



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2018 – 07:29 PM EDT

PDB ID : 4JK4  
Title : Crystal Structure of Bovine Serum Albumin in complex with 3,5-diiodosalicylic acid  
Authors : Zielinski, K.; Bujacz, A.; Sekula, B.; Bujacz, G.  
Deposited on : 2013-03-09  
Resolution : 2.65 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](mailto: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.

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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	:	rb-20031172
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)	:	rb-20031172

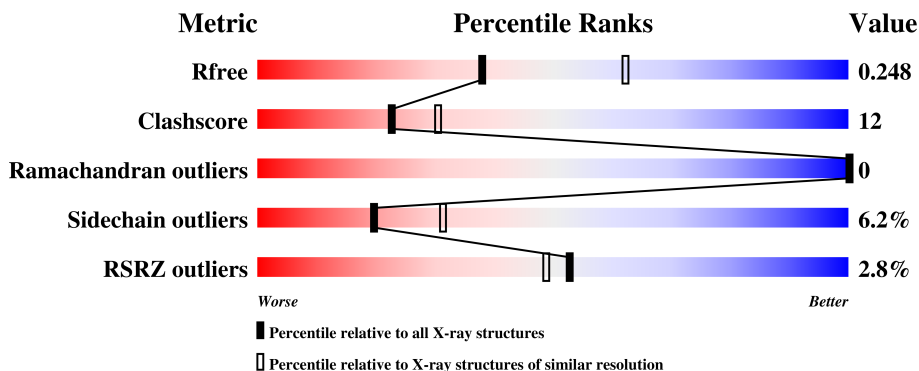
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1112 (2.68-2.64)
Clashscore	122126	1151 (2.68-2.64)
Ramachandran outliers	120053	1133 (2.68-2.64)
Sidechain outliers	120020	1133 (2.68-2.64)
RSRZ outliers	108989	1098 (2.68-2.64)

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  $\geq 3$ , 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	583	<div> <div>2%</div> <div>69%</div> <div>29%</div> <div>•</div> </div>
1	B	583	<div> <div>4%</div> <div>72%</div> <div>26%</div> <div>•</div> </div>

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
2	DIU	B	603	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9643 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.

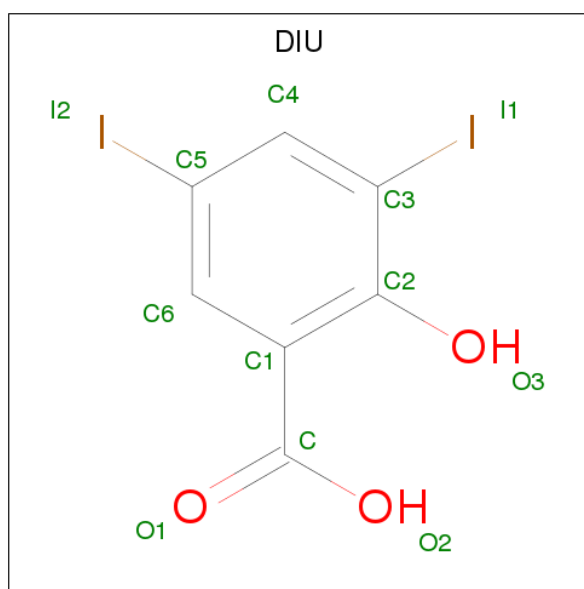
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	3	0
			4668	2944	782	903	39			
1	B	582	Total	C	N	O	S	0	0	0
			4645	2931	780	895	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	THR	ALA	VARIANT	UNP P02769
B	190	THR	ALA	VARIANT	UNP P02769

- Molecule 2 is 2-HYDROXY-3,5-DIIODO-BENZOIC ACID (three-letter code: DIU) (formula: C<sub>7</sub>H<sub>4</sub>I<sub>2</sub>O<sub>3</sub>).



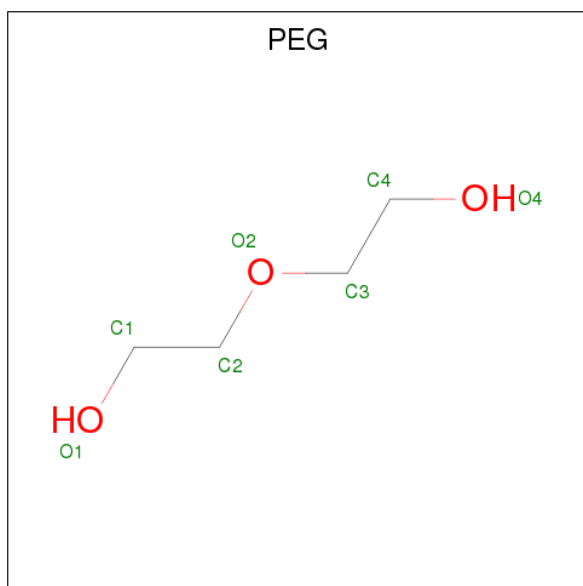
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			12	7	2	3		

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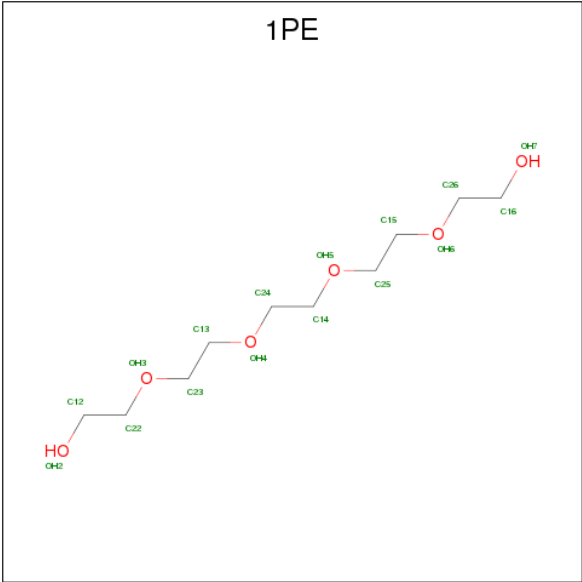
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	B	1	Total	C	I	O	0	0
			12	7	2	3		
2	B	1	Total	C	I	O	0	0
			12	7	2	3		
2	B	1	Total	C	I	O	0	0
			12	7	2	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



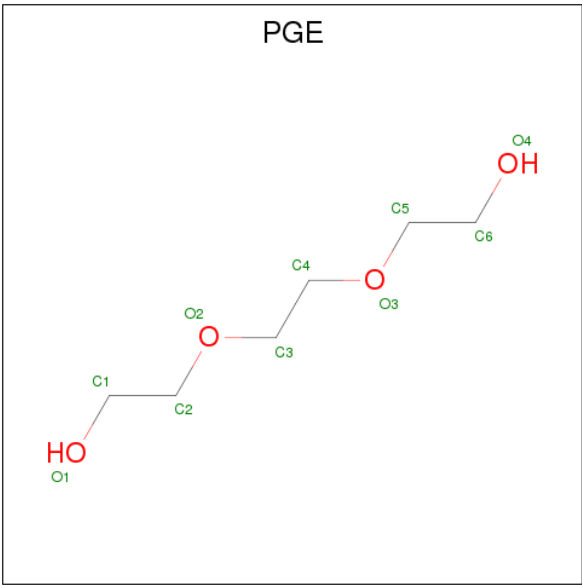
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Ca	0	0
			3	3		
6	A	4	Total	Ca	0	0
			4	4		

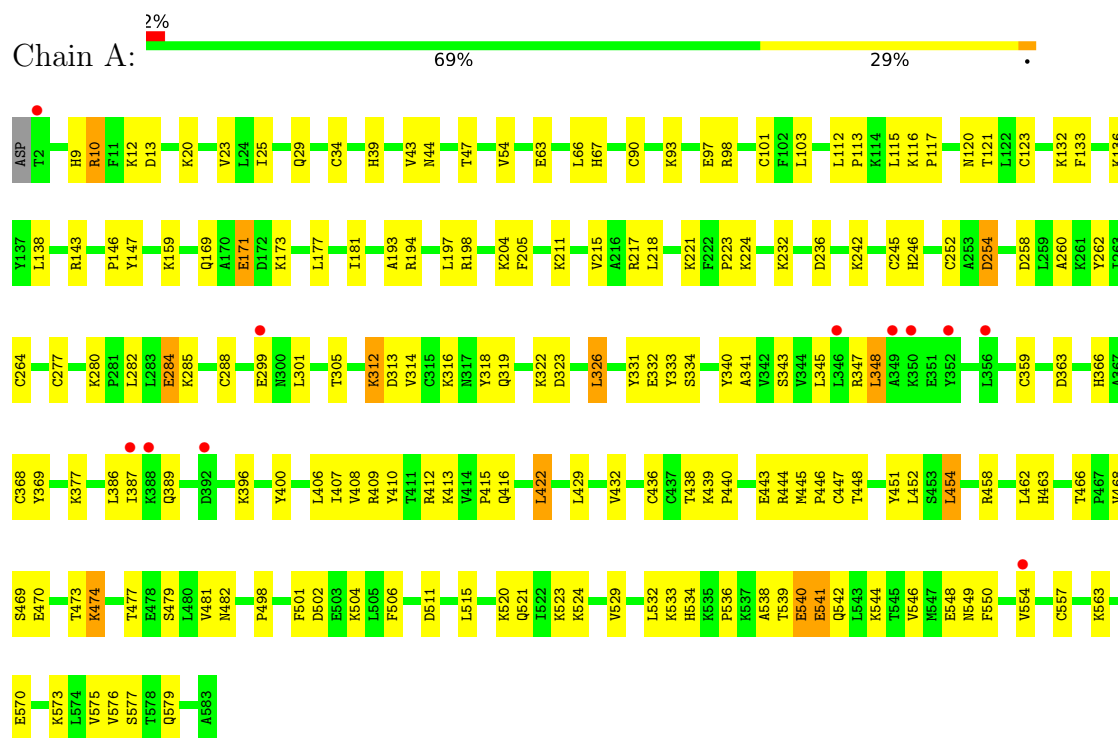
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	82	Total	O	0	0
			82	82		
7	B	63	Total	O	0	0
			63	63		

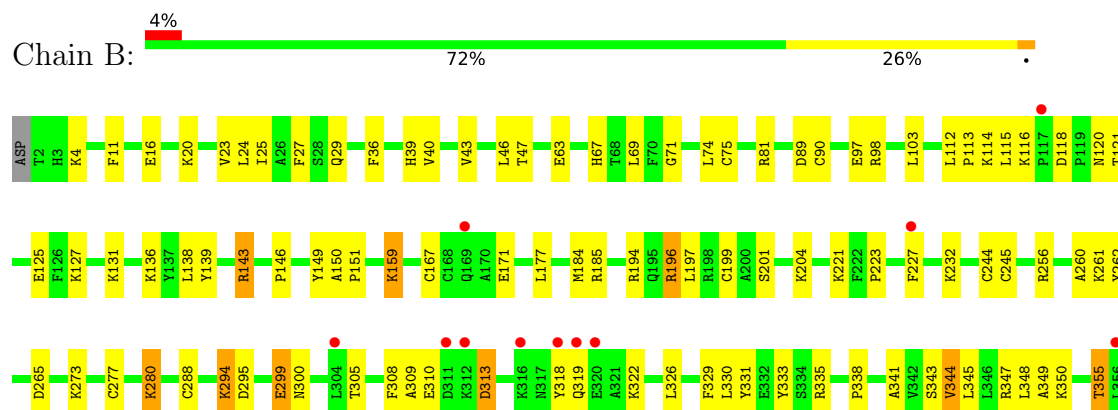
### 3 Residue-property plots

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.

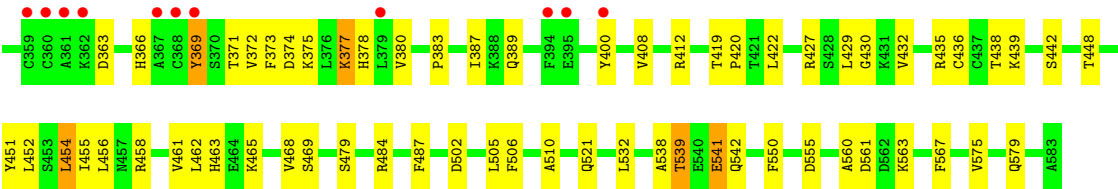
#### • Molecule 1: Serum albumin



#### • Molecule 1: Serum albumin







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.41Å 44.80Å 146.90Å 90.00° 115.77° 90.00°	Depositor
Resolution (Å)	36.53 – 2.65 44.10 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.53-2.65) 98.7 (44.10-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.188 , 0.246 0.191 , 0.248	Depositor DCC
$R_{free}$ test set	1844 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, DIU, CA, PGE, 1PE

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	0.99	3/4766 (0.1%)	0.97	4/6434 (0.1%)
1	B	0.91	3/4740 (0.1%)	0.91	2/6399 (0.0%)
All	All	0.95	6/9506 (0.1%)	0.94	6/12833 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	CYS	CB-SG	5.83	1.92	1.82
1	A	277	CYS	CB-SG	-5.66	1.72	1.81
1	B	199	CYS	CB-SG	5.40	1.91	1.82
1	A	245	CYS	CB-SG	5.29	1.91	1.82
1	A	147	TYR	CB-CG	-5.25	1.43	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	69	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	348	LEU	CA-CB-CG	-5.28	103.15	115.30
1	A	254	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	454	LEU	CB-CG-CD2	-5.23	102.12	111.00

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	4668	0	4573	116	0
1	B	4645	0	4559	115	0
2	A	48	0	8	5	0
2	B	48	0	9	10	0
3	A	7	0	10	2	0
3	B	7	0	10	3	0
4	A	32	0	44	3	0
4	B	16	0	22	0	0
5	A	10	0	14	1	0
5	B	10	0	14	2	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	82	0	0	6	0
7	B	63	0	0	9	0
All	All	9643	0	9263	232	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 12.

The worst 5 of 232 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:463:HIS:HE1	1:A:469:SER:H	1.15	0.93
1:B:432:VAL:HG22	1:B:451:TYR:CD2	2.16	0.80
1:B:11:PHE:HE2	1:B:47:THR:HG23	1.47	0.79
1:B:71:GLY:HA3	7:B:704:HOH:O	1.86	0.74
1:B:432:VAL:HG22	1:B:451:TYR:HD2	1.54	0.73

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	A	583/583 (100%)	570 (98%)	13 (2%)	0	100	100
1	B	580/583 (100%)	563 (97%)	17 (3%)	0	100	100
All	All	1163/1166 (100%)	1133 (97%)	30 (3%)	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	523/521 (100%)	491 (94%)	32 (6%)	20	33
1	B	520/521 (100%)	486 (94%)	34 (6%)	19	30
All	All	1043/1042 (100%)	977 (94%)	66 (6%)	20	31

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	540	GLU
1	B	159	LYS
1	B	479	SER
1	A	541	GLU
1	B	114	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN
1	A	463	HIS
1	B	366	HIS
1	A	366	HIS
1	B	241	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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
2	DIU	A	601	-	9,12,12	2.12	3 (33%)	12,17,17	1.56	2 (16%)
2	DIU	A	602	-	9,12,12	2.23	4 (44%)	12,17,17	0.82	0
2	DIU	A	603	-	9,12,12	2.33	4 (44%)	12,17,17	0.96	1 (8%)
2	DIU	A	604	-	9,12,12	3.45	6 (66%)	12,17,17	0.81	0
3	PEG	A	605	-	6,6,6	0.71	0	5,5,5	0.96	0
4	1PE	A	606	-	15,15,15	0.82	0	14,14,14	1.22	2 (14%)
4	1PE	A	607	-	15,15,15	0.97	0	14,14,14	0.94	0
5	PGE	A	608	-	9,9,9	0.60	0	8,8,8	0.80	0
2	DIU	B	601	-	9,12,12	2.72	5 (55%)	12,17,17	1.03	1 (8%)
2	DIU	B	602	-	9,12,12	1.78	3 (33%)	12,17,17	0.69	0
2	DIU	B	603	-	9,12,12	2.62	4 (44%)	12,17,17	1.17	2 (16%)
2	DIU	B	604	-	9,12,12	3.57	7 (77%)	12,17,17	1.02	0
3	PEG	B	605	-	6,6,6	0.64	0	5,5,5	0.64	0
4	1PE	B	606	-	15,15,15	0.80	0	14,14,14	0.67	0
5	PGE	B	607	-	9,9,9	0.67	0	8,8,8	0.33	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	DIU	A	601	-	-	0/0/4/4	0/1/1/1
2	DIU	A	602	-	-	0/0/4/4	0/1/1/1
2	DIU	A	603	-	-	0/0/4/4	0/1/1/1
2	DIU	A	604	-	-	0/0/4/4	0/1/1/1
3	PEG	A	605	-	-	0/4/4/4	0/0/0/0
4	1PE	A	606	-	-	0/13/13/13	0/0/0/0
4	1PE	A	607	-	-	0/13/13/13	0/0/0/0
5	PGE	A	608	-	-	0/7/7/7	0/0/0/0
2	DIU	B	601	-	-	0/0/4/4	0/1/1/1
2	DIU	B	602	-	-	0/0/4/4	0/1/1/1
2	DIU	B	603	-	-	0/0/4/4	0/1/1/1
2	DIU	B	604	-	-	0/0/4/4	0/1/1/1
3	PEG	B	605	-	-	0/4/4/4	0/0/0/0
4	1PE	B	606	-	-	0/13/13/13	0/0/0/0
5	PGE	B	607	-	-	0/7/7/7	0/0/0/0

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	DIU	C3-I1	-3.33	2.02	2.10
2	B	601	DIU	C5-I2	-3.07	2.02	2.10
2	B	601	DIU	O3-C2	-2.15	1.32	1.37
2	A	603	DIU	C3-I1	-2.15	2.05	2.10
2	A	601	DIU	C6-C1	2.07	1.43	1.39

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	1PE	OH5-C14-C24	-3.14	95.85	110.37
2	A	601	DIU	C4-C5-I2	-2.00	116.78	119.38
4	A	606	1PE	OH3-C22-C12	2.17	119.83	110.10
2	B	603	DIU	C6-C5-I2	2.22	122.26	119.38
2	A	603	DIU	C3-C4-C5	2.26	121.44	119.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	DIU	1	0
2	A	602	DIU	2	0
2	A	603	DIU	1	0
2	A	604	DIU	1	0
3	A	605	PEG	2	0
4	A	606	1PE	2	0
4	A	607	1PE	1	0
5	A	608	PGE	1	0
2	B	601	DIU	2	0
2	B	602	DIU	1	0
2	B	603	DIU	5	0
2	B	604	DIU	2	0
3	B	605	PEG	3	0
5	B	607	PGE	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	582/583 (99%)	0.00	11 (1%) 66 63	14, 40, 72, 103	0
1	B	582/583 (99%)	0.23	22 (3%) 40 36	17, 47, 92, 134	0
All	All	1164/1166 (99%)	0.12	33 (2%) 53 49	14, 43, 85, 134	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	ALA	6.7
1	B	367	ALA	5.5
1	B	316	LYS	4.9
1	B	117	PRO	4.5
1	B	379	LEU	3.9

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	1PE	B	606	16/16	0.69	0.33	52,69,81,81	0
5	PGE	B	607	10/10	0.81	0.47	62,65,68,69	0
2	DIU	B	602	12/12	0.82	0.30	48,50,91,123	12
6	CA	B	609	1/1	0.85	0.08	60,60,60,60	0
4	1PE	A	607	16/16	0.86	0.25	18,59,66,67	0
3	PEG	B	605	7/7	0.87	0.18	22,36,58,59	0
6	CA	B	610	1/1	0.89	0.08	65,65,65,65	0
2	DIU	A	603	12/12	0.89	0.18	61,64,76,120	0
2	DIU	A	602	12/12	0.90	0.15	48,53,96,98	0
5	PGE	A	608	10/10	0.91	0.22	40,44,47,49	0
3	PEG	A	605	7/7	0.92	0.20	13,26,31,32	0
4	1PE	A	606	16/16	0.92	0.17	12,31,40,40	0
6	CA	B	608	1/1	0.94	0.17	70,70,70,70	0
6	CA	A	612	1/1	0.94	0.08	48,48,48,48	0
6	CA	A	610	1/1	0.95	0.07	47,47,47,47	0
2	DIU	B	603	12/12	0.95	0.13	57,61,78,126	0
6	CA	A	611	1/1	0.96	0.16	74,74,74,74	0
6	CA	A	609	1/1	0.96	0.12	62,62,62,62	0
2	DIU	B	604	12/12	0.96	0.19	60,94,96,101	0
2	DIU	B	601	12/12	0.97	0.14	31,38,48,112	0
2	DIU	A	601	12/12	0.98	0.15	25,36,44,116	0
2	DIU	A	604	12/12	0.98	0.15	49,52,62,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.