



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2024 – 10:21 PM EDT

PDB ID : 5OW5
Title : p60p80-CAMSAP complex
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Deposited on : 2017-08-30
Resolution : 1.70 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  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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

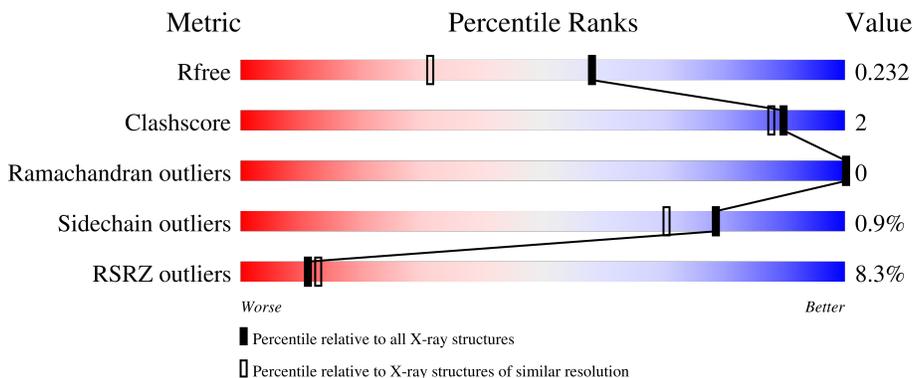
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	212	 79% 20%
1	C	212	 11% 74% 22%
2	B	80	 4% 90% 6%
2	D	80	 15% 76% 14% 10%
3	E	10	 100%

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Mol	Chain	Length	Quality of chain
3	F	10	 90% 10%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8601 atoms, of which 4211 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 Katanin p80 WD40 repeat-containing subunit B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	170	2759	852	1412	238	250	7	0	4	0
1	C	165	2642	822	1347	224	242	7	0	2	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	MET	-	initiating methionine	UNP Q8BG40
A	448	GLY	-	expression tag	UNP Q8BG40
A	449	SER	-	expression tag	UNP Q8BG40
A	450	SER	-	expression tag	UNP Q8BG40
A	451	HIS	-	expression tag	UNP Q8BG40
A	452	HIS	-	expression tag	UNP Q8BG40
A	453	HIS	-	expression tag	UNP Q8BG40
A	454	HIS	-	expression tag	UNP Q8BG40
A	455	HIS	-	expression tag	UNP Q8BG40
A	456	HIS	-	expression tag	UNP Q8BG40
A	457	SER	-	expression tag	UNP Q8BG40
A	458	SER	-	expression tag	UNP Q8BG40
A	459	GLY	-	expression tag	UNP Q8BG40
A	460	LEU	-	expression tag	UNP Q8BG40
A	461	VAL	-	expression tag	UNP Q8BG40
A	462	PRO	-	expression tag	UNP Q8BG40
A	463	ARG	-	expression tag	UNP Q8BG40
A	464	GLY	-	expression tag	UNP Q8BG40
A	465	SER	-	expression tag	UNP Q8BG40
A	466	HIS	-	expression tag	UNP Q8BG40
A	467	MET	-	expression tag	UNP Q8BG40
A	468	ALA	-	expression tag	UNP Q8BG40
A	469	SER	-	expression tag	UNP Q8BG40
A	470	MET	-	expression tag	UNP Q8BG40
A	471	THR	-	expression tag	UNP Q8BG40

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Chain	Residue	Modelled	Actual	Comment	Reference
A	472	GLY	-	expression tag	UNP Q8BG40
A	473	GLY	-	expression tag	UNP Q8BG40
A	474	GLN	-	expression tag	UNP Q8BG40
A	475	GLN	-	expression tag	UNP Q8BG40
A	476	MET	-	expression tag	UNP Q8BG40
A	477	GLY	-	expression tag	UNP Q8BG40
A	478	ARG	-	expression tag	UNP Q8BG40
A	479	GLY	-	expression tag	UNP Q8BG40
A	480	SER	-	expression tag	UNP Q8BG40
C	447	MET	-	initiating methionine	UNP Q8BG40
C	448	GLY	-	expression tag	UNP Q8BG40
C	449	SER	-	expression tag	UNP Q8BG40
C	450	SER	-	expression tag	UNP Q8BG40
C	451	HIS	-	expression tag	UNP Q8BG40
C	452	HIS	-	expression tag	UNP Q8BG40
C	453	HIS	-	expression tag	UNP Q8BG40
C	454	HIS	-	expression tag	UNP Q8BG40
C	455	HIS	-	expression tag	UNP Q8BG40
C	456	HIS	-	expression tag	UNP Q8BG40
C	457	SER	-	expression tag	UNP Q8BG40
C	458	SER	-	expression tag	UNP Q8BG40
C	459	GLY	-	expression tag	UNP Q8BG40
C	460	LEU	-	expression tag	UNP Q8BG40
C	461	VAL	-	expression tag	UNP Q8BG40
C	462	PRO	-	expression tag	UNP Q8BG40
C	463	ARG	-	expression tag	UNP Q8BG40
C	464	GLY	-	expression tag	UNP Q8BG40
C	465	SER	-	expression tag	UNP Q8BG40
C	466	HIS	-	expression tag	UNP Q8BG40
C	467	MET	-	expression tag	UNP Q8BG40
C	468	ALA	-	expression tag	UNP Q8BG40
C	469	SER	-	expression tag	UNP Q8BG40
C	470	MET	-	expression tag	UNP Q8BG40
C	471	THR	-	expression tag	UNP Q8BG40
C	472	GLY	-	expression tag	UNP Q8BG40
C	473	GLY	-	expression tag	UNP Q8BG40
C	474	GLN	-	expression tag	UNP Q8BG40
C	475	GLN	-	expression tag	UNP Q8BG40
C	476	MET	-	expression tag	UNP Q8BG40
C	477	GLY	-	expression tag	UNP Q8BG40
C	478	ARG	-	expression tag	UNP Q8BG40
C	479	GLY	-	expression tag	UNP Q8BG40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	480	SER	-	expression tag	UNP Q8BG40

- Molecule 2 is a protein called Katanin p60 ATPase-containing subunit A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	B	77	Total	C	H	N	O	S	0	1	0
			1316	421	661	109	121	4			
2	D	72	Total	C	H	N	O	S	0	2	0
			1229	392	616	103	114	4			

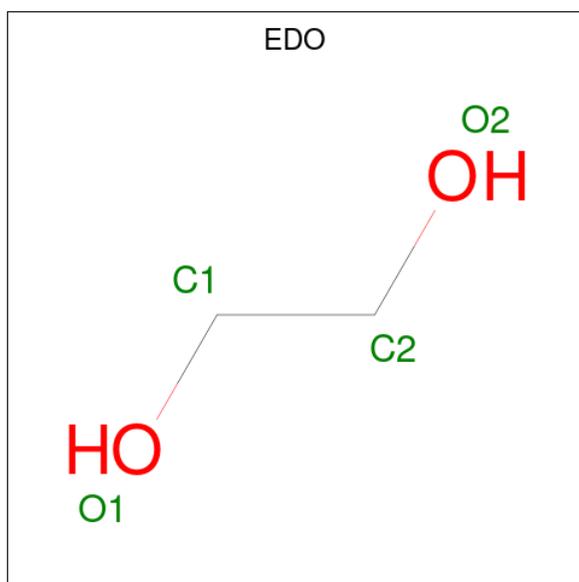
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP E9PZI6
B	0	GLY	-	expression tag	UNP E9PZI6
D	-1	MET	-	initiating methionine	UNP E9PZI6
D	0	GLY	-	expression tag	UNP E9PZI6

- Molecule 3 is a protein called Calmodulin-regulated spectrin-associated protein.

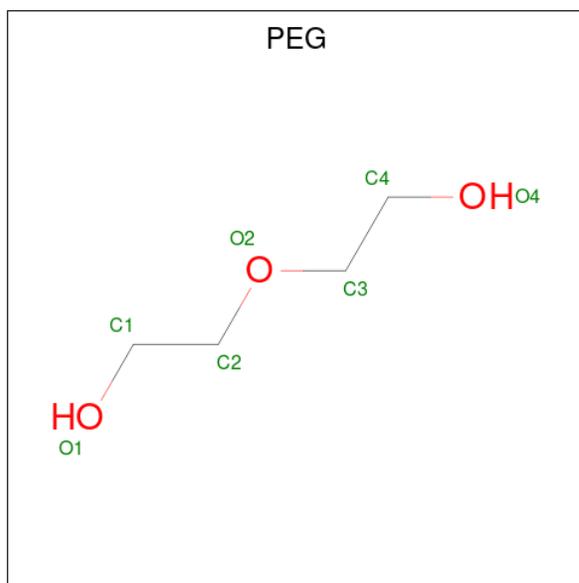
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	10	Total	C	H	N	O	0	0	0
			160	51	80	13	16			
3	F	10	Total	C	H	N	O	0	0	0
			159	51	79	13	16			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	D	1	10	2	6	2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	D	1	17	4	10	3	0	0

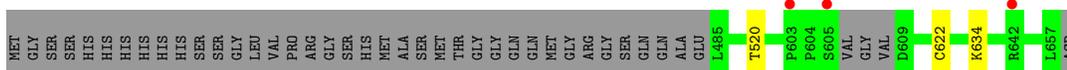
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	169	Total O 169 169	0	0
6	B	55	Total O 55 55	0	0
6	C	57	Total O 57 57	0	0
6	D	16	Total O 16 16	0	0
6	E	10	Total O 10 10	0	0
6	F	2	Total O 2 2	0	0

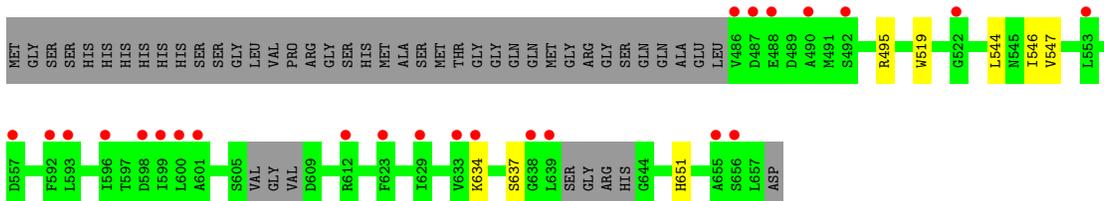
3 Residue-property plots [i](#)

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.

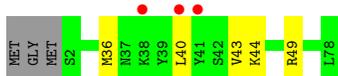
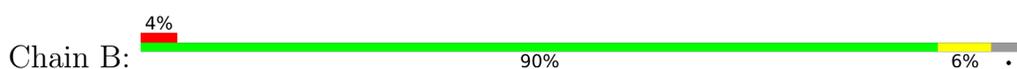
- Molecule 1: Katanin p80 WD40 repeat-containing subunit B1



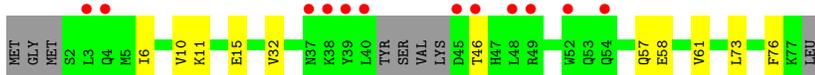
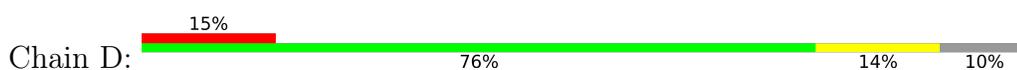
- Molecule 1: Katanin p80 WD40 repeat-containing subunit B1



- Molecule 2: Katanin p60 ATPase-containing subunit A1



- Molecule 2: Katanin p60 ATPase-containing subunit A1



- Molecule 3: Calmodulin-regulated spectrin-associated protein



There are no outlier residues recorded for this chain.

- Molecule 3: Calmodulin-regulated spectrin-associated protein

Chain F:  90% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.33Å 79.06Å 99.06Å 90.00° 94.97° 90.00°	Depositor
Resolution (Å)	41.86 – 1.70 41.86 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.86-1.70) 97.6 (41.86-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.70Å)	Xtrriage
Refinement program	PHENIX (dev_2875: ???)	Depositor
R, R_{free}	0.191 , 0.232 0.191 , 0.232	Depositor DCC
R_{free} test set	1019 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8601	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.21% 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, 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	0.53	1/1373 (0.1%)	0.62	0/1852
1	C	0.34	0/1316	0.52	0/1776
2	B	0.48	0/666	0.58	0/896
2	D	0.43	0/629	0.53	0/845
3	E	0.39	0/80	0.45	0/107
3	F	0.26	0/80	0.42	0/107
All	All	0.45	1/4144 (0.0%)	0.56	0/5583

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	CYS	CB-SG	-5.59	1.72	1.81

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	1347	1412	1410	1	0
1	C	1295	1347	1356	7	0
2	B	655	661	660	2	0
2	D	613	616	604	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	80	80	80	0	0
3	F	80	79	80	1	0
4	D	4	6	6	0	0
5	D	7	10	10	0	0
6	A	169	0	0	1	1
6	B	55	0	0	0	1
6	C	57	0	0	0	0
6	D	16	0	0	1	0
6	E	10	0	0	0	0
6	F	2	0	0	0	0
All	All	4390	4211	4206	15	1

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.

The worst 5 of 15 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:C:634:LYS:HZ2	1:C:651:HIS:CE1	2.16	0.63
1:C:634:LYS:NZ	1:C:651:HIS:CE1	2.67	0.63
1:A:634:LYS:NZ	6:A:704:HOH:O	2.39	0.55
2:D:6:ILE:HG23	2:D:32:VAL:CG2	2.39	0.52
2:D:11:LYS:NZ	6:D:201:HOH:O	2.43	0.52

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:862:HOH:O	6:B:152:HOH:O[2_1154]	1.93	0.27

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	170/212 (80%)	168 (99%)	2 (1%)	0	100	100
1	C	161/212 (76%)	160 (99%)	1 (1%)	0	100	100
2	B	76/80 (95%)	76 (100%)	0	0	100	100
2	D	70/80 (88%)	69 (99%)	1 (1%)	0	100	100
3	E	8/10 (80%)	8 (100%)	0	0	100	100
3	F	8/10 (80%)	8 (100%)	0	0	100	100
All	All	493/604 (82%)	489 (99%)	4 (1%)	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	158/186 (85%)	157 (99%)	1 (1%)	86	80
1	C	152/186 (82%)	151 (99%)	1 (1%)	84	77
2	B	72/73 (99%)	71 (99%)	1 (1%)	67	53
2	D	68/73 (93%)	67 (98%)	1 (2%)	65	51
3	E	9/9 (100%)	9 (100%)	0	100	100
3	F	9/9 (100%)	9 (100%)	0	100	100
All	All	468/536 (87%)	464 (99%)	4 (1%)	78	70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	520	THR
2	B	44	LYS
1	C	637	SER
2	D	46	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	511	ASN
1	C	651	HIS

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](#)

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	$\# Z > 2$
4	EDO	D	101	-	3,3,3	0.44	0	2,2,2	0.34	0
5	PEG	D	102	-	6,6,6	0.48	0	5,5,5	0.32	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	EDO	D	101	-	-	0/1/1/1	-
5	PEG	D	102	-	-	0/4/4/4	-

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	170/212 (80%)	0.29	3 (1%) 68 72	16, 28, 56, 78	0
1	C	165/212 (77%)	0.73	24 (14%) 2 2	33, 52, 87, 115	0
2	B	77/80 (96%)	0.26	3 (3%) 39 44	19, 31, 59, 82	0
2	D	72/80 (90%)	0.86	12 (16%) 1 1	28, 48, 84, 97	0
3	E	10/10 (100%)	0.23	0 100 100	24, 36, 54, 67	0
3	F	10/10 (100%)	0.23	0 100 100	39, 48, 76, 78	0
All	All	504/604 (83%)	0.51	42 (8%) 11 13	16, 40, 80, 115	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	38	LYS	7.2
1	C	639	LEU	5.5
2	B	40	LEU	4.8
1	C	638	GLY	4.7
2	D	3	LEU	4.7

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, 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
5	PEG	D	102	7/7	0.78	0.15	63,76,88,89	0
4	EDO	D	101	4/4	0.91	0.23	57,69,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.