Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2021 – 10:02 am GMT

PDB ID	:	7OYK
Title	:	DNA-binding domain of CggR in complex with the DNA operator
Authors	:	Novakova, M.; Rezacova, P.; Skerlova, J.; Brynda, J.
Deposited on	:	2021-06-24
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/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:

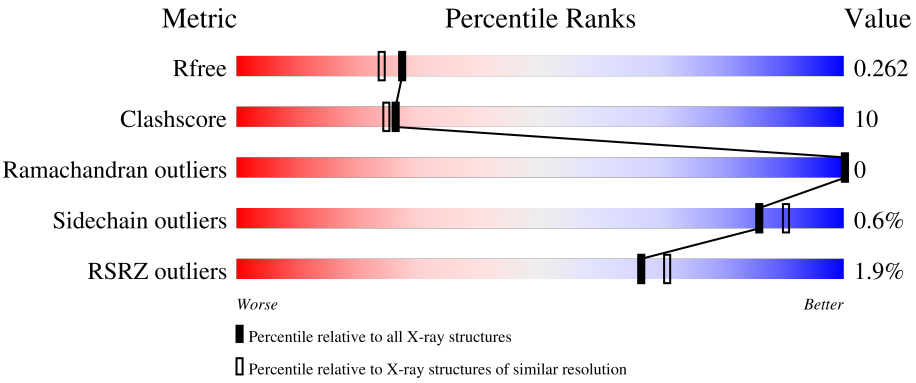
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	AAA	96	4% 81% 18%
1	BBB	96	% 83% 17%
1	CCC	96	2% 86% 12%
1	DDD	96	2% 78% 20%
2	EEE	16	75% 25%

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Mol	Chain	Length	Quality of chain
2	GGG	16	81% 19%
2	LLL	16	50% 50%
3	FFF	16	81% 19%
3	HHH	16	88% 12%
3	KKK	16	31% 69%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5175 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 Central glycolytic genes regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	96	Total	C	N	O	Se	0	1	0
			771	485	133	149	4			
1	DDD	95	Total	C	N	O	Se	0	0	0
			756	476	130	146	4			
1	CCC	96	Total	C	N	O	Se	0	1	0
			768	484	132	148	4			
1	BBB	96	Total	C	N	O	Se	0	2	0
			774	489	132	149	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-4	SER	-	expression tag	UNP O32253
AAA	-3	ASN	-	expression tag	UNP O32253
AAA	-2	ALA	-	expression tag	UNP O32253
AAA	-1	ALA	-	expression tag	UNP O32253
AAA	0	SER	-	expression tag	UNP O32253
DDD	-4	SER	-	expression tag	UNP O32253
DDD	-3	ASN	-	expression tag	UNP O32253
DDD	-2	ALA	-	expression tag	UNP O32253
DDD	-1	ALA	-	expression tag	UNP O32253
DDD	0	SER	-	expression tag	UNP O32253
CCC	-4	SER	-	expression tag	UNP O32253
CCC	-3	ASN	-	expression tag	UNP O32253
CCC	-2	ALA	-	expression tag	UNP O32253
CCC	-1	ALA	-	expression tag	UNP O32253
CCC	0	SER	-	expression tag	UNP O32253
BBB	-4	SER	-	expression tag	UNP O32253
BBB	-3	ASN	-	expression tag	UNP O32253
BBB	-2	ALA	-	expression tag	UNP O32253
BBB	-1	ALA	-	expression tag	UNP O32253
BBB	0	SER	-	expression tag	UNP O32253

- Molecule 2 is a DNA chain called DNA operator - strand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	EEE	16	Total	C	N	O	P	0	0	0
			325	155	67	88	15			
2	LLL	16	Total	C	N	O	P	0	16	0
			325	155	67	88	15			
2	GGG	16	Total	C	N	O	P	0	16	0
			325	155	67	88	15			

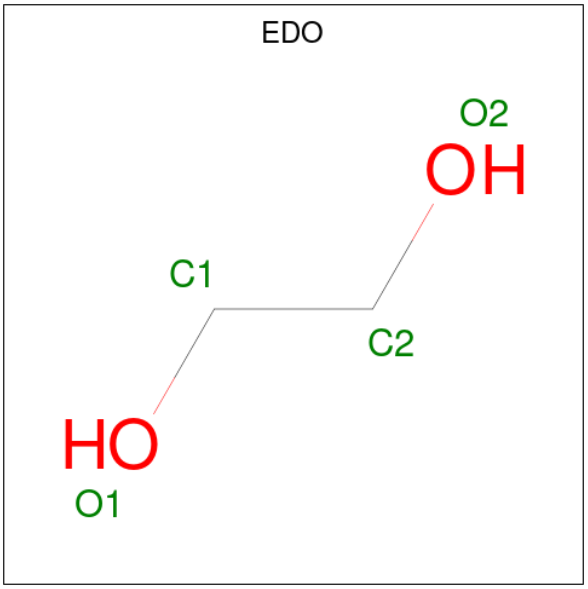
- Molecule 3 is a DNA chain called DNA operator - strand 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	FFF	16	Total	C	N	O	P	0	0	0
			325	157	53	100	15			
3	KKK	16	Total	C	N	O	P	0	16	0
			325	157	53	100	15			
3	HHH	16	Total	C	N	O	P	0	16	0
			325	157	53	100	15			

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

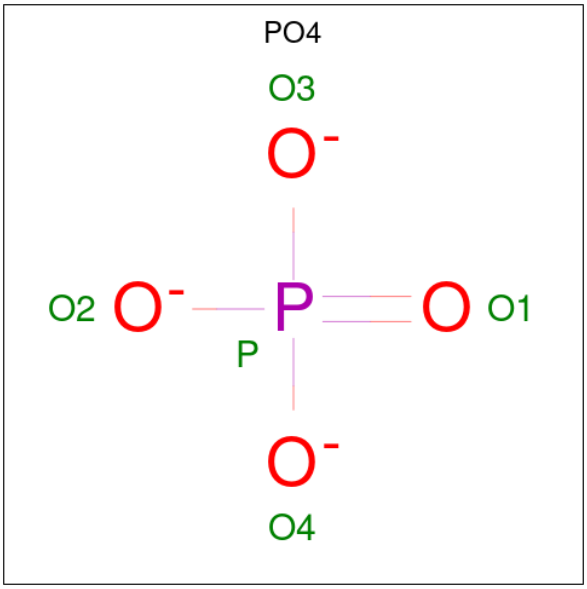
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Ca	0	0
			1	1		
4	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total C O 4 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	FFF	1	Total O P 5 4 1	0	0
6	GGG	1	Total O P 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	20	Total O 20 20	0	0
7	DDD	11	Total O 11 11	0	1
7	CCC	19	Total O 19 19	0	1
7	BBB	21	Total O 21 21	0	0
7	EEE	15	Total O 15 15	0	0
7	FFF	25	Total O 25 25	0	0
7	LLL	4	Total O 5 5	0	1

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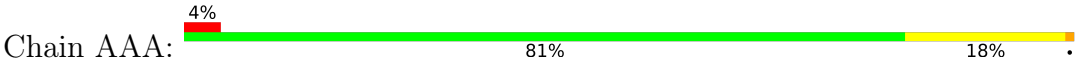
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	KKK	10	Total O 10 10	0	4
7	HHH	4	Total O 4 4	0	1
7	GGG	10	Total O 10 10	0	4

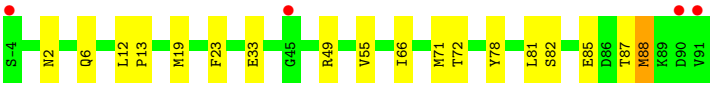
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Central glycolytic genes regulator

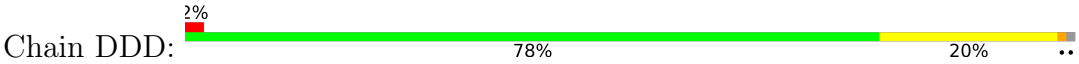
Chain AAA:

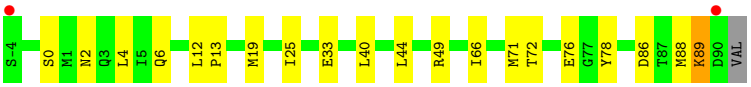




• Molecule 1: Central glycolytic genes regulator

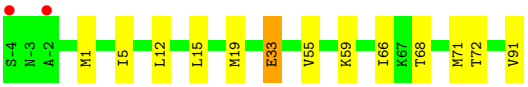
Chain DDD:





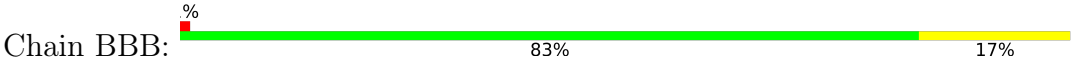
• Molecule 1: Central glycolytic genes regulator

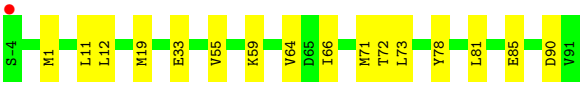
Chain CCC:



• Molecule 1: Central glycolytic genes regulator

Chain BBB:



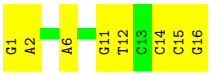


• Molecule 2: DNA operator - strand 1

Chain EEE:

• Molecule 2: DNA operator - strand 1

Chain LLL:

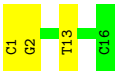


• Molecule 2: DNA operator - strand 1

Chain GGG:

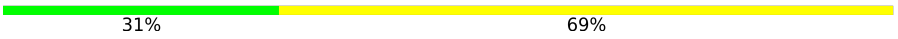
• Molecule 3: DNA operator - strand 2

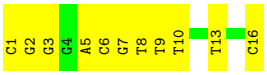
Chain FFF:



• Molecule 3: DNA operator - strand 2

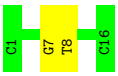
Chain KKK:





• Molecule 3: DNA operator - strand 2

Chain HHH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.97Å 103.14Å 51.11Å 90.00° 90.54° 90.00°	Depositor
Resolution (Å)	45.84 – 2.10 45.79 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.84-2.10) 95.8 (45.79-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.253 0.219 , 0.262	Depositor DCC
R_{free} test set	1726 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.349 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5175	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 6.46% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: EDO, PO4, CA

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	AAA	0.65	0/772	0.81	1/1030 (0.1%)
1	BBB	0.66	0/778	0.83	0/1039
1	CCC	0.65	0/772	0.83	1/1030 (0.1%)
1	DDD	0.66	0/757	0.80	0/1009
2	EEE	0.44	0/366	0.79	0/562
2	GGG	0.40	0/366	0.87	0/562
2	LLL	0.40	0/366	0.81	0/562
3	FFF	0.49	0/362	0.75	0/558
3	HHH	0.37	0/362	0.79	0/558
3	KKK	0.45	1/362 (0.3%)	0.72	0/558
All	All	0.57	1/5263 (0.0%)	0.81	2/7468 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	KKK	1[A]	DC	O3'-P	-5.24	1.54	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	88	MSE	CG-SE-CE	5.60	111.22	98.90
1	CCC	33	GLU	CB-CA-C	-5.22	99.95	110.40

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	AAA	771	0	811	22	0
1	BBB	774	0	821	17	0
1	CCC	768	0	812	21	0
1	DDD	756	0	797	30	0
2	EEE	325	0	179	2	0
2	GGG	325	0	161	3	0
2	LLL	325	0	161	8	0
3	FFF	325	0	185	3	0
3	HHH	325	0	175	1	0
3	KKK	325	0	173	10	0
4	AAA	1	0	0	0	0
4	DDD	1	0	0	0	0
5	CCC	4	0	6	0	0
6	FFF	5	0	0	0	0
6	GGG	5	0	0	0	0
7	AAA	20	0	0	1	0
7	BBB	21	0	0	0	0
7	CCC	19	0	0	1	0
7	DDD	11	0	0	1	0
7	EEE	15	0	0	0	0
7	FFF	25	0	0	0	0
7	GGG	10	0	0	0	0
7	HHH	4	0	0	0	0
7	KKK	10	0	0	2	0
7	LLL	5	0	0	1	0
All	All	5175	0	4281	93	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 10.

All (93) 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:DDD:19:MSE:HE2	1:CCC:12:LEU:HD12	1.26	1.16
1:DDD:19:MSE:CE	1:CCC:12:LEU:HD12	1.76	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:KKK:9[A]:DT:H2"	3:KKK:10[A]:DT:OP2	1.45	1.11
1:AAA:19:MSE:CE	1:BBB:12:LEU:HD12	1.80	1.10
1:AAA:19:MSE:HE2	1:BBB:12:LEU:HD12	1.35	1.08
2:LLL:6[A]:DA:H5"	7:LLL:102[A]:HOH:O	1.63	0.98
2:LLL:11[A]:DG:H2"	2:LLL:12[A]:DT:H5"	1.47	0.95
1:CCC:55:VAL:HG11	1:CCC:71:MSE:SE	2.26	0.86
3:KKK:9[A]:DT:C2'	3:KKK:10[A]:DT:OP2	2.25	0.83
1:DDD:19:MSE:HE3	1:CCC:12:LEU:HD12	1.61	0.82
1:DDD:40:LEU:HD23	1:DDD:71:MSE:HE1	1.63	0.78
1:CCC:33:GLU:HG2	1:CCC:72:THR:HA	1.67	0.76
1:AAA:19:MSE:HE3	1:BBB:12:LEU:HD12	1.66	0.73
2:LLL:11[A]:DG:C2'	2:LLL:12[A]:DT:H5"	2.18	0.73
1:DDD:40:LEU:O	1:DDD:44:LEU:HD13	1.91	0.71
1:DDD:86:ASP:O	1:DDD:89:LYS:HG3	1.90	0.70
2:EEE:11:DG:H2"	2:EEE:12:DT:H5"	1.75	0.69
1:AAA:23:PHE:CD2	1:AAA:88:MSE:HG2	2.28	0.68
1:AAA:12:LEU:HD11	1:BBB:19:MSE:CG	2.24	0.68
1:CCC:55:VAL:CG1	1:CCC:71:MSE:SE	2.92	0.67
1:DDD:76:GLU:HG3	7:DDD:206:HOH:O	1.94	0.66
3:HHH:7[B]:DG:H2"	3:HHH:8[B]:DT:OP2	1.96	0.65
1:DDD:0:SER:HB3	1:CCC:1:MSE:HE3	1.80	0.64
1:AAA:12:LEU:HD11	1:BBB:19:MSE:HG3	1.80	0.63
2:LLL:1[A]:DG:H2"	2:LLL:2[A]:DA:H5'	1.80	0.62
1:AAA:55:VAL:HG11	1:AAA:71:MSE:SE	2.50	0.62
2:LLL:11[A]:DG:H2"	2:LLL:12[A]:DT:C5'	2.26	0.61
2:GGG:14[B]:DC:H2'	2:GGG:15[B]:DC:C6	2.38	0.59
2:LLL:1[A]:DG:H2'	2:LLL:2[A]:DA:C8	2.37	0.59
1:DDD:19:MSE:HB2	1:CCC:12:LEU:CD1	2.32	0.59
1:DDD:40:LEU:CD2	1:DDD:71:MSE:HE1	2.33	0.58
1:DDD:19:MSE:CE	1:CCC:12:LEU:CD1	2.69	0.58
1:DDD:19:MSE:HE3	1:CCC:12:LEU:CD1	2.34	0.55
1:DDD:33:GLU:OE1	1:DDD:78:TYR:OH	2.24	0.55
1:BBB:33:GLU:OE1	1:BBB:78:TYR:OH	2.26	0.54
1:AAA:33:GLU:OE1	1:AAA:78:TYR:OH	2.24	0.54
3:KKK:16[A]:DC:C1'	7:KKK:101[A]:HOH:O	2.56	0.53
1:DDD:40:LEU:HD22	1:DDD:71:MSE:HE3	1.91	0.53
1:CCC:66:ILE:HG12	1:CCC:71:MSE:HG2	1.90	0.52
1:BBB:55:VAL:HG21	1:BBB:71:MSE:SE	2.59	0.52
1:DDD:49:ARG:CG	3:KKK:13[A]:DT:H2'	2.40	0.52
1:DDD:19:MSE:HG2	1:DDD:88:MSE:HE1	1.92	0.52
1:DDD:40:LEU:CD2	1:DDD:71:MSE:CE	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:2:ASN:O	1:DDD:6:GLN:HG2	2.09	0.52
1:DDD:25:ILE:HG12	1:DDD:44:LEU:CD2	2.41	0.51
1:AAA:12:LEU:HD11	1:BBB:19:MSE:HG2	1.92	0.51
1:BBB:64[A]:VAL:HG13	1:BBB:72[A]:THR:O	2.11	0.50
1:DDD:44:LEU:HD12	1:DDD:44:LEU:N	2.26	0.50
1:AAA:19:MSE:HE2	1:BBB:12:LEU:CD1	2.25	0.49
1:CCC:5:ILE:HD11	1:CCC:91:VAL:HG22	1.96	0.48
1:DDD:49:ARG:HG2	3:KKK:13[A]:DT:H2'	1.96	0.47
1:CCC:15:LEU:HG	1:CCC:19:MSE:CE	2.45	0.47
1:AAA:2:ASN:O	1:AAA:6:GLN:HG2	2.14	0.47
1:CCC:5:ILE:CD1	1:CCC:91:VAL:HG22	2.44	0.47
1:DDD:19:MSE:HB2	1:CCC:12:LEU:HD12	1.95	0.47
1:DDD:66:ILE:HG12	1:DDD:71:MSE:HG2	1.96	0.46
1:AAA:49:ARG:HG2	3:FFF:13:DT:H2'	1.98	0.46
1:DDD:19:MSE:HB2	1:CCC:12:LEU:HD11	1.95	0.46
3:KKK:7[A]:DG:H2"	3:KKK:8[A]:DT:OP2	2.15	0.46
1:DDD:44:LEU:N	1:DDD:44:LEU:CD1	2.79	0.45
3:KKK:7[A]:DG:C8	3:KKK:8[A]:DT:H72	2.51	0.45
1:AAA:55:VAL:CG1	1:AAA:71:MSE:SE	3.14	0.45
1:AAA:19:MSE:HG3	1:BBB:11:LEU:HD12	1.98	0.45
3:KKK:5[A]:DA:H2"	3:KKK:6[A]:DC:C6	2.52	0.45
1:AAA:49:ARG:CG	3:FFF:13:DT:H2'	2.47	0.45
2:GGG:15[B]:DC:H2"	2:GGG:16[B]:DG:H5'	1.99	0.45
1:CCC:68:THR:HG22	7:CCC:218:HOH:O	2.17	0.45
1:AAA:66:ILE:HG12	1:AAA:71:MSE:HG2	2.00	0.44
3:FFF:1:DC:H2'	3:FFF:2:DG:C8	2.53	0.44
1:AAA:23:PHE:CE1	1:AAA:81:LEU:HD23	2.52	0.44
1:CCC:59:LYS:HD3	1:CCC:66:ILE:HD12	1.99	0.43
1:DDD:12:LEU:N	1:DDD:13:PRO:CD	2.82	0.43
1:BBB:1:MSE:HE2	1:BBB:90:ASP:O	2.19	0.43
2:LLL:15[A]:DC:H2'	2:LLL:16[A]:DG:C8	2.52	0.43
1:CCC:15:LEU:HG	1:CCC:19:MSE:HE2	2.00	0.43
1:AAA:87:THR:HG23	7:AAA:205:HOH:O	2.17	0.43
1:AAA:19:MSE:HE3	1:BBB:12:LEU:CD1	2.43	0.43
1:DDD:0:SER:HB3	1:CCC:1:MSE:CE	2.48	0.43
2:LLL:14[A]:DC:H2'	2:LLL:15[A]:DC:C6	2.53	0.43
1:AAA:12:LEU:N	1:AAA:13:PRO:CD	2.82	0.43
3:KKK:2[A]:DG:H2"	3:KKK:3[A]:DG:C8	2.54	0.43
3:KKK:16[A]:DC:H1'	7:KKK:101[A]:HOH:O	2.15	0.43
1:BBB:33:GLU:HB2	1:BBB:72[B]:THR:HG22	1.99	0.43
1:AAA:33:GLU:HB2	1:AAA:72:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:40:LEU:HD22	1:DDD:71:MSE:CE	2.48	0.42
1:AAA:82:SER:O	1:AAA:85:GLU:HG2	2.20	0.42
1:BBB:81:LEU:O	1:BBB:85:GLU:HG3	2.20	0.41
2:GGG:15[B]:DC:H2'	2:GGG:16[B]:DG:C8	2.55	0.41
1:DDD:4:LEU:HD22	1:CCC:1:MSE:HG2	2.03	0.41
1:DDD:33:GLU:HB2	1:DDD:72:THR:HG22	2.03	0.41
1:BBB:66:ILE:HG12	1:BBB:71:MSE:HG2	2.01	0.41
1:BBB:64[B]:VAL:HG12	1:BBB:73:LEU:HD23	2.03	0.40
2:EEE:14:DC:H2'	2:EEE:15:DC:C6	2.56	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	AAA	95/96 (99%)	94 (99%)	1 (1%)	0	100	100
1	BBB	96/96 (100%)	95 (99%)	1 (1%)	0	100	100
1	CCC	95/96 (99%)	93 (98%)	2 (2%)	0	100	100
1	DDD	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
All	All	379/384 (99%)	370 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	88/83 (106%)	88 (100%)	0	100 100
1	BBB	89/83 (107%)	88 (99%)	1 (1%)	73 79
1	CCC	88/83 (106%)	88 (100%)	0	100 100
1	DDD	86/83 (104%)	85 (99%)	1 (1%)	71 77
All	All	351/332 (106%)	349 (99%)	2 (1%)	86 90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	89	LYS
1	BBB	59	LYS

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	AAA	92/96 (95%)	0.45	4 (4%)	35	41	29, 44, 70, 101	0
1	BBB	92/96 (95%)	0.28	1 (1%)	80	84	29, 44, 72, 77	0
1	CCC	92/96 (95%)	0.38	2 (2%)	62	66	31, 46, 73, 79	0
1	DDD	91/96 (94%)	0.27	2 (2%)	62	66	31, 46, 70, 98	0
2	EEE	16/16 (100%)	-0.44	0	100	100	32, 41, 51, 55	0
2	GGG	16/16 (100%)	-0.35	0	100	100	28, 39, 54, 57	16 (100%)
2	LLL	16/16 (100%)	-0.35	0	100	100	34, 41, 46, 53	16 (100%)
3	FFF	16/16 (100%)	-0.56	0	100	100	28, 39, 51, 52	0
3	HHH	16/16 (100%)	-0.36	0	100	100	26, 40, 54, 55	16 (100%)
3	KKK	16/16 (100%)	-0.20	0	100	100	27, 42, 52, 56	16 (100%)
All	All	463/480 (96%)	0.20	9 (1%)	66	71	26, 44, 70, 101	64 (13%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	91	VAL	7.3
1	AAA	-4	SER	5.7
1	DDD	-4	SER	3.5
1	CCC	-4	SER	3.4
1	BBB	-4	SER	3.1
1	DDD	90	ASP	2.6
1	AAA	45	GLY	2.5
1	AAA	90	ASP	2.3
1	CCC	-2	ALA	2.1

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 (i)

There are no monosaccharides 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^{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	B-factors(Å^2)	Q<0.9
5	EDO	CCC	101	4/4	0.61	0.21	62,64,64,65	0
6	PO4	GGG	101	5/5	0.78	0.24	44,49,50,60	5
6	PO4	FFF	101	5/5	0.90	0.11	49,52,59,67	0
4	CA	DDD	101	1/1	0.96	0.04	58,58,58,58	0
4	CA	AAA	101	1/1	0.99	0.12	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.