



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:34 PM GMT

PDB ID : 4CKE
Title : Vaccinia virus capping enzyme complexed with SAH in P1 form
Authors : Kyrieleis, O.J.P.; Chang, J.; de la Pena, M.; Shuman, S.; Cusack, S.
Deposited on : 2014-01-03
Resolution : 2.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

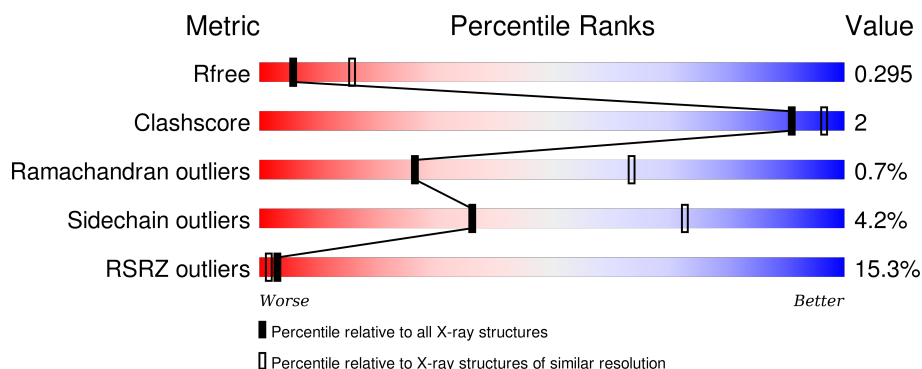
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 $\leq 5\%$. 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	844	<div> <div>20%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	D	844	<div> <div>14%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
2	B	287	<div> <div>7%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
2	E	287	<div> <div>10%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17794 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.

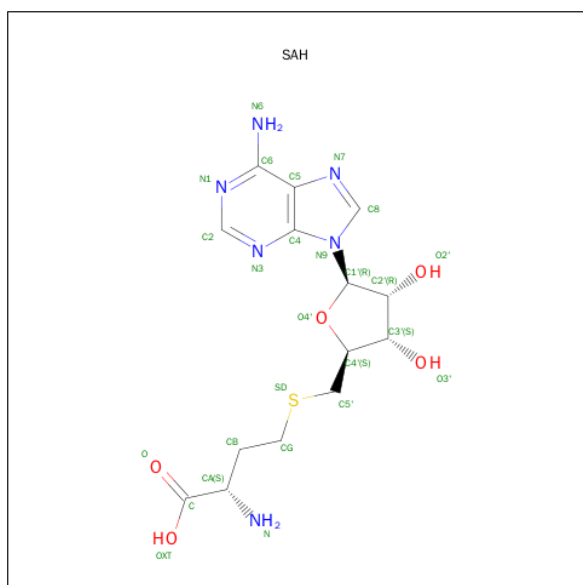
- Molecule 1 is a protein called MRNA-CAPPING ENZYME CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	802	Total	C	N	O	S	0	1	0
			6485	4181	1060	1226	18			
1	D	813	Total	C	N	O	S	0	1	0
			6583	4245	1080	1239	19			

- Molecule 2 is a protein called MRNA-CAPPING ENZYME REGULATORY SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2320	1492	385	430	13			
2	E	278	Total	C	N	O	S	0	0	0
			2278	1468	375	422	13			

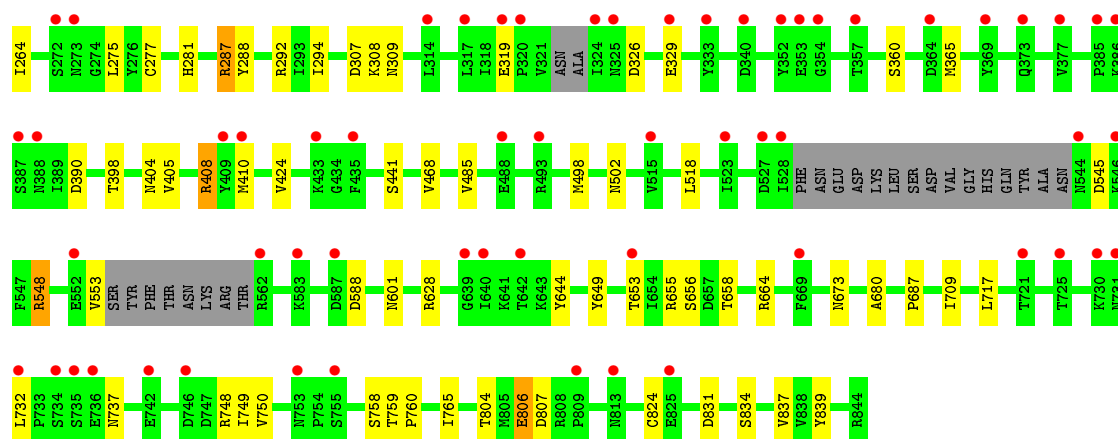
- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



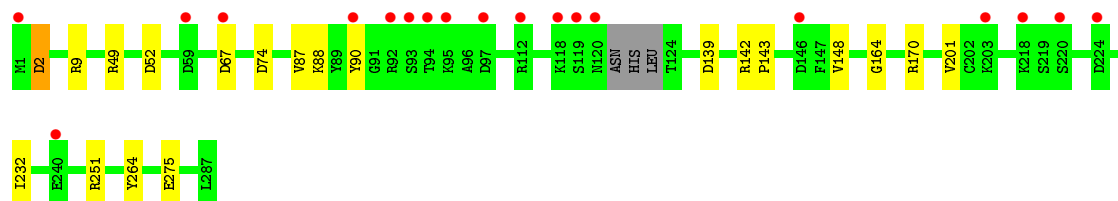
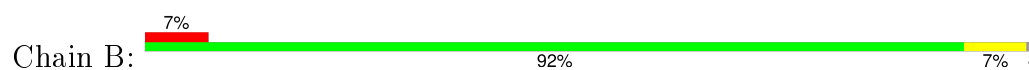
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is water.

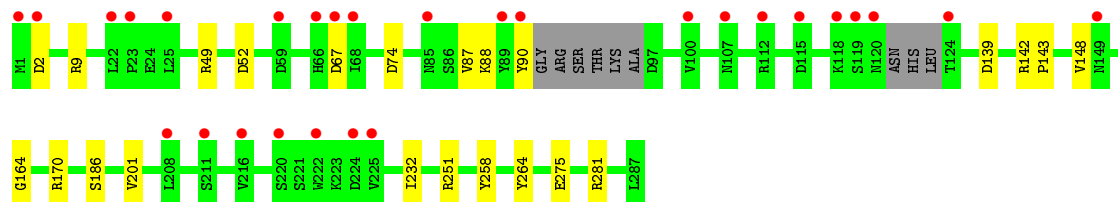
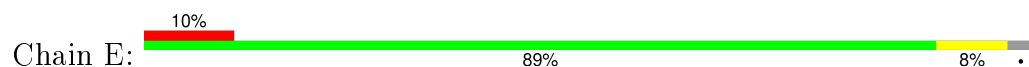
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	11	Total	O	0	0
			11	11		
4	D	37	Total	O	0	0
			37	37		
4	E	5	Total	O	0	0
			5	5		



• Molecule 2: MRNA-CAPPING ENZYME REGULATORY SUBUNIT



• Molecule 2: MRNA-CAPPING ENZYME REGULATORY SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.13Å 62.02Å 198.50Å 90.01° 85.53° 71.69°	Depositor
Resolution (Å)	41.81 – 2.90 48.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.8 (41.81-2.90) 94.1 (48.23-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.255 , 0.295 0.257 , 0.295	Depositor DCC
R_{free} test set	2919 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.7	EDS
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 57987 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17794	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH

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	0.23	0/6612	0.44	0/8936
1	D	0.24	0/6715	0.45	0/9078
2	B	0.23	0/2365	0.41	0/3189
2	E	0.23	0/2322	0.41	0/3131
All	All	0.23	0/18014	0.44	0/24334

There are no bond length outliers.

There are no bond angle outliers.

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	6485	0	6552	30	0
1	D	6583	0	6669	38	0
2	B	2320	0	2363	6	0
2	E	2278	0	2316	6	0
3	A	26	0	19	1	0
3	D	26	0	19	1	0
4	A	23	0	0	1	0
4	B	11	0	0	0	0
4	D	37	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	5	0	0	0	0
All	All	17794	0	17938	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 2.

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:A:87:GLY:O	1:A:89:ASP:N	2.30	0.64
1:D:87:GLY:O	1:D:89:ASP:N	2.30	0.64
1:A:485:VAL:HG11	1:A:518:LEU:HA	1.83	0.61
1:D:99:ILE:O	1:D:134:TYR:OH	2.18	0.61
1:A:99:ILE:O	1:A:134:TYR:OH	2.18	0.60
1:D:485:VAL:HG11	1:D:518:LEU:HA	1.81	0.60
1:D:226:ASN:OD1	1:D:287:ARG:NH1	2.38	0.56
1:A:588:ASP:O	1:A:592:ARG:NH2	2.38	0.56
1:D:545:ASP:OD1	1:D:655:ARG:NH1	2.41	0.53
2:B:74:ASP:OD1	2:B:74:ASP:N	2.43	0.52
1:A:545:ASP:OD1	1:A:655:ARG:NH1	2.42	0.52
1:D:548:ARG:NH2	4:D:2020:HOH:O	2.43	0.51
2:E:74:ASP:OD1	2:E:74:ASP:N	2.44	0.51
1:A:226:ASN:OD1	1:A:287:ARG:NH1	2.46	0.49
1:D:498:MET:O	1:D:502:ASN:ND2	2.45	0.49
1:A:19:ALA:HB3	1:A:209:ILE:HD11	1.95	0.49
1:A:685:PHE:N	4:A:2018:HOH:O	2.45	0.49
1:D:19:ALA:HB3	1:D:209:ILE:HD11	1.94	0.49
1:A:201:GLU:N	1:A:201:GLU:OE1	2.46	0.49
1:D:275:LEU:N	1:D:288:TYR:O	2.40	0.49
1:D:709:ILE:HB	1:D:839:TYR:HB2	1.97	0.47
1:D:2:ASP:N	1:D:2:ASP:OD1	2.46	0.47
1:A:709:ILE:HB	1:A:839:TYR:HB2	1.96	0.46
1:A:498:MET:O	1:A:502:ASN:ND2	2.47	0.46
1:A:759:THR:HB	1:A:760:PRO:HD2	1.98	0.45
1:D:206:ASP:OD1	1:D:206:ASP:N	2.49	0.45
1:A:264:ILE:HD11	1:A:281:HIS:HB3	1.98	0.45
2:B:2:ASP:N	2:B:2:ASP:OD1	2.50	0.45
1:A:307:ASP:O	1:A:309:ASN:N	2.50	0.45
1:A:271:THR:HG22	1:A:273:ASN:H	1.82	0.45
1:A:717:LEU:HD13	1:A:749:ILE:CD1	2.46	0.45
1:D:759:THR:HB	1:D:760:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:52:ASP:HB3	2:E:264:TYR:CE1	2.51	0.44
1:D:717:LEU:HD13	1:D:749:ILE:CD1	2.48	0.44
1:D:601:ASN:OD1	1:D:628:ARG:NH1	2.49	0.44
1:A:601:ASN:OD1	1:A:628:ARG:NH1	2.51	0.43
2:B:87:VAL:HG12	2:B:88:LYS:N	2.33	0.43
2:E:87:VAL:HG12	2:E:88:LYS:N	2.33	0.43
1:A:806:GLU:HA	2:B:49:ARG:HH12	1.83	0.43
1:A:2:ASP:N	1:A:2:ASP:OD1	2.47	0.43
1:A:806:GLU:OE1	1:A:807:ASP:N	2.52	0.43
2:E:258:TYR:OH	2:E:281:ARG:NH2	2.52	0.42
1:D:153:THR:O	1:D:155:ASN:N	2.43	0.42
1:A:749:ILE:HG22	1:A:750:VAL:N	2.34	0.42
1:D:748:ARG:NH2	4:D:2019:HOH:O	2.52	0.42
1:D:806:GLU:OE1	1:D:807:ASP:N	2.52	0.42
1:D:205:TYR:CZ	1:D:209:ILE:HG13	2.55	0.42
1:A:153:THR:O	1:A:155:ASN:N	2.44	0.41
1:D:56:ILE:HG23	1:D:218:HIS:NE2	2.35	0.41
1:D:656:SER:HG	1:D:658:THR:HG1	1.58	0.41
1:A:206:ASP:OD1	1:A:206:ASP:N	2.53	0.41
1:D:806:GLU:HA	2:E:49:ARG:HH12	1.86	0.41
1:D:405:VAL:HG13	1:D:424:VAL:HG22	2.02	0.41
1:D:655:ARG:NH2	3:D:1845:SAH:N7	2.68	0.41
1:A:749:ILE:HD11	1:A:765:ILE:HG12	2.03	0.41
1:D:264:ILE:HD11	1:D:281:HIS:HB3	2.03	0.41
1:D:114:ARG:HB2	1:D:120:LEU:HD23	2.02	0.41
1:A:732:LEU:HB3	1:A:737:ASN:HB3	2.03	0.41
1:A:580:TYR:O	1:A:592:ARG:NH1	2.54	0.41
1:D:408:ARG:C	1:D:410:MET:H	2.24	0.41
1:A:655:ARG:NH2	3:A:1845:SAH:N7	2.69	0.41
1:D:749:ILE:HD11	1:D:765:ILE:HG12	2.02	0.41
1:D:49:THR:HG21	1:D:191:LEU:HD22	2.03	0.41
1:D:732:LEU:HB3	1:D:737:ASN:HB3	2.02	0.41
2:B:52:ASP:HB3	2:B:264:TYR:CE1	2.56	0.41
1:A:732:LEU:HD23	1:A:733:PRO:HD2	2.03	0.41
2:B:142:ARG:N	2:B:143:PRO:CD	2.84	0.41
1:D:158:ILE:HD11	1:D:215:LEU:HD11	2.01	0.41
1:D:831:ASP:O	1:D:834:SER:OG	2.35	0.40
1:D:158:ILE:CD1	1:D:215:LEU:HD11	2.50	0.40
1:D:588:ASP:OD2	4:D:2024:HOH:O	2.22	0.40
1:D:307:ASP:O	1:D:309:ASN:N	2.54	0.40
1:A:405:VAL:HG13	1:A:424:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:749:ILE:HG22	1:D:750:VAL:N	2.35	0.40
1:A:158:ILE:CD1	1:A:215:LEU:HD11	2.52	0.40
1:D:326:ASP:OD2	1:D:329:GLU:N	2.50	0.40
2:E:142:ARG:N	2:E:143:PRO:CD	2.84	0.40
1:D:160:PHE:CZ	1:D:189:THR:HG23	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	787/844 (93%)	719 (91%)	62 (8%)	6 (1%)	24	60
1	D	804/844 (95%)	734 (91%)	65 (8%)	5 (1%)	30	67
2	B	280/287 (98%)	257 (92%)	21 (8%)	2 (1%)	26	63
2	E	272/287 (95%)	250 (92%)	20 (7%)	2 (1%)	26	63
All	All	2143/2262 (95%)	1960 (92%)	168 (8%)	15 (1%)	26	63

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	D	88	LEU
2	B	164	GLY
2	E	164	GLY
1	A	308	LYS
1	A	680	ALA
1	D	680	ALA
2	B	148	VAL
1	D	308	LYS
2	E	148	VAL

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Mol	Chain	Res	Type
1	A	248	VAL
1	A	564	PRO
1	A	687	PRO
1	D	248	VAL
1	D	687	PRO

5.3.2 Protein sidechains ⓘ

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	737/774 (95%)	708 (96%)	29 (4%)	39	75
1	D	748/774 (97%)	714 (96%)	34 (4%)	34	70
2	B	269/272 (99%)	259 (96%)	10 (4%)	41	77
2	E	265/272 (97%)	254 (96%)	11 (4%)	36	73
All	All	2019/2092 (96%)	1935 (96%)	84 (4%)	36	73

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	65	ARG
1	A	125	THR
1	A	190	SER
1	A	206	ASP
1	A	259	THR
1	A	277	CYS
1	A	287	ARG
1	A	294	ILE
1	A	319	GLU
1	A	360	SER
1	A	365	MET
1	A	390	ASP
1	A	398	THR
1	A	404	ASN
1	A	468	VAL

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Mol	Chain	Res	Type
1	A	548	ARG
1	A	553	VAL
1	A	619	THR
1	A	644	TYR
1	A	649	TYR
1	A	653	THR
1	A	664	ARG
1	A	673	ASN
1	A	758	SER
1	A	804	THR
1	A	806	GLU
1	A	824	CYS
1	A	837	VAL
2	B	2	ASP
2	B	9	ARG
2	B	67	ASP
2	B	90	TYR
2	B	139	ASP
2	B	170	ARG
2	B	201	VAL
2	B	232	ILE
2	B	251	ARG
2	B	275	GLU
1	D	49	THR
1	D	65	ARG
1	D	125	THR
1	D	188	ASN
1	D	190	SER
1	D	199	ASP
1	D	201	GLU
1	D	206	ASP
1	D	259	THR
1	D	277	CYS
1	D	287	ARG
1	D	292	ARG
1	D	294	ILE
1	D	319	GLU
1	D	360	SER
1	D	365	MET
1	D	390	ASP
1	D	398	THR
1	D	404	ASN

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Mol	Chain	Res	Type
1	D	408	ARG
1	D	441	SER
1	D	468	VAL
1	D	548	ARG
1	D	553	VAL
1	D	644	TYR
1	D	649	TYR
1	D	653	THR
1	D	664	ARG
1	D	673	ASN
1	D	758	SER
1	D	804	THR
1	D	806	GLU
1	D	824	CYS
1	D	837	VAL
2	E	2	ASP
2	E	9	ARG
2	E	67	ASP
2	E	90	TYR
2	E	139	ASP
2	E	170	ARG
2	E	186	SER
2	E	201	VAL
2	E	232	ILE
2	E	251	ARG
2	E	275	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	278	HIS
2	E	278	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

2 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	SAH	A	1845	-	20,28,28	1.13	2 (10%)	19,40,40	2.83	2 (10%)
3	SAH	D	1845	-	20,28,28	1.11	2 (10%)	19,40,40	2.76	2 (10%)

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	SAH	A	1845	-	-	0/7/31/31	0/3/3/3
3	SAH	D	1845	-	-	0/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1845	SAH	C2-N1	2.32	1.38	1.33
3	A	1845	SAH	C2-N1	2.40	1.38	1.33
3	D	1845	SAH	C2-N3	3.55	1.38	1.32
3	A	1845	SAH	C2-N3	3.59	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1845	SAH	N3-C2-N1	-11.23	120.30	128.89
3	D	1845	SAH	N3-C2-N1	-11.13	120.37	128.89
3	A	1845	SAH	C5'-SD-CG	-3.17	92.90	102.41

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	1845	SAH	C5'-SD-CG	-2.36	95.33	102.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1845	SAH	1	0
3	D	1845	SAH	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, 95th 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	802/844 (95%)	1.24	169 (21%) 1 1	17, 63, 107, 133	0
1	D	813/844 (96%)	0.96	117 (14%) 3 2	22, 49, 88, 114	0
2	B	284/287 (98%)	0.63	19 (6%) 21 15	15, 39, 78, 130	0
2	E	278/287 (96%)	0.96	28 (10%) 9 5	23, 54, 89, 131	0
All	All	2177/2262 (96%)	1.02	333 (15%) 3 1	15, 54, 97, 133	0

All (333) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	LEU	9.3
2	B	93	SER	8.9
2	B	120	ASN	7.2
1	A	200	ASN	7.1
2	B	94	THR	7.1
2	E	120	ASN	6.8
1	A	111	THR	6.5
1	A	2	ASP	6.3
1	A	153	THR	6.2
1	D	200	ASN	6.1
1	A	248	VAL	5.9
1	A	211	GLU	5.6
1	D	153	THR	5.6
1	A	91	LYS	5.5
1	A	330	GLU	5.5
2	E	211	SER	5.4
1	A	735	SER	5.3
1	A	730	LYS	5.3
1	D	71	LYS	5.0
1	A	35	ASN	5.0
1	A	552	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	203	VAL	4.7
1	A	154	LYS	4.7
1	A	734	SER	4.6
1	A	109	LEU	4.6
1	D	735	SER	4.6
1	A	373	GLN	4.5
1	A	341	ILE	4.4
1	A	294	ILE	4.4
2	E	112	ARG	4.4
1	D	528	ILE	4.3
1	A	119	CYS	4.3
1	D	133	ASP	4.3
1	A	338	LEU	4.3
2	E	118	LYS	4.3
1	D	435	PHE	4.2
1	D	27	GLN	4.2
1	A	125	THR	4.2
1	D	325	ASN	4.2
1	A	204	PRO	4.1
1	A	206	ASP	4.1
1	D	202	THR	4.1
1	D	373	GLN	4.1
1	A	22	ALA	4.1
1	A	131	PHE	4.0
1	D	154	LYS	4.0
2	E	222	TRP	4.0
1	A	352	TYR	4.0
1	D	249	GLY	4.0
1	D	639	GLY	3.9
1	A	155	ASN	3.9
1	A	435	PHE	3.9
1	D	142	ARG	3.9
1	D	742	GLU	3.9
1	D	527	ASP	3.9
1	D	22	ALA	3.9
1	D	731	ASN	3.9
1	A	39	GLU	3.8
1	D	109	LEU	3.8
1	D	126	GLU	3.8
2	E	1	MET	3.8
1	A	296	SER	3.8
1	A	325	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	640	ILE	3.8
1	A	317	LEU	3.8
1	A	92	ASN	3.8
1	A	36	ASN	3.8
2	E	115	ASP	3.8
2	E	100	VAL	3.8
2	E	89	TYR	3.7
1	A	136	LYS	3.7
1	A	72	GLU	3.7
1	A	1	MET	3.7
1	D	2	ASP	3.7
1	A	319	GLU	3.7
2	B	95	LYS	3.7
1	A	126	GLU	3.7
1	D	36	ASN	3.7
1	A	156	PHE	3.6
2	E	59	ASP	3.6
1	D	26	GLU	3.6
1	A	273	ASN	3.6
1	D	72	GLU	3.6
1	A	106	LYS	3.6
1	D	105	GLU	3.6
1	A	226	ASN	3.6
1	D	734	SER	3.6
1	D	35	ASN	3.6
1	A	218	HIS	3.6
1	A	731	ASN	3.6
1	A	544	ASN	3.5
1	A	199	ASP	3.5
1	D	18	LEU	3.5
1	A	195	PHE	3.5
1	A	13	THR	3.5
1	D	37	GLU	3.4
1	D	25	LEU	3.4
1	D	732	LEU	3.4
1	D	205	TYR	3.4
1	A	227	VAL	3.4
1	D	248	VAL	3.4
2	E	90	TYR	3.3
1	A	123	LEU	3.3
1	A	210	LYS	3.3
1	A	20	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLU	3.3
1	D	199	ASP	3.3
1	A	113	ASN	3.3
1	A	488	GLU	3.3
1	D	552	GLU	3.2
2	B	118	LYS	3.2
1	A	202	THR	3.2
1	A	101	ASN	3.2
1	D	825	GLU	3.2
2	E	67	ASP	3.2
1	D	111	THR	3.2
1	D	354	GLY	3.2
2	E	85	ASN	3.2
1	D	34	ILE	3.2
1	D	317	LEU	3.2
1	D	357	THR	3.2
2	B	203	LYS	3.2
2	E	119	SER	3.2
1	D	155	ASN	3.1
1	D	172	SER	3.1
1	D	19	ALA	3.1
1	A	371	PRO	3.1
1	A	105	GLU	3.1
1	A	433	LYS	3.1
2	B	59	ASP	3.1
1	A	334	VAL	3.1
1	D	329	GLU	3.1
1	A	24	GLU	3.1
2	E	225	VAL	3.1
1	A	271	THR	3.1
1	A	8	SER	3.0
1	A	23	SER	3.0
1	A	362	VAL	3.0
1	D	206	ASP	3.0
1	A	732	LEU	3.0
2	B	92	ARG	3.0
1	A	142	ARG	3.0
1	A	151	ALA	3.0
1	A	246	ASP	3.0
1	A	349	SER	3.0
1	A	357	THR	3.0
1	A	205	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	112	GLU	3.0
1	A	201	GLU	2.9
1	A	295	ASP	2.9
1	A	172	SER	2.9
1	A	354	GLY	2.9
1	A	324	ILE	2.9
1	A	344	ARG	2.9
2	E	107	ASN	2.9
1	A	669[A]	PHE	2.9
1	A	376	GLY	2.9
2	E	216	VAL	2.9
1	A	348	LYS	2.9
1	D	746	ASP	2.9
1	A	336	SER	2.9
1	D	131	PHE	2.9
1	A	377	VAL	2.8
1	A	26	GLU	2.8
1	D	515	VAL	2.8
1	A	17	ALA	2.8
1	D	721	THR	2.8
1	D	725	THR	2.8
1	A	639	GLY	2.8
2	E	2	ASP	2.8
1	D	753	ASN	2.7
1	A	642	THR	2.7
1	D	730	LYS	2.7
1	D	121	LEU	2.7
1	D	640	ILE	2.7
1	A	332	LYS	2.7
1	D	39	GLU	2.7
1	A	121	LEU	2.7
1	D	364	ASP	2.7
1	A	385	PRO	2.7
1	A	223	SER	2.7
2	B	119	SER	2.7
2	B	224	ASP	2.7
1	A	196	THR	2.7
1	D	69	THR	2.7
1	A	18	LEU	2.7
1	A	638	SER	2.7
1	A	314	LEU	2.7
2	B	220	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	70	ASN	2.6
1	A	34	ILE	2.6
1	D	736	GLU	2.6
1	D	587	ASP	2.6
1	A	104	TRP	2.6
1	D	272	SER	2.6
1	D	119	CYS	2.6
1	D	562	ARG	2.6
1	A	122	ARG	2.6
1	A	454	ASN	2.6
2	B	218	LYS	2.6
1	A	262	ASP	2.6
1	D	369	TYR	2.5
2	E	23	PRO	2.5
1	A	249	GLY	2.5
1	D	132	LEU	2.5
1	A	228	ILE	2.5
2	B	67	ASP	2.5
1	A	300	VAL	2.5
1	A	383	LYS	2.5
1	A	756	THR	2.5
1	D	262	ASP	2.5
1	D	211	GLU	2.5
1	A	87	GLY	2.5
1	A	212	LEU	2.5
1	A	267	THR	2.5
1	A	307	ASP	2.5
1	A	312	VAL	2.5
1	A	152	LYS	2.5
1	D	324	ILE	2.5
2	E	66	HIS	2.5
1	D	386	LYS	2.5
1	D	544	ASN	2.4
1	D	116	HIS	2.4
1	A	133	ASP	2.4
2	E	149	ASN	2.4
1	D	669[A]	PHE	2.4
1	A	75	LYS	2.4
1	A	120	LEU	2.4
1	D	204	PRO	2.4
1	D	410	MET	2.4
1	A	19	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	315	ILE	2.4
1	D	273	ASN	2.4
1	A	340	ASP	2.4
1	A	15	ILE	2.4
1	A	302	GLY	2.4
2	B	112	ARG	2.4
1	A	275	LEU	2.4
1	A	328	LEU	2.4
1	A	345	ILE	2.4
1	A	826	GLY	2.4
1	D	203	VAL	2.4
1	D	433	LYS	2.4
1	A	76	ILE	2.4
1	A	70	ASN	2.4
1	D	388	ASN	2.4
1	A	364	ASP	2.4
1	D	218	HIS	2.4
2	B	1	MET	2.3
1	D	152	LYS	2.3
1	D	755	SER	2.3
1	D	246	ASP	2.3
1	A	728	ILE	2.3
1	D	809	PRO	2.3
1	A	318	ILE	2.3
1	A	524	LYS	2.3
1	D	87	GLY	2.3
1	D	15	ILE	2.3
1	A	722	ASP	2.3
1	A	381	TYR	2.3
1	D	101	ASN	2.3
1	D	409	TYR	2.3
1	D	546	LYS	2.3
2	E	22	LEU	2.3
1	A	247	ILE	2.3
1	D	1	MET	2.3
1	A	16	ASP	2.2
1	A	308	LYS	2.3
1	D	385	PRO	2.3
2	B	146	ASP	2.2
1	A	823	LYS	2.2
1	A	256	TYR	2.2
1	A	412	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	760	PRO	2.2
1	D	156	PHE	2.2
1	A	331	SER	2.2
1	D	387	SER	2.2
1	A	432	ASP	2.2
1	D	642	THR	2.2
2	E	224	ASP	2.2
1	A	254	ASN	2.2
1	D	813	ASN	2.2
1	A	721	THR	2.2
1	D	523	ILE	2.2
1	D	333	TYR	2.2
1	D	75	LYS	2.2
1	A	494	ILE	2.2
1	D	201	GLU	2.2
1	D	352	TYR	2.2
1	D	314	LEU	2.2
2	B	97	ASP	2.2
1	D	259	THR	2.2
1	D	653	THR	2.2
1	A	333	TYR	2.2
1	D	493	ARG	2.2
1	A	825	GLU	2.2
1	D	76	ILE	2.2
1	A	753	ASN	2.2
1	D	98	ALA	2.2
1	D	226	ASN	2.2
1	A	356	PHE	2.1
1	A	824	CYS	2.1
1	A	339	VAL	2.1
1	A	108	SER	2.1
1	D	488	GLU	2.1
2	B	90	TYR	2.1
1	D	320	PRO	2.1
1	A	761	MET	2.1
1	A	225	GLU	2.1
1	A	276	TYR	2.1
1	A	526	GLY	2.1
1	D	353	GLU	2.1
2	E	25	LEU	2.1
1	D	583	LYS	2.1
1	D	125	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	124	SER	2.1
2	B	240	GLU	2.1
1	A	150	GLN	2.1
1	A	298	VAL	2.1
1	A	84	LYS	2.0
2	E	208	LEU	2.0
2	E	220	SER	2.0
1	A	3	ALA	2.0
1	A	737	ASN	2.0
1	D	377	VAL	2.0
1	D	251	ASP	2.0
1	D	319	GLU	2.0
1	D	340	ASP	2.0
1	A	523	ILE	2.0
2	E	68	ILE	2.0
1	A	257	ALA	2.0
1	A	259	THR	2.0
2	E	124	THR	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 [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, 95th 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	SAH	A	1845	26/26	0.92	0.22	-0.39	23,32,38,39	0
3	SAH	D	1845	26/26	0.88	0.21	-0.82	22,28,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.