



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 PM UTC

PDB ID : 7JWI / pdb_00007jwi
Title : Crystal structure of B17.R2 TCR in complex with H2D-b-NP366
Authors : Farenc, C.; Rossjohn, J.
Deposited on : 2020-08-25
Resolution : 3.02 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 ⓘ 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 ⓘ](#)) 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

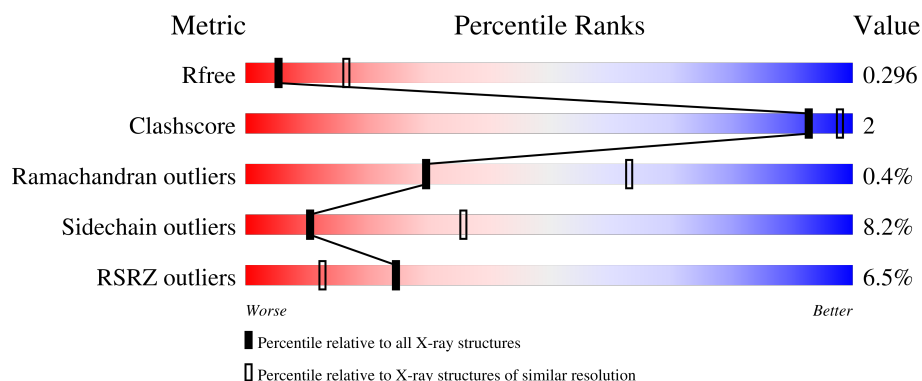
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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 $\leq 5\%$. 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	362	6% 65% 10% 23%
2	B	100	2% 84% 12% •
3	C	9	89% 11%
4	D	207	8% 91% 7% •
5	E	243	6% 88% 11% •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6864 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	5	0
			2317	1460	415	433	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			69	38	11	18	2			

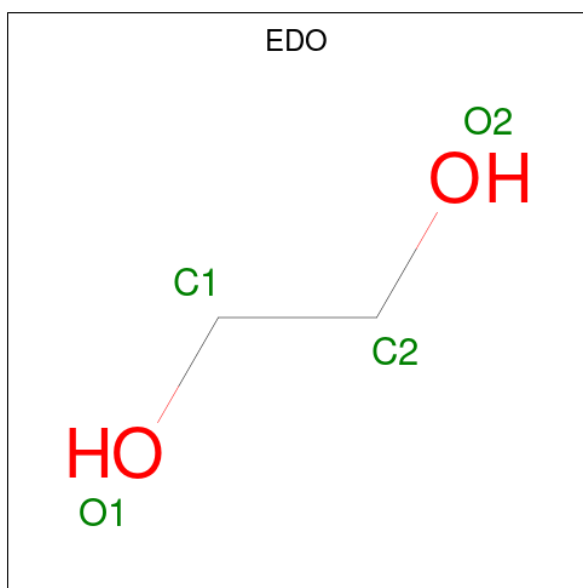
- Molecule 4 is a protein called B17.R2 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	203	Total	C	N	O	S	0	3	0
			1615	1011	265	329	10			

- Molecule 5 is a protein called B17.R2 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1940	1231	338	362	9			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

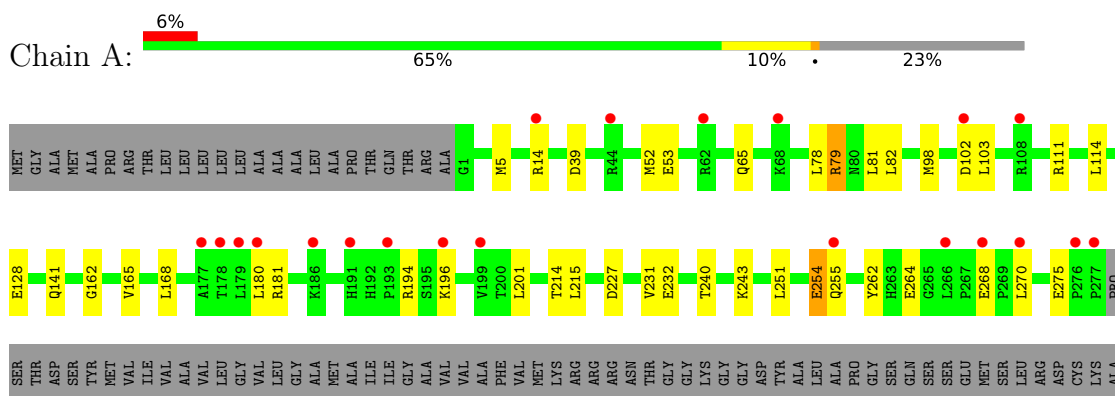
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	32	Total	O	0	0
			32	32		
7	B	14	Total	O	0	0
			14	14		
7	C	1	Total	O	0	0
			1	1		
7	D	21	Total	O	0	0
			21	21		
7	E	22	Total	O	0	0
			22	22		

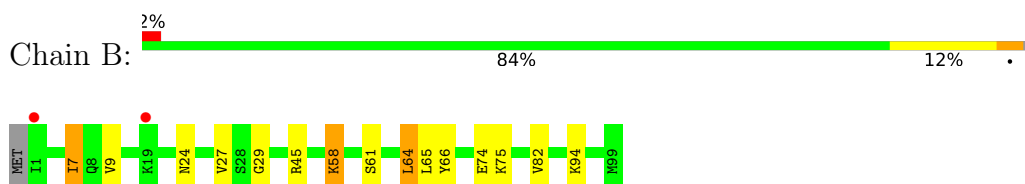
3 Residue-property plots [i](#)

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.

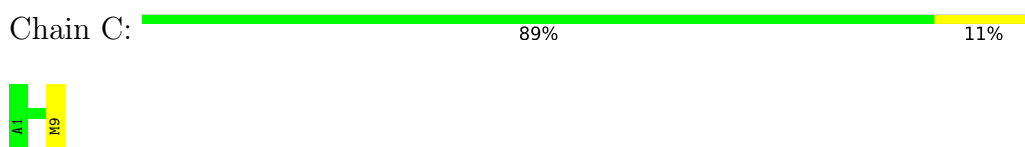
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



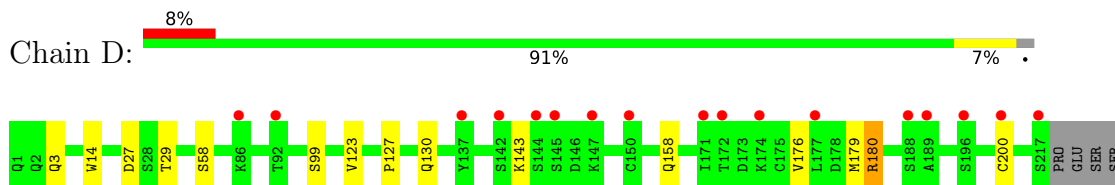
- Molecule 2: Beta-2-microglobulin



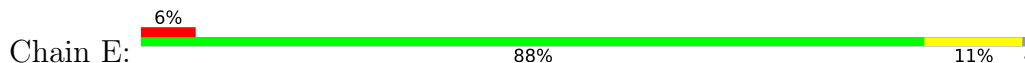
- Molecule 3: Nucleoprotein

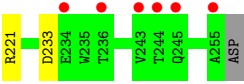
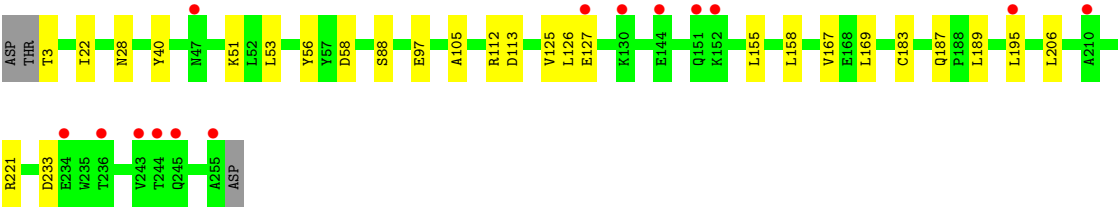


- Molecule 4: B17.R2 TCR alpha chain



- Molecule 5: B17.R2 TCR beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.67Å 141.00Å 217.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.27 – 3.02 44.27 – 3.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.27-3.02) 99.9 (44.27-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.239 , 0.281 0.250 , 0.296	Depositor DCC
R_{free} test set	1412 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6864	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.68	0/2385	1.13	4/3240 (0.1%)
2	B	0.69	0/852	1.06	0/1152
3	C	0.65	0/68	1.06	0/88
4	D	0.73	0/1654	1.05	2/2245 (0.1%)
5	E	0.69	0/1994	1.05	2/2711 (0.1%)
All	All	0.69	0/6953	1.08	8/9436 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	162	GLY	N-CA-C	6.54	116.16	110.21
5	E	113	ASP	CA-C-N	5.68	129.77	121.31
5	E	113	ASP	C-N-CA	5.68	129.77	121.31
4	D	179	MET	CA-C-N	5.56	128.00	120.38
4	D	179	MET	C-N-CA	5.56	128.00	120.38
1	A	102	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	162	GLY	CA-C-N	5.16	127.45	120.38
1	A	162	GLY	C-N-CA	5.16	127.45	120.38

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	A	2317	0	2193	9	0
2	B	829	0	794	5	0
3	C	69	0	61	0	0
4	D	1615	0	1503	4	0
5	E	1940	0	1868	3	0
6	E	4	0	6	0	0
7	A	32	0	0	0	0
7	B	14	0	0	0	0
7	C	1	0	0	0	0
7	D	21	0	0	0	0
7	E	22	0	0	0	0
All	All	6864	0	6425	20	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 2.

All (20) 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:7:ILE:HG12	2:B:82:VAL:HG21	1.77	0.66
1:A:79:ARG:HA	1:A:82:LEU:HD12	1.91	0.53
4:D:14:TRP:HZ2	4:D:158:GLN:HG3	1.75	0.52
1:A:98:MET:HE1	2:B:58:LYS:HG3	1.93	0.51
1:A:215:LEU:HD13	1:A:243:LYS:HD3	1.95	0.49
5:E:155:LEU:HD13	5:E:206:LEU:HD23	1.95	0.48
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.95	0.48
1:A:103:LEU:HD11	1:A:165:VAL:HG13	1.96	0.47
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.96	0.47
5:E:40:TYR:HB2	5:E:105:ALA:HB3	1.96	0.46
1:A:103:LEU:HD13	1:A:168:LEU:HD23	1.98	0.46
4:D:180:ARG:H	4:D:180:ARG:HD3	1.81	0.46
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.99	0.45
5:E:22:ILE:HD12	5:E:88:SER:HB3	1.99	0.44
4:D:127:PRO:HG3	4:D:176:VAL:HG11	2.00	0.43
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.00	0.43
1:A:214:THR:HB	1:A:262:TYR:HB2	2.00	0.42
1:A:111:ARG:HG3	1:A:128:GLU:HG3	2.01	0.42
4:D:27:ASP:HB3	4:D:29:THR:HG22	2.02	0.42
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.84	0.41

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	280/362 (77%)	269 (96%)	11 (4%)	0	100	100
2	B	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	204/207 (99%)	195 (96%)	7 (3%)	2 (1%)	12	43
5	E	238/243 (98%)	226 (95%)	11 (5%)	1 (0%)	30	63
All	All	826/921 (90%)	792 (96%)	31 (4%)	3 (0%)	30	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	58	ASP
4	D	99	SER
4	D	143	LYS

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	240/296 (81%)	214 (89%)	26 (11%)	6	25
2	B	94/95 (99%)	85 (90%)	9 (10%)	8	29
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	19
4	D	186/188 (99%)	180 (97%)	6 (3%)	34	66
5	E	212/215 (99%)	193 (91%)	19 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	740/802 (92%)	679 (92%)	61 (8%)	10	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14[A]	ARG
1	A	14[B]	ARG
1	A	39	ASP
1	A	52	MET
1	A	53	GLU
1	A	65	GLN
1	A	78	LEU
1	A	79	ARG
1	A	81	LEU
1	A	114	LEU
1	A	141	GLN
1	A	180	LEU
1	A	181	ARG
1	A	194	ARG
1	A	196	LYS
1	A	227	ASP
1	A	231	VAL
1	A	232	GLU
1	A	240	THR
1	A	251	LEU
1	A	254	GLU
1	A	255	GLN
1	A	264	GLU
1	A	268	GLU
1	A	270	LEU
1	A	275	GLU
2	B	7	ILE
2	B	9	VAL
2	B	27	VAL
2	B	45	ARG
2	B	58	LYS
2	B	64	LEU
2	B	74	GLU
2	B	75	LYS
2	B	94	LYS
3	C	9	MET
4	D	3	GLN

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Mol	Chain	Res	Type
4	D	58	SER
4	D	123	VAL
4	D	130	GLN
4	D	180	ARG
4	D	200	CYS
5	E	3	THR
5	E	28	ASN
5	E	51	LYS
5	E	53	LEU
5	E	56	TYR
5	E	97	GLU
5	E	112	ARG
5	E	125	VAL
5	E	126	LEU
5	E	127	GLU
5	E	158	LEU
5	E	167	VAL
5	E	169	LEU
5	E	183	CYS
5	E	187	GLN
5	E	189	LEU
5	E	195	LEU
5	E	221	ARG
5	E	233	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	127	ASN
1	A	256	ASN
2	B	89	GLN
4	D	3	GLN
4	D	22	ASN
4	D	31	ASN
4	D	43	GLN
4	D	95	GLN
4	D	138	GLN
4	D	158	GLN
4	D	206	ASN
5	E	83	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
6	EDO	E	301	-	3,3,3	0.50	0	2,2,2	0.40	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
6	EDO	E	301	-	-	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.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/362 (76%)	0.65	21 (7%) 20 10	20, 56, 92, 106	12 (4%)
2	B	99/100 (99%)	0.34	2 (2%) 65 41	35, 56, 75, 81	2 (2%)
3	C	9/9 (100%)	0.10	0 100 100	43, 46, 51, 54	0
4	D	203/207 (98%)	0.72	17 (8%) 17 8	24, 60, 85, 104	4 (1%)
5	E	240/243 (98%)	0.81	14 (5%) 29 14	41, 71, 99, 118	0
All	All	828/921 (89%)	0.67	54 (6%) 25 13	20, 61, 92, 118	18 (2%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	217	SER	5.4
1	A	14[A]	ARG	4.9
2	B	1	ILE	3.6
1	A	62[A]	ARG	3.5
4	D	150[A]	CYS	3.4
1	A	180	LEU	3.3
4	D	145	SER	3.2
4	D	92	THR	3.2
5	E	195	LEU	3.1
4	D	142	SER	3.1
1	A	178	THR	3.1
1	A	268	GLU	3.0
1	A	193	PRO	2.9
5	E	130	LYS	2.8
4	D	177	LEU	2.8
4	D	200	CYS	2.8
1	A	277	PRO	2.7
4	D	86	LYS	2.7
1	A	179	LEU	2.6
1	A	266	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	2.5
1	A	276	PRO	2.5
5	E	245	GLN	2.4
5	E	243	VAL	2.4
1	A	191	HIS	2.4
4	D	144	SER	2.4
5	E	255	ALA	2.3
1	A	255	GLN	2.3
4	D	196	SER	2.3
5	E	47	ASN	2.3
5	E	234	GLU	2.3
4	D	137	TYR	2.3
5	E	127	GLU	2.3
1	A	196	LYS	2.2
4	D	189	ALA	2.2
4	D	172	THR	2.2
5	E	244	THR	2.2
1	A	108[A]	ARG	2.2
1	A	199	VAL	2.2
5	E	151	GLN	2.2
5	E	236	THR	2.2
1	A	102	ASP	2.2
4	D	188	SER	2.2
1	A	186	LYS	2.1
4	D	147	LYS	2.1
5	E	210	ALA	2.1
1	A	68	LYS	2.1
5	E	152	LYS	2.1
4	D	171	ILE	2.1
1	A	44	ARG	2.1
1	A	177	ALA	2.1
4	D	174	LYS	2.0
2	B	19	LYS	2.0
5	E	144	GLU	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 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, 95th 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($\text{\AA}^2$)	Q<0.9
6	EDO	E	301	4/4	0.76	0.19	44,44,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.