



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:54 PM UTC

PDB ID : 3BG9 / pdb_00003bg9
Title : Crystal Structure of Human Pyruvate Carboxylase (missing the biotin carboxylase domain at the N-terminus) F1077A Mutant
Authors : Xiang, S.; Tong, L.
Deposited on : 2007-11-26
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 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
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

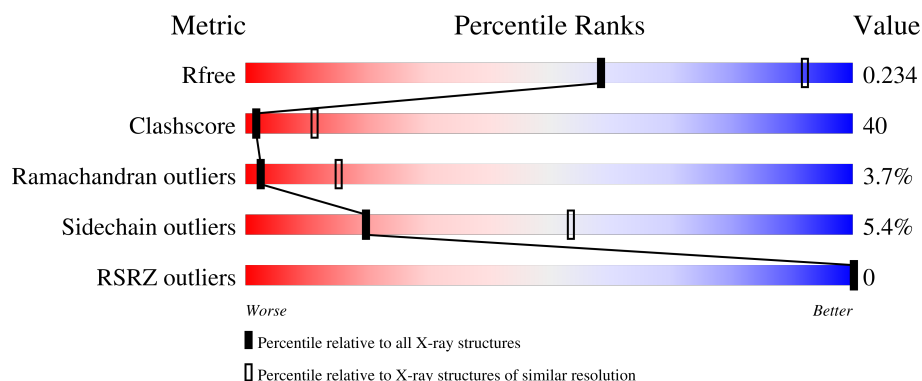
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	718	
1	B	718	
1	C	718	
1	D	718	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18516 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	B	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	C	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			
1	D	601	Total	C	N	O	S	0	0	0
			4628	2937	798	865	28			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	MET	-	expression tag	UNP P11498
A	462	GLY	-	expression tag	UNP P11498
A	463	SER	-	expression tag	UNP P11498
A	464	SER	-	expression tag	UNP P11498
A	465	HIS	-	expression tag	UNP P11498
A	466	HIS	-	expression tag	UNP P11498
A	467	HIS	-	expression tag	UNP P11498
A	468	HIS	-	expression tag	UNP P11498
A	469	HIS	-	expression tag	UNP P11498
A	470	HIS	-	expression tag	UNP P11498
A	471	SER	-	expression tag	UNP P11498
A	472	SER	-	expression tag	UNP P11498
A	473	GLY	-	expression tag	UNP P11498
A	474	LEU	-	expression tag	UNP P11498
A	475	VAL	-	expression tag	UNP P11498
A	476	PRO	-	expression tag	UNP P11498
A	477	ARG	-	expression tag	UNP P11498
A	478	GLY	-	expression tag	UNP P11498
A	479	SER	-	expression tag	UNP P11498
A	480	HIS	-	expression tag	UNP P11498
A	481	MET	-	expression tag	UNP P11498

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP P11498
B	461	MET	-	expression tag	UNP P11498
B	462	GLY	-	expression tag	UNP P11498
B	463	SER	-	expression tag	UNP P11498
B	464	SER	-	expression tag	UNP P11498
B	465	HIS	-	expression tag	UNP P11498
B	466	HIS	-	expression tag	UNP P11498
B	467	HIS	-	expression tag	UNP P11498
B	468	HIS	-	expression tag	UNP P11498
B	469	HIS	-	expression tag	UNP P11498
B	470	HIS	-	expression tag	UNP P11498
B	471	SER	-	expression tag	UNP P11498
B	472	SER	-	expression tag	UNP P11498
B	473	GLY	-	expression tag	UNP P11498
B	474	LEU	-	expression tag	UNP P11498
B	475	VAL	-	expression tag	UNP P11498
B	476	PRO	-	expression tag	UNP P11498
B	477	ARG	-	expression tag	UNP P11498
B	478	GLY	-	expression tag	UNP P11498
B	479	SER	-	expression tag	UNP P11498
B	480	HIS	-	expression tag	UNP P11498
B	481	MET	-	expression tag	UNP P11498
B	1077	ALA	PHE	engineered mutation	UNP P11498
C	461	MET	-	expression tag	UNP P11498
C	462	GLY	-	expression tag	UNP P11498
C	463	SER	-	expression tag	UNP P11498
C	464	SER	-	expression tag	UNP P11498
C	465	HIS	-	expression tag	UNP P11498
C	466	HIS	-	expression tag	UNP P11498
C	467	HIS	-	expression tag	UNP P11498
C	468	HIS	-	expression tag	UNP P11498
C	469	HIS	-	expression tag	UNP P11498
C	470	HIS	-	expression tag	UNP P11498
C	471	SER	-	expression tag	UNP P11498
C	472	SER	-	expression tag	UNP P11498
C	473	GLY	-	expression tag	UNP P11498
C	474	LEU	-	expression tag	UNP P11498
C	475	VAL	-	expression tag	UNP P11498
C	476	PRO	-	expression tag	UNP P11498
C	477	ARG	-	expression tag	UNP P11498
C	478	GLY	-	expression tag	UNP P11498
C	479	SER	-	expression tag	UNP P11498

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Chain	Residue	Modelled	Actual	Comment	Reference
C	480	HIS	-	expression tag	UNP P11498
C	481	MET	-	expression tag	UNP P11498
C	1077	ALA	PHE	engineered mutation	UNP P11498
D	461	MET	-	expression tag	UNP P11498
D	462	GLY	-	expression tag	UNP P11498
D	463	SER	-	expression tag	UNP P11498
D	464	SER	-	expression tag	UNP P11498
D	465	HIS	-	expression tag	UNP P11498
D	466	HIS	-	expression tag	UNP P11498
D	467	HIS	-	expression tag	UNP P11498
D	468	HIS	-	expression tag	UNP P11498
D	469	HIS	-	expression tag	UNP P11498
D	470	HIS	-	expression tag	UNP P11498
D	471	SER	-	expression tag	UNP P11498
D	472	SER	-	expression tag	UNP P11498
D	473	GLY	-	expression tag	UNP P11498
D	474	LEU	-	expression tag	UNP P11498
D	475	VAL	-	expression tag	UNP P11498
D	476	PRO	-	expression tag	UNP P11498
D	477	ARG	-	expression tag	UNP P11498
D	478	GLY	-	expression tag	UNP P11498
D	479	SER	-	expression tag	UNP P11498
D	480	HIS	-	expression tag	UNP P11498
D	481	MET	-	expression tag	UNP P11498
D	1077	ALA	PHE	engineered mutation	UNP P11498

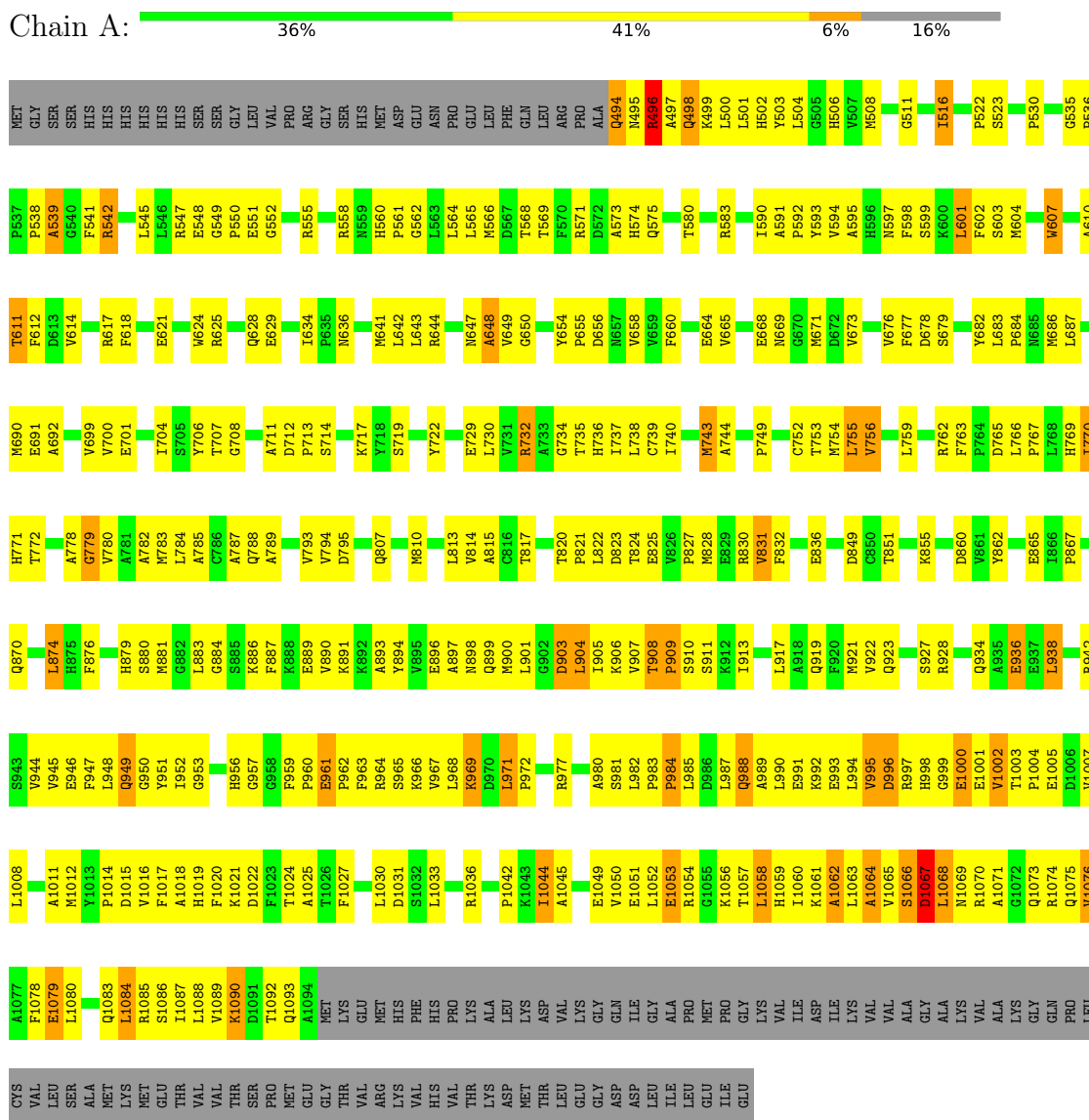
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

3 Residue-property plots

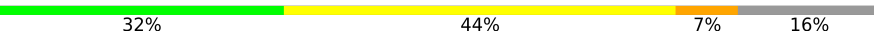
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pyruvate carboxylase, mitochondrial

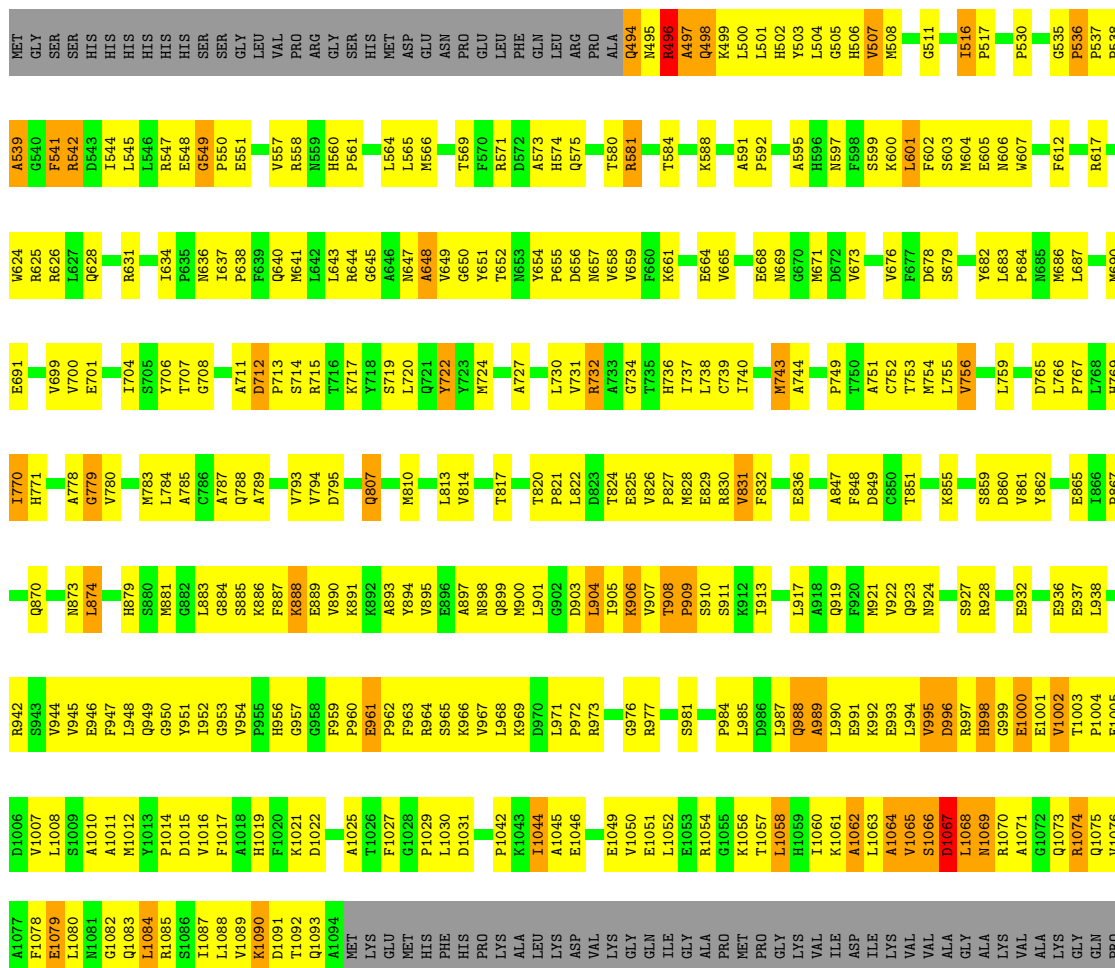
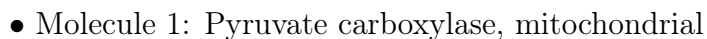


VAL	V1065	V995	R928	K855	F763	M686	F612	G535
ALA	D1066	D996		R856	P764	L687		P536
GLY	D1067	D996	R928	S856	P764	L687	F612	P536
ALA	D1068	H998	A935	S856	L766	G689	R617	P538
LYS	N1069	G999	E936	S859	P767	M690		A539
VAL	R1070	E1000	E937	D860	L768	E691	W624	G540
ALA	A1071	E1001	L938	V861	H769		R625	F541
LYS	G1072	V1002	S939	N864	T772	S695	Q628	R542
GLY	R1073	T1003	F940	E865		A696	E629	D543
GLN	R1074	P1004	R942	E865	M783	G697	Q628	D543
PRO	Q1075			Q870	L784	V699	L630	I544
LEU	V1076	V1007			A778	G779	R631	L545
CYS	A1077	L1008	V945		W779	V700	E632	L546
VAL	F1078	S1009	E946	M873		L633	E531	R547
LEU	E1079	A1010	F947	L874	M783	A702	L634	E548
SER	L1080	A1011	L948	Q877	L794	A703	P635	G549
ALA		M1012	Q949	A878	A785	I704	P635	P550
MET	Q1083	V1013		H879	C786	S705	I637	E551
LYS	L1084	P1014	I952	H879	C786	T706	P638	G552
MET	R1085	D1015	G953		Q788	T707	P639	R555
GLU	S1086	V1016	V954	L883	D792	G708	Q640	R558
THR	I1087	F1017	P955	G884	V793	D709	M641	
VAL	L1088	A1018	H956	S885	W794	A711	L642	P561
V1089		H1019	G957	K886		L643	R644	ASN
THR	K1090	F1020	G958	E889	S802	D712	G645	PRO
SER	D1091	K1021	F959	V890	Q807	P713	A646	GLU
PRO	T1092	D1022	P960	K891		S714	G645	LEU
MET	Q1093	F1023	E961	K892	P808	W719	N647	PHE
GLY	A1094	T1024	P962		S809		A648	GLN
MET		A1025	R963	A893	S809		V649	LEU
GLY		T1026	R964	R894	M810	Y722	G650	LEU
THR	LYS	F1027	S965	V895			Y651	ARG
VAL	GLY	F1027	S965	E896				PRO
ARG	MET	G1028	V967	E896	L813	L726	M652	ALA
LYS	HIS	P1029	R967	A897	W814		N653	Q494
VAL	PHE	L1030	L968	N898	A815	R732	Y654	N495
HIS	HIS	D1031	K969	Q899	C816	A733	P655	R496
VAL	PRO		D970	H900	T817	G734	D656	A497
VAL	LYS	T1035	L971	L901	R818	T735	N657	Q498
THR	LYS		P972	G902	G819	I737	V658	K499
ASP	ALA	P1042	R973	D903	T820	L738	K661	L501
MET	LYS	K1043	V974	L904	R821	C739		H502
THR	ASP	I1044		I905	L822			Y503
LEU	VAL	A1045	R977	K906	D823	D742	E664	L504
GLY	GLY	G1049	G979	T908	T824	M743	V665	G505
ASP	GLN	V1050	A980	P909	P827	L747	E668	H506
ILE	ILE	E1051	S981	S910	M828	K748	N669	V507
LEU	GLY	L1052	L982	S911	E829	P749	G670	M508
ILE	ALA	E1053	P983	R912	R830		M671	A595
LEU	PRO	R1054	P984	I913	W831	T750		H596
GLY	MET	G1055	L985	V914	F832	A751	V676	N510
ILE	PRO	K1056	D986	G915	D833			G511
GLY	GLY	T1057	L987	P916		T753	D678	
LYS	LYS	L1058	Q988	L917	E836	W754	S679	K600
VAL	VAL	H1059	A989	A918		L755	L680	L601
ILE	ILE	L1060	L990	Q919	A847	V756	N681	F602
ASP	ASP	K1061	E991	F920	F848			S603
ILE	ILE	A1062	K992	N921	D849	L759	V682	M604
LYS	LYS	L1063	V922	E993	C850		L683	E605
VAL	VAL	A1064	L904	O932	T851	P762	P654	N606
								P533
								I534

• Molecule 1: Pyruvate carboxylase, mitochondrial

Chain C:  32% 44% 7% 16%

MET		GLY		SER		SER		HIS		HIS		HIS		HIS		SER		SER		GLY		LEU		VAL		PRO		ARG		GLY		SER		HIS		MET		ASP		GLU		ASN		PRO		GLU		LEU		PHE		GLN		LEU		ARG		PRO		ALA		Q494		N495		R496		A497		Q498		K499		L500		L501		H502		Y503		L504		G505		H506		V507		M508		V509		N510		G511		I516		P517		P527		V528		V529		P530	
I534		G535		P536		P537		P538		A539		R542		D543		I544		L545		L546		R547		E548		G549		P550		E551		G552		P553		R555		A554		V557		R558		N559		H560		P561		G562		L563		L564		L565		M566		T569		F570		R571		D572		A573		H574		Q575		A579		T580		R581		V582		R583		D586		L587		I590		A591		P592		Y593		V594		A595		H596		N597		F598		S599			
K600		L601		F602		S603		M604		E605		M606		W607		F612		D613		V614		R617		W624		Q628		E632		L633		I634		P635		N636		I637		P638		M641		L642		L643		R644		G645		A646		N647		V649		G650		Y651		T652		N653		Y654		P655		D656		N657		V658		K659		F660		K661		E664		V665		E666		K667		E668		N669		M671		D672		V673											
V676		F677		D678		S679		L680		P681		Y682		L683		P684		M685		M686		L687		M690		E691		A696		V699		V700		E701		T704		S705		Y706		T707		G708		D709		V710		A711		D712		P713		S714		K717		Y718		S719		Y722		R732		A733		G734		T735		H736		I737		L738		C739		D740		M743		A744		K749		T750		A751		C752		T753		M754		L755									
W756		L759		R762		F763		P764		L765		L766		P767		L768		H769		T770		T771		T772		A778		G779		V780		M783		L784		A787		Q788		A789		V793		W794		D795		Q807		P808		S809		M810		L813		R814		A815		C816		T817		R818		G819		T820		P821		L822		D823		T824		E825		R826		M828		E829		R830		W831		F832		Y837		A847													



LEU	CYS	VAL	LEU	SER	ALA	MET	LYS	MET	GLU	THR	VAL	VAL	THR	SER	PRO	MET	GLU	GLY	THR	VAL	ARG	LYS	VAL	HIS	VAL	THR	LYS	ASP	MET	THR	LEU	GLU	GLY	ASP	ASP	LEU	ILE	LEU	GLU	ILE	GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.54Å 107.54Å 524.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	80.8 (30.00-3.00) 88.9 (30.00-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.236 0.193 , 0.234	Depositor DCC
R_{free} test set	2799 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.370 for -h,-k,l	Xtriage
Reported twinning fraction	0.366 for -h,-k,l	Depositor
Outliers	0 of 63285 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18516	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.58	0/4736	1.08	22/6428 (0.3%)
1	B	0.59	1/4736 (0.0%)	1.10	28/6428 (0.4%)
1	C	0.58	0/4736	1.09	32/6428 (0.5%)
1	D	0.60	0/4736	1.10	33/6428 (0.5%)
All	All	0.58	1/18944 (0.0%)	1.09	115/25712 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	536	PRO	CA-C	5.27	1.54	1.51

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	GLY	CA-C-N	13.55	129.56	119.66
1	B	535	GLY	C-N-CA	13.55	129.56	119.66
1	A	535	GLY	CA-C-N	8.91	129.56	120.38
1	A	535	GLY	C-N-CA	8.91	129.56	120.38
1	D	535	GLY	CA-C-N	8.74	129.38	120.38

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	4628	0	4579	375	1
1	B	4628	0	4579	379	0
1	C	4628	0	4579	395	1
1	D	4628	0	4579	353	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	18516	0	18316	1488	1

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 40.

The worst 5 of 1488 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:C:496:ARG:HB3	1:C:1052:LEU:HD11	1.27	1.12
1:D:1044:ILE:H	1:D:1044:ILE:HD12	1.18	1.07
1:D:496:ARG:HB3	1:D:1052:LEU:HD11	1.37	1.06
1:A:496:ARG:HB3	1:A:1052:LEU:HD11	1.38	1.02
1:A:700:VAL:H	1:A:736:HIS:HD2	1.11	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:LYS:NZ	1:C:970:ASP:OD1[1_565]	2.18	0.02

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	599/718 (83%)	505 (84%)	72 (12%)	22 (4%)	2	15
1	B	599/718 (83%)	495 (83%)	83 (14%)	21 (4%)	3	16
1	C	599/718 (83%)	497 (83%)	80 (13%)	22 (4%)	2	15
1	D	599/718 (83%)	499 (83%)	76 (13%)	24 (4%)	2	14
All	All	2396/2872 (83%)	1996 (83%)	311 (13%)	89 (4%)	2	15

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ALA
1	A	779	GLY
1	A	984	PRO
1	A	1002	VAL
1	A	1062	ALA

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	493/593 (83%)	466 (94%)	27 (6%)	19	53
1	B	493/593 (83%)	466 (94%)	27 (6%)	19	53
1	C	493/593 (83%)	467 (95%)	26 (5%)	20	54
1	D	493/593 (83%)	467 (95%)	26 (5%)	20	54
All	All	1972/2372 (83%)	1866 (95%)	106 (5%)	20	53

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	542	ARG
1	C	996	ASP
1	D	1044	ILE
1	C	601	LEU
1	C	765	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	879	HIS
1	D	628	GLN
1	C	899	GLN
1	D	498	GLN
1	D	736	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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 [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	601/718 (83%)	-1.61	0 100 100	47, 47, 47, 78	0
1	B	601/718 (83%)	-1.60	0 100 100	47, 47, 47, 78	0
1	C	601/718 (83%)	-1.61	0 100 100	1, 47, 47, 78	0
1	D	601/718 (83%)	-1.59	0 100 100	47, 47, 47, 78	0
All	All	2404/2872 (83%)	-1.60	0 100 100	1, 47, 47, 78	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	MN	D	2001	1/1	0.99	0.03	87,87,87,87	0
2	MN	B	2001	1/1	1.00	0.02	87,87,87,87	0
2	MN	C	2001	1/1	1.00	0.01	87,87,87,87	0
2	MN	A	2001	1/1	1.00	0.04	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.