



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 06:30 am BST

PDB ID : 4HNU
Title : crystal structure of K442E mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

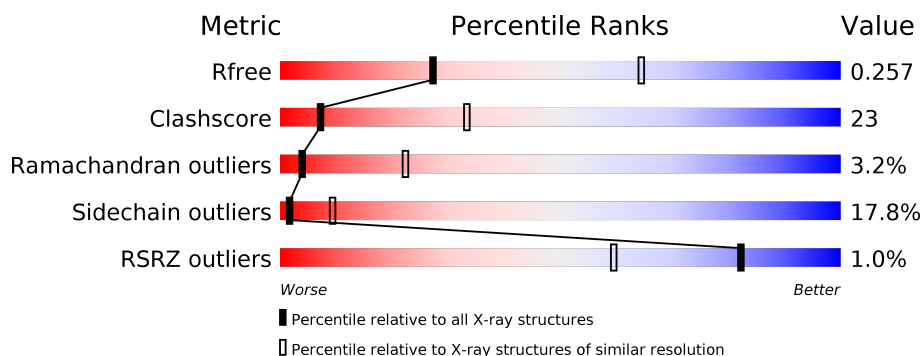
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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	1173	<div> <div>2%</div> <div> <div></div> <div>49%</div> <div>31%</div> <div>9%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	1173	<div> <div></div> <div> <div>47%</div> <div>31%</div> <div>6%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	1173	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>32%</div> <div>10%</div> <div>•</div> <div>10%</div> </div> </div>
1	D	1173	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>30%</div> <div>7%</div> <div>•</div> <div>16%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32443 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	0	0
			8342	5291	1403	1621	27			
1	B	989	Total	C	N	O	S	0	0	0
			7838	4974	1320	1518	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8379	5312	1411	1628	28			
1	D	989	Total	C	N	O	S	0	0	0
			7838	4974	1320	1518	26			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q99UY8
A	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	13	SER	-	EXPRESSION TAG	UNP Q99UY8
A	14	SER	-	EXPRESSION TAG	UNP Q99UY8
A	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	21	SER	-	EXPRESSION TAG	UNP Q99UY8
A	22	SER	-	EXPRESSION TAG	UNP Q99UY8
A	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
A	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
A	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
A	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
A	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	29	SER	-	EXPRESSION TAG	UNP Q99UY8
A	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	31	MET	-	EXPRESSION TAG	UNP Q99UY8

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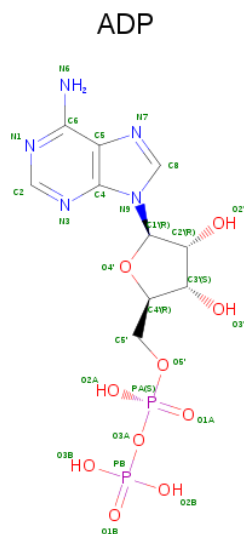
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
A	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	21	SER	-	EXPRESSION TAG	UNP Q99UY8
B	22	SER	-	EXPRESSION TAG	UNP Q99UY8
B	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
B	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
B	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
B	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
B	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	29	SER	-	EXPRESSION TAG	UNP Q99UY8
B	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	31	MET	-	EXPRESSION TAG	UNP Q99UY8
B	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
B	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8
C	11	MET	-	EXPRESSION TAG	UNP Q99UY8
C	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	13	SER	-	EXPRESSION TAG	UNP Q99UY8
C	14	SER	-	EXPRESSION TAG	UNP Q99UY8
C	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	21	SER	-	EXPRESSION TAG	UNP Q99UY8
C	22	SER	-	EXPRESSION TAG	UNP Q99UY8
C	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
C	25	VAL	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
C	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
D	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	13	SER	-	EXPRESSION TAG	UNP Q99UY8
D	14	SER	-	EXPRESSION TAG	UNP Q99UY8
D	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	21	SER	-	EXPRESSION TAG	UNP Q99UY8
D	22	SER	-	EXPRESSION TAG	UNP Q99UY8
D	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
D	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
D	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
D	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
D	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	29	SER	-	EXPRESSION TAG	UNP Q99UY8
D	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	31	MET	-	EXPRESSION TAG	UNP Q99UY8
D	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
D	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	442	GLU	LYS	ENGINEERED MUTATION	UNP Q99UY8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

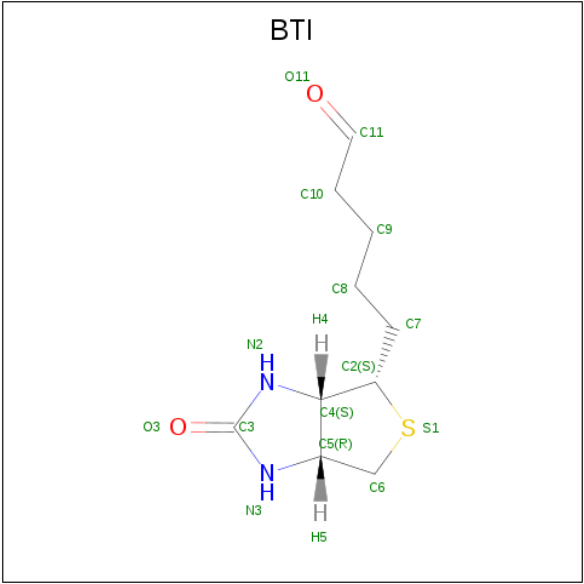


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).

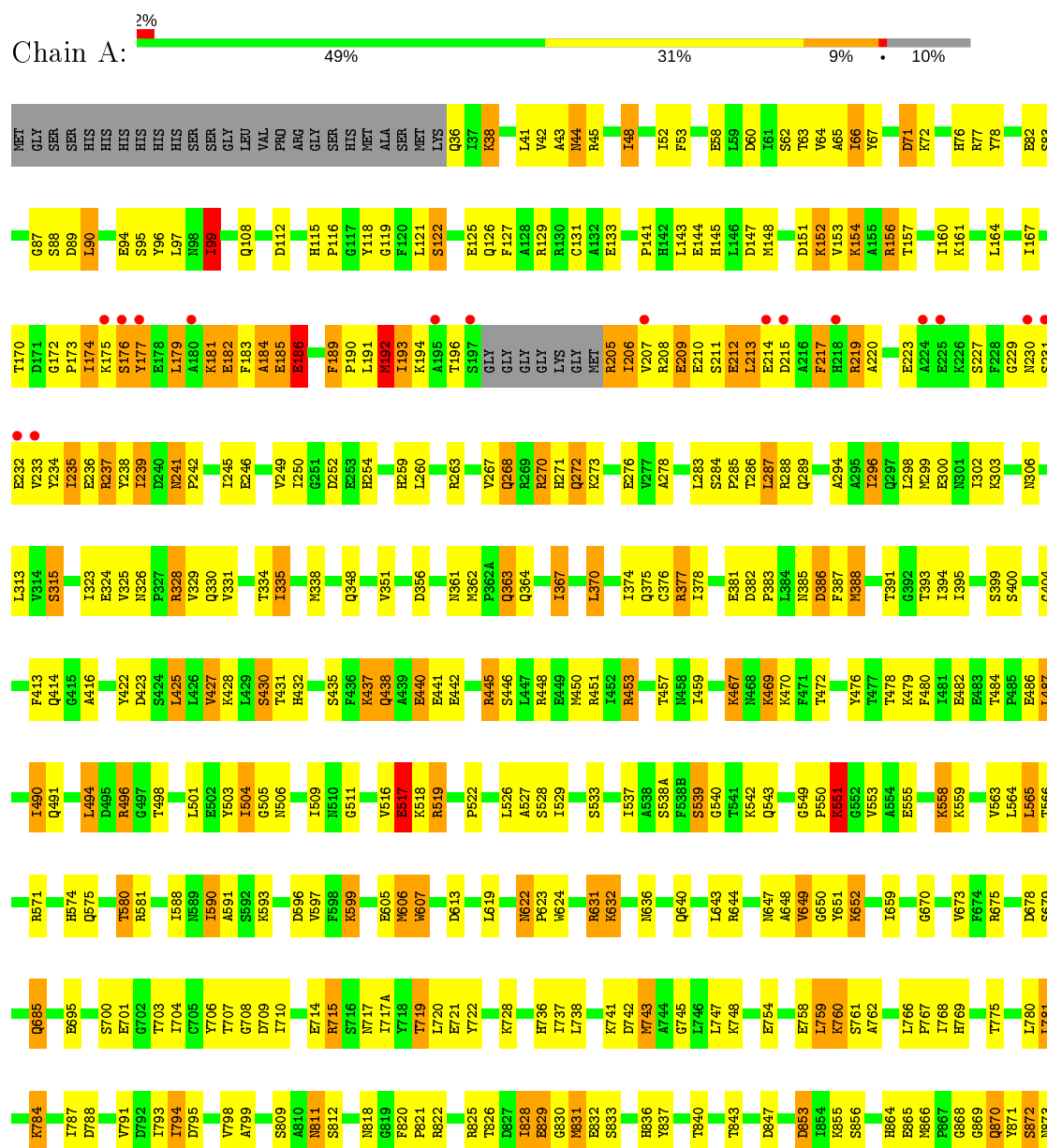


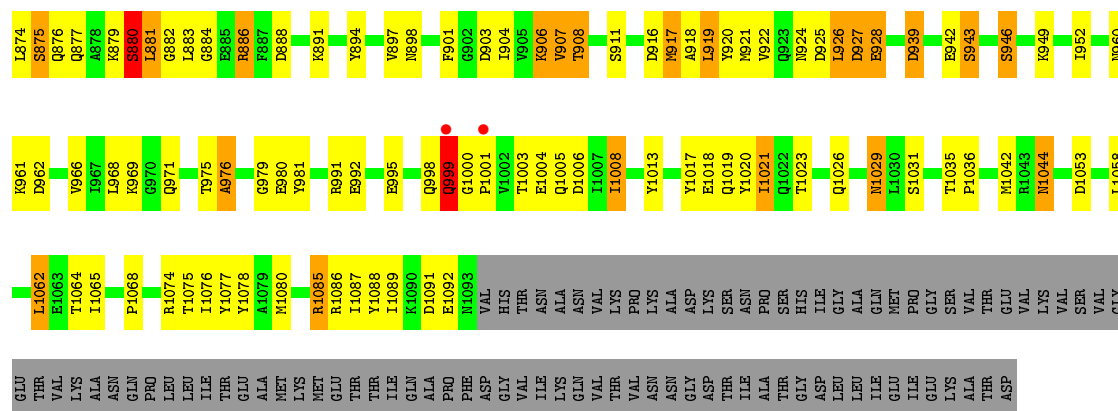
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	D	1	15	10	2	2	1	0	0

3 Residue-property plots

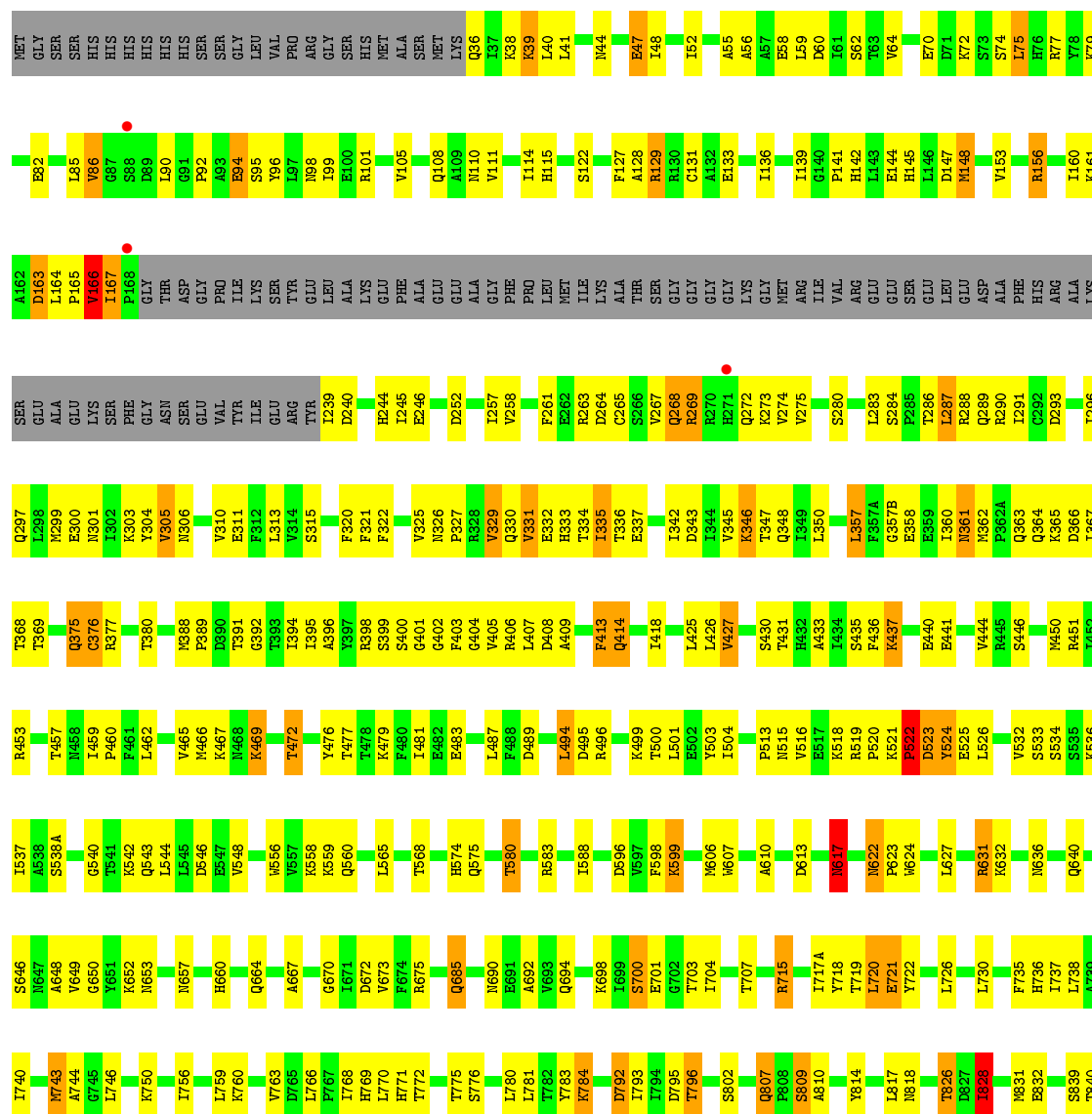
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Pyruvate carboxylase





• Molecule 1: Pyruvate carboxylase

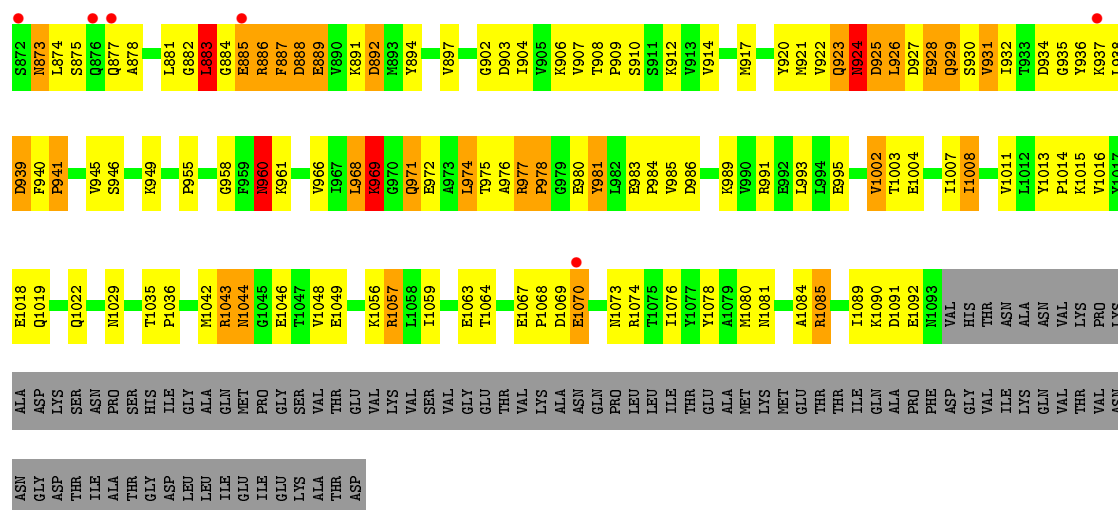


V841	V821	V1016	LYS
Y844	Y922	Y1017	ALA
Y845	Y923	Q1018	ASP
S846	Y924	Q1019	LYS
E849	D925	T1023	THR
S852	D926	R1024	ASN
D853	D927	R1024	PRO
I854	E928	Y1027	ALA
S855	Q929	Y1027	THR
S856	S930	L1030	GLY
P857	S931	S1031	ASP
	T932	L1032	LEU
	T933	L1032	ALA
I861	D934	M1042	ILE
H864	G935	R1043	GLU
H865	G935	N1044	GLY
H866	L938	N1044	VAL
P867	S943	E1049	THR
G868	Y944	I1050	GLU
G869	F948	E1051	VAL
Q870	T949	I1052	VAL
Y871	G950	D1053	VAL
	G951	K1056	SER
		R1057	VAL
S875	F959	GLY	GLY
Q876	N960	GLU	GLU
K879	L963	THR	THR
S880	L963	VAL	VAL
L881	Q964	L1065	LYS
	T969	I1065	ALA
	L982	D1069	ASN
		E1070	GLN
		N1071	PRO
		R1074	LEU
		T1075	LEU
		M1080	THR
		Q1083	GLU
		R1085	ALA
		R1086	MET
		I1087	MET
		Y1088	THR
		I1089	THR
		K1090	ILE
		D1091	GLN
		E1092	ALA
		N1093	PRO
		VAL	PHE
		HIS	ASP
		THR	GLY
		ASN	VAL
		ILE	VAL
		ALA	LYS
		ASN	LYS
		ASN	GLN
		VAL	THR
		PRO	VAL

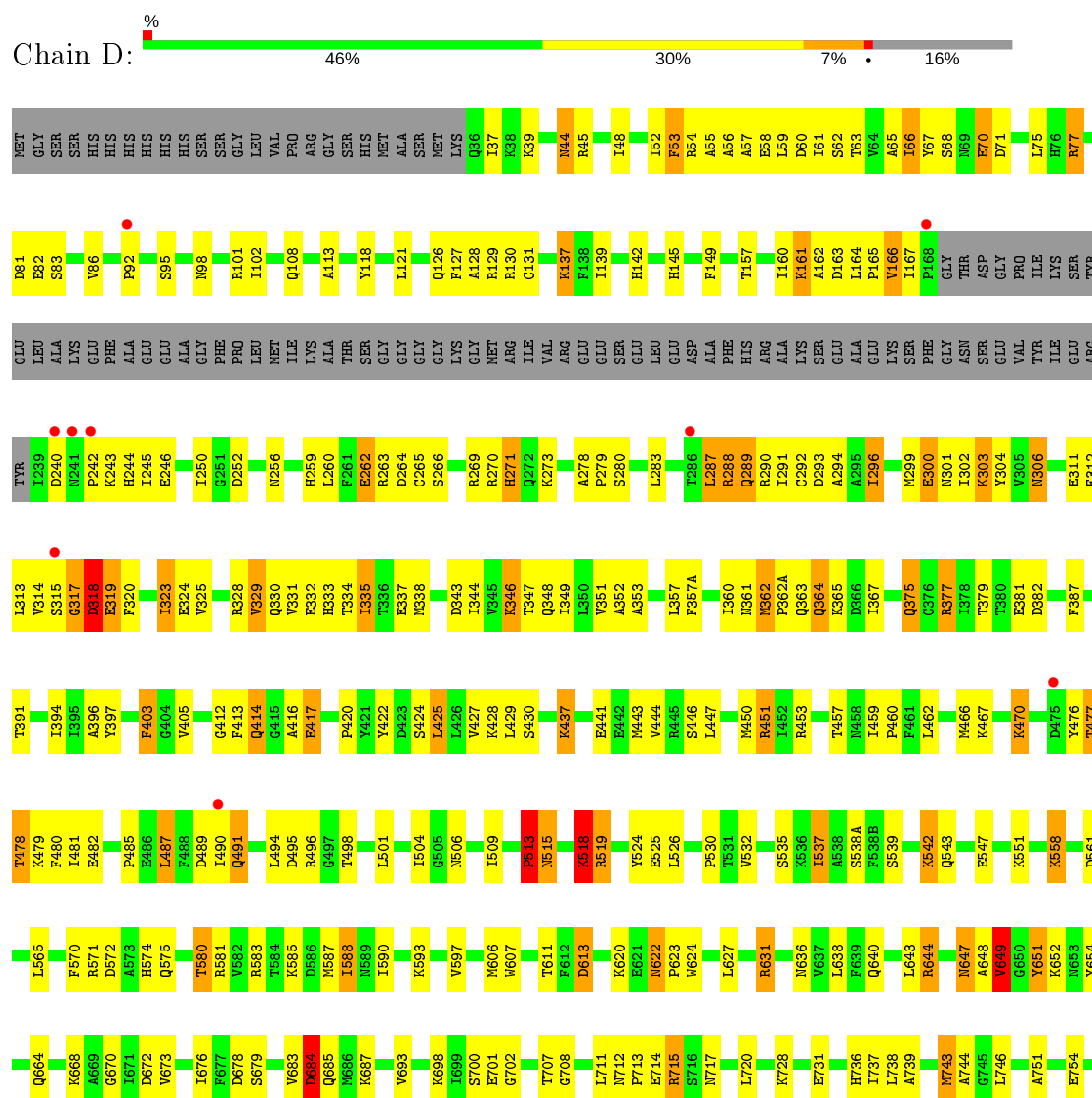
• Molecule 1: Pyruvate carboxylase



Y93	P165	K346	H432	V510	L578	S679	I793
E94	V166	T347	A433	Q511	A979	D684	I794
L97	P167	Q348	S434	P512	T580	Q685	D795
L99	P168	G354	S435	P513	S435	Q686	T796
T100	G169	E354	K436	N515	V582	V687	A797
R101	D171	E358	Q438	E517	T588	V688	A799
I102	G172	E359	A439	R519	N589	A689	G803
T103	G173	I360	E440	R519	I590	N690	L804
D104	I174	M362	E441	P520	E441	Q694	T805
K107	A180	K365	M443	V524	F598	K698	S806
Q108	E182	D366	V444	E525	E605	T699	P808
M110	F183	T369	M450	L526	M606	S700	S809
A113	A184	L370	R451	A527	M607	E701	A810
I114	E185	G371	R452	S528	V614	N712	N811
H115	F189	Y372	R453	P530	A615	T713	S812
P116	P190	A373	K456	T531	Y616	E714	L813
G117	L191	Q375	I459	S534	N617	R715	Y814
Y118	M192	C376	P460	S535	L619	T719	N818
F119	K194	R377	M466	K536	N622	L720	P821
G120	A195	I378	K467	S538A	P623	E721	R822
L121	T196	T379	M468	F538B	W624	E731	R823
S122	S197	T380	K469	S539	R629	H736	I828
E123	G198	E381	K472	G540	R631	L737	E832
N124	G199	D382	T472	T541	L738	A739	S833
E125	L41	P383	S473	Q474	K632	M743	L834
V42	Q126	L384	G475	Q543	L544	I756	Y837
A43	I206	N301	N306	V548	L643	L757	W838
M44	V207	I302	N306	G549	A645	A758	S839
R45	E208	Y304	Y306	P550	S646	G757	T840
R54	E210	V305	E306	G551	N647	E758	V841
E133	S211	E311	E306	G552	A648	L759	R842
E134	E212	E311	E306	G553	V649	T760	T843
G135	E213	E311	E306	G554	L644	S761	Y844
I136	E214	E311	E306	G555	A645	A762	S845
L139	E215	E311	E306	G556	G650	V763	Y846
H142	E216	E311	E306	G557	K558	D765	D847
L143	E217	E311	E306	G558	K559	F768	F848
E144	E218	E311	E306	G559	K560	L768	P849
H145	E219	E311	E306	G560	D561	L768	S852
D147	E220	E311	E306	G561	D562	L768	D853
M148	E221	E311	E306	G562	D563	L768	T854
F149	E222	E311	E306	G563	D564	L768	K855
G150	E223	E311	E306	G564	D565	L768	T861
L85	E224	E311	E306	G565	D566	L768	Y862
V86	E225	E311	E306	G566	D567	L768	Q863
G87	E226	E311	E306	G567	D568	L768	H864
S88	E227	E311	E306	G568	D569	L768	E865
D89	E228	E311	E306	G569	D570	L768	N866
R91	E229	E311	E306	G570	D571	L768	Q870
P92	E230	E311	E306	G571	D572	L768	Y871



• Molecule 1: Pyruvate carboxylase



GLY	HIS	E1051	I926	F848	E758
ASP	ILE	I1052	D927	E849	L759
LEU	GLY	D1053	Q928		K760
ILE	ALA	I1054	Q929	I854	S761
ILE	GLN	K1055	S930	K855	A762
PRO	MET	K1056	G935	S856	V763
GLY	PRO	K1057		P857	D765
LYS	GLY	L1058	I938	M858	L766
ALA	SER	L1059	D939	T859	P767
THR	VAL	I1060	F940	I861	I768
ASP	GLU	K1061		Y862	H769
	VAL	L1062	V944	Q863	T772
	LYS	E1063	V945	H863	H773
	VAL	T1064	S946	E865	D774
	SER	I1065	F947	M866	T775
	VAL	S1066	F948	P867	S776
	GLY	E1067	K949	G868	G777
	GLU	P1068	G950	G869	N778
	THR	D1069	E951	Q870	
	VAL	E1070	I952	Y871	L781
	LYS	N1071		S872	
	ALA	G1072	N960	N873	K784
	ASN	N1073	K961	L874	V791
	GLN	R1074	D962	S875	
	PRO	T1075	I963	Q876	
	LEU	I1076		Q877	A799
	ILE	Y1077	V966	A878	S800
	THR	A1079	I967	K879	S801
	GLU	M1080	T975	S880	S802
	ALA	N1081	A976	L881	
	MET	G1082	R977	G882	Q807
	LYS	Q1083		L883	P808
	MET	A1084	E983	G884	S809
	GLU	R1085		E885	A810
	THR	R1086		R886	N811
	THR	I1087	D986	F887	
	ILE	Y1088	R991		Y814
	GLN	I1089		K891	
	ALA	K1090	L994	N818	
	PRO		E995	G819	
	PHE		E996	F820	
	ASP		E997	P821	
	GLY		Q998	R822	
	VAL			E823	
	ILE		Q999	L824	
	LYS		G1000		
	ASN		P1001	I828	
	GLN			E829	
	VAL		Q1005		
	THR			P909	
	VAL				E832
	ASN		I1008	V914	
	ASN				Y837
	GLY		Y1013	M917	
	ASP		E1018	A918	T840
	THR			I919	V841
	ILE		T1035	Y920	E842
	ALA				T843
	THR			N924	
				D925	D847

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.57Å 258.52Å 126.90Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-3.00) 98.4 (29.72-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102, CNS	Depositor
R, R_{free}	0.194 , 0.262 0.192 , 0.257	Depositor DCC
R_{free} test set	5765 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32443	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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, 0.333 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: MN, BTI, ADP

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	0.60	0/8504	0.69	3/11500 (0.0%)
1	B	0.46	2/7990 (0.0%)	0.57	0/10811
1	C	0.53	5/8542 (0.1%)	0.61	3/11549 (0.0%)
1	D	0.59	2/7990 (0.0%)	0.68	4/10811 (0.0%)
All	All	0.55	9/33026 (0.0%)	0.64	10/44671 (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	3
1	B	0	2
1	C	0	1
1	D	0	3
All	All	0	9

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	515	ASN	N-CA	6.54	1.59	1.46
1	B	513	PRO	CA-C	6.53	1.66	1.52
1	C	513	PRO	CA-C	6.13	1.65	1.52
1	C	441	GLU	CG-CD	5.96	1.60	1.51
1	B	515	ASN	N-CA	5.89	1.58	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	GLU	CA-C-N	-7.39	100.94	117.20
1	C	513	PRO	CA-N-CD	7.06	121.59	111.70
1	C	513	PRO	N-CA-CB	-5.95	96.05	102.60
1	D	315	SER	N-CA-CB	-5.93	101.61	110.50
1	D	849	GLU	CA-C-N	5.54	129.38	117.20

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1092	GLU	Peptide
1	A	174	ILE	Peptide
1	A	215	ASP	Peptide
1	B	357(B)	GLY	Peptide
1	B	522	PRO	Peptide

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	8342	0	8246	393	0
1	B	7838	0	7764	331	0
1	C	8379	0	8284	385	0
1	D	7838	0	7764	365	0
2	A	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	15	0	16	4	0
All	All	32443	0	32086	1456	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 23.

The worst 5 of 1456 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:961:LYS:HD2	1:D:961:LYS:N	1.59	1.14
1:C:437:LYS:HD3	1:C:437:LYS:H	0.98	1.13
1:D:961:LYS:H	1:D:961:LYS:CD	1.59	1.12
1:A:864:HIS:CD2	1:A:866:MET:HG3	1.84	1.11
1:A:866:MET:HE3	1:A:870:GLN:HG2	1.26	1.11

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	1048/1173 (89%)	907 (86%)	111 (11%)	30 (3%)	4	24
1	B	985/1173 (84%)	847 (86%)	117 (12%)	21 (2%)	7	33
1	C	1057/1173 (90%)	896 (85%)	113 (11%)	48 (4%)	2	14
1	D	985/1173 (84%)	842 (86%)	110 (11%)	33 (3%)	3	20
All	All	4075/4692 (87%)	3492 (86%)	451 (11%)	132 (3%)	4	22

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	ALA
1	A	527	ALA
1	A	880	SER
1	A	999	GLN
1	B	94	GLU

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	908/1006 (90%)	730 (80%)	178 (20%)	1	7
1	B	856/1006 (85%)	721 (84%)	135 (16%)	2	12
1	C	910/1006 (90%)	721 (79%)	189 (21%)	1	5
1	D	856/1006 (85%)	728 (85%)	128 (15%)	3	14
All	All	3530/4024 (88%)	2900 (82%)	630 (18%)	2	9

5 of 630 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	907	VAL
1	C	226	LYS
1	D	766	LEU
1	B	934	ASP
1	C	73	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	960	ASN
1	C	241	ASN
1	D	778	ASN
1	B	999	GLN
1	B	1073	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BTI	D	1201	-	16,16,16	1.78	2 (12%)	21,21,21	2.13	6 (28%)
2	ADP	A	1201	-	24,29,29	1.02	2 (8%)	29,45,45	1.20	3 (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
4	BTI	D	1201	-	-	5/5/27/27	0/2/2/2
2	ADP	A	1201	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1201	BTI	O3-C3	5.17	1.34	1.23
4	D	1201	BTI	C2-S1	-4.08	1.76	1.82
2	A	1201	ADP	C5-C4	2.63	1.47	1.40
2	A	1201	ADP	O4'-C1'	2.02	1.43	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1201	BTI	C6-C5-N3	-4.99	106.68	113.03
4	D	1201	BTI	C5-C6-S1	4.55	110.21	106.31
4	D	1201	BTI	C2-C4-N2	-3.48	110.00	113.13
4	D	1201	BTI	C4-C2-S1	3.19	108.25	105.20
2	A	1201	ADP	N3-C2-N1	-2.85	124.22	128.68

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

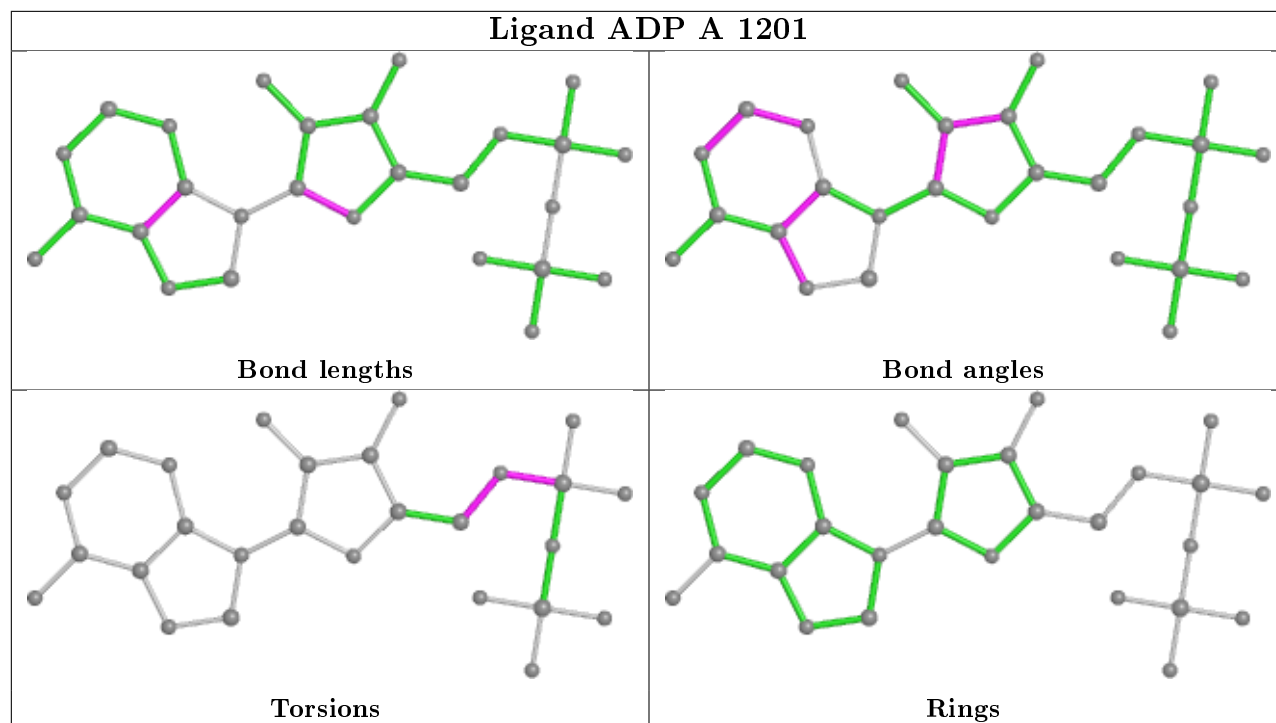
Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	C5'-O5'-PA-O1A
4	D	1201	BTI	C11-C10-C9-C8
4	D	1201	BTI	S1-C2-C7-C8
4	D	1201	BTI	C4-C2-C7-C8
4	D	1201	BTI	C2-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1201	BTI	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1052/1173 (89%)	-0.55	18 (1%) 70 41	36, 75, 131, 167	0
1	B	989/1173 (84%)	-0.41	3 (0%) 94 84	59, 105, 154, 233	0
1	C	1059/1173 (90%)	-0.42	10 (0%) 84 63	56, 101, 150, 197	0
1	D	989/1173 (84%)	-0.52	9 (0%) 84 63	41, 82, 173, 267	0
All	All	4089/4692 (87%)	-0.47	40 (0%) 82 59	36, 93, 151, 267	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	240	ASP	4.4
1	D	241	ASN	4.0
1	A	224	ALA	3.7
1	A	176	SER	3.7
1	D	490	ILE	3.6

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](#)

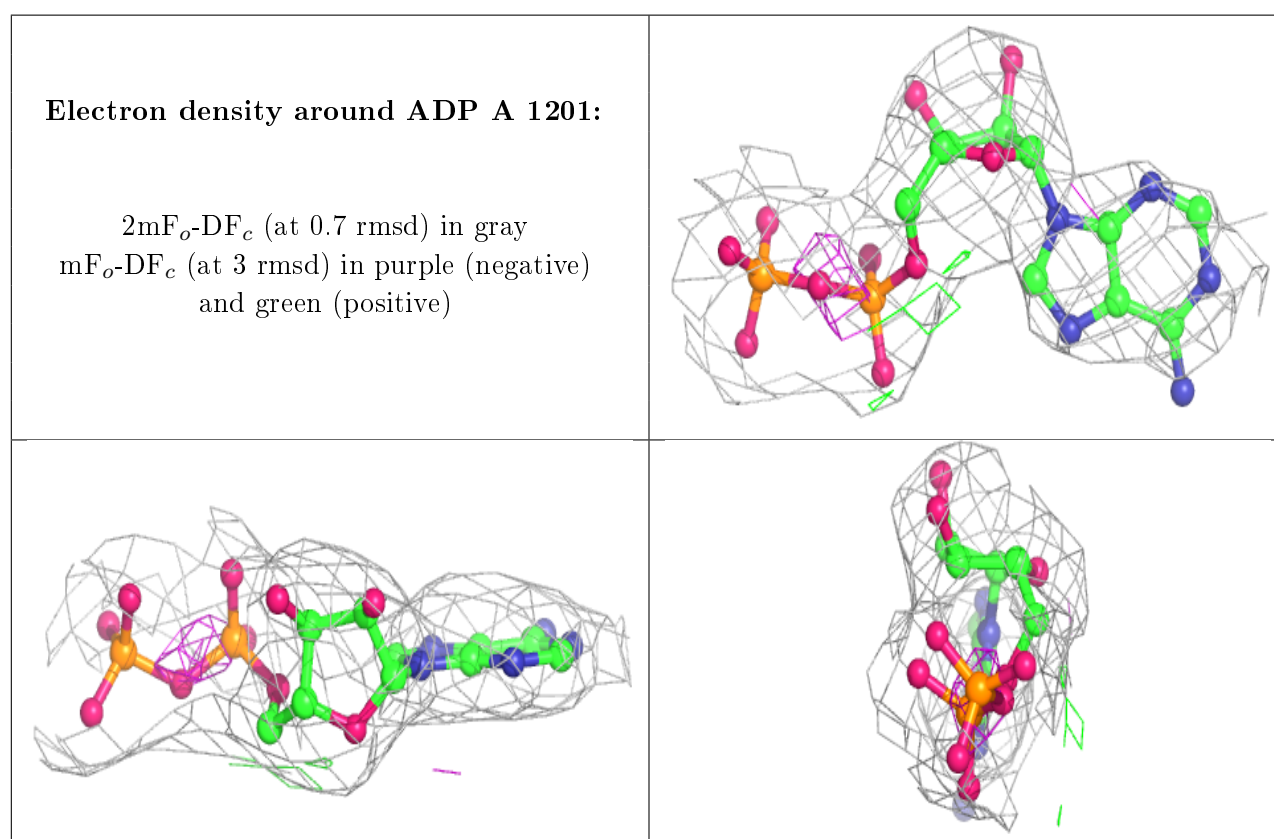
There are no carbohydrates in this entry.

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. 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	B-factors(\AA^2)	Q<0.9
4	BTI	D	1201	15/15	0.81	0.42	128,133,136,136	0
2	ADP	A	1201	27/27	0.87	0.20	108,112,144,146	0
3	MN	D	1202	1/1	0.97	0.18	79,79,79,79	0
3	MN	B	1201	1/1	0.97	0.18	108,108,108,108	0
3	MN	C	1201	1/1	0.97	0.29	105,105,105,105	0
3	MN	A	1202	1/1	0.98	0.30	83,83,83,83	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.