



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1I41  
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR APPA  
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.  
Deposited on : 2001-02-19  
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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

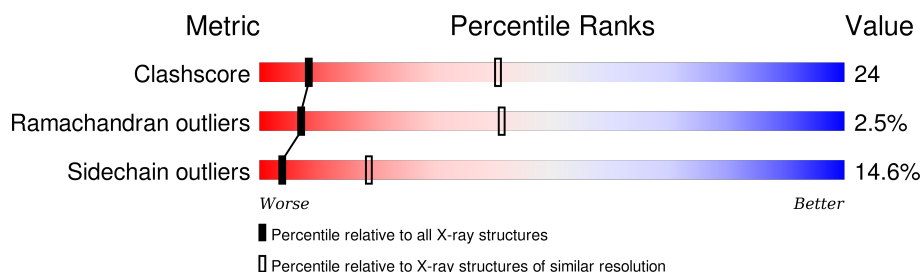
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	<div><div></div><div>42%41%7%11%</div></div>
1	I	445	<div><div></div><div>48%36%5%11%</div></div>
1	J	445	<div><div></div><div>43%40%6%11%</div></div>
1	K	445	<div><div></div><div>42%40%7%11%</div></div>
1	L	445	<div><div></div><div>47%36%6%11%</div></div>

## 2 Entry composition

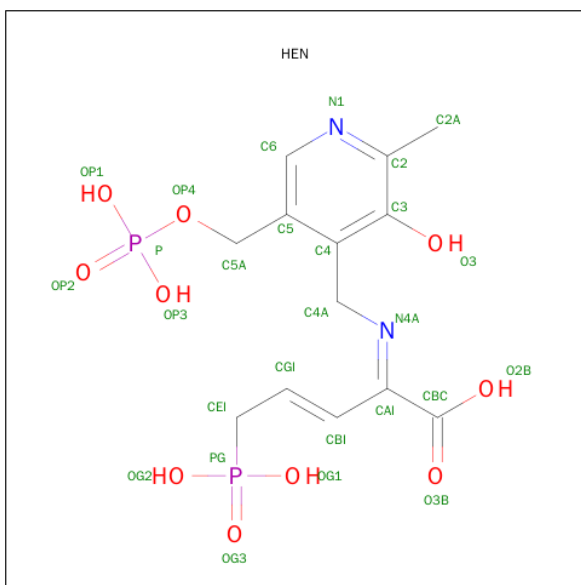
There are 2 unique types of molecules in this entry. The entry contains 36600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL)-IMINO]-5-PHOSPHONO-PENT-3-ENOIC ACID (three-letter code: HEN) (formula: C<sub>13</sub>H<sub>18</sub>N<sub>2</sub>O<sub>10</sub>P<sub>2</sub>).



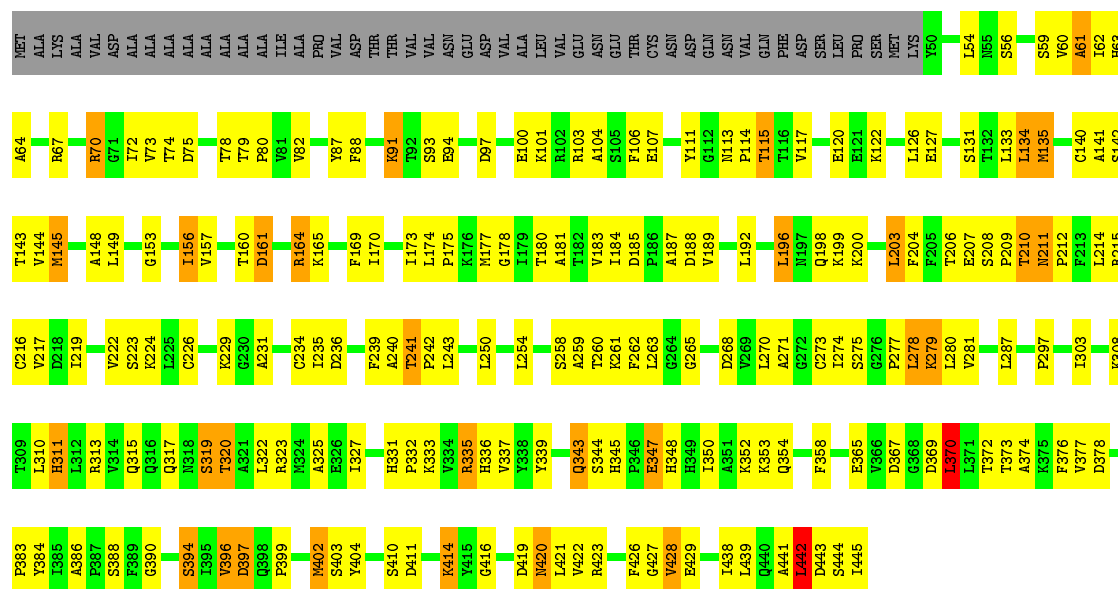
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	B	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	C	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	D	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	E	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	F	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	G	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	H	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	I	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	J	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	K	1	Total 27	C 13	N 2	O 10	P 2	0	0
2	L	1	Total 27	C 13	N 2	O 10	P 2	0	0





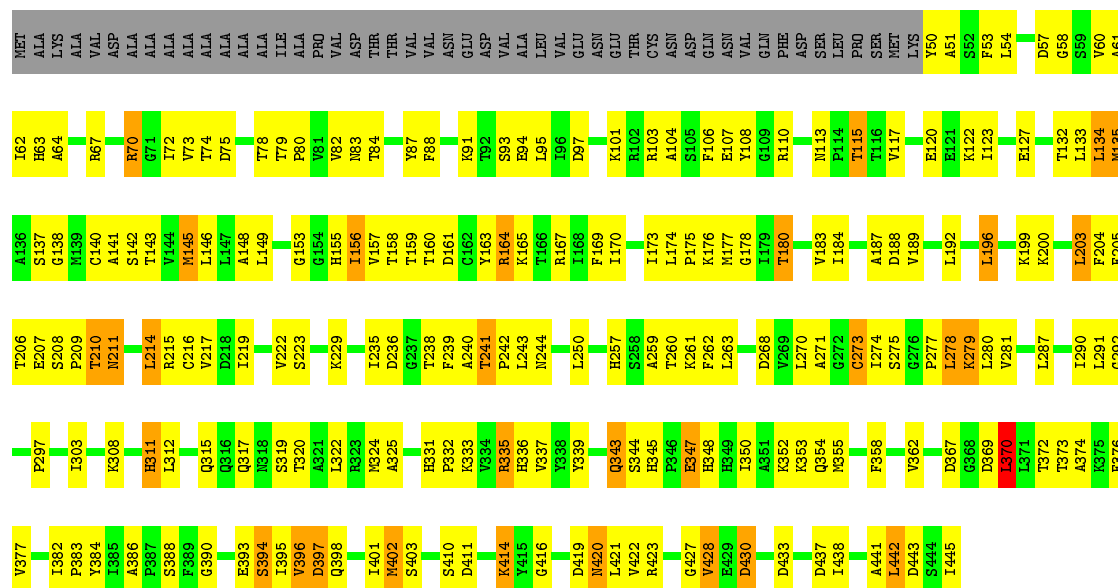
• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain C: 44% 38% 7% 11%

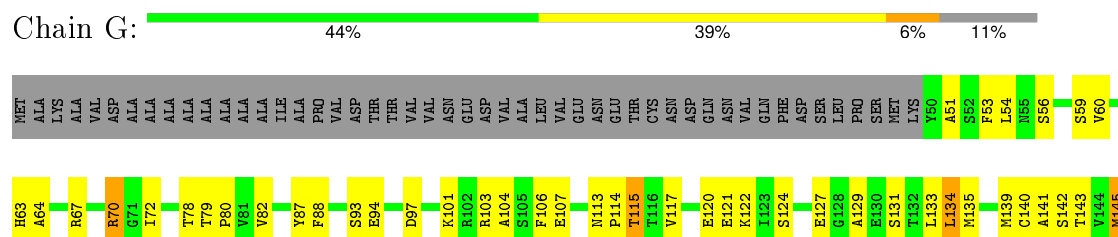


• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

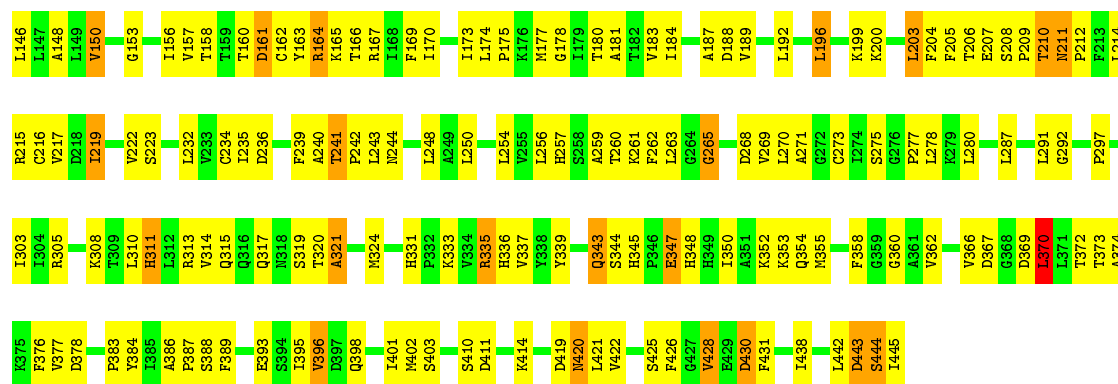
Chain D: 42% 40% 7% 11%



• Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

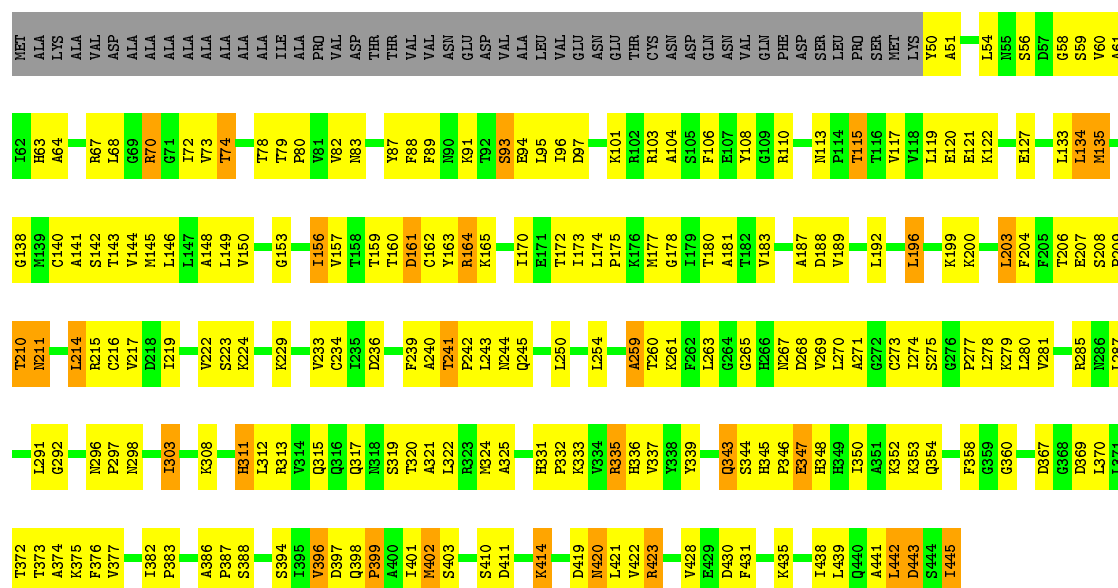






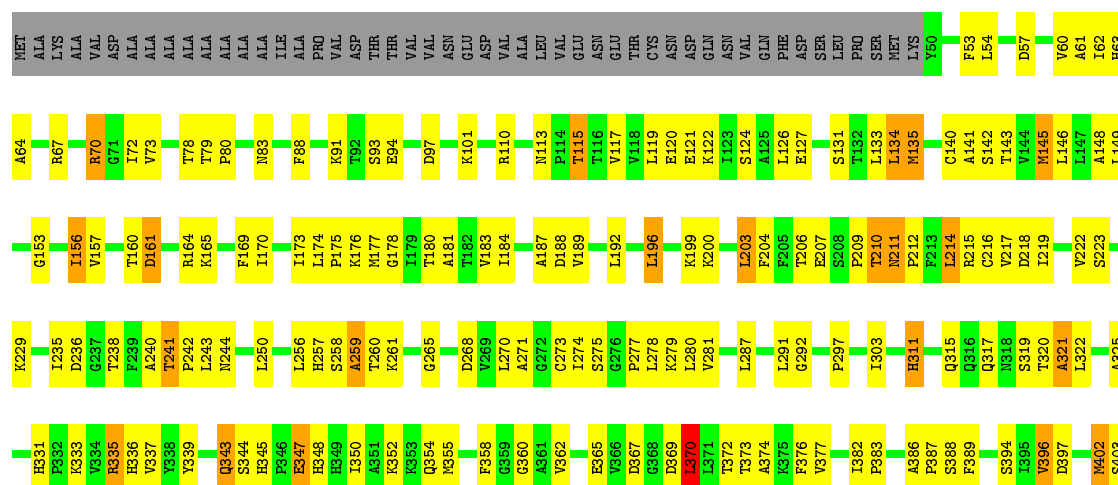
### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain H: 42% 41% 7% 11%



### • Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

Chain I: 48% 36% 5% 11%





A400	Q317	L232	L149	A64	ALA	MET
A401	R318	L233			ALA	
M402	S319	V233	G153	R67	LYS	
S403	T320	C234			VAL	
S410	A321	I235	I156	R70	ASP	
D411	L322	D236	V157	G71	ALA	
	R323	G237	T158	I72	ALA	
K414	K324	T338	T159	T73	ALA	
	A325	F239	F160	T74	ALA	
Y415		A240	D161	D75	ALA	
G416	H331	T241	C162	A76	ALA	
	F332	P242	F163	I77	ALA	
D419	K333	L243	R164	T78	ALA	
N420	V334		K165	T79	ALA	
L421	R335	L248		P80	ILE	
V422	H336	A249	I168		ALA	
R423	V337	L250	F169	K91	PRO	
F424	V338		I170	T92	VAL	
S425	V339	L254		E94	ASP	
F426					THR	
G427	Q343	E257	I173		THR	
V428	S344	S258	L174	D97	VAL	
A429	R345	A259	K176		VAL	
D430	F346	T260	M177	E100	ASN	
F431	E347	K261	G178	K101	GLU	
	H348	F262	I179	R102	ASP	
D437	H349	L263	T180	R103	VAL	
I438	I350		A181	A104	ALA	
		D268		S105	LEU	
L442	Q354	V269	I184	F106	VAL	
D443	R355	L270		E107	GLU	
I445	F358		A187	Y108	ASN	
		C273	D188		GLU	
	E365	T274	V189	M113	THR	
V366	V366	S275		P114	CYS	
	D367	G276	L192	T115	ASN	
		P277		T116	ASP	
			L196	V117	GLN	
		L280	K199	V118	ASN	
		V281	K200	E120	VAL	
T373	T373	L287		E121	GLN	
A374	R375			K122	PHF	
F376	F376	L291	L203	I123	ASP	
V377	V377		F204		SER	
		P297	F205		LEU	
			T206	E127	PRO	
		T303	E207		SER	
		T304	S208	L133	MET	
		R305	P209	L134	LYS	
				M135		
			M211			
		K308				
		T309	L214	C140		
		L310	R215	A141		
		H311	C216	S142		
		L312	T217	T143		
		R313		M145		
		V314	V222	L146		
		G315		I147		
		G316	V270			

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	312.20Å 166.00Å 161.80Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.239 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: HEN

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	0.33	0/3082	0.53	0/4179
1	B	0.31	0/3082	0.52	0/4179
1	C	0.32	0/3082	0.52	0/4179
1	D	0.32	0/3082	0.52	0/4179
1	E	0.33	0/3082	0.53	0/4179
1	F	0.32	0/3082	0.53	0/4179
1	G	0.33	0/3082	0.52	0/4179
1	H	0.33	0/3082	0.53	0/4179
1	I	0.32	0/3082	0.52	0/4179
1	J	0.31	0/3082	0.52	0/4179
1	K	0.31	0/3082	0.52	0/4179
1	L	0.31	0/3082	0.52	0/4179
All	All	0.32	0/36984	0.52	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	3054	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3054	167	0
1	C	3023	0	3054	159	0
1	D	3023	0	3054	159	0
1	E	3023	0	3054	155	0
1	F	3023	0	3054	160	0
1	G	3023	0	3054	156	0
1	H	3023	0	3054	164	0
1	I	3023	0	3054	141	0
1	J	3023	0	3054	155	0
1	K	3023	0	3054	153	0
1	L	3023	0	3054	131	0
2	A	27	0	12	3	0
2	B	27	0	12	1	0
2	C	27	0	12	0	0
2	D	27	0	12	2	0
2	E	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	1	0
2	H	27	0	12	2	0
2	I	27	0	12	2	0
2	J	27	0	12	1	0
2	K	27	0	12	1	0
2	L	27	0	12	1	0
All	All	36600	0	36792	1765	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 24.

The worst 5 of 1765 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:F:64:ALA:HB3	1:F:122:LYS:HG3	1.44	0.98
1:L:54:LEU:HD22	1:L:59:SER:HB3	1.45	0.97
1:A:145:MET:HE1	1:A:146:LEU:HD23	1.47	0.96
1:A:383:PRO:HB2	1:A:396:VAL:HG22	1.49	0.93
1:H:241:THR:HG22	1:H:243:LEU:H	1.31	0.92

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%)	322 (82%)	64 (16%)	8 (2%)	9	48
1	B	394/445 (88%)	320 (81%)	63 (16%)	11 (3%)	6	37
1	C	394/445 (88%)	324 (82%)	56 (14%)	14 (4%)	4	30
1	D	394/445 (88%)	331 (84%)	55 (14%)	8 (2%)	9	48
1	E	394/445 (88%)	327 (83%)	56 (14%)	11 (3%)	6	37
1	F	394/445 (88%)	316 (80%)	69 (18%)	9 (2%)	8	44
1	G	394/445 (88%)	332 (84%)	54 (14%)	8 (2%)	9	48
1	H	394/445 (88%)	327 (83%)	61 (16%)	6 (2%)	13	55
1	I	394/445 (88%)	329 (84%)	52 (13%)	13 (3%)	5	32
1	J	394/445 (88%)	328 (83%)	59 (15%)	7 (2%)	11	51
1	K	394/445 (88%)	325 (82%)	57 (14%)	12 (3%)	5	35
1	L	394/445 (88%)	325 (82%)	60 (15%)	9 (2%)	8	44
All	All	4728/5340 (88%)	3906 (83%)	706 (15%)	116 (2%)	7	41

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASP
1	B	188	ASP
1	C	188	ASP
1	D	164	ARG
1	D	188	ASP

### 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	327/364 (90%)	278 (85%)	49 (15%)	3	17
1	B	327/364 (90%)	283 (86%)	44 (14%)	5	22
1	C	327/364 (90%)	275 (84%)	52 (16%)	3	14
1	D	327/364 (90%)	279 (85%)	48 (15%)	4	18
1	E	327/364 (90%)	276 (84%)	51 (16%)	3	15
1	F	327/364 (90%)	274 (84%)	53 (16%)	3	14
1	G	327/364 (90%)	282 (86%)	45 (14%)	4	21
1	H	327/364 (90%)	279 (85%)	48 (15%)	4	18
1	I	327/364 (90%)	284 (87%)	43 (13%)	5	24
1	J	327/364 (90%)	281 (86%)	46 (14%)	4	20
1	K	327/364 (90%)	279 (85%)	48 (15%)	4	18
1	L	327/364 (90%)	283 (86%)	44 (14%)	5	22
All	All	3924/4368 (90%)	3353 (85%)	571 (15%)	4	19

5 of 571 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	161	ASP
1	G	223	SER
1	L	70	ARG
1	F	200	LYS
1	F	402	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	211	ASN
1	G	343	GLN
1	K	343	GLN
1	G	63	HIS
1	H	63	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

12 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	HEN	A	500	-	25,27,27	3.01	12 (48%)	29,39,39	2.08	10 (34%)
2	HEN	B	501	-	25,27,27	2.92	11 (44%)	29,39,39	1.96	9 (31%)
2	HEN	C	502	-	25,27,27	2.87	13 (52%)	29,39,39	2.01	11 (37%)
2	HEN	D	503	-	25,27,27	3.00	12 (48%)	29,39,39	1.93	11 (37%)
2	HEN	E	504	-	25,27,27	3.52	13 (52%)	29,39,39	2.19	10 (34%)
2	HEN	F	505	-	25,27,27	2.92	12 (48%)	29,39,39	2.00	10 (34%)
2	HEN	G	506	-	25,27,27	2.88	12 (48%)	29,39,39	1.95	8 (27%)
2	HEN	H	507	-	25,27,27	3.02	12 (48%)	29,39,39	2.00	9 (31%)
2	HEN	I	508	-	25,27,27	2.90	13 (52%)	29,39,39	2.02	9 (31%)
2	HEN	J	509	-	25,27,27	3.22	13 (52%)	29,39,39	2.06	9 (31%)
2	HEN	K	510	-	25,27,27	3.07	13 (52%)	29,39,39	1.99	8 (27%)
2	HEN	L	511	-	25,27,27	2.95	13 (52%)	29,39,39	1.96	11 (37%)

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	HEN	A	500	-	-	2/17/22/22	0/1/1/1
2	HEN	B	501	-	-	2/17/22/22	0/1/1/1
2	HEN	C	502	-	-	2/17/22/22	0/1/1/1
2	HEN	D	503	-	-	2/17/22/22	0/1/1/1
2	HEN	E	504	-	-	2/17/22/22	0/1/1/1
2	HEN	F	505	-	-	2/17/22/22	0/1/1/1
2	HEN	G	506	-	-	2/17/22/22	0/1/1/1
2	HEN	H	507	-	-	2/17/22/22	0/1/1/1
2	HEN	I	508	-	-	2/17/22/22	0/1/1/1
2	HEN	J	509	-	-	2/17/22/22	0/1/1/1
2	HEN	K	510	-	-	2/17/22/22	0/1/1/1
2	HEN	L	511	-	-	2/17/22/22	0/1/1/1

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	HEN	C4A-N4A	-5.63	1.38	1.46
2	A	500	HEN	C4A-N4A	-5.25	1.38	1.46
2	F	505	HEN	C4A-N4A	-5.14	1.38	1.46
2	D	503	HEN	CAI-N4A	-4.88	1.21	1.30
2	L	511	HEN	C4A-N4A	-4.84	1.39	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	HEN	C5-C6-N1	-3.31	118.11	123.86
2	B	501	HEN	C5-C6-N1	-3.26	118.21	123.86
2	G	506	HEN	C5-C6-N1	-3.25	118.23	123.86
2	F	505	HEN	C5-C6-N1	-3.24	118.24	123.86
2	K	510	HEN	C5-C6-N1	-3.23	118.25	123.86

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEN	C5-C4-C4A-N4A
2	E	504	HEN	C5-C4-C4A-N4A
2	J	509	HEN	C5-C4-C4A-N4A
2	E	504	HEN	C3-C4-C4A-N4A
2	A	500	HEN	C3-C4-C4A-N4A

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEN	3	0
2	B	501	HEN	1	0
2	D	503	HEN	2	0
2	E	504	HEN	1	0
2	F	505	HEN	1	0
2	G	506	HEN	1	0
2	H	507	HEN	2	0
2	I	508	HEN	2	0
2	J	509	HEN	1	0
2	K	510	HEN	1	0
2	L	511	HEN	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.