wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 01:47 am GMT

PDB ID	:	6R0E
Title	:	Structure of F11TCR in complex with DR1 MHC Class II presenting PKYVKQNTLKLAT
Authors	:	Rizkallah, P.J.; Greenshields-Watson, A.L.
Deposited on	:	2019-03-12
Resolution	:	1.91 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

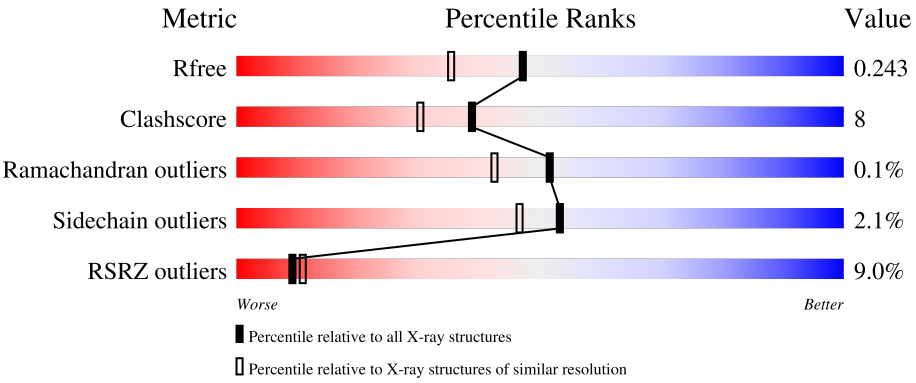
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	AAA	183	10% 85% 13%
2	BBB	191	24% 77% 23%
3	CCC	13	15% 92% 8%
4	DDD	202	2% 85% 14%
5	EEE	240	% 88% 12%

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	DDD	301	-	-	X	-
7	SO4	DDD	304	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6958 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	178	Total	C	N	O	S	0	0	0
			1447	940	234	268	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	190	Total	C	N	O	S	0	0	0
			1522	960	272	283	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	MET	-	initiating methionine	UNP P04229

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	13	Total	C	N	O	0	0	0
			106	69	18	19			

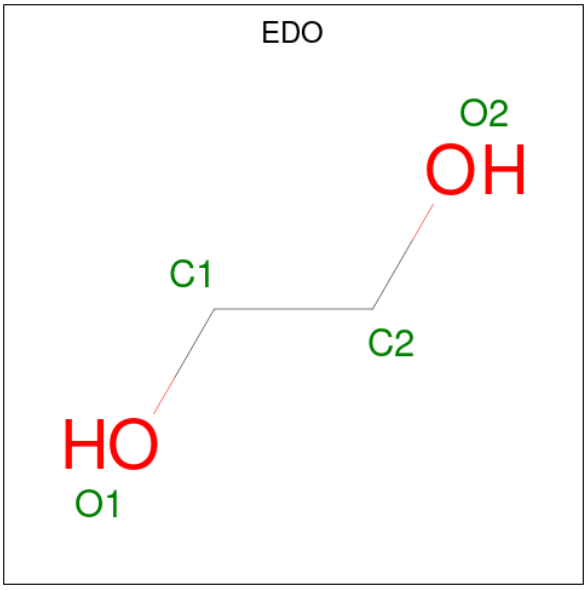
- Molecule 4 is a protein called F11-TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	202	Total	C	N	O	S	0	3	0
			1597	1007	263	317	10			

- Molecule 5 is a protein called F11-TCR Beta Chain.

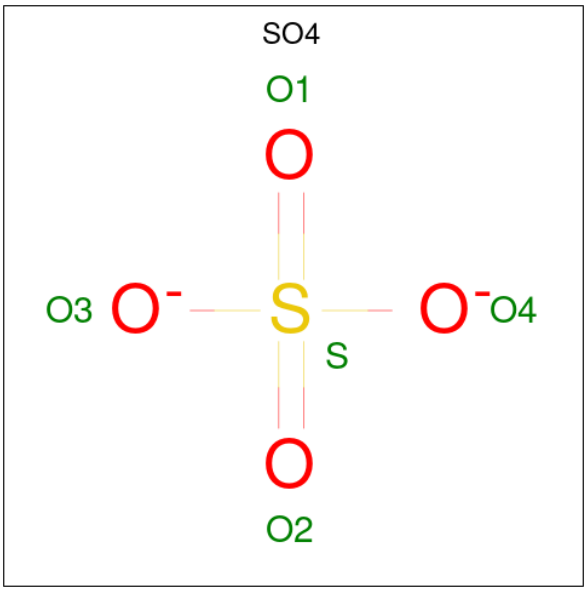
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	EEE	240	Total	C	N	O	S	0	3	0
			1935	1211	338	377	9			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



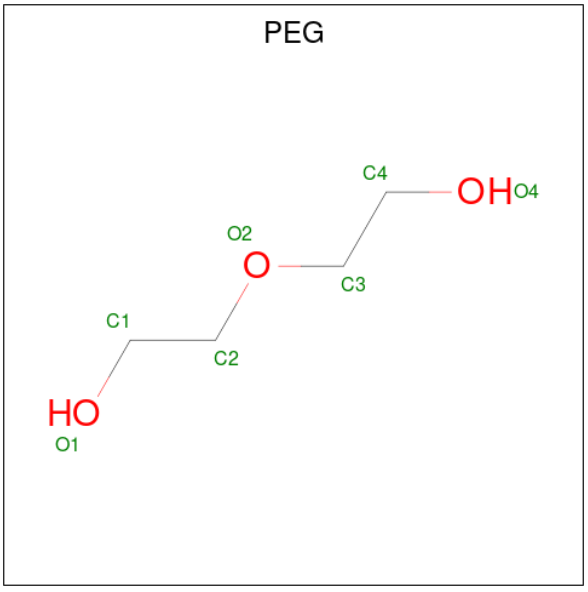
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	BBB	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	DDD	1	Total	C	O	0	0
			4	2	2		
6	EEE	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	DDD	1	Total O S 5 4 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	DDD	1	Total C O 7 4 3	0	0
8	EEE	1	Total C O 7 4 3	0	0

- Molecule 9 is water.

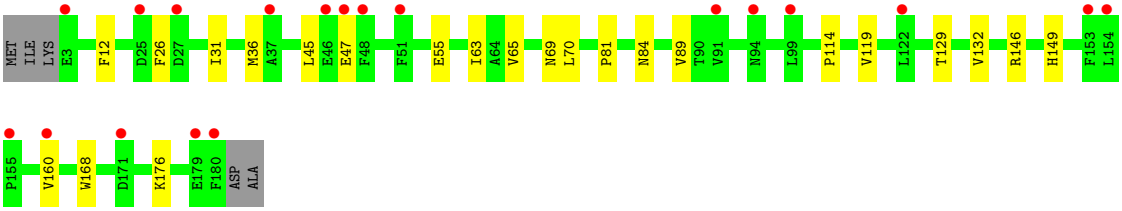
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	37	Total O 37 37	0	0
9	BBB	23	Total O 23 23	0	0
9	CCC	4	Total O 4 4	0	0
9	DDD	118	Total O 118 118	0	0
9	EEE	126	Total O 126 126	0	0

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.

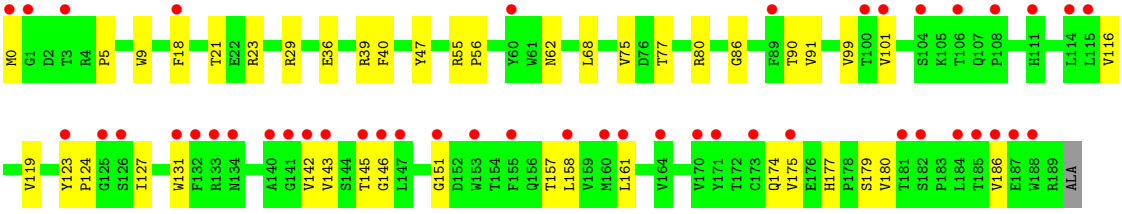
• Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain AAA:



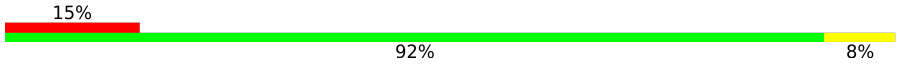
• Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain

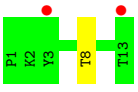
Chain BBB:



• Molecule 3: Hemagglutinin

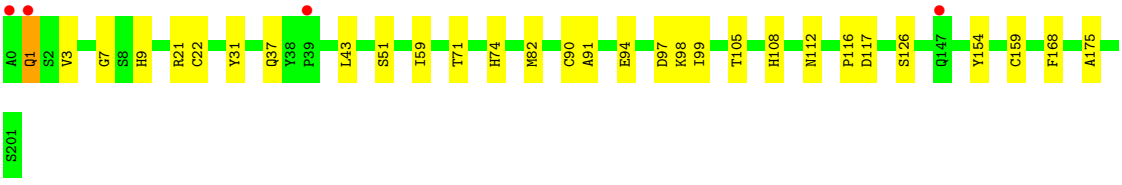
Chain CCC:





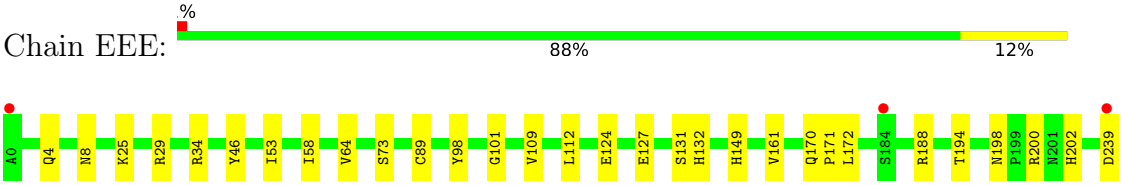
• Molecule 4: F11-TCR Alpha Chain

Chain DDD:



• Molecule 5: F11-TCR Beta Chain

Chain EEE:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.28Å 184.90Å 50.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.45 – 1.91 92.45 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.45-1.91) 99.9 (92.45-1.91)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.233 0.212 , 0.243	Depositor DCC
R_{free} test set	4762 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6958	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: PEG, EDO, SO4

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	AAA	0.74	0/1492	0.85	0/2038
2	BBB	0.75	0/1561	0.91	0/2124
3	CCC	0.66	0/107	0.83	0/141
4	DDD	0.82	0/1634	0.96	0/2216
5	EEE	0.76	1/1983 (0.1%)	0.94	0/2693
All	All	0.77	1/6777 (0.0%)	0.92	0/9212

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	BBB	0	1
4	DDD	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	EEE	124	GLU	CD-OE2	-5.26	1.19	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	151	GLY	Peptide
4	DDD	112	ASN	Mainchain

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	AAA	1447	0	1373	20	0
2	BBB	1522	0	1436	30	0
3	CCC	106	0	121	1	0
4	DDD	1597	0	1521	38	0
5	EEE	1935	0	1843	22	0
6	BBB	8	0	12	0	0
6	DDD	12	0	18	8	0
6	EEE	4	0	6	0	0
7	DDD	5	0	0	1	0
8	DDD	7	0	10	0	0
8	EEE	7	0	10	3	0
9	AAA	37	0	0	1	0
9	BBB	23	0	0	0	0
9	CCC	4	0	0	0	0
9	DDD	118	0	0	2	0
9	EEE	126	0	0	5	0
All	All	6958	0	6350	98	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.

The worst 5 of 98 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:DDD:3:VAL:CG2	4:DDD:90[B]:CYS:SG	2.60	0.90
4:DDD:3:VAL:HG21	4:DDD:90[B]:CYS:SG	2.18	0.84
4:DDD:3:VAL:HG23	4:DDD:22:CYS:SG	2.34	0.68
4:DDD:9:HIS:HD2	4:DDD:108:HIS:HE1	1.40	0.67
5:EEE:53:ILE:HD12	5:EEE:64:VAL:HG23	1.81	0.62

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	AAA	176/183 (96%)	170 (97%)	6 (3%)	0	100	100
2	BBB	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
3	CCC	11/13 (85%)	11 (100%)	0	0	100	100
4	DDD	203/202 (100%)	196 (97%)	6 (3%)	1 (0%)	29	18
5	EEE	241/240 (100%)	232 (96%)	9 (4%)	0	100	100
All	All	819/829 (99%)	791 (97%)	27 (3%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DDD	71	THR

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	AAA	159/167 (95%)	156 (98%)	3 (2%)	57	51
2	BBB	163/172 (95%)	160 (98%)	3 (2%)	59	53
3	CCC	12/12 (100%)	12 (100%)	0	100	100
4	DDD	182/180 (101%)	176 (97%)	6 (3%)	38	28
5	EEE	213/210 (101%)	209 (98%)	4 (2%)	57	51
All	All	729/741 (98%)	713 (98%)	16 (2%)	53	45

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	EEE	188	ARG
5	EEE	131	SER
4	DDD	116	PRO
5	EEE	25	LYS
4	DDD	59	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

9 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	BBB	201	-	3,3,3	0.15	0	2,2,2	0.34	0
6	EDO	DDD	303	-	3,3,3	0.11	0	2,2,2	0.38	0
8	PEG	DDD	305	-	6,6,6	0.32	0	5,5,5	0.27	0
6	EDO	BBB	202	-	3,3,3	0.17	0	2,2,2	0.25	0
6	EDO	DDD	301	-	3,3,3	0.24	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	EEE	302	-	3,3,3	0.12	0	2,2,2	0.39	0
8	PEG	EEE	301	-	6,6,6	0.29	0	5,5,5	0.26	0
7	SO4	DDD	304	-	4,4,4	0.36	0	6,6,6	0.10	0
6	EDO	DDD	302	-	3,3,3	0.18	0	2,2,2	0.21	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	BBB	201	-	-	0/1/1/1	-
6	EDO	DDD	303	-	-	0/1/1/1	-
8	PEG	DDD	305	-	-	1/4/4/4	-
6	EDO	BBB	202	-	-	0/1/1/1	-
6	EDO	DDD	301	-	-	1/1/1/1	-
6	EDO	EEE	302	-	-	1/1/1/1	-
8	PEG	EEE	301	-	-	2/4/4/4	-
6	EDO	DDD	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	DDD	305	PEG	O2-C3-C4-O4
6	DDD	301	EDO	O1-C1-C2-O2
6	EEE	302	EDO	O1-C1-C2-O2
8	EEE	301	PEG	O1-C1-C2-O2
8	EEE	301	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	DDD	303	EDO	1	0
6	DDD	301	EDO	6	0
8	EEE	301	PEG	3	0
7	DDD	304	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	DDD	302	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^{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	AAA	178/183 (97%)	0.74	19 (10%)	6	7	39, 63, 103, 114	0
2	BBB	190/191 (99%)	1.35	46 (24%)	0	0	40, 69, 94, 108	0
3	CCC	13/13 (100%)	0.83	2 (15%)	2	2	41, 48, 61, 72	0
4	DDD	202/202 (100%)	0.73	4 (1%)	65	68	22, 39, 69, 94	0
5	EEE	240/240 (100%)	0.56	3 (1%)	77	79	24, 42, 63, 91	0
All	All	823/829 (99%)	0.83	74 (8%)	9	11	22, 51, 92, 114	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	1	GLY	11.7
2	BBB	143	VAL	5.8
2	BBB	173	CYS	5.4
2	BBB	132	PHE	5.4
2	BBB	0	MET	5.0

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

There are no monosaccharides in this entry.

6.4 Ligands

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
7	SO4	DDD	304	5/5	0.61	0.45	38,47,59,62	5
8	PEG	EEE	301	7/7	0.65	0.22	48,64,74,76	0
8	PEG	DDD	305	7/7	0.70	0.31	62,67,73,75	0
6	EDO	DDD	303	4/4	0.74	0.19	63,65,65,68	0
6	EDO	BBB	201	4/4	0.82	0.22	56,60,62,65	0
6	EDO	EEE	302	4/4	0.86	0.15	54,63,67,75	0
6	EDO	DDD	301	4/4	0.88	0.14	48,54,60,66	0
6	EDO	BBB	202	4/4	0.90	0.43	52,55,60,60	0
6	EDO	DDD	302	4/4	0.93	0.27	50,55,55,61	0

6.5 Other polymers (i)

There are no such residues in this entry.