



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:09 pm BST

PDB ID : 5D7N  
Title : Crystal structure of human Sirt3 at an improved resolution  
Authors : Rumpf, T.; Gerhardt, S.; Einsle, O.; Jung, M.  
Deposited on : 2015-08-14  
Resolution : 1.83 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](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 : 1.8.5 (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

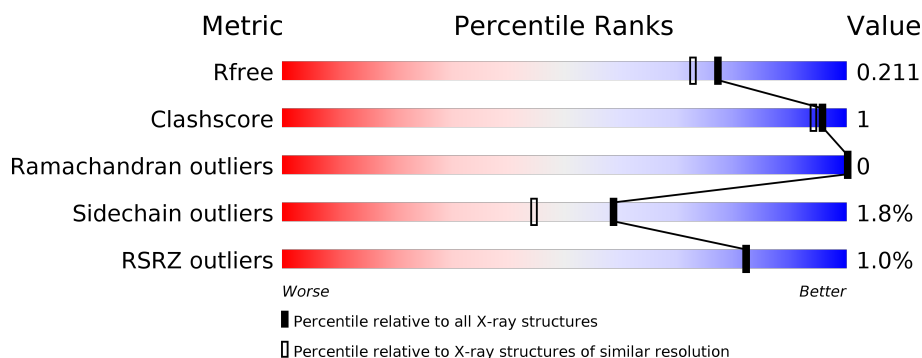
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 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	281	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>• •</div> </div> </div>
1	B	281	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> <div>• •</div> </div> </div>
1	C	281	<div> <div></div> <div> <div></div> <div>95%</div> <div></div> <div>• •</div> </div> </div>
1	D	281	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
1	E	281	<div> <div>%</div> <div> <div></div> <div>94%</div> <div></div> <div>• •</div> </div> </div>
1	F	281	<div> <div>%</div> <div> <div></div> <div>92%</div> <div></div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14318 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	5	0
			2149	1390	366	384	9			
1	B	272	Total	C	N	O	S	0	7	0
			2169	1401	370	389	9			
1	C	272	Total	C	N	O	S	0	10	0
			2186	1410	377	390	9			
1	D	272	Total	C	N	O	S	0	5	0
			2157	1392	368	387	10			
1	E	271	Total	C	N	O	S	0	7	0
			2159	1396	368	386	9			
1	F	270	Total	C	N	O	S	0	6	0
			2147	1389	365	384	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	GLY	-	expression tag	UNP Q9NTG7
A	116	HIS	-	expression tag	UNP Q9NTG7
A	117	MET	-	expression tag	UNP Q9NTG7
B	115	GLY	-	expression tag	UNP Q9NTG7
B	116	HIS	-	expression tag	UNP Q9NTG7
B	117	MET	-	expression tag	UNP Q9NTG7
C	115	GLY	-	expression tag	UNP Q9NTG7
C	116	HIS	-	expression tag	UNP Q9NTG7
C	117	MET	-	expression tag	UNP Q9NTG7
D	115	GLY	-	expression tag	UNP Q9NTG7
D	116	HIS	-	expression tag	UNP Q9NTG7
D	117	MET	-	expression tag	UNP Q9NTG7
E	115	GLY	-	expression tag	UNP Q9NTG7
E	116	HIS	-	expression tag	UNP Q9NTG7
E	117	MET	-	expression tag	UNP Q9NTG7
F	115	GLY	-	expression tag	UNP Q9NTG7
F	116	HIS	-	expression tag	UNP Q9NTG7

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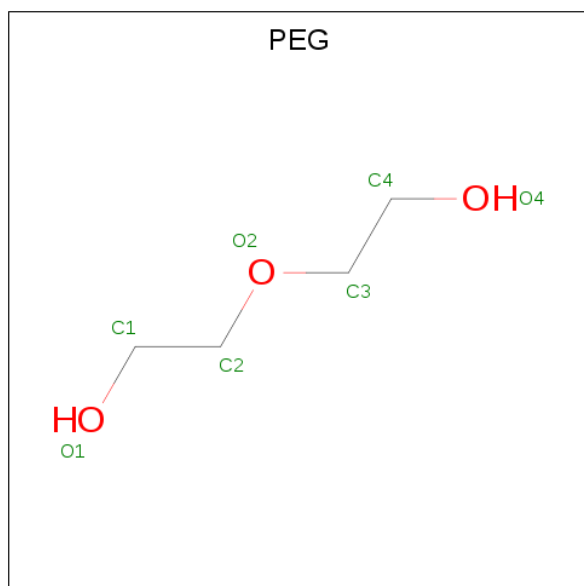
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Chain	Residue	Modelled	Actual	Comment	Reference
F	117	MET	-	expression tag	UNP Q9NTG7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- 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	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

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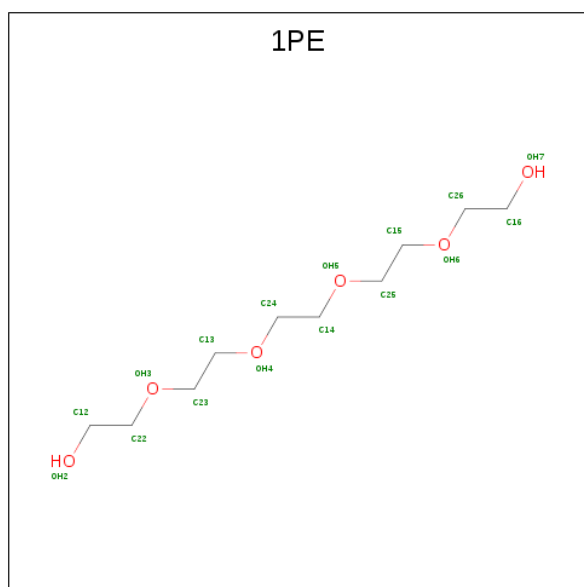
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 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
5	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



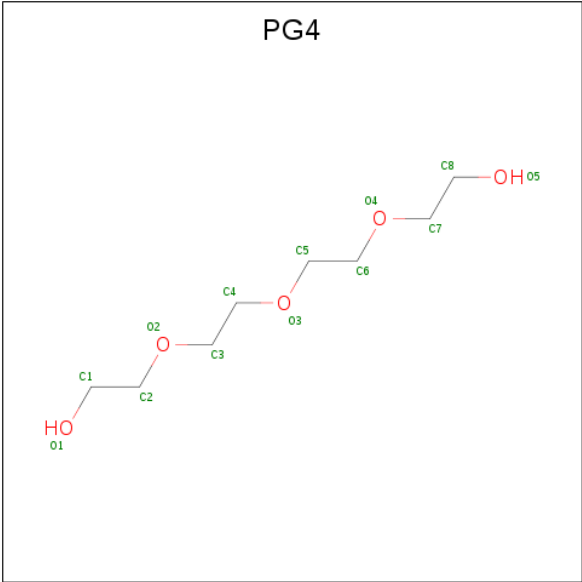
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			13	8	5		

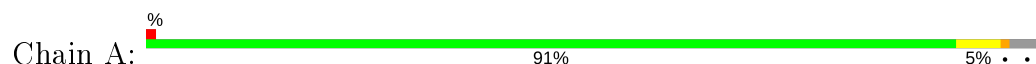
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	241	Total	O	0	0
			241	241		
9	B	216	Total	O	0	0
			216	216		
9	C	218	Total	O	0	0
			218	218		
9	D	205	Total	O	0	0
			205	205		
9	E	167	Total	O	0	0
			167	167		
9	F	210	Total	O	0	0
			210	210		

### 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.

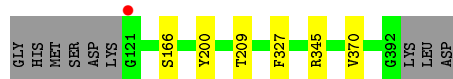
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



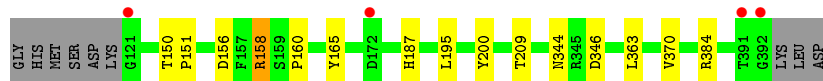
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

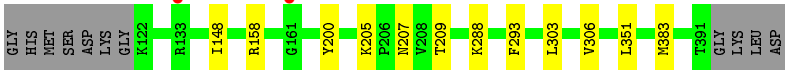


- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.99Å 143.85Å 89.46Å 90.00° 116.33° 90.00°	Depositor
Resolution (Å)	33.66 – 1.83 33.66 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.66-1.83) 99.8 (33.66-1.83)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.175 , 0.203 0.183 , 0.211	Depositor DCC
$R_{free}$ test set	8479 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: GOL, ZN, PGE, MG, 1PE, PG4, 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	0.44	0/2219	0.65	0/3025
1	B	0.44	0/2245	0.63	0/3059
1	C	0.44	0/2271	0.63	0/3093
1	D	0.43	0/2230	0.65	1/3038 (0.0%)
1	E	0.40	0/2235	0.63	0/3046
1	F	0.43	0/2220	0.64	0/3027
All	All	0.43	0/13420	0.64	1/18288 (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	D	384	ARG	NE-CZ-NH1	5.31	122.96	120.30

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	2149	0	2181	12	0
1	B	2169	0	2201	2	0
1	C	2186	0	2225	1	0
1	D	2157	0	2184	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2159	0	2196	3	0
1	F	2147	0	2181	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	21	0	30	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	7	0	10	0	0
4	A	1	0	0	0	0
5	D	16	0	22	0	0
6	D	6	0	8	0	0
7	E	10	0	14	0	0
8	F	13	0	18	0	0
9	A	241	0	0	1	0
9	B	216	0	0	0	0
9	C	218	0	0	0	0
9	D	205	0	0	1	0
9	E	167	0	0	0	0
9	F	210	0	0	0	0
All	All	14318	0	13290	28	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 (28) 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:F:148:ILE:HB	1:F:209[B]:THR:HG21	1.66	0.77
1:F:207:ASN:OD1	1:F:209[B]:THR:HG22	2.02	0.60
1:A:317[B]:ILE:CD1	1:A:351:LEU:HD11	2.35	0.57
1:A:316[A]:LEU:HD22	1:A:318:LEU:HD21	1.88	0.55
1:D:156:ASP:OD1	1:D:158:ARG:HG3	2.09	0.52
1:A:316[A]:LEU:CD2	1:A:318:LEU:HD21	2.40	0.51
1:A:135:ARG:HA	9:A:615:HOH:O	2.11	0.51
1:D:187:HIS:ND1	9:D:502:HOH:O	2.34	0.50
1:D:209[B]:THR:HG22	1:D:370:VAL:HG21	1.92	0.50
1:F:288:LYS:HE2	1:F:293:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317[B]:ILE:HD12	1:A:351:LEU:HD11	1.95	0.48
1:E:150:THR:N	1:E:151:PRO:CD	2.78	0.47
1:E:200:TYR:CG	1:E:201:PRO:HD2	2.51	0.46
1:F:303:LEU:O	1:F:306[A]:VAL:HG12	2.16	0.46
1:D:160:PRO:HA	1:D:165:TYR:CD2	2.51	0.46
1:C:209[A]:THR:HG22	1:C:370:VAL:HG21	1.97	0.45
1:F:383:MET:HB2	1:F:383:MET:HE2	1.79	0.45
1:A:266:GLU:CD	1:A:266:GLU:H	2.20	0.45
1:A:126:GLN:O	1:A:130:GLU:HG2	2.16	0.45
1:A:316[A]:LEU:HD22	1:A:318:LEU:CD2	2.46	0.45
1:A:135:ARG:HD3	1:A:135:ARG:HA	1.85	0.45
1:A:163:GLY:O	1:A:167:ASN:HB2	2.18	0.44
1:A:352:ALA:O	1:E:169:GLN:NE2	2.51	0.43
1:B:225[A]:LEU:HD21	1:B:234:GLU:HG2	2.02	0.42
1:A:317[B]:ILE:HD13	1:A:351:LEU:HD11	2.00	0.41
1:B:381:GLU:OE2	1:B:384:ARG:NH1	2.51	0.41
1:D:150:THR:N	1:D:151:PRO:CD	2.83	0.41
1:D:344:ASN:O	1:D:363:LEU:HA	2.21	0.41

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	274/281 (98%)	269 (98%)	5 (2%)	0	100	100
1	B	277/281 (99%)	274 (99%)	3 (1%)	0	100	100
1	C	280/281 (100%)	277 (99%)	3 (1%)	0	100	100
1	D	276/281 (98%)	273 (99%)	3 (1%)	0	100	100
1	E	276/281 (98%)	273 (99%)	3 (1%)	0	100	100
1	F	274/281 (98%)	273 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1657/1686 (98%)	1639 (99%)	18 (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	240/243 (99%)	232 (97%)	8 (3%)	38	20
1	B	243/243 (100%)	241 (99%)	2 (1%)	81	75
1	C	245/243 (101%)	241 (98%)	4 (2%)	62	49
1	D	241/243 (99%)	237 (98%)	4 (2%)	60	47
1	E	242/243 (100%)	238 (98%)	4 (2%)	60	47
1	F	241/243 (99%)	237 (98%)	4 (2%)	60	47
All	All	1452/1458 (100%)	1426 (98%)	26 (2%)	59	44

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	167	ASN
1	A	170	GLN
1	A	172	ASP
1	A	200	TYR
1	A	203	ASN
1	A	316[A]	LEU
1	A	316[B]	LEU
1	B	200	TYR
1	B	320	THR
1	C	166	SER
1	C	200	TYR
1	C	327	PHE
1	C	345	ARG

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Mol	Chain	Res	Type
1	D	158	ARG
1	D	195	LEU
1	D	200	TYR
1	D	346	ASP
1	E	200	TYR
1	E	320	THR
1	E	345	ARG
1	E	388	GLN
1	F	158	ARG
1	F	200	TYR
1	F	205	LYS
1	F	351	LEU

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

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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
7	PGE	E	402	-	9,9,9	0.52	0	8,8,8	0.43	0
3	PEG	A	403	-	6,6,6	0.44	0	5,5,5	0.24	0
5	1PE	D	403	-	15,15,15	0.53	0	14,14,14	0.40	0
3	PEG	A	404	-	6,6,6	0.49	0	5,5,5	0.22	0
8	PG4	F	402	-	12,12,12	0.41	0	11,11,11	0.46	0
6	GOL	D	404	-	5,5,5	0.37	0	5,5,5	0.19	0
3	PEG	B	402	-	6,6,6	0.30	0	5,5,5	0.45	0
3	PEG	D	402	-	6,6,6	0.46	0	5,5,5	0.25	0
3	PEG	C	402	-	6,6,6	0.45	0	5,5,5	0.17	0
3	PEG	A	402	-	6,6,6	0.45	0	5,5,5	0.17	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
7	PGE	E	402	-	-	5/7/7/7	-
3	PEG	A	403	-	-	1/4/4/4	-
5	1PE	D	403	-	-	9/13/13/13	-
3	PEG	A	404	-	-	2/4/4/4	-
8	PG4	F	402	-	-	2/10/10/10	-
6	GOL	D	404	-	-	2/4/4/4	-
3	PEG	B	402	-	-	1/4/4/4	-
3	PEG	D	402	-	-	3/4/4/4	-
3	PEG	C	402	-	-	0/4/4/4	-
3	PEG	A	402	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	404	GOL	O1-C1-C2-C3
7	E	402	PGE	O2-C3-C4-O3
7	E	402	PGE	O1-C1-C2-O2
5	D	403	1PE	OH2-C12-C22-OH3
3	A	404	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	402	PEG	O1-C1-C2-O2
6	D	404	GOL	O1-C1-C2-O2
3	A	404	PEG	O2-C3-C4-O4
5	D	403	1PE	OH4-C13-C23-OH3
5	D	403	1PE	OH7-C16-C26-OH6
3	D	402	PEG	O1-C1-C2-O2
5	D	403	1PE	C25-C15-OH6-C26
3	B	402	PEG	O1-C1-C2-O2
3	A	402	PEG	O2-C3-C4-O4
7	E	402	PGE	C3-C4-O3-C5
5	D	403	1PE	C13-C23-OH3-C22
7	E	402	PGE	C4-C3-O2-C2
8	F	402	PG4	O4-C7-C8-O5
3	D	402	PEG	O2-C3-C4-O4
5	D	403	1PE	C24-C14-OH5-C25
5	D	403	1PE	OH6-C15-C25-OH5
7	E	402	PGE	C1-C2-O2-C3
3	A	403	PEG	C4-C3-O2-C2
5	D	403	1PE	C23-C13-OH4-C24
3	D	402	PEG	C1-C2-O2-C3
8	F	402	PG4	O1-C1-C2-O2
5	D	403	1PE	OH5-C14-C24-OH4

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

### 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, 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	271/281 (96%)	-0.43	3 (1%) 80 80	12, 22, 36, 50	1 (0%)
1	B	272/281 (96%)	-0.34	3 (1%) 80 80	12, 21, 37, 70	0
1	C	272/281 (96%)	-0.38	1 (0%) 92 92	12, 22, 37, 53	0
1	D	272/281 (96%)	-0.39	4 (1%) 73 73	11, 21, 38, 59	0
1	E	271/281 (96%)	-0.30	4 (1%) 73 73	15, 26, 47, 63	1 (0%)
1	F	270/281 (96%)	-0.34	2 (0%) 87 87	11, 23, 41, 52	0
All	All	1628/1686 (96%)	-0.36	17 (1%) 82 82	11, 23, 41, 70	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	392	GLY	5.9
1	D	121	GLY	3.7
1	B	393	LYS	3.6
1	C	121	GLY	3.0
1	D	392	GLY	2.9
1	D	391	THR	2.9
1	B	122	LYS	2.5
1	D	172	ASP	2.4
1	A	391	THR	2.3
1	E	345	ARG	2.3
1	A	388	GLN	2.2
1	E	391	THR	2.2
1	E	388	GLN	2.2
1	E	381	GLU	2.1
1	F	133	ARG	2.1
1	F	161	GLY	2.1
1	A	161	GLY	2.0

## 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
6	GOL	D	404	6/6	0.70	0.20	54,56,57,58	0
3	PEG	A	403	7/7	0.73	0.18	45,45,49,50	0
3	PEG	A	404	7/7	0.79	0.19	51,52,54,55	0
7	PGE	E	402	10/10	0.79	0.16	47,50,53,55	0
5	1PE	D	403	16/16	0.82	0.16	36,41,50,50	0
3	PEG	C	402	7/7	0.85	0.13	34,35,38,41	0
3	PEG	D	402	7/7	0.86	0.11	53,55,57,57	0
3	PEG	A	402	7/7	0.89	0.12	42,42,45,49	0
3	PEG	B	402	7/7	0.90	0.13	34,35,40,41	0
8	PG4	F	402	13/13	0.94	0.10	27,28,34,39	0
4	MG	A	405	1/1	0.98	0.08	11,11,11,11	1
2	ZN	D	401	1/1	0.99	0.05	23,23,23,23	0
2	ZN	A	401	1/1	1.00	0.04	21,21,21,21	0
2	ZN	B	401	1/1	1.00	0.07	13,13,13,13	0
2	ZN	C	401	1/1	1.00	0.04	22,22,22,22	0
2	ZN	E	401	1/1	1.00	0.06	18,18,18,18	0
2	ZN	F	401	1/1	1.00	0.05	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.