

# Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2023 – 12:26 pm GMT

PDB ID	:	8BCA
Title	:	Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and com-
		pound 26
Authors	:	Vester, K.; Loll, B.; Wahl, M.C.
Deposited on	:	2022-10-15
Resolution	:	2.80  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.32.1
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)	:	2.32.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	73%	25%	
2	J	263	<mark>6%</mark> 77%	22%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Q96	В	5802	-	Х	-	-
4	EDO	В	5806	-	-	Х	-



#### 8BCA

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16236 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		A	toms			ZeroOcc	AltConf	Trace
1	В	1724	Total 13870	C 8864	N 2372	O 2562	S 72	0	1	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		At	oms			ZeroOcc	AltConf	Trace
2	J	263	Total 2123	C 1358	N 365	O 388	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 3-azanyl-  $\{N\}$ -methyl-4-(methylamino)benzenesulfonamide (three-letter code: Q96) (formula:  $C_8H_{13}N_3O_2S$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
3	В	1	Total	С	Ν	0	S	0	0
0	9 D	1	14	8	3	2	1	0	0
2	В	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
0	3 B	1	14	8	3	2	1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	155	Total O 155 155	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	18	Total O 18 18	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.













## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	100.41Å 119.36Å 187.76Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	48.53 - 2.80	Depositor
Resolution (A)	48.53 - 2.80	EDS
% Data completeness	99.4 (48.53-2.80)	Depositor
(in resolution range)	$99.4 \ (48.53-2.80)$	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.17 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
P. P.	0.199 , $0.258$	Depositor
$n, n_{free}$	0.205 , $0.259$	DCC
$R_{free}$ test set	2100 reflections $(3.75%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	66.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , $35.2$	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16236	wwPDB-VP
Average B, all atoms $(Å^2)$	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: GOL, Q96, EDO

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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	В	0.34	0/14164	0.55	0/19192
2	J	0.35	0/2190	0.55	0/2981
All	All	0.35	0/16354	0.55	0/22173

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	В	13870	0	14008	258	1
2	J	2123	0	2063	32	0
3	В	28	0	0	0	0
4	В	36	0	53	6	0
5	В	6	0	8	0	0
6	В	155	0	0	7	0
6	J	18	0	0	0	0
All	All	16236	0	16132	289	1

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.



A		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1900:SER:HG	1:B:1954:TRP:HE1	1.17	0.90
1:B:1227:ASP:HB2	4:B:5806:EDO:H11	1.55	0.88
1:B:1558:PRO:HD2	1:B:1693:ARG:HH12	1.42	0.82
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.63	0.81
1:B:1229:ASP:HB2	1:B:1231:GLU:HG2	1.65	0.78
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.65	0.77
1:B:1481:ILE:HG22	1:B:1483:ARG:H	1.51	0.76
1:B:1586:ARG:HH12	1:B:1588:ARG:HD3	1.48	0.76
1:B:1894:LEU:HB3	1:B:1912:THR:HG22	1.68	0.75
1:B:525:ILE:HG12	1:B:531:ILE:HG13	1.69	0.74
1:B:436:ARG:HG2	1:B:445:VAL:HG22	1.73	0.71
2:J:2087:THR:HB	2:J:2112:LYS:HD3	1.72	0.71
1:B:2019:LEU:HB3	1:B:2041:LEU:HD23	1.71	0.71
2:J:2141:GLU:OE1	2:J:2143:ARG:NH2	2.23	0.71
2:J:2164:PRO:HB3	2:J:2296:LEU:HD11	1.73	0.69
1:B:1869:ARG:HD3	1:B:1884:PHE:HZ	1.57	0.69
1:B:1298:PRO:HB3	1:B:1515:HIS:CG	2.27	0.69
1:B:1259:PHE:HE2	4:B:5806:EDO:H22	1.58	0.69
1:B:1672:LYS:NZ	1:B:1856:GLU:OE1	2.24	0.69
1:B:1862:HIS:CG	1:B:1863:HIS:H	2.11	0.68
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.75	0.68
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.09	0.68
1:B:1406:VAL:HB	1:B:1418:LEU:HD22	1.75	0.68
1:B:420:SER:HB3	1:B:622:ASP:HA	1.75	0.68
1:B:1072:LEU:HD13	1:B:1077:LEU:HB3	1.76	0.68
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.76	0.67
1:B:1361:GLU:OE2	1:B:1393:TRP:NE1	2.26	0.67
1:B:2017:ILE:HD11	1:B:2041:LEU:HB3	1.75	0.67
1:B:406:ARG:HD3	1:B:954:LEU:HD22	1.76	0.67
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.75	0.66
1:B:1944:GLU:HA	1:B:1947:GLN:HE21	1.60	0.66
1:B:546:SER:OG	6:B:5901:HOH:O	2.15	0.64
1:B:421:HIS:ND1	6:B:5902:HOH:O	2.30	0.63
1:B:444:GLU:HG2	1:B:690:VAL:HG22	1.80	0.63
1:B:1501:ALA:HB1	1:B:1506:CYS:HB2	1.79	0.63
1:B:1607:SER:O	1:B:1611:GLU:HG2	1.98	0.63
1:B:1269:ARG:HG2	1:B:1281:GLN:HG3	1.80	0.63
1:B:1586:ARG:NH1	1:B:1588:ARG:HD3	2.13	0.63
1:B:1670:ASN:HB3	1:B:1673:ILE:HD11	1.80	0.63
2:J:2105:ILE:HD13	2:J:2262:LEU:HB2	1.81	0.63

All (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:971:LYS:HB2	1:B:980:GLN:HB3	1.81	0.63
1:B:1883:LYS:HB2	1:B:1889:VAL:HG21	1.80	0.62
1:B:624:ARG:O	1:B:627:VAL:HG13	1.99	0.62
1:B:1819:ALA:HB2	1:B:1829:ILE:HG21	1.82	0.62
1:B:636:ILE:HD13	1:B:666:ARG:HD2	1.82	0.62
1:B:2043:ARG:HB3	1:B:2086:GLN:HA	1.81	0.62
1:B:920:LEU:HD23	1:B:953:ARG:HG2	1.83	0.60
2:J:2141:GLU:OE2	2:J:2266:ARG:NH2	2.32	0.60
1:B:2029:ILE:HG13	1:B:2126:VAL:HA	1.83	0.60
1:B:690:VAL:HG11	1:B:707:ILE:HD13	1.84	0.60
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.40	0.60
1:B:2030:ARG:HA	1:B:2126:VAL:HG13	1.84	0.59
1:B:991:TYR:OH	1:B:1097:GLU:OE1	2.19	0.59
1:B:448:PRO:HA	1:B:686[A]:GLU:HG3	1.84	0.59
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.35	0.58
1:B:1900:SER:OG	1:B:1954:TRP:NE1	2.26	0.58
1:B:1195:ARG:NH1	1:B:1260:GLU:OE1	2.37	0.57
2:J:2059:PRO:HB2	2:J:2063:MET:HB2	1.85	0.57
1:B:1944:GLU:O	1:B:1947:GLN:HG2	2.05	0.57
1:B:639:ILE:HD11	1:B:646:VAL:HB	1.86	0.57
2:J:2284:MET:HB3	2:J:2287:ARG:HD3	1.85	0.57
1:B:789:MET:HE2	1:B:794:ARG:HG2	1.87	0.57
1:B:1456:VAL:HG21	1:B:1489:ALA:HB1	1.86	0.57
2:J:2252:LEU:HB2	2:J:2255:HIS:CE1	2.41	0.56
1:B:1620:LEU:HD22	1:B:1629:ARG:HG3	1.87	0.56
1:B:1156:LEU:HD13	1:B:1160:GLU:HG3	1.87	0.56
2:J:2212:ILE:HG22	2:J:2229:LYS:HB3	1.87	0.56
1:B:1435:LEU:O	1:B:1442:ARG:NH1	2.39	0.55
1:B:1515:HIS:CE1	1:B:1721:PRO:HG3	2.41	0.55
1:B:721:VAL:HG12	1:B:825:THR:HB	1.88	0.55
1:B:446:HIS:HB3	6:B:6008:HOH:O	2.07	0.55
1:B:1131:GLN:O	4:B:5812:EDO:H12	2.06	0.55
2:J:2212:ILE:HG21	2:J:2259:VAL:HG21	1.87	0.55
1:B:2051:VAL:HG22	1:B:2062:GLU:HG3	1.87	0.55
1:B:1696:GLN:NE2	6:B:5903:HOH:O	2.36	0.54
1:B:1156:LEU:HD22	1:B:1160:GLU:HG2	1.88	0.54
1:B:545:ARG:NH2	1:B:549:GLN:OE1	2.40	0.54
2:J:2194:THR:O	2:J:2198:LYS:HG2	2.07	0.54
1:B:1764:MET:HE3	1:B:1773:LEU:HD11	1.90	0.54
1:B:2041:LEU:O	1:B:2087:LYS:HA	2.07	0.54
1:B:1037:LEU:HD13	1:B:1052:ILE:HD11	1.89	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1269:ARG:NH1	1:B:1279:GLU:OE2	2.31	0.54
1:B:1438:ARG:HB2	1:B:1442:ARG:HD3	1.89	0.53
1:B:1588:ARG:HG3	1:B:1590:LEU:H	1.72	0.53
1:B:1909:GLN:O	1:B:1912:THR:OG1	2.20	0.53
1:B:1195:ARG:HD3	1:B:1260:GLU:OE2	2.09	0.53
1:B:1457:HIS:CE1	1:B:1492:SER:HB2	2.43	0.53
1:B:1456:VAL:O	1:B:1459:ILE:HG12	2.09	0.53
1:B:1307:LEU:HD23	1:B:1328:PHE:HD2	1.73	0.53
1:B:1396:LYS:O	1:B:1400:ARG:HB2	2.09	0.53
1:B:1973:ARG:HH12	1:B:1998:GLN:HB2	1.73	0.53
1:B:893:MET:HB3	1:B:925:LEU:HD22	1.91	0.52
1:B:1593:THR:HG22	1:B:1595:LYS:H	1.75	0.52
1:B:1660:LEU:HA	1:B:1701:ARG:O	2.10	0.52
1:B:1539:LEU:HD21	1:B:1665:ASP:HB2	1.92	0.52
2:J:2123:GLN:HB2	2:J:2157:VAL:HG22	1.90	0.52
1:B:1715:LYS:NZ	6:B:5905:HOH:O	2.42	0.52
2:J:2167:GLU:HG3	2:J:2170:LYS:NZ	2.25	0.52
2:J:2199:ILE:O	2:J:2203:ASN:ND2	2.34	0.52
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.45	0.52
1:B:1838:ALA:HA	1:B:1938:PRO:HG3	1.92	0.52
1:B:1475:ARG:HD2	1:B:1504:LEU:HA	1.91	0.52
1:B:1783:ASP:O	1:B:1787:GLU:HG3	2.11	0.51
1:B:815:LEU:HD11	1:B:821:LEU:HD23	1.90	0.51
1:B:828:ILE:HD12	1:B:869:LEU:HD12	1.92	0.51
1:B:1224:LEU:HD23	1:B:1236:HIS:HB2	1.92	0.51
1:B:1616:GLY:HA2	1:B:1641:ILE:HG22	1.92	0.51
1:B:421:HIS:NE2	1:B:875:GLU:OE1	2.32	0.51
2:J:2264:SER:OG	2:J:2265:ASP:N	2.43	0.51
2:J:2243:ASP:HB3	2:J:2248:PRO:HB3	1.91	0.51
1:B:689:TYR:HE2	1:B:883:LEU:HD12	1.75	0.50
1:B:1930:LEU:HD13	1:B:1938:PRO:HB2	1.92	0.50
1:B:1338:THR:O	1:B:1342:SER:HB2	2.11	0.50
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.93	0.50
1:B:1137:GLU:HA	1:B:1140:VAL:HG22	1.93	0.50
1:B:1946:ALA:O	1:B:1950:THR:HG23	2.12	0.50
1:B:656:PRO:O	1:B:657:ASN:HB2	2.11	0.50
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.92	0.50
1:B:969:LEU:HD21	1:B:998:VAL:HG23	1.93	0.50
1:B:1943:MET:CE	1:B:2109:MET:HB2	2.41	0.50
1:B:774:LEU:HD22	1:B:778:LEU:HG	1.93	0.49
1:B:1604:LEU:HD23	1:B:1628:GLU:HG2	1.92	0.49



	<b>A A D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:J:2149:PRO:HB3	2:J:2281:TYR:CE1	2.47	0.49
1:B:1968:SER:HA	1:B:1971:ILE:HD12	1.93	0.49
1:B:1963:LEU:HD21	1:B:1982:VAL:HG13	1.93	0.49
1:B:770:LYS:HE2	1:B:796:LEU:HD22	1.94	0.49
1:B:1923:ILE:O	1:B:1927:VAL:HG13	2.12	0.49
1:B:1869:ARG:HD3	1:B:1884:PHE:CZ	2.42	0.49
1:B:1438:ARG:HB2	1:B:1442:ARG:NH1	2.28	0.49
2:J:2072:GLU:OE1	2:J:2072:GLU:N	2.46	0.49
1:B:545:ARG:NH1	1:B:568:GLU:OE1	2.46	0.49
1:B:1725:GLU:OE1	1:B:1763:ARG:HD3	2.12	0.49
1:B:726:HIS:HB3	1:B:833:VAL:HG23	1.93	0.49
1:B:1346:VAL:HB	1:B:1488:VAL:HG22	1.95	0.49
1:B:2065:TRP:CD1	1:B:2081:ARG:HG2	2.48	0.48
1:B:607:GLN:O	1:B:610:ARG:NH2	2.46	0.48
1:B:1841:LYS:O	1:B:1845:LEU:HG	2.13	0.48
1:B:933:PRO:HG3	1:B:943:LEU:HD22	1.96	0.48
1:B:1911:ASP:O	1:B:1915:ILE:HG12	2.13	0.48
1:B:1157:ASN:O	1:B:1161:ILE:HG12	2.14	0.48
1:B:1891:THR:HG23	1:B:1915:ILE:HD12	1.96	0.48
1:B:1138:GLU:O	1:B:1142:LYS:HG2	2.14	0.48
1:B:1153:LEU:HD22	1:B:1161:ILE:HD12	1.96	0.48
1:B:1862:HIS:CG	1:B:1863:HIS:N	2.79	0.48
1:B:1897:ALA:HA	1:B:1902:MET:HG3	1.96	0.48
2:J:2280:ASN:HB3	2:J:2309:HIS:CD2	2.49	0.48
1:B:1205:THR:HG23	1:B:1249:GLU:HG2	1.96	0.48
1:B:1222:TRP:O	1:B:1270:VAL:HA	2.14	0.48
1:B:1190:LEU:HD21	1:B:1284:VAL:HG11	1.96	0.47
1:B:513:ALA:O	1:B:517:MET:HG3	2.14	0.47
1:B:542:ALA:O	1:B:589:THR:HA	2.13	0.47
1:B:1712:ASP:HB3	6:B:5992:HOH:O	2.14	0.47
1:B:709:TYR:OH	1:B:745:LYS:HD2	2.14	0.47
1:B:1113:ASN:O	1:B:1117:MET:HG3	2.14	0.47
1:B:429:GLN:O	4:B:5807:EDO:H21	2.14	0.47
1:B:2064:TRP:CZ3	1:B:2110:SER:HB3	2.50	0.47
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.95	0.47
1:B:502:CYS:HA	1:B:652:SER:O	2.15	0.47
1:B:526:ASN:HB2	1:B:528:ASP:OD1	2.15	0.47
1:B:1018:PHE:HE1	1:B:1088:ALA:HA	1.79	0.47
2:J:2189:SER:HB2	2:J:2192:ASP:H	1.80	0.47
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.97	0.47
1:B:1271:VAL:HG12	1:B:1279:GLU:HB2	1.97	0.47



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:609:VAL:O	1:B:610:ARG:NH1	2.48	0.46
1:B:436:ARG:HE	1:B:443:GLU:CD	2.19	0.46
1:B:752:LEU:HB3	1:B:759:THR:HG22	1.96	0.46
1:B:850:LEU:HD23	1:B:883:LEU:HD23	1.98	0.46
1:B:1961:LYS:HG2	1:B:1971:ILE:HD11	1.97	0.46
1:B:442:TYR:CD2	1:B:707:ILE:HD11	2.51	0.46
2:J:2149:PRO:O	2:J:2160:PRO:HD3	2.16	0.46
1:B:984:LEU:CD1	1:B:998:VAL:HB	2.45	0.46
1:B:1453:VAL:HG22	1:B:1456:VAL:HG22	1.98	0.46
1:B:1225:VAL:HG11	1:B:1256:VAL:HG11	1.98	0.46
1:B:654:THR:HG21	1:B:676:PHE:O	2.16	0.45
1:B:2077:ILE:HG13	1:B:2094:PHE:CZ	2.52	0.45
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.17	0.45
1:B:2105:THR:HG22	1:B:2121:LYS:HG2	1.97	0.45
1:B:580:ILE:HG23	1:B:586:ILE:HD11	1.98	0.45
1:B:757:ALA:O	1:B:761:VAL:HG23	2.16	0.45
1:B:929:MET:HE3	1:B:949:LEU:HD13	1.98	0.45
1:B:1009:LEU:HG	1:B:1013:GLU:HB3	1.98	0.45
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.98	0.45
1:B:1824:ILE:HD13	1:B:1922:LEU:HD23	1.98	0.45
1:B:1022:SER:O	1:B:1025:LYS:HB2	2.16	0.45
1:B:1041:LEU:HD11	1:B:1048:VAL:HB	1.98	0.45
1:B:1772:ASN:O	1:B:1772:ASN:ND2	2.50	0.45
1:B:461:LEU:HB3	1:B:480:THR:OG1	2.16	0.45
1:B:771:ASN:O	1:B:775:LYS:N	2.43	0.45
1:B:1664:MET:O	1:B:1705:MET:HB2	2.17	0.45
1:B:2109:MET:HE2	1:B:2109:MET:HB3	1.85	0.45
1:B:1258:VAL:HG12	1:B:1259:PHE:H	1.83	0.44
1:B:1566:ARG:HG3	1:B:1621:HIS:CG	2.52	0.44
2:J:2147:MET:O	2:J:2274:PRO:HD3	2.17	0.44
1:B:1259:PHE:CE2	4:B:5806:EDO:H22	2.46	0.44
1:B:804:LYS:HE3	1:B:861:TYR:CE2	2.53	0.44
1:B:1228:VAL:HG13	4:B:5806:EDO:H12	1.99	0.44
2:J:2280:ASN:HB3	2:J:2309:HIS:CG	2.52	0.44
1:B:715:HIS:CD2	1:B:825:THR:HG21	2.53	0.44
1:B:1006:LYS:H	1:B:1009:LEU:HD13	1.83	0.44
1:B:726:HIS:NE2	1:B:830:GLY:O	2.47	0.44
1:B:1183:LYS:HG2	1:B:1207:ASP:HB3	2.00	0.44
1:B:1953:MET:HE3	1:B:2114:MET:SD	2.58	0.44
1:B:1307:LEU:HD23	1:B:1328:PHE:CD2	2.52	0.44
1:B:1456:VAL:HG23	1:B:1490:LEU:O	2.18	0.44



	<b>A A A</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:1514:PHE:HB3	1:B:1518:VAL:CG2	2.40	0.44
1:B:2103:ASN:HA	1:B:2123:SER:HA	1.99	0.44
1:B:603:ARG:HH22	1:B:1861:ARG:HA	1.83	0.43
1:B:1146:LYS:HB3	1:B:1148:PHE:HD1	1.83	0.43
1:B:1187:SER:OG	1:B:1203:THR:HB	2.17	0.43
1:B:1606:ASP:HB3	1:B:1609:LEU:HB3	2.00	0.43
1:B:1673:ILE:H	1:B:1673:ILE:HG13	1.66	0.43
1:B:2068:ILE:O	1:B:2076:LEU:HD12	2.18	0.43
1:B:2077:ILE:HG23	1:B:2094:PHE:CG	2.53	0.43
2:J:2098:LYS:NZ	2:J:2101:GLY:HA3	2.34	0.43
1:B:1964:PRO:HD2	1:B:2007:VAL:HA	1.99	0.43
1:B:1997:LEU:HD13	1:B:2004:ILE:HG12	1.99	0.43
1:B:708:VAL:HG21	1:B:829:LYS:HG3	2.01	0.43
1:B:1940:LEU:HA	1:B:1943:MET:HB2	2.00	0.43
1:B:769:CYS:SG	1:B:775:LYS:HE2	2.59	0.43
1:B:1375:ARG:HD3	1:B:1419:LEU:O	2.18	0.43
1:B:1745:ILE:HA	1:B:1750:ASP:HB3	2.00	0.43
1:B:1044:VAL:O	2:J:2074:ARG:NH1	2.46	0.43
1:B:1357:THR:O	1:B:1361:GLU:HG3	2.19	0.43
2:J:2229:LYS:O	2:J:2256:TYR:HA	2.18	0.43
1:B:1071:LYS:HD3	1:B:1071:LYS:HA	1.73	0.42
1:B:621:HIS:HB2	1:B:889:ILE:HG23	2.02	0.42
1:B:1368:LEU:HD22	1:B:1403:LYS:HE3	2.02	0.42
1:B:1406:VAL:HG21	1:B:1418:LEU:HB3	2.00	0.42
1:B:1574:ILE:HD11	1:B:1608:THR:HG21	2.01	0.42
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	2.01	0.42
1:B:1899:LEU:HA	1:B:1899:LEU:HD23	1.74	0.42
2:J:2306:HIS:ND1	2:J:2308:VAL:HG22	2.34	0.42
1:B:1018:PHE:CE2	1:B:1063:LEU:HD22	2.54	0.42
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.19	0.42
1:B:1535:THR:HG21	1:B:1676:TYR:CE2	2.54	0.42
1:B:1269:ARG:HD2	1:B:1279:GLU:OE2	2.19	0.42
1:B:1590:LEU:HD22	1:B:1614:LEU:O	2.19	0.42
1:B:1735:HIS:O	1:B:1739:GLU:HG2	2.19	0.42
1:B:635:ALA:O	1:B:639:ILE:HG13	2.20	0.42
1:B:1225:VAL:HG21	1:B:1254:PHE:CE1	2.54	0.42
1:B:1515:HIS:O	1:B:1517:ASN:N	2.53	0.42
1:B:542:ALA:HB3	1:B:548:VAL:HG23	2.01	0.42
1:B:1553:HIS:HB3	1:B:1701:ARG:HD2	2.00	0.42
1:B:1836:LEU:HD23	1:B:1848:ILE:HD13	2.01	0.42
1:B:1933:ASN:HB3	1:B:1935:TRP:CD1	2.54	0.42



	<b>A A D</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:2076:LEU:HD11	1:B:2079:ILE:HG23	2.01	0.42
1:B:695:LYS:HD3	1:B:695:LYS:HA	1.66	0.42
1:B:988:ALA:HB2	1:B:998:VAL:HG21	2.02	0.42
1:B:1356:LYS:HB2	1:B:1356:LYS:HE2	1.89	0.42
1:B:1132:PHE:HE1	1:B:1214:VAL:HG11	1.84	0.42
1:B:1589:PHE:HB3	1:B:1642:GLN:HB3	2.01	0.42
1:B:2093:ASP:OD1	1:B:2093:ASP:N	2.53	0.42
1:B:1957:ASP:HB3	1:B:1961:LYS:HD2	2.02	0.41
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	2.01	0.41
1:B:1129:LEU:HD23	1:B:1129:LEU:HA	1.80	0.41
1:B:1725:GLU:HB3	1:B:1771:TYR:OH	2.19	0.41
1:B:827:ILE:HG12	1:B:868:ILE:HB	2.03	0.41
1:B:1960:LEU:HD12	1:B:1971:ILE:HG23	2.03	0.41
2:J:2216:CYS:HA	2:J:2225:LEU:HD23	2.03	0.41
1:B:984:LEU:HD12	1:B:998:VAL:HB	2.03	0.41
1:B:1494:LEU:O	1:B:1513:ASN:ND2	2.50	0.41
1:B:1666:THR:HG21	1:B:1714:PHE:CE2	2.56	0.41
1:B:1858:ILE:HG12	1:B:1915:ILE:HD11	2.01	0.41
1:B:1093:ARG:NH2	1:B:1273:ASP:OD1	2.53	0.41
1:B:1910:SER:O	1:B:1914:GLU:HG2	2.21	0.41
1:B:1957:ASP:N	1:B:1957:ASP:OD1	2.53	0.41
1:B:1375:ARG:HH21	1:B:1447:ASN:CB	2.34	0.41
1:B:488:LEU:HD22	1:B:501:LEU:HD22	2.02	0.41
1:B:973:ASP:O	1:B:977:GLY:N	2.51	0.41
1:B:1567:LYS:O	1:B:1571:LEU:HG	2.21	0.41
1:B:694:GLU:HG2	1:B:699:LYS:CG	2.50	0.41
1:B:770:LYS:HE3	1:B:793:ASP:OD1	2.21	0.41
1:B:1733:HIS:HB3	1:B:1796:LEU:HD21	2.02	0.41
1:B:1875:VAL:HG12	1:B:1877:HIS:HB3	2.03	0.41
1:B:1912:THR:O	1:B:1916:LEU:HG	2.21	0.41
2:J:2167:GLU:HG3	2:J:2170:LYS:HZ1	1.85	0.41
1:B:666:ARG:HA	6:B:5948:HOH:O	2.20	0.40
1:B:2077:ILE:HG23	1:B:2094:PHE:CD1	2.56	0.40
1:B:1122:MET:HE3	1:B:1126:MET:HB2	2.02	0.40
2:J:2084:HIS:O	2:J:2087:THR:OG1	2.37	0.40
1:B:509:LYS:HD2	1:B:651:LEU:HB3	2.02	0.40
1:B:1174:ILE:O	1:B:1178:VAL:HG23	2.20	0.40
1:B:1200:VAL:O	1:B:1253:THR:HA	2.20	0.40
1:B:1515:HIS:NE2	1:B:1721:PRO:HG3	2.36	0.40
1:B:2099:THR:HG22	1:B:2126:VAL:HG11	2.04	0.40
1:B:1419:LEU:HG	1:B:1444:ASN:HB3	2.03	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HB2	1:B:954:LEU:CD1	2.50	0.40
1:B:626:PRO:HB2	1:B:896:LYS:HD2	2.03	0.40
1:B:1092:MET:SD	1:B:1114:LEU:HD23	2.61	0.40

All (1) 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-1 Atom-2		Clash overlap (Å)
1:B:1720:GLU:OE2	1:B:2000:THR:OG1[3_554]	2.12	0.08

#### 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	1723/1747~(99%)	1658 (96%)	61 (4%)	4 (0%)	47	78
2	J	261/263~(99%)	247 (95%)	12 (5%)	2 (1%)	19	49
All	All	1984/2010 (99%)	1905 (96%)	73 (4%)	6 (0%)	41	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	657	ASN
2	J	2135	ASP
1	В	1863	HIS
2	J	2059	PRO
1	В	1326	PRO
1	В	2097	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	В	1544/1560~(99%)	1492~(97%)	52 (3%)	37 71		
2	J	236/236~(100%)	230~(98%)	6(2%)	47 80		
All	All	1780/1796~(99%)	1722~(97%)	58~(3%)	38 72		

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	418	GLN
1	В	459	GLU
1	В	489	TYR
1	В	546	SER
1	В	561	THR
1	В	610	ARG
1	В	720	GLN
1	В	727	SER
1	В	728	ARG
1	В	832	GLN
1	В	835	SER
1	В	877	GLN
1	В	914	LYS
1	В	941	ASP
1	В	954	LEU
1	В	969	LEU
1	В	970	VAL
1	В	984	LEU
1	В	992	TYR
1	В	1009	LEU
1	В	1039	LYS
1	В	1087	SER
1	В	1167	MET
1	В	1277	SER
1	В	1293	GLU
1	В	1357	THR
1	В	1371	SER



Mol	Chain	Res	Type
1	В	1402	ASN
1	В	1411	GLU
1	В	1412	THR
1	В	1458	LEU
1	В	1537	THR
1	В	1559	VAL
1	В	1596	ASP
1	В	1699	GLU
1	В	1731	CYS
1	В	1763	ARG
1	В	1788	LEU
1	В	1797	GLU
1	В	1829	ILE
1	В	1831	LEU
1	В	1857	ASN
1	В	1858	ILE
1	В	1861	ARG
1	В	1926	CYS
1	В	1937	SER
1	В	1966	PHE
1	В	1979	VAL
1	В	1980	GLU
1	В	2017	ILE
1	В	2055	LEU
1	В	2072	LYS
2	J	2066	THR
2	J	2121	ARG
2	J	2156	THR
2	J	2223	CYS
2	J	2226	THR
2	J	2239	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	В	524	HIS

#### 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)

12 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).

Mal	Turne	Chain	Dec	T inl.	Bo	ond leng	ths	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	В	5810	1	3,3,3	0.50	0	2,2,2	0.28	0
4	EDO	В	5809	-	3,3,3	0.62	0	2,2,2	0.05	0
4	EDO	В	5803	-	3,3,3	0.44	0	2,2,2	0.40	0
4	EDO	В	5808	-	3,3,3	0.44	0	2,2,2	0.66	0
3	Q96	В	5801	-	13,14,14	2.13	5 (38%)	19,20,20	4.10	8 (42%)
4	EDO	В	5805	-	3,3,3	0.54	0	2,2,2	0.39	0
4	EDO	В	5811	-	3,3,3	0.61	0	2,2,2	0.08	0
4	EDO	В	5812	-	3,3,3	0.47	0	2,2,2	0.16	0
4	EDO	В	5807	-	3,3,3	0.48	0	2,2,2	0.29	0
5	GOL	В	5804	-	$5,\!5,\!5$	1.26	0	$5,\!5,\!5$	0.73	0
3	Q96	В	5802	-	13,14,14	2.35	5 (38%)	19,20,20	<mark>3.97</mark>	9 (47%)
4	EDO	В	5806	-	3,3,3	0.53	0	2,2,2	0.20	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
4	EDO	В	5810	1	-	0/1/1/1	-
4	EDO	В	5809	-	-	0/1/1/1	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	В	5803	-	-	0/1/1/1	-
4	EDO	В	5808	-	-	1/1/1/1	-
3	Q96	В	5801	-	-	2/11/11/11	0/1/1/1
4	EDO	В	5805	-	-	1/1/1/1	-
4	EDO	В	5811	-	-	1/1/1/1	-
4	EDO	В	5812	-	-	0/1/1/1	-
4	EDO	В	5807	-	-	0/1/1/1	-
5	GOL	В	5804	-	-	4/4/4/4	-
3	Q96	В	5802	-	-	5/11/11/11	0/1/1/1
4	EDO	В	5806	-	-	1/1/1/1	-

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All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	В	5802	Q96	C03-N02	4.50	1.46	1.37
3	В	5801	Q96	C03-N02	4.22	1.45	1.37
3	В	5802	Q96	O11-S10	3.81	1.47	1.43
3	В	5802	Q96	C07-S10	3.77	1.82	1.76
3	В	5802	Q96	O12-S10	3.73	1.47	1.43
3	В	5801	Q96	O12-S10	3.62	1.47	1.43
3	В	5801	Q96	C07-S10	3.34	1.81	1.76
3	В	5801	Q96	O11-S10	3.10	1.47	1.43
3	В	5802	Q96	C04-N05	2.65	1.46	1.37
3	В	5801	Q96	C04-N05	2.50	1.46	1.37

All	(17)	) bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	5801	Q96	O12-S10-O11	-14.82	101.33	119.55
3	В	5802	Q96	O12-S10-O11	-13.31	103.19	119.55
3	В	5802	Q96	C04-C03-N02	5.88	123.49	118.47
3	В	5801	Q96	O11-S10-N13	5.38	113.15	107.08
3	В	5801	Q96	C04-C03-N02	4.83	122.60	118.47
3	В	5802	Q96	O12-S10-N13	4.81	112.51	107.08
3	В	5802	Q96	C09-C03-N02	-4.20	115.97	121.23
3	В	5802	Q96	C01-N02-C03	-3.66	116.70	122.44
3	В	5801	Q96	C01-N02-C03	-3.32	117.23	122.44
3	В	5801	Q96	C09-C03-N02	-3.32	117.07	121.23
3	В	5802	Q96	C06-C07-S10	2.80	122.21	119.08
3	В	5801	Q96	O12-S10-N13	2.69	110.11	107.08
3	В	5802	Q96	C07-S10-N13	2.61	111.16	107.56



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	В	5802	Q96	C08-C07-S10	-2.51	117.04	119.77
3	В	5801	Q96	O12-S10-C07	2.46	111.00	107.97
3	В	5801	Q96	O11-S10-C07	2.40	110.93	107.97
3	В	5802	Q96	O11-S10-N13	2.30	109.67	107.08

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
3	В	5801	Q96	C14-N13-S10-C07
3	В	5801	Q96	C14-N13-S10-O11
3	В	5802	Q96	C14-N13-S10-O12
5	В	5804	GOL	O1-C1-C2-O2
5	В	5804	GOL	O1-C1-C2-C3
5	В	5804	GOL	C1-C2-C3-O3
3	В	5802	Q96	C08-C07-S10-O11
3	В	5802	Q96	C06-C07-S10-O11
3	В	5802	Q96	C08-C07-S10-N13
3	В	5802	Q96	C06-C07-S10-N13
5	В	5804	GOL	O2-C2-C3-O3
4	В	5805	EDO	O1-C1-C2-O2
4	В	5808	EDO	O1-C1-C2-O2
4	В	5811	EDO	O1-C1-C2-O2
4	В	5806	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	5812	EDO	1	0
4	В	5807	EDO	1	0
4	В	5806	EDO	4	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	$OWAB(Å^2)$	Q<0.9
1	В	1724/1747~(98%)	-0.04	72 (4%) 36 26	40, 70, 147, 263	0
2	J	263/263~(100%)	-0.04	15 (5%) 23 15	44, 66, 141, 186	0
All	All	1987/2010~(98%)	-0.04	87 (4%) 34 24	40, 69, 146, 263	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	2058	GLY	12.0
1	В	1880	ASN	10.6
2	J	2061	GLY	8.2
1	В	2124	VAL	7.3
1	В	2123	SER	6.7
1	В	1873	GLN	6.6
1	В	1879	LEU	6.5
2	J	2320	LEU	6.3
1	В	1584	ILE	6.2
1	В	1977	LYS	5.4
1	В	1878	LYS	5.0
1	В	2122	PHE	4.9
1	В	1996	LEU	4.8
2	J	2060	LEU	4.8
1	В	805	HIS	4.8
2	J	2317	PHE	4.8
1	В	1870	GLN	4.6
1	В	782	PHE	4.2
2	J	2062	SER	4.1
1	В	2022	GLU	4.0
1	В	2095	VAL	4.0
1	В	1587	GLN	3.8
1	В	456	GLY	3.8
1	В	1877	HIS	3.8



Mol	Chain	Res	Type	RSRZ
1	В	2034	PRO	3.8
2	J	2065	GLN	3.6
2	J	2319	LEU	3.5
2	J	2098	LYS	3.5
1	В	2104	TYR	3.5
2	J	2097	ILE	3.4
1	В	770	LYS	3.4
1	В	1601	LEU	3.4
1	В	1135	LEU	3.4
1	В	1748	LYS	3.4
1	В	726	HIS	3.3
1	В	800	LEU	3.3
1	В	1973	ARG	3.3
1	В	2092	LEU	3.3
1	В	1985	ILE	3.3
1	В	756	SER	3.2
1	В	2029	ILE	3.2
1	В	1926	CYS	3.2
2	J	2066	THR	3.2
1	В	601	GLY	3.1
1	В	1603	LYS	3.1
1	В	458	GLU	3.0
1	В	573	HIS	3.0
2	J	2100	THR	2.9
1	В	1876	PRO	2.9
1	В	1868	LEU	2.8
1	В	754	GLU	2.8
1	В	1044	VAL	2.8
1	В	2077	ILE	2.7
1	В	821	LEU	2.7
1	В	2035	VAL	2.7
1	В	2105	THR	2.7
1	В	2038	LEU	2.7
1	В	806	ILE	2.6
1	В	2120	TYR	2.6
1	В	2017	ILE	2.6
2	J	2261	MET	2.6
1	В	1815	LEU	2.5
1	В	576	CYS	2.5
1	В	2108	PHE	2.5
1	В	1964	PRO	2.5
1	В	1170	MET	2.5



Mol	Chain	Res	Type	RSRZ
1	В	2098	ALA	2.4
1	В	1590	LEU	2.4
1	В	1886	ASP	2.3
1	В	2012	ASN	2.3
1	В	1903	GLN	2.3
2	J	2068	SER	2.2
1	В	2036	VAL	2.2
2	J	2059	PRO	2.2
1	В	1883	LYS	2.2
1	В	1963	LEU	2.2
1	В	1988	MET	2.2
1	В	1874	LYS	2.1
1	В	1597	LEU	2.1
1	В	404	ALA	2.1
1	В	484	ILE	2.1
1	В	704	MET	2.1
1	В	459	GLU	2.1
1	В	1839	LYS	2.0
1	В	2024	VAL	2.0
1	В	1843	ARG	2.0
1	В	1614	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 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	EDO	В	5810	4/4	0.65	0.21	81,88,94,97	0
4	EDO	В	5809	4/4	0.81	0.25	59,61,65,66	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	В	5806	4/4	0.83	0.30	$55,\!60,\!63,\!63$	0
4	EDO	В	5807	4/4	0.85	0.15	70,71,73,73	0
4	EDO	В	5805	4/4	0.88	0.20	56,58,62,64	0
4	EDO	В	5811	4/4	0.90	0.23	67,68,68,70	0
4	EDO	В	5808	4/4	0.91	0.26	$50,\!53,\!55,\!63$	0
3	Q96	В	5802	14/14	0.91	0.33	43,61,83,88	0
4	EDO	В	5812	4/4	0.92	0.27	70,73,75,76	0
5	GOL	В	5804	6/6	0.93	0.17	48,62,64,65	0
4	EDO	В	5803	4/4	0.97	0.14	45,46,48,52	0
3	Q96	В	5801	14/14	0.97	0.12	45,52,58,59	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.

