Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:33 PM GMT

PDB ID	:	1KTW
Title	:	IOTA-CARRAGEENASE COMPLEXED TO IOTA-CARRAGEENAN FRAGMENTS
Authors	:	Michel, G.; Kahn, R.; Dideberg, O.
Deposited on	:	2002-01-18
Resolution	:	2.00 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

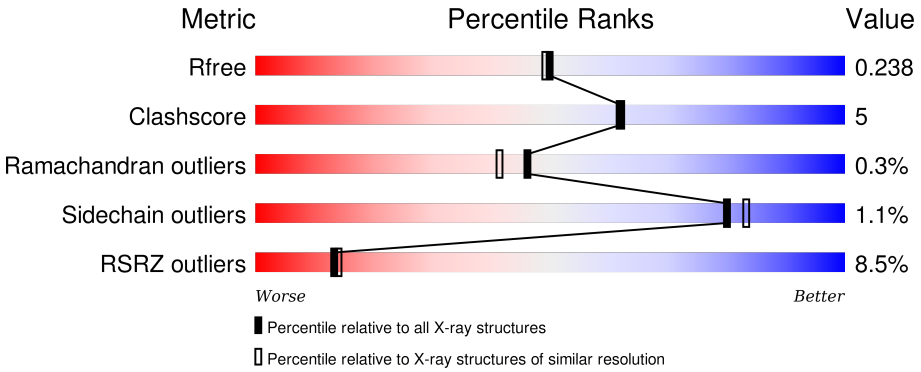
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	464	5%, 88%, 9%
1	B	464	11%, 88%, 10%

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	G4S	A	2	-	-	-	X
6	CL	B	531	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7837 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 IOTA-CARRAGEENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	16	0	0
			3605	2259	639	692	15			
1	B	457	Total	C	N	O	S	37	0	0
			3605	2259	639	692	15			

- Molecule 2 is a polymer of unknown type called SUGAR (DGS-G4S).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	O	S	0	0
			30	12	16	2		

- Molecule 3 is a polymer of unknown type called SUGAR (DGS-G4S-DGS-G4S).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	O	S	0	0
			59	24	31	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	Ca	0	0
			5	5		
4	A	5	Total	Ca	0	0
			5	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

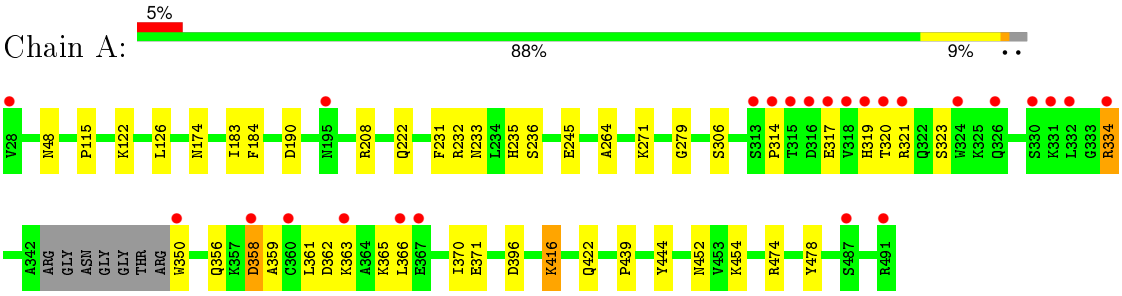
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	289	Total O 289 289	0	0
7	B	233	Total O 233 233	0	0

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 errors 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.

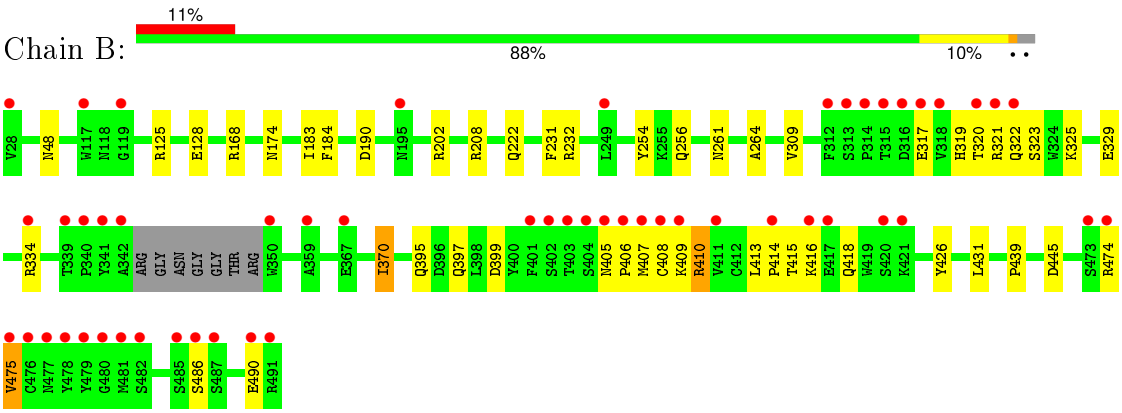
- Molecule 1: IOTA-CARRAGEENASE

Chain A:



- Molecule 1: IOTA-CARRAGEENASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.73Å 122.31Å 91.94Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	23.17 – 2.00 23.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (23.17-2.00) 97.2 (23.17-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 1.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.203 , 0.238 0.203 , 0.238	Depositor DCC
R_{free} test set	3986 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 83.7	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 79185 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7837	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, G4S, DGS, CL

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	0.54	0/3678	0.69	0/4970
1	B	0.48	0/3678	0.67	0/4970
All	All	0.51	0/7356	0.68	0/9940

There are no bond length outliers.

There are no bond angle outliers.

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	3605	0	3500	37	0
1	B	3605	0	3500	37	0
2	A	30	0	18	3	0
3	A	59	0	32	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	1	0
7	A	289	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	233	0	0	2	0
All	All	7837	0	7050	77	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 5.

All (77) 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:405:ASN:HD21	1:B:409:LYS:H	1.01	0.95
1:B:320:THR:HG22	1:B:321:ARG:N	1.97	0.80
1:B:405:ASN:ND2	1:B:409:LYS:H	1.83	0.73
1:B:320:THR:CG2	1:B:321:ARG:H	2.03	0.71
1:A:334:ARG:CD	1:A:334:ARG:H	2.03	0.71
1:A:320:THR:H	1:A:323:SER:HB3	1.56	0.70
2:A:1:DGS:H3	2:A:1:DGS:O8	1.91	0.70
1:B:405:ASN:HD21	1:B:409:LYS:N	1.82	0.69
1:B:320:THR:CG2	1:B:321:ARG:N	2.56	0.68
1:B:415:THR:OG1	1:B:418:GLN:HG3	1.94	0.68
1:A:334:ARG:H	1:A:334:ARG:HD3	1.58	0.67
1:B:261:ASN:HB3	7:B:738:HOH:O	1.94	0.67
1:B:320:THR:HG22	1:B:321:ARG:H	1.59	0.67
1:A:334:ARG:N	1:A:334:ARG:HD3	2.12	0.65
1:A:416:LYS:H	1:A:416:LYS:CE	2.09	0.65
1:B:416:LYS:HD3	1:B:416:LYS:H	1.63	0.64
1:B:254:TYR:O	1:B:256:GLN:HG3	1.99	0.63
1:B:125:ARG:HD3	1:B:128:GLU:OE2	1.99	0.61
1:B:320:THR:H	1:B:323:SER:HB3	1.65	0.60
1:A:115:PRO:HB3	1:A:126:LEU:HD21	1.84	0.60
1:B:399:ASP:OD1	1:B:474:ARG:HA	2.02	0.59
1:B:416:LYS:H	1:B:416:LYS:CD	2.16	0.58
1:B:416:LYS:HD3	1:B:416:LYS:N	2.20	0.57
1:B:409:LYS:O	1:B:410:ARG:HB2	2.06	0.56
1:A:365:LYS:CD	1:A:371:GLU:HG2	2.36	0.56
3:A:494:DGS:O8	3:A:494:DGS:H3	2.07	0.55
1:A:314:PRO:HG2	1:A:317:GLU:HB3	1.87	0.55
1:A:321:ARG:NH1	1:A:350:TRP:HZ3	2.05	0.55
1:A:365:LYS:HE2	1:A:371:GLU:HG2	1.89	0.54
1:B:183:ILE:O	1:B:184:PHE:HB2	2.07	0.53
1:A:365:LYS:CE	1:A:371:GLU:HG2	2.38	0.53
1:B:413:LEU:HD12	1:B:414:PRO:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:HD3	1:A:422:GLN:NE2	2.25	0.51
1:A:416:LYS:H	1:A:416:LYS:CD	2.22	0.51
1:A:334:ARG:CD	1:A:334:ARG:N	2.72	0.50
1:B:168:ARG:NE	1:B:202:ARG:HD3	2.26	0.50
1:A:416:LYS:HE2	1:A:416:LYS:H	1.75	0.50
1:B:329:GLU:OE1	1:B:334:ARG:HA	2.12	0.49
1:A:231:PHE:O	1:A:264:ALA:HA	2.13	0.49
1:B:395:GLN:NE2	1:B:426:TYR:OH	2.37	0.49
1:A:271:LYS:HE2	7:A:818:HOH:O	2.12	0.48
1:A:365:LYS:HD3	1:A:371:GLU:HG2	1.96	0.48
1:A:361:LEU:O	1:A:365:LYS:HG3	2.13	0.48
1:B:486:SER:HB3	1:B:490:GLU:OE2	2.13	0.48
1:A:416:LYS:HD3	1:A:416:LYS:N	2.29	0.48
1:A:365:LYS:NZ	1:A:444:TYR:HE2	2.13	0.47
1:A:362:ASP:O	1:A:366:LEU:HG	2.14	0.47
2:A:1:DGS:C3	2:A:1:DGS:O8	2.62	0.47
1:A:416:LYS:N	1:A:416:LYS:CD	2.78	0.46
1:A:317:GLU:CD	1:A:319:HIS:HE2	2.19	0.46
1:B:317:GLU:HB3	1:B:319:HIS:CD2	2.50	0.46
1:B:168:ARG:CZ	1:B:202:ARG:HD3	2.45	0.46
1:B:309:VAL:HG13	1:B:370:ILE:HG21	1.98	0.46
1:A:356:GLN:HG3	1:A:356:GLN:O	2.15	0.45
1:B:174:ASN:HA	1:B:208:ARG:O	2.15	0.45
1:A:306:SER:HB2	1:A:439:PRO:HD3	1.98	0.45
1:A:174:ASN:HA	1:A:208:ARG:O	2.16	0.45
1:B:320:THR:HG22	1:B:322:GLN:H	1.82	0.45
1:A:122:LYS:HA	2:A:1:DGS:O7	2.17	0.45
1:B:325:LYS:HE2	1:B:329:GLU:OE2	2.17	0.44
1:A:365:LYS:HG2	1:A:370:ILE:O	2.17	0.44
1:A:232:ARG:HG2	1:A:233:ASN:ND2	2.33	0.44
1:B:231:PHE:O	1:B:264:ALA:HA	2.19	0.43
1:B:222:GLN:NE2	6:B:531:CL:CL	2.88	0.43
1:A:183:ILE:O	1:A:184:PHE:HB2	2.17	0.43
1:B:397:GLN:HB3	1:B:431:LEU:CD1	2.49	0.43
1:A:222:GLN:NE2	6:A:530:CL:CL	2.89	0.43
1:B:406:PRO:O	1:B:475:VAL:HB	2.18	0.42
1:A:474:ARG:HH21	1:A:478:TYR:H	1.66	0.42
1:A:359:ALA:O	1:A:363:LYS:HG3	2.20	0.42
1:A:245:GLU:HA	1:A:279:GLY:O	2.20	0.42
1:B:232:ARG:HD2	7:B:615:HOH:O	2.19	0.42
1:A:235:HIS:HD2	1:A:236:SER:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:OD1	1:A:454:LYS:HE2	2.20	0.41
1:B:407:MET:O	1:B:408:CYS:C	2.59	0.41
1:B:439:PRO:O	1:B:445:ASP:HB2	2.20	0.40
1:B:409:LYS:O	1:B:410:ARG:CB	2.69	0.40

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	453/464 (98%)	429 (95%)	23 (5%)	1 (0%)	52	48
1	B	453/464 (98%)	418 (92%)	33 (7%)	2 (0%)	39	33
All	All	906/928 (98%)	847 (94%)	56 (6%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ASP
1	B	410	ARG
1	B	475	VAL

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 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	395/399 (99%)	389 (98%)	6 (2%)	72 75
1	B	395/399 (99%)	392 (99%)	3 (1%)	86 89
All	All	790/798 (99%)	781 (99%)	9 (1%)	80 83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	190	ASP
1	A	334	ARG
1	A	358	ASP
1	A	396	ASP
1	A	416	LYS
1	B	48	ASN
1	B	190	ASP
1	B	370	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	222	GLN
1	A	422	GLN
1	B	60	ASN
1	B	195	ASN
1	B	222	GLN
1	B	235	HIS
1	B	395	GLN
1	B	405	ASN

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)

6 carbohydrates 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	DGS	A	1	2	15,15,16	1.02	1 (6%)	19,23,25	1.40	3 (15%)
2	G4S	A	2	2	16,16,16	0.55	0	22,24,24	0.53	0
3	DGS	A	492	3	15,15,16	0.87	0	19,23,25	1.28	3 (15%)
3	G4S	A	493	3	15,15,16	0.72	0	20,22,24	0.72	0
3	DGS	A	494	3	15,15,16	0.89	0	19,23,25	1.18	1 (5%)
3	G4S	A	495	3	16,16,16	0.50	0	22,24,24	0.63	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	DGS	A	1	2	-	0/5/27/30	0/0/2/2
2	G4S	A	2	2	-	0/7/27/27	0/1/1/1
3	DGS	A	492	3	-	0/5/27/30	0/0/2/2
3	G4S	A	493	3	-	0/7/24/27	0/1/1/1
3	DGS	A	494	3	-	0/5/27/30	0/0/2/2
3	G4S	A	495	3	-	0/7/27/27	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	DGS	C1-C2	2.44	1.55	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	494	DGS	O5-C5-C6	-2.57	109.20	113.33
2	A	1	DGS	C4-C3-C2	-2.46	107.35	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	492	DGS	O5-C5-C6	-2.27	109.68	113.33
3	A	492	DGS	O9-S-O8	-2.22	102.79	112.46
2	A	1	DGS	O5-C5-C6	-2.08	109.99	113.33
3	A	492	DGS	C1-O5-C5	2.47	115.39	112.25
2	A	1	DGS	C1-O5-C5	3.30	116.44	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	DGS	3	0
3	A	494	DGS	1	0

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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^{th} 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	457/464 (98%)	0.01	25 (5%) 29 30	7, 16, 51, 61	7 (1%)
1	B	457/464 (98%)	0.41	53 (11%) 6 7	8, 19, 57, 71	12 (2%)
All	All	914/928 (98%)	0.21	78 (8%) 13 14	7, 17, 55, 71	19 (2%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	MET	9.1
1	B	316	ASP	7.5
1	B	476	CYS	7.5
1	A	315	THR	7.4
1	B	318	VAL	7.2
1	B	315	THR	6.0
1	B	475	VAL	6.0
1	B	350	TRP	6.0
1	B	490	GLU	5.9
1	B	477	ASN	5.4
1	B	314	PRO	5.3
1	B	480	GLY	5.2
1	A	316	ASP	5.1
1	B	402	SER	4.9
1	B	473	SER	4.8
1	B	408	CYS	4.6
1	B	342	ALA	4.5
1	B	341	TYR	4.2
1	B	479	TYR	4.2
1	A	318	VAL	4.1
1	B	486	SER	4.1
1	B	482	SER	4.1
1	B	409	LYS	4.1
1	B	406	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	474	ARG	3.9
1	A	350	TRP	3.9
1	B	401	PHE	3.8
1	B	487	SER	3.8
1	A	366	LEU	3.8
1	A	360	CYS	3.7
1	A	317	GLU	3.7
1	B	478	TYR	3.7
1	B	317	GLU	3.6
1	A	314	PRO	3.5
1	B	334	ARG	3.5
1	B	420	SER	3.4
1	A	334	ARG	3.4
1	A	367	GLU	3.4
1	B	416	LYS	3.3
1	A	320	THR	3.3
1	B	411	VAL	3.1
1	B	313	SER	3.1
1	A	358	ASP	3.1
1	B	421	LYS	3.0
1	A	330	SER	3.0
1	B	481	MET	3.0
1	A	324	TRP	2.9
1	A	363	LYS	2.8
1	B	491	ARG	2.7
1	B	417	GLU	2.7
1	B	367	GLU	2.6
1	B	320	THR	2.6
1	B	340	PRO	2.6
1	B	405	ASN	2.6
1	B	414	PRO	2.6
1	A	487	SER	2.5
1	B	485	SER	2.5
1	A	319	HIS	2.5
1	B	117	TRP	2.5
1	B	321	ARG	2.5
1	A	28	VAL	2.5
1	A	332	LEU	2.4
1	B	249	LEU	2.4
1	B	339	THR	2.4
1	B	119	GLY	2.4
1	B	403	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLN	2.4
1	A	321	ARG	2.4
1	B	404	SER	2.3
1	B	28	VAL	2.3
1	B	195	ASN	2.3
1	A	195	ASN	2.2
1	A	313	SER	2.2
1	B	359	ALA	2.1
1	A	331	LYS	2.1
1	B	312	PHE	2.1
1	A	491	ARG	2.0
1	A	326	GLN	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)

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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	G4S	A	2	16/16	0.70	0.39	13.38	66,67,68,69	16
3	DGS	A	492	14/15	0.95	0.12	0.43	17,21,21,22	0
3	DGS	A	494	14/15	0.86	0.17	0.20	27,37,50,50	0
3	G4S	A	493	15/16	0.96	0.08	-1.62	17,20,24,26	0
2	DGS	A	1	14/15	0.62	0.40	-	69,70,70,70	14
3	G4S	A	495	16/16	0.85	0.22	-	47,52,54,56	0

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. 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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
6	CL	B	531	1/1	0.98	0.15	6.41	37,37,37,37	0
5	NA	A	11	1/1	0.99	0.11	-0.22	13,13,13,13	0
4	CA	A	3	1/1	0.99	0.03	-1.38	15,15,15,15	0
4	CA	B	4	1/1	0.98	0.03	-1.60	17,17,17,17	0
4	CA	B	8	1/1	0.99	0.06	-1.94	24,24,24,24	0
4	CA	A	7	1/1	1.00	0.04	-2.91	15,15,15,15	0
5	NA	B	12	1/1	0.99	0.05	-3.81	19,19,19,19	0
6	CL	A	530	1/1	0.99	0.07	-3.96	30,30,30,30	0
5	NA	B	14	1/1	0.98	0.07	-	19,19,19,19	0
4	CA	A	496	1/1	0.99	0.04	-	14,14,14,14	0
4	CA	A	9	1/1	0.97	0.05	-	22,22,22,22	0
4	CA	B	2	1/1	0.99	0.04	-	16,16,16,16	0
4	CA	A	5	1/1	0.99	0.04	-	15,15,15,15	0
4	CA	B	10	1/1	0.96	0.07	-	27,27,27,27	0
4	CA	B	6	1/1	0.99	0.03	-	18,18,18,18	0
5	NA	A	13	1/1	0.98	0.11	-	14,14,14,14	0

6.5 Other polymers

There are no such residues in this entry.