



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:50 PM UTC

PDB ID : 8EM1 / pdb\_00008em1  
Title : Type IIS Restriction Endonuclease PqCI, DNA Unbound  
Authors : Kennedy, M.A.; Stoddard, B.L.  
Deposited on : 2022-09-26  
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

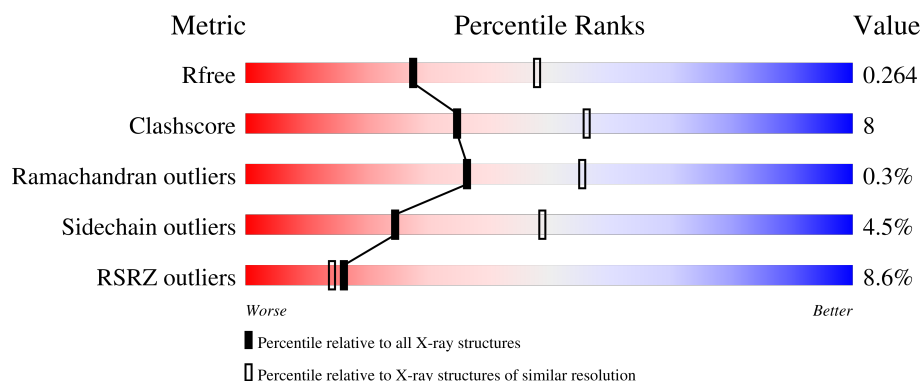
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	510	<div> <div>8%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>
1	B	510	<div> <div>9%</div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>

## 2 Entry composition [i](#)

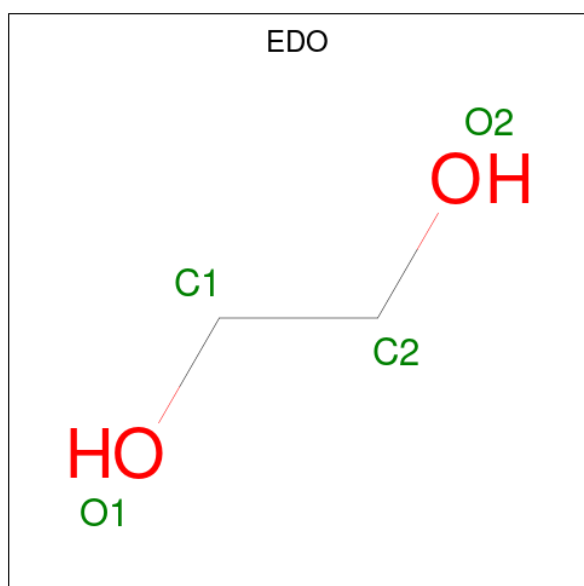
There are 3 unique types of molecules in this entry. The entry contains 7353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PaqCI, DNA Unbound.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3696	2363	640	684	9			
1	B	482	Total	C	N	O	S	0	0	0
			3580	2291	624	655	10			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0
3	B	31	Total 31	O 31	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.62Å 136.62Å 106.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.58 – 2.50 49.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.58-2.50) 97.7 (49.58-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.89 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.20	Depositor
R, $R_{free}$	0.211 , 0.267 0.208 , 0.264	Depositor DCC
$R_{free}$ test set	2000 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtrriage
Anisotropy	0.431	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 35.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7364e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/3792	0.61	1/5175 (0.0%)
1	B	0.39	0/3673	0.57	0/5017
All	All	0.40	0/7465	0.59	1/10192 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	223	ARG	CA-CB-CG	5.35	124.80	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	ARG	Sidechain

### 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	A	3696	0	3467	48	0
1	B	3580	0	3326	63	0
2	B	8	0	12	1	0
3	A	38	0	0	3	0
3	B	31	0	0	2	0
All	All	7353	0	6805	106	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:MET:HE2	1:A:312:ILE:HD13	1.61	0.81
1:A:75:LYS:HB2	1:A:106:ILE:HG22	1.70	0.71
1:B:293:GLU:HB2	1:B:300:LYS:HD3	1.73	0.71
1:A:356:ARG:NH1	3:A:602:HOH:O	2.25	0.68
1:B:359:GLU:HG2	1:B:363:LEU:O	1.93	0.68
1:A:499:TRP:O	1:A:503:VAL:HG23	1.96	0.66
1:B:49:GLY:H	1:B:97:LYS:HE3	1.62	0.65
1:B:76:ARG:HG3	1:B:79:GLU:OE2	1.98	0.64
1:A:293:GLU:HG3	1:A:300:LYS:HE3	1.80	0.64
1:A:81:ILE:HG22	1:B:50:TRP:CZ2	2.33	0.64
1:B:75:LYS:HB2	1:B:106:ILE:HG22	1.79	0.62
1:B:211:PRO:O	1:B:231:ILE:HD11	1.99	0.62
1:B:408:ASN:HB2	1:B:499:TRP:HZ2	1.63	0.62
1:B:394:LEU:HD13	1:B:477:LEU:HD21	1.80	0.62
1:B:235:THR:HG22	1:B:251:TRP:HD1	1.65	0.61
1:A:354:GLN:NE2	3:A:605:HOH:O	2.33	0.60
1:B:133:ILE:O	1:B:157:ARG:NH1	2.33	0.60
1:B:247:TRP:CD2	1:B:345:ARG:HG3	2.37	0.60
1:B:198:VAL:HG12	1:B:246:VAL:HG23	1.83	0.60
1:B:443:GLN:O	1:B:447:THR:HG23	2.01	0.59
1:B:447:THR:HA	1:B:450:THR:HG22	1.84	0.57
1:B:194:ARG:NH2	3:B:703:HOH:O	2.32	0.56
1:B:221:ILE:HG21	1:B:230:PRO:HA	1.87	0.56
1:B:40:SER:OG	1:B:457:ARG:HG3	2.06	0.55
1:A:263:PRO:HB2	1:A:264:TRP:CE3	2.42	0.55
1:B:39:ALA:HA	1:B:58:SER:O	2.07	0.55
1:A:446:GLU:O	1:A:450:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ASP:HB2	1:A:506:LEU:HD22	1.88	0.54
1:A:73:GLU:OE1	3:A:601:HOH:O	2.19	0.53
1:B:220:ALA:O	1:B:224:LEU:HD12	2.09	0.53
1:B:307:LEU:HD12	1:B:308:ASN:N	2.23	0.53
1:A:214:ARG:NH2	1:A:262:THR:OG1	2.41	0.53
1:A:438:TYR:CZ	1:A:442:LEU:HD11	2.44	0.52
1:A:205:ASP:OD1	1:A:209:PRO:HD3	2.10	0.52
1:B:392:ALA:O	1:B:396:GLN:HG3	2.10	0.52
1:A:81:ILE:HD11	1:A:110:TYR:HB2	1.93	0.51
1:B:221:ILE:HG23	1:B:233:TYR:CD2	2.46	0.50
1:B:449:LEU:HD23	1:B:453:LEU:HD22	1.93	0.50
1:B:295:ARG:O	1:B:300:LYS:HG3	2.11	0.50
1:A:392:ALA:HA	1:A:505:ALA:HB1	1.94	0.50
1:A:81:ILE:HG22	1:B:50:TRP:CH2	2.48	0.49
1:A:115:THR:HB	1:A:118:GLU:OE1	2.13	0.49
1:B:52:LYS:NZ	3:B:707:HOH:O	2.45	0.49
1:B:410:LEU:HD22	1:B:448:LYS:HG2	1.95	0.49
1:A:435:GLU:CD	1:A:488:ARG:HH22	2.21	0.49
1:A:424:LYS:HE3	1:A:436:GLU:HB3	1.95	0.49
1:B:110:TYR:HD1	1:B:116:PRO:HG3	1.79	0.48
1:B:435:GLU:OE2	1:B:488:ARG:NH2	2.43	0.47
1:A:414:LYS:HD3	1:A:422:TYR:OH	2.14	0.47
1:A:92:HIS:HD2	1:B:127:ILE:HG22	1.79	0.47
1:A:249:PHE:O	1:A:253:GLU:HB2	2.14	0.47
1:A:11:PHE:CD2	1:A:148:PRO:HG2	2.50	0.47
1:A:313:SER:HB3	1:A:316:GLN:HG3	1.97	0.47
1:A:44:GLU:OE1	1:A:99:TYR:OH	2.17	0.47
1:B:235:THR:HG22	1:B:251:TRP:CD1	2.48	0.46
1:B:292:TRP:CZ2	1:B:337:VAL:HA	2.49	0.46
1:A:403:PHE:CZ	1:A:407:ILE:HD11	2.50	0.46
1:B:60:LEU:HD23	1:B:67:GLN:HB3	1.97	0.46
1:A:222:GLY:O	1:A:226:PRO:HA	2.16	0.46
1:B:15:GLU:OE2	1:B:15:GLU:HA	2.16	0.45
1:B:392:ALA:HA	1:B:505:ALA:HB1	1.99	0.45
1:B:438:TYR:CZ	1:B:442:LEU:HD11	2.51	0.45
1:B:30:ALA:O	1:B:33:LEU:HD12	2.17	0.45
1:B:446:GLU:O	1:B:450:THR:HG22	2.17	0.45
1:B:304:ALA:O	1:B:307:LEU:HG	2.17	0.44
1:A:106:ILE:HD11	1:A:117:ALA:HB2	2.00	0.44
1:A:306:MET:CE	1:A:312:ILE:HD13	2.40	0.44
1:B:229:ASP:OD2	1:B:232:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PRO:HA	1:A:110:TYR:CE2	2.53	0.44
1:B:249:PHE:O	1:B:253:GLU:HB2	2.17	0.44
1:A:43:TYR:CE2	1:A:180:VAL:HA	2.53	0.43
1:A:106:ILE:HD11	1:A:117:ALA:CA	2.48	0.43
1:B:115:THR:HB	1:B:118:GLU:HB2	2.00	0.43
1:A:410:LEU:HD22	1:A:448:LYS:HG2	2.00	0.43
1:B:49:GLY:N	1:B:97:LYS:HE3	2.32	0.43
1:A:50:TRP:HZ3	1:B:119:TYR:CE2	2.37	0.43
1:A:441:TYR:CZ	1:A:445:LEU:HD11	2.54	0.42
1:B:95:LEU:HD11	1:B:133:ILE:HG13	2.01	0.42
1:B:447:THR:HA	1:B:450:THR:CG2	2.48	0.42
1:B:239:ASP:CG	1:B:244:THR:HG21	2.44	0.42
1:A:67:GLN:HB3	1:A:170:PRO:O	2.18	0.42
1:B:256:ALA:HB1	1:B:261:LEU:HD21	2.02	0.42
1:B:356:ARG:HH11	2:B:602:EDO:H21	1.84	0.42
1:A:234:ILE:HD12	1:A:234:ILE:HA	1.87	0.42
1:B:177:THR:OG1	1:B:179:TRP:O	2.36	0.42
1:A:53:ALA:HA	1:A:94:TYR:OH	2.20	0.42
1:B:260:VAL:HG21	1:B:278:THR:HG22	2.00	0.42
1:A:495:ILE:HA	1:A:496:PRO:HD3	1.94	0.42
1:A:53:ALA:HA	1:A:94:TYR:CZ	2.55	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.93	0.41
1:B:50:TRP:CD1	1:B:50:TRP:C	2.92	0.41
1:B:243:LEU:O	1:B:246:VAL:HG12	2.21	0.41
1:B:108:GLY:HA2	1:B:137:SER:HB2	2.02	0.41
1:B:245:LYS:O	1:B:249:PHE:HD1	2.03	0.41
1:A:15:GLU:OE2	1:A:150:ALA:HA	2.20	0.41
1:A:82:HIS:NE2	1:B:86:THR:HG21	2.36	0.41
1:B:106:ILE:O	1:B:137:SER:HA	2.20	0.41
1:A:81:ILE:HD12	1:A:81:ILE:HG23	1.53	0.41
1:B:51:PRO:HD2	1:B:97:LYS:HD2	2.01	0.41
1:B:384:ARG:HA	1:B:384:ARG:HD2	1.88	0.41
1:B:435:GLU:CD	1:B:488:ARG:NH2	2.79	0.41
1:A:37:ILE:HA	1:A:60:LEU:O	2.21	0.40
1:B:359:GLU:HG2	1:B:359:GLU:H	1.76	0.40
1:A:209:PRO:HB2	1:A:249:PHE:CE2	2.57	0.40
1:A:142:ASP:OD1	1:A:144:THR:HB	2.21	0.40
1:B:377:ARG:HB2	1:B:378:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/510 (95%)	469 (97%)	12 (2%)	2 (0%)	30	49
1	B	472/510 (92%)	452 (96%)	19 (4%)	1 (0%)	43	63
All	All	955/1020 (94%)	921 (96%)	31 (3%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	ASP
1	B	185	GLY
1	A	170	PRO

### 5.3.2 Protein sidechains

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	A	347/408 (85%)	330 (95%)	17 (5%)	22	45
1	B	327/408 (80%)	314 (96%)	13 (4%)	28	54
All	All	674/816 (83%)	644 (96%)	30 (4%)	24	49

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	118	GLU
1	A	144	THR

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Mol	Chain	Res	Type
1	A	180	VAL
1	A	212	THR
1	A	229	ASP
1	A	234	ILE
1	A	284	ASP
1	A	313	SER
1	A	326	SER
1	A	358	ILE
1	A	377	ARG
1	A	413	ARG
1	A	450	THR
1	A	459	VAL
1	A	500	GLU
1	A	508	VAL
1	B	40	SER
1	B	64	THR
1	B	97	LYS
1	B	106	ILE
1	B	143	THR
1	B	221	ILE
1	B	244	THR
1	B	361	ASP
1	B	370	ARG
1	B	432	VAL
1	B	447	THR
1	B	484	VAL
1	B	485	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	GLN
1	A	405	HIS
1	B	167	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	B	601	-	3,3,3	0.57	0	2,2,2	0.17	0
2	EDO	B	602	-	3,3,3	0.51	0	2,2,2	0.30	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
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	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	491/510 (96%)	0.46	39 (7%)	18 16	33, 50, 89, 125	0
1	B	482/510 (94%)	0.62	45 (9%)	14 12	33, 54, 97, 120	0
All	All	973/1020 (95%)	0.54	84 (8%)	16 14	33, 52, 96, 125	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	TYR	5.5
1	B	204	ALA	5.1
1	A	208	ALA	5.1
1	B	4	ASP	5.0
1	B	427	PRO	4.8
1	B	467	VAL	4.6
1	B	227	GLY	3.9
1	B	273	ALA	3.8
1	B	296	VAL	3.8
1	B	186	SER	3.8
1	A	2	PRO	3.6
1	B	184	GLU	3.6
1	B	287	ASP	3.6
1	B	302	THR	3.5
1	A	3	TYR	3.5
1	B	183	ARG	3.4
1	B	272	SER	3.3
1	A	162	ASP	3.3
1	A	35	ALA	3.3
1	B	205	ASP	3.2
1	B	312	ILE	3.2
1	B	265	LYS	3.1
1	B	298	SER	3.1
1	A	82	HIS	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	182	MET	3.0
1	A	170	PRO	3.0
1	A	168	LEU	3.0
1	A	62	GLY	3.0
1	A	240	ASN	3.0
1	A	459	VAL	2.9
1	A	239	ASP	2.8
1	A	112	SER	2.8
1	A	163	ALA	2.8
1	A	452	GLU	2.8
1	A	209	PRO	2.7
1	B	297	ASN	2.7
1	B	200	LYS	2.7
1	A	29	ASP	2.6
1	A	32	SER	2.6
1	B	203	SER	2.6
1	A	37	ILE	2.6
1	B	459	VAL	2.5
1	A	64	THR	2.5
1	B	307	LEU	2.5
1	A	22	ALA	2.5
1	B	218	VAL	2.5
1	A	65	SER	2.5
1	A	172	ASN	2.4
1	A	210	ARG	2.4
1	A	439	TRP	2.4
1	B	238	ALA	2.4
1	A	69	ALA	2.4
1	B	51	PRO	2.4
1	A	186	SER	2.4
1	B	240	ASN	2.3
1	A	46	SER	2.3
1	B	509	ASP	2.3
1	B	49	GLY	2.3
1	B	29	ASP	2.3
1	B	316	GLN	2.2
1	A	33	LEU	2.2
1	B	300	LYS	2.2
1	B	510	LEU	2.2
1	A	503	VAL	2.2
1	B	308	ASN	2.2
1	A	5	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	163	ALA	2.2
1	A	469	THR	2.2
1	A	184	GLU	2.2
1	A	66	THR	2.1
1	B	286	THR	2.1
1	B	333	ASP	2.1
1	B	318	TRP	2.1
1	B	5	HIS	2.1
1	A	63	GLY	2.1
1	B	239	ASP	2.1
1	A	223	ARG	2.0
1	B	31	ALA	2.0
1	B	217	LEU	2.0
1	A	47	ALA	2.0
1	A	238	ALA	2.0
1	B	304	ALA	2.0
1	B	164	GLY	2.0
1	B	32	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	EDO	B	601	4/4	0.81	0.13	55,58,59,61	0
2	EDO	B	602	4/4	0.85	0.27	53,53,57,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.