wwPDB EM Validation Summary Report

Nov 5, 2024 – 10:57 AM JST

PDB ID	:	8ZBE
EMDB ID	:	EMD-39901
Title	:	cryo-EM structure of the octreotide-bound SSTR5-Gi complex
Authors	:	Li, Y.G.; Meng, X.Y.; Yang, X.R.; Ling, S.L.; Shi, P.; Tian, C.L.; Yang, F.
Deposited on	:	2024-04-26
Resolution	:	3.24 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

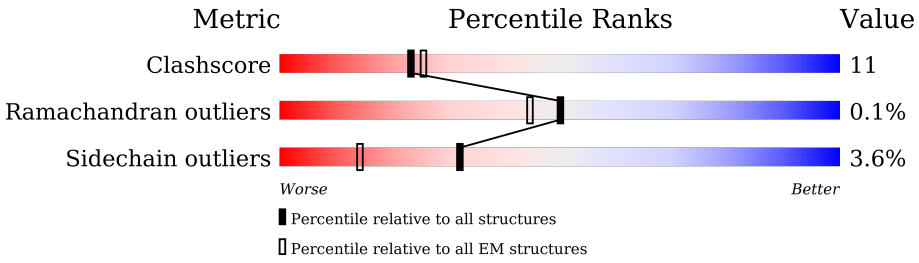
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	570	40% 6% • 54%
2	B	354	50% 10% • 40%
3	D	71	63% 18% 18%
4	E	304	62% 15% 23%
5	P	8	25% 25% 25% 25%
6	C	377	63% 27% • 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7489 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Beta-2 adrenergic receptor,Somatostatin receptor type 5,lgbit (fusion protein).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	263	Total	C	N	O	S	0	0
			1648	1045	293	304	6		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-47	MET	-	initiating methionine	UNP P07550
A	-46	LYS	-	expression tag	UNP P07550
A	-45	THR	-	expression tag	UNP P07550
A	-44	ILE	-	expression tag	UNP P07550
A	-43	ILE	-	expression tag	UNP P07550
A	-42	ALA	-	expression tag	UNP P07550
A	-41	LEU	-	expression tag	UNP P07550
A	-40	SER	-	expression tag	UNP P07550
A	-39	TYR	-	expression tag	UNP P07550
A	-38	ILE	-	expression tag	UNP P07550
A	-37	PHE	-	expression tag	UNP P07550
A	-36	CYS	-	expression tag	UNP P07550
A	-35	LEU	-	expression tag	UNP P07550
A	-34	VAL	-	expression tag	UNP P07550
A	-33	PHE	-	expression tag	UNP P07550
A	-32	ALA	-	expression tag	UNP P07550
A	-31	ASP	-	expression tag	UNP P07550
A	-30	TYR	-	expression tag	UNP P07550
A	-29	LYS	-	expression tag	UNP P07550
A	-28	ASP	-	expression tag	UNP P07550
A	-27	ASP	-	expression tag	UNP P07550
A	-26	ASP	-	expression tag	UNP P07550
A	-25	ASP	-	expression tag	UNP P07550
A	-24	LYS	-	expression tag	UNP P07550

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	213	Total	C	N	O	S	0	0
			1414	890	246	272	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	ALA	GLY	conflict	UNP P63096
B	326	SER	ALA	conflict	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein subunit gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	58	Total	C	N	O	0	0
			329	203	60	66		

- Molecule 4 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	233	Total	C	N	O	S	0	0
			1602	1009	271	313	9		

- Molecule 5 is a protein called octreotide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	6	Total	C	N	O	S	0	0
			53	36	8	7	2		

- Molecule 6 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	341	Total	C	N	O	S	0	0
			2443	1509	447	475	12		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP P54311
C	-9	HIS	-	expression tag	UNP P54311
C	-8	HIS	-	expression tag	UNP P54311
C	-7	HIS	-	expression tag	UNP P54311
C	-6	HIS	-	expression tag	UNP P54311

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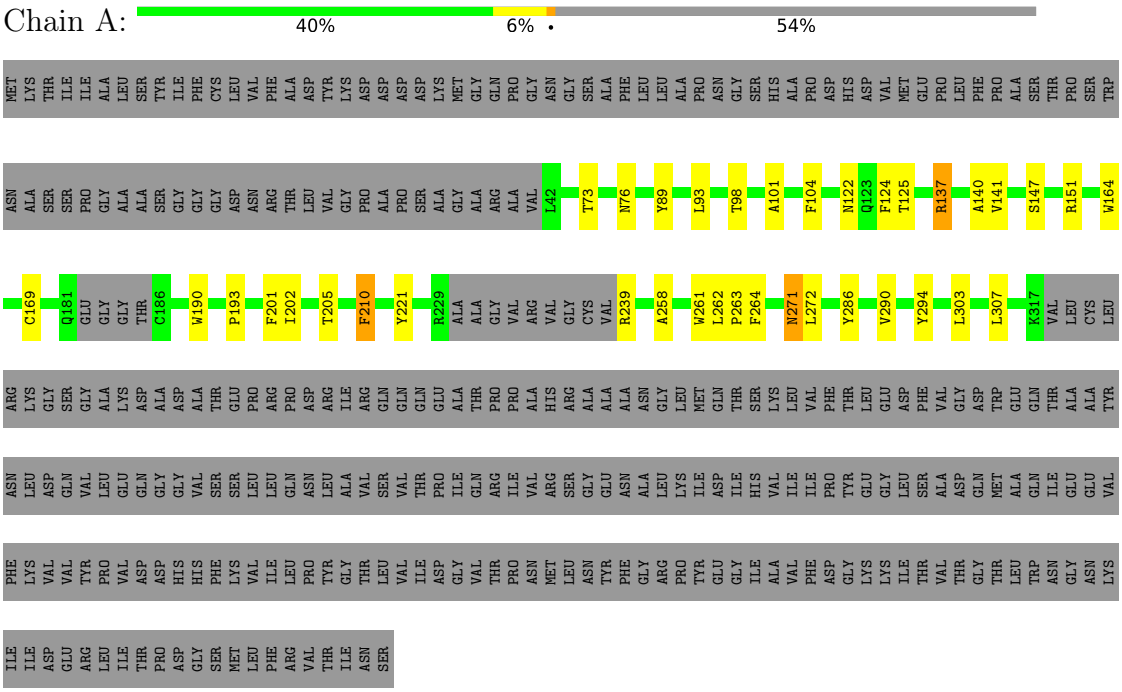
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P54311
C	-4	HIS	-	expression tag	UNP P54311
C	-3	GLY	-	expression tag	UNP P54311
C	-2	SER	-	expression tag	UNP P54311
C	-1	LEU	-	expression tag	UNP P54311
C	0	LEU	-	expression tag	UNP P54311
C	1	GLN	-	expression tag	UNP P54311
C	341	GLY	-	expression tag	UNP P54311
C	342	SER	-	expression tag	UNP P54311
C	343	SER	-	expression tag	UNP P54311
C	344	GLY	-	expression tag	UNP P54311
C	345	GLY	-	expression tag	UNP P54311
C	346	GLY	-	expression tag	UNP P54311
C	347	GLY	-	expression tag	UNP P54311
C	348	SER	-	expression tag	UNP P54311
C	349	GLY	-	expression tag	UNP P54311
C	350	GLY	-	expression tag	UNP P54311
C	351	GLY	-	expression tag	UNP P54311
C	352	GLY	-	expression tag	UNP P54311
C	353	SER	-	expression tag	UNP P54311
C	354	SER	-	expression tag	UNP P54311
C	355	GLY	-	expression tag	UNP P54311
C	356	VAL	-	expression tag	UNP P54311
C	357	SER	-	expression tag	UNP P54311
C	358	GLY	-	expression tag	UNP P54311
C	359	TRP	-	expression tag	UNP P54311
C	360	ARG	-	expression tag	UNP P54311
C	361	LEU	-	expression tag	UNP P54311
C	362	PHE	-	expression tag	UNP P54311
C	363	LYS	-	expression tag	UNP P54311
C	364	LYS	-	expression tag	UNP P54311
C	365	ILE	-	expression tag	UNP P54311
C	366	SER	-	expression tag	UNP P54311

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. 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. 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.

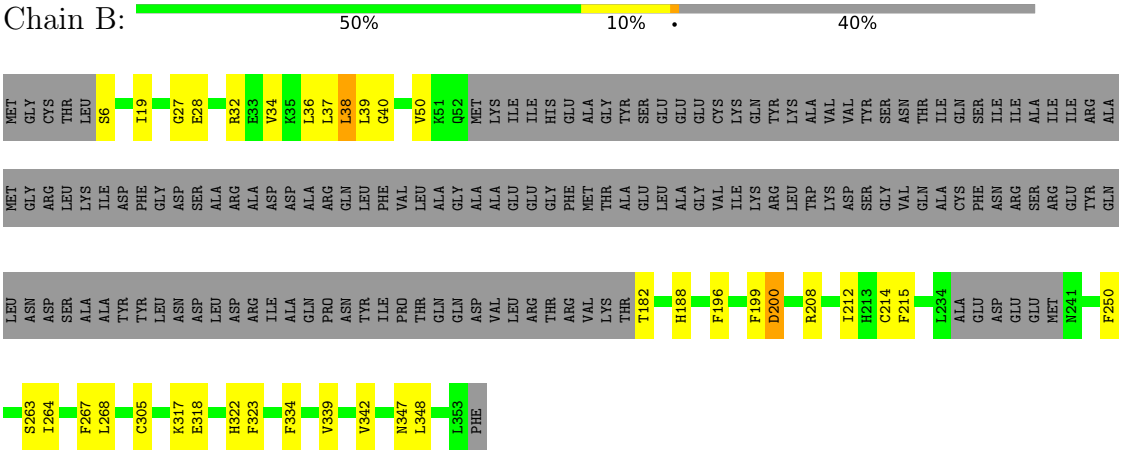
• Molecule 1: Beta-2 adrenergic receptor,Somatostatin receptor type 5,lgbit (fusion protein)

Chain A:



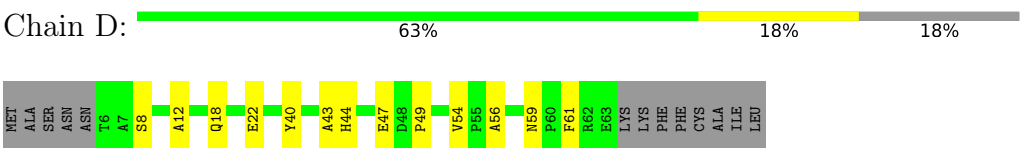
• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain B:



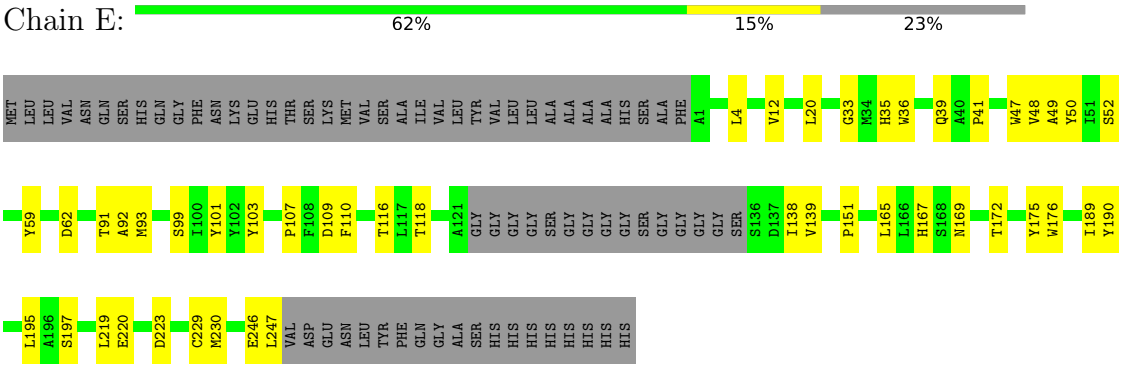
• Molecule 3: Guanine nucleotide-binding protein subunit gamma

Chain D:



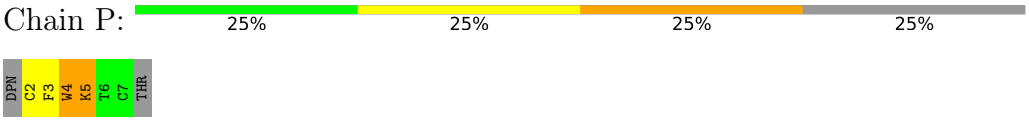
• Molecule 4: ScFv16

Chain E:



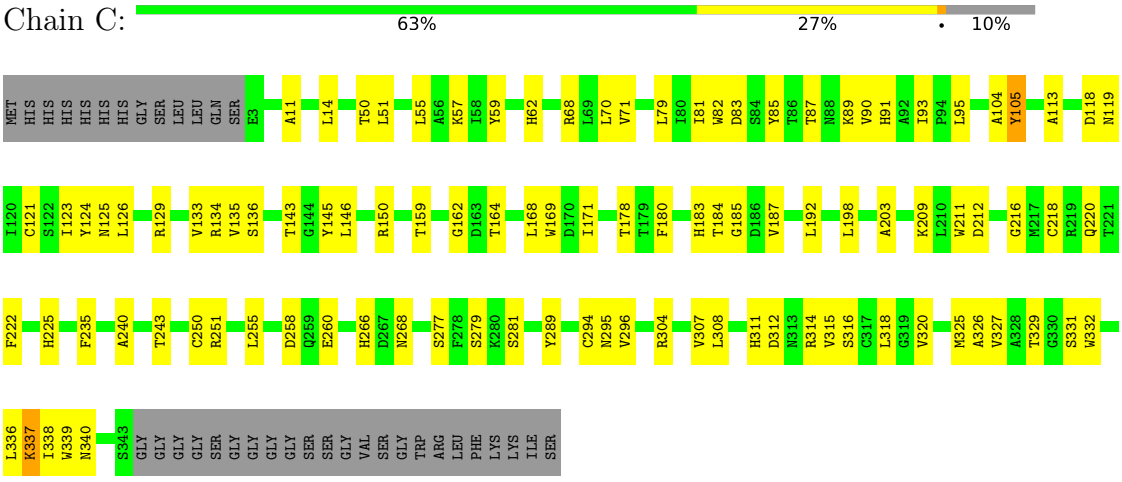
• Molecule 5: octreotide

Chain P:



• Molecule 6: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	452725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTR

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	0.29	0/1676	0.53	0/2322
2	B	0.26	0/1433	0.46	0/1960
3	D	0.39	0/334	0.75	0/467
4	E	0.28	0/1640	0.54	0/2242
5	P	0.52	0/38	1.34	1/47 (2.1%)
6	C	0.30	0/2488	0.58	0/3393
All	All	0.29	0/7609	0.55	1/10431 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	5	LYS	N-CA-CB	5.49	120.47	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1648	0	1347	25	0
2	B	1414	0	1155	23	0
3	D	329	0	225	10	0
4	E	1602	0	1367	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	53	0	45	5	0
6	C	2443	0	2191	75	0
All	All	7489	0	6330	149	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 11.

The worst 5 of 149 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)
6:C:150:ARG:HB2	6:C:192:LEU:HD13	1.68	0.76
6:C:164:THR:HG22	6:C:185:GLY:O	1.87	0.74
6:C:164:THR:HG22	6:C:185:GLY:C	2.13	0.68
6:C:235:PHE:HB2	6:C:240:ALA:HB3	1.75	0.67
1:A:137:ARG:NH1	1:A:221:TYR:OH	2.29	0.66

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 PDB entries followed by that with respect to all EM entries.

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	257/570 (45%)	240 (93%)	17 (7%)	0	100 100
2	B	207/354 (58%)	194 (94%)	13 (6%)	0	100 100
3	D	56/71 (79%)	51 (91%)	5 (9%)	0	100 100
4	E	229/304 (75%)	219 (96%)	10 (4%)	0	100 100
5	P	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0 0
6	C	339/377 (90%)	316 (93%)	23 (7%)	0	100 100
All	All	1091/1684 (65%)	1021 (94%)	69 (6%)	1 (0%)	50 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	3	PHE

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 PDB entries followed by that with respect to all EM entries.

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	118/471 (25%)	112 (95%)	6 (5%)	20 50
2	B	110/306 (36%)	103 (94%)	7 (6%)	14 43
3	D	15/58 (26%)	15 (100%)	0	100 100
4	E	142/246 (58%)	138 (97%)	4 (3%)	38 65
5	P	5/6 (83%)	5 (100%)	0	100 100
6	C	229/308 (74%)	224 (98%)	5 (2%)	47 71
All	All	619/1395 (44%)	597 (96%)	22 (4%)	32 59

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	52	SER
6	C	105	TYR
4	E	109	ASP
6	C	118	ASP
2	B	6	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	167	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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
5	DTR	P	4	5	13,15,16	1.14	0	13,20,22	2.45	4 (30%)

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
5	DTR	P	4	5	-	1/4/6/8	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	4	DTR	CB-CA-C	-5.79	100.62	111.47
5	P	4	DTR	CG-CB-CA	-4.83	107.06	114.53
5	P	4	DTR	CE3-CD2-CE2	2.61	121.63	118.17
5	P	4	DTR	CZ3-CE3-CD2	-2.45	117.50	120.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	4	DTR	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	4	DTR	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.