



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:59 PM GMT

PDB ID : 1I7M  
Title : HUMAN S-ADENOSYLMETHIONINE DECARBOXYLASE WITH COVALENTLY BOUND PYRUVOYL GROUP AND COMPLEXED WITH 4-AMIDINOINDAN-1-ONE-2'-AMIDINOHYDRAZONE  
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Deposited on : 2001-03-09  
Resolution : 2.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

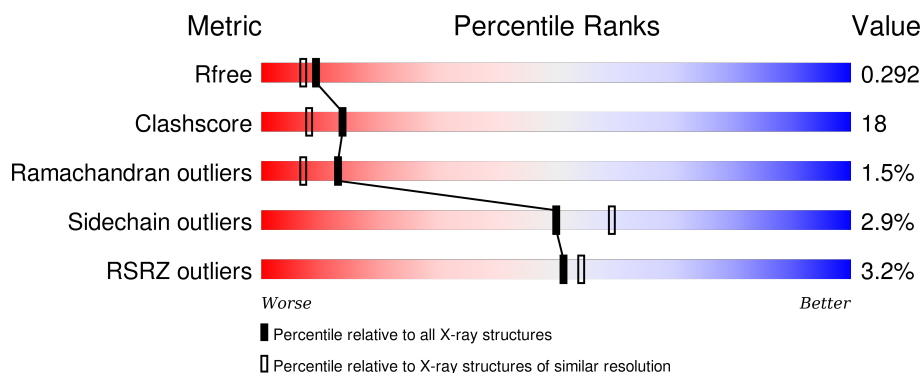
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.24 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))
$R_{free}$	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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.

Mol	Chain	Length	Quality of chain
1	B	67	<div> <div>3%</div> <div>60% 16% 7% 15%</div> </div>
1	D	67	<div> <div>4%</div> <div>61% 15% 6% 18%</div> </div>
2	A	267	<div> <div>2%</div> <div>61% 31% 7%</div> </div>
2	C	267	<div> <div>3%</div> <div>65% 27% 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CG	D	1375	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5225 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 S-ADENOSYLMETHIONINE DECARBOXYLASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	57	Total	C	N	O	S	0	0	0
			464	296	76	91	1			
1	D	55	Total	C	N	O	S	0	0	0
			448	287	71	89	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	MET	MODIFIED RESIDUE	UNP P17707
D	1001	MSE	MET	MODIFIED RESIDUE	UNP P17707

- Molecule 2 is a protein called S-ADENOSYLMETHIONINE DECARBOXYLASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	249	Total	C	N	O	S	Se	0	0	0
			2012	1295	325	375	6	11			
2	C	249	Total	C	N	O	S	Se	0	0	0
			2012	1295	325	375	6	11			

There are 24 discrepancies between the modelled and reference sequences:

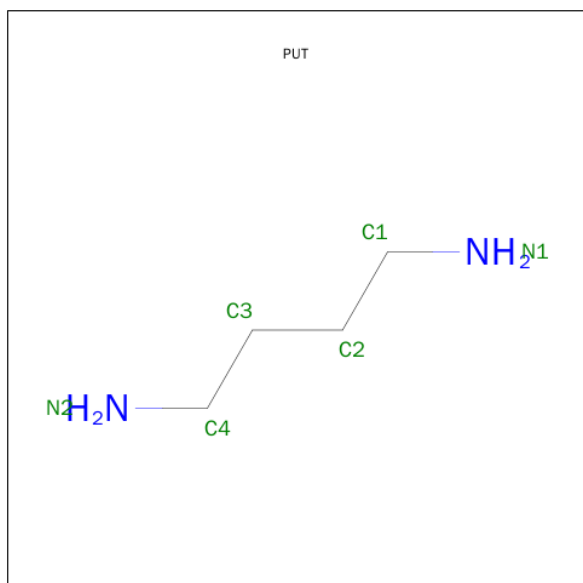
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	PYR	SER	SEE REMARK 999	UNP P17707
A	70	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	118	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	149	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	152	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	181	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	189	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	194	MSE	MET	MODIFIED RESIDUE	UNP P17707

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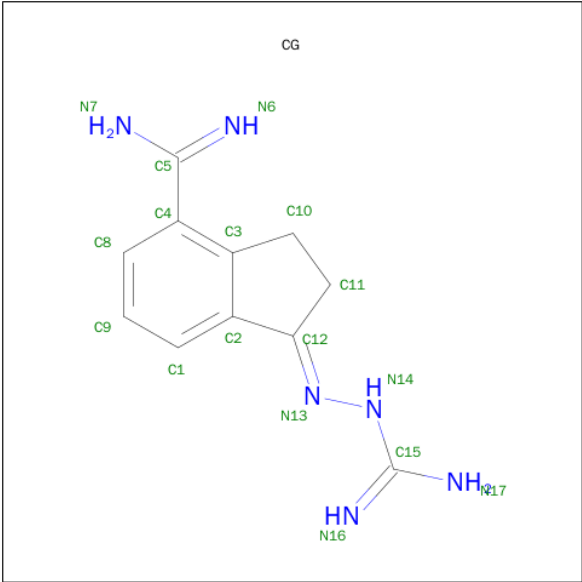
Chain	Residue	Modelled	Actual	Comment	Reference
A	222	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	230	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	233	MSE	MET	MODIFIED RESIDUE	UNP P17707
A	314	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1068	PYR	SER	SEE REMARK 999	UNP P17707
C	1070	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1118	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1149	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1152	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1181	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1189	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1194	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1222	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1230	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1233	MSE	MET	MODIFIED RESIDUE	UNP P17707
C	1314	MSE	MET	MODIFIED RESIDUE	UNP P17707

- Molecule 3 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			6	4	2		
3	D	1	Total	C	N	0	0
			6	4	2		

- Molecule 4 is 4-AMIDINOINDAN-1-ONE-2'-AMIDINOHYDRAZONE (three-letter code: CG) (formula:  $C_{11}H_{14}N_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			17	11	6		
4	D	1	Total	C	N	0	0
			17	11	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total	O	0	0
			109	109		
5	B	23	Total	O	0	0
			23	23		
5	C	92	Total	O	0	0
			92	92		
5	D	19	Total	O	0	0
			19	19		

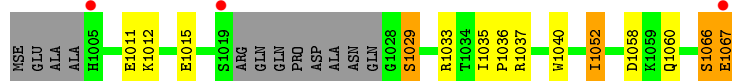
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

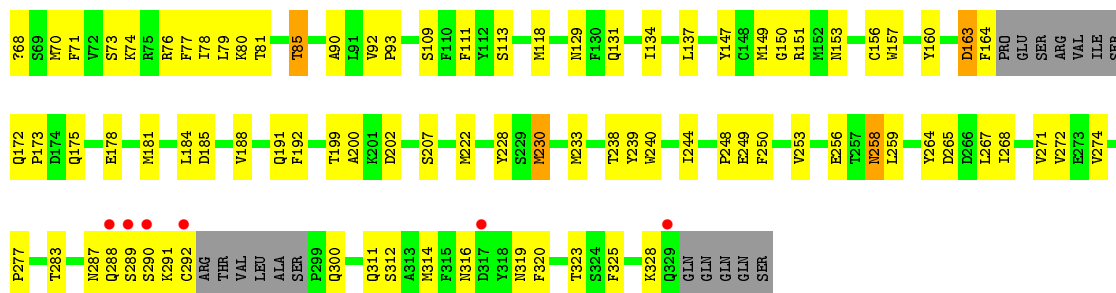
- Molecule 1: S-ADENOSYLMETHIONINE DECARBOXYLASE BETA CHAIN



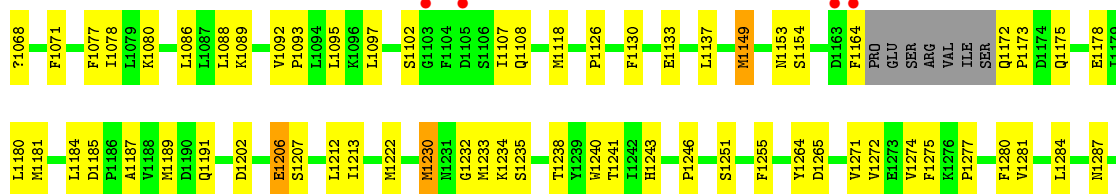
- Molecule 1: S-ADENOSYLMETHIONINE DECARBOXYLASE BETA CHAIN

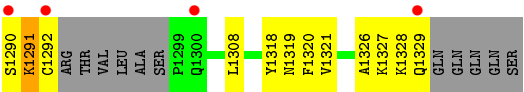


- Molecule 2: S-ADENOSYLMETHIONINE DECARBOXYLASE ALPHA CHAIN



- Molecule 2: S-ADENOSYLMETHIONINE DECARBOXYLASE ALPHA CHAIN







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.90 Å 55.67 Å 96.09 Å 90.00° 110.39° 90.00°	Depositor
Resolution (Å)	29.41 – 2.24 29.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.41-2.24) 87.8 (29.41-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.00 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.242 , 0.294 0.242 , 0.292	Depositor DCC
$R_{free}$ test set	3542 reflections (10.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 25.2	EDS
Estimated twinning fraction	0.196 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 48878 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	5225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PUT, PYR, CG

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	B	1.42	4/472 (0.8%)	1.57	10/634 (1.6%)
1	D	2.16	7/456 (1.5%)	2.34	8/613 (1.3%)
2	A	0.46	0/2046	0.65	0/2738
2	C	0.46	2/2046 (0.1%)	0.71	1/2738 (0.0%)
All	All	0.89	13/5020 (0.3%)	1.05	19/6723 (0.3%)

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	B	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1066	SER	C-O	-29.34	0.67	1.23
1	D	1067	GLU	N-CA	25.79	1.98	1.46
1	B	47	VAL	C-N	-19.99	0.88	1.34
1	D	1066	SER	C-N	15.60	1.70	1.34
1	B	48	GLN	C-N	-14.48	1.00	1.34
1	B	49	CYS	N-CA	13.95	1.74	1.46
1	D	1067	GLU	CA-CB	-11.42	1.28	1.53
1	B	49	CYS	C-N	-8.47	1.14	1.34
1	D	1067	GLU	CD-OE1	7.64	1.34	1.25
1	D	1067	GLU	CA-C	7.17	1.71	1.52
1	D	1067	GLU	CD-OE2	-7.01	1.18	1.25
2	C	1328	LYS	C-N	5.62	1.47	1.34
2	C	1280	PHE	C-N	-5.58	1.21	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1066	SER	O-C-N	-43.26	53.48	122.70
1	D	1067	GLU	CB-CA-C	24.56	159.53	110.40
1	B	48	GLN	CA-C-O	-19.32	79.53	120.10
1	B	47	VAL	C-N-CA	15.71	160.98	121.70
1	B	47	VAL	O-C-N	-15.63	97.69	122.70
1	D	1067	GLU	CA-CB-CG	11.88	139.54	113.40
2	C	1328	LYS	C-N-CA	11.77	151.11	121.70
1	D	1066	SER	CA-C-O	-11.59	95.76	120.10
1	D	1066	SER	CA-C-N	-11.09	92.81	117.20
1	B	47	VAL	CA-C-N	10.67	140.68	117.20
1	D	1066	SER	C-N-CA	-10.38	95.75	121.70
1	B	48	GLN	C-N-CA	9.68	145.91	121.70
1	D	1067	GLU	N-CA-C	-9.35	85.76	111.00
1	B	48	GLN	O-C-N	7.85	135.27	122.70
1	B	49	CYS	O-C-N	-5.83	113.37	122.70
1	B	48	GLN	N-CA-C	5.43	125.66	111.00
1	B	48	GLN	CA-C-N	5.38	129.03	117.20
1	D	1012	LYS	N-CA-C	-5.14	97.12	111.00
1	B	49	CYS	CA-C-N	5.03	128.26	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	47	VAL	Peptide
1	B	48	GLN	Mainchain,Peptide

## 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	B	464	0	452	20	0
1	D	448	0	437	34	0
2	A	2012	0	1958	72	0
2	C	2012	0	1957	65	0
3	B	6	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	12	0	0
4	A	17	0	13	1	0
4	D	17	0	14	14	0
5	A	109	0	0	1	0
5	B	23	0	0	3	0
5	C	92	0	0	0	0
5	D	19	0	0	3	0
All	All	5225	0	4855	182	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 18.

All (182) 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:B:49:CYS:N	1:B:49:CYS:CA	1.74	1.46
1:D:1066:SER:C	1:D:1067:GLU:N	1.69	1.46
4:D:1375:CG:N14	4:D:1375:CG:N13	1.65	1.43
1:D:1066:SER:O	1:D:1066:SER:CA	1.73	1.35
4:D:1375:CG:C12	4:D:1375:CG:C2	1.79	1.33
1:D:1067:GLU:N	1:D:1067:GLU:CA	1.97	1.26
2:C:1327:LYS:CG	2:C:1329:GLN:HG3	1.80	1.11
2:C:1327:LYS:HG3	2:C:1329:GLN:HG3	1.22	1.09
1:D:1067:GLU:HG2	4:D:1375:CG:H112	1.36	1.02
2:C:1327:LYS:HG2	2:C:1329:GLN:HE21	1.21	1.01
2:C:1327:LYS:HG2	2:C:1329:GLN:NE2	1.74	1.00
1:D:1066:SER:HB2	1:D:1067:GLU:N	1.81	0.95
1:D:1066:SER:CB	1:D:1067:GLU:N	2.31	0.94
1:D:1066:SER:C	1:D:1067:GLU:C	2.27	0.92
2:C:1327:LYS:CG	2:C:1329:GLN:CG	2.47	0.92
1:D:1066:SER:HB2	1:D:1067:GLU:H	1.32	0.92
2:C:1291:LYS:HD3	2:C:1291:LYS:H	1.36	0.91
2:C:1327:LYS:HG2	2:C:1329:GLN:CG	2.03	0.88
1:D:1066:SER:C	1:D:1066:SER:O	0.67	0.87
2:A:164:PHE:H	2:A:316:ASN:HD21	1.23	0.86
1:D:1066:SER:O	1:D:1067:GLU:CA	2.25	0.85
1:D:1067:GLU:CG	4:D:1375:CG:H112	2.06	0.84
1:D:1066:SER:O	1:D:1067:GLU:C	2.17	0.83
4:D:1375:CG:N13	4:D:1375:CG:C2	2.41	0.83
1:B:45:LYS:O	1:B:48:GLN:NE2	2.11	0.83
4:D:1375:CG:C12	4:D:1375:CG:N14	2.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1327:LYS:CG	2:C:1329:GLN:HE21	1.92	0.81
1:D:1067:GLU:OXT	4:D:1375:CG:H101	1.80	0.80
1:D:1029:SER:HB3	2:C:1102:SER:HA	1.63	0.77
1:D:1060:GLN:HG3	2:C:1233:MSE:SE	2.36	0.75
4:D:1375:CG:C15	4:D:1375:CG:N13	2.49	0.75
2:A:238:THR:HA	2:A:258:ASN:HD21	1.52	0.75
1:D:1066:SER:CA	1:D:1067:GLU:N	2.34	0.74
2:C:1088:LEU:HD22	2:C:1137:LEU:HD21	1.69	0.72
2:C:1181:MSE:HE2	2:C:1277:PRO:HG3	1.70	0.72
4:D:1375:CG:N6	4:D:1375:CG:C10	2.53	0.71
2:C:1181:MSE:HE2	2:C:1277:PRO:CG	2.21	0.71
2:A:131:GLN:HE22	2:C:1153:ASN:HD21	1.37	0.71
2:A:222:MSE:HE3	2:A:228:TYR:HB2	1.73	0.70
2:C:1189:MSE:HE2	2:C:1251:SER:HB2	1.74	0.69
5:B:1559:HOH:O	2:A:118:MSE:HE2	1.92	0.69
2:A:68:PYR:H33	2:A:80:LYS:O	1.93	0.69
2:C:1327:LYS:HG3	2:C:1329:GLN:CG	2.09	0.69
2:C:1327:LYS:HG2	2:C:1329:GLN:CD	2.13	0.68
2:A:150:GLY:H	2:A:311:GLN:NE2	1.93	0.67
2:A:164:PHE:H	2:A:316:ASN:ND2	1.92	0.67
1:D:1066:SER:C	1:D:1067:GLU:O	2.33	0.66
2:A:323:THR:HG1	2:A:325:PHE:HE2	1.44	0.66
2:A:164:PHE:N	2:A:316:ASN:HD21	1.92	0.65
2:C:1149:MSE:HG2	2:C:1320:PHE:HE2	1.62	0.65
2:A:268:ILE:O	2:A:272:VAL:HG23	1.96	0.65
1:B:60:GLN:HE22	2:A:76:ARG:HH22	1.43	0.64
2:A:184:LEU:HD13	2:A:253:VAL:HG23	1.79	0.64
2:C:1180:LEU:HB2	2:C:1281:VAL:CG2	2.28	0.63
1:D:1067:GLU:N	1:D:1067:GLU:C	2.52	0.63
2:C:1212:LEU:HD13	2:C:1271:VAL:HG22	1.80	0.63
1:D:1067:GLU:O	5:D:1591:HOH:O	2.15	0.63
2:C:1191:GLN:HE22	2:C:1207:SER:HA	1.64	0.63
1:D:1066:SER:O	1:D:1066:SER:HA	1.94	0.62
2:C:1181:MSE:HE1	2:C:1272:VAL:HA	1.82	0.62
2:A:150:GLY:H	2:A:311:GLN:HE22	1.47	0.61
1:B:60:GLN:NE2	2:A:76:ARG:HH22	1.99	0.60
1:B:60:GLN:NE2	2:A:76:ARG:NH2	2.49	0.60
2:C:1172:GLN:N	2:C:1173:PRO:HD3	2.17	0.60
2:A:244:ILE:HG12	2:A:253:VAL:HG22	1.83	0.60
1:B:57:THR:HG22	1:B:58:ASP:H	1.65	0.60
2:A:192:PHE:HA	2:A:222:MSE:HE1	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:199:THR:HG23	2:A:202:ASP:H	1.66	0.59
2:A:85:THR:HG23	5:A:1451:HOH:O	2.03	0.59
1:D:1052:ILE:HG13	1:D:1066:SER:HB3	1.86	0.57
2:A:131:GLN:HA	2:A:134:ILE:HD12	1.85	0.57
1:B:60:GLN:HE22	2:A:76:ARG:NH2	2.03	0.57
2:A:191:GLN:HE22	2:A:207:SER:HA	1.67	0.57
1:B:57:THR:HG22	1:B:58:ASP:N	2.19	0.57
1:D:1066:SER:C	1:D:1067:GLU:CA	2.73	0.56
1:B:28:GLY:O	1:B:29:SER:HB3	2.04	0.56
2:C:1189:MSE:HE3	2:C:1246:PRO:HA	1.87	0.56
2:A:81:THR:HB	2:A:85:THR:HG21	1.88	0.55
1:B:49:CYS:N	1:B:49:CYS:CB	2.64	0.55
2:C:1230:MSE:O	2:C:1241:THR:HG23	2.04	0.55
2:C:1086:LEU:HD13	2:C:1089:LYS:NZ	2.21	0.55
2:A:178:GLU:HB2	2:A:283:THR:OG1	2.07	0.55
1:B:31:ASP:OD1	2:A:74:LYS:HA	2.07	0.54
2:C:1181:MSE:CE	2:C:1277:PRO:HG3	2.35	0.54
2:A:181:MSE:HB3	2:A:277:PRO:HB3	1.88	0.54
2:C:1180:LEU:HB2	2:C:1281:VAL:HG23	1.89	0.54
2:C:1093:PRO:O	2:C:1097:LEU:HG	2.07	0.54
2:C:1071:PHE:HB2	2:C:1078:ILE:HB	1.88	0.54
2:A:150:GLY:N	2:A:311:GLN:NE2	2.57	0.53
2:A:68:PYR:H33	2:A:80:LYS:C	2.29	0.53
2:A:131:GLN:NE2	2:C:1153:ASN:HD21	2.06	0.53
1:B:60:GLN:HG3	2:A:233:MSE:SE	2.59	0.53
4:D:1375:CG:H102	4:D:1375:CG:N6	2.23	0.53
2:C:1184:LEU:CD2	2:C:1275:PHE:HB3	2.39	0.52
2:C:1185:ASP:OD2	2:C:1187:ALA:HB3	2.10	0.52
2:C:1284:LEU:HB3	2:C:1321:VAL:HG13	1.90	0.52
1:B:13:LEU:HD13	2:A:80:LYS:HD3	1.93	0.51
2:C:1202:ASP:O	2:C:1206:GLU:HB2	2.10	0.51
2:A:147:TYR:HB3	2:A:149:MSE:HE2	1.93	0.51
2:C:1068:PYR:H33	2:C:1080:LYS:O	2.11	0.51
1:B:32:LEU:HD11	5:B:1507:HOH:O	2.10	0.51
2:A:77:PHE:CE2	2:A:79:LEU:HB2	2.46	0.50
1:B:63:TYR:HB2	2:A:70:MSE:HB3	1.94	0.50
2:C:1327:LYS:CB	2:C:1329:GLN:HE21	2.24	0.50
2:A:290:SER:C	2:A:292:CYS:H	2.15	0.50
1:D:1011:GLU:CD	2:C:1080:LYS:HE2	2.32	0.49
1:D:1037:ARG:HH11	1:D:1037:ARG:HG3	1.76	0.49
2:C:1092:VAL:HB	2:C:1093:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1068:PYR:H33	2:C:1080:LYS:C	2.33	0.49
2:A:258:ASN:HD22	2:A:258:ASN:H	1.61	0.49
1:D:1067:GLU:HA	4:D:1375:CG:C11	2.43	0.48
2:C:1089:LYS:HE3	2:C:1126:PRO:HD3	1.94	0.48
5:D:1411:HOH:O	2:C:1118:MSE:HE1	2.12	0.48
2:A:240:TRP:HA	2:A:256:GLU:O	2.14	0.48
1:D:1040:TRP:HA	1:D:1040:TRP:CE3	2.48	0.48
2:C:1178:GLU:HA	2:C:1255:PHE:O	2.13	0.48
2:C:1184:LEU:HD23	2:C:1275:PHE:HB3	1.95	0.48
2:A:175:GLN:HG3	2:A:292:CYS:SG	2.54	0.48
2:A:153:ASN:N	2:A:153:ASN:HD22	2.12	0.48
2:A:109:SER:HB3	2:A:111:PHE:CE2	2.49	0.47
2:A:314:MSE:SE	2:A:319:ASN:OD1	2.82	0.47
2:C:1287:ASN:HA	2:C:1318:TYR:HA	1.95	0.47
2:A:73:SER:OG	2:A:76:ARG:HB3	2.14	0.47
2:A:118:MSE:HE1	2:A:250:PHE:HB2	1.95	0.47
1:B:44:LEU:O	1:B:49:CYS:HB3	2.14	0.47
2:A:113:SER:HB2	2:A:157:TRP:CZ2	2.50	0.47
2:A:137:LEU:HD13	2:A:160:TYR:CG	2.50	0.47
2:A:185:ASP:O	2:A:188:VAL:HG22	2.14	0.47
2:C:1189:MSE:CE	2:C:1251:SER:HB2	2.42	0.47
2:A:71:PHE:HB2	2:A:78:ILE:HB	1.96	0.47
2:C:1234:LYS:HB2	2:C:1238:THR:HB	1.96	0.46
1:D:1067:GLU:HB2	5:D:1435:HOH:O	2.15	0.46
2:A:163:ASP:HA	2:A:316:ASN:HD21	1.80	0.46
2:A:239:TYR:H	2:A:258:ASN:ND2	2.13	0.46
2:A:287:ASN:OD1	2:A:290:SER:HB2	2.15	0.46
2:A:259:LEU:HD23	2:A:267:LEU:HD22	1.98	0.45
1:B:56:LYS:HD3	5:B:1560:HOH:O	2.17	0.45
2:C:1175:GLN:HG3	2:C:1264:TYR:OH	2.17	0.45
2:A:230:MSE:HE1	2:A:240:TRP:CD2	2.52	0.45
1:D:1066:SER:CB	1:D:1067:GLU:H	2.07	0.44
2:C:1095:LEU:HD21	2:C:1107:ILE:HD11	1.99	0.44
1:B:11:GLU:HG2	2:A:80:LYS:HG2	1.97	0.44
2:C:1241:THR:HG21	2:C:1243:HIS:HE2	1.82	0.44
2:A:172:GLN:HA	2:A:173:PRO:HD3	1.88	0.44
2:A:271:VAL:O	2:A:274:VAL:HG22	2.17	0.43
1:D:1033:ARG:NH1	1:D:1058:ASP:O	2.51	0.43
2:A:92:VAL:HB	2:A:93:PRO:HD3	2.00	0.43
2:C:1230:MSE:SE	2:C:1230:MSE:C	3.07	0.43
2:C:1130:PHE:HA	2:C:1133:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:151:ARG:O	2:A:156:CYS:HB3	2.19	0.43
2:C:1108:GLN:HA	2:C:1164:PHE:CE1	2.53	0.43
1:D:1067:GLU:CG	4:D:1375:CG:C11	2.89	0.43
2:A:153:ASN:N	2:A:153:ASN:ND2	2.67	0.43
2:C:1212:LEU:HD21	2:C:1274:VAL:HG21	2.01	0.42
1:B:32:LEU:HB2	2:A:73:SER:O	2.19	0.42
2:C:1234:LYS:NZ	2:C:1234:LYS:HB3	2.35	0.42
2:A:175:GLN:HG3	2:A:264:TYR:OH	2.19	0.42
2:A:81:THR:HB	2:A:85:THR:CG2	2.49	0.42
2:A:248:PRO:HG2	2:A:249:GLU:OE2	2.19	0.41
4:D:1375:CG:N13	4:D:1375:CG:C1	2.84	0.41
2:A:239:TYR:H	2:A:258:ASN:HD21	1.67	0.41
2:A:244:ILE:O	4:A:375:CG:H11	2.20	0.41
2:A:312:SER:HA	2:A:320:PHE:O	2.20	0.41
2:A:258:ASN:HD22	2:A:258:ASN:N	2.17	0.41
2:C:1232:GLY:N	2:C:1240:TRP:O	2.51	0.41
1:D:1015:GLU:HA	2:C:1077:PHE:O	2.21	0.41
2:A:163:ASP:HA	2:A:316:ASN:ND2	2.35	0.41
1:B:12:LYS:O	2:A:113:SER:O	2.39	0.41
2:A:90:ALA:C	2:A:93:PRO:HD2	2.39	0.41
1:D:1067:GLU:N	1:D:1067:GLU:CB	2.70	0.41
1:D:1035:ILE:HA	1:D:1036:PRO:HD3	1.81	0.41
2:C:1290:SER:OG	2:C:1292:CYS:SG	2.78	0.41
2:C:1181:MSE:HB3	2:C:1277:PRO:HB3	2.01	0.41
2:C:1180:LEU:HB2	2:C:1281:VAL:HG22	2.01	0.41
2:A:137:LEU:HB3	2:A:160:TYR:CZ	2.55	0.41
2:C:1181:MSE:HE2	2:C:1277:PRO:CB	2.51	0.41
2:C:1308:LEU:HD11	2:C:1326:ALA:HB2	2.02	0.41
2:C:1191:GLN:O	2:C:1222:MSE:HE1	2.21	0.41
2:C:1213:ILE:HB	2:C:1240:TRP:CE2	2.56	0.41
1:D:1067:GLU:HA	4:D:1375:CG:H112	2.03	0.40
2:C:1327:LYS:HB3	2:C:1329:GLN:HE21	1.87	0.40
2:A:199:THR:OG1	2:A:200:ALA:N	2.54	0.40

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	B	53/67 (79%)	47 (89%)	3 (6%)	3 (6%)	2	0
1	D	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	9	4
2	A	242/267 (91%)	225 (93%)	13 (5%)	4 (2%)	11	5
2	C	242/267 (91%)	222 (92%)	19 (8%)	1 (0%)	39	42
All	All	588/668 (88%)	542 (92%)	37 (6%)	9 (2%)	13	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
1	B	48	GLN
2	A	288	GLN
2	A	300	GLN
1	D	1029	SER
2	C	1154	SER
1	B	29	SER
2	A	291	LYS
2	A	289	SER

### 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	B	52/59 (88%)	51 (98%)	1 (2%)	65	75
1	D	51/59 (86%)	50 (98%)	1 (2%)	63	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	225/231 (97%)	218 (97%)	7 (3%)	47	57
2	C	225/231 (97%)	218 (97%)	7 (3%)	47	57
All	All	553/580 (95%)	537 (97%)	16 (3%)	50	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	ASP
2	A	85	THR
2	A	129	ASN
2	A	163	ASP
2	A	230	MSE
2	A	258	ASN
2	A	265	ASP
2	A	328	LYS
1	D	1052	ILE
2	C	1149	MSE
2	C	1206	GLU
2	C	1230	MSE
2	C	1235	SER
2	C	1265	ASP
2	C	1291	LYS
2	C	1319	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	60	GLN
2	A	108	GLN
2	A	191	GLN
2	A	231	ASN
2	A	258	ASN
2	A	311	GLN
2	A	316	ASN
2	C	1153	ASN
2	C	1191	GLN
2	C	1319	ASN
2	C	1329	GLN

### 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 ⓘ

4 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	$\# Z  > 2$
4	CG	A	375	-	14,18,18	5.41	4 (28%)	13,25,25	2.70	5 (38%)
3	PUT	B	350	-	5,5,5	0.72	0	4,4,4	0.37	0
3	PUT	D	1350	-	5,5,5	0.63	0	4,4,4	0.44	0
4	CG	D	1375	-	14,18,18	5.04	10 (71%)	13,25,25	4.98	9 (69%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CG	A	375	-	-	0/7/18/18	0/2/2/2
3	PUT	B	350	-	-	0/3/3/3	0/0/0/0
3	PUT	D	1350	-	-	0/3/3/3	0/0/0/0
4	CG	D	1375	-	-	2/7/18/18	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	375	CG	C11-C12	-15.92	1.37	1.51
4	D	1375	CG	C11-C12	-3.77	1.47	1.51
4	D	1375	CG	C10-C3	-3.37	1.45	1.51
4	D	1375	CG	C2-C3	-2.26	1.32	1.39
4	D	1375	CG	C10-C11	-2.07	1.51	1.54
4	D	1375	CG	C9-C8	2.07	1.43	1.38
4	D	1375	CG	C5-N6	2.31	1.36	1.28
4	D	1375	CG	C1-C2	2.99	1.44	1.39
4	D	1375	CG	C4-C3	3.21	1.43	1.40
4	A	375	CG	C5-N6	3.82	1.42	1.28
4	A	375	CG	C5-N7	4.40	1.44	1.33
4	D	1375	CG	C12-N13	8.29	1.39	1.29
4	A	375	CG	C12-N13	10.59	1.42	1.29
4	D	1375	CG	C2-C12	14.85	1.79	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1375	CG	C12-N13-N14	-7.07	104.06	116.95
4	D	1375	CG	C11-C10-C3	-6.07	101.72	104.54
4	A	375	CG	C11-C10-C3	-5.43	102.01	104.54
4	D	1375	CG	C10-C3-C4	-3.96	123.50	130.08
4	A	375	CG	C12-N13-N14	-3.83	109.97	116.95
4	A	375	CG	C10-C3-C2	-2.98	109.32	111.36
4	D	1375	CG	C8-C4-C3	-2.82	116.18	119.86
4	A	375	CG	C8-C4-C3	-2.79	116.22	119.86
4	D	1375	CG	C9-C1-C2	-2.08	115.86	119.87
4	D	1375	CG	C4-C5-N7	2.27	121.69	118.05
4	D	1375	CG	C8-C4-C5	3.72	129.19	118.78
4	D	1375	CG	C10-C3-C2	4.54	114.47	111.36
4	A	375	CG	C10-C11-C12	5.11	111.10	104.33
4	D	1375	CG	C10-C11-C12	12.78	121.28	104.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1375	CG	C2-C12-N13-N14
4	D	1375	CG	C11-C12-N13-N14

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	375	CG	1	0
4	D	1375	CG	14	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	57/67 (85%)	-0.08	2 (3%) 48 50	5, 19, 29, 37	0
1	D	55/67 (82%)	0.32	3 (5%) 29 30	7, 25, 36, 41	0
2	A	237/267 (88%)	-0.21	6 (2%) 61 64	0, 12, 32, 49	0
2	C	237/267 (88%)	0.03	8 (3%) 49 51	3, 16, 36, 56	0
All	All	586/668 (87%)	-0.05	19 (3%) 51 54	0, 16, 35, 56	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1164	PHE	10.4
2	C	1329	GLN	7.9
1	D	1067	GLU	3.8
2	A	290	SER	3.3
2	C	1105	ASP	3.2
2	A	288	GLN	2.8
2	C	1163	ASP	2.6
2	C	1292	CYS	2.6
2	A	289	SER	2.5
2	C	1103	GLY	2.5
1	B	28	GLY	2.4
2	A	329	GLN	2.3
2	C	1290	SER	2.3
2	C	1300	GLN	2.2
2	A	292	CYS	2.2
1	D	1005	HIS	2.2
1	B	67	GLU	2.1
1	D	1019	SER	2.1
2	A	317	ASP	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CG	A	375	17/17	0.87	0.17	0.78	15,17,22,23	0
3	PUT	B	350	6/6	0.96	0.12	0.33	0,1,1,3	0
4	CG	D	1375	17/17	0.80	0.16	0.25	16,22,25,25	0
3	PUT	D	1350	6/6	0.90	0.10	-1.23	0,0,2,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.