Full wwPDB X-ray Structure Validation Report (i)

May 12, 2016 – 06:15 AM EDT

PDB ID	:	5EQU
Title	:	Crystal structure of the epimerase SnoN in complex with Fe3+, alpha ketoglutarate and nogalamycin RO
Authors	:	Selvaraj, B.; Lindqvist, Y.; Siitonen, V.; Metsa-Ketela, M.; Schneider, G.
Deposited on	:	2015-11-13
Resolution	:	2.20 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:

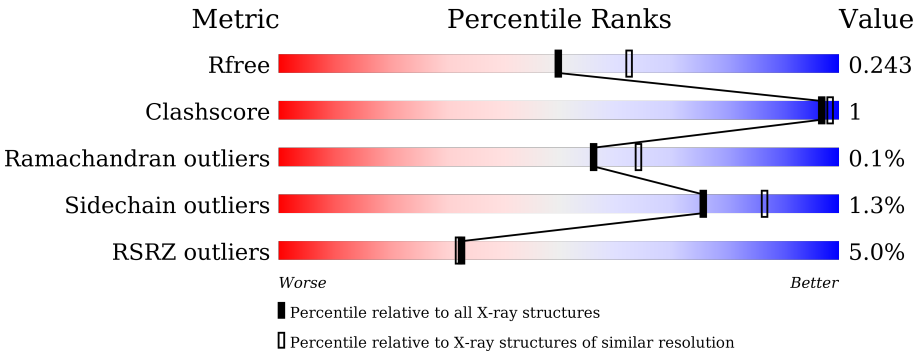
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	305	2% 80% • 16%
1	B	305	4% 76% 6% • 16%
1	C	305	4% 80% • 16%
1	D	305	7% 83% 16%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	5R6	B	302	-	-	-	X
4	5R6	C	302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8337 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 SnoN,SnoN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	1	0
			1954	1232	351	364	7			
1	B	256	Total	C	N	O	S	0	0	0
			1946	1227	348	364	7			
1	C	256	Total	C	N	O	S	0	0	0
			1946	1227	348	364	7			
1	D	256	Total	C	N	O	S	0	1	0
			1954	1232	351	364	7			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9RN67
A	-10	ALA	-	expression tag	UNP Q9RN67
A	-9	HIS	-	expression tag	UNP Q9RN67
A	-8	HIS	-	expression tag	UNP Q9RN67
A	-7	HIS	-	expression tag	UNP Q9RN67
A	-6	HIS	-	expression tag	UNP Q9RN67
A	-5	HIS	-	expression tag	UNP Q9RN67
A	-4	HIS	-	expression tag	UNP Q9RN67
A	-3	HIS	-	expression tag	UNP Q9RN67
A	-2	ARG	-	expression tag	UNP Q9RN67
A	-1	SER	-	expression tag	UNP Q9RN67
A	0	ALA	-	expression tag	UNP Q9RN67
A	1	ASP	-	expression tag	UNP Q9RN67
B	-11	MET	-	initiating methionine	UNP Q9RN67
B	-10	ALA	-	expression tag	UNP Q9RN67
B	-9	HIS	-	expression tag	UNP Q9RN67
B	-8	HIS	-	expression tag	UNP Q9RN67
B	-7	HIS	-	expression tag	UNP Q9RN67
B	-6	HIS	-	expression tag	UNP Q9RN67
B	-5	HIS	-	expression tag	UNP Q9RN67
B	-4	HIS	-	expression tag	UNP Q9RN67

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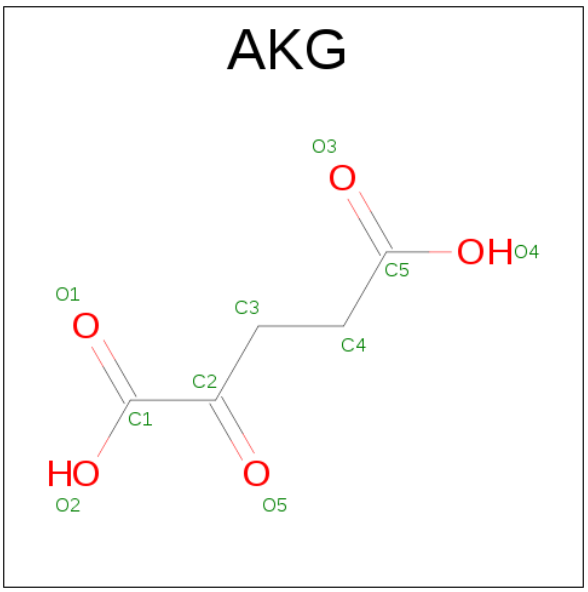
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9RN67
B	-2	ARG	-	expression tag	UNP Q9RN67
B	-1	SER	-	expression tag	UNP Q9RN67
B	0	ALA	-	expression tag	UNP Q9RN67
B	1	ASP	-	expression tag	UNP Q9RN67
C	-11	MET	-	initiating methionine	UNP Q9RN67
C	-10	ALA	-	expression tag	UNP Q9RN67
C	-9	HIS	-	expression tag	UNP Q9RN67
C	-8	HIS	-	expression tag	UNP Q9RN67
C	-7	HIS	-	expression tag	UNP Q9RN67
C	-6	HIS	-	expression tag	UNP Q9RN67
C	-5	HIS	-	expression tag	UNP Q9RN67
C	-4	HIS	-	expression tag	UNP Q9RN67
C	-3	HIS	-	expression tag	UNP Q9RN67
C	-2	ARG	-	expression tag	UNP Q9RN67
C	-1	SER	-	expression tag	UNP Q9RN67
C	0	ALA	-	expression tag	UNP Q9RN67
C	1	ASP	-	expression tag	UNP Q9RN67
D	-11	MET	-	initiating methionine	UNP Q9RN67
D	-10	ALA	-	expression tag	UNP Q9RN67
D	-9	HIS	-	expression tag	UNP Q9RN67
D	-8	HIS	-	expression tag	UNP Q9RN67
D	-7	HIS	-	expression tag	UNP Q9RN67
D	-6	HIS	-	expression tag	UNP Q9RN67
D	-5	HIS	-	expression tag	UNP Q9RN67
D	-4	HIS	-	expression tag	UNP Q9RN67
D	-3	HIS	-	expression tag	UNP Q9RN67
D	-2	ARG	-	expression tag	UNP Q9RN67
D	-1	SER	-	expression tag	UNP Q9RN67
D	0	ALA	-	expression tag	UNP Q9RN67
D	1	ASP	-	expression tag	UNP Q9RN67

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

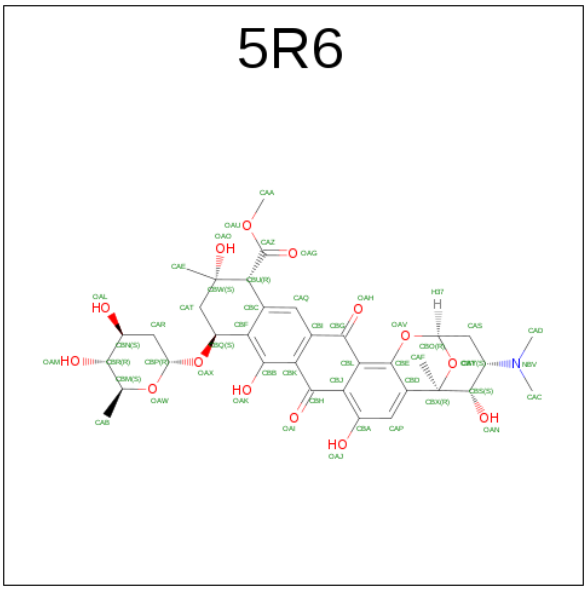
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

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



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

- Molecule 4 is Nogalamycin RO (three-letter code: 5R6) (formula: $C_{35}H_{41}NO_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			50	35	1	14		
4	B	1	Total	C	N	O	0	0
			50	35	1	14		
4	C	1	Total	C	N	O	0	0
			50	35	1	14		
4	D	1	Total	C	N	O	0	0
			50	35	1	14		

- Molecule 5 is water.

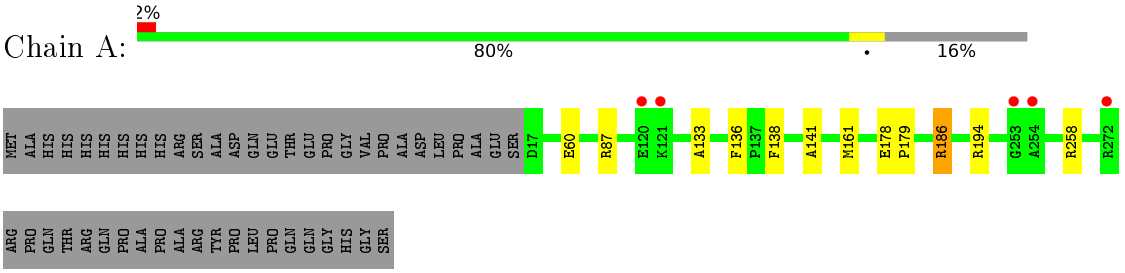
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total	O	0	0
			102	102		
5	B	70	Total	O	0	0
			70	70		
5	C	69	Total	O	0	0
			69	69		
5	D	52	Total	O	0	0
			52	52		

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.

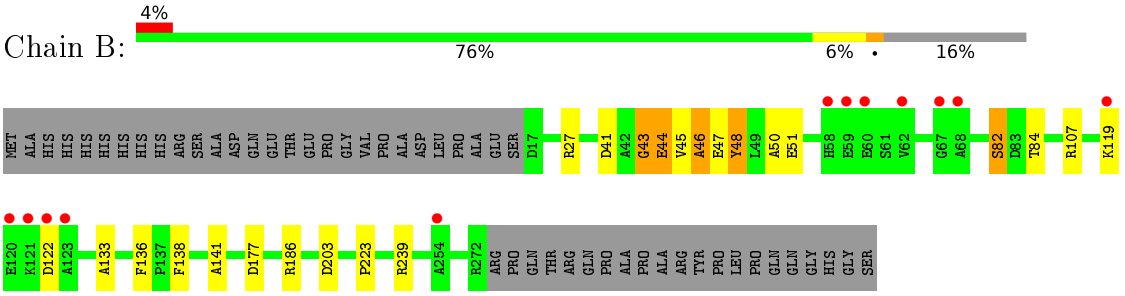
- Molecule 1: SnoN,SnoN

Chain A:



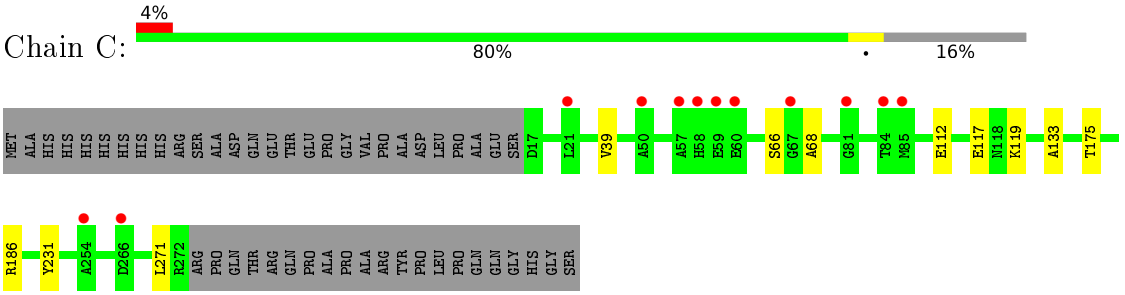
- Molecule 1: SnoN,SnoN

Chain B:



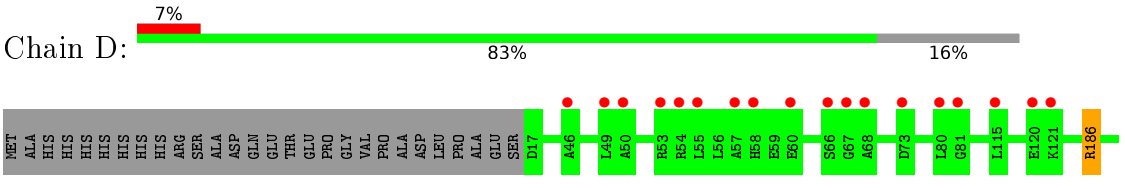
- Molecule 1: SnoN,SnoN

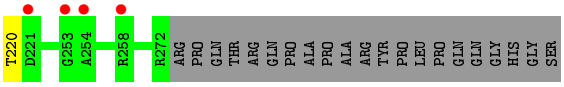
Chain C:



- Molecule 1: SnoN,SnoN

Chain D:




T220
D221
G253
A254
R258
R272
ARG
PRO
GLN
THR
ARG
GLN
PRO
ALA
PRO
ALA
ARG
TYR
PRO
LEU
PRO
GLN
GLN
GLY
HIS
GLY
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.91Å 119.74Å 159.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.75 – 2.20 48.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (95.75-2.20) 99.0 (48.77-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.199 , 0.238 0.211 , 0.243	Depositor DCC
R_{free} test set	3423 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8337	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: 5R6, AKG, FE

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	0.67	0/2010	0.87	5/2746 (0.2%)
1	B	1.21	8/1999 (0.4%)	1.00	14/2732 (0.5%)
1	C	0.64	0/1999	0.83	0/2732
1	D	0.58	0/2010	0.78	1/2746 (0.0%)
All	All	0.81	8/8018 (0.1%)	0.88	20/10956 (0.2%)

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	B	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	SER	CB-OG	30.77	1.82	1.42
1	B	47	GLU	CD-OE1	23.54	1.51	1.25
1	B	46	ALA	CA-CB	8.96	1.71	1.52
1	B	44	GLU	CA-C	7.18	1.71	1.52
1	B	48	TYR	C-N	7.15	1.50	1.34
1	B	43	GLY	C-N	6.85	1.49	1.34
1	B	46	ALA	N-CA	5.26	1.56	1.46
1	B	50	ALA	C-O	5.04	1.32	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	41	ASP	CB-CG-OD2	-13.16	106.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	43	GLY	CA-C-O	8.75	136.35	120.60
1	B	46	ALA	CB-CA-C	7.46	121.29	110.10
1	B	46	ALA	O-C-N	-7.39	110.87	122.70
1	B	44	GLU	CA-C-N	-6.99	101.82	117.20
1	B	43	GLY	O-C-N	-6.82	111.79	122.70
1	A	87	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	27	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	43	GLY	CA-C-N	-5.82	104.40	117.20
1	A	194	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	203	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	194	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	48	TYR	CA-C-N	-5.47	105.16	117.20
1	A	87	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	47	GLU	CG-CD-OE2	5.43	129.17	118.30
1	B	44	GLU	CA-C-O	5.38	131.41	120.10
1	A	186	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	186	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	239	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	107	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	GLY	Mainchain
1	B	46	ALA	Mainchain
1	B	48	TYR	Mainchain

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	1954	0	1905	4	0
1	B	1946	0	1892	6	0
1	C	1946	0	1892	5	0
1	D	1954	0	1905	0	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	50	0	0	2	0
4	B	50	0	0	1	0
4	C	50	0	0	2	0
4	D	50	0	0	2	0
5	A	102	0	0	1	0
5	B	70	0	0	0	0
5	C	69	0	0	1	0
5	D	52	0	0	0	0
All	All	8337	0	7610	21	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 (21) 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:82:SER:OG	1:B:82:SER:CB	1.82	1.26
1:C:175:THR:HG22	5:C:469:HOH:O	2.03	0.56
4:A:302:5R6:OAX	4:A:302:5R6:OAK	2.24	0.54
1:B:44:GLU:O	1:B:45:VAL:C	2.48	0.51
1:A:136:PHE:HB3	1:A:138:PHE:CE2	2.45	0.51
1:B:133:ALA:O	1:B:141:ALA:HB1	2.12	0.48
1:B:136:PHE:HB3	1:B:138:PHE:CE2	2.49	0.48
4:D:302:5R6:CAT	4:D:302:5R6:CBM	2.91	0.48
1:C:66:SER:OG	1:C:68:ALA:HB3	2.14	0.46
1:C:112:GLU:OE1	4:C:302:5R6:NBV	2.49	0.46
4:C:302:5R6:OAI	4:C:302:5R6:OAK	2.33	0.46
4:B:302:5R6:OAK	4:B:302:5R6:OAX	2.34	0.46
1:C:231:TYR:CD1	1:C:271:LEU:HD11	2.52	0.45
4:A:302:5R6:OAJ	4:A:302:5R6:OAI	2.35	0.44
1:C:117:GLU:HG3	1:C:119:LYS:HE2	1.99	0.44
1:B:51:GLU:HG2	1:B:84:THR:HB	2.01	0.42
1:A:133:ALA:O	1:A:141:ALA:HB1	2.20	0.41
4:D:302:5R6:OAI	4:D:302:5R6:OAJ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HB2	1:B:122:ASP:HB3	2.02	0.41
1:A:161:MET:HE2	5:A:407:HOH:O	2.20	0.41
1:A:178:GLU:HA	1:A:179:PRO:HD3	1.94	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	255/305 (84%)	248 (97%)	7 (3%)	0	100	100
1	B	254/305 (83%)	248 (98%)	6 (2%)	0	100	100
1	C	254/305 (83%)	246 (97%)	7 (3%)	1 (0%)	39	42
1	D	255/305 (84%)	251 (98%)	4 (2%)	0	100	100
All	All	1018/1220 (83%)	993 (98%)	24 (2%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	133	ALA

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	198/237 (84%)	195 (98%)	3 (2%)	72	84
1	B	197/237 (83%)	194 (98%)	3 (2%)	72	84
1	C	197/237 (83%)	195 (99%)	2 (1%)	82	91
1	D	198/237 (84%)	196 (99%)	2 (1%)	82	91
All	All	790/948 (83%)	780 (99%)	10 (1%)	76	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	186	ARG
1	A	258	ARG
1	B	177	ASP
1	B	186	ARG
1	B	223	PRO
1	C	39	VAL
1	C	186	ARG
1	D	186	ARG
1	D	220	THR

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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	AKG	A	301	2	3,9,9	1.20	0	4,11,11	1.65	1 (25%)
4	5R6	A	302	-	50,56,56	1.84	13 (26%)	67,91,91	1.53	10 (14%)
3	AKG	B	301	2	3,9,9	0.65	0	4,11,11	0.49	0
4	5R6	B	302	-	50,56,56	1.95	13 (26%)	67,91,91	1.34	8 (11%)
3	AKG	C	301	2	3,9,9	1.05	0	4,11,11	0.78	0
4	5R6	C	302	-	50,56,56	1.89	12 (24%)	67,91,91	1.81	14 (20%)
3	AKG	D	301	2	3,9,9	0.78	0	4,11,11	1.08	0
4	5R6	D	302	-	50,56,56	1.74	9 (18%)	67,91,91	1.99	14 (20%)

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	A	301	2	-	0/3/9/9	0/0/0/0
4	5R6	A	302	-	-	0/14/94/94	1/1/7/7
3	AKG	B	301	2	-	0/3/9/9	0/0/0/0
4	5R6	B	302	-	-	0/14/94/94	0/1/7/7
3	AKG	C	301	2	-	0/3/9/9	0/0/0/0
4	5R6	C	302	-	-	0/14/94/94	0/1/7/7
3	AKG	D	301	2	-	0/3/9/9	0/0/0/0
4	5R6	D	302	-	-	0/14/94/94	0/1/7/7

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	5R6	CBF-CBQ	-6.44	1.38	1.51
4	D	302	5R6	CBF-CBQ	-5.37	1.41	1.51
4	B	302	5R6	CBC-CBU	-4.88	1.43	1.51
4	A	302	5R6	CBC-CBU	-4.67	1.44	1.51
4	C	302	5R6	CBF-CBQ	-4.66	1.42	1.51
4	C	302	5R6	CBC-CBU	-4.41	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	5R6	CBI-CBG	-4.40	1.38	1.48
4	D	302	5R6	CBI-CBG	-4.18	1.39	1.48
4	D	302	5R6	CBC-CBU	-4.12	1.45	1.51
4	C	302	5R6	CBI-CBG	-4.01	1.39	1.48
4	A	302	5R6	CBF-CBQ	-3.96	1.43	1.51
4	A	302	5R6	CAR-CBN	-3.41	1.47	1.52
4	A	302	5R6	CBI-CBG	-3.32	1.41	1.48
4	A	302	5R6	CBK-CBH	-3.24	1.39	1.47
4	D	302	5R6	CBJ-CBH	-3.22	1.39	1.47
4	B	302	5R6	CBL-CBG	-3.17	1.39	1.47
4	C	302	5R6	CBK-CBH	-3.15	1.39	1.47
4	B	302	5R6	CBJ-CBH	-3.13	1.39	1.47
4	A	302	5R6	CBL-CBG	-2.93	1.40	1.47
4	B	302	5R6	CBK-CBH	-2.85	1.40	1.47
4	D	302	5R6	CBK-CBH	-2.60	1.41	1.47
4	A	302	5R6	CBJ-CBH	-2.60	1.41	1.47
4	D	302	5R6	OAV-CBE	-2.25	1.33	1.37
4	D	302	5R6	OAX-CBQ	-2.09	1.40	1.44
4	C	302	5R6	CBL-CBG	-2.04	1.42	1.47
4	D	302	5R6	CBN-CBR	-2.03	1.49	1.52
4	A	302	5R6	OAL-CBN	2.00	1.47	1.43
4	B	302	5R6	CAC-NBV	2.04	1.53	1.46
4	B	302	5R6	OAX-CBP	2.07	1.47	1.41
4	C	302	5R6	OAL-CBN	2.08	1.48	1.43
4	B	302	5R6	CAS-CBT	2.08	1.58	1.53
4	B	302	5R6	CAF-CBX	2.13	1.56	1.52
4	A	302	5R6	OAW-CBP	2.16	1.48	1.42
4	B	302	5R6	OAU-CAZ	2.40	1.39	1.33
4	C	302	5R6	OAU-CAZ	2.53	1.39	1.33
4	A	302	5R6	CBR-CBM	2.64	1.58	1.53
4	C	302	5R6	CAT-CBQ	2.65	1.58	1.52
4	A	302	5R6	OAU-CAZ	2.72	1.40	1.33
4	B	302	5R6	OAW-CBP	2.75	1.49	1.42
4	C	302	5R6	CAS-CBT	3.04	1.60	1.53
4	A	302	5R6	CBN-CBR	3.07	1.56	1.52
4	A	302	5R6	CAS-CBO	3.14	1.58	1.51
4	C	302	5R6	CAR-CBP	3.14	1.58	1.51
4	C	302	5R6	CAR-CBN	3.42	1.58	1.52
4	C	302	5R6	CBN-CBR	3.52	1.57	1.52
4	D	302	5R6	OAN-CBS	4.16	1.51	1.42
4	B	302	5R6	CBR-CBM	4.26	1.61	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	302	5R6	CAC-NBV-CBT	-4.02	101.35	113.14
4	D	302	5R6	OAW-CBP-CAR	-4.00	104.63	110.88
4	D	302	5R6	CAB-CBM-CBR	-3.75	105.77	113.02
4	B	302	5R6	CAR-CBN-CBR	-3.53	105.82	110.54
4	A	302	5R6	OAM-CBR-CBN	-3.50	103.59	110.01
4	D	302	5R6	OAH-CBG-CBI	-3.03	116.15	120.89
4	D	302	5R6	CAA-OAU-CAZ	-2.99	108.86	115.97
4	C	302	5R6	OAX-CBP-OAW	-2.95	100.22	110.20
3	A	301	AKG	C3-C2-C1	-2.88	115.25	121.63
4	C	302	5R6	CAD-NBV-CAC	-2.77	101.54	110.45
4	C	302	5R6	CBC-CBF-CBQ	-2.56	112.76	120.24
4	C	302	5R6	OAH-CBG-CBI	-2.46	117.05	120.89
4	B	302	5R6	OAX-CBP-CAR	-2.46	103.84	108.38
4	C	302	5R6	OAI-CBH-CBK	-2.42	117.17	121.46
4	C	302	5R6	OAK-CBB-CBK	-2.31	115.85	120.99
4	A	302	5R6	OAM-CBR-CBM	-2.29	104.43	109.67
4	A	302	5R6	CBW-CAT-CBQ	-2.21	108.63	114.42
4	D	302	5R6	OAJ-CBA-CBJ	-2.21	116.94	121.18
4	B	302	5R6	CBW-CAT-CBQ	-2.19	108.70	114.42
4	A	302	5R6	OAJ-CBA-CBJ	-2.15	117.06	121.18
4	A	302	5R6	OAV-CBE-CBD	-2.13	117.38	122.05
4	D	302	5R6	CAS-CBT-NBV	-2.05	109.52	115.68
4	D	302	5R6	CAS-CBT-CBS	2.01	113.04	109.95
4	C	302	5R6	CBF-CBC-CBU	2.05	125.34	116.56
4	D	302	5R6	OAO-CBW-CAE	2.07	112.56	108.08
4	C	302	5R6	CAP-CBD-CBX	2.19	124.64	121.17
4	D	302	5R6	OAX-CBP-CAR	2.63	113.23	108.38
4	C	302	5R6	CAR-CBN-CBR	2.63	114.06	110.54
4	B	302	5R6	OAX-CBQ-CBF	2.63	113.28	107.76
4	B	302	5R6	OAU-CAZ-CBU	2.92	116.22	111.17
4	A	302	5R6	CBN-CBR-CBM	3.03	116.26	110.75
4	B	302	5R6	OAW-CBM-CBR	3.05	114.85	109.58
4	D	302	5R6	CBN-CBR-CBM	3.08	116.35	110.75
4	A	302	5R6	OAL-CBN-CBR	3.36	116.95	110.19
4	D	302	5R6	OAW-CBM-CBR	3.40	115.46	109.58
4	B	302	5R6	CAD-NBV-CAC	3.52	121.74	110.45
4	C	302	5R6	OAW-CBP-CAR	3.61	116.54	110.88
4	B	302	5R6	CBP-OAW-CBM	3.86	123.49	114.31
4	A	302	5R6	OAW-CBP-CAR	3.91	117.00	110.88
4	A	302	5R6	OAU-CAZ-CBU	4.04	118.14	111.17
4	A	302	5R6	OAX-CBQ-CAT	4.44	121.02	110.22
4	D	302	5R6	CAR-CBN-CBR	4.72	116.86	110.54
4	C	302	5R6	OAU-CAZ-CBU	4.76	119.39	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	302	5R6	CAC-NBV-CBT	4.79	127.20	113.14
4	C	302	5R6	OAX-CBP-CAR	5.04	117.68	108.38
4	C	302	5R6	OAX-CBQ-CBF	5.37	119.00	107.76
4	D	302	5R6	OAX-CBQ-CBF	8.39	125.34	107.76

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	5R6	CAR-CBM-CBN-CBP-CBR-OAW

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	5R6	2	0
4	B	302	5R6	1	0
4	C	302	5R6	2	0
4	D	302	5R6	2	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	256/305 (83%)	-0.02	5 (1%)	68	67	35, 50, 78, 101	0
1	B	256/305 (83%)	0.36	12 (4%)	35	34	37, 60, 100, 126	0
1	C	256/305 (83%)	0.25	12 (4%)	35	34	40, 60, 92, 111	0
1	D	256/305 (83%)	0.54	22 (8%)	13	12	41, 67, 99, 123	0
All	All	1024/1220 (83%)	0.28	51 (4%)	32	32	35, 58, 95, 126	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	67	GLY	7.6
1	B	67	GLY	6.5
1	B	68	ALA	6.0
1	B	120	GLU	4.7
1	B	123	ALA	4.7
1	D	68	ALA	4.7
1	D	66	SER	4.5
1	D	54	ARG	4.2
1	D	50	ALA	4.1
1	D	58	HIS	3.8
1	D	254	ALA	3.8
1	A	120	GLU	3.8
1	A	254	ALA	3.7
1	C	67	GLY	3.6
1	B	122	ASP	3.6
1	D	121	LYS	3.6
1	B	121	LYS	3.5
1	B	60	GLU	3.3
1	B	58	HIS	3.3
1	D	60	GLU	3.3
1	D	120	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	57	ALA	3.0
1	D	57	ALA	2.9
1	C	58	HIS	2.9
1	B	254	ALA	2.7
1	A	253	GLY	2.7
1	C	84	THR	2.7
1	D	81	GLY	2.7
1	D	115	LEU	2.7
1	C	81	GLY	2.6
1	D	80	LEU	2.6
1	D	46	ALA	2.6
1	D	221	ASP	2.5
1	C	60	GLU	2.5
1	D	49	LEU	2.5
1	C	85	MET	2.5
1	B	119	LYS	2.5
1	C	254	ALA	2.4
1	D	258	ARG	2.4
1	C	21	LEU	2.3
1	A	121	LYS	2.3
1	B	62	VAL	2.3
1	D	55	LEU	2.2
1	D	253	GLY	2.2
1	B	59	GLU	2.2
1	D	73	ASP	2.1
1	C	266	ASP	2.1
1	A	272	ARG	2.1
1	C	59	GLU	2.0
1	D	53	ARG	2.0
1	C	50	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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
4	5R6	C	302	50/50	0.85	0.22	3.83	27,39,54,56	0
4	5R6	B	302	50/50	0.81	0.23	2.95	29,34,44,47	0
4	5R6	D	302	50/50	0.82	0.28	1.63	29,41,59,63	0
4	5R6	A	302	50/50	0.91	0.13	0.27	24,29,45,49	0
3	AKG	B	301	10/10	0.95	0.12	-0.90	25,27,29,29	0
3	AKG	D	301	10/10	0.95	0.11	-1.34	23,24,25,25	0
3	AKG	C	301	10/10	0.95	0.10	-1.52	20,25,26,26	0
3	AKG	A	301	10/10	0.97	0.07	-3.12	24,27,28,30	0
2	FE	A	300	1/1	0.99	0.08	-	26,26,26,26	0
2	FE	B	300	1/1	0.96	0.06	-	25,25,25,25	0
2	FE	D	300	1/1	0.98	0.06	-	24,24,24,24	0
2	FE	C	300	1/1	0.97	0.07	-	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.