

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

Feb 28, 2023 – 12:23 pm GMT

PDB ID	:	8BC8
Title	:	Human Brr2 Helicase Region in complex with C-tail deleted Jab1 and com-
		pound 18
Authors	:	Vester, K.; Loll, B.; Wahl, M.C.
Deposited on	:	2022-10-15
Resolution	:	2.39 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 2.39 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	75%	22%	••
2	J	263	81%	17%	•

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	QB6	В	5802	-	Х	-	-
3	QB6	В	5803	-	Х	-	-
3	QB6	J	2402	-	Х	-	-



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# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16467 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	1724	Total 13901	C 8881	N 2381	O 2567	S 72	0	4	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	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-4-oxidanyl-benzenesulfonamide (three-letter code: QB6) (formula:  $C_6H_8N_2O_3S$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	В	1	Total	С	Ν	0	$\mathbf{S}$	0	0
0	D	1	12	6	2	3	1	0	0
3	В	1	Total	С	Ν	0	$\mathbf{S}$	0	0
0	D	1	12	6	2	3	1	0	0
3	В	1	Total	С	Ν	0	$\mathbf{S}$	0	0
0	D	1	12	6	2	3	1	0	0
3	т	1	Total	С	Ν	0	S	0	0
5	J	1	12	6	2	3	1	0	0

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





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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
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
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	TotalCO422	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	288	Total         O           288         288	0	2
5	J	43	Total O 43 43	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	100.60Å 119.06Å 187.03Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	46.33 - 2.39	Depositor
Resolution (A)	46.33 - 2.39	EDS
% Data completeness	99.7 (46.33-2.39)	Depositor
(in resolution range)	$99.7 \ (46.33 - 2.39)$	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.13 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
B B.	0.207 , $0.245$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.205 , $0.244$	DCC
$R_{free}$ test set	2100 reflections $(2.34\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29 , $40.5$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16467	wwPDB-VP
Average B, all atoms $(Å^2)$	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.20% 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: QB6, 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	0.44	0/14196	0.61	0/19233
2	J	0.50	0/2190	0.65	0/2981
All	All	0.45	0/16386	0.62	0/22214

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	13901	0	14035	252	1
2	J	2123	0	2063	35	0
3	В	36	0	0	1	0
3	J	12	0	0	0	0
4	В	56	0	84	7	0
4	J	8	0	12	1	0
5	В	288	0	0	5	0
5	J	43	0	0	2	0
All	All	16467	0	16194	281	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.



Atom-1	Atom-2	Interatomic distance $(\hat{A})$	Clash overlap (Å)
1·B·1542·MET·HE3	1.B.1664.MET.HG2	1.51	
1.B.1253.THR.H	4·B·5816·EDO·H22	1.34	0.91
1:B:1672:LYS:HG3	1.B.1859.PRO.HB3	1.61	0.80
1:B:1010:SEB:OG	1:B:1013:GLU:OE1	2.01	0.78
2:J:2141:GLU:OE1	2:J:2143:ABG:NH2	2.18	0.77
1:B:570:THB:OG1	1:B:576:CYS:SG	2.42	0.76
1:B:2067:VAL:HG13	1:B:2107:TYB:HB2	1.70	0.74
1:B:708:VAL:O	1:B:712:ILE:HG12	1.90	0.72
1:B:993:ILE:HD12	1:B:1091:LEU:HD23	1.69	0.71
1:B:1894:LEU:HG	1:B:1912:THR:HG22	1.71	0.71
1:B:1628:GLU:HA	1:B:1631:LEU:HD12	1.73	0.71
2:J:2072:GLU:HG2	2:J:2076:ARG:HH21	1.56	0.71
1:B:1195:ARG:H	4:B:5810:EDO:H22	1.56	0.70
1:B:2017:ILE:HG12	1:B:2043:ARG:HD2	1.74	0.70
2:J:2133:PRO:HG2	2:J:2136:ASN:HB3	1.74	0.69
1:B:1229:ASP:HB2	1:B:1231:GLU:HG2	1.74	0.69
1:B:984:LEU:HD21	1:B:1002:ASN:HB2	1.76	0.68
1:B:1843:ARG:HH12	1:B:1876:PRO:HB2	1.61	0.66
1:B:1126:MET:HB3	1:B:1130:ARG:HD2	1.77	0.65
4:B:5813:EDO:O2	5:B:5901:HOH:O	2.15	0.64
1:B:1877:HIS:CE1	1:B:1879:LEU:HD23	2.33	0.64
2:J:2236:GLU:OE2	2:J:2239:ARG:NH1	2.30	0.64
1:B:1629:ARG:NH2	1:B:1653:GLY:O	2.31	0.63
2:J:2092:VAL:HG13	2:J:2261:MET:HE3	1.80	0.63
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.81	0.63
1:B:1188:VAL:HG21	1:B:1284:VAL:HG13	1.80	0.63
1:B:1604:LEU:HD23	1:B:1628:GLU:HG2	1.80	0.63
1:B:1868:LEU:HB3	1:B:1893:LEU:HD13	1.80	0.63
1:B:790:THR:HG22	1:B:792:VAL:H	1.64	0.62
1:B:654:THR:HG21	1:B:676:PHE:O	1.98	0.62
1:B:1886:ASP:O	1:B:1889:VAL:HG12	1.99	0.62
1:B:1030:ARG:HH21	1:B:1076:ALA:HB1	1.65	0.62
1:B:1507:SER:O	1:B:1511:THR:HG23	1.99	0.62
1:B:1586:ARG:HD2	1:B:1587:GLN:H	1.64	0.62
1:B:1127:CYS:O	1:B:1130:ARG:HG2	1.99	0.62
1:B:1009:LEU:HG	1:B:1013:GLU:HB2	1.81	0.62
1:B:1542:MET:HE1	1:B:1665:ASP:HB2	1.80	0.62
1:B:1156:LEU:HB2	1:B:1161:ILE:HG13	1.81	0.61
2:J:2147:MET:O	2:J:2274:PRO:HD3	1.99	0.61
1:B:1030:ARG:O	1:B:1033:GLU:HG2	2.01	0.61

All (281) 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	distance $(\text{\AA})$	overlap (Å)
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.82	0.61
1:B:1892:ASN:O	1:B:1896:GLN:NE2	2.34	0.61
1:B:2043:ARG:HB2	1:B:2086:GLN:HA	1.82	0.61
1:B:1861:ARG:HG2	1:B:1864:GLU:H	1.67	0.59
1:B:1804:ILE:HG12	1:B:1810:VAL:HG12	1.85	0.59
1:B:2051:VAL:HG22	1:B:2062:GLU:HG2	1.85	0.59
1:B:694:GLU:HG2	1:B:699:LYS:HB3	1.85	0.58
1:B:1542:MET:CE	1:B:1664:MET:HG2	2.31	0.58
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	1.85	0.58
1:B:1678:ASP:OD1	1:B:1710:LYS:HE3	2.04	0.58
1:B:1898:HIS:HD2	1:B:1899:LEU:HD12	1.68	0.58
1:B:712:ILE:HD12	1:B:721:VAL:HG21	1.85	0.57
1:B:1950:THR:HG21	1:B:2060:ARG:HH21	1.70	0.57
1:B:484:ILE:HD11	1:B:501:LEU:HD21	1.86	0.57
1:B:1846:ILE:HD11	1:B:1945:LEU:HD21	1.86	0.57
1:B:1861:ARG:HD3	1:B:1864:GLU:HB2	1.85	0.57
1:B:1864:GLU:O	1:B:1868:LEU:HG	2.04	0.57
1:B:1881:ASN:HD22	1:B:1883:LYS:NZ	2.03	0.57
2:J:2207:ASP:HB3	2:J:2210:LYS:HB2	1.87	0.56
1:B:1190:LEU:HD21	1:B:1284:VAL:HG11	1.87	0.56
1:B:1846:ILE:O	1:B:1850:SER:OG	2.19	0.56
1:B:482:ASN:OD1	1:B:484:ILE:HG22	2.05	0.56
2:J:2106:LEU:HD12	2:J:2107:PRO:HD2	1.86	0.56
1:B:1566:ARG:HG2	1:B:1621:HIS:CG	2.41	0.56
1:B:2098:ALA:O	1:B:2126:VAL:HG21	2.06	0.56
1:B:1042:GLU:HG3	2:J:2069:SER:O	2.06	0.55
1:B:1456:VAL:HG12	1:B:1490:LEU:O	2.07	0.55
2:J:2106:LEU:HD21	2:J:2111:LEU:HD13	1.87	0.55
1:B:548:VAL:HG13	1:B:587:VAL:HG12	1.89	0.55
1:B:1837:ASN:OD1	1:B:1838:ALA:N	2.41	0.54
1:B:1843:ARG:HB3	1:B:1877:HIS:HB2	1.89	0.54
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.90	0.54
1:B:1947:GLN:HB3	1:B:2114:MET:HG2	1.89	0.54
1:B:1429:PRO:HG3	1:B:1467:LEU:HD13	1.90	0.54
1:B:1586:ARG:HD2	1:B:1587:GLN:N	2.22	0.54
1:B:1843:ARG:HD2	1:B:1877:HIS:HB2	1.89	0.54
1:B:639:ILE:HD11	1:B:646:VAL:HB	1.90	0.54
1:B:2043:ARG:NH2	1:B:2062:GLU:OE1	2.40	0.54
1:B:1933:ASN:HB3	1:B:1935:TRP:CE2	2.43	0.53
1:B:1044:VAL:O	2:J:2074:ARG:NH2	2.40	0.53
1:B:1364:ILE:HG21	1:B:1424:ILE:HD11	1.91	0.53



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1225:VAL:HG21	1:B:1254:PHE:CE1	2.44	0.53
1:B:526:ASN:ND2	1:B:532:ASN:OD1	2.42	0.53
1:B:1156:LEU:HB3	1:B:1160:GLU:HB2	1.90	0.52
1:B:1954:TRP:HB2	1:B:1956:LYS:HE3	1.90	0.52
1:B:1868:LEU:HA	1:B:1871:LEU:HB3	1.90	0.52
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.08	0.52
1:B:2013:ARG:NH1	1:B:2048:THR:H	2.07	0.52
1:B:416:PHE:HB2	1:B:892:GLN:HE22	1.73	0.52
1:B:1319:SER:O	1:B:1400:ARG:NH1	2.43	0.52
2:J:2089:HIS:O	2:J:2222:SER:HB2	2.10	0.52
1:B:721:VAL:HG12	1:B:825:THR:HB	1.91	0.52
1:B:1174:ILE:O	1:B:1178:VAL:HG23	2.10	0.52
1:B:2030:ARG:NE	1:B:2127:LYS:HE3	2.25	0.52
1:B:1513:ASN:OD1	5:B:5902:HOH:O	2.19	0.52
1:B:1979:VAL:HG11	1:B:1985:ILE:HG22	1.92	0.52
1:B:2029:ILE:O	1:B:2127:LYS:N	2.43	0.52
2:J:2165:GLN:NE2	5:J:2503:HOH:O	2.39	0.52
4:J:2403:EDO:H21	5:J:2540:HOH:O	2.10	0.51
1:B:1123:TRP:HB2	1:B:1126:MET:HE3	1.92	0.51
1:B:531:ILE:HD13	1:B:562:TYR:O	2.11	0.51
1:B:547:LEU:O	1:B:551:MET:HG2	2.11	0.51
1:B:1515:HIS:CD2	1:B:1516:PRO:HD2	2.46	0.51
1:B:1712:ASP:OD2	1:B:1716:LYS:HE2	2.11	0.50
1:B:1045:PRO:HD3	2:J:2317:PHE:CD2	2.46	0.50
1:B:1357:THR:O	1:B:1361:GLU:HG3	2.12	0.50
1:B:1438:ARG:HB2	1:B:1442:ARG:HD2	1.93	0.50
1:B:1890:LYS:O	1:B:1894:LEU:HB2	2.11	0.50
1:B:509:LYS:HB3	1:B:651:LEU:HD22	1.93	0.49
1:B:1130:ARG:NH2	1:B:1137:GLU:OE2	2.43	0.49
1:B:1997:LEU:HD12	1:B:1999:LEU:HB3	1.94	0.49
1:B:406:ARG:HD3	1:B:954:LEU:HG	1.94	0.49
1:B:1043:ARG:HH22	2:J:2313:HIS:HA	1.76	0.49
1:B:589:THR:HG23	4:B:5804:EDO:H22	1.93	0.49
1:B:771:ASN:HB3	1:B:774:LEU:HB2	1.94	0.49
1:B:484:ILE:HD11	1:B:501:LEU:HD11	1.94	0.49
1:B:457:SER:O	1:B:459:GLU:N	2.45	0.49
1:B:566:VAL:HG13	1:B:585:ILE:HB	1.94	0.49
1:B:1139:VAL:HA	1:B:1142:LYS:HG3	1.93	0.49
1:B:811:SER:OG	1:B:812:THR:N	2.46	0.49
1:B:1043:ARG:HG3	2:J:2317:PHE:HD1	1.78	0.49
1:B:1672:LYS:HG3	1:B:1859:PRO:CB	2.37	0.49



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
2:J:2086:ARG:NH1	2:J:2219:THR:O	2.44	0.49
1:B:1581:ALA:HA	1:B:1586:ARG:HD3	1.94	0.48
1:B:1813:LEU:O	1:B:1817:MET:HG3	2.14	0.48
1:B:1122:MET:SD	1:B:1130:ARG:HG3	2.54	0.48
1:B:777:LEU:HB3	1:B:782:PHE:O	2.13	0.48
1:B:1732:MET:CE	1:B:1788:LEU:HD12	2.43	0.48
1:B:1909:GLN:O	1:B:1912:THR:OG1	2.26	0.48
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.96	0.48
1:B:2030:ARG:HE	1:B:2127:LYS:HE3	1.77	0.48
1:B:1512:PHE:HB3	1:B:1514:PHE:CE2	2.49	0.47
1:B:421:HIS:ND1	5:B:5905:HOH:O	2.35	0.47
1:B:420:SER:HB3	1:B:622:ASP:HA	1.95	0.47
1:B:709:TYR:CE1	1:B:713:MET:HE3	2.49	0.47
1:B:1210:TRP:HE1	1:B:1212:GLU:HG3	1.80	0.47
1:B:2031:SER:HA	1:B:2096:ALA:HB3	1.96	0.47
1:B:2058:GLN:OE1	1:B:2058:GLN:N	2.48	0.47
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.54	0.47
1:B:475:PHE:CE2	1:B:481:LEU:HD22	2.50	0.47
1:B:757:ALA:O	1:B:761:VAL:HG23	2.15	0.47
1:B:2094:PHE:CZ	1:B:2097:PRO:HD3	2.50	0.47
2:J:2076:ARG:HB3	2:J:2305:TYR:OH	2.14	0.47
1:B:1499:ASP:OD2	1:B:1766:GLN:HG3	2.15	0.46
1:B:1607:SER:O	1:B:1611:GLU:HG2	2.15	0.46
1:B:1138:GLU:O	1:B:1142:LYS:HG2	2.15	0.46
2:J:2280:ASN:HB3	2:J:2309:HIS:CG	2.50	0.46
1:B:1191:GLN:OE1	1:B:1199:LYS:HE3	2.15	0.46
1:B:682:PRO:HG2	5:B:6122:HOH:O	2.16	0.46
1:B:987:ILE:HD13	1:B:1098:ILE:HG13	1.96	0.46
1:B:1452:VAL:HG22	1:B:1488:VAL:HB	1.98	0.46
1:B:1436:SER:O	1:B:1473:ARG:HD3	2.15	0.46
1:B:1905:SER:CB	1:B:1908:LEU:HB3	2.46	0.46
1:B:1905:SER:HB2	1:B:1908:LEU:HB3	1.98	0.46
1:B:1142:LYS:O	1:B:1146:LYS:HG2	2.16	0.46
1:B:1967:THR:HG22	1:B:1968:SER:H	1.81	0.46
1:B:1335:VAL:O	1:B:1339:VAL:HG23	2.15	0.46
2:J:2113:LYS:O	2:J:2117:ILE:HG23	2.16	0.46
2:J:2200:MET:HE1	2:J:2230:LEU:HD22	1.96	0.46
1:B:1331:ILE:HD12	1:B:1354:SER:HB3	1.98	0.46
1:B:1648:ARG:HD2	1:B:1679:TYR:CE1	2.52	0.45
1:B:1735:HIS:O	1:B:1739:GLU:HG2	2.16	0.45
1:B:2033:GLY:O	1:B:2095:VAL:HA	2.16	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:2133:PRO:HD3	2:J:2141:GLU:HG3	1.98	0.45
1:B:1049:LYS:HB2	1:B:1049:LYS:HE3	1.73	0.45
1:B:1050:GLU:CD	1:B:1050:GLU:H	2.20	0.45
1:B:1127:CYS:SG	1:B:1129:LEU:HB2	2.57	0.45
1:B:790:THR:HG21	1:B:792:VAL:HG12	1.98	0.45
1:B:1868:LEU:HD22	1:B:1871:LEU:HD22	1.98	0.45
1:B:1908:LEU:O	1:B:1912:THR:HG23	2.16	0.45
2:J:2188:LEU:O	2:J:2251:TYR:OH	2.33	0.45
1:B:537:LYS:NZ	1:B:580:ILE:O	2.29	0.45
1:B:2029:ILE:H	1:B:2127:LYS:HA	1.81	0.45
1:B:576:CYS:O	1:B:580:ILE:HG13	2.17	0.45
1:B:1093:ARG:NH1	1:B:1115:CYS:HB3	2.31	0.45
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.98	0.45
1:B:758:SER:HA	1:B:805:HIS:CD2	2.52	0.45
1:B:1146:LYS:NZ	1:B:1166:ARG:HG3	2.32	0.45
1:B:1583:ASP:OD1	1:B:1584:ILE:N	2.43	0.45
1:B:2101:ALA:HB1	1:B:2125:ASP:CG	2.36	0.45
1:B:430:LEU:HD12	1:B:430:LEU:H	1.82	0.45
1:B:660:ASP:OD2	1:B:928:ARG:NH1	2.48	0.45
1:B:739:ARG:HH22	1:B:776:ASP:CG	2.20	0.45
1:B:1395:GLU:O	1:B:1400:ARG:HG3	2.16	0.45
2:J:2229:LYS:NZ	2:J:2230:LEU:O	2.50	0.45
1:B:1225:VAL:HG11	1:B:1256:VAL:HG11	1.98	0.45
1:B:1999:LEU:HB2	1:B:2004:ILE:HG23	1.99	0.45
1:B:538:ILE:HG23	1:B:611:LEU:HD23	1.99	0.44
1:B:1945:LEU:O	1:B:1949:VAL:HG22	2.17	0.44
1:B:1538:ARG:O	1:B:1542:MET:HG3	2.17	0.44
1:B:548:VAL:HG11	4:B:5804:EDO:H12	1.99	0.44
1:B:1045:PRO:HB2	2:J:2314:PHE:CE2	2.53	0.44
1:B:1253:THR:N	4:B:5816:EDO:H22	2.17	0.44
1:B:1077:LEU:HD23	1:B:1077:LEU:HA	1.83	0.44
1:B:1550:ILE:HG12	1:B:1559:VAL:HG11	2.00	0.44
1:B:2071:ALA:C	1:B:2073:SER:H	2.21	0.44
2:J:2095:ASP:N	2:J:2095:ASP:OD1	2.49	0.44
1:B:793:ASP:O	1:B:797:VAL:HG13	2.17	0.44
1:B:800:LEU:O	1:B:805:HIS:HB2	2.17	0.44
1:B:1998:GLN:HA	1:B:1998:GLN:OE1	2.18	0.44
1:B:2066:VAL:O	1:B:2079:ILE:HA	2.17	0.44
2:J:2149:PRO:HD3	2:J:2274:PRO:HG3	2.00	0.44
1:B:1306:PRO:HB2	1:B:1327:PHE:CD2	2.52	0.44
1:B:1648:ARG:HG3	1:B:1649:SER:N	2.33	0.44



Atom_1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1660:LEU:HA	1:B:1701:ARG:O	2.18	0.43
1:B:573:HIS:O	1:B:577:LYS:HG2	2.19	0.43
1:B:1977:LYS:HD3	1:B:1996:LEU:HD22	2.00	0.43
2:J:2197:ALA:HA	2:J:2200:MET:HE3	1.98	0.43
1:B:1986:MET:HE2	1:B:1986:MET:HB3	1.84	0.43
1:B:1138:GLU:OE1	1:B:1138:GLU:N	2.40	0.43
1:B:1601:LEU:O	1:B:1610:LYS:HD3	2.18	0.43
1:B:2103:ASN:HA	1:B:2123:SER:HA	2.01	0.43
1:B:2118:GLN:HB3	1:B:2120:TYR:HE1	1.84	0.43
1:B:1192:PRO:HB2	1:B:1292:PRO:HD3	2.01	0.43
1:B:752:LEU:HD11	1:B:780:TYR:HA	2.01	0.43
1:B:736[A]:ARG:NH1	1:B:773:GLU:HG2	2.34	0.43
1:B:1364:ILE:HD13	1:B:1424:ILE:HD13	2.01	0.43
1:B:2050:PRO:HA	1:B:2061:GLU:OE2	2.18	0.43
1:B:2103:ASN:HD21	1:B:2121:LYS:HG2	1.84	0.43
1:B:690:VAL:HG11	1:B:707:ILE:HD13	2.01	0.43
1:B:1460:GLY:HA2	1:B:1725:GLU:O	2.19	0.43
1:B:1539:LEU:HD23	1:B:1542:MET:CE	2.48	0.43
1:B:1985:ILE:HD11	1:B:2011:CYS:SG	2.59	0.43
1:B:2000:THR:HB	1:B:2003:GLN:HG3	2.00	0.43
1:B:993:ILE:CD1	1:B:1091:LEU:HD23	2.44	0.42
1:B:1981:SER:O	1:B:1984:ASP:HB2	2.18	0.42
1:B:1262:LEU:HD23	1:B:1262:LEU:HA	1.90	0.42
1:B:1583:ASP:CG	1:B:1584:ILE:H	2.20	0.42
1:B:1953:MET:HG3	1:B:2114:MET:SD	2.60	0.42
1:B:1954:TRP:HB3	1:B:1955:SER:H	1.71	0.42
1:B:971:LYS:HB2	1:B:980:GLN:HB3	2.02	0.42
2:J:2090:ILE:HG21	2:J:2111:LEU:HD21	2.01	0.42
2:J:2130:GLY:HA3	2:J:2141:GLU:O	2.20	0.42
1:B:1356:LYS:N	3:B:5803:QB6:O11	2.48	0.42
1:B:1881:ASN:HD22	1:B:1883:LYS:HZ3	1.66	0.42
2:J:2235:TYR:O	2:J:2239:ARG:HG2	2.20	0.42
1:B:569:LEU:HD13	1:B:596:ILE:CD1	2.50	0.42
1:B:1081:MET:O	1:B:1085:THR:HG23	2.20	0.42
1:B:1961:LYS:HG2	1:B:1971:ILE:HD11	2.01	0.42
1:B:1583:ASP:CG	1:B:1584:ILE:N	2.73	0.42
1:B:1314:ASN:O	1:B:1318:GLU:HG3	2.19	0.42
1:B:1737:ASN:O	1:B:1741:VAL:HG23	2.20	0.42
1:B:1977:LYS:HD2	1:B:1996:LEU:HD13	2.02	0.42
2:J:2170:LYS:HA	2:J:2170:LYS:HD3	1.87	0.42
1:B:1158:HIS:O	1:B:1171:GLY:HA3	2.20	0.41



Atom-1	Atom-2	Interatomic	Clash
	1100m <b>2</b>	distance (Å)	overlap (Å)
1:B:2099:THR:HA	1:B:2126:VAL:HG21	2.02	0.41
1:B:1043:ARG:HB3	2:J:2317:PHE:CE1	2.55	0.41
1:B:1777:SER:HG	1:B:1780:HIS:CG	2.39	0.41
1:B:1448:ILE:O	1:B:1485:ILE:HG12	2.21	0.41
1:B:1931:SER:HA	1:B:2076:LEU:HD13	2.02	0.41
1:B:467:LEU:HD11	1:B:481:LEU:HD21	2.02	0.41
1:B:502:CYS:HA	1:B:652:SER:O	2.20	0.41
1:B:1167:MET:HE3	1:B:1167:MET:HB3	1.97	0.41
1:B:1356:LYS:HB2	1:B:1356:LYS:HE2	1.94	0.41
1:B:784:ILE:HA	1:B:810:VAL:O	2.21	0.41
1:B:1016:ARG:NH1	5:B:5931:HOH:O	2.53	0.41
1:B:1043:ARG:HB3	2:J:2317:PHE:HE1	1.85	0.41
1:B:2017:ILE:HD13	1:B:2084:LEU:HD23	2.02	0.41
1:B:484:ILE:HG13	1:B:676:PHE:CE2	2.56	0.41
1:B:489:TYR:HB2	1:B:515:MET:HE1	2.03	0.41
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.21	0.41
2:J:2091:TYR:O	2:J:2224:THR:HA	2.21	0.41
1:B:769:CYS:SG	1:B:774:LEU:HD23	2.61	0.41
1:B:1577:LEU:HD11	1:B:1612:THR:HA	2.02	0.41
1:B:1953:MET:SD	1:B:1962:GLN:HG3	2.61	0.41
1:B:1973:ARG:HG2	1:B:1996:LEU:HD12	2.03	0.41
1:B:1477:ILE:O	1:B:1481:ILE:HG12	2.21	0.40
1:B:1953:MET:HE2	1:B:1961:LYS:HB2	2.03	0.40
1:B:1269:ARG:NH1	1:B:1279[A]:GLU:OE1	2.55	0.40
1:B:2045:GLU:O	1:B:2046:GLU:HG3	2.21	0.40
1:B:531:ILE:HD12	1:B:531:ILE:N	2.36	0.40
1:B:699:LYS:O	1:B:703:ILE:HG13	2.21	0.40
1:B:705:ASN:HA	1:B:708:VAL:HG12	2.02	0.40
1:B:1043:ARG:HA	1:B:1043:ARG:HD2	1.85	0.40
1:B:1046:ILE:HB	1:B:1064:GLN:NE2	2.35	0.40
1:B:1415:ASP:HB3	1:B:1435:LEU:HD11	2.02	0.40
1:B:1971:ILE:O	1:B:1975:THR:OG1	2.31	0.40
1:B:513:ALA:O	1:B:517:MET:HG3	2.21	0.40
1:B:615:ASP:HA	1:B:651:LEU:HB2	2.04	0.40
1:B:1872:ALA:O	1:B:1875:VAL:HG22	2.21	0.40
1:B:1194:THR:HB	4:B:5810:EDO:H22	2.02	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-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LYS:NZ	1:B:1695:LEU:O[2_455]	2.08	0.12

### 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	1726/1747~(99%)	1656~(96%)	64 (4%)	6 (0%)	41	55
2	J	261/263~(99%)	249~(95%)	11 (4%)	1 (0%)	34	48
All	All	1987/2010~(99%)	1905 (96%)	75 (4%)	7 (0%)	34	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	458	GLU
1	В	1859	PRO
1	В	2086	GLN
2	J	2059	PRO
1	В	405	PRO
1	В	528	ASP
1	В	1882	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	1547/1560~(99%)	1485~(96%)	62~(4%)	31 49	

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Continued	trom	previous	<i>paae</i>
• • • • • • • • • • • •	J	<i>r</i> · · · · · · · · · · · · · · · · · · ·	r ~g ····

Mol	Chain	Analysed	Rotameric	Outliers	Percentile	$\mathbf{s}$
2	J	236/236~(100%)	231~(98%)	5 (2%)	53 72	
All	All	1783/1796~(99%)	1716 (96%)	67(4%)	33 51	

All (67) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	426	LYS
1	В	429	GLN
1	В	432	ASP
1	В	437	ARG
1	В	439	ARG
1	В	457	SER
1	В	489	TYR
1	В	490	ARG
1	В	510	THR
1	В	526	ASN
1	В	530	THR
1	В	545	ARG
1	В	551	MET
1	В	554	SER
1	В	696	LYS
1	В	699	LYS
1	В	739	ARG
1	В	743	LEU
1	В	759	THR
1	В	760	GLU
1	В	893	MET
1	В	992	TYR
1	В	1044	VAL
1	В	1051	SER
1	В	1113	ASN
1	В	1126	MET
1	В	1137	GLU
1	В	1147	ASN
1	В	1187	SER
1	В	1212	GLU
1	В	1310	SER
1	В	1342	SER
1	В	1357	THR
1	В	1414	THR
1	В	1507	SER
1	В	1566	ARG



Mol	Chain	Res	Type
1	В	1597	LEU
1	В	1603	LYS
1	В	1625	SER
1	В	1699	GLU
1	В	1710	LYS
1	В	1731	CYS
1	В	1742	THR
1	В	1772	ASN
1	В	1788	LEU
1	В	1791	GLN
1	В	1831	LEU
1	В	1847	GLU
1	В	1848	ILE
1	В	1856	GLU
1	В	1860	ILE
1	В	1877	HIS
1	В	1904	LEU
1	В	1907	GLU
1	В	1958	SER
1	В	1966	PHE
1	В	1980	GLU
1	В	1985	ILE
1	В	1990	ASP
1	В	2067	VAL
1	В	2073	SER
1	В	2095	VAL
2	J	2095	ASP
2	J	2219	THR
2	J	2233	SER
2	J	2239	ARG
2	J	2258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	805	HIS
1	В	892	GLN
1	В	980	GLN
1	В	1370	GLN
1	В	1591	HIS
1	В	1772	ASN
1	В	1798	GLN



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Mol	Chain	Res	Type
1	В	1881	ASN
1	В	1994	ASN
1	В	2103	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

20 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	ol Type Chain Bos Link		Timle	Bo	Bond lengths			Bond angles		
NIOI	Moi Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	QB6	В	5802	-	12,12,12	2.27	6 (50%)	18,18,18	2.44	5 (27%)
4	EDO	В	5810	-	3,3,3	0.57	0	2,2,2	0.49	0
4	EDO	В	5808	-	3, 3, 3	0.51	0	2,2,2	0.38	0
3	QB6	В	5803	-	12,12,12	2.53	4 (33%)	18,18,18	4.62	8 (44%)
4	EDO	В	5814	-	3,3,3	0.81	0	2,2,2	0.26	0
3	QB6	J	2402	-	12,12,12	2.46	5 (41%)	18,18,18	3.13	6 (33%)
4	EDO	В	5817	-	3,3,3	0.60	0	2,2,2	0.37	0
3	QB6	В	5801	-	12,12,12	2.43	5 (41%)	18,18,18	2.64	4 (22%)
4	EDO	В	5813	-	3,3,3	0.51	0	2,2,2	0.66	0
4	EDO	В	5804	-	3,3,3	0.32	0	2,2,2	1.05	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
IVIOI	wor Type Chain	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	EDO	В	5806	-	3,3,3	0.39	0	$2,\!2,\!2$	1.45	0
4	EDO	В	5816	-	3,3,3	0.67	0	2,2,2	0.36	0
4	EDO	J	2403	-	3,3,3	0.58	0	$2,\!2,\!2$	0.14	0
4	EDO	В	5805	-	3,3,3	0.36	0	$2,\!2,\!2$	0.95	0
4	EDO	В	5811	-	3,3,3	0.68	0	2,2,2	0.29	0
4	EDO	В	5809	-	3,3,3	0.51	0	$2,\!2,\!2$	0.43	0
4	EDO	В	5815	-	3,3,3	0.38	0	$2,\!2,\!2$	0.93	0
4	EDO	В	5807	-	3,3,3	0.70	0	2,2,2	0.35	0
4	EDO	J	2401	-	3,3,3	0.49	0	$2,\!2,\!2$	0.41	0
4	EDO	В	5812	-	3,3,3	0.50	0	2,2,2	0.39	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
3	QB6	В	5802	-	-	4/6/6/6	0/1/1/1
4	EDO	В	5810	-	-	0/1/1/1	-
4	EDO	В	5808	-	-	1/1/1/1	-
3	QB6	В	5803	-	-	4/6/6/6	0/1/1/1
4	EDO	В	5814	-	-	1/1/1/1	-
3	QB6	J	2402	-	-	4/6/6/6	0/1/1/1
4	EDO	В	5817	-	-	1/1/1/1	-
3	QB6	В	5801	-	-	4/6/6/6	0/1/1/1
4	EDO	В	5813	-	-	1/1/1/1	-
4	EDO	В	5804	-	-	1/1/1/1	-
4	EDO	В	5806	-	-	1/1/1/1	-
4	EDO	В	5816	-	-	0/1/1/1	-
4	EDO	J	2403	-	-	1/1/1/1	-
4	EDO	В	5805	-	-	0/1/1/1	-
4	EDO	В	5811	-	-	1/1/1/1	-
4	EDO	В	5809	-	-	0/1/1/1	-
4	EDO	В	5815	-	-	1/1/1/1	_
4	EDO	В	5807	-	-	1/1/1/1	-
4	EDO	J	2401	-	-	1/1/1/1	-
4	EDO	В	5812	-	-	0/1/1/1	-

All (20) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2402	QB6	S09-N10	5.84	1.71	1.60
3	В	5803	QB6	S09-N10	5.83	1.71	1.60
3	В	5801	QB6	S09-N10	5.73	1.71	1.60
3	В	5802	QB6	S09-N10	5.52	1.71	1.60
3	В	5803	QB6	C07-S09	4.95	1.84	1.77
3	В	5801	QB6	C07-S09	3.89	1.83	1.77
3	J	2402	QB6	C07-S09	3.81	1.83	1.77
3	В	5802	QB6	C07-S09	2.93	1.81	1.77
3	В	5801	QB6	O12-S09	2.77	1.48	1.43
3	В	5803	QB6	O04-C03	2.76	1.42	1.36
3	J	2402	QB6	C02-N01	2.75	1.47	1.37
3	В	5803	QB6	C02-N01	2.57	1.46	1.37
3	J	2402	QB6	O12-S09	2.50	1.48	1.43
3	J	2402	QB6	O04-C03	2.45	1.41	1.36
3	В	5802	QB6	C02-N01	2.45	1.46	1.37
3	В	5802	QB6	O11-S09	2.32	1.48	1.43
3	В	5801	QB6	O04-C03	2.26	1.41	1.36
3	В	5802	QB6	O12-S09	2.25	1.47	1.43
3	В	5801	QB6	C02-N01	2.19	1.45	1.37
3	В	5802	QB6	O04-C03	2.17	1.40	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	5803	QB6	O12-S09-O11	-14.13	95.53	118.76
3	J	2402	QB6	O12-S09-O11	-11.10	100.51	118.76
3	В	5803	QB6	O12-S09-C07	11.01	119.63	107.35
3	В	5801	QB6	O12-S09-O11	-9.36	103.38	118.76
3	В	5802	QB6	O12-S09-O11	-8.17	105.33	118.76
3	В	5803	QB6	O12-S09-N10	4.10	113.44	107.36
3	J	2402	QB6	O11-S09-C07	4.05	111.87	107.35
3	В	5803	QB6	O04-C03-C02	3.67	122.39	116.25
3	J	2402	QB6	O12-S09-N10	3.56	112.64	107.36
3	В	5802	QB6	C07-S09-N10	3.43	113.23	108.38
3	В	5801	QB6	O11-S09-N10	3.32	112.29	107.36
3	J	2402	QB6	C07-S09-N10	2.90	112.48	108.38
3	В	5803	QB6	C08-C07-S09	2.87	125.02	119.31
3	В	5801	QB6	O12-S09-C07	2.87	110.55	107.35
3	В	5803	QB6	C05-C06-C07	2.79	122.34	119.45
3	В	5802	QB6	O04-C03-C02	2.74	120.83	116.25
3	J	2402	QB6	O04-C03-C02	2.56	120.54	116.25
3	В	5802	QB6	C03-C02-N01	2.52	122.78	118.77
3	J	2402	QB6	O11-S09-N10	2.36	110.87	107.36



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	В	5801	QB6	O12-S09-N10	2.33	110.81	107.36
3	В	5803	QB6	C06-C07-S09	-2.16	116.60	119.73
3	В	5802	QB6	O12-S09-N10	2.09	110.46	107.36
3	В	5803	QB6	O11-S09-N10	2.00	110.33	107.36

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	5806	EDO	O1-C1-C2-O2
4	В	5807	EDO	O1-C1-C2-O2
4	В	5811	EDO	O1-C1-C2-O2
4	В	5815	EDO	O1-C1-C2-O2
4	В	5817	EDO	O1-C1-C2-O2
3	В	5801	QB6	C06-C07-S09-O12
3	В	5801	QB6	C08-C07-S09-N10
3	В	5802	QB6	C06-C07-S09-N10
3	В	5802	QB6	C08-C07-S09-N10
3	В	5803	QB6	C08-C07-S09-N10
3	В	5801	QB6	C08-C07-S09-O12
3	В	5803	QB6	C06-C07-S09-N10
3	J	2402	QB6	C08-C07-S09-N10
3	В	5801	QB6	C06-C07-S09-N10
3	J	2402	QB6	C06-C07-S09-N10
4	J	2403	EDO	O1-C1-C2-O2
3	В	5803	QB6	C06-C07-S09-O11
4	В	5808	EDO	O1-C1-C2-O2
4	В	5813	EDO	O1-C1-C2-O2
4	В	5814	EDO	O1-C1-C2-O2
3	В	5803	QB6	C08-C07-S09-O11
3	J	2402	QB6	C08-C07-S09-O11
4	В	5804	EDO	O1-C1-C2-O2
4	J	2401	EDO	O1-C1-C2-O2
3	В	5802	QB6	C06-C07-S09-O11
3	J	2402	QB6	C06-C07-S09-O11
3	В	5802	QB6	C08-C07-S09-O11

There are no ring outliers.

6 monomers are involved in 9 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	5810	EDO	2	0
3	В	5803	QB6	1	0
4	В	5813	EDO	1	0
4	В	5804	EDO	2	0
4	В	5816	EDO	2	0
4	J	2403	EDO	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 sufficient must be 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	1724/1747~(98%)	0.59	178 (10%) 6 6	34, 66, 142, 226	0
2	J	263/263~(100%)	0.43	19 (7%) 15 14	36, 59, 122, 203	0
All	All	1987/2010~(98%)	0.57	197 (9%) 7 6	34, 65, 140, 226	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	1879	LEU	17.7
1	В	1880	ASN	10.0
2	J	2061	GLY	9.1
1	В	1870	GLN	8.9
1	В	1601	LEU	8.3
1	В	2124	VAL	8.2
2	J	2319	LEU	7.8
1	В	1996	LEU	7.8
1	В	1873	GLN	7.7
1	В	1871	LEU	7.2
1	В	1858	ILE	7.1
1	В	1603	LYS	7.0
2	J	2098	LYS	6.8
1	В	2102	HIS	6.7
2	J	2060	LEU	6.6
2	J	2058	GLY	6.6
1	В	404	ALA	6.5
1	В	1940	LEU	6.4
1	В	805	HIS	6.3
1	В	2045	GLU	6.3
1	В	1936	LEU	6.3
1	В	1877	HIS	6.0
1	В	2120	TYR	5.9
2	J	2099	GLU	5.9



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Mol	Chain	$\operatorname{Res}$	Type	RSRZ
1	В	1863	HIS	5.9
1	В	1893	LEU	5.9
2	J	2062	SER	5.8
1	В	1882	PRO	5.8
1	В	1604	LEU	5.6
1	В	1597	LEU	5.6
1	В	753	ARG	5.5
1	В	1868	LEU	5.3
1	В	1874	LYS	5.1
1	В	1841	LYS	5.1
1	В	1869	ARG	5.0
1	В	2035	VAL	4.9
1	В	2047	VAL	4.9
1	В	1997	LEU	4.9
1	В	2046	GLU	4.9
1	В	602	GLU	4.7
1	В	2107	TYR	4.7
1	В	2096	ALA	4.7
1	В	2122	PHE	4.6
1	В	1307	LEU	4.5
1	В	1865	ASP	4.5
1	В	1899	LEU	4.5
1	В	1584	ILE	4.5
1	В	2033	GLY	4.5
1	В	1977	LYS	4.4
1	В	755	GLY	4.4
1	В	1044	VAL	4.4
1	В	1872	ALA	4.4
1	В	2077	ILE	4.4
1	В	782	PHE	4.4
1	В	2038	LEU	4.4
1	В	571	GLY	4.3
1	В	1987	GLU	4.2
1	В	1586	ARG	4.2
1	В	2121	LYS	4.2
1	В	1954	TRP	4.1
1	В	2095	VAL	4.1
1	В	2022	GLU	4.1
1	В	456	GLY	4.0
1	В	2103	ASN	4.0
1	В	1174	ILE	3.9
2	J	2320	LEU	3.7



8BC8

Mol	Chain	Res	Type	RSRZ
1	В	2098	ALA	3.7
1	В	1876	PRO	3.7
1	В	1321	TYR	3.7
1	В	1963	LEU	3.7
2	J	2317	PHE	3.6
2	J	2066	THR	3.6
1	В	2008	ALA	3.6
1	В	754	GLU	3.6
1	В	2072	LYS	3.6
1	В	2104	TYR	3.5
2	J	2096	ASP	3.5
1	В	2076	LEU	3.5
1	В	2040	GLN	3.4
1	В	1890	LYS	3.4
2	J	2097	ILE	3.4
1	В	603	ARG	3.4
1	В	2024	VAL	3.3
1	В	2123	SER	3.3
1	В	2097	PRO	3.2
1	В	1878	LYS	3.2
1	В	601	GLY	3.2
1	В	1943	MET	3.2
1	В	861	TYR	3.2
1	В	715	HIS	3.2
1	В	1041	LEU	3.1
1	В	457	SER	3.1
1	В	1135	LEU	3.1
1	В	575	LEU	3.1
1	В	1985	ILE	3.0
1	В	726	HIS	3.0
2	J	2070	LYS	3.0
1	В	573	HIS	3.0
1	В	1170	MET	3.0
1	В	743	LEU	3.0
1	В	1043	ARG	3.0
2	J	2063	MET	3.0
1	В	716	ALA	3.0
1	В	2010	PHE	3.0
1	В	1164	LEU	2.9
1	В	1590	LEU	2.9
1	В	1598	ILE	2.9
1	В	1585	GLN	2.9

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1

SP	2.9
YR	2.9
HR	2.8
LΕ	2.8
SP	2.8
LΕ	2.8
LA	2.7
RG	2.7
TD	

Continued from previous page... Mol Chain Res

1988

В

Type RSRZ

2.9

MET

1         B         1931         SER         2.9           1         B         1973         ARG         2.9           2         J         2318         ALA         2.9           1         B         746         ASP         2.9           1         B         1959         TYR         2.9           1         B         2048         THR         2.8           1         B         2027         ASP         2.8           1         B         10641         ILE         2.8           1         B         1076         ALA         2.7           1         B         1075         THR         2.7           1         B         2105         THR         2.7           1         B         774         LEU         2.6           2         J         2286         VAL         2.6           1         B         1313         ILE         2.6           1         B         1320         LEU         2.6           1         B         1348         VAL         2.5           1         B         1402         ASN         2.5 <th>1</th> <th>В</th> <th>2119</th> <th>GLU</th> <th>2.9</th>	1	В	2119	GLU	2.9
1         B         1973         ARG         2.9           2         J         2318         ALA         2.9           1         B         746         ASP         2.9           1         B         1959         TYR         2.9           1         B         2048         THR         2.8           1         B         2027         ASP         2.8           1         B         1641         ILE         2.8           1         B         1076         ALA         2.7           1         B         1993         ARG         2.7           1         B         2105         THR         2.7           1         B         751         PHE         2.7           1         B         774         LEU         2.6           2         J         2286         VAL         2.6           1         B         1320         LEU         2.6           1         B         1320         LEU         2.6           1         B         1348         VAL         2.5           1         B         1402         ASN         2.5	1	В	1931	SER	2.9
2         J         2318         ALA         2.9           1         B         746         ASP         2.9           1         B         1959         TYR         2.9           1         B         2048         THR         2.8           1         B         2027         ASP         2.8           1         B         1641         ILE         2.8           1         B         1076         ALA         2.7           1         B         1993         ARG         2.7           1         B         1055         THR         2.7           1         B         2105         THR         2.7           1         B         714         LEU         2.6           2         J         2286         VAL         2.6           1         B         1320         LEU         2.6           1         B         1320         LEU         2.6           1         B         1348         VAL         2.5           1         B         1402         ASN         2.5           1         B         1402         ASN         2.5	1	В	1973	ARG	2.9
1       B       746       ASP       2.9         1       B       1959       TYR       2.9         1       B       2048       THR       2.8         1       B       2027       ASP       2.8         1       B       10641       ILE       2.8         1       B       1076       ALA       2.7         1       B       1993       ARG       2.7         1       B       2105       THR       2.7         1       B       2105       THR       2.7         1       B       751       PHE       2.7         1       B       774       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         1       B       1957       ASP       2.6         1       B       1920       LEU       2.6         1       B       1320       LEU       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B<	2	J	2318	ALA	2.9
1       B       1959       TYR       2.9         1       B       2048       THR       2.8         1       B       2027       ASP       2.8         1       B       1641       ILE       2.8         1       B       1641       ILE       2.8         1       B       1076       ALA       2.7         1       B       1993       ARG       2.7         1       B       2105       THR       2.7         1       B       751       PHE       2.7         1       B       751       PHE       2.7         1       B       774       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         1       B       1957       ASP       2.6         1       B       1920       LEU       2.6         1       B       1320       LEU       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B </td <td>1</td> <td>В</td> <td>746</td> <td>ASP</td> <td>2.9</td>	1	В	746	ASP	2.9
1       B       2048       THR       2.8         1       B       2027       ASP       2.8         1       B       1641       ILE       2.8         1       B       1076       ALA       2.7         1       B       1993       ARG       2.7         1       B       2105       THR       2.7         1       B       2105       THR       2.7         1       B       71       ARG       2.7         1       B       71       PHE       2.7         1       B       71       PHE       2.7         1       B       74       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B	1	В	1959	TYR	2.9
1       B       806       ILE       2.8         1       B       1641       ILE       2.8         1       B       1076       ALA       2.7         1       B       1993       ARG       2.7         1       B       2105       THR       2.7         1       B       2105       THR       2.7         2       J       2121       ARG       2.7         1       B       751       PHE       2.7         1       B       751       PHE       2.7         1       B       74       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B	1	В	2048	THR	2.8
1B $2027$ ASP $2.8$ 1B $1641$ ILE $2.8$ 1B $1076$ ALA $2.7$ 1B $1993$ ARG $2.7$ 1B $2105$ THR $2.7$ 2J $2121$ ARG $2.7$ 1B $751$ PHE $2.7$ 1B $751$ PHE $2.7$ 1B $751$ PHE $2.7$ 1B $774$ LEU $2.6$ 2J $2286$ VAL $2.6$ 2J $2266$ ARG $2.6$ 1B $1957$ ASP $2.6$ 1B $1957$ ASP $2.6$ 1B $1320$ LEU $2.6$ 1B $1348$ VAL $2.5$ 1B $1402$ ASN $2.5$ 1B $1402$ ASN $2.5$ 1B $1402$ ASN $2.5$ 1B $1402$ ASN $2.5$ 1B $1884$ PHE $2.5$ 1B $1866$ ASN $2.5$ 1B $1983$ PHE $2.5$ 1B $1908$ LEU $2.5$ 1B $1908$ LEU $2.5$ 1B $1908$ LEU $2.5$ 1B $1908$ LEU $2.5$ 1B $108$ $2042$ $GLU$ $2.5$ 1B $108$ $148$ $PHE$ <td>1</td> <td>В</td> <td>806</td> <td>ILE</td> <td>2.8</td>	1	В	806	ILE	2.8
1B1641ILE $2.8$ 1B1076ALA $2.7$ 1B1993ARG $2.7$ 1B2105THR $2.7$ 2J2121ARG $2.7$ 1B751PHE $2.7$ 1B1143ILE $2.7$ 1B1143ILE $2.7$ 1B774LEU $2.6$ 2J2286VAL $2.6$ 2J2266ARG $2.6$ 1B1957ASP $2.6$ 1B1957ASP $2.6$ 1B1967ASP $2.6$ 1B1974CYS $2.5$ 1B1974CYS $2.5$ 1B1402ASN $2.5$ 1B1402ASN $2.5$ 1B1402ASN $2.5$ 1B1884PHE $2.5$ 1B1884PHE $2.5$ 1B1613LEU $2.5$ 1B1613LEU $2.5$ 1B1983PHE $2.5$ 1B1908LEU $2.5$ 1B1908LEU $2.5$ 1B106LEU $2.5$ 1B709TYR $2.4$ 1B148PHE $2.4$ 1B1317PHE $2.4$ </td <td>1</td> <td>В</td> <td>2027</td> <td>ASP</td> <td>2.8</td>	1	В	2027	ASP	2.8
1       B       1076       ALA       2.7         1       B       2105       THR       2.7         2       J       2121       ARG       2.7         1       B       751       PHE       2.7         1       B       751       PHE       2.7         1       B       751       PHE       2.7         1       B       774       LEU       2.6         2       J       2286       VAL       2.6         2       J       2266       ARG       2.6         1       B       531       ILE       2.6         1       B       1957       ASP       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.5         1       B       1402       ASN       2.5         1       B <td>1</td> <td>В</td> <td>1641</td> <td>ILE</td> <td>2.8</td>	1	В	1641	ILE	2.8
1       B       1993       ARG       2.7         1       B       2105       THR       2.7         2       J       2121       ARG       2.7         1       B       751       PHE       2.7         1       B       1143       ILE       2.7         1       B       751       PHE       2.7         1       B       774       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         2       J       2266       ARG       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.5         1       B       1348       VAL       2.5         1       B       1402       ASN       2.5         1       B <td>1</td> <td>В</td> <td>1076</td> <td>ALA</td> <td>2.7</td>	1	В	1076	ALA	2.7
1       B       2105       THR       2.7         2       J       2121       ARG       2.7         1       B       751       PHE       2.7         1       B       1143       ILE       2.7         1       B       1143       ILE       2.7         1       B       1143       ILE       2.7         1       B       774       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         2       J       2266       ARG       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.5         1       B       1348       VAL       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1613       LEU       2.5         1       B </td <td>1</td> <td>В</td> <td>1993</td> <td>ARG</td> <td>2.7</td>	1	В	1993	ARG	2.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	2105	THR	2.7
1B751PHE $2.7$ 1B1143ILE $2.7$ 1B774LEU $2.6$ 2J2286VAL $2.6$ 1B531ILE $2.6$ 2J2266ARG $2.6$ 1B1957ASP $2.6$ 1B1320LEU $2.6$ 1B1320LEU $2.6$ 1B1348VAL $2.5$ 1B1974CYS $2.5$ 1B1402ASN $2.5$ 1B1402ASN $2.5$ 1B1884PHE $2.5$ 1B1884PHE $2.5$ 1B1613LEU $2.5$ 1B1613LEU $2.5$ 1B1983PHE $2.5$ 1B1983PHE $2.5$ 1B1908LEU $2.5$ 1B1908LEU $2.5$ 1B1908LEU $2.5$ 1B2042GLU $2.5$ 1B709TYR $2.4$ 1B1148PHE $2.4$ 1B1317PHE $2.4$	2	J	2121	ARG	2.7
1B1143ILE $2.7$ 1B $774$ LEU $2.6$ 2J $2286$ VAL $2.6$ 1B $531$ ILE $2.6$ 2J $2266$ ARG $2.6$ 1B $1957$ ASP $2.6$ 1B $1320$ LEU $2.6$ 1B $1320$ LEU $2.6$ 1B $1320$ LEU $2.6$ 1B $1348$ VAL $2.5$ 1B $1974$ CYS $2.5$ 1B $1402$ ASN $2.5$ 1B $1776$ ILE $2.5$ 1B $1884$ PHE $2.5$ 1B $2034$ PRO $2.5$ 1B $1866$ ASN $2.5$ 1B $1613$ LEU $2.5$ 1B $1983$ PHE $2.5$ 1B $1908$ LEU $2.5$ 1B $1908$ LEU $2.5$ 1B $2042$ GLU $2.5$ 1B $762$ LEU $2.5$ 1B $709$ TYR $2.4$ 1B $1148$ PHE $2.4$ 1B $1317$ PHE $2.4$	1	В	751	PHE	2.7
1       B       774       LEU       2.6         2       J       2286       VAL       2.6         1       B       531       ILE       2.6         2       J       2266       ARG       2.6         1       B       1957       ASP       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1849       PHE       2.5         1       B       2034       PRO       2.5         1       B       1613       LEU       2.5         1       B       1613       LEU       2.5         1       B       1908       LEU       2.5         1       B<	1	В	1143	ILE	2.7
2       J       2286       VAL       2.6         1       B       531       ILE       2.6         2       J       2266       ARG       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       1866       ASN       2.5         1       B       1866       ASN       2.5         1       B       1849       ILEU       2.5         1       B       1849       ILEU       2.5         1 <td< td=""><td>1</td><td>В</td><td>774</td><td>LEU</td><td>2.6</td></td<>	1	В	774	LEU	2.6
1       B       531       ILE       2.6         2       J       2266       ARG       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.6         1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1833       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILEU       2.5         1	2	J	2286	VAL	2.6
2       J       2266       ARG       2.6         1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1776       ILE       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2042       GLU       2.5         1	1	В	531	ILE	2.6
1       B       1957       ASP       2.6         1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1844       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1833       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2042       GLU       2.5         1	2	J	2266	266 ARG 2	
1       B       1320       LEU       2.6         1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1776       ILE       2.5         1       B       1776       ILE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1866       ASN       2.5         1       B       1613       LEU       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2042       GLU       2.5         1       B       709       TYR       2.4         1       B	1	В	1957	ASP	2.6
1       B       1348       VAL       2.5         1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1402       ASN       2.5         1       B       1776       ILE       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1866       ASN       2.5         1       B       1866       ASN       2.5         1       B       183       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2042       GLU       2.5         1       B       709       TYR       2.4         1       B<	1	В	1320	LEU	2.6
1       B       1974       CYS       2.5         1       B       1402       ASN       2.5         1       B       1776       ILE       2.5         1       B       1884       PHE       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1866       ASN       2.5         1       B       1863       PHE       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       709       TYR       2.4         1       B       148       PHE       2.4         1       B<	1	В	1348	VAL	2.5
1       B       1402       ASN       2.5         1       B       1776       ILE       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       2068       ILE       2.5         1       B       1613       LEU       2.5         1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B </td <td>1</td> <td>В</td> <td>1974</td> <td>CYS</td> <td>2.5</td>	1	В	1974	CYS	2.5
1       B       1776       ILE       2.5         1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1866       ASN       2.5         1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B </td <td>1</td> <td>В</td> <td>1402</td> <td>ASN</td> <td>2.5</td>	1	В	1402	ASN	2.5
1       B       1884       PHE       2.5         1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1613       LEU       2.5         1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B       1317       PHE       2.4	1	В	1776	ILE	2.5
1       B       2034       PRO       2.5         1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1613       LEU       2.5         1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B       1317       PHE       2.4	1	В	1884	PHE	2.5
1       B       2068       ILE       2.5         1       B       1866       ASN       2.5         1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B       1317       PHE       2.4	1	В	2034	PRO	2.5
1       B       1866       ASN       2.5         1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B       1317       PHE       2.4	1	В	2068	ILE	2.5
1       B       1613       LEU       2.5         1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       1908       LEU       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       1148       PHE       2.4         1       B       528       ASP       2.4         1       B       1317       PHE       2.4	1	В	1866	ASN	2.5
1       B       1983       PHE       2.5         1       B       1849       ILE       2.5         1       B       1908       LEU       2.5         1       B       2106       LEU       2.5         1       B       2042       GLU       2.5         1       B       762       LEU       2.5         1       B       709       TYR       2.4         1       B       528       ASP       2.4         1       B       1317       PHE       2.4	1	В	1613	LEU	2.5
1         B         1849         ILE         2.5           1         B         1908         LEU         2.5           1         B         2106         LEU         2.5           1         B         2042         GLU         2.5           1         B         762         LEU         2.5           1         B         762         LEU         2.5           1         B         709         TYR         2.4           1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	1983	PHE	2.5
1         B         1908         LEU         2.5           1         B         2106         LEU         2.5           1         B         2042         GLU         2.5           1         B         762         LEU         2.5           1         B         762         LEU         2.5           1         B         709         TYR         2.4           1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	1849	ILE	2.5
1         B         2106         LEU         2.5           1         B         2042         GLU         2.5           1         B         762         LEU         2.5           1         B         709         TYR         2.4           1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	1908	LEU	2.5
1         B         2042         GLU         2.5           1         B         762         LEU         2.5           1         B         709         TYR         2.4           1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	2106	LEU	2.5
1         B         762         LEU         2.5           1         B         709         TYR         2.4           1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	2042	GLU	2.5
1         B         709         TYR         2.4           1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	762	LEU	2.5
1         B         1148         PHE         2.4           1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	709	TYR	2.4
1         B         528         ASP         2.4           1         B         1317         PHE         2.4	1	В	1148	PHE	2.4
1 B 1317 PHE 2.4	1	В	528	ASP	2.4
	1	В	1317	PHE	2.4



Mol	Chain	Res	Type	RSRZ	
1	В	1394	TYR	2.4	
1	В	1886	1886 ASP		
1	В	1748	LYS	2.4	
1	В	2036	VAL	2.4	
1	В	2090 VAL		2.4	
1	В	1152	ARG	2.3	
1	В	1894	LEU	2.3	
1	В	1964	PRO	2.3	
1	В	1159	ASN	2.3	
1	В	2005	ALA	2.3	
1	В	1627	MET	2.3	
1	В	1989	GLU	2.3	
1	В	526	ASN	2.3	
1	В	1843	ARG	2.3	
1	В	2101	ALA	2.3	
1	В	1053	GLU	2.3	
1	В	1800	LYS	2.3	
1	В	821	LEU	2.2	
1	В	1145 LYS		2.2	
1	В	801	PHE	2.2	
1	В	2092	LEU	2.2	
1	В	572	ASP	2.2	
1	В	770	LYS	2.2	
1	В	1035	LEU	2.2	
1	В	1837	ASN	2.2	
1	В	1992	GLU	2.2	
1	В	2029	ILE	2.2	
1	В	518	LEU	2.2	
1	В	998	VAL	2.1	
1	В	1922	LEU	2.1	
1	В	1347	PHE	2.1	
1	В	2118	GLN	2.1	
1	В	1630	ARG	2.1	
2	J	2090	ILE	2.1	
1	В	718	LYS	2.1	
1	В	1511	THR	2.1	
1	В	1881	ASN	2.1	
1	В	2108	PHE	2.1	
1	В	455	PHE	2.1	
1	В	2125	ASP	2.1	
1	В	1349	GLY	2.1	
1	В	1262	LEU	2.0	



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	В	2041	LEU	2.0
1	В	2066	VAL	2.0
1	В	1052	ILE	2.0
1	В	1302	LEU	2.0
1	В	2084	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	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	В	5809	4/4	0.81	0.26	57,60,62,67	0
4	EDO	В	5810	4/4	0.85	0.19	53,59,60,60	0
4	EDO	В	5813	4/4	0.85	0.21	42,46,51,51	0
4	EDO	В	5807	4/4	0.86	0.26	42,46,54,55	0
4	EDO	J	2401	4/4	0.88	0.45	66,70,72,79	0
4	EDO	В	5814	4/4	0.89	0.28	41,46,51,56	0
4	EDO	В	5816	4/4	0.89	0.28	44,58,60,67	0
3	QB6	В	5803	12/12	0.89	0.19	56,67,74,74	0
4	EDO	В	5817	4/4	0.90	0.18	56,58,58,61	0
3	QB6	В	5802	12/12	0.90	0.23	62,69,74,76	0
4	EDO	В	5806	4/4	0.91	0.19	39,41,42,48	0
4	EDO	В	5812	4/4	0.92	0.18	60,63,63,69	0
3	QB6	J	2402	12/12	0.92	0.31	60,65,68,74	0
4	EDO	В	5804	4/4	0.93	0.21	46,52,61,72	0
4	EDO	В	5805	4/4	0.93	0.25	43,48,50,65	0
4	EDO	В	5811	4/4	0.93	0.15	54,54,55,57	0
4	EDO	J	2403	4/4	0.93	0.18	47,48,54,58	0
4	EDO	В	5808	4/4	0.94	0.14	61,63,65,70	0



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Mol	Type	Chain	$\mathbf{Res}$	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	EDO	В	5815	4/4	0.94	0.26	$51,\!52,\!66,\!66$	0
3	QB6	В	5801	12/12	0.95	0.12	48,54,58,60	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.

