



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:24 pm BST

PDB ID : 6BCR
Title : Complex of 14-3-3 theta with an IRSp53 peptide phosphorylated at T340
Authors : Kast, D.J.; Dominguez, R.
Deposited on : 2017-10-20
Resolution : 1.99 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 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

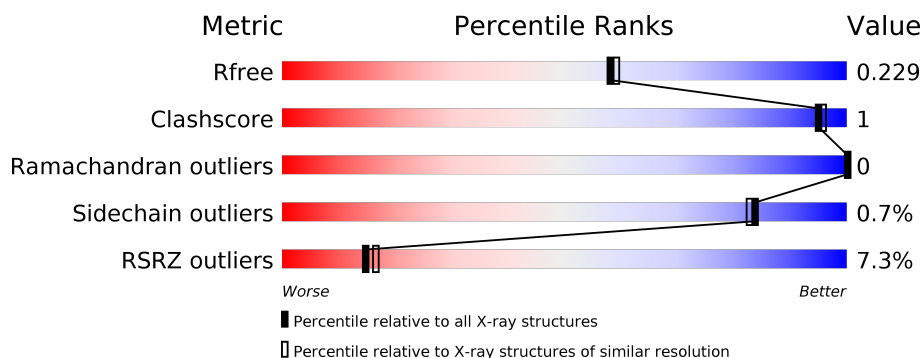
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 ≥ 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	245	<div> <div>5%</div> <div>89%</div> <div>6%</div> </div>
1	B	245	<div> <div>7%</div> <div>90%</div> <div>6%</div> </div>
1	E	245	<div> <div>8%</div> <div>92%</div> <div>6%</div> </div>
1	F	245	<div> <div>3%</div> <div>91%</div> <div>6%</div> </div>
2	C	14	<div> <div>14%</div> <div>64%</div> <div>36%</div> </div>
2	D	14	<div> <div>21%</div> <div>64%</div> <div>36%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	14	
2	H	14	

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	PEG	E	303	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16436 atoms, of which 7959 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 14-3-3 protein theta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	11	0
			3823	1202	1910	314	387	10			
1	B	230	Total	C	H	N	O	S	0	3	0
			3722	1169	1859	310	374	10			
1	E	231	Total	C	H	N	O	S	0	7	0
			3780	1187	1892	311	379	11			
1	F	230	Total	C	H	N	O	S	0	4	0
			3735	1173	1868	310	374	10			

- Molecule 2 is a protein called Insulin receptor substrate protein of 53 kDa, peptide (IRSp53).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	9	Total	C	H	N	O	P	0	1	0
			173	56	85	14	17	1			
2	D	9	Total	C	H	N	O	P	0	0	0
			157	48	78	14	16	1			
2	G	10	Total	C	H	N	O	P	0	0	0
			167	51	82	15	18	1			
2	H	10	Total	C	H	N	O	P	0	0	0
			167	51	82	15	18	1			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

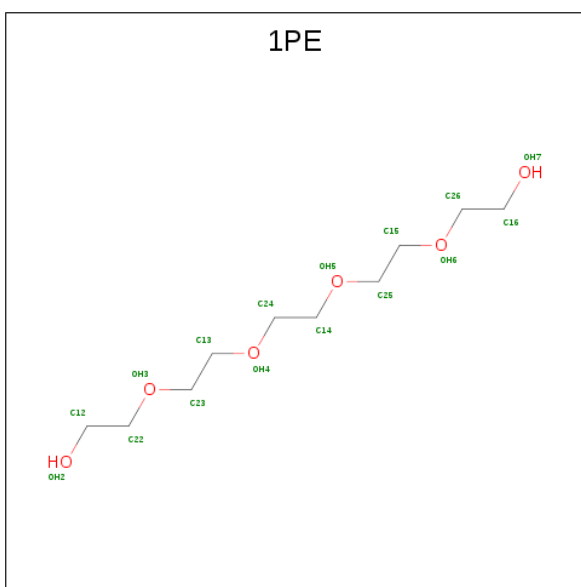
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			16	4	9	3		
4	A	1	Total	C	H	O	0	0
			16	4	9	3		
4	E	1	Total	C	H	O	0	0
			16	4	9	3		
4	E	1	Total	C	H	O	0	0
			16	4	9	3		
4	F	1	Total	C	H	O	0	0
			16	4	9	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



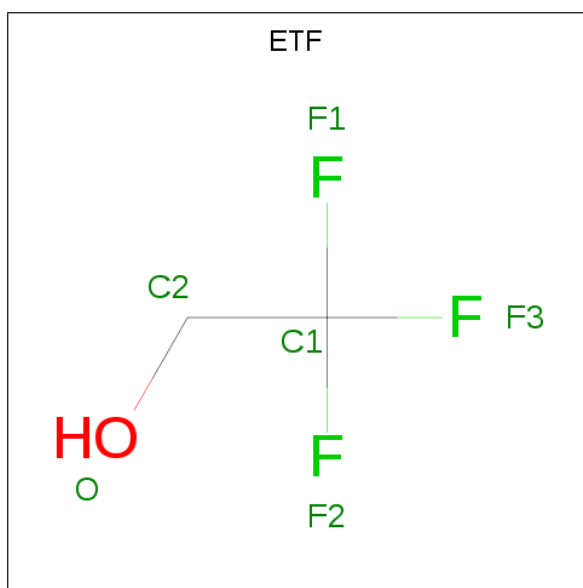
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			37	10	21	6		
5	F	1	Total	C	H	O	0	0
			37	10	21	6		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			9	2	5	2		
6	F	1	Total	C	H	O	0	0
			9	2	5	2		

- Molecule 7 is TRIFLUOROETHANOL (three-letter code: ETF) (formula: $C_2H_3F_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	F	H	O	0	0
			9	2	3	3	1		
7	F	1	Total	C	F	H	O	0	0
			9	2	3	3	1		

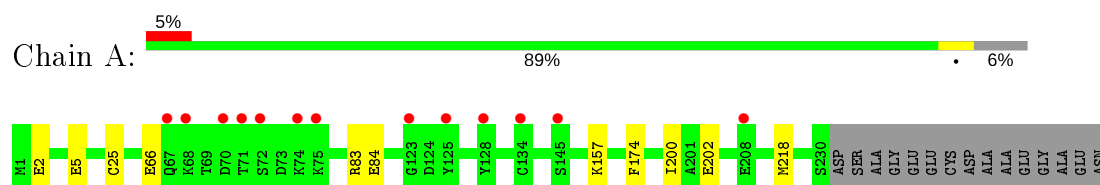
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	143	Total	O	0	0
			143	143		
8	B	109	Total	O	0	0
			109	109		
8	C	13	Total	O	0	0
			13	13		
8	D	7	Total	O	0	0
			7	7		
8	E	120	Total	O	0	0
			120	120		
8	F	107	Total	O	0	0
			107	107		
8	G	11	Total	O	0	0
			11	11		
8	H	7	Total	O	0	0
			7	7		

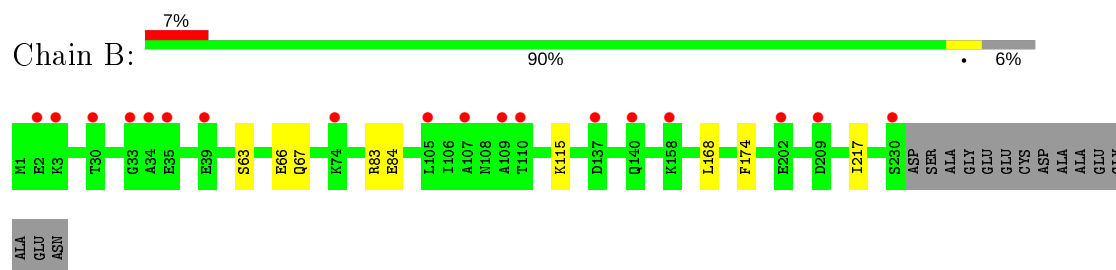
3 Residue-property plots [i](#)

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.

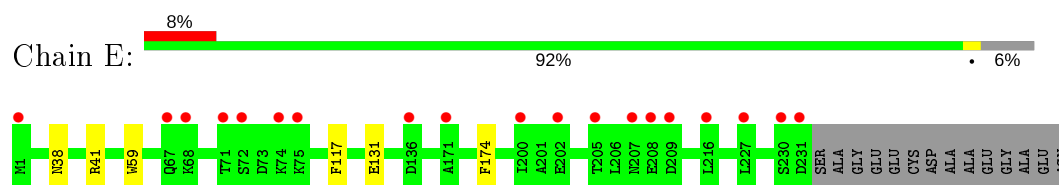
- Molecule 1: 14-3-3 protein theta



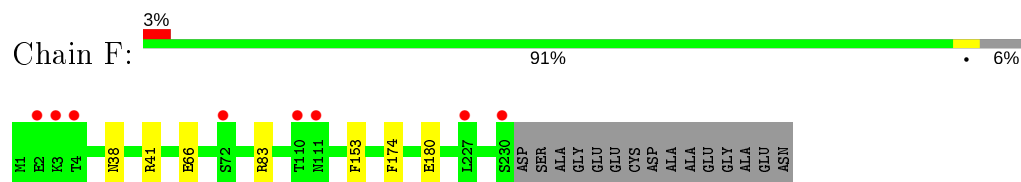
- Molecule 1: 14-3-3 protein theta



- Molecule 1: 14-3-3 protein theta

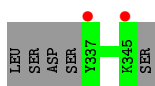


- Molecule 1: 14-3-3 protein theta

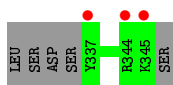


- Molecule 2: Insulin receptor substrate protein of 53 kDa, peptide (IRSp53)

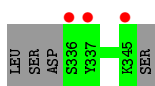




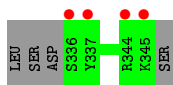
- Molecule 2: Insulin receptor substrate protein of 53 kDa, peptide (IRSp53)



- Molecule 2: Insulin receptor substrate protein of 53 kDa, peptide (IRSp53)



- Molecule 2: Insulin receptor substrate protein of 53 kDa, peptide (IRSp53)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.01Å 69.11Å 84.56Å 105.25° 95.72° 115.04°	Depositor
Resolution (Å)	31.29 – 1.99 31.29 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.7 (31.29-1.99) 95.7 (31.29-1.99)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.195 , 0.229 0.195 , 0.229	Depositor DCC
R_{free} test set	3820 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.3	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	0.95	EDS
Total number of atoms	16436	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: MG, TPO, EDO, 1PE, ETF, PEG

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	0.27	0/1965	0.40	0/2649
1	B	0.25	0/1894	0.40	0/2555
1	E	0.26	0/1934	0.39	0/2607
1	F	0.26	0/1904	0.41	0/2567
2	C	0.23	0/81	0.35	0/107
2	D	0.24	0/68	0.46	0/89
2	G	0.23	0/74	0.36	0/97
2	H	0.23	0/74	0.37	0/97
All	All	0.26	0/7994	0.40	0/10768

There are no bond length outliers.

There are no bond angle outliers.

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	1913	1910	1916	7	0
1	B	1863	1859	1860	5	0
1	E	1888	1892	1898	5	0
1	F	1867	1868	1871	2	0
2	C	88	85	85	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	79	78	77	0	0
2	G	85	82	82	0	0
2	H	85	82	82	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	14	18	20	1	0
4	E	14	18	20	3	0
4	F	7	9	10	0	0
5	B	16	21	22	0	0
5	F	16	21	22	0	0
6	B	4	5	6	0	0
6	F	4	5	6	0	0
7	E	6	3	3	0	0
7	F	6	3	3	0	0
8	A	143	0	0	1	0
8	B	109	0	0	1	0
8	C	13	0	0	0	0
8	D	7	0	0	0	0
8	E	120	0	0	0	0
8	F	107	0	0	0	0
8	G	11	0	0	0	0
8	H	7	0	0	0	0
All	All	8477	7959	7983	19	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 (19) 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:157:LYS:NZ	8:A:401:HOH:O	2.25	0.69
1:A:84[B]:GLU:HA	1:A:84[B]:GLU:OE1	1.98	0.62
1:E:38:ASN:OD1	1:E:41:ARG:NH1	2.32	0.62
1:B:115:LYS:NZ	8:B:404:HOH:O	2.34	0.60
1:E:41:ARG:HD2	1:E:117:PHE:CG	2.40	0.56
1:A:66:GLU:OE2	1:A:83:ARG:HD3	2.09	0.53
1:E:131:GLU:OE1	4:E:303:PEG:H22	2.10	0.52
1:B:83:ARG:NH1	1:B:84:GLU:OE1	2.43	0.51
1:E:59:TRP:CE3	4:E:303:PEG:H12	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HG23	1:A:218:MET:CE	2.47	0.45
1:F:66:GLU:OE1	1:F:83:ARG:HD3	2.16	0.45
1:B:63:SER:O	1:B:67:GLN:HG2	2.16	0.44
1:B:66:GLU:OE1	1:B:83:ARG:HD3	2.18	0.44
1:A:2[A]:GLU:HG2	1:A:5[A]:GLU:OE2	2.20	0.41
1:A:25:CYS:SG	4:A:302:PEG:H22	2.60	0.41
1:B:168:LEU:HB3	1:B:217:ILE:HG21	2.02	0.41
1:E:59:TRP:CZ3	4:E:303:PEG:H31	2.55	0.41
1:F:38:ASN:OD1	1:F:41:ARG:NH2	2.48	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	239/245 (98%)	237 (99%)	2 (1%)	0	100	100
1	B	231/245 (94%)	229 (99%)	2 (1%)	0	100	100
1	E	236/245 (96%)	233 (99%)	3 (1%)	0	100	100
1	F	232/245 (95%)	231 (100%)	1 (0%)	0	100	100
2	C	6/14 (43%)	6 (100%)	0	0	100	100
2	D	6/14 (43%)	6 (100%)	0	0	100	100
2	G	7/14 (50%)	7 (100%)	0	0	100	100
2	H	7/14 (50%)	7 (100%)	0	0	100	100
All	All	964/1036 (93%)	956 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	214/212 (101%)	213 (100%)	1 (0%)	88	87
1	B	206/212 (97%)	205 (100%)	1 (0%)	88	87
1	E	211/212 (100%)	210 (100%)	1 (0%)	88	87
1	F	207/212 (98%)	203 (98%)	4 (2%)	57	50
2	C	9/13 (69%)	9 (100%)	0	100	100
2	D	8/13 (62%)	8 (100%)	0	100	100
2	G	9/13 (69%)	9 (100%)	0	100	100
2	H	9/13 (69%)	9 (100%)	0	100	100
All	All	873/900 (97%)	866 (99%)	7 (1%)	84	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	PHE
1	B	174	PHE
1	E	174	PHE
1	F	153	PHE
1	F	174	PHE
1	F	180[A]	GLU
1	F	180[B]	GLU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	TPO	D	340	2	8,10,11	1.52	1 (12%)	10,14,16	1.39	1 (10%)
2	TPO	C	340	2	8,10,11	1.60	1 (12%)	10,14,16	1.46	2 (20%)
2	TPO	H	340	2	8,10,11	1.10	0	10,14,16	1.32	1 (10%)
2	TPO	G	340	2	8,10,11	1.11	0	10,14,16	1.41	1 (10%)

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	TPO	D	340	2	-	3/9/11/13	-
2	TPO	C	340	2	-	2/9/11/13	-
2	TPO	H	340	2	-	2/9/11/13	-
2	TPO	G	340	2	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	340	TPO	P-O1P	3.45	1.61	1.50
2	D	340	TPO	P-O1P	3.16	1.60	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	340	TPO	P-OG1-CB	-3.53	112.55	123.21
2	D	340	TPO	P-OG1-CB	-3.40	112.94	123.21
2	G	340	TPO	P-OG1-CB	-3.38	113.00	123.21
2	H	340	TPO	P-OG1-CB	-3.21	113.53	123.21
2	C	340	TPO	CG2-CB-CA	-2.11	108.99	113.16

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	340	TPO	CB-OG1-P-O3P
2	C	340	TPO	CB-OG1-P-O3P
2	D	340	TPO	CB-OG1-P-O2P
2	H	340	TPO	CB-OG1-P-O2P
2	G	340	TPO	CB-OG1-P-O2P
2	D	340	TPO	O-C-CA-CB
2	C	340	TPO	O-C-CA-CB
2	H	340	TPO	O-C-CA-CB
2	G	340	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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	PEG	F	302	-	6,6,6	0.49	0	5,5,5	0.34	0
6	EDO	B	303	-	3,3,3	0.59	0	2,2,2	0.28	0
4	PEG	A	302	-	6,6,6	0.48	0	5,5,5	0.31	0
7	ETF	E	301	-	5,5,5	0.39	0	7,7,7	0.71	0
4	PEG	E	302	-	6,6,6	0.49	0	5,5,5	0.27	0
5	1PE	F	303	-	15,15,15	0.66	0	14,14,14	0.23	0
4	PEG	A	303	-	6,6,6	0.51	0	5,5,5	0.26	0
4	PEG	E	303	-	6,6,6	0.58	0	5,5,5	1.20	1 (20%)
5	1PE	B	302	-	15,15,15	0.66	0	14,14,14	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ETF	F	301	-	5,5,5	0.44	0	7,7,7	0.64	0
6	EDO	F	304	-	3,3,3	0.53	0	2,2,2	0.41	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	PEG	F	302	-	-	1/4/4/4	-
6	EDO	B	303	-	-	0/1/1/1	-
4	PEG	A	302	-	-	0/4/4/4	-
7	ETF	E	301	-	-	0/3/3/3	-
4	PEG	E	302	-	-	2/4/4/4	-
5	1PE	F	303	-	-	4/13/13/13	-
4	PEG	A	303	-	-	2/4/4/4	-
4	PEG	E	303	-	-	3/4/4/4	-
5	1PE	B	302	-	-	6/13/13/13	-
7	ETF	F	301	-	-	3/3/3/3	-
6	EDO	F	304	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	303	PEG	C3-O2-C2	2.21	122.87	113.29

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	303	PEG	C1-C2-O2-C3
4	E	303	PEG	O2-C3-C4-O4
5	F	303	1PE	OH5-C14-C24-OH4
4	A	303	PEG	O1-C1-C2-O2
4	F	302	PEG	O2-C3-C4-O4
5	B	302	1PE	OH2-C12-C22-OH3
6	F	304	EDO	O1-C1-C2-O2
5	F	303	1PE	OH7-C16-C26-OH6
5	B	302	1PE	OH7-C16-C26-OH6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	303	PEG	C4-C3-O2-C2
5	B	302	1PE	C24-C14-OH5-C25
5	F	303	1PE	C23-C13-OH4-C24
4	A	303	PEG	O2-C3-C4-O4
4	E	302	PEG	C1-C2-O2-C3
5	F	303	1PE	C16-C26-OH6-C15
5	B	302	1PE	C23-C13-OH4-C24
4	E	302	PEG	O1-C1-C2-O2
7	F	301	ETF	F1-C1-C2-O
7	F	301	ETF	F3-C1-C2-O
5	B	302	1PE	OH6-C15-C25-OH5
7	F	301	ETF	F2-C1-C2-O
5	B	302	1PE	C15-C25-OH5-C14

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	PEG	1	0
4	E	303	PEG	3	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, 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	230/245 (93%)	0.35	13 (5%) 23 25	22, 34, 62, 79	0
1	B	230/245 (93%)	0.49	18 (7%) 13 14	27, 42, 78, 91	0
1	E	231/245 (94%)	0.40	19 (8%) 11 13	25, 38, 74, 105	0
1	F	230/245 (93%)	0.38	8 (3%) 44 46	24, 38, 62, 83	0
2	C	8/14 (57%)	1.25	2 (25%) 0 0	37, 47, 75, 76	0
2	D	8/14 (57%)	2.03	3 (37%) 0 0	39, 49, 77, 83	0
2	G	9/14 (64%)	1.96	3 (33%) 0 0	43, 48, 82, 87	0
2	H	9/14 (64%)	2.27	4 (44%) 0 0	35, 42, 76, 90	0
All	All	955/1036 (92%)	0.46	70 (7%) 15 16	22, 38, 73, 105	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	337	TYR	6.8
1	B	110	THR	6.3
2	G	336	SER	6.1
2	D	337	TYR	6.1
1	B	33	GLY	5.5
1	B	34	ALA	5.2
1	E	207	ASN	5.0
1	A	208	GLU	5.0
2	D	345	LYS	4.9
1	F	230	SER	4.8
2	H	345	LYS	4.7
2	C	345	LYS	4.6
2	H	336	SER	4.4
1	E	231	ASP	4.0
1	B	109	ALA	3.8
1	E	205	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	THR	3.6
2	G	345	LYS	3.6
1	E	208	GLU	3.5
1	A	74	LYS	3.5
2	G	337	TYR	3.5
1	B	3	LYS	3.4
2	C	337[A]	TYR	3.4
1	E	209	ASP	3.4
1	B	230	SER	3.3
1	E	68	LYS	3.1
1	A	67	GLN	3.0
1	B	105	LEU	2.9
1	E	216	LEU	2.9
1	F	227	LEU	2.9
1	B	140	GLN	2.8
1	E	71	THR	2.8
1	F	2	GLU	2.7
2	D	344	ARG	2.7
1	E	230	SER	2.6
2	H	344	ARG	2.6
1	E	1	MET	2.6
1	B	137	ASP	2.6
1	E	136	ASP	2.6
1	B	209	ASP	2.5
1	E	202	GLU	2.5
1	E	67	GLN	2.5
1	B	107	ALA	2.5
1	B	202	GLU	2.5
1	B	35	GLU	2.4
1	A	72	SER	2.4
1	A	145	SER	2.4
1	B	158	LYS	2.4
1	A	68	LYS	2.4
1	A	134	CYS	2.4
1	A	125	TYR	2.3
1	F	72	SER	2.3
1	E	200	ILE	2.3
1	A	123	GLY	2.3
1	F	110	THR	2.3
1	E	171	ALA	2.3
1	E	72	SER	2.2
1	A	75	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	4	THR	2.2
1	E	227	LEU	2.1
1	A	70	ASP	2.1
1	B	39	GLU	2.1
1	E	74	LYS	2.1
1	F	3	LYS	2.1
1	B	30	THR	2.1
1	B	2	GLU	2.1
1	A	128	TYR	2.0
1	F	111	ASN	2.0
1	B	74	LYS	2.0
1	E	75	LYS	2.0

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

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(Å ²)	Q<0.9
2	TPO	D	340	11/12	0.97	0.14	26,30,38,40	0
2	TPO	C	340	11/12	0.98	0.16	22,27,34,36	0
2	TPO	H	340	11/12	0.98	0.19	23,27,34,40	0
2	TPO	G	340	11/12	0.99	0.16	27,34,43,47	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 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(Å ²)	Q<0.9
6	EDO	B	303	4/4	0.68	0.19	54,60,73,73	0
4	PEG	E	303	7/7	0.71	0.45	43,56,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PEG	A	303	7/7	0.84	0.18	51,63,66,66	0
4	PEG	E	302	7/7	0.86	0.13	52,63,72,72	0
4	PEG	F	302	7/7	0.86	0.15	51,61,68,69	0
7	ETF	E	301	6/6	0.88	0.18	53,59,65,78	0
4	PEG	A	302	7/7	0.88	0.17	50,61,74,74	0
5	1PE	B	302	16/16	0.91	0.16	40,58,71,75	0
6	EDO	F	304	4/4	0.91	0.29	45,53,60,63	0
5	1PE	F	303	16/16	0.93	0.14	39,52,63,66	0
3	MG	A	300	1/1	0.94	0.10	36,36,36,36	0
3	MG	A	301	1/1	0.95	0.06	58,58,58,58	0
3	MG	F	300	1/1	0.96	0.05	60,60,60,60	0
7	ETF	F	301	6/6	0.96	0.07	43,49,52,58	0
3	MG	E	300	1/1	0.96	0.08	36,36,36,36	0
3	MG	B	301	1/1	0.98	0.07	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.