Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2017 – 05:01 PM EST

PDB ID	:	5MAC
Title	:	Crystal structure of decameric Methanococcoides burtonii Rubisco complexed with 2-carboxyarabinitol bisphosphate
Authors	:	Gunn, L.H.; Valegard, K.; Andersson, I.
Deposited on	:	2016-11-03
Resolution	:	2.60 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:

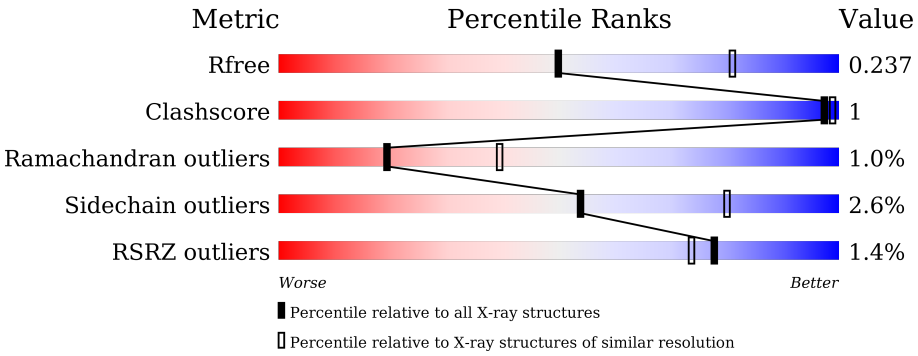
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	474	92% 8%
1	B	474	93% 7%
1	C	474	94% 5%
1	D	474	93% 7%
1	E	474	4% 93% 6%

2 Entry composition

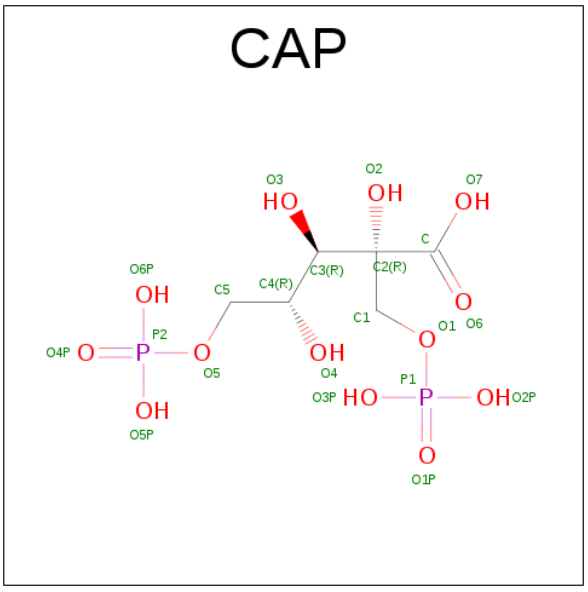
There are 5 unique types of molecules in this entry. The entry contains 19036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-1,5-bisphosphate carboxylase-oxygenase type III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	3	0
			3732	2382	621	703	26			
1	B	473	Total	C	N	O	S	0	2	0
			3721	2376	617	702	26			
1	C	472	Total	C	N	O	S	0	3	0
			3724	2378	619	701	26			
1	D	473	Total	C	N	O	S	0	2	0
			3721	2376	617	702	26			
1	E	472	Total	C	N	O	S	0	3	0
			3724	2377	620	702	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			21	6	13	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O P 21 6 13 2	0	0
2	C	1	Total C O P 21 6 13 2	0	0
2	D	1	Total C O P 21 6 13 2	0	0
2	E	1	Total C O P 21 6 13 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	A	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	E	2	Total Mg 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	86	Total O 86 86	0	0

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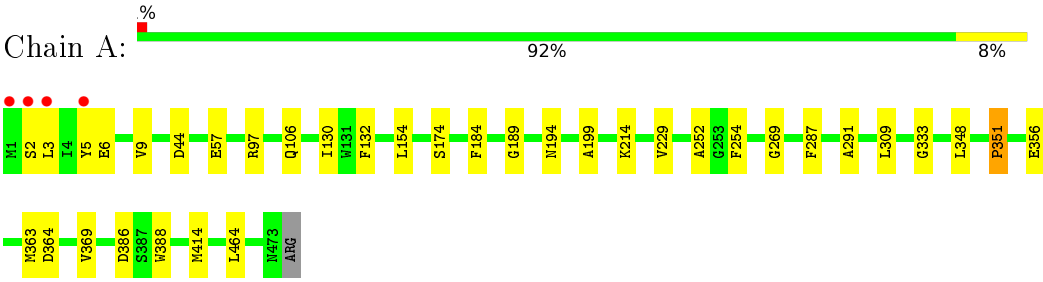
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	85	Total O 85 85	0	0
5	C	50	Total O 50 50	0	0
5	D	45	Total O 45 45	0	0
5	E	28	Total O 28 28	0	0

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.

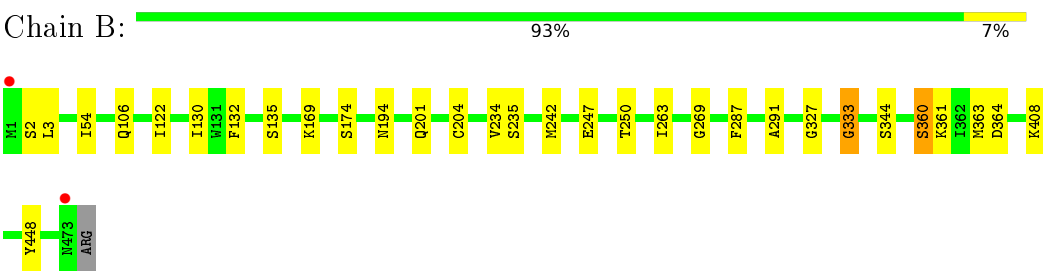
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

Chain A:



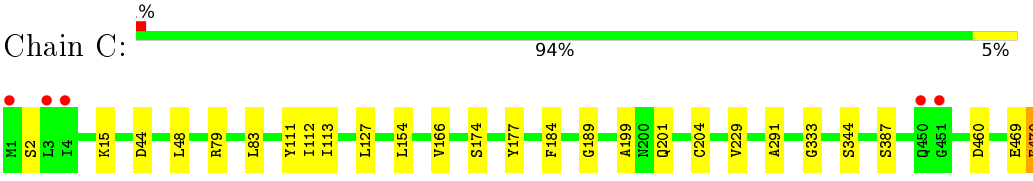
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

Chain B:



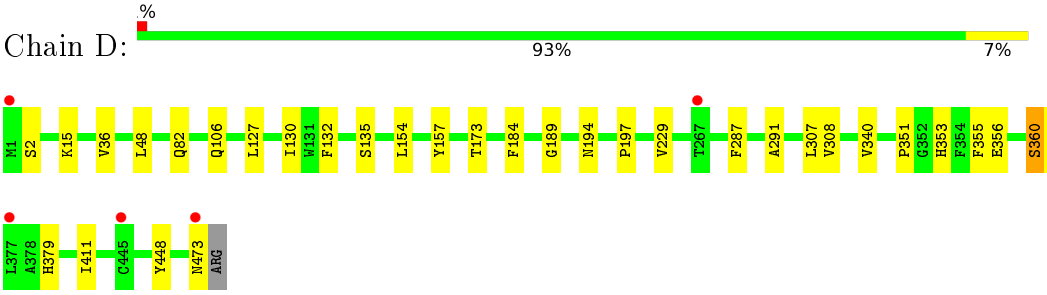
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

Chain C:



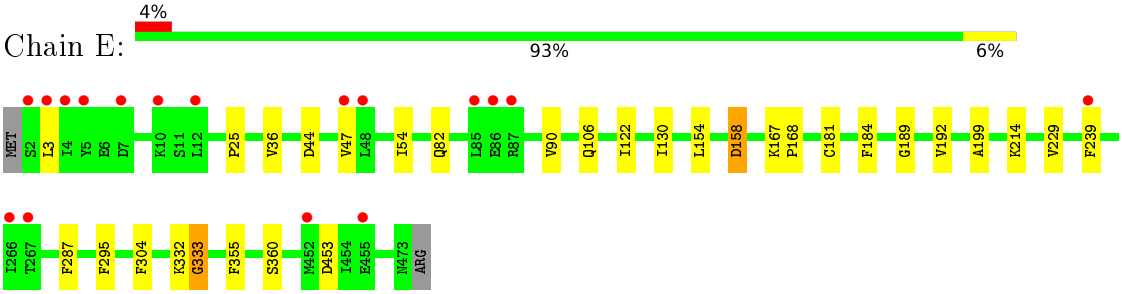
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

Chain D:



• Molecule 1: Ribulose-1,5-bisphosphate carboxylase-oxygenase type III

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	273.76Å 273.76Å 96.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 2.60 48.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.37-2.60) 99.7 (48.37-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.189 , 0.225 0.199 , 0.237	Depositor DCC
R_{free} test set	6337 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19036	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: MG, CAP, KCX, 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	0.52	0/3810	0.75	2/5161 (0.0%)
1	B	0.52	0/3799	0.74	1/5147 (0.0%)
1	C	0.49	0/3802	0.69	0/5150
1	D	0.49	0/3799	0.73	1/5147 (0.0%)
1	E	0.48	0/3802	0.69	2/5151 (0.0%)
All	All	0.50	0/19012	0.72	6/25756 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	2
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	SER	C-N-CA	9.47	145.37	121.70
1	D	360	SER	C-N-CA	9.31	144.97	121.70
1	B	360	SER	C-N-CA	9.26	144.85	121.70
1	E	360	SER	C-N-CA	8.03	141.78	121.70
1	E	158	ASP	N-CA-C	-5.68	95.68	111.00
1	A	351	PRO	CA-C-N	5.42	127.04	116.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	SER	Mainchain,Peptide
1	B	360	SER	Mainchain,Peptide
1	D	360	SER	Mainchain,Peptide

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	3732	0	3651	11	0
1	B	3721	0	3639	12	0
1	C	3724	0	3645	9	0
1	D	3721	0	3639	10	0
1	E	3724	0	3639	8	0
2	A	21	0	7	0	0
2	B	21	0	8	0	0
2	C	21	0	7	0	0
2	D	21	0	8	0	0
2	E	21	0	9	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	86	0	0	0	0
5	B	85	0	0	0	0
5	C	50	0	0	0	0
5	D	45	0	0	0	0
5	E	28	0	0	0	0
All	All	19036	0	18252	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (46) 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:E:154:LEU:HD21	1:E:229:VAL:HG23	1.80	0.63
1:D:36:VAL:HG23	1:D:355:PHE:CE2	2.36	0.60
1:A:154:LEU:HD21	1:A:229:VAL:HG23	1.85	0.57
1:C:48:LEU:HD13	1:C:83:LEU:HD11	1.87	0.56
1:A:386:ASP:HA	1:A:388:TRP:CZ3	2.43	0.53
1:E:36:VAL:HG23	1:E:355:PHE:CE2	2.45	0.52
1:D:154:LEU:HD21	1:D:229:VAL:HG23	1.91	0.51
1:B:54:ILE:HD11	1:B:122:ILE:HG21	1.92	0.51
1:A:5:TYR:O	1:A:9:VAL:HG23	2.12	0.49
1:D:127:LEU:HD23	1:D:308:VAL:HG11	1.94	0.49
1:B:135:SER:HA	1:D:173:THR:HG21	1.93	0.49
1:D:351:PRO:O	1:D:356:GLU:HA	2.14	0.47
1:D:184:PHE:CE2	1:D:189:GLY:HA3	2.50	0.46
1:E:295:PHE:CD1	1:E:304:PHE:CE2	3.03	0.46
1:B:201:GLN:HB2	1:B:204[A]:CYS:SG	2.56	0.45
1:B:327:GLY:HA3	1:B:333:GLY:O	2.17	0.45
1:C:469:GLU:O	1:C:470:PHE:CB	2.64	0.45
1:C:154:LEU:HD21	1:C:229:VAL:HG23	1.99	0.45
1:B:130:ILE:HD13	1:B:132:PHE:CZ	2.52	0.45
1:B:242:MET:HE1	1:B:263:ILE:HD13	1.98	0.44
1:E:181:CYS:SG	1:E:192:VAL:HG11	2.58	0.44
1:A:130:ILE:HD13	1:A:132:PHE:CZ	2.53	0.44
1:E:54:ILE:HD11	1:E:122:ILE:HG21	2.00	0.44
1:E:167:LYS:HA	1:E:168:PRO:C	2.38	0.43
1:A:184:PHE:CE2	1:A:189:GLY:HA3	2.53	0.43
1:E:184:PHE:CE2	1:E:189:GLY:HA3	2.53	0.43
1:B:54:ILE:HD11	1:B:122:ILE:CG2	2.48	0.43
1:C:166:VAL:HG11	1:C:177:TYR:CD1	2.53	0.43
1:B:411:ILE:HG21	1:B:448:TYR:CZ	2.54	0.43
1:B:242:MET:CE	1:B:263:ILE:HD13	2.49	0.42
1:C:113:ILE:O	1:C:113:ILE:HD12	2.20	0.42
1:A:364:ASP:HA	1:A:369:VAL:HG11	2.01	0.42
1:D:130:ILE:HD13	1:D:132:PHE:CZ	2.53	0.42
1:D:340:VAL:HG11	1:D:353:HIS:ND1	2.34	0.42
1:A:252:ALA:HB3	1:A:254:PHE:CD2	2.55	0.42
1:B:247:GLU:HA	1:B:250:THR:HB	2.02	0.42
1:C:111:TYR:CZ	1:D:197:PRO:HB2	2.54	0.42
1:C:112:ILE:HD12	1:C:127:LEU:HD21	2.02	0.42
1:C:201:GLN:HB2	1:C:204[A]:CYS:SG	2.60	0.41
1:E:332:LYS:HA	1:E:333:GLY:HA3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:O	1:A:356:GLU:HA	2.21	0.41
1:C:184:PHE:CE2	1:C:189:GLY:HA3	2.56	0.41
1:A:269:GLY:HA3	1:B:269:GLY:HA3	2.01	0.41
1:D:411:ILE:HG21	1:D:448:TYR:CZ	2.56	0.41
1:A:348:LEU:O	1:A:358:THR:HA	2.21	0.41
1:A:57:GLU:O	1:B:169:LYS:HE3	2.20	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	473/474 (100%)	446 (94%)	22 (5%)	5 (1%)	17	36
1	B	472/474 (100%)	443 (94%)	25 (5%)	4 (1%)	24	46
1	C	472/474 (100%)	452 (96%)	14 (3%)	6 (1%)	15	30
1	D	472/474 (100%)	441 (93%)	28 (6%)	3 (1%)	30	56
1	E	472/474 (100%)	443 (94%)	24 (5%)	5 (1%)	17	36
All	All	2361/2370 (100%)	2225 (94%)	113 (5%)	23 (1%)	19	39

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	B	2	SER
1	B	361	LYS
1	C	2	SER
1	C	470	PHE
1	D	2	SER
1	D	361	LYS
1	C	44	ASP

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Mol	Chain	Res	Type
1	E	3	LEU
1	A	44	ASP
1	A	291	ALA
1	A	333	GLY
1	B	333	GLY
1	C	333	GLY
1	B	291	ALA
1	C	291	ALA
1	D	291	ALA
1	E	44	ASP
1	E	199	ALA
1	A	199	ALA
1	C	199	ALA
1	E	333	GLY
1	E	25	PRO

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	397/395 (100%)	385 (97%)	12 (3%)	48	76
1	B	396/395 (100%)	384 (97%)	12 (3%)	48	76
1	C	396/395 (100%)	389 (98%)	7 (2%)	66	87
1	D	396/395 (100%)	384 (97%)	12 (3%)	48	76
1	E	396/395 (100%)	385 (97%)	11 (3%)	51	78
All	All	1981/1975 (100%)	1927 (97%)	54 (3%)	54	79

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	GLU
1	A	97	ARG
1	A	106	GLN

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Mol	Chain	Res	Type
1	A	174	SER
1	A	194	ASN
1	A	214	LYS
1	A	287	PHE
1	A	309	LEU
1	A	363	MET
1	A	414	MET
1	A	464	LEU
1	B	3	LEU
1	B	106	GLN
1	B	174	SER
1	B	194	ASN
1	B	234	VAL
1	B	235	SER
1	B	287	PHE
1	B	344	SER
1	B	363	MET
1	B	364	ASP
1	B	408	LYS
1	B	414	MET
1	C	15	LYS
1	C	79[A]	ARG
1	C	79[B]	ARG
1	C	174	SER
1	C	344	SER
1	C	387	SER
1	C	460	ASP
1	D	15	LYS
1	D	48	LEU
1	D	82	GLN
1	D	106	GLN
1	D	135	SER
1	D	157	TYR
1	D	194	ASN
1	D	287	PHE
1	D	307	LEU
1	D	364	ASP
1	D	379	HIS
1	D	473	ASN
1	E	47	VAL
1	E	82	GLN
1	E	90	VAL

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Mol	Chain	Res	Type
1	E	106	GLN
1	E	130	ILE
1	E	158	ASP
1	E	214	LYS
1	E	239[A]	PHE
1	E	239[B]	PHE
1	E	287	PHE
1	E	453	ASP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

5 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	KCX	A	193	1,3	6,11,12	1.16	0	7,12,14	1.31	1 (14%)
1	KCX	B	193	1,3	6,11,12	0.96	0	7,12,14	0.73	0
1	KCX	C	193	1,3	6,11,12	0.64	0	7,12,14	1.32	1 (14%)
1	KCX	D	193	1,3	6,11,12	1.27	1 (16%)	7,12,14	1.28	0
1	KCX	E	193	1,3	6,11,12	0.56	0	7,12,14	1.20	1 (14%)

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	KCX	A	193	1,3	-	0/6/10/12	0/0/0/0
1	KCX	B	193	1,3	-	0/6/10/12	0/0/0/0
1	KCX	C	193	1,3	-	0/6/10/12	0/0/0/0
1	KCX	D	193	1,3	-	0/6/10/12	0/0/0/0
1	KCX	E	193	1,3	-	0/6/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	KCX	CB-CA	2.82	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	193	KCX	CE-NZ-CX	-2.15	121.27	123.53
1	A	193	KCX	CB-CA-N	2.26	116.89	110.54
1	C	193	KCX	CD-CE-NZ	2.42	117.88	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 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	$\#\|Z\|>2$
2	CAP	A	501	3	14,20,20	0.62	0	16,31,31	1.15	1 (6%)
2	CAP	B	501	3	14,20,20	0.69	0	16,31,31	1.22	1 (6%)
2	CAP	C	501	3	14,20,20	0.63	0	16,31,31	1.26	1 (6%)
2	CAP	D	501	3	14,20,20	0.67	0	16,31,31	1.23	2 (12%)
2	CAP	E	501	3	14,20,20	0.65	0	16,31,31	1.18	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	CAP	A	501	3	-	0/23/29/29	0/0/0/0
2	CAP	B	501	3	-	0/23/29/29	0/0/0/0
2	CAP	C	501	3	-	0/23/29/29	0/0/0/0
2	CAP	D	501	3	-	0/23/29/29	0/0/0/0
2	CAP	E	501	3	-	0/23/29/29	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	CAP	O5-P2-O4P	-2.05	101.94	107.08
2	A	501	CAP	O6P-P2-O4P	2.14	117.61	110.63
2	B	501	CAP	O6P-P2-O5P	2.14	115.31	107.44
2	C	501	CAP	O3-C3-C4	2.25	113.63	109.07
2	D	501	CAP	O1-C1-C2	2.72	114.83	109.53

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

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	472/474 (99%)	-0.40	4 (0%)	87 85	43, 55, 75, 107	0
1	B	472/474 (99%)	-0.40	2 (0%)	93 91	43, 55, 73, 98	0
1	C	471/474 (99%)	-0.22	5 (1%)	82 79	51, 64, 84, 110	0
1	D	472/474 (99%)	-0.22	5 (1%)	82 79	48, 62, 81, 121	0
1	E	471/474 (99%)	-0.06	17 (3%)	46 38	56, 72, 92, 113	0
All	All	2358/2370 (99%)	-0.26	33 (1%)	78 74	43, 61, 84, 121	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.1
1	A	3	LEU	4.2
1	E	12	LEU	3.1
1	E	5	TYR	3.1
1	E	239[A]	PHE	3.1
1	C	3	LEU	3.0
1	C	1	MET	2.9
1	E	4	ILE	2.8
1	D	1	MET	2.8
1	E	267	THR	2.8
1	E	3	LEU	2.8
1	E	10	LYS	2.7
1	A	2	SER	2.7
1	D	445	CYS	2.5
1	E	266	ILE	2.5
1	C	4	ILE	2.4
1	E	2	SER	2.4
1	E	47	VAL	2.4
1	B	473	ASN	2.3
1	D	267	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	48	LEU	2.2
1	E	85	LEU	2.2
1	E	86	GLU	2.1
1	A	5	TYR	2.1
1	E	455	GLU	2.1
1	C	450	GLN	2.1
1	B	1	MET	2.1
1	E	452	MET	2.1
1	D	377	LEU	2.0
1	E	87	ARG	2.0
1	D	473	ASN	2.0
1	E	7	ASP	2.0
1	C	451	GLY	2.0

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	KCX	B	193	12/13	0.98	0.16	-	45,47,51,52	0
1	KCX	A	193	12/13	0.97	0.14	-	47,52,55,56	0
1	KCX	D	193	12/13	0.97	0.16	-	48,48,52,55	0
1	KCX	C	193	12/13	0.96	0.18	-	60,63,63,65	0
1	KCX	E	193	12/13	0.97	0.18	-	57,61,66,66	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
3	MG	C	503	1/1	0.99	0.16	1.07	50,50,50,50	0
2	CAP	C	501	21/21	0.96	0.17	0.42	62,66,73,74	0
3	MG	A	503	1/1	0.99	0.13	0.12	41,41,41,41	0
2	CAP	E	501	21/21	0.97	0.16	0.10	75,78,80,80	0
2	CAP	B	501	21/21	0.98	0.16	0.01	52,60,65,67	0
2	CAP	A	501	21/21	0.98	0.14	-0.39	50,55,60,63	0
2	CAP	D	501	21/21	0.98	0.13	-0.50	54,61,63,64	0
4	CL	A	504	1/1	0.99	0.11	-0.82	49,49,49,49	0
3	MG	E	502	1/1	0.93	0.15	-0.97	62,62,62,62	0
3	MG	B	502	1/1	0.96	0.15	-1.06	59,59,59,59	0
3	MG	A	502	1/1	0.98	0.12	-1.35	46,46,46,46	0
4	CL	B	504	1/1	1.00	0.12	-1.40	48,48,48,48	0
4	CL	D	504	1/1	0.88	0.08	-1.45	61,61,61,61	0
3	MG	C	502	1/1	0.92	0.13	-1.45	58,58,58,58	0
3	MG	B	503	1/1	0.97	0.08	-1.77	46,46,46,46	0
3	MG	D	502	1/1	0.99	0.09	-1.86	55,55,55,55	0
3	MG	D	503	1/1	0.98	0.07	-4.53	53,53,53,53	0
4	CL	E	504	1/1	0.94	0.10	-	63,63,63,63	0
4	CL	C	504	1/1	0.98	0.10	-	49,49,49,49	0
3	MG	E	503	1/1	0.97	0.11	-	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.