Full wwPDB X-ray Structure Validation Report (i)

Apr 16, 2025 – 01:09 pm BST

PDB ID	:	9GV7 / pdb_00009gv7
Title	:	Structure of reverse docking TCR in complex with peptide-HLA
Authors	:	Karuppiah, V.
Deposited on	:	2024-09-23
Resolution	:	1.86 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 (i)) were used in the production of this report:

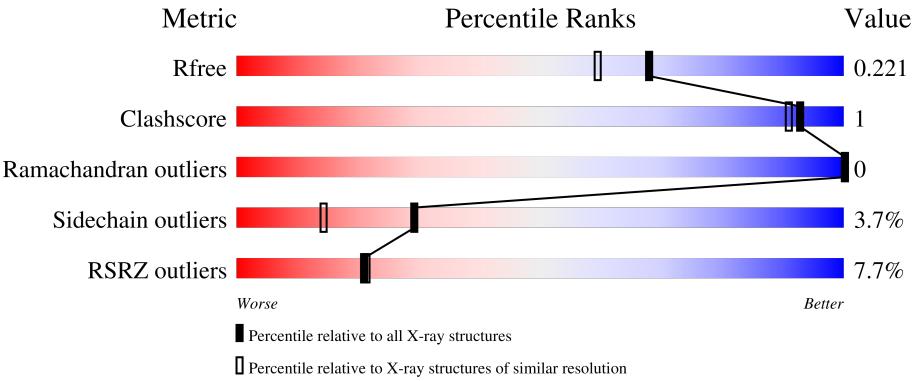
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	A	276	7% 89% 9% ••
2	B	100	% 93% 7%
3	C	11	100%
4	D	200	16% 88% 5% • 6%
5	E	244	5% 95% • •

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
6	EDO	E	301	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7022 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			844	537	142	161	4			

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 Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	S	0	0	0
			74	44	12	17	1			

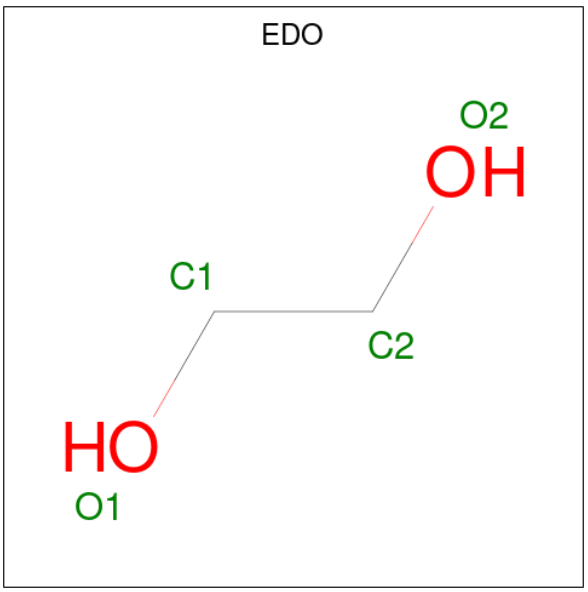
- Molecule 4 is a protein called TCR Alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	187	Total	C	N	O	S	0	1	0
			1455	906	245	296	8			

- Molecule 5 is a protein called TCR Beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	0	0	0
			1921	1212	336	364	9			

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



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

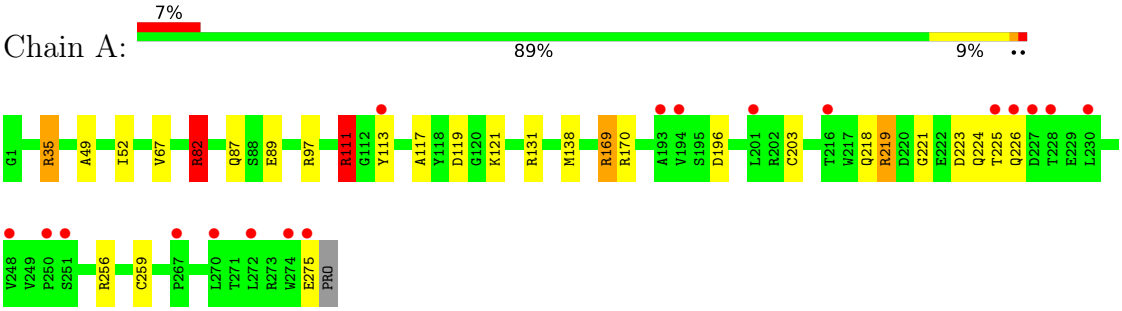
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	176	Total O 176 176	0	0
7	B	63	Total O 63 63	0	0
7	C	11	Total O 11 11	0	0
7	D	78	Total O 78 78	0	0
7	E	146	Total O 146 146	0	0

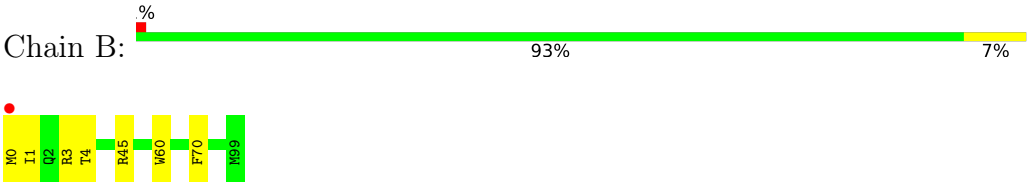
3 Residue-property plots (i)

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: MHC class I antigen



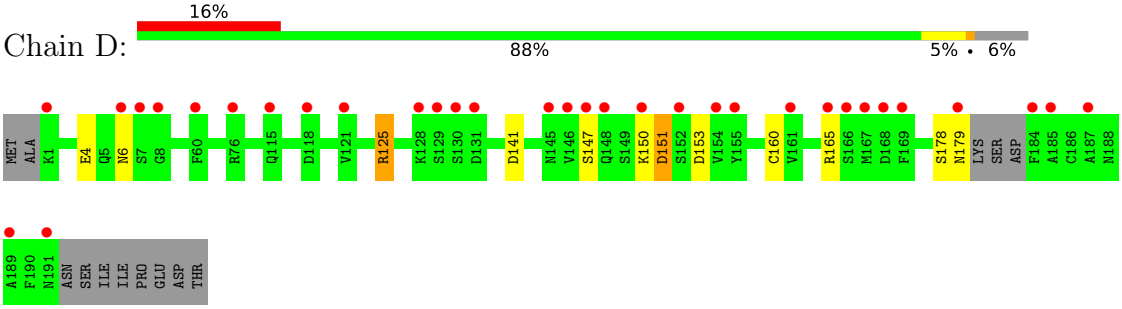
• Molecule 2: Beta-2-microglobulin



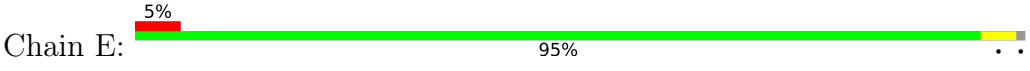
• Molecule 3: Peptide

There are no outlier residues recorded for this chain.

• Molecule 4: TCR Alpha



• Molecule 5: TCR Beta




MET
ASN
ALA
G3
Q22
R36
Q37
D38
P39
G40
M41
G42
I46
H47
R50
S67
N118
C170
L176
P180
A181
L182
R192
R208
R241
A242
D243

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	144.13Å 144.13Å 106.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	124.82 – 1.86 124.82 – 1.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (124.82-1.86) 100.0 (124.82-1.86)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.180 , 0.212 0.193 , 0.221	Depositor DCC
R_{free} test set	5187 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7022	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.62	0/2311	1.06	10/3137 (0.3%)
2	B	0.48	0/867	0.86	1/1173 (0.1%)
3	C	0.86	0/73	1.11	0/94
4	D	0.54	0/1485	0.88	0/2007
5	E	0.55	0/1976	0.98	4/2688 (0.1%)
All	All	0.57	0/6712	0.98	15/9099 (0.2%)

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	4
2	B	0	1
4	D	0	1
5	E	0	1
All	All	0	7

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	50	ARG	NE-CZ-NH2	-14.89	112.86	120.30
1	A	131	ARG	NE-CZ-NH2	14.55	127.58	120.30
5	E	50	ARG	NE-CZ-NH1	14.09	127.34	120.30
1	A	131	ARG	NE-CZ-NH1	-13.61	113.50	120.30
1	A	111	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	A	131	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	111	ARG	CD-NE-CZ	6.43	132.60	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	ARG	NE-CZ-NH2	6.38	123.49	120.30
5	E	50	ARG	CD-NE-CZ	6.14	132.19	123.60
1	A	82	ARG	CA-CB-CG	5.93	126.45	113.40
1	A	97	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	170	ARG	NE-CZ-NH2	-5.29	117.65	120.30
5	E	208	ARG	CD-NE-CZ	5.20	130.88	123.60
2	B	3	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	169	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	169	ARG	Sidechain
1	A	219	ARG	Sidechain
1	A	82	ARG	Sidechain
2	B	45	ARG	Sidechain
4	D	165	ARG	Sidechain
5	E	36	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	2246	0	2098	10	0
2	B	844	0	810	4	0
3	C	74	0	75	0	0
4	D	1455	0	1396	5	0
5	E	1921	0	1822	1	0
6	A	4	0	6	0	0
6	E	4	0	6	0	0
7	A	176	0	0	1	0
7	B	63	0	0	1	0
7	C	11	0	0	0	0
7	D	78	0	0	0	0
7	E	146	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7022	0	6213	17	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 1.

All (17) 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)
4:D:153:ASP:O	4:D:178:SER:HB2	1.88	0.72
1:A:219:ARG:HH11	1:A:256:ARG:HH21	1.42	0.67
4:D:125:ARG:HH21	4:D:125:ARG:HG2	1.60	0.67
1:A:138:MET:HE2	7:A:499:HOH:O	2.05	0.57
2:B:4[B]:THR:HG21	7:B:160:HOH:O	2.08	0.54
1:A:119:ASP:HB3	2:B:0:MET:HA	1.89	0.53
1:A:82:ARG:HA	1:A:87:GLN:HE21	1.76	0.49
1:A:121:LYS:HG3	2:B:1:ILE:HG23	1.95	0.48
4:D:151:ASP:N	4:D:151:ASP:OD1	2.48	0.47
4:D:153:ASP:O	4:D:178:SER:CB	2.63	0.45
1:A:49:ALA:O	1:A:52:ILE:HG22	2.17	0.45
5:E:46:ILE:HG22	5:E:47:HIS:CD2	2.52	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
1:A:203:CYS:SG	1:A:259:CYS:CB	3.05	0.43
4:D:151:ASP:C	4:D:153:ASP:H	2.21	0.43
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.84	0.42
1:A:219:ARG:HH11	1:A:256:ARG:NH2	2.13	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	
1	A	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
3	C	9/11 (82%)	9 (100%)	0	0	100	100
4	D	184/200 (92%)	180 (98%)	4 (2%)	0	100	100
5	E	239/244 (98%)	231 (97%)	8 (3%)	0	100	100
All	All	804/831 (97%)	785 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	231/232 (100%)	220 (95%)	11 (5%)	21	8
2	B	96/95 (101%)	95 (99%)	1 (1%)	73	67
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	165/176 (94%)	156 (94%)	9 (6%)	18	6
5	E	207/209 (99%)	202 (98%)	5 (2%)	44	29
All	All	706/719 (98%)	680 (96%)	26 (4%)	29	14

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	67	VAL
1	A	89	GLU
1	A	111	ARG
1	A	113	TYR
1	A	196	ASP
1	A	223	ASP
1	A	224	GLN
1	A	225	THR
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	275	GLU
2	B	70	PHE
4	D	4	GLU
4	D	6	ASN
4	D	125	ARG
4	D	141	ASP
4	D	147	SER
4	D	150	LYS
4	D	151	ASP
4	D	160	CYS
4	D	179	ASN
5	E	22	GLN
5	E	38	ASP
5	E	67	SER
5	E	192	ARG
5	E	241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	141	GLN
1	A	218	GLN
4	D	69	GLN
4	D	179	ASN
5	E	102	GLN

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)

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	$\#\|Z\| > 2$
6	EDO	A	301	-	3,3,3	0.11	0	2,2,2	0.14	0
6	EDO	E	301	-	3,3,3	2.24	2 (66%)	2,2,2	2.05	2 (100%)

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	A	301	-	-	0/1/1/1	-
6	EDO	E	301	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	301	EDO	O1-C1	2.74	1.56	1.42
6	E	301	EDO	O2-C2	2.68	1.55	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	301	EDO	O2-C2-C1	2.06	126.71	111.91
6	E	301	EDO	O1-C1-C2	2.04	126.55	111.91

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	301	EDO	O1-C1-C2-O2

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	275/276 (99%)	0.24	18 (6%) 26 27	28, 39, 89, 107	0
2	B	100/100 (100%)	0.27	1 (1%) 79 82	18, 47, 68, 77	1 (1%)
3	C	11/11 (100%)	-0.30	0 100 100	30, 32, 35, 40	0
4	D	187/200 (93%)	0.86	33 (17%) 4 4	29, 50, 97, 124	1 (0%)
5	E	241/244 (98%)	0.33	11 (4%) 38 40	29, 43, 73, 101	0
All	All	814/831 (97%)	0.40	63 (7%) 21 21	18, 43, 88, 124	2 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	40	GLY	5.3
5	E	41	MET	4.6
5	E	182	LEU	4.4
1	A	225	THR	4.2
4	D	179	ASN	4.2
4	D	146	VAL	3.9
5	E	181	ALA	3.8
1	A	194	VAL	3.8
4	D	148	GLN	3.7
4	D	168	ASP	3.6
4	D	166	SER	3.6
4	D	6	ASN	3.6
1	A	228	THR	3.5
5	E	176	LEU	3.5
1	A	250	PRO	3.4
5	E	39	PRO	3.4
4	D	191	ASN	3.1
4	D	167	MET	3.0
1	A	230	LEU	2.9
4	D	184	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	169	PHE	2.9
4	D	185	ALA	2.9
4	D	7	SER	2.8
4	D	130	SER	2.8
5	E	38	ASP	2.8
4	D	150	LYS	2.8
4	D	187	ALA	2.8
4	D	152	SER	2.7
5	E	42	GLY	2.7
2	B	0	MET	2.7
5	E	180	PRO	2.6
5	E	118	ASN	2.6
1	A	226	GLN	2.6
4	D	128	LYS	2.6
4	D	131	ASP	2.5
4	D	60	PHE	2.5
4	D	154	VAL	2.5
1	A	227	ASP	2.5
1	A	193	ALA	2.4
4	D	165	ARG	2.4
1	A	272	LEU	2.4
1	A	270	LEU	2.3
1	A	251	SER	2.3
1	A	275	GLU	2.3
4	D	145	ASN	2.3
4	D	1	LYS	2.3
4	D	121	VAL	2.3
1	A	113	TYR	2.3
4	D	155	TYR	2.3
4	D	147	SER	2.2
1	A	274	TRP	2.2
5	E	170	CYS	2.2
4	D	115	GLN	2.2
1	A	267	PRO	2.2
4	D	76	ARG	2.2
4	D	189	ALA	2.1
1	A	248	VAL	2.1
4	D	161	VAL	2.1
1	A	201	LEU	2.1
1	A	216	THR	2.1
4	D	129	SER	2.1
4	D	8	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	118	ASP	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^2)	Q<0.9
6	EDO	E	301	4/4	0.92	0.13	30,31,41,44	0
6	EDO	A	301	4/4	0.93	0.11	40,47,48,53	0

6.5 Other polymers (i)

There are no such residues in this entry.