



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 12:19 pm GMT

PDB ID : 5U3Z
Title : Human PPARdelta ligand-binding domain in complexed with specific agonist
10
Authors : Wu, C.-C.; Baiga, T.J.; Downes, M.; La Clair, J.J.; Atkins, A.R.; Richard,
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Deposited on : 2016-12-03
Resolution : 1.72 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

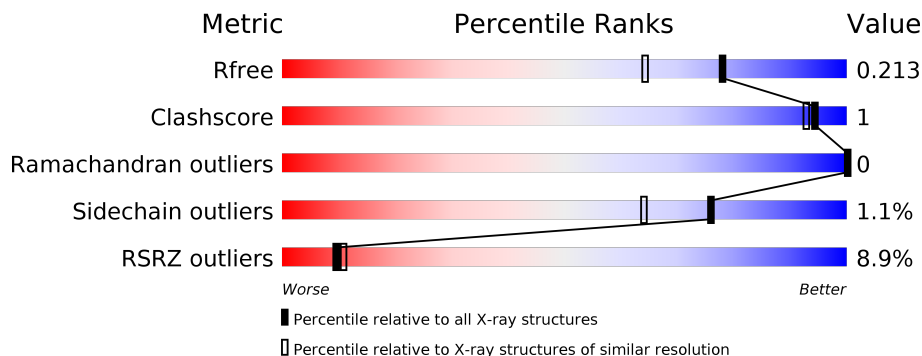
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	111664	4894 (1.74-1.70)
Clashscore	122126	5296 (1.74-1.70)
Ramachandran outliers	120053	5219 (1.74-1.70)
Sidechain outliers	120020	5219 (1.74-1.70)
RSRZ outliers	108989	4804 (1.74-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	272	<div> <div>10%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	272	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div></div> </div> </div>

2 Entry composition [i](#)

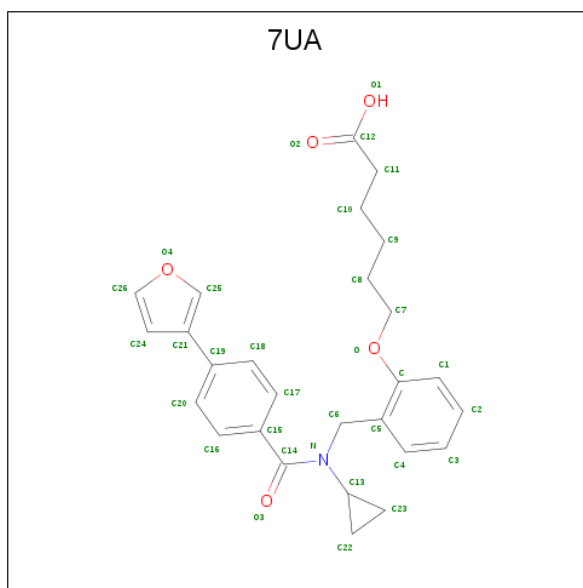
There are 6 unique types of molecules in this entry. The entry contains 9494 atoms, of which 4708 are hydrogens and 0 are deuteriums.

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 Peroxisome proliferator-activated receptor delta.

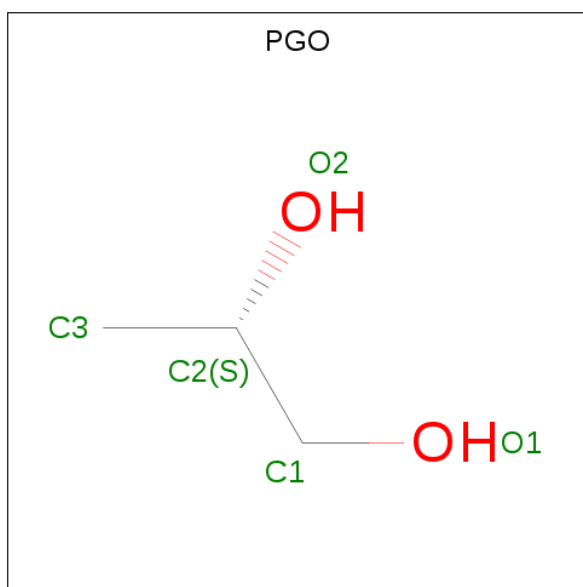
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	H	N	O	S	0	19	0
			4502	1436	2277	378	401	10			
1	B	261	Total	C	H	N	O	S	0	15	0
			4353	1394	2199	361	390	9			

- Molecule 2 is 6-[2-({cyclopropyl[4-(furan-3-yl)benzene-1-carbonyl]amino}methyl)phenoxy]hexanoic acid (three-letter code: 7UA) (formula: C₂₇H₂₉NO₅).



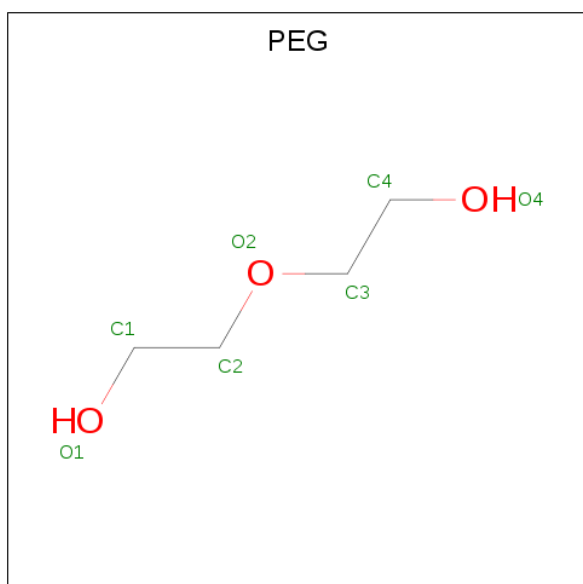
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			61	27	28	1	5		
2	B	1	Total	C	H	N	O	0	0
			61	27	28	1	5		

- Molecule 3 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



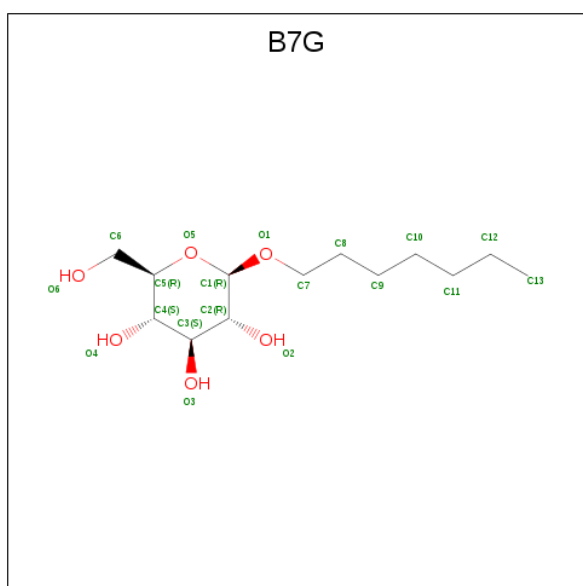
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	3	8	2		
3	A	1	Total	C	H	O	0	0
			13	3	8	2		
3	A	1	Total	C	H	O	0	0
			13	3	8	2		
3	A	1	Total	C	H	O	0	1
			26	6	16	4		
3	B	1	Total	C	H	O	0	0
			13	3	8	2		

- 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 17 4 10 3	0	0
4	A	1	Total C H O 17 4 10 3	0	0
4	B	1	Total C H O 17 4 10 3	0	0
4	B	1	Total C H O 17 4 10 3	0	0
4	B	1	Total C H O 17 4 10 3	0	0

- Molecule 5 is HEPTYL-BETA-D-GLUCOPYRANOSIDE (three-letter code: B7G) (formula: $C_{13}H_{26}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 45 13 26 6	0	0
5	A	1	Total C H O 45 13 26 6	0	0
5	B	1	Total C H O 45 13 26 6	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	121	Total O 121 121	0	0

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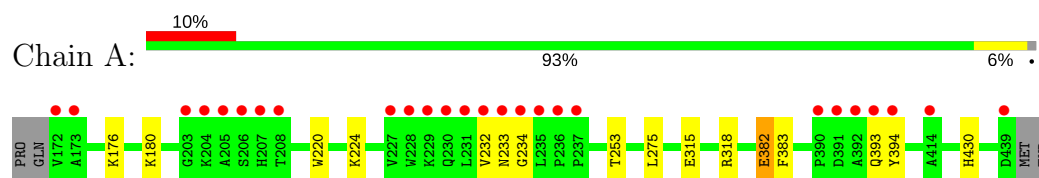
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	98	Total	O	0	0
			98	98		

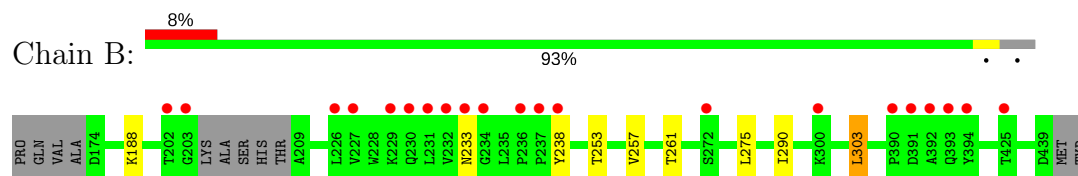
3 Residue-property plots [i](#)

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: Peroxisome proliferator-activated receptor delta



- Molecule 1: Peroxisome proliferator-activated receptor delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.43Å 94.75Å 96.05Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	42.53 – 1.72 42.53 – 1.72	Depositor EDS
% Data completeness (in resolution range)	95.3 (42.53-1.72) 95.4 (42.53-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.9pre_1665	Depositor
R, R_{free}	0.172 , 0.214 0.175 , 0.213	Depositor DCC
R_{free} test set	1933 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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: PGO, 7UA, PEG, B7G

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	0.56	0/2353	0.64	0/3182
1	B	0.52	0/2275	0.64	1/3075 (0.0%)
All	All	0.54	0/4628	0.64	1/6257 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	LEU	CA-CB-CG	7.52	132.59	115.30

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	2225	2277	2184	8	1
1	B	2154	2199	2110	6	1
2	A	33	28	0	1	0
2	B	33	28	0	1	0
3	A	25	40	40	1	0
3	B	5	8	8	0	0
4	A	14	20	20	0	0
4	B	21	30	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	38	52	52	1	0
5	B	19	26	26	0	0
6	A	121	0	0	0	0
6	B	98	0	0	1	0
All	All	4786	4708	4470	13	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 1.

The worst 5 of 13 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:B:253[A]:THR:HG21	2:B:502:7UA:O1	1.98	0.64
1:A:253[A]:THR:HG21	2:A:501:7UA:O1	2.01	0.61
1:A:393:GLN:HG3	1:A:394:TYR:CD2	2.46	0.50
1:A:315[A]:GLU:OE2	1:A:318:ARG:NH1	2.45	0.49
1:A:220:TRP:CZ2	1:A:224:LYS:HD2	2.52	0.44

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)
1:A:382:GLU:OE1	1:B:238[B]:TYR:OH[2_547]	2.13	0.07

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	285/272 (105%)	277 (97%)	8 (3%)	0	100	100
1	B	272/272 (100%)	268 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	557/544 (102%)	545 (98%)	12 (2%)	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	253/240 (105%)	250 (99%)	3 (1%)	74	60
1	B	244/240 (102%)	242 (99%)	2 (1%)	83	75
All	All	497/480 (104%)	492 (99%)	5 (1%)	76	68

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
1	A	232	VAL
1	A	382	GLU
1	B	233	ASN
1	B	303	LEU

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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
2	7UA	A	501	-	30,36,36	0.93	1 (3%)	38,48,48	1.46	4 (10%)
3	PGO	A	502	-	4,4,4	0.48	0	4,4,4	0.91	0
4	PEG	A	503	-	6,6,6	0.56	0	5,5,5	0.39	0
3	PGO	A	504	-	4,4,4	0.27	0	4,4,4	0.66	0
5	B7G	A	505	-	19,19,19	0.95	1 (5%)	24,24,24	0.89	0
4	PEG	A	506	-	6,6,6	0.62	0	5,5,5	0.32	0
3	PGO	A	507	-	4,4,4	0.28	0	4,4,4	1.04	0
5	B7G	A	508	-	19,19,19	0.81	0	24,24,24	0.94	1 (4%)
3	PGO	A	509[A]	-	4,4,4	0.38	0	4,4,4	0.35	0
3	PGO	A	509[B]	-	4,4,4	0.31	0	4,4,4	0.74	0
5	B7G	B	501	-	19,19,19	0.71	0	24,24,24	1.15	2 (8%)
2	7UA	B	502	-	30,36,36	0.91	1 (3%)	38,48,48	1.52	6 (15%)
4	PEG	B	503	-	6,6,6	0.58	0	5,5,5	0.31	0
4	PEG	B	504	-	6,6,6	0.62	0	5,5,5	0.34	0
3	PGO	B	505	-	4,4,4	0.30	0	4,4,4	1.27	1 (25%)
4	PEG	B	506	-	6,6,6	0.64	0	5,5,5	0.53	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
2	7UA	A	501	-	-	0/27/31/31	0/3/4/4
3	PGO	A	502	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	503	-	-	0/4/4/4	0/0/0/0
3	PGO	A	504	-	-	0/2/2/2	0/0/0/0
5	B7G	A	505	-	-	0/10/30/30	0/1/1/1
4	PEG	A	506	-	-	0/4/4/4	0/0/0/0
3	PGO	A	507	-	-	0/2/2/2	0/0/0/0
5	B7G	A	508	-	-	0/10/30/30	0/1/1/1
3	PGO	A	509[A]	-	-	0/2/2/2	0/0/0/0
3	PGO	A	509[B]	-	-	0/2/2/2	0/0/0/0
5	B7G	B	501	-	-	0/10/30/30	0/1/1/1
2	7UA	B	502	-	-	0/27/31/31	0/3/4/4
4	PEG	B	503	-	-	0/4/4/4	0/0/0/0
4	PEG	B	504	-	-	0/4/4/4	0/0/0/0
3	PGO	B	505	-	-	0/2/2/2	0/0/0/0
4	PEG	B	506	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	7UA	C24-C21	-2.47	1.38	1.42
5	A	505	B7G	O5-C1	2.30	1.47	1.41
2	B	502	7UA	C22-C13	2.36	1.53	1.49

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	7UA	C23-C13-N	-4.90	111.46	119.93
2	A	501	7UA	C23-C13-N	-4.17	112.72	119.93
2	A	501	7UA	O3-C14-C15	-2.50	115.42	120.19
3	B	505	PGO	O1-C1-C2	-2.48	104.95	111.23
2	B	502	7UA	C20-C16-C15	-2.33	118.14	120.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	7UA	1	0
5	A	505	B7G	1	0
3	A	509[A]	PGO	1	0
2	B	502	7UA	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 [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	268/272 (98%)	0.69	26 (9%) 8 8	19, 33, 70, 102	0
1	B	261/272 (95%)	0.57	21 (8%) 12 14	20, 37, 71, 115	0
All	All	529/544 (97%)	0.63	47 (8%) 9 11	19, 35, 72, 115	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	VAL	9.4
1	A	229	LYS	7.6
1	A	394	TYR	6.9
1	A	233	ASN	6.8
1	B	233	ASN	6.3

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 carbohydrates 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(\AA^2)	Q<0.9
4	PEG	A	506	7/7	0.50	0.27	76,91,96,96	0
4	PEG	B	504	7/7	0.58	0.26	63,78,91,91	0
3	PGO	A	509[B]	5/5	0.61	0.25	56,70,84,84	13
3	PGO	A	509[A]	5/5	0.61	0.25	51,63,75,76	13
5	B7G	A	505	19/19	0.66	0.19	27,93,166,174	0
4	PEG	B	503	7/7	0.68	0.26	59,86,100,101	0
3	PGO	A	507	5/5	0.77	0.34	60,73,83,92	0
4	PEG	A	503	7/7	0.78	0.13	59,77,98,98	0
3	PGO	A	504	5/5	0.80	0.18	48,61,75,77	0
4	PEG	B	506	7/7	0.81	0.16	43,78,95,95	0
5	B7G	A	508	19/19	0.88	0.11	32,43,52,67	0
5	B7G	B	501	19/19	0.88	0.12	32,42,50,52	0
3	PGO	B	505	5/5	0.90	0.14	44,64,71,81	0
3	PGO	A	502	5/5	0.91	0.20	48,62,69,75	0
2	7UA	B	502	33/33	0.95	0.10	22,30,41,44	0
2	7UA	A	501	33/33	0.97	0.11	16,25,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.