



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:17 am BST

PDB ID : 3BRG  
Title : CSL (RBP-Jk) bound to DNA  
Authors : Friedmann, D.R.; Kovall, R.A.  
Deposited on : 2007-12-21  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

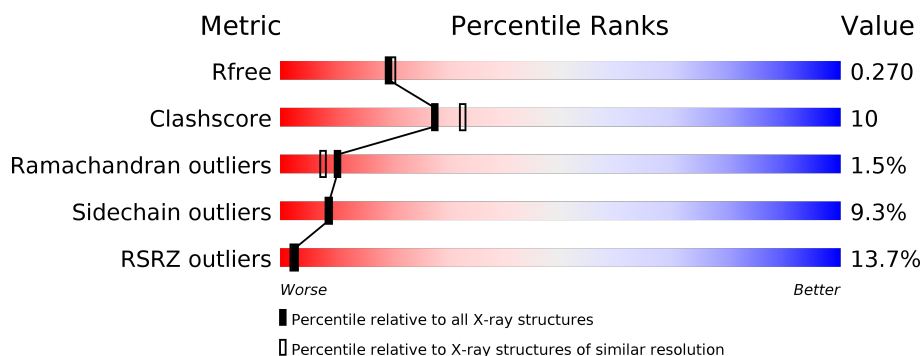
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	15	<div> <div>7%</div> <div> <div></div> <div>47%</div> <div>40%</div> <div>13%</div> </div> </div>
2	B	15	<div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
3	C	427	<div> <div>14%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• •</div> </div> </div>

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
4	EDO	C	9	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4081 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 DNA chain called DNA (5'-D(\*DAP\*DAP\*DTP\*DCP\*DTP\*DTP\*DTP\*D CP\*DCP\*DCP\*DAP\*DCP\*DAP\*DGP\*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			298	145	50	89	14			

- Molecule 2 is a DNA chain called DNA (5'-D(\*DTP\*DTP\*DAP\*DCP\*DTP\*DGP\*DTP\*D GP\*DGP\*DGP\*DAP\*DAP\*DAP\*DGP\*DA)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			311	149	61	87	14			

- Molecule 3 is a protein called Recombining binding protein suppressor of hairless.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	414	Total	C	N	O	S	0	0	0
			3290	2084	567	614	25			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLY	-	EXPRESSION TAG	UNP P31266
C	49	PRO	-	EXPRESSION TAG	UNP P31266
C	50	LEU	-	EXPRESSION TAG	UNP P31266
C	51	GLY	-	EXPRESSION TAG	UNP P31266
C	52	SER	-	EXPRESSION TAG	UNP P31266

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	2	Total 2	O 2	0	0
5	C	128	Total 128	O 128	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

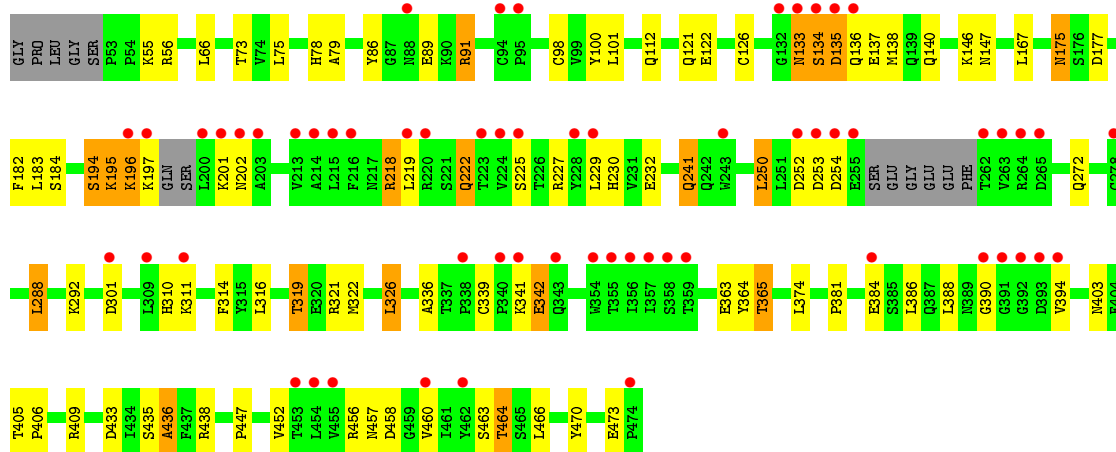
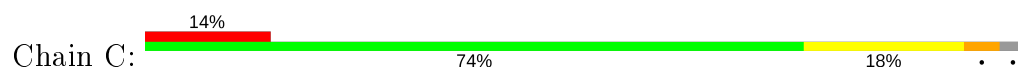
- Molecule 1: DNA (5'-D(\*DAP\*DAP\*DTP\*DCP\*DTP\*DTP\*DTP\*DCP\*DCP\*DCP\*DAP\*DCP\*DAP\*DGP\*DT)-3')



- Molecule 2: DNA (5'-D(\*DTP\*DTP\*DAP\*DCP\*DTP\*DGP\*DTP\*DGP\*DGP\*DGP\*DAP\*DA\*AP\*DAP\*DGP\*DA)-3')



- Molecule 3: Recombining binding protein suppressor of hairless



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.77Å 95.39Å 113.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.06 – 2.20 32.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.06-2.20) 99.9 (32.05-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3.0020	Depositor
R, $R_{free}$	0.219 , 0.255 0.247 , 0.270	Depositor DCC
$R_{free}$ test set	1876 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4081	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.76	8/332 (2.4%)	1.84	10/509 (2.0%)
2	B	1.73	5/350 (1.4%)	1.76	8/540 (1.5%)
3	C	0.64	0/3360	0.76	4/4538 (0.1%)
All	All	0.92	13/4042 (0.3%)	1.04	22/5587 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	2
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	DT	O5'-C5'	15.24	1.80	1.42
1	A	1	DA	N3-C4	14.86	1.43	1.34
2	B	1	DT	N1-C2	12.13	1.47	1.38
2	B	1	DT	C4-C5	11.24	1.55	1.45
1	A	1	DA	N1-C2	9.40	1.42	1.34
1	A	2	DA	C5-C4	9.23	1.45	1.38
2	B	1	DT	N1-C6	8.53	1.44	1.38
1	A	1	DA	C6-N1	-7.79	1.30	1.35
1	A	2	DA	N3-C4	-6.58	1.30	1.34
1	A	2	DA	N7-C5	-6.46	1.35	1.39
1	A	1	DA	N9-C8	-6.32	1.32	1.37
1	A	2	DA	C8-N7	5.80	1.35	1.31
2	B	1	DT	N3-C4	5.20	1.42	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	DG	O4'-C1'-N9	10.17	115.12	108.00
1	A	1	DA	C4-C5-N7	-10.14	105.63	110.70
2	B	5	DT	O4'-C1'-N1	-9.90	101.07	108.00
1	A	1	DA	N9-C4-C5	9.52	109.61	105.80
1	A	13	DA	P-O3'-C3'	6.83	127.89	119.70
2	B	1	DT	C4-C5-C7	6.74	123.04	119.00
1	A	2	DA	C8-N9-C4	-6.71	103.11	105.80
1	A	1	DA	C8-N9-C4	-6.62	103.15	105.80
3	C	438	ARG	NE-CZ-NH2	-6.40	117.10	120.30
2	B	1	DT	C6-C5-C7	-6.40	119.06	122.90
2	B	14	DG	P-O3'-C3'	6.37	127.34	119.70
3	C	326	LEU	CA-CB-CG	6.31	129.81	115.30
2	B	5	DT	C4-C5-C7	6.07	122.64	119.00
1	A	1	DA	C4-C5-C6	5.98	119.99	117.00
3	C	438	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	2	DA	N9-C4-C5	5.59	108.03	105.80
1	A	1	DA	C2-N3-C4	-5.40	107.90	110.60
2	B	14	DG	C8-N9-C4	-5.24	104.31	106.40
1	A	2	DA	C4-C5-N7	-5.22	108.09	110.70
1	A	2	DA	N1-C2-N3	5.19	131.90	129.30
3	C	91	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	B	5	DT	C6-C5-C7	-5.07	119.86	122.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	15	DA	Sidechain
3	C	218	ARG	Peptide
3	C	435	SER	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	298	0	172	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	311	0	171	3	0
3	C	3290	0	3278	68	0
4	C	48	0	72	13	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	128	0	0	0	0
All	All	4081	0	3693	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:DT:O5'	2:B:1:DT:C5'	1.80	1.29
3:C:194:SER:HB2	3:C:195:LYS:HA	1.31	1.06
3:C:230:HIS:HE1	4:C:8:EDO:H12	1.11	1.06
3:C:464:THR:HG22	3:C:466:LEU:H	1.28	0.97
3:C:230:HIS:CE1	4:C:8:EDO:H12	2.02	0.94
3:C:433:ASP:O	3:C:436:ALA:HB3	1.70	0.91
3:C:182:PHE:HA	4:C:6:EDO:H21	1.54	0.88
3:C:227:ARG:HH11	3:C:227:ARG:HG2	1.43	0.82
3:C:319:THR:HG21	3:C:322:MET:HB2	1.62	0.82
3:C:194:SER:HB2	3:C:195:LYS:CA	2.11	0.81
3:C:194:SER:CB	3:C:195:LYS:HA	2.09	0.80
3:C:230:HIS:HD2	3:C:232:GLU:OE2	1.65	0.79
3:C:464:THR:CG2	3:C:466:LEU:H	1.94	0.79
3:C:195:LYS:HB2	3:C:196:LYS:HA	1.68	0.74
3:C:288:LEU:HG	3:C:314:PHE:HB3	1.69	0.74
3:C:405:THR:HG22	3:C:406:PRO:HD2	1.75	0.68
3:C:86:TYR:O	3:C:89:GLU:HB2	1.94	0.68
3:C:126:CYS:HB3	4:C:5:EDO:H21	1.77	0.67
3:C:319:THR:CG2	3:C:322:MET:H	2.09	0.65
2:B:8:DG:N7	3:C:91:ARG:NH2	2.44	0.65
3:C:457:ASN:HB2	4:C:3:EDO:O2	1.97	0.65
1:A:1:DA:H2''	1:A:2:DA:C8	2.33	0.64
3:C:364:TYR:CZ	4:C:6:EDO:H22	2.33	0.63
3:C:56:ARG:HH22	3:C:409:ARG:HH11	1.48	0.61
3:C:227:ARG:NH1	3:C:227:ARG:HG2	2.14	0.61
3:C:241:GLN:HG3	4:C:2:EDO:O2	2.02	0.60
1:A:4:DC:H2''	1:A:5:DT:O5'	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:LYS:CB	3:C:196:LYS:HA	2.32	0.59
3:C:464:THR:HG22	3:C:466:LEU:N	2.11	0.59
3:C:456:ARG:HD2	3:C:458:ASP:OD1	2.03	0.58
3:C:195:LYS:H	3:C:195:LYS:HZ3	1.52	0.57
3:C:98:CYS:SG	3:C:100:TYR:CE1	2.88	0.56
3:C:241:GLN:HA	3:C:241:GLN:HE21	1.71	0.55
1:A:4:DC:H2'	1:A:5:DT:H72	1.87	0.55
3:C:319:THR:CG2	3:C:322:MET:HB2	2.35	0.55
3:C:122:GLU:HB3	3:C:175:ASN:HB3	1.87	0.55
3:C:316:LEU:O	3:C:319:THR:HB	2.07	0.54
3:C:183:LEU:H	4:C:6:EDO:C2	2.21	0.54
3:C:405:THR:HG22	3:C:406:PRO:CD	2.38	0.53
3:C:167:LEU:HB2	3:C:184:SER:HB3	1.91	0.52
3:C:195:LYS:HB2	3:C:196:LYS:CA	2.37	0.52
3:C:56:ARG:HH22	3:C:409:ARG:NH1	2.09	0.51
3:C:452:VAL:O	3:C:464:THR:HB	2.09	0.51
3:C:78:HIS:HD2	3:C:79:ALA:O	1.94	0.51
3:C:112:GLN:HG2	4:C:9:EDO:H22	1.93	0.50
3:C:319:THR:HG23	3:C:322:MET:H	1.77	0.50
3:C:133:ASN:ND2	3:C:134:SER:O	2.45	0.49
2:B:14:DG:H2"	2:B:15:DA:OP2	2.12	0.49
3:C:140:GLN:HG3	4:C:5:EDO:H22	1.95	0.49
3:C:230:HIS:CD2	3:C:232:GLU:OE2	2.55	0.48
3:C:136:GLN:C	3:C:138:MET:H	2.15	0.48
1:A:10:DC:H2"	1:A:11:DA:C8	2.49	0.48
3:C:135:ASP:C	3:C:137:GLU:H	2.17	0.48
3:C:310:HIS:CD2	3:C:311:LYS:O	2.67	0.47
3:C:341:LYS:HB2	3:C:342:GLU:HG2	1.96	0.47
3:C:75:LEU:HD23	3:C:363:GLU:HG3	1.97	0.47
3:C:175:ASN:ND2	3:C:177:ASP:H	2.13	0.47
3:C:219:LEU:HB2	3:C:222:GLN:HG2	1.98	0.46
1:A:8:DC:H41	4:C:7:EDO:C2	2.29	0.46
3:C:195:LYS:HG2	3:C:292:LYS:NZ	2.31	0.45
3:C:381:PRO:HA	3:C:403:ASN:HB2	1.96	0.45
3:C:310:HIS:HD2	3:C:311:LYS:O	1.99	0.45
3:C:138:MET:HG2	4:C:10:EDO:H22	1.99	0.45
3:C:196:LYS:O	3:C:197:LYS:HB2	2.17	0.45
3:C:195:LYS:HD2	3:C:196:LYS:HG3	2.00	0.44
3:C:219:LEU:HG	3:C:222:GLN:HE21	1.83	0.43
3:C:91:ARG:NH1	4:C:7:EDO:H21	2.33	0.43
3:C:75:LEU:CD2	3:C:363:GLU:HG3	2.47	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:DA:H1'	1:A:2:DA:H5'	2.00	0.43
3:C:101:LEU:O	3:C:147:ASN:OD1	2.36	0.42
3:C:195:LYS:HE2	3:C:195:LYS:O	2.19	0.42
3:C:447:PRO:HA	3:C:470:TYR:O	2.19	0.42
3:C:250:LEU:HD21	3:C:272:GLN:HB3	2.02	0.42
3:C:321:ARG:NH1	3:C:336:ALA:O	2.49	0.42
3:C:195:LYS:HZ3	3:C:195:LYS:N	2.19	0.41
3:C:73:THR:OG1	3:C:365:THR:HB	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	408/427 (96%)	387 (95%)	15 (4%)	6 (2%)	10 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	194	SER
3	C	253	ASP
3	C	436	ALA
3	C	390	GLY
3	C	252	ASP
3	C	339	CYS

### 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
3	C	365/375 (97%)	331 (91%)	34 (9%)	9 8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	55	LYS
3	C	66	LEU
3	C	121	GLN
3	C	133	ASN
3	C	134	SER
3	C	135	ASP
3	C	146	LYS
3	C	175	ASN
3	C	195	LYS
3	C	196	LYS
3	C	201	LYS
3	C	202	ASN
3	C	218	ARG
3	C	222	GLN
3	C	225	SER
3	C	229	LEU
3	C	241	GLN
3	C	250	LEU
3	C	254	ASP
3	C	288	LEU
3	C	301	ASP
3	C	319	THR
3	C	326	LEU
3	C	342	GLU
3	C	365	THR
3	C	374	LEU
3	C	384	GLU
3	C	386	LEU
3	C	388	LEU
3	C	394	VAL
3	C	460	VAL
3	C	463	SER
3	C	464	THR
3	C	473	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	64	ASN
3	C	72	GLN
3	C	78	HIS
3	C	83	GLN
3	C	140	GLN
3	C	164	HIS
3	C	175	ASN
3	C	222	GLN
3	C	230	HIS
3	C	241	GLN
3	C	310	HIS
3	C	389	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 carbohydrates 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	C	12	-	3,3,3	0.63	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	5	-	3,3,3	0.34	0	2,2,2	0.74	0
4	EDO	C	8	-	3,3,3	0.56	0	2,2,2	0.10	0
4	EDO	C	1	-	3,3,3	0.54	0	2,2,2	0.38	0
4	EDO	C	6	-	3,3,3	0.37	0	2,2,2	0.57	0
4	EDO	C	10	-	3,3,3	0.50	0	2,2,2	0.22	0
4	EDO	C	7	-	3,3,3	0.40	0	2,2,2	0.49	0
4	EDO	C	2	-	3,3,3	0.62	0	2,2,2	0.22	0
4	EDO	C	9	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	C	3	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	C	11	-	3,3,3	0.35	0	2,2,2	0.56	0
4	EDO	C	4	-	3,3,3	0.59	0	2,2,2	0.08	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	C	12	-	-	0/1/1/1	-
4	EDO	C	5	-	-	1/1/1/1	-
4	EDO	C	8	-	-	1/1/1/1	-
4	EDO	C	1	-	-	1/1/1/1	-
4	EDO	C	6	-	-	1/1/1/1	-
4	EDO	C	10	-	-	1/1/1/1	-
4	EDO	C	7	-	-	0/1/1/1	-
4	EDO	C	2	-	-	1/1/1/1	-
4	EDO	C	9	-	-	1/1/1/1	-
4	EDO	C	3	-	-	1/1/1/1	-
4	EDO	C	11	-	-	1/1/1/1	-
4	EDO	C	4	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	6	EDO	O1-C1-C2-O2
4	C	10	EDO	O1-C1-C2-O2
4	C	9	EDO	O1-C1-C2-O2
4	C	4	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	C	5	EDO	O1-C1-C2-O2
4	C	8	EDO	O1-C1-C2-O2
4	C	3	EDO	O1-C1-C2-O2
4	C	11	EDO	O1-C1-C2-O2
4	C	1	EDO	O1-C1-C2-O2
4	C	2	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5	EDO	2	0
4	C	8	EDO	2	0
4	C	6	EDO	3	0
4	C	10	EDO	1	0
4	C	7	EDO	2	0
4	C	2	EDO	1	0
4	C	9	EDO	1	0
4	C	3	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	15/15 (100%)	0.10	1 (6%) 17 16	37, 44, 66, 67	0
2	B	15/15 (100%)	0.36	0 100 100	33, 44, 55, 58	0
3	C	414/427 (96%)	0.71	60 (14%) 2 2	14, 31, 47, 59	1 (0%)
All	All	444/457 (97%)	0.68	61 (13%) 3 2	14, 32, 49, 67	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	391	GLY	8.0
3	C	135	ASP	7.2
3	C	134	SER	7.1
3	C	390	GLY	6.6
3	C	263	VAL	6.3
3	C	133	ASN	6.2
3	C	254	ASP	6.0
3	C	255	GLU	5.3
3	C	219	LEU	5.3
3	C	393	ASP	5.2
3	C	252	ASP	4.6
3	C	357	ILE	4.5
3	C	136	GLN	4.3
3	C	94	CYS	4.3
3	C	356	ILE	4.2
3	C	309	LEU	4.1
3	C	262	THR	4.0
3	C	394	VAL	4.0
3	C	338	PRO	3.8
3	C	359	THR	3.7
3	C	355	THR	3.6
3	C	341	LYS	3.4
3	C	132	GLY	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	C	196	LYS	3.3
3	C	264	ARG	3.2
3	C	265	ASP	3.1
3	C	343	GLN	3.1
3	C	214	ALA	3.0
3	C	340	PRO	3.0
3	C	301	ASP	3.0
3	C	201	LYS	2.9
3	C	224	VAL	2.9
3	C	392	GLY	2.9
3	C	216	PHE	2.9
3	C	220	ARG	2.7
3	C	215	LEU	2.7
3	C	358	SER	2.7
3	C	202	ASN	2.6
3	C	454	LEU	2.6
3	C	460	VAL	2.6
3	C	253	ASP	2.6
3	C	225	SER	2.4
3	C	384	GLU	2.4
3	C	88	ASN	2.4
3	C	95	PRO	2.4
3	C	197	LYS	2.4
3	C	203	ALA	2.4
3	C	462	TYR	2.4
3	C	223	THR	2.4
3	C	474	PRO	2.4
3	C	455	VAL	2.4
3	C	213	VAL	2.3
3	C	354	TRP	2.3
3	C	229	LEU	2.2
3	C	278	CYS	2.1
1	A	3	DT	2.1
3	C	243	TRP	2.1
3	C	311	LYS	2.1
3	C	453	THR	2.1
3	C	200	LEU	2.0
3	C	228	TYR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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	C	8	4/4	0.68	0.38	71,71,71,72	0
4	EDO	C	12	4/4	0.73	0.19	61,63,63,64	0
4	EDO	C	10	4/4	0.74	0.27	62,62,63,65	0
4	EDO	C	2	4/4	0.76	0.24	63,64,64,65	0
4	EDO	C	9	4/4	0.78	0.49	69,69,70,70	0
4	EDO	C	1	4/4	0.80	0.20	50,51,52,53	0
4	EDO	C	3	4/4	0.80	0.24	54,56,57,57	0
4	EDO	C	4	4/4	0.81	0.34	50,53,54,56	0
4	EDO	C	11	4/4	0.87	0.18	35,41,43,46	0
4	EDO	C	7	4/4	0.93	0.36	43,44,45,45	0
4	EDO	C	6	4/4	0.93	0.28	37,39,40,40	0
4	EDO	C	5	4/4	0.94	0.29	41,47,48,49	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.