wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:45 PM GMT

PDB ID	:	1UWA
Title	:	L290F MUTANT RUBISCO FROM CHLAMYDOMONAS
Authors	:	Karkehabadi, S.; Taylor, T.C.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2004-02-03
Resolution	:	2.30 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
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:

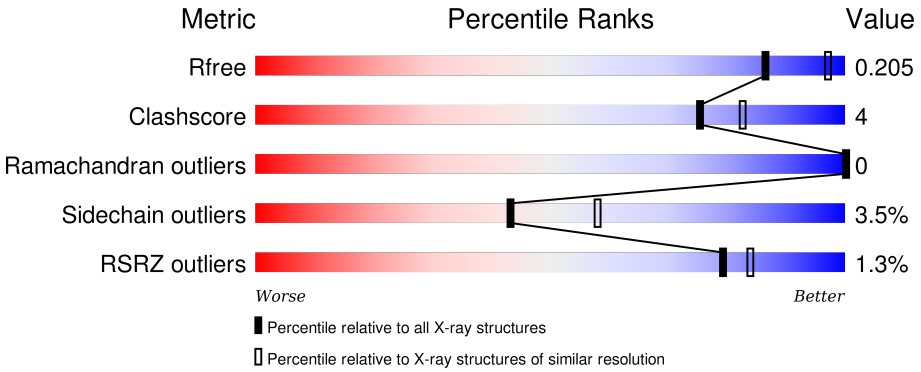
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	475	88% 9%
1	B	475	85% 12%
1	E	475	88% 10%
1	H	475	87% 11%
1	K	475	87% 11%

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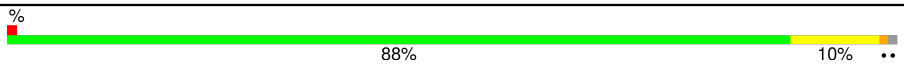
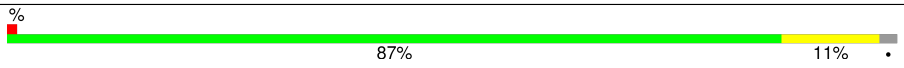
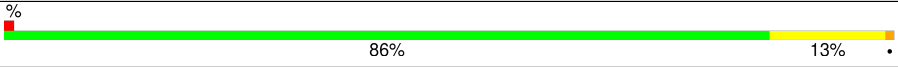
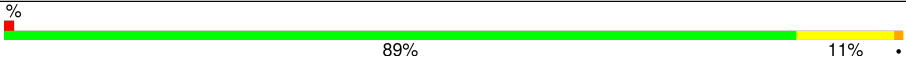
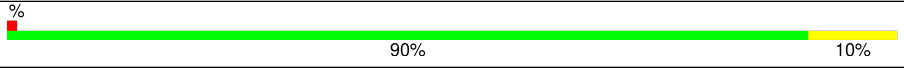
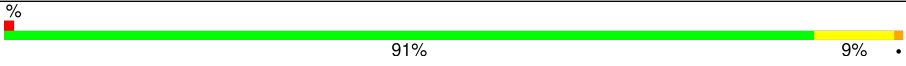
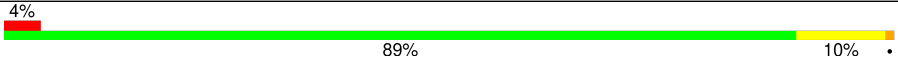
Mol	Chain	Length	Quality of chain
1	O	475	
1	R	475	
1	V	475	
2	C	140	
2	F	140	
2	I	140	
2	J	140	
2	M	140	
2	P	140	
2	T	140	
2	W	140	

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
5	EDO	D	13	-	-	-	X
5	EDO	D	14	-	-	-	X
5	EDO	D	19	-	-	-	X
5	EDO	D	21	-	-	-	X
5	EDO	D	22	-	-	-	X
5	EDO	D	25	-	-	-	X
5	EDO	D	27	-	-	-	X
5	EDO	D	3	-	-	-	X
5	EDO	D	34	-	-	-	X
5	EDO	D	4	-	-	-	X
5	EDO	D	40	-	-	-	X
5	EDO	D	45	-	-	-	X
5	EDO	D	47	-	-	-	X
5	EDO	D	48	-	-	-	X
5	EDO	D	49	-	-	-	X
5	EDO	D	51	-	-	-	X
5	EDO	D	53	-	-	-	X
5	EDO	D	56	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	D	57	-	-	-	X
5	EDO	D	58	-	-	-	X
5	EDO	D	59	-	-	-	X
5	EDO	D	7	-	-	-	X
5	EDO	D	9	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 41073 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 RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	2	0
			3640	2302	641	673	24			
1	B	465	Total	C	N	O	S	0	3	0
			3643	2303	641	675	24			
1	E	469	Total	C	N	O	S	0	4	0
			3671	2319	646	682	24			
1	H	469	Total	C	N	O	S	0	4	0
			3674	2321	649	680	24			
1	K	469	Total	C	N	O	S	0	3	0
			3669	2319	646	680	24			
1	O	469	Total	C	N	O	S	0	4	0
			3672	2320	646	682	24			
1	R	465	Total	C	N	O	S	0	2	0
			3639	2302	641	672	24			
1	V	465	Total	C	N	O	S	0	1	0
			3635	2300	640	671	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	PRO	LEU	CONFLICT	UNP P00877
B	46	PRO	LEU	CONFLICT	UNP P00877
E	46	PRO	LEU	CONFLICT	UNP P00877
H	46	PRO	LEU	CONFLICT	UNP P00877
K	46	PRO	LEU	CONFLICT	UNP P00877
O	46	PRO	LEU	CONFLICT	UNP P00877
R	46	PRO	LEU	CONFLICT	UNP P00877
V	46	PRO	LEU	CONFLICT	UNP P00877
A	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
B	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
E	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
H	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877

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Chain	Residue	Modelled	Actual	Comment	Reference
K	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
O	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
R	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877
V	290	PHE	LEU	ENGINEERED MUTATION	UNP P00877

- Molecule 2 is a protein called RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	1	0
			1142	737	192	202	11			
2	F	140	Total	C	N	O	S	0	1	0
			1138	736	187	203	12			
2	I	140	Total	C	N	O	S	0	1	0
			1133	732	188	202	11			
2	J	140	Total	C	N	O	S	0	1	0
			1142	737	190	203	12			
2	M	140	Total	C	N	O	S	0	1	0
			1140	736	189	203	12			
2	P	140	Total	C	N	O	S	0	1	0
			1138	734	189	203	12			
2	T	140	Total	C	N	O	S	0	1	0
			1134	733	186	203	12			
2	W	140	Total	C	N	O	S	0	1	0
			1141	737	189	203	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	128	SER	THR	CONFLICT	UNP P00873
I	132	TRP	PHE	CONFLICT	UNP P00873
C	128	SER	THR	CONFLICT	UNP P00873
C	132	TRP	PHE	CONFLICT	UNP P00873
F	128	SER	THR	CONFLICT	UNP P00873
F	132	TRP	PHE	CONFLICT	UNP P00873
J	128	SER	THR	CONFLICT	UNP P00873
J	132	TRP	PHE	CONFLICT	UNP P00873
P	128	SER	THR	CONFLICT	UNP P00873
P	132	TRP	PHE	CONFLICT	UNP P00873
T	128	SER	THR	CONFLICT	UNP P00873
T	132	TRP	PHE	CONFLICT	UNP P00873
M	128	SER	THR	CONFLICT	UNP P00873
M	132	TRP	PHE	CONFLICT	UNP P00873

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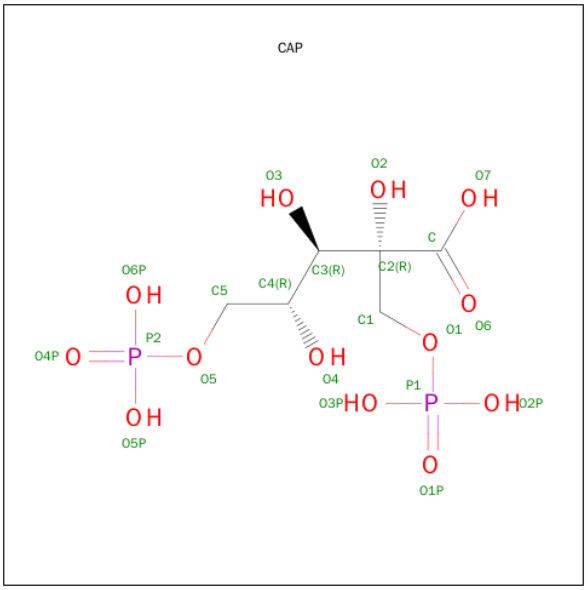
Chain	Residue	Modelled	Actual	Comment	Reference
W	128	SER	THR	CONFLICT	UNP P00873
W	132	TRP	PHE	CONFLICT	UNP P00873

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

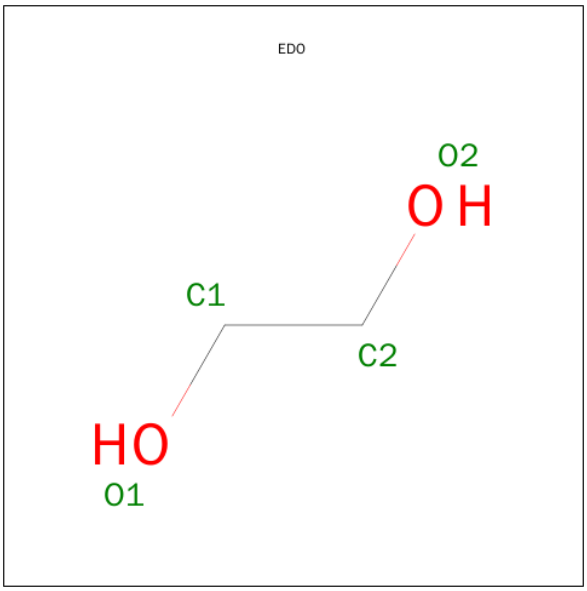
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	V	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	O	1	Total Mg 1 1	0	0
3	R	1	Total Mg 1 1	0	0

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 21 6 13 2	0	0
4	B	1	Total C O P 21 6 13 2	0	0
4	E	1	Total C O P 21 6 13 2	0	0
4	H	1	Total C O P 21 6 13 2	0	0
4	K	1	Total C O P 21 6 13 2	0	0
4	O	1	Total C O P 21 6 13 2	0	0
4	R	1	Total C O P 21 6 13 2	0	0
4	V	1	Total C O P 21 6 13 2	0	0

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



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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	245	Total O 245 245	0	0
6	B	247	Total O 247 247	0	0
6	C	46	Total O 46 46	0	0
6	D	53	Total O 53 53	0	0
6	E	248	Total O 248 248	0	0
6	F	47	Total O 47 47	0	0

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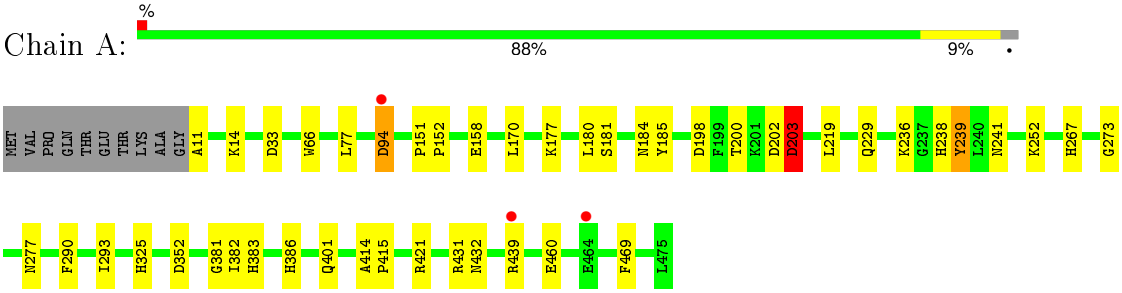
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	189	Total O 189 189	0	0
6	I	57	Total O 57 57	0	0
6	J	44	Total O 44 44	0	0
6	K	238	Total O 238 238	0	0
6	M	62	Total O 62 62	0	0
6	O	228	Total O 228 228	0	0
6	P	59	Total O 59 59	0	0
6	R	215	Total O 215 215	0	0
6	T	50	Total O 50 50	0	0
6	V	214	Total O 214 214	0	0
6	W	68	Total O 68 68	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.

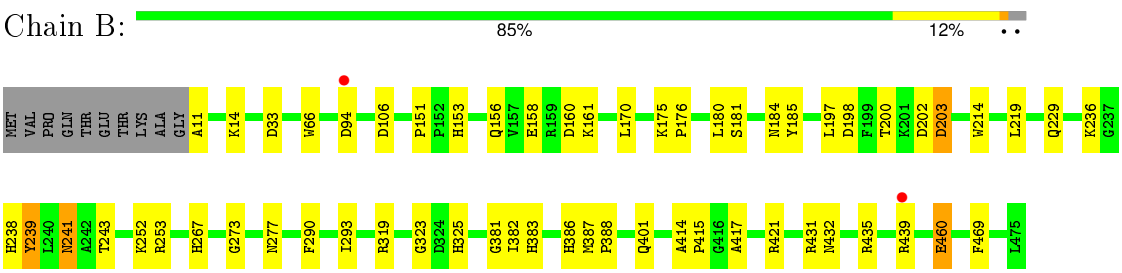
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain A:



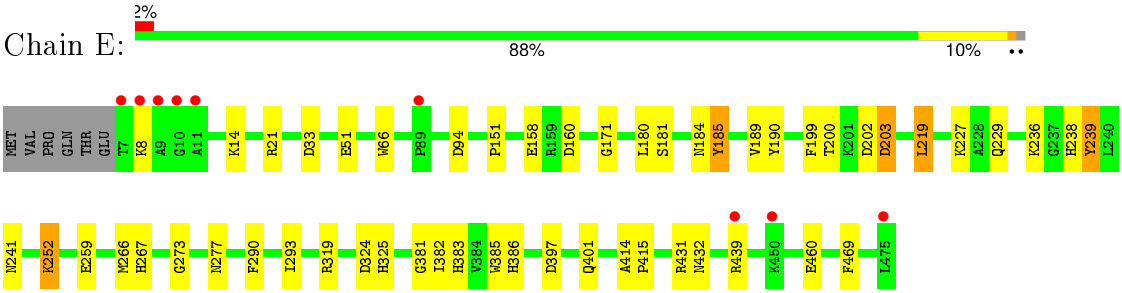
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain B:



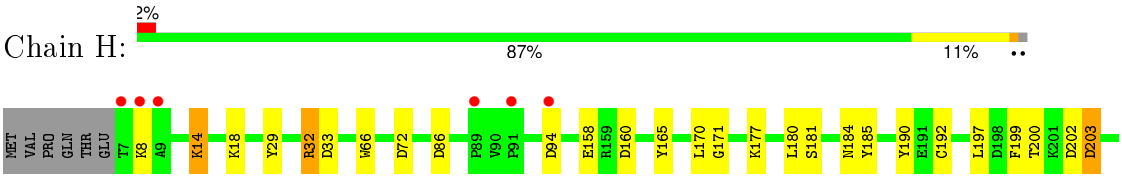
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

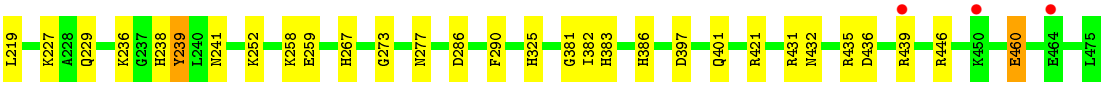
Chain E:



- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

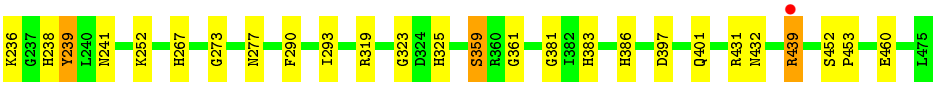
Chain H:





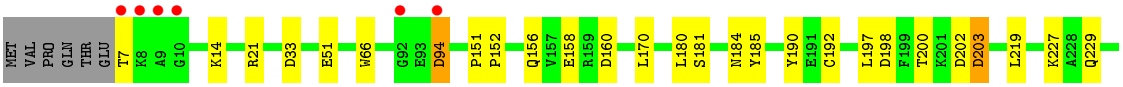
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

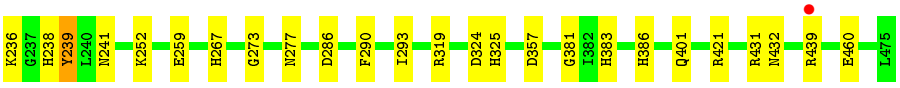
Chain K:



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

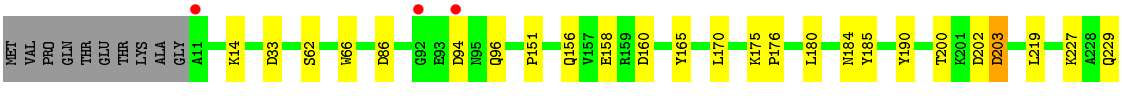
Chain O:





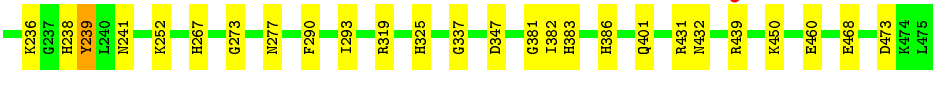
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain R:



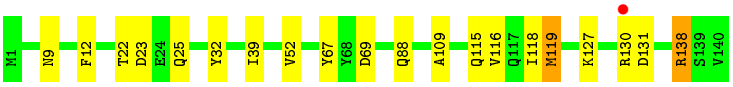
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE LARGE CHAIN

Chain V:



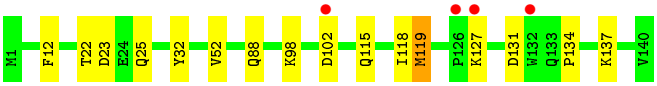
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain C:



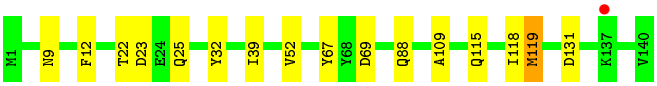
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain F:



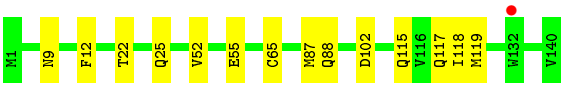
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain I:



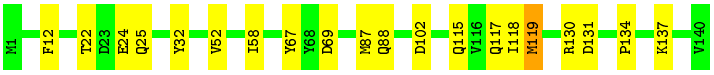
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain J:



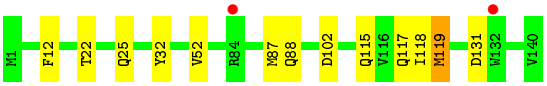
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain M:



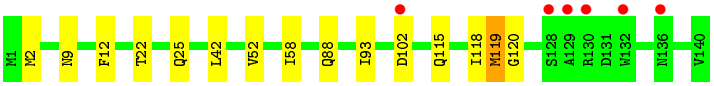
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain P:



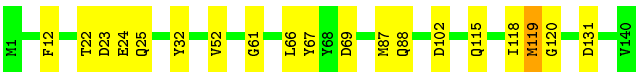
• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain T:



• Molecule 2: RIBULOSE BISPHOSPHATE CARBOXYLASE SMALL CHAIN 1

Chain W:


M1
F12
T22
D23
E24
Q25
Y32
V52
G61
L66
Y67
Y68
D69
M87
Q88
D102
Q115
I118
M119
G120
D131
V140

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.98Å 177.71Å 122.66Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.30) 95.7 (29.97-2.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.171 , 0.205 0.170 , 0.205	Depositor DCC
R_{free} test set	10117 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.4	EDS
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-l,-k,l 0.158 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	1 of 255592 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	41073	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: MG, CAP, EDO, HYP, SMC, KCX

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	0.56	0/3690	0.75	5/4986 (0.1%)
1	B	0.55	0/3699	0.74	5/4998 (0.1%)
1	E	0.54	0/3733	0.73	5/5043 (0.1%)
1	H	0.57	0/3735	0.74	7/5045 (0.1%)
1	K	0.65	1/3722 (0.0%)	0.74	7/5025 (0.1%)
1	O	0.54	0/3733	0.73	8/5043 (0.2%)
1	R	0.55	0/3690	0.74	6/4986 (0.1%)
1	V	0.55	0/3680	0.74	4/4974 (0.1%)
2	C	0.56	0/1181	1.06	6/1605 (0.4%)
2	F	0.57	0/1177	0.69	3/1600 (0.2%)
2	I	0.58	0/1172	0.71	3/1595 (0.2%)
2	J	0.54	0/1181	0.68	1/1605 (0.1%)
2	M	0.55	0/1179	0.72	3/1603 (0.2%)
2	P	0.55	0/1177	0.71	2/1601 (0.1%)
2	T	0.57	0/1173	0.69	1/1596 (0.1%)
2	W	0.55	0/1180	0.72	4/1604 (0.2%)
All	All	0.56	1/39102 (0.0%)	0.74	70/52909 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	359	SER	C-N	21.06	1.82	1.34

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	138	ARG	NE-CZ-NH1	-21.02	109.79	120.30
2	C	138	ARG	NE-CZ-NH2	20.39	130.50	120.30
2	C	138	ARG	CD-NE-CZ	9.92	137.49	123.60
1	O	203	ASP	CB-CG-OD2	7.07	124.66	118.30
1	E	203	ASP	CB-CG-OD2	6.68	124.32	118.30

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	3640	0	3542	28	0
1	B	3643	0	3540	37	0
1	E	3671	0	3566	33	1
1	H	3674	0	3577	34	1
1	K	3669	0	3571	36	1
1	O	3672	0	3570	30	0
1	R	3639	0	3540	33	1
1	V	3635	0	3538	33	0
2	C	1142	0	1110	10	0
2	F	1138	0	1103	8	0
2	I	1133	0	1090	8	0
2	J	1142	0	1110	8	0
2	M	1140	0	1103	12	0
2	P	1138	0	1099	7	0
2	T	1134	0	1092	9	0
2	W	1141	0	1105	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	7	0	0
4	E	21	0	7	0	0
4	H	21	0	7	0	0
4	K	21	0	7	0	0
4	O	21	0	7	0	0
4	R	21	0	7	0	0
4	V	21	0	7	0	0
5	D	236	0	354	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	245	0	0	1	0
6	B	247	0	0	3	0
6	C	46	0	0	1	0
6	D	53	0	0	4	0
6	E	248	0	0	1	0
6	F	47	0	0	1	0
6	H	189	0	0	5	0
6	I	57	0	0	0	0
6	J	44	0	0	1	0
6	K	238	0	0	4	0
6	M	62	0	0	2	0
6	O	228	0	0	4	0
6	P	59	0	0	1	0
6	R	215	0	0	7	0
6	T	50	0	0	0	0
6	V	214	0	0	5	0
6	W	68	0	0	3	0
All	All	41073	0	37666	299	2

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 4.

The worst 5 of 299 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:267:HIS:HD2	1:B:277:ASN:HD22	1.09	0.97
1:R:267:HIS:HD2	1:R:277:ASN:HD22	1.06	0.97
1:V:267:HIS:HD2	1:V:277:ASN:HD22	1.07	0.96
2:J:87:MET:HE3	6:J:2034:HOH:O	1.64	0.96
1:K:267:HIS:HD2	1:K:277:ASN:HD22	1.12	0.95

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	Interatomic distance (Å)	Clash overlap (Å)
1:E:51[A]:GLU:OE2	1:K:439:ARG:NH2[1_554]	1.95	0.25
1:H:14:LYS:CE	1:R:460:GLU:OE1[2_547]	2.00	0.20

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	460/475 (97%)	446 (97%)	14 (3%)	0	100	100
1	B	461/475 (97%)	448 (97%)	13 (3%)	0	100	100
1	E	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	H	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	K	462/475 (97%)	449 (97%)	13 (3%)	0	100	100
1	O	466/475 (98%)	452 (97%)	14 (3%)	0	100	100
1	R	460/475 (97%)	446 (97%)	14 (3%)	0	100	100
1	V	459/475 (97%)	445 (97%)	14 (3%)	0	100	100
2	C	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	F	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	I	139/140 (99%)	133 (96%)	6 (4%)	0	100	100
2	J	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	M	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	P	139/140 (99%)	134 (96%)	5 (4%)	0	100	100
2	T	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
2	W	139/140 (99%)	132 (95%)	7 (5%)	0	100	100
All	All	4812/4920 (98%)	4652 (97%)	160 (3%)	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	A	370/376 (98%)	360 (97%)	10 (3%)	52	70
1	B	371/376 (99%)	360 (97%)	11 (3%)	48	65
1	E	374/376 (100%)	363 (97%)	11 (3%)	50	66
1	H	374/376 (100%)	358 (96%)	16 (4%)	35	47
1	K	373/376 (99%)	361 (97%)	12 (3%)	46	62
1	O	374/376 (100%)	361 (96%)	13 (4%)	43	58
1	R	370/376 (98%)	359 (97%)	11 (3%)	48	65
1	V	369/376 (98%)	359 (97%)	10 (3%)	52	70
2	C	122/123 (99%)	114 (93%)	8 (7%)	21	27
2	F	122/123 (99%)	116 (95%)	6 (5%)	31	41
2	I	120/123 (98%)	114 (95%)	6 (5%)	30	41
2	J	123/123 (100%)	117 (95%)	6 (5%)	31	41
2	M	122/123 (99%)	116 (95%)	6 (5%)	31	41
2	P	122/123 (99%)	117 (96%)	5 (4%)	37	50
2	T	121/123 (98%)	115 (95%)	6 (5%)	30	41
2	W	122/123 (99%)	117 (96%)	5 (4%)	37	50
All	All	3949/3992 (99%)	3807 (96%)	142 (4%)	43	57

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	52	VAL
1	K	203	ASP
1	V	219	LEU
2	I	118	ILE
2	J	118	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	115	GLN
1	K	386	HIS
1	V	277	ASN
2	J	9	ASN
1	K	229	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

40 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HYP	A	104	1	7,8,9	0.71	0	5,10,12	3.21	3 (60%)
1	HYP	A	151	1	7,8,9	0.96	0	5,10,12	4.10	4 (80%)
1	KCX	A	201	1,3	7,11,12	1.12	1 (14%)	7,12,14	0.87	0
1	SMC	A	256	1	5,6,7	1.11	1 (20%)	2,6,8	1.42	0
1	SMC	A	369	1	5,6,7	1.22	1 (20%)	2,6,8	1.29	0
1	HYP	B	104	1	7,8,9	0.91	0	5,10,12	3.26	4 (80%)
1	HYP	B	151	1	7,8,9	1.31	1 (14%)	5,10,12	3.90	4 (80%)
1	KCX	B	201	1,3	7,11,12	0.80	0	7,12,14	0.92	0
1	SMC	B	256	1	5,6,7	1.66	1 (20%)	2,6,8	1.65	1 (50%)
1	SMC	B	369	1	5,6,7	0.72	0	2,6,8	1.61	0
1	HYP	E	104	1	7,8,9	0.82	0	5,10,12	3.26	3 (60%)
1	HYP	E	151	1	7,8,9	1.01	1 (14%)	5,10,12	3.66	4 (80%)
1	KCX	E	201	1,3	7,11,12	0.92	0	7,12,14	0.88	0
1	SMC	E	256	1	5,6,7	1.23	1 (20%)	2,6,8	1.68	1 (50%)
1	SMC	E	369	1	5,6,7	0.98	0	2,6,8	1.07	0
1	HYP	H	104	1	7,8,9	0.71	0	5,10,12	3.63	3 (60%)
1	HYP	H	151	1	7,8,9	1.23	1 (14%)	5,10,12	4.11	4 (80%)
1	KCX	H	201	1,3	7,11,12	0.70	0	7,12,14	1.26	1 (14%)
1	SMC	H	256	1	5,6,7	0.74	0	2,6,8	1.78	1 (50%)
1	SMC	H	369	1	5,6,7	0.71	0	2,6,8	1.52	0
1	HYP	K	104	1	7,8,9	0.80	0	5,10,12	3.34	4 (80%)
1	HYP	K	151	1	7,8,9	1.11	1 (14%)	5,10,12	3.53	4 (80%)
1	KCX	K	201	1,3	7,11,12	0.69	0	7,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SMC	K	256	1	5,6,7	1.68	1 (20%)	2,6,8	1.73	1 (50%)
1	SMC	K	369	1	5,6,7	1.31	1 (20%)	2,6,8	1.59	1 (50%)
1	HYP	O	104	1	7,8,9	0.78	0	5,10,12	3.23	3 (60%)
1	HYP	O	151	1	7,8,9	1.17	1 (14%)	5,10,12	3.97	3 (60%)
1	KCX	O	201	1,3	7,11,12	0.95	0	7,12,14	1.24	1 (14%)
1	SMC	O	256	1	5,6,7	0.85	0	2,6,8	1.83	1 (50%)
1	SMC	O	369	1	5,6,7	0.81	0	2,6,8	1.17	0
1	HYP	R	104	1	6,7,9	0.69	0	7,8,12	1.51	2 (28%)
1	HYP	R	151	1	7,8,9	1.13	1 (14%)	5,10,12	3.35	4 (80%)
1	KCX	R	201	1,3	7,11,12	0.80	0	7,12,14	1.11	1 (14%)
1	SMC	R	256	1	5,6,7	0.49	0	2,6,8	1.64	1 (50%)
1	SMC	R	369	1	5,6,7	0.77	0	2,6,8	1.80	1 (50%)
1	HYP	V	104	1	7,8,9	0.52	0	5,10,12	3.18	3 (60%)
1	HYP	V	151	1	7,8,9	1.36	1 (14%)	5,10,12	3.17	4 (80%)
1	KCX	V	201	1,3	7,11,12	0.59	0	7,12,14	1.03	0
1	SMC	V	256	1	5,6,7	0.60	0	2,6,8	1.20	0
1	SMC	V	369	1	5,6,7	1.06	1 (20%)	2,6,8	1.31	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
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	KCX	A	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	A	256	1	-	0/3/5/7	0/0/0/0
1	SMC	A	369	1	-	0/3/5/7	0/0/0/0
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	B	256	1	-	0/3/5/7	0/0/0/0
1	SMC	B	369	1	-	0/3/5/7	0/0/0/0
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	E	256	1	-	0/3/5/7	0/0/0/0
1	SMC	E	369	1	-	0/3/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	KCX	H	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	H	256	1	-	0/3/5/7	0/0/0/0
1	SMC	H	369	1	-	0/3/5/7	0/0/0/0
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	KCX	K	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	K	256	1	-	0/3/5/7	0/0/0/0
1	SMC	K	369	1	-	0/3/5/7	0/0/0/0
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	KCX	O	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	O	256	1	-	0/3/5/7	0/0/0/0
1	SMC	O	369	1	-	0/3/5/7	0/0/0/0
1	HYP	R	104	1	-	0/0/9/13	0/1/1/1
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	KCX	R	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	R	256	1	-	0/3/5/7	0/0/0/0
1	SMC	R	369	1	-	0/3/5/7	0/0/0/0
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	KCX	V	201	1,3	-	0/6/10/12	0/0/0/0
1	SMC	V	256	1	-	0/3/5/7	0/0/0/0
1	SMC	V	369	1	-	0/3/5/7	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	256	SMC	CB-SG	-3.69	1.76	1.80
1	B	256	SMC	CB-SG	-3.63	1.76	1.80
1	V	151	HYP	CA-N	-3.04	1.43	1.47
1	B	151	HYP	CA-N	-2.90	1.43	1.47
1	H	151	HYP	CA-N	-2.75	1.44	1.47

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	151	HYP	OD1-CG-CD	-5.84	97.79	110.47
1	O	151	HYP	OD1-CG-CD	-5.40	98.74	110.47
1	B	151	HYP	OD1-CG-CD	-5.12	99.35	110.47
1	A	151	HYP	OD1-CG-CD	-4.94	99.74	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	151	HYP	OD1-CG-CD	-4.70	100.25	110.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	151	HYP	1	0
1	B	151	HYP	2	0
1	E	151	HYP	1	0
1	K	151	HYP	3	0
1	O	151	HYP	2	0
1	R	151	HYP	1	0
1	V	151	HYP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 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	$\#\|Z\| > 2$
4	CAP	A	477	3	14,20,20	0.83	1 (7%)	15,31,31	0.90	0
4	CAP	B	477	3	14,20,20	0.81	0	15,31,31	0.79	0
5	EDO	D	1	-	3,3,3	0.36	0	2,2,2	0.21	0
5	EDO	D	10	-	3,3,3	0.30	0	2,2,2	0.29	0
5	EDO	D	11	-	3,3,3	0.37	0	2,2,2	0.31	0
5	EDO	D	12	-	3,3,3	0.35	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	D	13	-	3,3,3	0.36	0	2,2,2	0.35	0
5	EDO	D	14	-	3,3,3	0.32	0	2,2,2	0.16	0
5	EDO	D	15	-	3,3,3	0.26	0	2,2,2	0.52	0
5	EDO	D	16	-	3,3,3	0.24	0	2,2,2	0.52	0
5	EDO	D	18	-	3,3,3	0.32	0	2,2,2	0.51	0
5	EDO	D	19	-	3,3,3	0.37	0	2,2,2	0.20	0
5	EDO	D	2	-	3,3,3	0.33	0	2,2,2	0.14	0
5	EDO	D	20	-	3,3,3	0.38	0	2,2,2	0.21	0
5	EDO	D	21	-	3,3,3	0.34	0	2,2,2	0.15	0
5	EDO	D	22	-	3,3,3	0.43	0	2,2,2	0.22	0
5	EDO	D	23	-	3,3,3	0.33	0	2,2,2	0.60	0
5	EDO	D	24	-	3,3,3	0.25	0	2,2,2	0.68	0
5	EDO	D	25	-	3,3,3	0.36	0	2,2,2	0.28	0
5	EDO	D	26	-	3,3,3	0.22	0	2,2,2	0.19	0
5	EDO	D	27	-	3,3,3	0.30	0	2,2,2	0.60	0
5	EDO	D	28	-	3,3,3	0.41	0	2,2,2	0.27	0
5	EDO	D	29	-	3,3,3	0.35	0	2,2,2	0.20	0
5	EDO	D	3	-	3,3,3	0.37	0	2,2,2	0.20	0
5	EDO	D	30	-	3,3,3	0.41	0	2,2,2	0.19	0
5	EDO	D	31	-	3,3,3	0.49	0	2,2,2	0.35	0
5	EDO	D	32	-	3,3,3	0.39	0	2,2,2	0.13	0
5	EDO	D	33	-	3,3,3	0.34	0	2,2,2	0.11	0
5	EDO	D	34	-	3,3,3	0.33	0	2,2,2	0.39	0
5	EDO	D	35	-	3,3,3	0.38	0	2,2,2	0.16	0
5	EDO	D	36	-	3,3,3	0.46	0	2,2,2	0.12	0
5	EDO	D	37	-	3,3,3	0.30	0	2,2,2	0.50	0
5	EDO	D	38	-	3,3,3	0.36	0	2,2,2	0.31	0
5	EDO	D	39	-	3,3,3	0.32	0	2,2,2	0.32	0
5	EDO	D	4	-	3,3,3	0.38	0	2,2,2	0.16	0
5	EDO	D	40	-	3,3,3	0.37	0	2,2,2	0.15	0
5	EDO	D	41	-	3,3,3	0.36	0	2,2,2	0.28	0
5	EDO	D	42	-	3,3,3	0.34	0	2,2,2	0.22	0
5	EDO	D	43	-	3,3,3	0.27	0	2,2,2	0.79	0
5	EDO	D	44	-	3,3,3	0.38	0	2,2,2	0.31	0
5	EDO	D	45	-	3,3,3	0.31	0	2,2,2	0.37	0
5	EDO	D	46	-	3,3,3	0.44	0	2,2,2	0.26	0
5	EDO	D	47	-	3,3,3	0.37	0	2,2,2	0.27	0
5	EDO	D	48	-	3,3,3	0.31	0	2,2,2	0.37	0
5	EDO	D	49	-	3,3,3	0.35	0	2,2,2	0.06	0
5	EDO	D	5	-	3,3,3	0.49	0	2,2,2	0.04	0
5	EDO	D	50	-	3,3,3	0.27	0	2,2,2	0.49	0
5	EDO	D	51	-	3,3,3	0.33	0	2,2,2	0.18	0
5	EDO	D	52	-	3,3,3	0.26	0	2,2,2	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	D	53	-	3,3,3	0.43	0	2,2,2	0.12	0
5	EDO	D	54	-	3,3,3	0.51	0	2,2,2	0.09	0
5	EDO	D	56	-	3,3,3	0.36	0	2,2,2	0.12	0
5	EDO	D	57	-	3,3,3	0.39	0	2,2,2	0.14	0
5	EDO	D	58	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	D	59	-	3,3,3	0.30	0	2,2,2	0.48	0
5	EDO	D	6	-	3,3,3	0.34	0	2,2,2	0.32	0
5	EDO	D	61	-	3,3,3	0.36	0	2,2,2	0.13	0
5	EDO	D	62	-	3,3,3	0.29	0	2,2,2	0.36	0
5	EDO	D	7	-	3,3,3	0.32	0	2,2,2	0.29	0
5	EDO	D	8	-	3,3,3	0.41	0	2,2,2	0.30	0
5	EDO	D	9	-	3,3,3	0.46	0	2,2,2	0.13	0
4	CAP	E	477	3	14,20,20	0.73	0	15,31,31	0.85	0
4	CAP	H	477	3	14,20,20	0.63	0	15,31,31	0.83	0
4	CAP	K	477	3	14,20,20	1.16	1 (7%)	15,31,31	0.78	0
4	CAP	O	477	3	14,20,20	0.80	1 (7%)	15,31,31	0.93	0
4	CAP	R	477	3	14,20,20	0.62	0	15,31,31	0.79	0
4	CAP	V	477	3	14,20,20	0.65	0	15,31,31	0.78	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
4	CAP	A	477	3	-	0/23/29/29	0/0/0/0
4	CAP	B	477	3	-	0/23/29/29	0/0/0/0
5	EDO	D	1	-	-	0/1/1/1	0/0/0/0
5	EDO	D	10	-	-	0/1/1/1	0/0/0/0
5	EDO	D	11	-	-	0/1/1/1	0/0/0/0
5	EDO	D	12	-	-	0/1/1/1	0/0/0/0
5	EDO	D	13	-	-	0/1/1/1	0/0/0/0
5	EDO	D	14	-	-	0/1/1/1	0/0/0/0
5	EDO	D	15	-	-	0/1/1/1	0/0/0/0
5	EDO	D	16	-	-	0/1/1/1	0/0/0/0
5	EDO	D	18	-	-	0/1/1/1	0/0/0/0
5	EDO	D	19	-	-	0/1/1/1	0/0/0/0
5	EDO	D	2	-	-	0/1/1/1	0/0/0/0
5	EDO	D	20	-	-	0/1/1/1	0/0/0/0
5	EDO	D	21	-	-	0/1/1/1	0/0/0/0
5	EDO	D	22	-	-	0/1/1/1	0/0/0/0
5	EDO	D	23	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	24	-	-	0/1/1/1	0/0/0/0
5	EDO	D	25	-	-	0/1/1/1	0/0/0/0
5	EDO	D	26	-	-	0/1/1/1	0/0/0/0
5	EDO	D	27	-	-	0/1/1/1	0/0/0/0
5	EDO	D	28	-	-	0/1/1/1	0/0/0/0
5	EDO	D	29	-	-	0/1/1/1	0/0/0/0
5	EDO	D	3	-	-	0/1/1/1	0/0/0/0
5	EDO	D	30	-	-	0/1/1/1	0/0/0/0
5	EDO	D	31	-	-	0/1/1/1	0/0/0/0
5	EDO	D	32	-	-	0/1/1/1	0/0/0/0
5	EDO	D	33	-	-	0/1/1/1	0/0/0/0
5	EDO	D	34	-	-	0/1/1/1	0/0/0/0
5	EDO	D	35	-	-	0/1/1/1	0/0/0/0
5	EDO	D	36	-	-	0/1/1/1	0/0/0/0
5	EDO	D	37	-	-	0/1/1/1	0/0/0/0
5	EDO	D	38	-	-	0/1/1/1	0/0/0/0
5	EDO	D	39	-	-	0/1/1/1	0/0/0/0
5	EDO	D	4	-	-	0/1/1/1	0/0/0/0
5	EDO	D	40	-	-	0/1/1/1	0/0/0/0
5	EDO	D	41	-	-	0/1/1/1	0/0/0/0
5	EDO	D	42	-	-	0/1/1/1	0/0/0/0
5	EDO	D	43	-	-	0/1/1/1	0/0/0/0
5	EDO	D	44	-	-	0/1/1/1	0/0/0/0
5	EDO	D	45	-	-	0/1/1/1	0/0/0/0
5	EDO	D	46	-	-	0/1/1/1	0/0/0/0
5	EDO	D	47	-	-	0/1/1/1	0/0/0/0
5	EDO	D	48	-	-	0/1/1/1	0/0/0/0
5	EDO	D	49	-	-	0/1/1/1	0/0/0/0
5	EDO	D	5	-	-	0/1/1/1	0/0/0/0
5	EDO	D	50	-	-	0/1/1/1	0/0/0/0
5	EDO	D	51	-	-	0/1/1/1	0/0/0/0
5	EDO	D	52	-	-	0/1/1/1	0/0/0/0
5	EDO	D	53	-	-	0/1/1/1	0/0/0/0
5	EDO	D	54	-	-	0/1/1/1	0/0/0/0
5	EDO	D	56	-	-	0/1/1/1	0/0/0/0
5	EDO	D	57	-	-	0/1/1/1	0/0/0/0
5	EDO	D	58	-	-	0/1/1/1	0/0/0/0
5	EDO	D	59	-	-	0/1/1/1	0/0/0/0
5	EDO	D	6	-	-	0/1/1/1	0/0/0/0
5	EDO	D	61	-	-	0/1/1/1	0/0/0/0
5	EDO	D	62	-	-	0/1/1/1	0/0/0/0
5	EDO	D	7	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	8	-	-	0/1/1/1	0/0/0/0
5	EDO	D	9	-	-	0/1/1/1	0/0/0/0
4	CAP	E	477	3	-	0/23/29/29	0/0/0/0
4	CAP	H	477	3	-	0/23/29/29	0/0/0/0
4	CAP	K	477	3	-	0/23/29/29	0/0/0/0
4	CAP	O	477	3	-	0/23/29/29	0/0/0/0
4	CAP	R	477	3	-	0/23/29/29	0/0/0/0
4	CAP	V	477	3	-	0/23/29/29	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	477	CAP	O2-C2	2.11	1.46	1.43
4	A	477	CAP	O2-C2	2.42	1.46	1.43
4	K	477	CAP	O2-C2	3.41	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1	EDO	1	0
5	D	12	EDO	1	0
5	D	13	EDO	1	0
5	D	18	EDO	1	0
5	D	35	EDO	1	0
5	D	39	EDO	3	0
5	D	40	EDO	3	0
5	D	42	EDO	1	0
5	D	44	EDO	2	0
5	D	52	EDO	3	0
5	D	53	EDO	1	0
5	D	61	EDO	1	0
5	D	8	EDO	1	0

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^{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	460/475 (96%)	-0.60	3 (0%) 89 92	24, 31, 46, 63	0
1	B	460/475 (96%)	-0.63	2 (0%) 93 95	24, 31, 46, 63	0
1	E	464/475 (97%)	-0.55	9 (1%) 70 76	24, 31, 47, 92	0
1	H	464/475 (97%)	-0.54	9 (1%) 70 76	24, 31, 47, 95	0
1	K	464/475 (97%)	-0.51	7 (1%) 76 81	24, 31, 47, 90	0
1	O	464/475 (97%)	-0.54	7 (1%) 76 81	24, 31, 47, 87	0
1	R	460/475 (96%)	-0.58	5 (1%) 82 86	24, 31, 46, 63	0
1	V	460/475 (96%)	-0.60	5 (1%) 82 86	24, 31, 46, 63	0
2	C	140/140 (100%)	-0.24	1 (0%) 89 92	30, 40, 52, 64	0
2	F	140/140 (100%)	-0.22	4 (2%) 55 64	30, 40, 52, 60	0
2	I	140/140 (100%)	-0.31	1 (0%) 89 92	30, 40, 52, 56	0
2	J	140/140 (100%)	-0.17	1 (0%) 89 92	30, 40, 52, 63	1 (0%)
2	M	140/140 (100%)	-0.41	0 100 100	30, 40, 52, 57	1 (0%)
2	P	140/140 (100%)	-0.31	2 (1%) 78 83	30, 40, 52, 60	0
2	T	140/140 (100%)	-0.11	6 (4%) 39 48	30, 40, 52, 57	0
2	W	140/140 (100%)	-0.47	0 100 100	30, 40, 52, 56	1 (0%)
All	All	4816/4920 (97%)	-0.50	62 (1%) 79 84	24, 32, 50, 95	3 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	92	GLY	7.3
1	H	7	THR	5.4
1	E	8	LYS	5.0
1	K	7	THR	4.7
1	K	8	LYS	4.6

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	HYP	E	104	8/9	0.92	0.10	-	26,28,30,30	0
1	SMC	H	256	7/8	0.99	0.05	-	27,29,29,30	0
1	SMC	R	369	7/8	0.98	0.07	-	28,30,32,37	0
1	KCX	E	201	12/13	0.98	0.12	-	23,26,28,29	0
1	HYP	R	151	8/9	0.95	0.09	-	24,28,29,30	0
1	HYP	H	104	8/9	0.94	0.09	-	26,29,30,30	0
1	HYP	V	104	8/9	0.95	0.07	-	26,28,30,30	0
1	KCX	K	201	12/13	0.97	0.12	-	23,26,28,29	0
1	SMC	E	256	7/8	0.98	0.07	-	27,29,29,31	0
1	KCX	H	201	12/13	0.97	0.10	-	23,26,28,29	0
1	KCX	B	201	12/13	0.96	0.11	-	23,26,28,29	0
1	SMC	V	256	7/8	0.98	0.06	-	27,29,30,31	0
1	SMC	B	256	7/8	0.97	0.07	-	27,28,29,30	0
1	HYP	A	104	8/9	0.96	0.08	-	26,28,30,30	0
1	HYP	B	104	8/9	0.94	0.09	-	26,28,30,30	0
1	KCX	R	201	12/13	0.97	0.12	-	23,26,28,29	0
1	SMC	A	369	7/8	0.98	0.06	-	28,30,32,37	0
1	HYP	K	104	8/9	0.96	0.08	-	26,29,30,30	0
1	SMC	K	256	7/8	0.98	0.07	-	27,29,29,31	0
1	SMC	A	256	7/8	0.96	0.09	-	27,29,29,31	0
1	HYP	B	151	8/9	0.92	0.10	-	24,27,29,30	0
1	SMC	E	369	7/8	0.97	0.06	-	28,30,32,37	0
1	HYP	O	151	8/9	0.94	0.09	-	24,28,29,30	0
1	KCX	V	201	12/13	0.97	0.12	-	23,26,28,29	0
1	HYP	A	151	8/9	0.94	0.08	-	24,28,29,30	0
1	HYP	V	151	8/9	0.93	0.10	-	24,28,29,30	0
1	HYP	E	151	8/9	0.97	0.06	-	24,28,29,30	0
1	HYP	H	151	8/9	0.96	0.06	-	24,28,29,30	0
1	SMC	B	369	7/8	0.98	0.06	-	28,30,32,36	0
1	SMC	O	256	7/8	0.97	0.08	-	27,29,30,30	0
1	SMC	R	256	7/8	0.97	0.07	-	27,29,29,31	0
1	HYP	K	151	8/9	0.96	0.07	-	24,28,29,30	0
1	SMC	V	369	7/8	0.97	0.07	-	28,30,32,37	0
1	KCX	O	201	12/13	0.97	0.13	-	23,26,28,29	0
1	HYP	O	104	8/9	0.95	0.07	-	26,28,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	KCX	A	201	12/13	0.96	0.12	-	23,26,28,29	0
1	SMC	K	369	7/8	0.97	0.08	-	28,30,32,37	0
1	SMC	O	369	7/8	0.97	0.07	-	28,30,32,36	0
1	SMC	H	369	7/8	0.96	0.07	-	28,31,32,37	0
1	HYP	R	104	7/9	0.95	0.08	-	26,28,30,30	0

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. 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
5	EDO	D	47	4/4	0.58	0.36	16.03	61,64,65,67	0
5	EDO	D	40	4/4	0.29	0.41	13.98	62,63,63,67	0
5	EDO	D	9	4/4	0.65	0.26	10.25	52,55,55,57	0
5	EDO	D	4	4/4	0.67	0.38	9.82	56,59,61,63	0
5	EDO	D	56	4/4	0.78	0.28	9.17	59,60,60,61	0
5	EDO	D	45	4/4	0.82	0.23	8.92	56,63,64,66	0
5	EDO	D	48	4/4	0.79	0.20	8.13	55,65,66,72	0
5	EDO	D	21	4/4	0.75	0.22	7.22	59,62,62,63	0
5	EDO	D	27	4/4	0.89	0.16	7.19	58,64,67,67	0
5	EDO	D	57	4/4	0.67	0.26	6.82	55,57,58,59	0
5	EDO	D	3	4/4	0.75	0.15	5.40	55,55,56,58	0
5	EDO	D	7	4/4	0.78	0.17	5.27	48,53,53,55	0
5	EDO	D	59	4/4	0.48	0.29	4.98	88,89,91,92	0
5	EDO	D	19	4/4	0.76	0.30	4.67	59,62,62,63	0
5	EDO	D	49	4/4	0.84	0.23	4.45	56,60,61,63	0
5	EDO	D	51	4/4	0.78	0.31	3.84	59,61,62,62	0
5	EDO	D	14	4/4	0.90	0.26	3.41	51,53,53,56	0
5	EDO	D	13	4/4	0.88	0.15	3.39	48,53,56,56	0
5	EDO	D	58	4/4	0.89	0.31	2.67	53,54,57,60	0
5	EDO	D	22	4/4	0.90	0.13	2.55	40,45,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	EDO	D	34	4/4	0.91	0.14	2.51	40,43,43,46	0
5	EDO	D	53	4/4	0.89	0.17	2.32	38,41,46,48	0
5	EDO	D	25	4/4	0.91	0.14	2.25	35,40,40,43	0
5	EDO	D	61	4/4	0.85	0.17	1.69	44,46,48,49	0
5	EDO	D	42	4/4	0.63	0.20	1.65	66,69,70,71	0
5	EDO	D	29	4/4	0.75	0.20	1.64	62,64,69,70	0
5	EDO	D	62	4/4	0.87	0.22	1.39	74,74,74,76	0
5	EDO	D	50	4/4	0.92	0.20	1.24	64,64,64,65	0
5	EDO	D	23	4/4	0.94	0.10	1.00	32,33,35,36	0
5	EDO	D	38	4/4	0.80	0.14	0.85	51,54,58,58	0
3	MG	E	476	1/1	0.99	0.14	0.80	27,27,27,27	0
5	EDO	D	26	4/4	0.94	0.11	0.77	33,34,35,39	0
5	EDO	D	5	4/4	0.90	0.11	0.77	30,31,37,37	0
5	EDO	D	30	4/4	0.94	0.12	0.64	31,31,34,35	0
5	EDO	D	24	4/4	0.94	0.15	0.56	41,47,51,58	0
5	EDO	D	54	4/4	0.93	0.11	0.51	31,32,32,36	0
5	EDO	D	1	4/4	0.93	0.11	0.48	33,35,36,37	0
5	EDO	D	11	4/4	0.97	0.09	0.43	28,33,34,35	0
4	CAP	A	477	21/21	0.98	0.12	0.28	27,31,32,37	0
5	EDO	D	15	4/4	0.92	0.12	0.25	49,53,53,55	0
5	EDO	D	10	4/4	0.96	0.09	0.24	29,35,36,39	0
4	CAP	K	477	21/21	0.99	0.13	0.22	27,31,33,37	0
5	EDO	D	41	4/4	0.87	0.15	0.13	50,56,60,63	0
5	EDO	D	31	4/4	0.94	0.12	0.06	22,22,25,29	0
5	EDO	D	6	4/4	0.97	0.09	-0.03	33,33,35,37	0
5	EDO	D	18	4/4	0.96	0.10	-0.05	39,40,42,43	0
5	EDO	D	52	4/4	0.71	0.15	-0.07	57,57,58,61	0
4	CAP	R	477	21/21	0.98	0.10	-0.17	27,31,33,37	0
4	CAP	O	477	21/21	0.99	0.10	-0.36	27,31,33,37	0
5	EDO	D	37	4/4	0.96	0.09	-0.36	39,41,41,46	0
4	CAP	B	477	21/21	0.98	0.11	-0.37	28,31,32,37	0
5	EDO	D	33	4/4	0.95	0.08	-0.39	36,37,40,42	0
4	CAP	V	477	21/21	0.97	0.09	-0.39	28,31,33,37	0
5	EDO	D	43	4/4	0.95	0.09	-0.46	38,44,45,46	0
4	CAP	H	477	21/21	0.99	0.09	-0.47	28,32,33,37	0
5	EDO	D	2	4/4	0.97	0.09	-0.49	33,34,41,42	0
5	EDO	D	32	4/4	0.96	0.10	-0.53	34,34,36,37	0
4	CAP	E	477	21/21	0.98	0.11	-0.56	28,31,33,37	0
5	EDO	D	36	4/4	0.94	0.09	-0.58	30,35,38,40	0
3	MG	A	476	1/1	0.97	0.10	-1.20	27,27,27,27	0
3	MG	K	476	1/1	0.96	0.08	-1.20	27,27,27,27	0
3	MG	O	476	1/1	0.98	0.09	-1.21	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	B	476	1/1	0.97	0.09	-1.54	27,27,27,27	0
5	EDO	D	16	4/4	0.97	0.05	-1.64	33,33,34,37	0
3	MG	H	476	1/1	0.99	0.05	-2.12	28,28,28,28	0
3	MG	R	476	1/1	0.97	0.06	-3.59	28,28,28,28	0
3	MG	V	476	1/1	0.99	0.07	-3.89	27,27,27,27	0
5	EDO	D	28	4/4	0.91	0.19	-	42,51,52,57	0
5	EDO	D	46	4/4	0.88	0.16	-	39,41,45,49	0
5	EDO	D	12	4/4	0.88	0.15	-	46,49,49,51	0
5	EDO	D	39	4/4	0.76	0.35	-	53,62,67,69	0
5	EDO	D	44	4/4	0.91	0.21	-	49,59,61,63	0
5	EDO	D	20	4/4	0.90	0.24	-	49,51,52,55	0
5	EDO	D	8	4/4	0.95	0.15	-	29,39,39,41	0
5	EDO	D	35	4/4	0.94	0.18	-	46,47,49,54	0

6.5 Other polymers

There are no such residues in this entry.