



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:56 AM GMT

PDB ID : 1UMP  
Title : GEOMETRY OF TRITERPENE CONVERSION TO PENTACARBO-  
CYCLIC HOPENE  
Authors : Reinert, D.J.; Balliano, G.; Schulz, G.E.  
Deposited on : 2003-08-27  
Resolution : 2.13 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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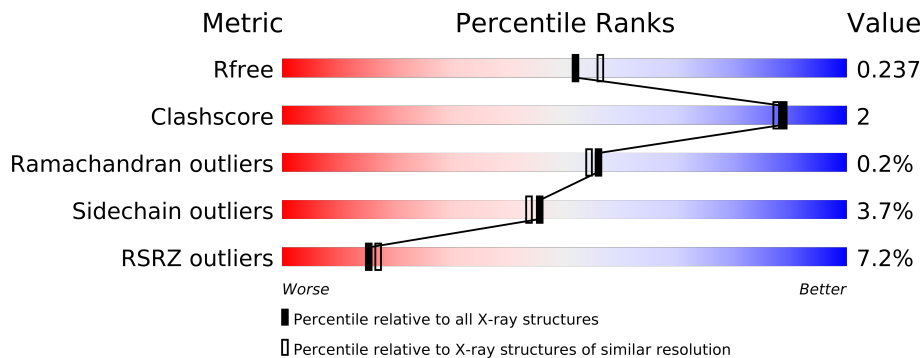
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.13 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))
$R_{free}$	66092	1116 (2.16-2.12)
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)
RSRZ outliers	66119	1116 (2.16-2.12)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	631	
1	B	631	
1	C	631	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	C8E	B	1629	-	X
2	C8E	B	1630[A]	-	X
2	C8E	B	1630[B]	-	X
2	C8E	C	1629	-	X
2	C8E	C	1630[A]	-	X
2	C8E	C	1630[B]	-	X

## 2 Entry composition i

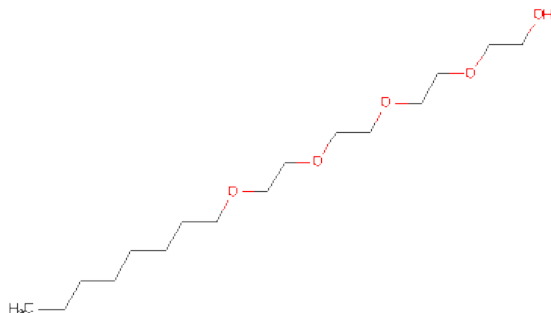
There are 4 unique types of molecules in this entry. The entry contains 16339 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SQUALENE-HOPENE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			
1	B	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			
1	C	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



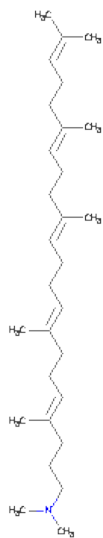
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	1
			42	32	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	1
			42	32	10		

- Molecule 3 is 2-AZASQUALENE (three-letter code: SQA) (formula: C<sub>29</sub>H<sub>51</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			30	29	1		
3	B	1	Total	C	N	0	0
			30	29	1		
3	C	1	Total	C	N	0	0
			30	29	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	526	Total	O	0	0
			526	526		
4	C	366	Total	O	0	0
			366	366		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.14Å 139.14Å 240.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.73 – 2.13 19.55 – 2.13	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.73-2.13) 99.6 (19.55-2.13)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 2.13Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.186 , 0.228 0.200 , 0.237	Depositor DCC
$R_{free}$ test set	3691 reflections (2.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.0	EDS
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 149920 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.9592e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQA, C8E

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	0.60	1/5117 (0.0%)	0.78	10/6967 (0.1%)
1	B	0.64	0/5117	0.81	16/6967 (0.2%)
1	C	0.59	0/5117	0.79	10/6967 (0.1%)
All	All	0.61	1/15351 (0.0%)	0.79	36/20901 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	SER	CB-OG	10.74	1.56	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	ASP	CB-CG-OD2	7.62	125.16	118.30
1	C	57	ASP	CB-CG-OD2	7.37	124.93	118.30
1	C	398	ASP	CB-CG-OD2	7.17	124.76	118.30
1	B	628	ILE	O-C-N	-6.88	111.68	122.70
1	A	276	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	298	ASP	CB-CG-OD2	6.59	124.24	118.30
1	A	331	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	222	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	368	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	427	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	368	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	377	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	106	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	423	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	521	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	604	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	222	ASP	CB-CG-OD2	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	331	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	377	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	397	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	510	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	628	ILE	O-C-N	-5.54	113.83	122.70
1	C	246	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	423	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	350	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	298	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	329	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	313	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	342	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	592	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	219	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	202	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	592	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	276	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	482	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4964	0	0	14	0
1	B	4964	0	0	7	0
1	C	4964	0	0	10	0
2	A	21	0	34	2	0
2	B	63	0	102	0	0
2	C	63	0	102	0	0
3	A	30	0	51	4	0
3	B	30	0	51	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	30	0	51	1	0
4	A	318	0	0	7	1
4	B	526	0	0	3	1
4	C	366	0	0	4	1
All	All	16339	0	391	36	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:276:ASP:OD2	4:C:2169:HOH:O	2.05	0.74
1:C:143:GLU:OE2	1:C:230:LYS:NZ	2.29	0.66
1:A:526:HIS:NE2	4:A:2260:HOH:O	2.30	0.64
1:A:74:GLU:O	1:A:112:LYS:NZ	2.33	0.61
1:C:296:GLU:O	4:C:2192:HOH:O	2.17	0.57
1:C:414:ASN:ND2	1:C:474:TYR:CE1	2.73	0.56
1:C:511:THR:O	1:C:517:GLN:NE2	2.39	0.56
1:A:568:ARG:O	1:A:571:SER:OG	2.25	0.55
1:C:211:LYS:NZ	1:C:604:ASP:OD2	2.40	0.54
1:A:402:LYS:NZ	4:A:2211:HOH:O	2.41	0.53
1:B:139:GLU:O	1:B:199:TYR:OH	2.26	0.53
1:A:157:LYS:NZ	2:A:1629:C8E:H13	2.26	0.51
1:C:344:GLN:OE1	4:C:2209:HOH:O	2.19	0.51
3:A:1630:SQA:C7	3:A:1630:SQA:H3C2	2.40	0.50
1:C:309:SER:N	1:C:310:PRO:CD	2.74	0.49
1:C:573:ALA:N	4:C:2330:HOH:O	2.46	0.48
1:A:99:LYS:NZ	1:A:197:GLU:OE2	2.47	0.48
1:A:211:LYS:NZ	1:A:604:ASP:OD2	2.47	0.47
1:B:62:GLU:OE1	1:B:65:ARG:NH1	2.48	0.47
1:B:192:ARG:NH2	4:B:2175:HOH:O	2.48	0.47
1:B:388:LEU:O	1:B:389:ARG:NH1	2.48	0.46
1:A:45:GLU:OE2	1:A:93:GLU:OE1	2.34	0.46
1:A:324:ALA:O	1:A:625:LYS:NZ	2.49	0.45
1:B:481:PRO:O	1:B:518:LYS:NZ	2.50	0.44
1:B:288:GLU:CD	4:B:2246:HOH:O	2.55	0.44
1:A:312:TRP:CZ2	3:A:1630:SQA:H1C1	2.52	0.44
3:A:1630:SQA:H283	3:A:1630:SQA:H11	2.01	0.43
1:A:63:LYS:NZ	4:A:2047:HOH:O	2.52	0.43
1:A:66:ARG:NH1	4:A:2048:HOH:O	2.51	0.43
2:A:1629:C8E:H31	4:A:2135:HOH:O	2.19	0.42
3:C:1631:SQA:H261	3:C:1631:SQA:H8C2	1.80	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1630:SQA:H121	3:A:1630:SQA:H271	1.82	0.41
1:A:142:TRP:N	4:A:2096:HOH:O	2.53	0.41
1:A:273:LYS:NZ	4:A:2145:HOH:O	2.54	0.41
1:C:45:GLU:OE2	1:C:93:GLU:OE1	2.40	0.40
1:B:625:LYS:NZ	4:B:2524:HOH:O	2.55	0.40

All (2) 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	Distance(Å)	Clash(Å)
4:A:2212:HOH:O	4:C:2274:HOH:O[5_565]	2.10	0.10
4:B:2130:HOH:O	4:B:2272:HOH:O[5_555]	2.17	0.03

## 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	618/631 (98%)	600 (97%)	18 (3%)	0	100	100
1	B	618/631 (98%)	603 (98%)	14 (2%)	1 (0%)	56	54
1	C	618/631 (98%)	597 (97%)	19 (3%)	2 (0%)	50	46
All	All	1854/1893 (98%)	1800 (97%)	51 (3%)	3 (0%)	56	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	414	ASN
1	C	309	SER
1	B	309	SER

### 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	503/513 (98%)	477 (95%)	26 (5%)	32	27
1	B	503/513 (98%)	488 (97%)	15 (3%)	53	53
1	C	503/513 (98%)	488 (97%)	15 (3%)	53	53
All	All	1509/1539 (98%)	1453 (96%)	56 (4%)	45	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	28	ASP
1	A	69	LEU
1	A	111	GLN
1	A	208	ARG
1	A	217	ILE
1	A	223	ARG
1	A	230	LYS
1	A	233	VAL
1	A	346	THR
1	A	376	ASP
1	A	388	LEU
1	A	397	ARG
1	A	422	VAL
1	A	427	ASP
1	A	430	ASN
1	A	448	VAL
1	A	477	ARG
1	A	502	SER
1	A	504	LEU
1	A	512	ARG
1	A	513	GLU
1	A	560	LEU
1	A	572	GLU
1	A	575	ARG
1	A	625	LYS
1	B	15	LEU
1	B	27	LYS
1	B	69	LEU
1	B	104	SER
1	B	114	LEU
1	B	194	ARG

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Mol	Chain	Res	Type
1	B	208	ARG
1	B	233	VAL
1	B	376	ASP
1	B	394	ARG
1	B	398	ASP
1	B	453	LEU
1	B	494	LEU
1	B	541	GLU
1	B	560	LEU
1	C	15	LEU
1	C	20	GLU
1	C	27	LYS
1	C	37	LEU
1	C	157	LYS
1	C	217	ILE
1	C	335	LYS
1	C	370	VAL
1	C	376	ASP
1	C	394	ARG
1	C	413	SER
1	C	517	GLN
1	C	560	LEU
1	C	570	GLU
1	C	625	LYS

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 chains 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 ⓘ

10 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	C8E	A	1629	-	20,20,20	0.43	0	19,19,19	0.57	0
3	SQA	A	1630	-	29,29,29	0.61	0	34,34,34	1.37	3 (8%)
2	C8E	B	1629	-	20,20,20	0.46	0	19,19,19	0.70	0
2	C8E	B	1630[A]	-	20,20,20	0.54	0	19,19,19	0.42	0
2	C8E	B	1630[B]	-	20,20,20	0.45	0	19,19,19	0.37	0
3	SQA	B	1631	-	29,29,29	0.74	0	34,34,34	0.86	0
2	C8E	C	1629	-	20,20,20	0.38	0	19,19,19	0.75	0
2	C8E	C	1630[A]	-	20,20,20	0.53	0	19,19,19	0.45	0
2	C8E	C	1630[B]	-	20,20,20	0.40	0	19,19,19	0.41	0
3	SQA	C	1631	-	29,29,29	0.61	0	34,34,34	1.27	4 (11%)

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	C8E	A	1629	-	-	0/18/18/18	0/0/0/0
3	SQA	A	1630	-	-	0/31/31/31	0/0/0/0
2	C8E	B	1629	-	-	0/18/18/18	0/0/0/0
2	C8E	B	1630[A]	-	-	0/18/18/18	0/0/0/0
2	C8E	B	1630[B]	-	-	0/18/18/18	0/0/0/0
3	SQA	B	1631	-	-	0/31/31/31	0/0/0/0
2	C8E	C	1629	-	-	0/18/18/18	0/0/0/0
2	C8E	C	1630[A]	-	-	0/18/18/18	0/0/0/0
2	C8E	C	1630[B]	-	-	0/18/18/18	0/0/0/0
3	SQA	C	1631	-	-	0/31/31/31	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1630	SQA	C28-C15-C16	3.38	120.52	115.39
3	C	1631	SQA	C28-C15-C16	2.87	119.76	115.39
3	A	1630	SQA	C12-C11-C10	-2.73	121.91	127.80
3	C	1631	SQA	C8-C9-C10	-2.53	104.37	112.74
3	C	1631	SQA	C8-C7-C6	-2.35	122.72	127.80
3	C	1631	SQA	C4-C5-C6	-2.25	107.42	112.78
3	A	1630	SQA	C4-C5-C6	-2.21	107.54	112.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	620/631 (98%)	0.43	58 (9%) 9 9	17, 25, 32, 39	0
1	B	620/631 (98%)	-0.15	20 (3%) 45 48	18, 23, 34, 45	0
1	C	620/631 (98%)	0.24	57 (9%) 9 10	18, 24, 32, 44	0
All	All	1860/1893 (98%)	0.17	135 (7%) 15 17	17, 24, 33, 45	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	10.3
1	A	214	GLY	7.2
1	A	212	GLY	6.8
1	C	212	GLY	6.5
1	C	214	GLY	6.3
1	A	158	ARG	6.1
1	C	514	PRO	5.2
1	C	464	ALA	5.2
1	A	204	PRO	5.1
1	B	158	ARG	4.8
1	A	394	ARG	4.6
1	B	212	GLY	4.4
1	C	158	ARG	4.3
1	C	512	ARG	4.3
1	A	475	LEU	4.3
1	C	626	GLN	4.2
1	A	213	GLY	4.1
1	C	567	GLY	4.0
1	A	575	ARG	4.0
1	C	570	GLU	3.9
1	C	202	ASP	3.8
1	A	207	ARG	3.8
1	C	207	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	331	ASP	3.8
1	A	232	SER	3.8
1	A	397	ARG	3.8
1	B	213	GLY	3.8
1	A	629	GLU	3.6
1	A	211	LYS	3.6
1	A	233	VAL	3.6
1	A	469	ARG	3.6
1	A	507	VAL	3.5
1	A	427	ASP	3.4
1	B	394	ARG	3.4
1	A	466	LYS	3.4
1	C	572	GLU	3.3
1	A	572	GLU	3.3
1	A	543	PRO	3.3
1	A	504	LEU	3.3
1	C	332	ARG	3.3
1	B	10	ALA	3.2
1	A	191	GLU	3.2
1	B	191	GLU	3.2
1	A	217	ILE	3.2
1	C	628	ILE	3.2
1	C	568	ARG	3.1
1	C	325	GLY	3.1
1	C	106	ASP	3.1
1	C	390	LEU	3.1
1	B	209	GLY	3.1
1	A	559	ALA	3.0
1	A	206	ARG	3.0
1	A	485	TRP	3.0
1	B	207	ARG	3.0
1	A	482	ASP	3.0
1	C	625	LYS	2.9
1	A	202	ASP	2.9
1	C	508	GLY	2.9
1	A	481	PRO	2.8
1	A	115	ARG	2.8
1	A	392	ASP	2.8
1	A	218	PHE	2.8
1	C	469	ARG	2.8
1	A	565	ALA	2.8
1	A	628	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	143	GLU	2.7
1	B	202	ASP	2.7
1	B	106	ASP	2.7
1	A	407	ILE	2.7
1	C	471	ALA	2.7
1	A	201	THR	2.7
1	A	512	ARG	2.7
1	C	210	ALA	2.6
1	A	210	ALA	2.6
1	C	334	VAL	2.6
1	A	395	ARG	2.6
1	A	144	LYS	2.6
1	A	626	GLN	2.6
1	C	232	SER	2.6
1	C	504	LEU	2.6
1	B	204	PRO	2.5
1	C	391	PRO	2.5
1	C	213	GLY	2.5
1	C	204	PRO	2.5
1	B	427	ASP	2.5
1	C	394	ARG	2.5
1	B	232	SER	2.5
1	A	627	ALA	2.5
1	B	104	SER	2.5
1	C	233	VAL	2.5
1	C	329	ASP	2.5
1	C	18	ALA	2.5
1	A	106	ASP	2.5
1	B	208	ARG	2.4
1	C	28	ASP	2.4
1	C	467	VAL	2.4
1	C	473	GLU	2.4
1	B	230	LYS	2.4
1	C	211	LYS	2.4
1	C	11	TYR	2.4
1	C	383	TRP	2.3
1	A	208	ARG	2.3
1	C	191	GLU	2.3
1	C	206	ARG	2.3
1	A	514	PRO	2.3
1	A	499	ALA	2.3
1	A	141	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	328	ALA	2.3
1	B	628	ILE	2.3
1	A	340	LEU	2.3
1	A	515	TYR	2.3
1	C	157	LYS	2.2
1	A	230	LYS	2.2
1	C	236	PHE	2.2
1	C	465	TRP	2.2
1	C	318	VAL	2.2
1	C	392	ASP	2.2
1	C	327	PRO	2.2
1	C	510	ASP	2.2
1	A	517	GLN	2.1
1	A	357	ASN	2.1
1	B	215	GLY	2.1
1	C	581	LEU	2.1
1	C	517	GLN	2.1
1	C	459	PHE	2.1
1	B	231	LEU	2.1
1	A	391	PRO	2.1
1	A	215	GLY	2.1
1	A	470	ARG	2.1
1	A	157	LYS	2.0
1	C	461	TYR	2.0
1	C	10	ALA	2.0
1	C	14	THR	2.0
1	C	314	THR	2.0
1	A	10	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	C8E	B	1629	21/21	0.23	7.02	31,43,46,46	21
2	C8E	C	1630[B]	21/21	0.30	6.70	30,32,34,34	21
2	C8E	B	1630[B]	21/21	0.31	6.31	31,32,34,35	21
2	C8E	B	1630[A]	21/21	0.31	5.23	40,43,46,47	21
2	C8E	C	1629	21/21	0.25	5.08	33,41,43,45	21
2	C8E	C	1630[A]	21/21	0.30	4.07	43,47,48,49	21
2	C8E	A	1629	21/21	0.22	1.87	36,43,45,47	21
3	SQA	C	1631	30/30	0.09	-0.08	29,30,36,38	0
3	SQA	A	1630	30/30	0.09	-0.30	36,39,42,45	0
3	SQA	B	1631	30/30	0.08	-0.36	28,30,32,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.