Full wwPDB X-ray Structure Validation Report

Jun 17, 2024 – 07:30 PM EDT

PDB ID	:	5Y2V
Title	:	Strcutrue of the full-length CcmR complexed with 2-OG from Synechocystis PCC6803
Authors	:	Jiang, Y.L.; Wang, X.P.; Sun, H.; Cheng, W.; Han, S.J.; Li, W.F.; Chen, Y.; Zhou, C.Z.
Deposited on	:	2017-07-27
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

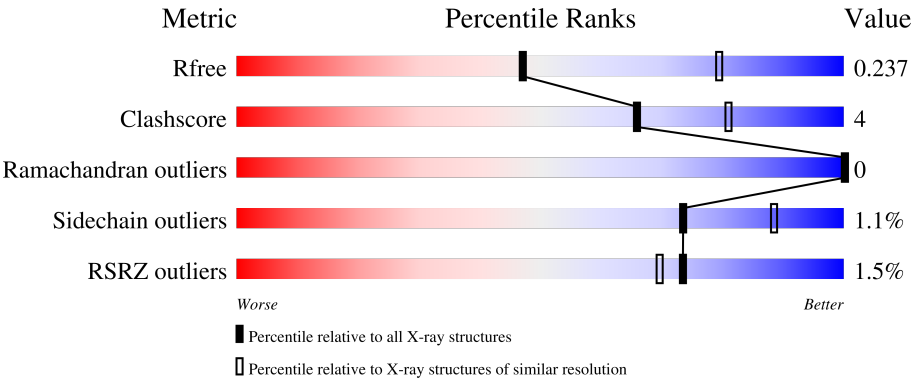
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	A	324	88% 6% 6%
1	B	324	2% 82% 12% 6%
1	C	324	% 79% 13% 8%
1	D	324	2% 84% 9% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	C	401	-	X	-	-
3	AKG	B	401	-	X	-	-
3	AKG	D	401	-	X	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9770 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 Rubisco operon transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2423	1543	429	443	8			
1	B	303	Total	C	N	O	S	0	0	0
			2417	1539	428	442	8			
1	C	299	Total	C	N	O	S	0	0	0
			2384	1516	422	438	8			
1	D	302	Total	C	N	O	S	0	0	0
			2407	1533	425	441	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P73862
A	-6	GLY	-	expression tag	UNP P73862
A	-5	HIS	-	expression tag	UNP P73862
A	-4	HIS	-	expression tag	UNP P73862
A	-3	HIS	-	expression tag	UNP P73862
A	-2	HIS	-	expression tag	UNP P73862
A	-1	HIS	-	expression tag	UNP P73862
A	0	HIS	-	expression tag	UNP P73862
B	-7	MET	-	expression tag	UNP P73862
B	-6	GLY	-	expression tag	UNP P73862
B	-5	HIS	-	expression tag	UNP P73862
B	-4	HIS	-	expression tag	UNP P73862
B	-3	HIS	-	expression tag	UNP P73862
B	-2	HIS	-	expression tag	UNP P73862
B	-1	HIS	-	expression tag	UNP P73862
B	0	HIS	-	expression tag	UNP P73862
C	-7	MET	-	expression tag	UNP P73862
C	-6	GLY	-	expression tag	UNP P73862
C	-5	HIS	-	expression tag	UNP P73862
C	-4	HIS	-	expression tag	UNP P73862
C	-3	HIS	-	expression tag	UNP P73862

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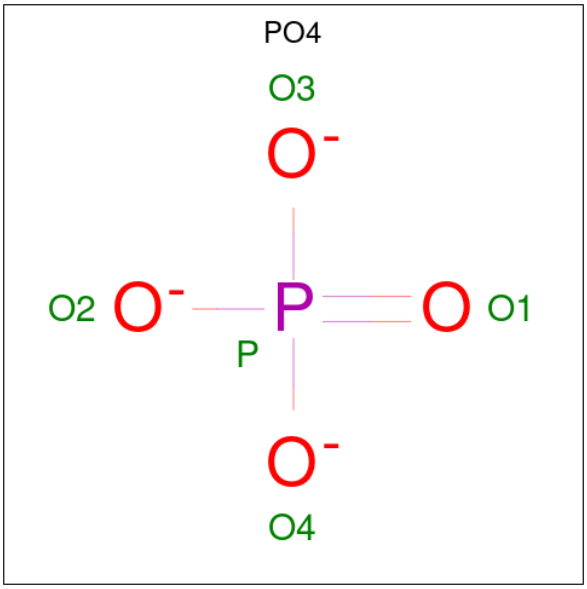
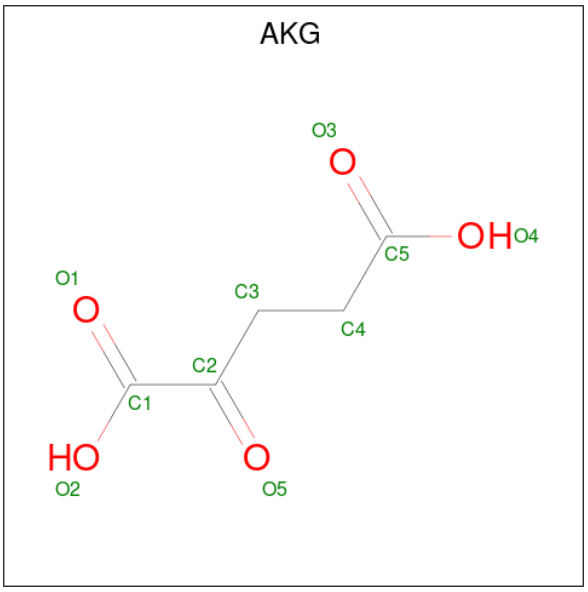
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP P73862
C	-1	HIS	-	expression tag	UNP P73862
C	0	HIS	-	expression tag	UNP P73862
D	-7	MET	-	expression tag	UNP P73862
D	-6	GLY	-	expression tag	UNP P73862
D	-5	HIS	-	expression tag	UNP P73862
D	-4	HIS	-	expression tag	UNP P73862
D	-3	HIS	-	expression tag	UNP P73862
D	-2	HIS	-	expression tag	UNP P73862
D	-1	HIS	-	expression tag	UNP P73862
D	0	HIS	-	expression tag	UNP P73862

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0

- Molecule 4 is water.

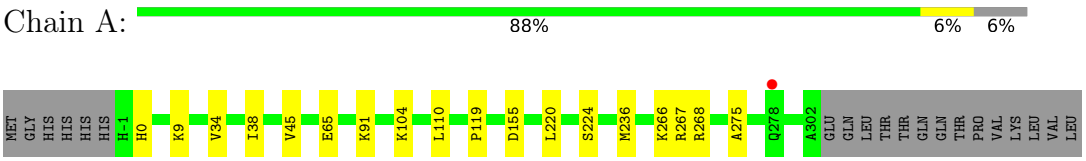
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	25	Total O 25 25	0	0
4	C	30	Total O 30 30	0	0
4	D	28	Total O 28 28	0	0

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.

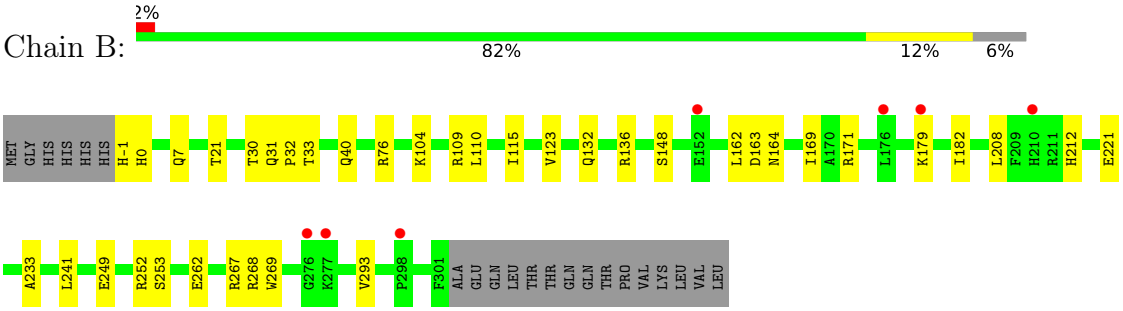
• Molecule 1: Rubisco operon transcriptional regulator

Chain A:



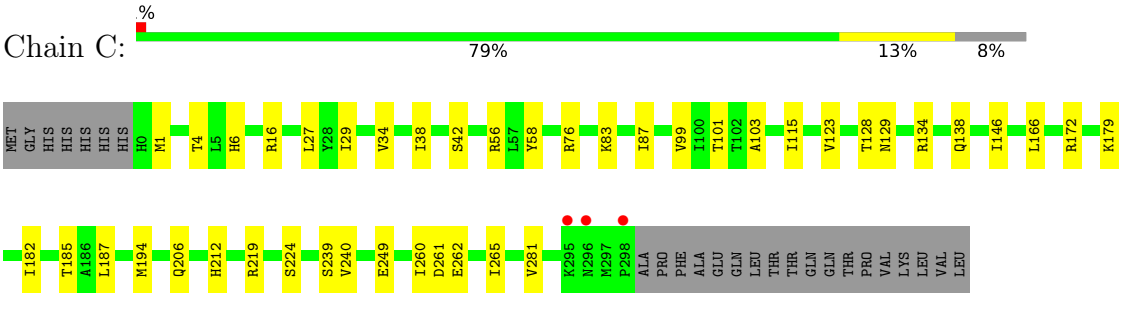
• Molecule 1: Rubisco operon transcriptional regulator

Chain B:



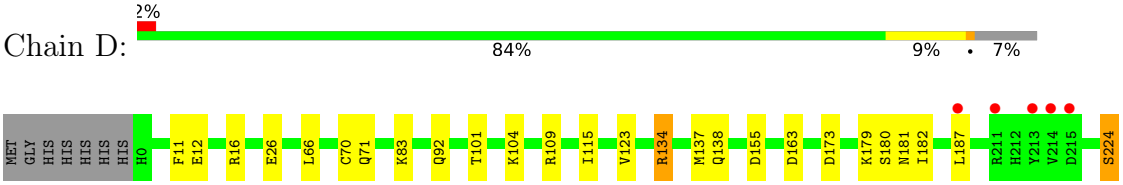
• Molecule 1: Rubisco operon transcriptional regulator

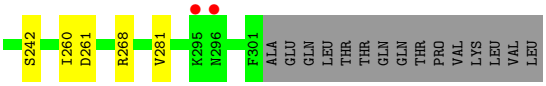
Chain C:



• Molecule 1: Rubisco operon transcriptional regulator

Chain D:




S242
I260
D261
R268
V281
K295
N296
F301
ALA
GLU
GLN
LEU
THR
THR
GLN
GLN
THR
PRO
VAL
LYS
LEU
VAL
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.77Å 109.16Å 178.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 37.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-2.60) 94.9 (37.56-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.197 , 0.234 0.202 , 0.237	Depositor DCC
R_{free} test set	2632 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	64.2	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9770	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9721e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: AKG, PO4

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	0.77	0/2469	0.87	2/3341 (0.1%)
1	B	0.75	0/2461	0.88	2/3330 (0.1%)
1	C	0.82	0/2425	0.92	1/3280 (0.0%)
1	D	0.79	0/2450	0.93	5/3315 (0.2%)
All	All	0.78	0/9805	0.90	10/13266 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	134	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	D	173	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	16	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	109	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	268	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	110	LEU	CA-CB-CG	5.56	128.10	115.30
1	D	268	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	267	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	163	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	109	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2423	0	2471	11	0
1	B	2417	0	2464	27	0
1	C	2384	0	2436	26	0
1	D	2407	0	2457	18	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	B	10	0	4	0	0
3	D	10	0	4	4	0
4	A	26	0	0	1	0
4	B	25	0	0	6	0
4	C	30	0	0	3	0
4	D	28	0	0	2	0
All	All	9770	0	9836	78	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 4.

All (78) 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:D:224:SER:OG	3:D:401:AKG:O3	1.67	1.10
1:D:224:SER:CB	3:D:401:AKG:O3	2.25	0.84
1:B:268:ARG:HA	4:B:501:HOH:O	1.81	0.80
1:B:76:ARG:NH2	4:B:503:HOH:O	2.16	0.79
1:D:83:LYS:HE3	1:D:92:GLN:HE22	1.54	0.72
1:B:162:LEU:O	4:B:501:HOH:O	2.05	0.72
1:B:269:TRP:O	4:B:502:HOH:O	2.09	0.69
1:A:220:LEU:HD22	1:A:236:MET:SD	2.35	0.66
1:C:261:ASP:HB3	4:C:503:HOH:O	1.97	0.65
1:C:187:LEU:HD21	1:C:260:ILE:CD1	2.27	0.65
1:D:16:ARG:NH2	1:D:26:GLU:OE2	2.30	0.64
1:B:30:THR:HG22	1:B:32:PRO:HD2	1.81	0.62
1:D:179:LYS:HB2	1:D:182:ILE:HD11	1.82	0.60
1:D:242:SER:OG	4:D:501:HOH:O	2.16	0.59
1:C:115:ILE:HD11	1:C:123:VAL:HG11	1.85	0.58
1:C:99:VAL:HG22	1:C:146:ILE:HB	1.86	0.58
1:C:56:ARG:HD3	1:C:58:TYR:CZ	2.37	0.58
1:A:34:VAL:O	1:A:38:ILE:HG12	2.04	0.57
1:B:179:LYS:HB2	1:B:182:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:O	4:A:501:HOH:O	2.18	0.56
1:C:87:ILE:O	1:C:281:VAL:HG21	2.05	0.56
1:C:212:HIS:NE2	1:C:262:GLU:HG2	2.21	0.55
1:B:110:LEU:HD13	1:B:293:VAL:HG11	1.89	0.55
1:C:99:VAL:HG13	1:C:103:ALA:HB3	1.89	0.55
1:B:249:GLU:HG3	1:B:253:SER:OG	2.08	0.54
1:B:221:GLU:OE2	1:B:221:GLU:CG	2.55	0.54
1:A:104:LYS:NZ	3:D:401:AKG:H42	2.23	0.53
1:B:164:ASN:N	4:B:501:HOH:O	2.41	0.53
1:B:115:ILE:HD11	1:B:123:VAL:HG13	1.90	0.53
1:B:115:ILE:HG23	1:C:219:ARG:NH2	2.25	0.52
1:A:0:HIS:NE2	1:A:45:VAL:HG22	2.25	0.52
1:A:65:GLU:HG3	4:C:517:HOH:O	2.11	0.50
1:C:179:LYS:HB2	1:C:182:ILE:HD11	1.93	0.50
1:C:261:ASP:O	1:C:262:GLU:HB2	2.10	0.50
1:C:115:ILE:HD11	1:C:123:VAL:CG1	2.41	0.50
1:B:171:ARG:NH1	1:B:233:ALA:O	2.43	0.49
1:B:30:THR:HB	1:B:33:THR:OG1	2.13	0.49
1:B:163:ASP:C	4:B:501:HOH:O	2.51	0.48
1:C:34:VAL:O	1:C:38:ILE:HG12	2.13	0.48
1:D:12:GLU:OE1	1:D:16:ARG:NH1	2.49	0.46
1:B:212:HIS:NE2	1:B:262:GLU:HG3	2.31	0.46
1:C:27:LEU:O	1:C:29:ILE:HG23	2.15	0.46
1:B:249:GLU:HG3	1:B:253:SER:CB	2.46	0.45
1:D:101:THR:O	1:D:104:LYS:HE2	2.16	0.45
1:A:65:GLU:HG2	1:C:83:LYS:HG2	1.98	0.45
1:B:208:LEU:O	1:B:208:LEU:HG	2.17	0.45
1:D:187:LEU:HD21	1:D:260:ILE:CD1	2.46	0.45
1:B:-1:HIS:CG	1:B:0:HIS:H	2.35	0.45
1:D:260:ILE:HG22	1:D:261:ASP:O	2.16	0.45
1:C:239:SER:OG	1:C:240:VAL:N	2.50	0.45
1:B:252:ARG:HD3	1:C:249:GLU:O	2.16	0.44
1:C:128:THR:OG1	1:C:129:ASN:N	2.46	0.44
1:A:9:LYS:HE2	1:C:1:MET:HB3	1.98	0.44
1:C:187:LEU:HD21	1:C:260:ILE:HD12	1.99	0.44
1:B:30:THR:HG22	1:B:32:PRO:CD	2.46	0.44
1:D:83:LYS:HE3	1:D:92:GLN:NE2	2.26	0.43
1:D:66:LEU:HD23	1:D:70:CYS:SG	2.59	0.42
1:B:132:GLN:O	1:B:136:ARG:HG3	2.20	0.42
1:C:4:THR:HG22	1:C:6:HIS:N	2.34	0.42
1:C:166:LEU:HB2	1:C:265:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:THR:HG22	1:B:31:GLN:HG3	2.00	0.42
1:C:134:ARG:O	1:C:138:GLN:HG2	2.20	0.42
1:D:115:ILE:HD11	1:D:123:VAL:HG11	2.02	0.42
1:D:180:SER:O	1:D:181:ASN:C	2.56	0.42
1:D:71:GLN:NE2	4:D:503:HOH:O	2.33	0.42
1:A:91:LYS:HE3	1:A:119:PRO:O	2.20	0.42
1:B:169:ILE:HD12	1:B:241:LEU:HB2	2.01	0.42
1:A:104:LYS:CE	3:D:401:AKG:H42	2.50	0.41
1:B:249:GLU:HG3	1:B:253:SER:HB2	2.02	0.41
1:D:134:ARG:O	1:D:138:GLN:HG2	2.20	0.41
1:B:110:LEU:CD1	1:B:293:VAL:HG11	2.50	0.41
1:A:155:ASP:HB3	1:A:275:ALA:HB2	2.02	0.41
1:C:4:THR:HG22	1:C:6:HIS:H	1.85	0.41
1:D:137:MET:HB2	1:D:137:MET:HE2	1.91	0.41
1:C:172:ARG:NH1	4:C:507:HOH:O	2.53	0.40
1:D:11:PHE:CE2	1:D:66:LEU:HD22	2.56	0.40
1:B:7:GLN:HE22	1:B:40:GLN:HG3	1.87	0.40
1:C:194:MET:CE	1:C:206:GLN:HG3	2.52	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	302/324 (93%)	289 (96%)	13 (4%)	0	100	100
1	B	301/324 (93%)	290 (96%)	11 (4%)	0	100	100
1	C	297/324 (92%)	285 (96%)	12 (4%)	0	100	100
1	D	300/324 (93%)	289 (96%)	11 (4%)	0	100	100
All	All	1200/1296 (93%)	1153 (96%)	47 (4%)	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	263/282 (93%)	261 (99%)	2 (1%)	81 92
1	B	262/282 (93%)	260 (99%)	2 (1%)	81 92
1	C	259/282 (92%)	254 (98%)	5 (2%)	57 79
1	D	261/282 (93%)	258 (99%)	3 (1%)	73 88
All	All	1045/1128 (93%)	1033 (99%)	12 (1%)	73 88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	SER
1	A	267	ARG
1	B	104	LYS
1	B	148	SER
1	C	42	SER
1	C	76	ARG
1	C	101	THR
1	C	185	THR
1	C	224	SER
1	D	155	ASP
1	D	224	SER
1	D	281	VAL

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

Mol	Chain	Res	Type
1	A	92	GLN
1	A	140	ASN
1	A	206	GLN
1	A	212	HIS
1	A	284	GLN
1	B	7	GLN
1	C	37	GLN

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Mol	Chain	Res	Type
1	C	159	GLN
1	D	92	GLN

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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AKG	B	401	-	9,9,9	3.30	3 (33%)	11,11,11	4.50	8 (72%)
2	PO4	A	401	-	4,4,4	2.68	2 (50%)	6,6,6	1.95	1 (16%)
2	PO4	C	401	-	4,4,4	1.37	1 (25%)	6,6,6	1.78	3 (50%)
3	AKG	D	401	-	9,9,9	2.80	4 (44%)	11,11,11	4.08	7 (63%)

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
3	AKG	B	401	-	-	7/9/9/9	-
3	AKG	D	401	-	-	3/9/9/9	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	AKG	C2-C1	-9.11	1.41	1.53
3	D	401	AKG	C2-C1	-6.64	1.44	1.53
2	A	401	PO4	P-O1	4.25	1.60	1.50
3	D	401	AKG	C3-C2	-3.18	1.47	1.51
3	D	401	AKG	C4-C5	-2.56	1.44	1.50
3	D	401	AKG	O2-C1	-2.41	1.23	1.30
2	A	401	PO4	P-O4	2.33	1.61	1.54
2	C	401	PO4	P-O1	2.33	1.56	1.50
3	B	401	AKG	O3-C5	2.15	1.29	1.22
3	B	401	AKG	O1-C1	2.09	1.28	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	AKG	O1-C1-C2	-10.17	108.14	121.72
3	D	401	AKG	O1-C1-C2	-6.72	112.74	121.72
3	D	401	AKG	C3-C4-C5	-5.90	100.92	113.60
3	B	401	AKG	O5-C2-C1	-5.89	110.90	119.43
3	D	401	AKG	O5-C2-C1	5.05	126.75	119.43
3	D	401	AKG	C4-C3-C2	-4.99	103.63	113.03
3	D	401	AKG	O2-C1-C2	4.80	127.09	113.97
3	B	401	AKG	O2-C1-O1	4.30	133.46	123.61
3	B	401	AKG	C4-C3-C2	-4.26	105.00	113.03
3	B	401	AKG	O4-C5-O3	4.24	133.87	123.30
3	D	401	AKG	O4-C5-O3	4.17	133.68	123.30
2	A	401	PO4	O3-P-O1	-3.36	98.62	110.89
3	B	401	AKG	C3-C2-C1	3.20	121.92	115.97
3	B	401	AKG	O3-C5-C4	-2.66	114.54	123.08
3	D	401	AKG	O3-C5-C4	-2.63	114.63	123.08
3	B	401	AKG	O5-C2-C3	2.60	126.97	121.20
2	C	401	PO4	O4-P-O3	-2.42	100.20	107.97
2	C	401	PO4	O3-P-O2	2.07	114.61	107.97
2	C	401	PO4	O2-P-O1	-2.02	103.51	110.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	AKG	O2-C1-C2-C3
3	B	401	AKG	C2-C3-C4-C5
3	D	401	AKG	O1-C1-C2-O5
3	D	401	AKG	O1-C1-C2-C3
3	D	401	AKG	O2-C1-C2-C3
3	B	401	AKG	O5-C2-C3-C4
3	B	401	AKG	O2-C1-C2-O5
3	B	401	AKG	C3-C4-C5-O4
3	B	401	AKG	C3-C4-C5-O3
3	B	401	AKG	O1-C1-C2-O5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	AKG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	304/324 (93%)	-0.25	1 (0%)	94	93	54, 76, 115, 135	1 (0%)
1	B	303/324 (93%)	-0.19	7 (2%)	60	54	55, 80, 120, 161	1 (0%)
1	C	299/324 (92%)	-0.33	3 (1%)	82	80	52, 73, 104, 125	0
1	D	302/324 (93%)	-0.15	7 (2%)	60	54	54, 77, 116, 151	0
All	All	1208/1296 (93%)	-0.23	18 (1%)	73	70	52, 76, 117, 161	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	GLY	5.6
1	D	213	TYR	5.2
1	C	296	ASN	4.3
1	D	296	ASN	3.6
1	D	295	LYS	3.3
1	B	179	LYS	2.8
1	D	187	LEU	2.7
1	D	214	VAL	2.5
1	C	295	LYS	2.4
1	C	298	PRO	2.2
1	D	215	ASP	2.2
1	B	176	LEU	2.2
1	A	278	GLN	2.1
1	B	152	GLU	2.1
1	D	211	ARG	2.1
1	B	210	HIS	2.1
1	B	277	LYS	2.1
1	B	298	PRO	2.1

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

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

6.3 Carbohydrates (i)

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
3	AKG	D	401	10/10	0.87	0.22	59,69,78,88	0
3	AKG	B	401	10/10	0.90	0.18	55,63,71,78	0
2	PO4	A	401	5/5	0.94	0.09	66,67,76,107	0
2	PO4	C	401	5/5	0.98	0.09	69,72,85,100	0

6.5 Other polymers (i)

There are no such residues in this entry.