



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:58 am GMT

PDB ID : 1I48  
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR CTCPO  
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.  
Deposited on : 2001-02-20  
Resolution : 3.25 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

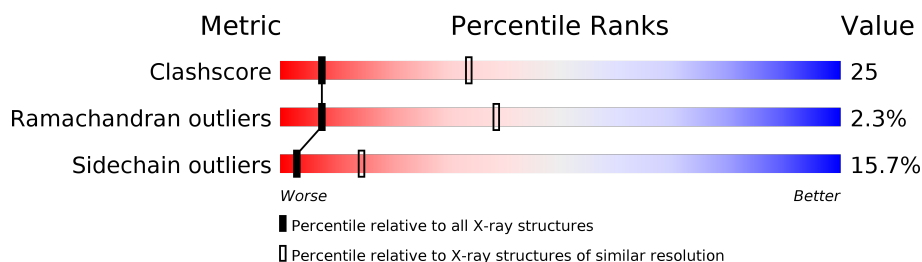
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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))
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)




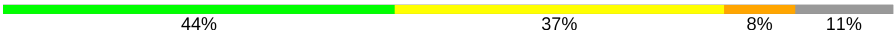
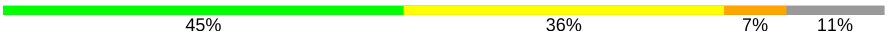
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	
1	B	445	
1	C	445	
1	D	445	
1	E	445	
1	F	445	
1	G	445	

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Mol	Chain	Length	Quality of chain
1	H	445	
1	I	445	
1	J	445	
1	K	445	
1	L	445	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36660 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 CYSTATHIONINE GAMMA-SYNTHASE.

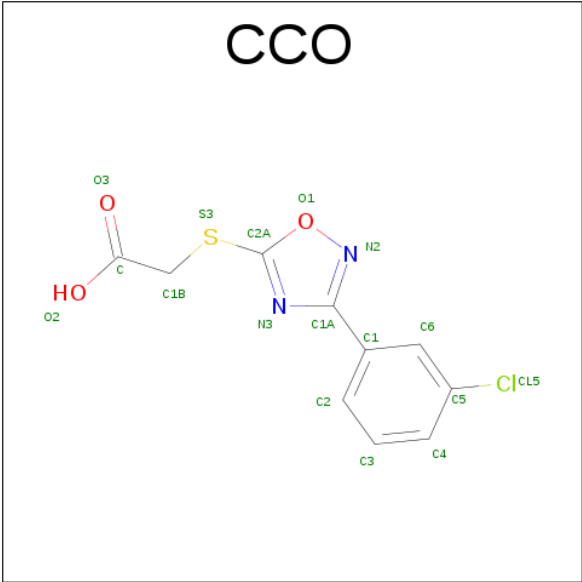
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	B	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	C	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	D	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	E	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	F	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	G	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	H	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	I	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	J	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	K	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	L	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



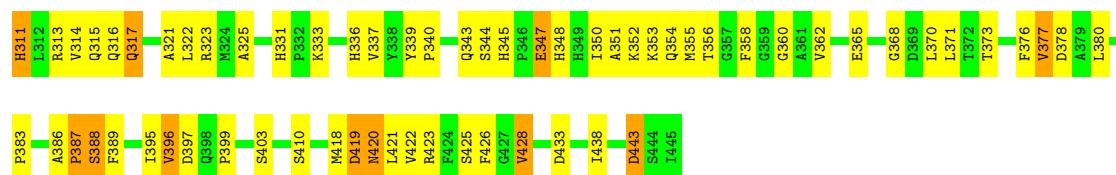
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CARBOXYMETHYLTHIO-3-(3-CHLOROPHENYL)-1,2,4-OXADIAZOL (three-letter code: CCO) (formula: C<sub>10</sub>H<sub>7</sub>ClN<sub>2</sub>O<sub>3</sub>S).



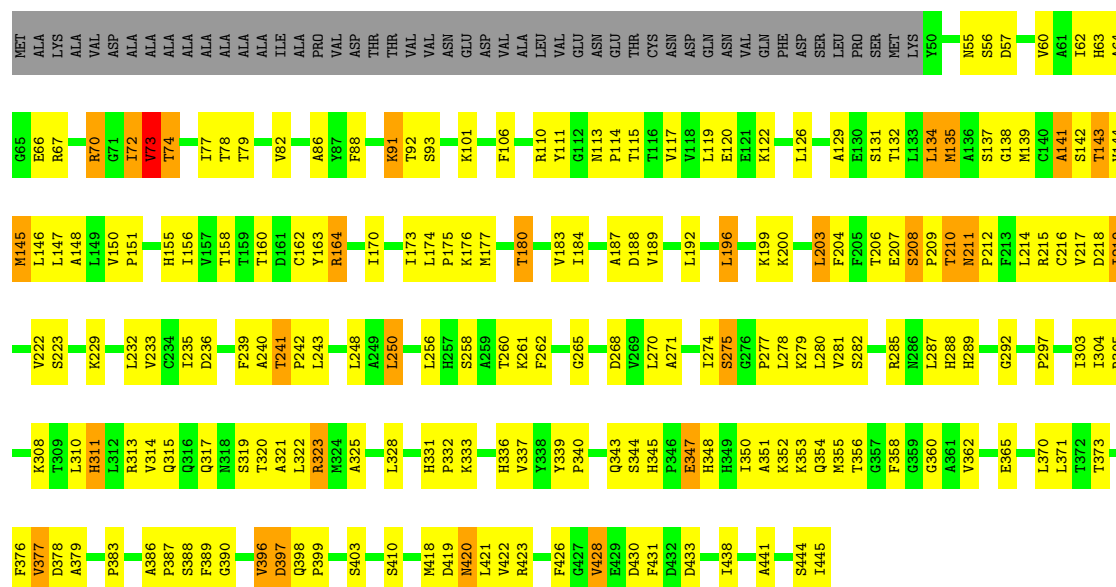
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	E	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	F	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	G	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	H	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	I	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	J	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	K	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		
3	L	1	Total	C	Cl	N	O	S	0	0
			17	10	1	2	3	1		





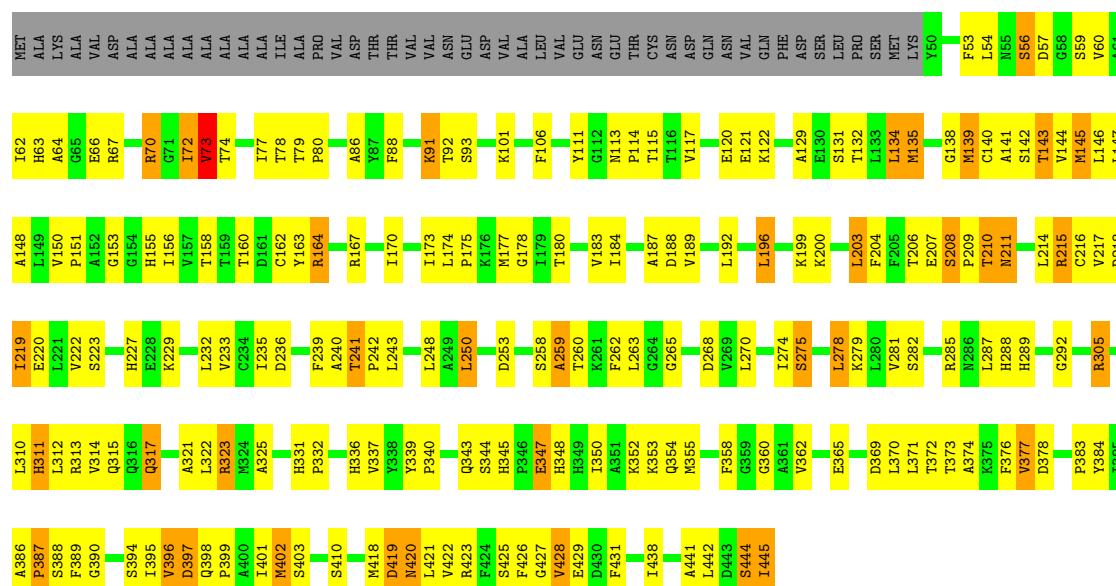
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain C: 44% 39% 6% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

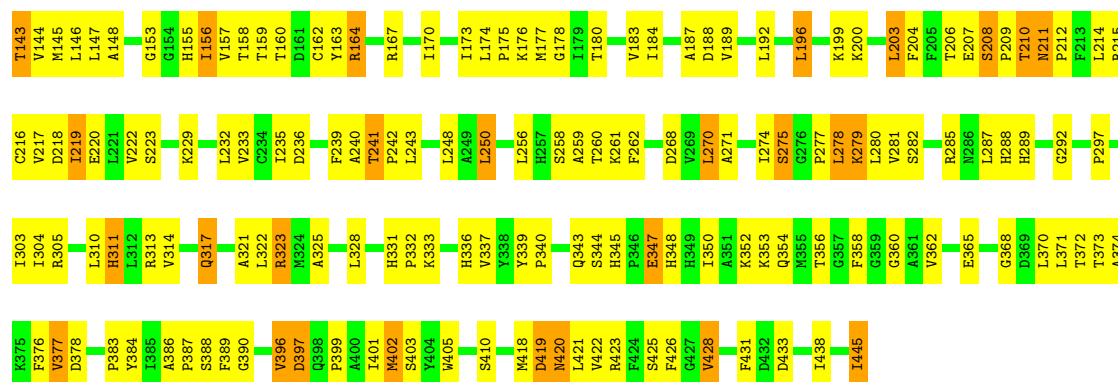
Chain D: 44% 37% 8% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

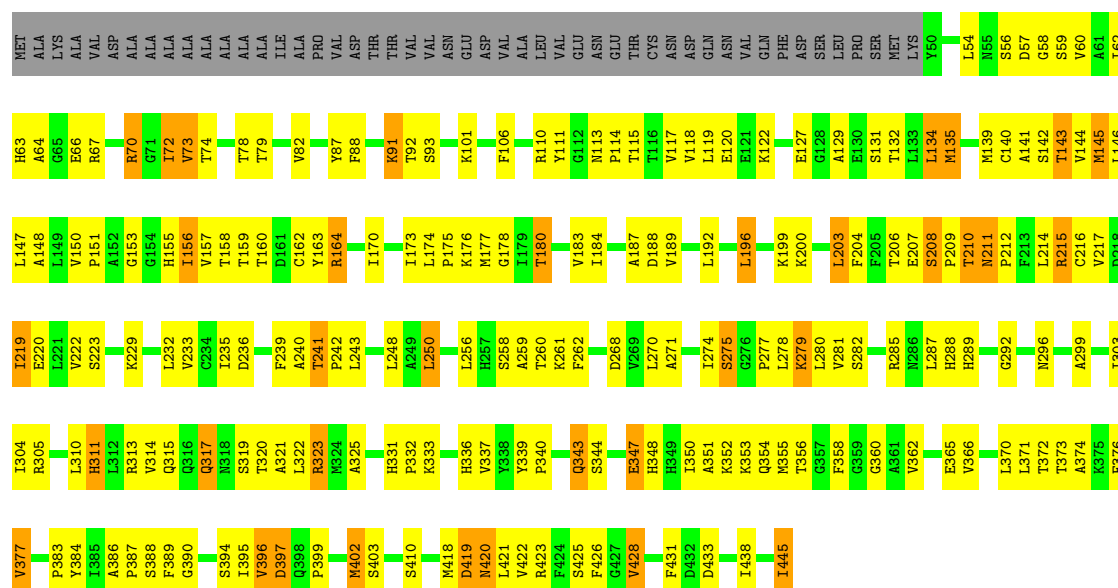






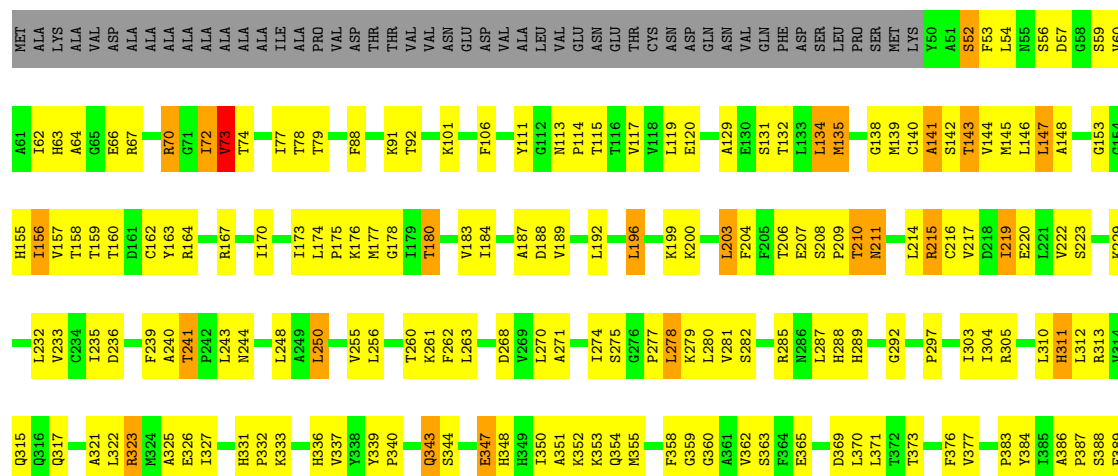
### • Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

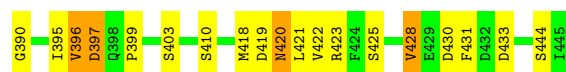
Chain H: 43% 38% 8% 11%



### • Molecule 1: CYSTATHIONINE GAMMA-SYNTASE

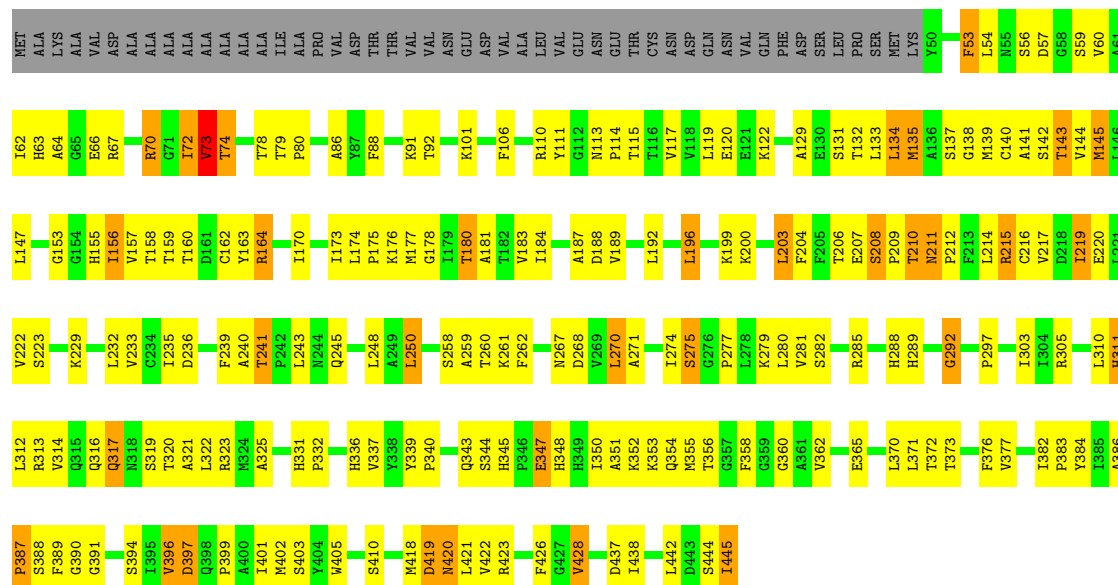
Chain I: 45% 38% 6% 11%





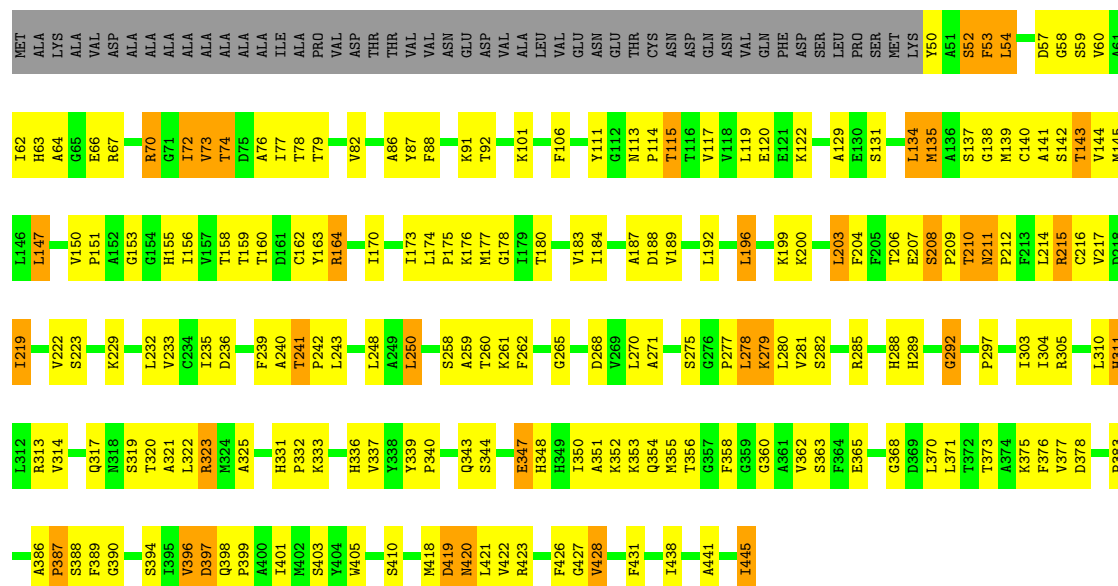
● Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain J: 44% 38% 7% 11%



● Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain K: 44% 37% 8% 11%



● Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain L: 45% 36% 7% 11%

MET	H63	A148	L310	D378
ALA	A64	L149	H311	P383
LYS	G65	G153	L312	A386
ALA	E66	G154	R313	S388
VAL	R67	H155	V314	F389
ASP		I156	Q317	G390
ALA	R70	I157	H318	V396
ALA	G71	T158	S319	D397
ALA	T72	T159	T320	G398
ALA	V73	T160	A321	F399
ALA	T74	D161	L322	A400
ALA	I77	C162	R323	M402
ALA	T78	Y163	H324	S403
ILE	T79	R164	A325	Y404
ALA	P80	L243		W405
PRO	V81	I170	L328	S410
VAL	V82	L248	H331	M418
ASP		A249	P332	D419
THR	A86	L250	K333	M420
THR	Y87	G251		L421
VAL	F88	S258	H336	V422
VAL	K91	T259	V337	F424
ASN	T92	T260	Y338	S425
GLU		K261	Y339	F426
ASP	K101	F262	P340	G427
VAL		L263		V428
ALA	F106	L266	Q343	D430
LEU	Y111	G264	H345	F431
VAL		G265	F346	I438
GLU	P114	D268	E347	T445
ASN	T115	V269	H349	
THR	T116	L270	I350	
CYS	V117	I274	A351	
ASN		S275	K352	
ASP	E120	K199	K353	
GLN	E121	K200	Q354	
ASN	K122	L278	M355	
VAL		K279		
GLN	A129	L280	F358	
PHE	F130	V281	G359	
ASP	E131	S282	G360	
SER	T132	R285	A361	
LEU	L133	H288	V362	
PRO	M135	H289	S363	
SER	A136	G292	F364	
MET	S137		E365	
LYS	G138	F213	G368	
V60	M139	L214	D369	
	C140	R215	L370	
L54	A141	C216	L371	
N55	S142	T217	T372	
S56	T143	I218	T373	
D57	V144	V222	F376	
G58	M145	S223	V377	
S59	L146			
V60	A61			
I62	L147			

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	312.40Å 165.60Å 162.20Å 90.00° 89.80° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.25)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.226 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 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: CCO, PLP

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	0.30	0/3082	0.49	0/4179
1	B	0.30	0/3082	0.50	0/4179
1	C	0.29	0/3082	0.49	0/4179
1	D	0.30	0/3082	0.49	0/4179
1	E	0.30	0/3082	0.49	0/4179
1	F	0.29	0/3082	0.49	0/4179
1	G	0.29	0/3082	0.48	0/4179
1	H	0.29	0/3082	0.49	0/4179
1	I	0.29	0/3082	0.49	0/4179
1	J	0.29	0/3082	0.48	0/4179
1	K	0.29	0/3082	0.48	0/4179
1	L	0.29	0/3082	0.49	0/4179
All	All	0.29	0/36984	0.49	0/50148

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	3023	0	3052	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3052	157	0
1	C	3023	0	3052	160	0
1	D	3023	0	3052	155	0
1	E	3023	0	3052	155	0
1	F	3023	0	3052	165	0
1	G	3023	0	3052	172	0
1	H	3023	0	3052	160	0
1	I	3023	0	3052	151	0
1	J	3023	0	3052	163	0
1	K	3023	0	3052	165	0
1	L	3023	0	3052	156	0
2	A	15	0	6	2	0
2	B	15	0	6	0	0
2	C	15	0	6	2	0
2	D	15	0	6	0	0
2	E	15	0	6	0	0
2	F	15	0	6	1	0
2	G	15	0	6	1	0
2	H	15	0	6	0	0
2	I	15	0	6	1	0
2	J	15	0	6	1	0
2	K	15	0	6	1	0
2	L	15	0	6	1	0
3	A	17	0	6	1	0
3	B	17	0	6	1	0
3	C	17	0	6	1	0
3	D	17	0	6	1	0
3	E	17	0	6	1	0
3	F	17	0	6	2	0
3	G	17	0	6	1	0
3	H	17	0	6	2	0
3	I	17	0	6	1	0
3	J	17	0	6	2	0
3	K	17	0	6	2	0
3	L	17	0	6	1	0
All	All	36660	0	36768	1810	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 25.

The worst 5 of 1810 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:H:241:THR:HG22	1:H:243:LEU:H	1.33	0.94
1:E:370:LEU:HD23	1:E:419:ASP:HB3	1.49	0.92
1:G:241:THR:HG22	1:G:243:LEU:H	1.33	0.92
1:A:241:THR:HG22	1:A:243:LEU:H	1.34	0.92
1:A:370:LEU:HD23	1:A:419:ASP:HB3	1.50	0.91

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	394/445 (88%)	324 (82%)	62 (16%)	8 (2%)	9	42
1	B	394/445 (88%)	327 (83%)	61 (16%)	6 (2%)	12	49
1	C	394/445 (88%)	320 (81%)	65 (16%)	9 (2%)	7	38
1	D	394/445 (88%)	312 (79%)	73 (18%)	9 (2%)	7	38
1	E	394/445 (88%)	310 (79%)	75 (19%)	9 (2%)	7	38
1	F	394/445 (88%)	319 (81%)	65 (16%)	10 (2%)	6	36
1	G	394/445 (88%)	319 (81%)	65 (16%)	10 (2%)	6	36
1	H	394/445 (88%)	316 (80%)	69 (18%)	9 (2%)	7	38
1	I	394/445 (88%)	316 (80%)	71 (18%)	7 (2%)	10	45
1	J	394/445 (88%)	316 (80%)	68 (17%)	10 (2%)	6	36
1	K	394/445 (88%)	312 (79%)	70 (18%)	12 (3%)	5	32
1	L	394/445 (88%)	318 (81%)	67 (17%)	9 (2%)	7	38
All	All	4728/5340 (88%)	3809 (81%)	811 (17%)	108 (2%)	7	38

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	VAL

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Mol	Chain	Res	Type
1	A	188	ASP
1	B	73	VAL
1	B	188	ASP
1	C	73	VAL

### 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	327/364 (90%)	280 (86%)	47 (14%)	4	18
1	B	327/364 (90%)	275 (84%)	52 (16%)	3	14
1	C	327/364 (90%)	277 (85%)	50 (15%)	3	15
1	D	327/364 (90%)	273 (84%)	54 (16%)	2	13
1	E	327/364 (90%)	272 (83%)	55 (17%)	2	12
1	F	327/364 (90%)	277 (85%)	50 (15%)	3	15
1	G	327/364 (90%)	274 (84%)	53 (16%)	3	13
1	H	327/364 (90%)	276 (84%)	51 (16%)	3	14
1	I	327/364 (90%)	277 (85%)	50 (15%)	3	15
1	J	327/364 (90%)	273 (84%)	54 (16%)	2	13
1	K	327/364 (90%)	276 (84%)	51 (16%)	3	14
1	L	327/364 (90%)	278 (85%)	49 (15%)	3	16
All	All	3924/4368 (90%)	3308 (84%)	616 (16%)	3	14

5 of 616 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	196	LEU
1	G	317	GLN
1	L	72	ILE
1	F	245	GLN
1	G	73	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	211	ASN
1	G	343	GLN
1	L	63	HIS
1	F	317	GLN
1	F	420	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

24 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	$\# Z  > 2$
2	PLP	A	500	1	15,15,16	4.28	4 (26%)	20,22,23	2.39	10 (50%)
3	CCO	A	600	-	11,18,18	1.65	3 (27%)	13,24,24	1.86	3 (23%)
2	PLP	B	500	1	15,15,16	3.67	5 (33%)	20,22,23	2.37	8 (40%)
3	CCO	B	601	-	11,18,18	1.59	2 (18%)	13,24,24	1.83	2 (15%)
2	PLP	C	500	1	15,15,16	3.98	5 (33%)	20,22,23	2.43	9 (45%)
3	CCO	C	602	-	11,18,18	1.66	2 (18%)	13,24,24	1.95	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	D	500	1	15,15,16	3.90	4 (26%)	20,22,23	2.37	9 (45%)
3	CCO	D	603	-	11,18,18	1.65	2 (18%)	13,24,24	1.90	2 (15%)
2	PLP	E	500	1	15,15,16	4.03	4 (26%)	20,22,23	2.39	8 (40%)
3	CCO	E	604	-	11,18,18	1.64	3 (27%)	13,24,24	1.91	3 (23%)
2	PLP	F	500	1	15,15,16	3.90	5 (33%)	20,22,23	2.37	8 (40%)
3	CCO	F	605	-	11,18,18	1.63	3 (27%)	13,24,24	1.86	3 (23%)
2	PLP	G	500	1	15,15,16	3.97	5 (33%)	20,22,23	2.43	9 (45%)
3	CCO	G	606	-	11,18,18	1.64	2 (18%)	13,24,24	1.91	3 (23%)
2	PLP	H	500	1	15,15,16	3.90	4 (26%)	20,22,23	2.39	9 (45%)
3	CCO	H	607	-	11,18,18	1.58	2 (18%)	13,24,24	1.81	3 (23%)
2	PLP	I	500	1	15,15,16	3.84	4 (26%)	20,22,23	2.35	8 (40%)
3	CCO	I	608	-	11,18,18	1.59	2 (18%)	13,24,24	1.96	3 (23%)
2	PLP	J	500	1	15,15,16	3.95	4 (26%)	20,22,23	2.32	8 (40%)
3	CCO	J	609	-	11,18,18	1.66	2 (18%)	13,24,24	1.92	2 (15%)
2	PLP	K	500	1	15,15,16	4.13	4 (26%)	20,22,23	2.40	9 (45%)
3	CCO	K	610	-	11,18,18	1.54	2 (18%)	13,24,24	1.78	3 (23%)
2	PLP	L	500	1	15,15,16	3.79	4 (26%)	20,22,23	2.34	8 (40%)
3	CCO	L	611	-	11,18,18	1.67	3 (27%)	13,24,24	1.95	2 (15%)

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
2	PLP	A	500	1	-	0/6/6/8	0/1/1/1
3	CCO	A	600	-	-	0/5/9/9	0/1/2/2
2	PLP	B	500	1	-	0/6/6/8	0/1/1/1
3	CCO	B	601	-	-	0/5/9/9	0/1/2/2
2	PLP	C	500	1	-	0/6/6/8	0/1/1/1
3	CCO	C	602	-	-	0/5/9/9	0/1/2/2
2	PLP	D	500	1	-	0/6/6/8	0/1/1/1
3	CCO	D	603	-	-	0/5/9/9	0/1/2/2
2	PLP	E	500	1	-	0/6/6/8	0/1/1/1
3	CCO	E	604	-	-	0/5/9/9	0/1/2/2
2	PLP	F	500	1	-	0/6/6/8	0/1/1/1
3	CCO	F	605	-	-	0/5/9/9	0/1/2/2
2	PLP	G	500	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CCO	G	606	-	-	0/5/9/9	0/1/2/2
2	PLP	H	500	1	-	0/6/6/8	0/1/1/1
3	CCO	H	607	-	-	0/5/9/9	0/1/2/2
2	PLP	I	500	1	-	0/6/6/8	0/1/1/1
3	CCO	I	608	-	-	0/5/9/9	0/1/2/2
2	PLP	J	500	1	-	0/6/6/8	0/1/1/1
3	CCO	J	609	-	-	0/5/9/9	0/1/2/2
2	PLP	K	500	1	-	0/6/6/8	0/1/1/1
3	CCO	K	610	-	-	0/5/9/9	0/1/2/2
2	PLP	L	500	1	-	0/6/6/8	0/1/1/1
3	CCO	L	611	-	-	0/5/9/9	0/1/2/2

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	PLP	C4A-C4	-2.93	1.45	1.51
2	I	500	PLP	C4A-C4	-2.81	1.45	1.51
2	J	500	PLP	C4A-C4	-2.69	1.46	1.51
2	H	500	PLP	C4A-C4	-2.68	1.46	1.51
2	L	500	PLP	C4A-C4	-2.60	1.46	1.51

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	PLP	C3-C2-N1	-3.35	116.35	120.75
2	H	500	PLP	C3-C2-N1	-3.31	116.40	120.75
2	B	500	PLP	C3-C2-N1	-3.28	116.44	120.75
2	E	500	PLP	C3-C2-N1	-3.26	116.47	120.75
2	J	500	PLP	C3-C2-N1	-3.24	116.49	120.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLP	2	0
3	A	600	CCO	1	0
3	B	601	CCO	1	0
2	C	500	PLP	2	0
3	C	602	CCO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	CCO	1	0
3	E	604	CCO	1	0
2	F	500	PLP	1	0
3	F	605	CCO	2	0
2	G	500	PLP	1	0
3	G	606	CCO	1	0
3	H	607	CCO	2	0
2	I	500	PLP	1	0
3	I	608	CCO	1	0
2	J	500	PLP	1	0
3	J	609	CCO	2	0
2	K	500	PLP	1	0
3	K	610	CCO	2	0
2	L	500	PLP	1	0
3	L	611	CCO	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.