAL:HG13	2.00	0.44
1:B:822:PRO:HG2	1:B:858:ARG:HG3	2.00	0.44
1:B:1836:LEU:HD22	1:B:1930:LEU:HD21	1.99	0.44
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	2.00	0.43
1:B:1006:LYS:O	1:B:1009:LEU:HB2	2.18	0.43
1:B:2084:LEU:HD13	1:B:2086:GLN:N	2.33	0.43
1:B:1630:ARG:NH2	1:B:1634:GLN:HG3	2.33	0.43
1:B:1835:SER:HB3	1:B:1848:ILE:HG21	2.00	0.43
1:B:1999:LEU:O	1:B:2003:GLN:HB2	2.18	0.43
1:B:1532:ILE:HD13	1:B:1537:THR:HG22	2.00	0.43
1:B:681:ARG:HG2	1:B:682:PRO:HD2	2.01	0.43
1:B:1894:LEU:HD22	1:B:1908:LEU:HD21	2.00	0.43
1:B:406:ARG:HH21	1:B:954:LEU:HG	1.83	0.42
1:B:748:LEU:HB3	1:B:780:TYR:CE1	2.54	0.42
1:B:1491:SER:OG	1:B:1492:SER:O	2.36	0.42
1:B:2065:TRP:CZ3	1:B:2111:ASP:HB3	2.54	0.42
1:B:789:MET:O	1:B:794:ARG:NH1	2.52	0.42
1:B:794:ARG:O	1:B:798:GLU:HG2	2.19	0.42
1:B:1958:SER:HB2	1:B:1960:LEU:HD23	2.00	0.42
1:B:762:LEU:HD21	1:B:781:GLY:HA2	2.00	0.42
1:B:1445:VAL:O	1:B:1448:ILE:HG12	2.19	0.42
2:J:2280:ASN:HB3	2:J:2309:HIS:CG	2.54	0.42



	A O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:569:LEU:HD13	1:B:572:ASP:OD2	2.19	0.42
1:B:2037:VAL:HG13	1:B:2092:LEU:HB2	2.01	0.42
1:B:2105:THR:HG22	1:B:2121:LYS:HE3	2.01	0.42
1:B:1084:VAL:HG13	1:B:1085:THR:HG23	2.01	0.42
1:B:1334:GLN:HE21	1:B:1334:GLN:HB3	1.61	0.42
1:B:1842:VAL:HA	1:B:1845:LEU:HD12	2.02	0.42
1:B:1135:LEU:HD13	1:B:1177:TYR:CD2	2.55	0.42
1:B:1346:VAL:HG13	1:B:1488:VAL:HG13	2.02	0.42
1:B:1351:PRO:CG	1:B:1516:PRO:HA	2.48	0.42
1:B:1556:LYS:HG2	1:B:1557:LYS:HG3	2.01	0.42
1:B:1989:GLU:O	1:B:1993:ARG:HB3	2.19	0.42
2:J:2191:GLN:HG2	2:J:2244:LYS:HD2	2.02	0.42
1:B:636:ILE:HD13	1:B:666:ARG:HD2	2.02	0.41
1:B:1499:ASP:OD2	1:B:1763:ARG:NH1	2.45	0.41
1:B:626:PRO:HG3	1:B:893:MET:HA	2.03	0.41
1:B:1769:ASN:HD22	1:B:1769:ASN:HA	1.69	0.41
1:B:603:ARG:NE	1:B:607:GLN:H	2.18	0.41
1:B:1856:GLU:OE1	1:B:1888:HIS:NE2	2.54	0.41
2:J:2306:HIS:ND1	2:J:2308:VAL:HG22	2.36	0.41
1:B:605:TYR:HD1	1:B:606:THR:HG1	1.65	0.41
1:B:944:LYS:HD2	1:B:944:LYS:HA	1.81	0.41
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	2.02	0.41
1:B:1993:ARG:C	1:B:1995:ALA:N	2.74	0.41
1:B:428:CYS:HB3	1:B:877:GLN:OE1	2.21	0.41
1:B:1451:PHE:O	1:B:1487:ILE:HA	2.21	0.41
1:B:1672:LYS:HZ1	1:B:1858:ILE:CA	2.34	0.41
1:B:1339:VAL:HA	1:B:1486:ARG:HH22	1.85	0.41
1:B:1981:SER:OG	1:B:1984:ASP:N	2.39	0.41
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.55	0.41
2:J:2237:TRP:O	2:J:2240:GLN:HG3	2.21	0.41
1:B:502:CYS:HA	1:B:652:SER:O	2.21	0.41
1:B:725:VAL:HG12	1:B:829:LYS:HB3	2.03	0.41
1:B:1262:LEU:HD23	1:B:1262:LEU:HA	1.91	0.41
1:B:1378:TYR:OH	1:B:1454:ASP:OD2	2.31	0.41
1:B:1566:ARG:O	1:B:1569:THR:OG1	2.30	0.41
1:B:547:LEU:O	1:B:551:MET:HG2	2.21	0.41
1:B:1123:TRP:HB3	2:J:2307:GLU:OE2	2.21	0.41
1:B:1995:ALA:O	1:B:1996:LEU:HB2	2.21	0.40
3:B:2202:TGB:O10	3:B:2202:TGB:O14	2.39	0.40
1:B:1080:ASP:O	1:B:1084:VAL:HG12	2.20	0.40
1:B:1381:PRO:HB2	1:B:1458:LEU:HD12	2.03	0.40



Atom-1	Atom-2	${f Interatomic} \ {f distance} \ ({ m \AA})$	Clash overlap (Å)
1:B:1871:LEU:HD11	1:B:1897:ALA:HB2	2.02	0.40
1:B:1967:THR:OG1	1:B:1970:HIS:CD2	2.74	0.40
1:B:436:ARG:HG2	1:B:445:VAL:HG22	2.04	0.40
1:B:572:ASP:HB3	1:B:592:LYS:HE3	2.03	0.40
1:B:1515:HIS:NE2	1:B:1721:PRO:HG3	2.36	0.40
1:B:2039:VAL:HB	1:B:2090:VAL:CG1	2.52	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	Perce	entiles
1	В	1718/1747~(98%)	1593~(93%)	112 (6%)	13 (1%)	19	39
2	J	260/263~(99%)	244 (94%)	15~(6%)	1 (0%)	34	57
All	All	1978/2010 (98%)	1837 (93%)	127 (6%)	14 (1%)	22	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	1261	PRO
1	В	1967	THR
1	В	1171	GLY
1	В	1994	ASN
1	В	2086	GLN
1	В	1141	LYS
1	В	1973	ARG
2	J	2098	LYS
1	В	404	ALA
1	В	2085	GLN
1	В	1157	ASN
1	В	1982	VAL



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Mol	Chain	Res	Type
1	В	1326	PRO
1	В	2057	PRO

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	В	1541/1560~(99%)	1491~(97%)	50 (3%)	39 65
2	J	236/236~(100%)	235~(100%)	1 (0%)	91 97
All	All	1777/1796~(99%)	1726~(97%)	51 (3%)	42 68

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	406	ARG
1	В	429	GLN
1	В	438	GLN
1	В	545	ARG
1	В	603	ARG
1	В	641	MET
1	В	652	SER
1	В	696	LYS
1	В	753	ARG
1	В	780	TYR
1	В	858	ARG
1	В	941	ASP
1	В	992	TYR
1	В	1043	ARG
1	В	1051	SER
1	В	1126	MET
1	В	1315	SER
1	В	1375	ARG
1	В	1443	LYS
1	В	1515	HIS
1	В	1556	LYS



Mol	Chain	Res	Type
1	В	1575	ASP
1	В	1580	CYS
1	В	1586	ARG
1	В	1603	LYS
1	В	1627	MET
1	В	1630	ARG
1	В	1648	ARG
1	В	1699	GLU
1	В	1762	ARG
1	В	1797	GLU
1	В	1841	LYS
1	В	1843	ARG
1	В	1863	HIS
1	В	1909	GLN
1	В	1956	LYS
1	В	1958	SER
1	В	1966	PHE
1	В	1969	GLU
1	В	1970	HIS
1	В	1972	LYS
1	В	1973	ARG
1	В	1983	PHE
1	В	1993	ARG
1	В	2026	LYS
1	В	2072	LYS
1	В	2078	SER
1	В	2082	LEU
1	В	2106	LEU
1	В	2110	SER
2	J	2246	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	526	ASN
1	В	1147	ASN
1	В	1157	ASN
1	В	1870	GLN
1	В	2086	GLN
2	J	2065	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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).

Mal	Tuno	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	gles
	туре	Chain	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	TGB	В	2201	4	35,44,44	<mark>3.70</mark>	13 (37%)	41,67,67	1.66	6 (14%)
3	TGB	В	2202	4	35,44,44	<mark>3.68</mark>	13 (37%)	41,67,67	1.53	5 (12%)

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
3	TGB	В	2201	4	-	7/26/48/48	0/4/4/4
3	TGB	В	2202	4	-	8/26/48/48	0/4/4/4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	2201	TGB	C13-C15	-12.31	1.35	1.53



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	В	2202	TGB	C13-C15	-12.04	1.35	1.53
3	В	2202	TGB	O26-C15	10.81	1.56	1.41
3	В	2201	TGB	O26-C15	10.70	1.56	1.41
3	В	2202	TGB	C12-C27	-6.31	1.36	1.52
3	В	2201	TGB	C12-C27	-6.14	1.36	1.52
3	В	2202	TGB	C03-N02	5.97	1.48	1.37
3	В	2201	TGB	C03-N02	5.88	1.48	1.37
3	В	2201	TGB	O26-C27	5.41	1.57	1.45
3	В	2202	TGB	O26-C27	4.99	1.56	1.45
3	В	2202	TGB	O11-C09	4.78	1.44	1.34
3	В	2201	TGB	O11-C09	4.65	1.44	1.34
3	В	2202	TGB	P38-O39	4.24	1.67	1.56
3	В	2201	TGB	P38-O39	4.23	1.67	1.56
3	В	2202	TGB	C20-N21	4.04	1.48	1.34
3	В	2201	TGB	C20-N21	3.94	1.48	1.34
3	В	2201	TGB	C08-C09	3.80	1.58	1.50
3	В	2202	TGB	C08-C09	3.54	1.57	1.50
3	В	2202	TGB	C13-C12	3.42	1.60	1.52
3	В	2201	TGB	C13-C12	3.22	1.60	1.52
3	В	2201	TGB	O10-C09	-2.34	1.16	1.22
3	В	2202	TGB	O10-C09	-2.32	1.16	1.22
3	В	2202	TGB	C28-C27	2.26	1.58	1.51
3	В	2201	TGB	C28-C27	2.26	1.58	1.51
3	В	2202	TGB	C19-N18	-2.12	1.32	1.39
3	В	2201	TGB	C19-N18	-2.10	1.32	1.39

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All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	2202	TGB	O11-C09-C08	5.99	121.02	111.69
3	В	2201	TGB	O11-C09-C08	5.65	120.50	111.69
3	В	2201	TGB	O26-C15-C13	-4.55	100.27	106.93
3	В	2201	TGB	N24-C23-N22	-4.33	121.90	128.68
3	В	2202	TGB	N24-C23-N22	-4.26	122.02	128.68
3	В	2201	TGB	P34-O33-P30	-3.06	122.34	132.83
3	В	2202	TGB	P34-O33-P30	-2.64	123.77	132.83
3	В	2201	TGB	O11-C09-O10	-2.38	119.65	123.53
3	В	2202	TGB	O26-C15-C13	-2.28	103.59	106.93
3	В	2202	TGB	C25-C19-N18	-2.10	107.21	109.40
3	В	2201	TGB	C25-C19-N18	-2.04	107.28	109.40

There are no chirality outliers.



Mol	Chain	Res	Type	Atoms
3	В	2201	TGB	C08-C09-O11-C12
3	В	2201	TGB	O10-C09-O11-C12
3	В	2201	TGB	P34-O37-P38-O39
3	В	2202	TGB	C08-C09-O11-C12
3	В	2202	TGB	O10-C09-O11-C12
3	В	2202	TGB	P34-O37-P38-O39
3	В	2201	TGB	O26-C27-C28-O29
3	В	2202	TGB	O26-C27-C28-O29
3	В	2202	TGB	C04-C03-N02-C01
3	В	2201	TGB	C08-C03-N02-C01
3	В	2202	TGB	C08-C03-N02-C01
3	В	2201	TGB	C12-C27-C28-O29
3	В	2202	TGB	C12-C27-C28-O29
3	В	2201	TGB	C04-C03-N02-C01
3	В	2202	TGB	P38-O37-P34-O35

All (15) torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	2202	TGB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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, 95^{th} 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		$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	В	1722/1747~(98%)	0.39	132 (7%) 13	10	31,61,108,133	0
2	J	262/263~(99%)	0.18	16 (6%) 21 1	l6	35, 57, 90, 118	0
All	All	1984/2010 (98%)	0.36	148 (7%) 14	10	31,60,107,133	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	2059	PRO	11.8
1	В	1889	VAL	10.1
1	В	2123	SER	8.8
1	В	1904	LEU	8.3
1	В	2038	LEU	7.9
1	В	753	ARG	7.6
1	В	2124	VAL	7.4
1	В	2027	ASP	7.2
1	В	1881	ASN	7.0
1	В	1880	ASN	6.9
1	В	1879	LEU	6.8
1	В	2106	LEU	6.7
2	J	2100	THR	6.6
2	J	2320	LEU	6.6
1	В	2122	PHE	6.2
1	В	2033	GLY	6.2
1	В	2035	VAL	6.1
1	В	749	GLY	5.9
1	В	1859	PRO	5.6
2	J	2099	GLU	5.2
1	В	2036	VAL	5.2
1	В	2097	PRO	5.1
2	J	2061	GLY	5.1
1	В	2020	SER	5.0



Mol	Chain	Res	Type	RSRZ
2	J	2062	SER	4.9
1	В	1873	GLN	4.9
1	В	1601	LEU	4.9
1	В	1876	PRO	4.8
1	В	2028	SER	4.8
1	В	1877	HIS	4.8
1	В	454	PRO	4.7
1	В	2101	ALA	4.5
1	В	1893	LEU	4.5
1	В	2034	PRO	4.4
1	В	1858	ILE	4.3
1	В	2040	GLN	4.3
1	В	1895	LEU	4.3
1	В	1996	LEU	4.3
1	В	757	ALA	4.3
1	В	456	GLY	4.2
1	В	1584	ILE	4.2
1	В	2026	LYS	4.0
1	В	1599	PRO	4.0
1	В	754	GLU	3.9
1	В	457	SER	3.9
1	В	1868	LEU	3.9
1	В	2069	GLY	3.9
1	В	2032	GLY	3.9
1	В	1915	ILE	3.8
1	В	1842	VAL	3.8
1	В	404	ALA	3.8
1	В	2008	ALA	3.8
1	В	750	LEU	3.8
1	В	1600	TYR	3.7
1	В	573	HIS	3.6
1	В	2082	LEU	3.6
2	J	2060	LEU	3.6
1	В	780	TYR	3.6
1	В	1971	ILE	3.5
1	В	2029	ILE	3.5
2	J	2095	ASP	3.5
1	В	1841	LYS	3.5
1	В	861	TYR	3.5
2	J	2094	SER	3.5
2	J	2097	ILE	3.5
2	J	2098	LYS	3.5



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Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	2108	PHE	3.5
1	В	1849	ILE	3.4
1	В	1896	GLN	3.4
1	В	1940	LEU	3.4
1	В	1995	ALA	3.4
1	В	2120	TYR	3.3
1	В	1155	ASP	3.3
1	В	2107	TYR	3.3
1	В	859	PRO	3.2
1	В	1936	LEU	3.2
1	В	805	HIS	3.2
1	В	2001	ASP	3.1
2	J	2063	MET	3.1
1	В	769	CYS	3.1
1	В	2090	VAL	3.0
1	В	1860	ILE	3.0
1	В	2037	VAL	3.0
1	В	2066	VAL	3.0
1	В	640	GLU	3.0
1	В	1962	GLN	3.0
2	J	2157	VAL	2.9
1	В	755	GLY	2.9
1	В	762	LEU	2.9
1	В	1604	LEU	2.8
1	В	1980	GLU	2.8
1	В	764	THR	2.8
1	В	1878	LYS	2.8
1	В	1959	TYR	2.8
1	В	1605	SER	2.8
1	В	2046	GLU	2.7
1	В	2039	VAL	2.7
1	В	1587	GLN	2.7
1	В	1585	GLN	2.7
1	B	1843	ARG	2.7
1	В	1886	ASP	2.7
1	B	1171	GLY	2.6
1	В	1911	ASP	2.6
1	В	1597	LEU	2.6
1	B	1908	LEU	2.6
1	В	765	GLU	2.6
1	В	1954	TRP	2.6
1	В	1075	PHE	2.5



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Mol	Chain	Res	Type	RSRZ
1	В	1963	LEU	2.5
1	В	1883	LYS	2.5
1	В	1912	THR	2.5
1	В	1905	SER	2.5
1	В	1614	LEU	2.4
1	В	1586	ARG	2.4
1	В	1869	ARG	2.4
1	В	1885	ASN	2.3
1	В	779	PRO	2.3
1	В	1072	LEU	2.3
1	В	2030	ARG	2.3
1	В	2047	VAL	2.3
1	В	1872	ALA	2.3
1	В	1960	LEU	2.3
1	В	1997	LEU	2.3
1	В	1874	LYS	2.2
1	В	1602	GLU	2.2
1	В	940	HIS	2.2
1	В	1983	PHE	2.2
1	В	774	LEU	2.2
2	J	2121	ARG	2.2
1	В	1972	LYS	2.2
1	В	1906	ALA	2.1
1	В	1976	ASP	2.1
1	В	1135	LEU	2.1
2	J	2065	GLN	2.1
2	J	2139	VAL	2.1
1	В	580	ILE	2.1
1	В	1307	LEU	2.1
1	B	2031	SER	2.1
1	В	1998	GLN	2.1
1	В	2024	VAL	2.1
1	В	458	GLU	2.1
1	В	1836	LEU	2.1
1	В	2086	GLN	2.1
1	В	405	PRO	2.0
1	В	1875	VAL	2.0
1	В	2048	THR	2.0
1	B	798	GLU	2.0
1	В	2104	TYR	2.0

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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 monosaccharides 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, 95^{th} 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
3	TGB	В	2201	41/41	0.89	0.21	$53,\!83,\!101,\!105$	0
4	MG	В	2204	1/1	0.89	0.21	64,64,64,64	0
3	TGB	В	2202	41/41	0.93	0.14	47,74,89,91	0
4	MG	В	2203	1/1	0.98	0.24	70,70,70,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









6.5 Other polymers (i)

There are no such residues in this entry.

