



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 03:05 PM UTC

PDB ID : 3N6R / pdb_00003n6r
Title : CRYSTAL STRUCTURE OF the holoenzyme of PROPIONYL-COA CARBOXYLASE (PCC)
Authors : Huang, C.S.; Sadre-Bazzaz, K.; Tong, L.
Deposited on : 2010-05-26
Resolution : 3.20 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

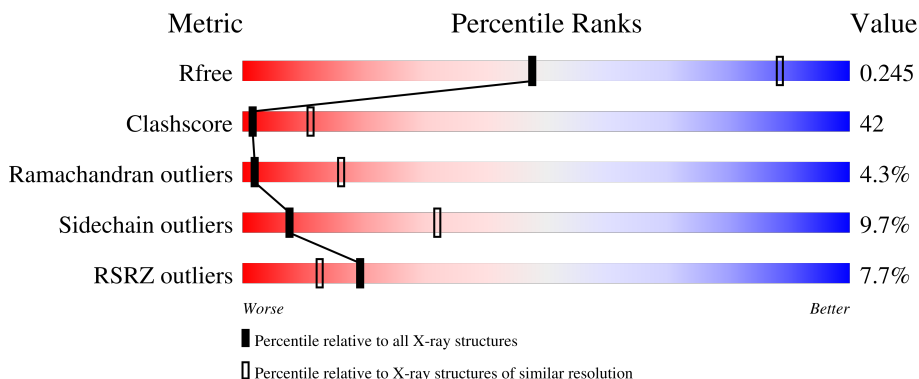
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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 $\leq 5\%$. 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	681	12% 29% 46% 11% • 13%
1	C	681	11% 28% 46% 12% • 13%
1	E	681	13% 30% 45% 12% • 13%
1	G	681	12% 31% 51% 12% • 5%
1	I	681	15% 30% 52% 12% • 5%

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Mol	Chain	Length	Quality of chain
1	K	681	12%32%51%11%5%
2	B	531	%45%43%7%5%
2	D	531	%44%45%6%5%
2	F	531	47%40%7%5%
2	H	531	45%43%6%5%
2	J	531	%45%43%7%5%
2	L	531	%45%44%6%5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51921 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 Propionyl-CoA carboxylase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	C	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	E	591	Total	C	N	O	S	0	0	0
			4507	2828	794	857	28			
1	G	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	I	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			
1	K	646	Total	C	N	O	S	0	0	0
			4950	3108	869	942	31			

- Molecule 2 is a protein called Propionyl-CoA carboxylase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	D	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	F	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	H	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	J	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			
2	L	506	Total	C	N	O	S	0	0	0
			3910	2462	683	744	21			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	MET	-	expression tag	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	GLY	-	expression tag	UNP Q168G2
B	13	SER	-	expression tag	UNP Q168G2
B	14	SER	-	expression tag	UNP Q168G2
B	15	HIS	-	expression tag	UNP Q168G2
B	16	HIS	-	expression tag	UNP Q168G2
B	17	HIS	-	expression tag	UNP Q168G2
B	18	HIS	-	expression tag	UNP Q168G2
B	19	HIS	-	expression tag	UNP Q168G2
B	20	HIS	-	expression tag	UNP Q168G2
B	21	SER	-	expression tag	UNP Q168G2
B	22	SER	-	expression tag	UNP Q168G2
B	23	GLY	-	expression tag	UNP Q168G2
B	24	LEU	-	expression tag	UNP Q168G2
B	25	VAL	-	expression tag	UNP Q168G2
B	26	PRO	-	expression tag	UNP Q168G2
B	27	ARG	-	expression tag	UNP Q168G2
B	28	GLY	-	expression tag	UNP Q168G2
B	29	SER	-	expression tag	UNP Q168G2
B	30	HIS	-	expression tag	UNP Q168G2
B	31	MET	-	expression tag	UNP Q168G2
D	11	MET	-	expression tag	UNP Q168G2
D	12	GLY	-	expression tag	UNP Q168G2
D	13	SER	-	expression tag	UNP Q168G2
D	14	SER	-	expression tag	UNP Q168G2
D	15	HIS	-	expression tag	UNP Q168G2
D	16	HIS	-	expression tag	UNP Q168G2
D	17	HIS	-	expression tag	UNP Q168G2
D	18	HIS	-	expression tag	UNP Q168G2
D	19	HIS	-	expression tag	UNP Q168G2
D	20	HIS	-	expression tag	UNP Q168G2
D	21	SER	-	expression tag	UNP Q168G2
D	22	SER	-	expression tag	UNP Q168G2
D	23	GLY	-	expression tag	UNP Q168G2
D	24	LEU	-	expression tag	UNP Q168G2
D	25	VAL	-	expression tag	UNP Q168G2
D	26	PRO	-	expression tag	UNP Q168G2
D	27	ARG	-	expression tag	UNP Q168G2
D	28	GLY	-	expression tag	UNP Q168G2
D	29	SER	-	expression tag	UNP Q168G2
D	30	HIS	-	expression tag	UNP Q168G2
D	31	MET	-	expression tag	UNP Q168G2
F	11	MET	-	expression tag	UNP Q168G2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	12	GLY	-	expression tag	UNP Q168G2
F	13	SER	-	expression tag	UNP Q168G2
F	14	SER	-	expression tag	UNP Q168G2
F	15	HIS	-	expression tag	UNP Q168G2
F	16	HIS	-	expression tag	UNP Q168G2
F	17	HIS	-	expression tag	UNP Q168G2
F	18	HIS	-	expression tag	UNP Q168G2
F	19	HIS	-	expression tag	UNP Q168G2
F	20	HIS	-	expression tag	UNP Q168G2
F	21	SER	-	expression tag	UNP Q168G2
F	22	SER	-	expression tag	UNP Q168G2
F	23	GLY	-	expression tag	UNP Q168G2
F	24	LEU	-	expression tag	UNP Q168G2
F	25	VAL	-	expression tag	UNP Q168G2
F	26	PRO	-	expression tag	UNP Q168G2
F	27	ARG	-	expression tag	UNP Q168G2
F	28	GLY	-	expression tag	UNP Q168G2
F	29	SER	-	expression tag	UNP Q168G2
F	30	HIS	-	expression tag	UNP Q168G2
F	31	MET	-	expression tag	UNP Q168G2
H	11	MET	-	expression tag	UNP Q168G2
H	12	GLY	-	expression tag	UNP Q168G2
H	13	SER	-	expression tag	UNP Q168G2
H	14	SER	-	expression tag	UNP Q168G2
H	15	HIS	-	expression tag	UNP Q168G2
H	16	HIS	-	expression tag	UNP Q168G2
H	17	HIS	-	expression tag	UNP Q168G2
H	18	HIS	-	expression tag	UNP Q168G2
H	19	HIS	-	expression tag	UNP Q168G2
H	20	HIS	-	expression tag	UNP Q168G2
H	21	SER	-	expression tag	UNP Q168G2
H	22	SER	-	expression tag	UNP Q168G2
H	23	GLY	-	expression tag	UNP Q168G2
H	24	LEU	-	expression tag	UNP Q168G2
H	25	VAL	-	expression tag	UNP Q168G2
H	26	PRO	-	expression tag	UNP Q168G2
H	27	ARG	-	expression tag	UNP Q168G2
H	28	GLY	-	expression tag	UNP Q168G2
H	29	SER	-	expression tag	UNP Q168G2
H	30	HIS	-	expression tag	UNP Q168G2
H	31	MET	-	expression tag	UNP Q168G2
J	11	MET	-	expression tag	UNP Q168G2

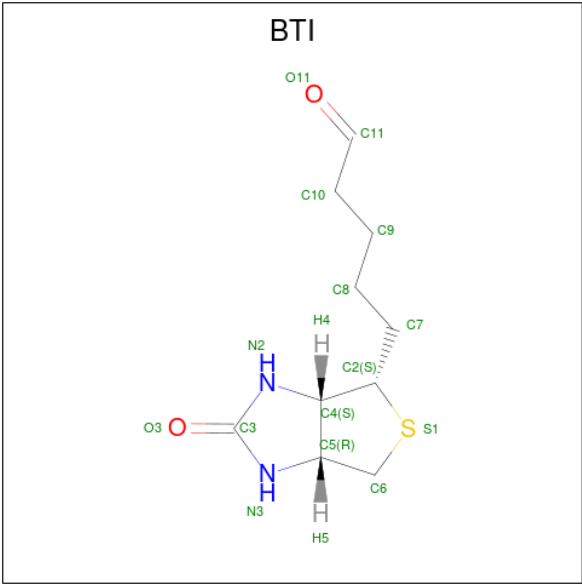
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Chain	Residue	Modelled	Actual	Comment	Reference
J	12	GLY	-	expression tag	UNP Q168G2
J	13	SER	-	expression tag	UNP Q168G2
J	14	SER	-	expression tag	UNP Q168G2
J	15	HIS	-	expression tag	UNP Q168G2
J	16	HIS	-	expression tag	UNP Q168G2
J	17	HIS	-	expression tag	UNP Q168G2
J	18	HIS	-	expression tag	UNP Q168G2
J	19	HIS	-	expression tag	UNP Q168G2
J	20	HIS	-	expression tag	UNP Q168G2
J	21	SER	-	expression tag	UNP Q168G2
J	22	SER	-	expression tag	UNP Q168G2
J	23	GLY	-	expression tag	UNP Q168G2
J	24	LEU	-	expression tag	UNP Q168G2
J	25	VAL	-	expression tag	UNP Q168G2
J	26	PRO	-	expression tag	UNP Q168G2
J	27	ARG	-	expression tag	UNP Q168G2
J	28	GLY	-	expression tag	UNP Q168G2
J	29	SER	-	expression tag	UNP Q168G2
J	30	HIS	-	expression tag	UNP Q168G2
J	31	MET	-	expression tag	UNP Q168G2
L	11	MET	-	expression tag	UNP Q168G2
L	12	GLY	-	expression tag	UNP Q168G2
L	13	SER	-	expression tag	UNP Q168G2
L	14	SER	-	expression tag	UNP Q168G2
L	15	HIS	-	expression tag	UNP Q168G2
L	16	HIS	-	expression tag	UNP Q168G2
L	17	HIS	-	expression tag	UNP Q168G2
L	18	HIS	-	expression tag	UNP Q168G2
L	19	HIS	-	expression tag	UNP Q168G2
L	20	HIS	-	expression tag	UNP Q168G2
L	21	SER	-	expression tag	UNP Q168G2
L	22	SER	-	expression tag	UNP Q168G2
L	23	GLY	-	expression tag	UNP Q168G2
L	24	LEU	-	expression tag	UNP Q168G2
L	25	VAL	-	expression tag	UNP Q168G2
L	26	PRO	-	expression tag	UNP Q168G2
L	27	ARG	-	expression tag	UNP Q168G2
L	28	GLY	-	expression tag	UNP Q168G2
L	29	SER	-	expression tag	UNP Q168G2
L	30	HIS	-	expression tag	UNP Q168G2
L	31	MET	-	expression tag	UNP Q168G2

- Molecule 3 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL

(CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	E	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	G	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	I	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
3	K	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

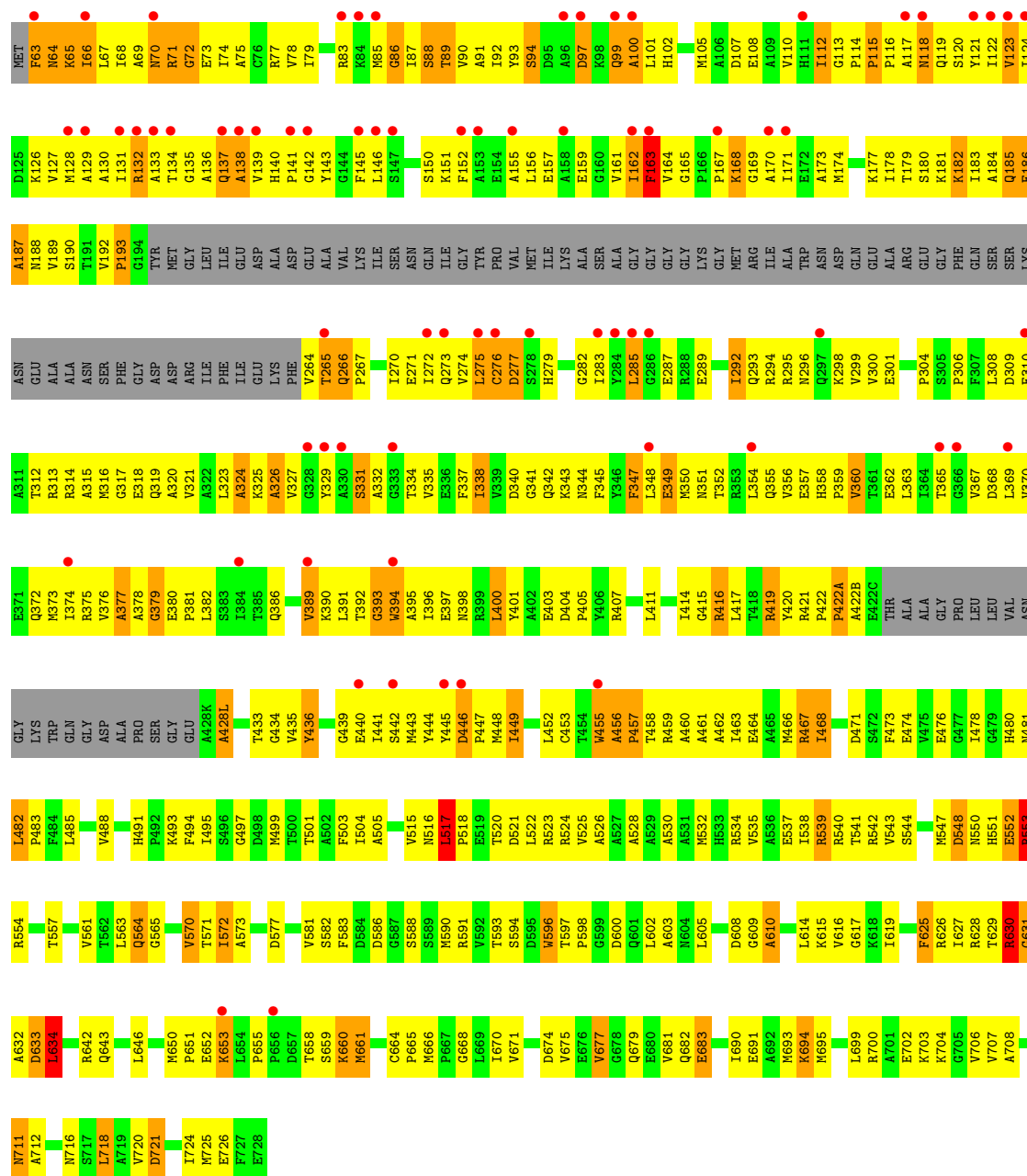
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

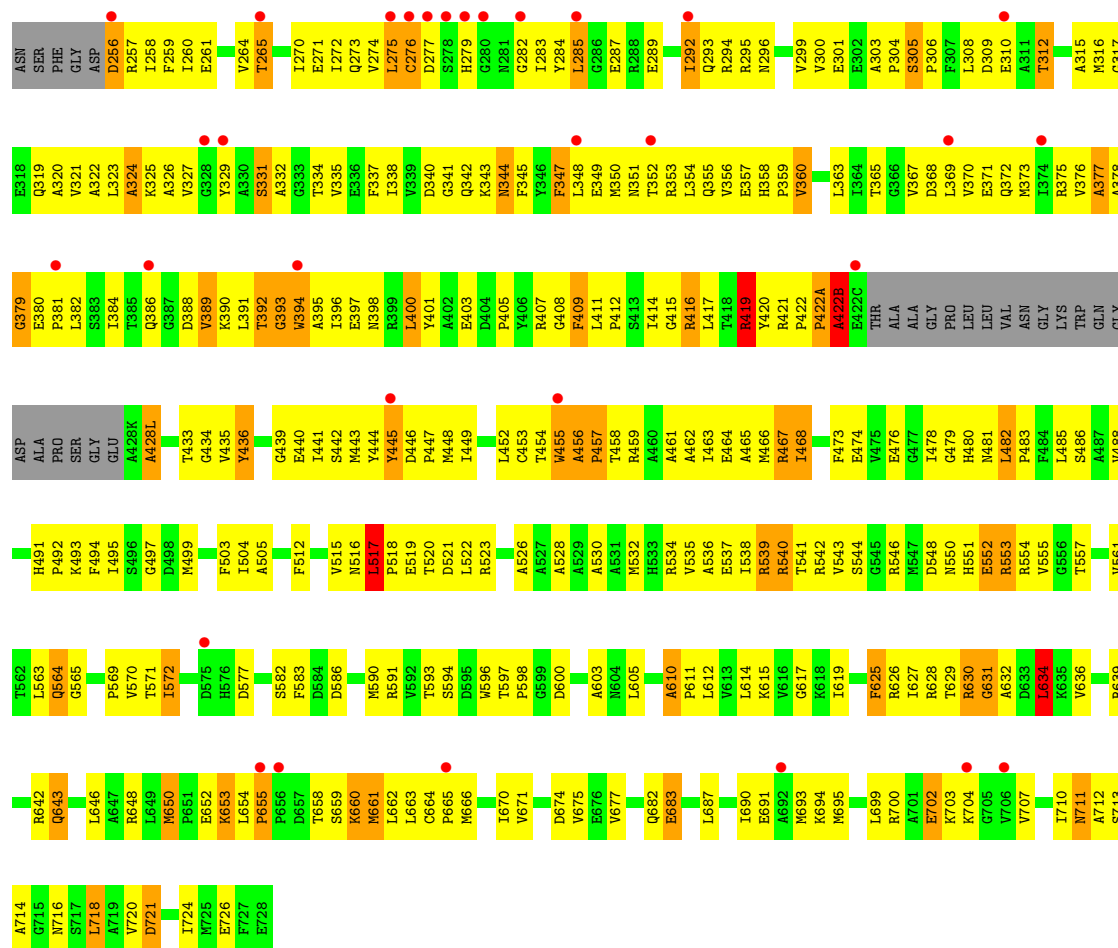
- [illegible]

M725
E726
E727
E728

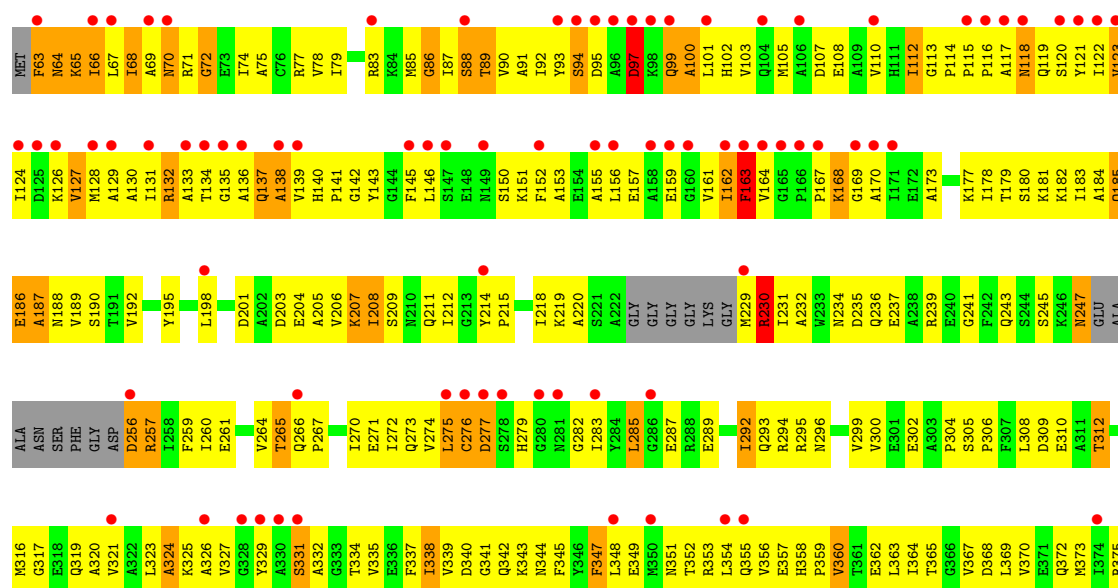
• Molecule 1: Propionyl-CoA carboxylase, alpha subunit

Chain C: 11% 28% 46% 12% 13%

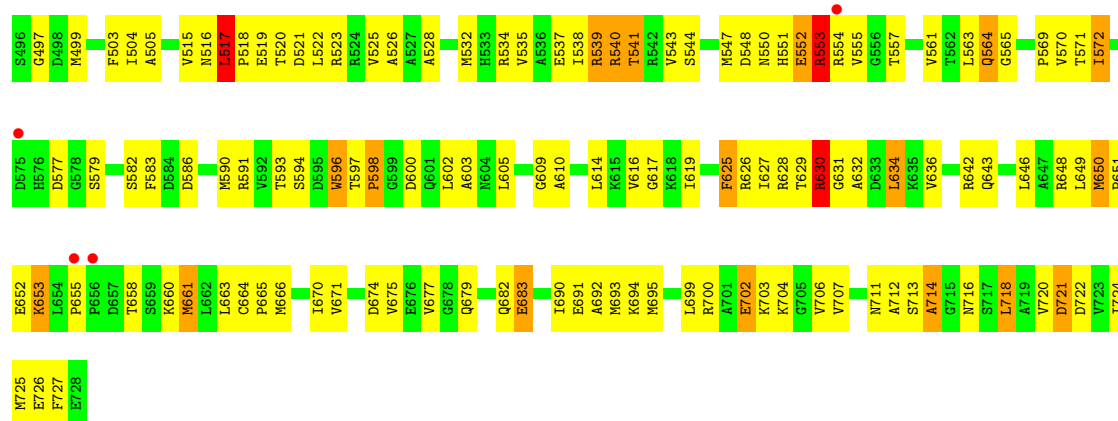




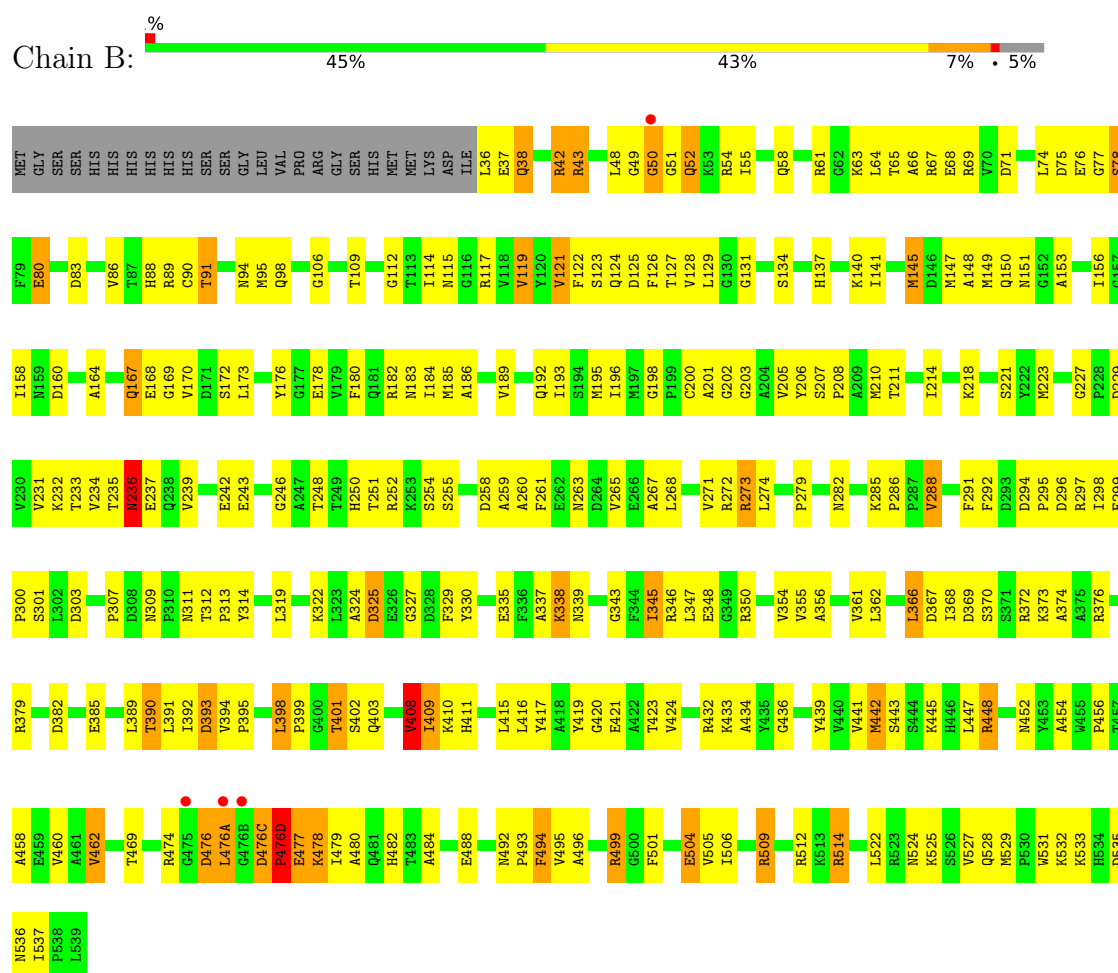
● Molecule 1: Propionyl-CoA carboxylase, alpha subunit



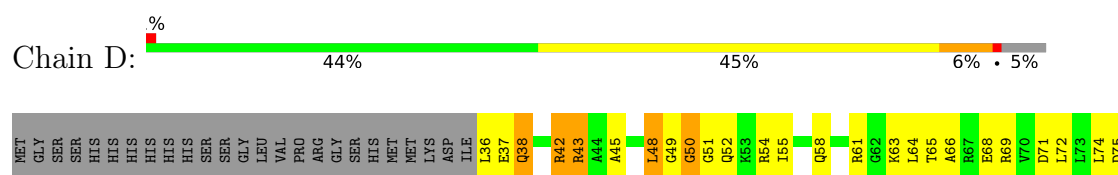




• Molecule 2: Propionyl-CoA carboxylase, beta subunit



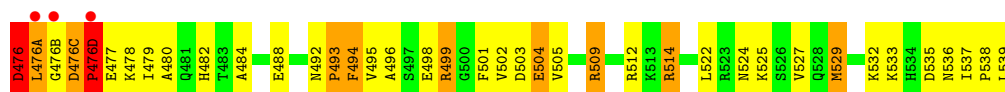
• Molecule 2: Propionyl-CoA carboxylase, beta subunit



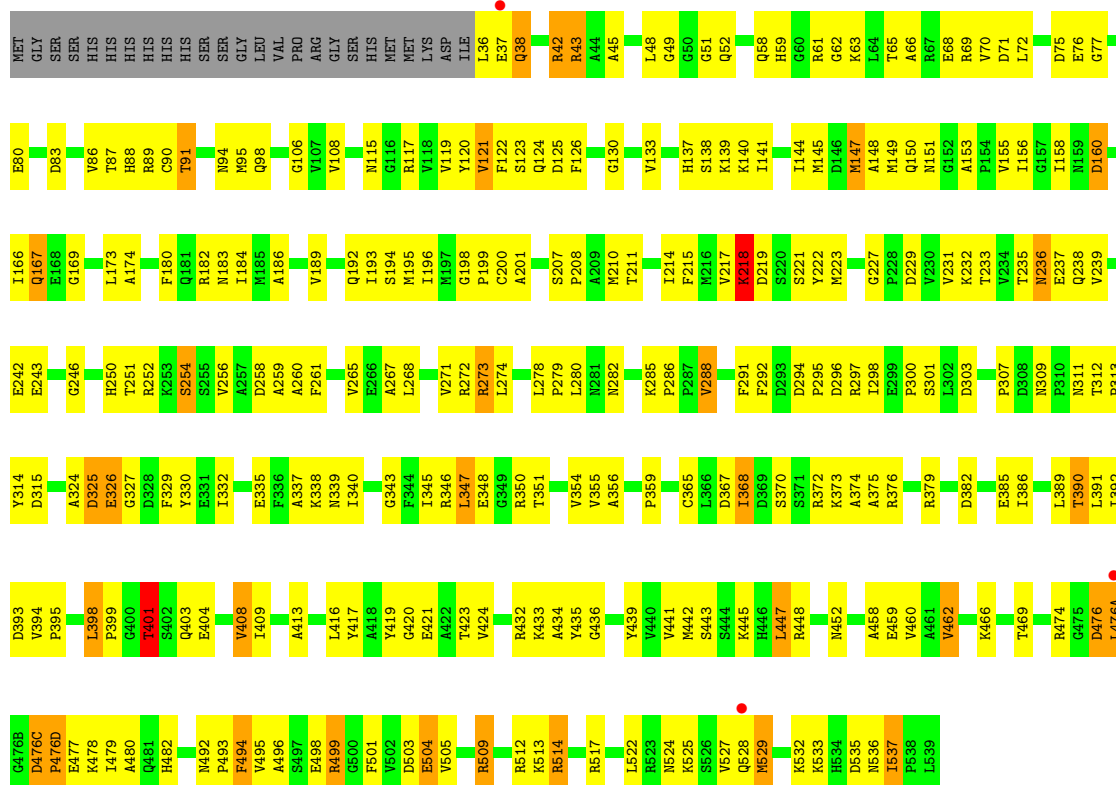
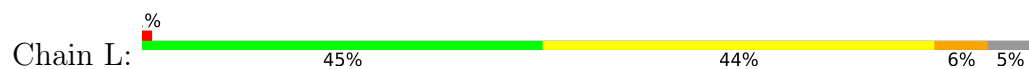
D476C	P395	K322	E243	G169	D83	MET
P476D	L398	L323	E244	V170		GLY
E477	L398	A324	G245	L173	V86	SER
K478	T404	D325	G245	A174	T87	SER
L479	S402	G327	H250	F180	R88	HIS
A480		D328	T251	F181	R89	HIS
G481	V408	F329	R252	Q181	C90	HIS
T483	I409	F330	K253	R182	T91	HIS
A484	K410	E331	S254	N183		HIS
		I332	S255	N184	N94	HIS
	L415		V256	M185	M95	SER
E488	L416	E335		A186	Q98	SER
M492	A417	F336	A260		G106	GLY
P493	P493	A337	F261	V189	V107	LEU
F494	Y419	K338	E262	V190	V108	VAL
V495	G420	N339	N263	P191	T109	ARG
A496	E421			Q192		GLY
S497	T422	G343	A267	S193	G112	SER
A498	T423	F344	L268	S194		SER
R499		T345		M195		MET
G500	M426	R346	V271	N196	G116	MET
F501		L347	R272	M197	R117	LYS
	R432	E348	R273	G198	V118	LYS
E504	K433	G349	L274	P199	V119	ASP
V505	A434	R350		C200		ASP
I506	Y435	T351	L278	A201	V120	L36
O507	G436		P279	G202	V121	E37
F508		V354	L280	G203	F122	Q38
		V355	N281	A204	Q124	
R509	Y439	F356	N282	V205		R42
	V440	A356		D125	F126	R43
R512	V441		K285	S207	T127	L48
R514	M442	L362	P286	P208		G49
	S443	A363	P287	A209	S138	G50
	S444		V288	N210	K139	G51
L522	K445			T211	K140	Q52
	H446	L366	F291		I141	K53
K525	L447	D367	F292			R54
S526	R448	I368		L214		
V527		D369	D296		T144	
	M452	R297	R297	V217	M45	Q58
		S371		R218	D146	
A458		R372	T298	S221	M147	R61
K532	E459	K373	E299	R221	A148	G62
V460	V460	A374	P300	Y222	M149	K63
	A461	A375	S301	M223	Q150	L64
D535	V462		L302	N151	N151	T65
		V378	D303	G227	G152	A66
L539		R379		P228	A153	R67
	K466		P307	D229	E154	R68
	G467	E385	D308	V230	V155	
	T469	I386	N309	V231	I156	D71
		P387	P310	K232	G157	L72
		L388	N311	T233	T158	
T472		L389	T312	V234	N159	D75
H473		T390		E237		
R474	D475	L391	Y314	N236		S78
G476	G476	I392	D315	Q237	T166	F79
L476A	D393	K392	M316	Q238	Q167	E80
C476B		I394		V239	S169	

Chain J: 45% 43% 7% 5%

L389	N311	D229	I158	E80	MET
T390	T312	V230	N159	D83	GLY
L391	P313	V231	D160	M84	SER
I392	Y314	K232		F85	SER
D393	D315	K233	A164	V86	HIS
		V234		T87	HIS
L398	A324	T235	Q167	H88	HIS
P399	D325	N236	E168	R89	HIS
G400	E326	E237	G169	C90	HIS
T401	G327	Q238		T91	HIS
V408	T328	V239	L173		SER
I409	F329		A174	N94	SER
L410	Y330	E243	G175	M95	GLY
H411	E331	L244	Y176	Q98	LEU
	I332	G245	G177		VAL
			E178		PRO
L415	E335	T248		V108	ARG
L416	F336	T249	R182	T109	GLY
I417	A337	H250	M183		SER
A418	K338	T251	I184	G112	HIS
Y419	N339	R252	M185		HIS
G420	I340	K253	A186	M115	MET
E421		S254	S187	G116	LYS
A422	G343		G188	R117	ASP
T423	F344	A260	V118	V118	ILE
V424	I345	F261	V190	V119	L36
	R346	E262	P191	Y120	E37
T428	L347		Q192	V121	Q38
	E348	V265	I193	F122	L39
R432	G349	E266	S194	S123	
K433	R350	A267	M195	Q124	
A434	T351	L268	I196	D125	
Y435			M197	F126	
G436	V354	R272	G198	T127	
	V355	R273	P199		L48
Y439	A356	L274	C200	G131	G49
V440			A201	S132	G50
V441	V361	L278	G202	V133	G51
H442	L362	P279	G203	S134	Q52
S443	A363	L280	A204	T135	
A444	G364	M281	V205	E136	Q58
K445	C365	N282	Y206	H137	H59
H446	L366		S207	S138	G60
L447	D367	V288	P208	K139	R61
R448	I368		A209	K63	G62
	D369	F291	M210	I141	K63
N452	S370	F292	T211	L144	L64
		D293	D212	I145	T65
	A374		F213	M146	A66
A458	R375	D296	I214	D146	R67
E459	A376	R297	K218	A148	E68
V460	R377	L298	D219	M149	R69
A461	E299	F299	D219	Q150	V70
V462	R379	P300	S220	Q150	D71
		S301	Y221	M151	L72
	D382		Y222	L74	L73
K466	A383	P307	M223	P154	D75
T469	F384	D308	P155	V155	
	E385	N309	G157	T157	S78
R474	I386	R340	P208		F79
T475					



• Molecule 2: Propionyl-CoA carboxylase, beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	133.89Å 159.17Å 153.74Å 113.87° 101.03° 108.99°	Depositor
Resolution (Å)	29.36 – 3.20 29.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.36-3.20) 92.3 (29.36-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.245 0.211 , 0.245	Depositor DCC
R_{free} test set	12641 reflections (7.45%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,h+k+l,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51921	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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: BTI

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	0.65	0/4586	1.11	32/6209 (0.5%)
1	C	0.65	0/4586	1.12	35/6209 (0.6%)
1	E	0.66	1/4586 (0.0%)	1.10	26/6209 (0.4%)
1	G	0.68	1/5036 (0.0%)	1.13	39/6811 (0.6%)
1	I	0.68	0/5036	1.11	33/6811 (0.5%)
1	K	0.65	0/5036	1.12	37/6811 (0.5%)
2	B	0.77	0/3990	1.18	26/5399 (0.5%)
2	D	0.77	0/3990	1.20	32/5399 (0.6%)
2	F	0.77	0/3990	1.19	24/5399 (0.4%)
2	H	0.78	1/3990 (0.0%)	1.18	25/5399 (0.5%)
2	J	0.76	1/3990 (0.0%)	1.19	31/5399 (0.6%)
2	L	0.77	0/3990	1.19	33/5399 (0.6%)
All	All	0.71	4/52806 (0.0%)	1.15	373/71454 (0.5%)

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	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	149	MET	SD-CE	-5.72	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	426	MET	SD-CE	5.34	1.92	1.79
1	E	629	THR	CA-C	-5.18	1.49	1.52
1	G	536	ALA	CA-CB	-5.15	1.45	1.53

The worst 5 of 373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	517	LEU	CA-C-N	9.41	130.12	120.14
1	G	517	LEU	C-N-CA	9.41	130.12	120.14
1	I	517	LEU	CA-C-N	9.31	130.00	120.14
1	I	517	LEU	C-N-CA	9.31	130.00	120.14
2	L	392	ILE	N-CA-C	8.97	121.54	108.53

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	420	TYR	Sidechain
1	E	420	TYR	Sidechain
1	G	420	TYR	Sidechain
1	I	420	TYR	Sidechain
1	K	420	TYR	Sidechain

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	4507	0	4511	462	0
1	C	4507	0	4512	476	0
1	E	4507	0	4512	485	0
1	G	4950	0	4944	525	0
1	I	4950	0	4943	523	0
1	K	4950	0	4943	510	0
2	B	3910	0	3851	285	0
2	D	3910	0	3851	267	0
2	F	3910	0	3851	246	0
2	H	3910	0	3851	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	3910	0	3851	251	0
2	L	3910	0	3851	251	0
3	A	15	0	15	1	0
3	C	15	0	15	0	0
3	E	15	0	15	1	0
3	G	15	0	15	0	0
3	I	15	0	15	2	0
3	K	15	0	15	0	0
All	All	51921	0	51561	4296	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 42.

The worst 5 of 4296 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:HD11	1:E:348:LEU:HB2	1.25	1.17
1:A:338:ILE:HD11	1:A:348:LEU:HB2	1.26	1.16
1:C:115:PRO:HG2	1:C:116:PRO:HD3	1.29	1.14
1:A:433:THR:HG22	1:A:435:VAL:H	1.06	1.11
1:G:400:LEU:HD13	1:G:449:ILE:HD11	1.33	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	585/681 (86%)	451 (77%)	99 (17%)	35 (6%)	1	10
1	C	585/681 (86%)	456 (78%)	94 (16%)	35 (6%)	1	10
1	E	585/681 (86%)	449 (77%)	98 (17%)	38 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	638/681 (94%)	502 (79%)	100 (16%)	36 (6%)	1	11
1	I	638/681 (94%)	504 (79%)	94 (15%)	40 (6%)	1	8
1	K	638/681 (94%)	505 (79%)	92 (14%)	41 (6%)	1	8
2	B	504/531 (95%)	444 (88%)	49 (10%)	11 (2%)	5	29
2	D	504/531 (95%)	445 (88%)	47 (9%)	12 (2%)	4	28
2	F	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	6	31
2	H	504/531 (95%)	451 (90%)	43 (8%)	10 (2%)	6	31
2	J	504/531 (95%)	452 (90%)	43 (8%)	9 (2%)	6	34
2	L	504/531 (95%)	455 (90%)	39 (8%)	10 (2%)	6	31
All	All	6693/7272 (92%)	5565 (83%)	841 (13%)	287 (4%)	2	16

5 of 287 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	137	GLN
1	A	138	ALA
1	A	277	ASP
1	A	331	SER

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	474/540 (88%)	415 (88%)	59 (12%)	4	21
1	C	474/540 (88%)	422 (89%)	52 (11%)	6	26
1	E	474/540 (88%)	419 (88%)	55 (12%)	5	24
1	G	520/540 (96%)	462 (89%)	58 (11%)	6	25
1	I	520/540 (96%)	457 (88%)	63 (12%)	5	22
1	K	520/540 (96%)	460 (88%)	60 (12%)	5	24
2	B	415/437 (95%)	389 (94%)	26 (6%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	415/437 (95%)	386 (93%)	29 (7%)	14	45
2	F	415/437 (95%)	382 (92%)	33 (8%)	11	40
2	H	415/437 (95%)	385 (93%)	30 (7%)	13	44
2	J	415/437 (95%)	379 (91%)	36 (9%)	9	36
2	L	415/437 (95%)	385 (93%)	30 (7%)	13	44
All	All	5472/5862 (93%)	4941 (90%)	531 (10%)	8	32

5 of 531 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	400	LEU
1	K	547	MET
1	K	388	ASP
2	L	448	ARG
1	E	488	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	100	GLN
2	L	100	GLN
2	J	183	ASN
1	K	119	GLN
2	L	482	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	BTI	G	801	1	15,16,16	1.86	1 (6%)	20,21,21	2.33	7 (35%)
3	BTI	K	801	1	15,16,16	1.76	1 (6%)	20,21,21	2.08	5 (25%)
3	BTI	C	801	1	15,16,16	1.72	1 (6%)	20,21,21	2.10	6 (30%)
3	BTI	I	801	1	15,16,16	1.77	1 (6%)	20,21,21	2.11	6 (30%)
3	BTI	A	801	1	15,16,16	1.72	1 (6%)	20,21,21	2.05	7 (35%)
3	BTI	E	801	1	15,16,16	1.76	1 (6%)	20,21,21	2.22	7 (35%)

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	BTI	G	801	1	-	5/6/27/27	0/2/2/2
3	BTI	K	801	1	-	3/6/27/27	0/2/2/2
3	BTI	C	801	1	-	0/6/27/27	0/2/2/2
3	BTI	I	801	1	-	3/6/27/27	0/2/2/2
3	BTI	A	801	1	-	2/6/27/27	0/2/2/2
3	BTI	E	801	1	-	1/6/27/27	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	801	BTI	O3-C3	6.63	1.37	1.23
3	I	801	BTI	O3-C3	6.37	1.36	1.23
3	E	801	BTI	O3-C3	6.36	1.36	1.23
3	K	801	BTI	O3-C3	6.31	1.36	1.23
3	C	801	BTI	O3-C3	6.22	1.36	1.23

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	801	BTI	C6-C5-N3	-4.53	107.34	113.18
3	E	801	BTI	C6-C5-N3	-4.24	107.72	113.18
3	G	801	BTI	C4-N2-C3	-4.09	107.49	112.56
3	I	801	BTI	C6-S1-C2	4.03	98.37	89.98
3	E	801	BTI	C4-N2-C3	-3.98	107.62	112.56

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	801	BTI	S1-C2-C7-C8
3	G	801	BTI	C4-C2-C7-C8
3	I	801	BTI	C9-C10-C11-O11
3	K	801	BTI	C2-C7-C8-C9
3	A	801	BTI	C2-C7-C8-C9

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	801	BTI	2	0
3	A	801	BTI	1	0
3	E	801	BTI	1	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 [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	591/681 (86%)	0.79	83 (14%) 6 5	17, 65, 113, 128	0
1	C	591/681 (86%)	0.77	72 (12%) 8 6	17, 65, 113, 128	0
1	E	591/681 (86%)	0.82	86 (14%) 6 4	17, 66, 113, 128	0
1	G	646/681 (94%)	0.79	79 (12%) 8 6	15, 67, 112, 128	0
1	I	646/681 (94%)	0.85	99 (15%) 5 4	16, 67, 112, 127	0
1	K	646/681 (94%)	0.76	79 (12%) 8 6	16, 68, 112, 128	0
2	B	506/531 (95%)	-0.44	4 (0%) 82 67	10, 26, 57, 101	0
2	D	506/531 (95%)	-0.43	3 (0%) 85 73	11, 26, 58, 101	0
2	F	506/531 (95%)	-0.42	2 (0%) 88 79	12, 27, 58, 100	0
2	H	506/531 (95%)	-0.44	2 (0%) 88 79	10, 26, 58, 101	0
2	J	506/531 (95%)	-0.45	5 (0%) 79 63	11, 26, 58, 100	0
2	L	506/531 (95%)	-0.47	3 (0%) 85 73	11, 26, 57, 100	0
All	All	6747/7272 (92%)	0.24	517 (7%) 19 13	10, 43, 108, 128	0

The worst 5 of 517 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ILE	6.9
1	E	162	ILE	6.1
1	C	162	ILE	6.0
1	C	286	GLY	6.0
1	I	70	ASN	5.2

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	BTI	I	801	15/15	0.92	0.12	57,65,68,69	0
3	BTI	E	801	15/15	0.94	0.10	31,39,49,50	0
3	BTI	G	801	15/15	0.94	0.14	43,49,56,60	0
3	BTI	A	801	15/15	0.94	0.11	30,42,56,62	0
3	BTI	K	801	15/15	0.94	0.12	39,50,57,62	0
3	BTI	C	801	15/15	0.96	0.08	30,38,46,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.