



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:34 PM GMT

PDB ID : 1XPM  
Title : Crystal Structure of Staphylococcus aureus HMG-CoA Synthase with HMG-CoA and Acetoacetyl-CoA and Acetylated Cysteine  
Authors : Theisen, M.J.; Misra, I.; Saadat, D.; Campobasso, N.; Miziorko, H.M.; Harrison, D.H.T.  
Deposited on : 2004-10-08  
Resolution : 1.60 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

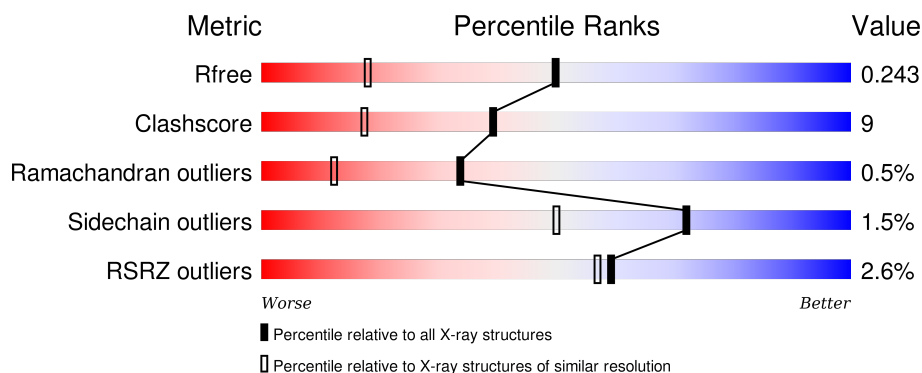
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	A	397	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	397	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	397	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	D	397	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15324 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 3-hydroxy-3-methylglutaryl CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	33	0
			3458	2202	576	664	16			
1	B	389	Total	C	N	O	S	0	33	0
			3431	2188	569	658	16			
1	C	389	Total	C	N	O	S	0	33	0
			3425	2184	571	654	16			
1	D	389	Total	C	N	O	S	0	33	0
			3439	2191	571	661	16			

There are 44 discrepancies between the modelled and reference sequences:

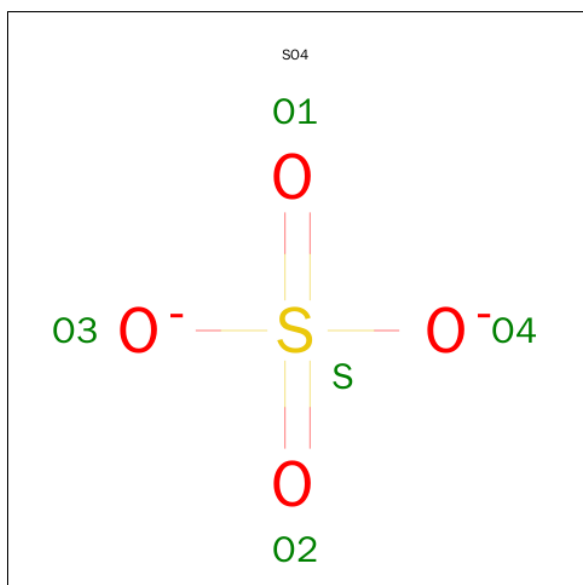
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
A	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
A	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
A	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
A	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
A	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
A	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
B	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
B	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
B	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
B	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
B	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
B	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6

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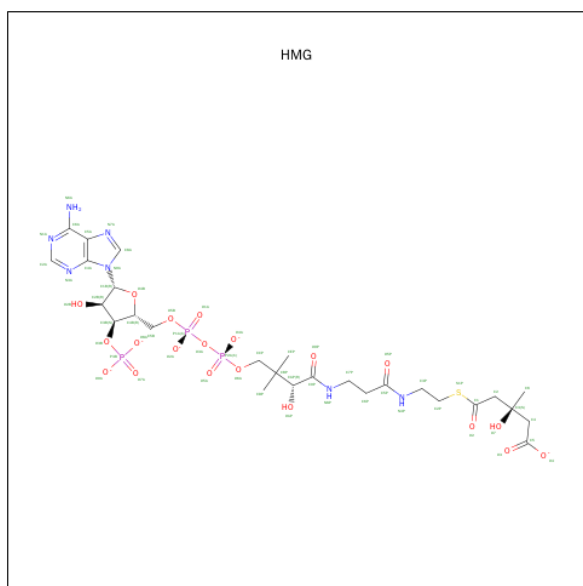
Chain	Residue	Modelled	Actual	Comment	Reference
B	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
C	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
C	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
C	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
C	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
C	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
C	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	1	MET	-	INITIATING METHIONINE	UNP Q79ZY6
D	2	ALA	-	CLONING ARTIFACT	UNP Q79ZY6
D	111	SCY	CYS	MICROHETEROGENEITY	UNP Q79ZY6
D	389	LEU	-	CLONING ARTIFACT	UNP Q79ZY6
D	390	GLU	-	CLONING ARTIFACT	UNP Q79ZY6
D	391	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	392	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	393	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	394	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	395	HIS	-	EXPRESSION TAG	UNP Q79ZY6
D	396	HIS	-	EXPRESSION TAG	UNP Q79ZY6

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is 3-HYDROXY-3-METHYLGLUTARYL-COENZYME A (three-letter code: HMG) (formula:  $C_{27}H_{39}N_7O_{20}P_3S$ ).



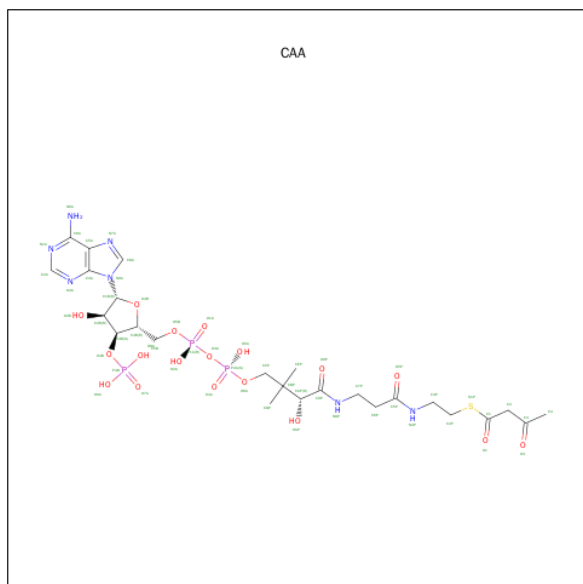
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 58 27 7 20 3 1	0	1
3	B	1	Total C N O P S 58 27 7 20 3 1	0	1
3	C	1	Total C N O P S 58 27 7 20 3 1	0	1

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	1
			58	27	7	20	3	1		

- Molecule 4 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula:  $C_{25}H_{40}N_7O_{18}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		
4	B	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		
4	C	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		
4	D	1	Total	C	N	O	P	S	0	1
			54	25	7	18	3	1		

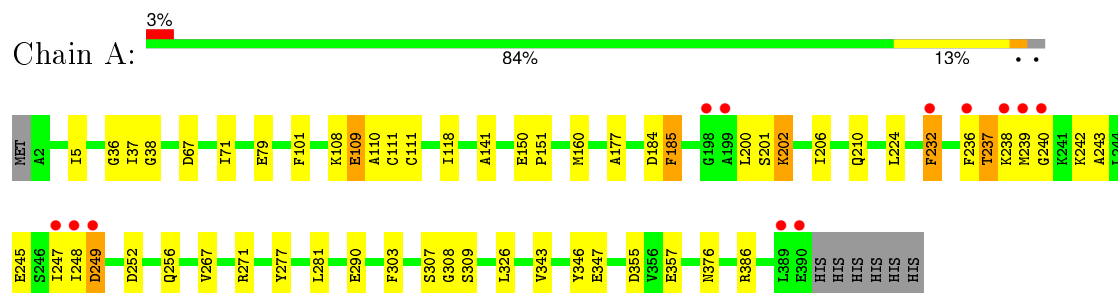
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	1
			265	265		
5	B	277	Total	O	0	1
			277	277		
5	C	278	Total	O	0	1
			278	278		
5	D	263	Total	O	0	1
			263	263		

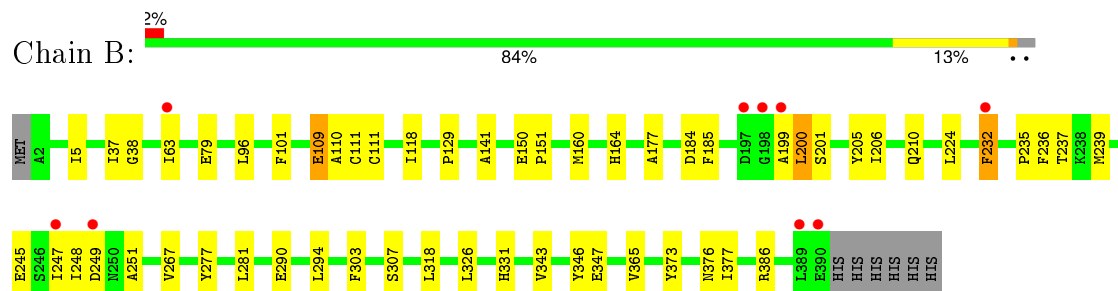
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

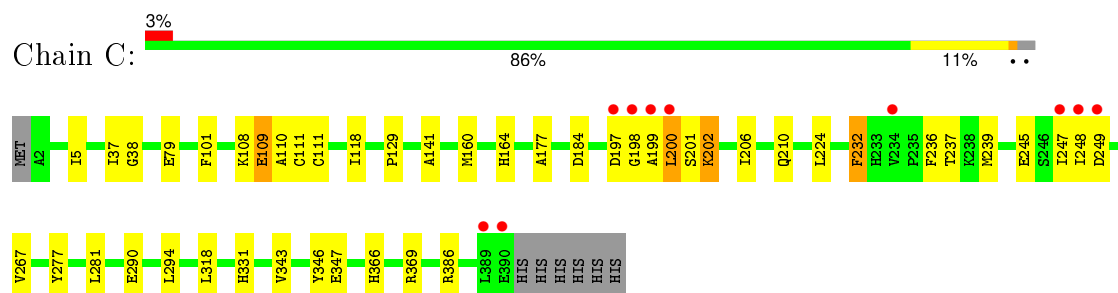
- Molecule 1: 3-hydroxy-3-methylglutaryl CoA synthase



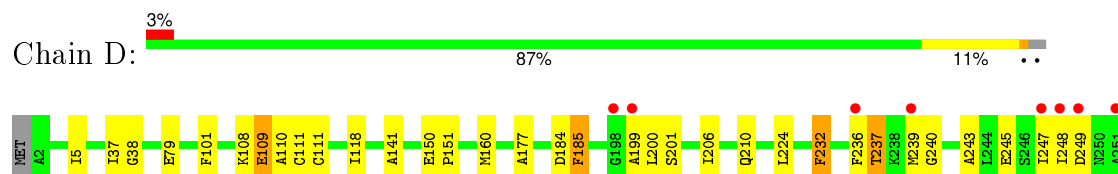
- Molecule 1: 3-hydroxy-3-methylglutaryl CoA synthase

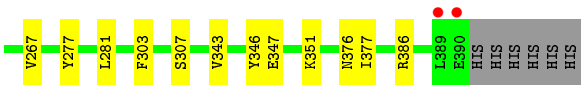


- Molecule 1: 3-hydroxy-3-methylglutaryl CoA synthase



- Molecule 1: 3-hydroxy-3-methylglutaryl CoA synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.12Å 118.77Å 121.30Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 24.96 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-1.60) 89.1 (24.96-1.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.226 0.229 , 0.243	Depositor DCC
$R_{free}$ test set	10669 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.4	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.459 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 216697 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1581e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CAA, HMG, SCY, SO4

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	4.51	9/3586 (0.3%)	1.33	15/4857 (0.3%)
1	B	1.09	3/3547 (0.1%)	0.66	3/4808 (0.1%)
1	C	1.72	6/3543 (0.2%)	0.84	6/4801 (0.1%)
1	D	1.13	3/3564 (0.1%)	0.66	3/4831 (0.1%)
All	All	2.54	21/14240 (0.1%)	0.91	27/19297 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202[A]	LYS	CD-CE	147.32	5.19	1.51
1	A	202[B]	LYS	CD-CE	147.32	5.19	1.51
1	A	202[C]	LYS	CD-CE	147.32	5.19	1.51
1	C	202[A]	LYS	CG-CD	44.16	3.02	1.52
1	C	202[B]	LYS	CG-CD	44.16	3.02	1.52
1	C	202[C]	LYS	CG-CD	44.16	3.02	1.52
1	A	249[A]	ASP	CG-OD2	43.32	2.25	1.25
1	A	249[B]	ASP	CG-OD2	43.32	2.25	1.25
1	A	249[C]	ASP	CG-OD2	43.32	2.25	1.25
1	C	249[A]	ASP	CB-CG	37.95	2.31	1.51
1	C	249[B]	ASP	CB-CG	37.95	2.31	1.51
1	C	249[C]	ASP	CB-CG	37.95	2.31	1.51
1	D	249[A]	ASP	CB-CG	37.29	2.30	1.51
1	D	249[B]	ASP	CB-CG	37.29	2.30	1.51
1	D	249[C]	ASP	CB-CG	37.29	2.30	1.51
1	B	249[A]	ASP	CB-CG	35.87	2.27	1.51
1	B	249[B]	ASP	CB-CG	35.87	2.27	1.51
1	B	249[C]	ASP	CB-CG	35.87	2.27	1.51
1	A	249[A]	ASP	CG-OD1	24.51	1.81	1.25
1	A	249[B]	ASP	CG-OD1	24.51	1.81	1.25
1	A	249[C]	ASP	CG-OD1	24.51	1.81	1.25

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249[A]	ASP	OD1-CG-OD2	-30.98	64.44	123.30
1	A	249[B]	ASP	OD1-CG-OD2	-30.98	64.44	123.30
1	A	249[C]	ASP	OD1-CG-OD2	-30.98	64.44	123.30
1	A	249[A]	ASP	CB-CG-OD2	-22.70	97.87	118.30
1	A	249[B]	ASP	CB-CG-OD2	-22.70	97.87	118.30
1	A	249[C]	ASP	CB-CG-OD2	-22.70	97.87	118.30
1	A	202[A]	LYS	CG-CD-CE	-21.92	46.15	111.90
1	A	202[B]	LYS	CG-CD-CE	-21.92	46.15	111.90
1	A	202[C]	LYS	CG-CD-CE	-21.92	46.15	111.90
1	C	202[A]	LYS	CB-CG-CD	-20.75	57.65	111.60
1	C	202[B]	LYS	CB-CG-CD	-20.75	57.65	111.60
1	C	202[C]	LYS	CB-CG-CD	-20.75	57.65	111.60
1	A	249[A]	ASP	CB-CG-OD1	15.81	132.53	118.30
1	A	249[B]	ASP	CB-CG-OD1	15.81	132.53	118.30
1	A	249[C]	ASP	CB-CG-OD1	15.81	132.53	118.30
1	B	249[A]	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	B	249[B]	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	B	249[C]	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	D	249[A]	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	D	249[B]	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	D	249[C]	ASP	CB-CG-OD2	-10.43	108.92	118.30
1	C	249[A]	ASP	CB-CG-OD2	-10.35	108.99	118.30
1	C	249[B]	ASP	CB-CG-OD2	-10.35	108.99	118.30
1	C	249[C]	ASP	CB-CG-OD2	-10.35	108.99	118.30
1	A	202[A]	LYS	CD-CE-NZ	9.45	133.44	111.70
1	A	202[B]	LYS	CD-CE-NZ	9.45	133.44	111.70
1	A	202[C]	LYS	CD-CE-NZ	9.45	133.44	111.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3310	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3431	0	3252	62	0
1	C	3425	0	3257	57	0
1	D	3439	0	3277	48	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	58	0	39	5	0
3	B	58	0	39	1	0
3	C	58	0	39	4	0
3	D	58	0	39	2	0
4	A	54	0	36	0	0
4	B	54	0	36	0	0
4	C	54	0	36	4	0
4	D	54	0	36	1	0
5	A	265	0	0	6	0
5	B	277	0	0	4	0
5	C	278	0	0	5	0
5	D	263	0	0	2	0
All	All	15324	0	13396	238	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 9.

All (238) 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:118:ILE:HG21	1:C:160[C]:MET:HE2	1.51	0.93
1:B:386[C]:ARG:HD3	5:B:2630:HOH:O	1.84	0.76
1:B:118:ILE:HG21	1:B:160[C]:MET:HE2	1.68	0.75
1:A:202[C]:LYS:HG3	1:A:239[C]:MET:SD	2.27	0.74
1:D:236[B]:PHE:HE1	3:D:4401[B]:HMG:H3P2	1.55	0.70
1:B:5:ILE:HG12	1:B:160[C]:MET:HE3	1.73	0.70
1:A:36:GLY:O	1:A:238[A]:LYS:HG3	1.93	0.69
1:A:36:GLY:O	1:A:238[B]:LYS:HG3	1.93	0.69
1:A:118:ILE:HG21	1:A:160[C]:MET:HE2	1.75	0.69
3:C:3401[B]:HMG:H131	3:C:3401[B]:HMG:H8	1.58	0.67
1:A:36:GLY:O	1:A:238[C]:LYS:HG3	1.96	0.65
1:A:236[B]:PHE:CZ	1:A:239[B]:MET:HB2	2.32	0.64
1:A:236[A]:PHE:CZ	1:A:239[A]:MET:HB2	2.32	0.64
1:D:236[B]:PHE:CZ	1:D:239[B]:MET:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HG21	1:B:160[C]:MET:CE	2.28	0.64
1:B:63:ILE:HD11	1:B:96:LEU:HD22	1.79	0.63
1:C:236[A]:PHE:CZ	1:C:239[A]:MET:HB2	2.33	0.63
1:C:5:ILE:HG12	1:C:160[C]:MET:HE3	1.81	0.63
1:D:236[A]:PHE:CZ	1:D:239[A]:MET:HB2	2.34	0.63
1:B:365:VAL:HG13	1:B:373:TYR:CZ	2.33	0.63
1:A:236[B]:PHE:HE1	3:A:1401[B]:HMG:H3P2	1.63	0.63
1:C:236[B]:PHE:CZ	1:C:239[B]:MET:HB2	2.34	0.63
1:B:236[A]:PHE:CZ	1:B:239[A]:MET:HB2	2.34	0.62
1:C:110[A]:ALA:HB1	1:C:111[A]:SCY:CE	2.30	0.62
1:B:111[A]:SCY:CD	1:B:111[A]:SCY:H	2.13	0.62
1:C:111[A]:SCY:H	1:C:111[A]:SCY:CD	2.13	0.62
1:B:236[B]:PHE:CZ	1:B:239[B]:MET:HB2	2.35	0.62
1:A:111[A]:SCY:H	1:A:111[A]:SCY:CD	2.13	0.61
1:C:202[C]:LYS:HG3	1:C:239[C]:MET:HE1	1.82	0.61
1:D:111[A]:SCY:CD	1:D:111[A]:SCY:H	2.14	0.60
1:B:110[A]:ALA:HB1	1:B:111[A]:SCY:CE	2.31	0.60
1:D:224:LEU:HD11	1:D:247[C]:ILE:HG22	1.82	0.60
1:C:206:ILE:O	1:C:210[B]:GLN:HG3	2.02	0.59
1:C:236[A]:PHE:CE1	1:C:239[A]:MET:HB2	2.38	0.59
1:C:236[B]:PHE:CE1	1:C:239[B]:MET:HB2	2.38	0.59
1:C:118:ILE:HG21	1:C:160[C]:MET:CE	2.30	0.58
3:C:3401[B]:HMG:H8	3:C:3401[B]:HMG:CDP	2.16	0.58
1:A:37:ILE:HG23	1:A:236[C]:PHE:CD2	2.39	0.58
1:B:236[B]:PHE:CE1	1:B:239[B]:MET:HB2	2.38	0.58
1:B:236[A]:PHE:CE1	1:B:239[A]:MET:HB2	2.38	0.57
1:C:206:ILE:O	1:C:210[A]:GLN:HG3	2.03	0.57
1:B:224:LEU:HD11	1:B:247[C]:ILE:HG22	1.85	0.57
1:D:206:ILE:O	1:D:210[B]:GLN:HG3	2.05	0.56
1:D:110[A]:ALA:HB1	1:D:111[A]:SCY:CE	2.34	0.56
1:D:206:ILE:O	1:D:210[A]:GLN:HG3	2.05	0.56
1:A:5:ILE:CD1	1:A:160[C]:MET:HE3	2.36	0.56
1:A:110[A]:ALA:HB1	1:A:111[A]:SCY:CE	2.35	0.56
1:C:129:PRO:HA	1:C:164:HIS:CD2	2.42	0.55
1:A:206:ILE:O	1:A:210[B]:GLN:HG3	2.06	0.54
1:C:237[A]:THR:HG22	1:C:267:VAL:HB	1.88	0.54
1:C:237[B]:THR:HG22	1:C:267:VAL:HB	1.88	0.54
1:C:386[C]:ARG:HD3	5:C:3773:HOH:O	2.07	0.54
1:B:199[C]:ALA:O	1:B:200[C]:LEU:HD23	2.06	0.54
1:B:206:ILE:O	1:B:210[A]:GLN:HG3	2.08	0.54
1:C:224:LEU:HD11	1:C:247[C]:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:3402[A]:CAA:H141	4:C:3402[A]:CAA:HN8	1.73	0.53
1:A:206:ILE:O	1:A:210[A]:GLN:HG3	2.07	0.53
1:B:129:PRO:HA	1:B:164:HIS:CD2	2.44	0.53
1:D:199[C]:ALA:O	1:D:200[C]:LEU:HD23	2.09	0.53
1:A:118:ILE:HG21	1:A:160[C]:MET:CE	2.38	0.53
1:A:202[C]:LYS:HG3	1:A:239[C]:MET:CE	2.40	0.52
1:B:206:ILE:O	1:B:210[B]:GLN:HG3	2.09	0.52
1:D:5:ILE:CD1	1:D:160[C]:MET:HE3	2.39	0.52
1:B:5:ILE:CD1	1:B:160[C]:MET:HE3	2.40	0.52
1:B:237[A]:THR:HG22	1:B:267:VAL:HB	1.91	0.52
1:B:37:ILE:HG23	1:B:236[C]:PHE:CD2	2.45	0.52
1:C:290:GLU:OE2	1:C:331:HIS:ND1	2.42	0.52
1:C:202[C]:LYS:HG3	1:C:239[C]:MET:CE	2.40	0.51
1:D:184:ASP:HB2	1:D:201[B]:SER:HA	1.92	0.51
1:C:294:LEU:HB2	1:C:318:LEU:HD11	1.92	0.51
1:B:386[A]:ARG:HH11	1:B:386[A]:ARG:HG3	1.76	0.51
1:B:386[B]:ARG:HH11	1:B:386[B]:ARG:HG3	1.76	0.51
1:B:237[B]:THR:HG22	1:B:267:VAL:HB	1.91	0.51
1:D:184:ASP:HB2	1:D:201[A]:SER:HA	1.92	0.51
3:A:1401[B]:HMG:H8	3:A:1401[B]:HMG:H131	1.76	0.51
1:B:184:ASP:HB2	1:B:201[C]:SER:HA	1.93	0.51
1:D:386[B]:ARG:HH11	1:D:386[B]:ARG:HG3	1.76	0.50
1:D:386[A]:ARG:HG3	1:D:386[A]:ARG:HH11	1.76	0.50
1:D:79:GLU:OE2	1:D:111[A]:SCY:HE2	2.12	0.50
4:C:3402[A]:CAA:N8P	4:C:3402[A]:CAA:H141	2.26	0.50
1:A:252:ASP:O	1:A:256:GLN:HG3	2.11	0.50
1:A:245[B]:GLU:CD	1:A:248[B]:ILE:HD11	2.32	0.50
1:A:245[A]:GLU:CD	1:A:248[A]:ILE:HD11	2.32	0.50
1:B:5:ILE:CG1	1:B:160[C]:MET:HE3	2.40	0.50
1:B:184:ASP:HB2	1:B:201[B]:SER:HA	1.93	0.50
1:A:79:GLU:OE2	1:A:111[A]:SCY:HE2	2.12	0.49
4:C:3402[A]:CAA:CEP	4:C:3402[A]:CAA:HN8	2.25	0.49
1:A:224:LEU:HD11	1:A:247[C]:ILE:HG22	1.93	0.49
1:C:247[A]:ILE:HB	5:C:3749:HOH:O	2.12	0.49
1:C:236[C]:PHE:CZ	1:C:239[C]:MET:HB2	2.48	0.49
1:A:386[C]:ARG:HG3	1:A:386[C]:ARG:HH11	1.78	0.49
1:C:247[B]:ILE:HB	5:C:3749:HOH:O	2.13	0.48
1:C:184:ASP:HB2	1:C:201[B]:SER:HA	1.95	0.48
1:D:236[C]:PHE:CZ	1:D:239[C]:MET:HB2	2.49	0.48
1:B:184:ASP:HB2	1:B:201[A]:SER:HA	1.93	0.48
1:D:232[B]:PHE:N	1:D:232[B]:PHE:CD1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLY:HA3	1:D:237[B]:THR:OG1	2.13	0.48
1:D:343:VAL:O	1:D:347:GLU:HG3	2.14	0.48
1:A:5:ILE:HG12	1:A:160[C]:MET:HE3	1.96	0.48
1:C:247[A]:ILE:HG13	1:C:248[A]:ILE:N	2.28	0.48
1:D:232[A]:PHE:CD1	1:D:232[A]:PHE:N	2.82	0.48
1:C:247[B]:ILE:HG13	1:C:248[B]:ILE:N	2.28	0.48
1:D:247[A]:ILE:HG13	1:D:248[A]:ILE:N	2.28	0.47
1:B:247[A]:ILE:HG13	1:B:248[A]:ILE:N	2.29	0.47
1:B:247[B]:ILE:HG13	1:B:248[B]:ILE:N	2.29	0.47
1:C:386[A]:ARG:HH11	1:C:386[A]:ARG:HG3	1.79	0.47
1:D:247[B]:ILE:HG13	1:D:248[B]:ILE:N	2.28	0.47
1:D:37:ILE:HG23	1:D:236[C]:PHE:CD2	2.50	0.47
1:D:184:ASP:HB2	1:D:201[C]:SER:HA	1.95	0.47
1:A:386[B]:ARG:HH11	1:A:386[B]:ARG:HG3	1.78	0.47
1:C:141:ALA:HA	1:C:277:TYR:CE2	2.50	0.47
1:C:386[B]:ARG:HH11	1:C:386[B]:ARG:HG3	1.79	0.47
1:A:386[A]:ARG:HG3	1:A:386[A]:ARG:HH11	1.78	0.47
1:B:294:LEU:HB2	1:B:318:LEU:HD11	1.97	0.47
1:D:38:GLY:HA3	1:D:237[A]:THR:OG1	2.13	0.47
1:A:108[B]:LYS:HE2	5:A:1722:HOH:O	2.14	0.47
1:A:108[A]:LYS:HE2	5:A:1722:HOH:O	2.14	0.47
1:B:365:VAL:HG13	1:B:373:TYR:OH	2.15	0.47
1:D:347:GLU:HB3	1:D:351:LYS:NZ	2.30	0.47
1:A:38:GLY:HA3	1:A:237[C]:THR:OG1	2.15	0.46
1:A:355:ASP:HB2	1:A:357:GLU:HG3	1.96	0.46
1:C:232[B]:PHE:N	1:C:232[B]:PHE:CD1	2.82	0.46
1:B:38:GLY:HA3	1:B:237[B]:THR:OG1	2.15	0.46
1:A:238[C]:LYS:HD3	5:A:1633:HOH:O	2.14	0.46
1:C:79:GLU:OE2	1:C:111[A]:SCY:HE2	2.15	0.46
1:C:184:ASP:HB2	1:C:201[A]:SER:HA	1.96	0.46
1:B:343:VAL:O	1:B:347:GLU:HG3	2.16	0.46
1:C:232[A]:PHE:CD1	1:C:232[A]:PHE:N	2.83	0.46
1:D:245[B]:GLU:CD	1:D:248[B]:ILE:HD11	2.36	0.46
1:C:38:GLY:HA3	1:C:237[C]:THR:OG1	2.15	0.46
1:D:245[A]:GLU:CD	1:D:248[A]:ILE:HD11	2.36	0.46
1:A:247[B]:ILE:HG13	1:A:248[B]:ILE:N	2.30	0.46
1:B:245[B]:GLU:CD	1:B:248[B]:ILE:HD11	2.35	0.46
1:B:247[A]:ILE:HB	5:B:2671:HOH:O	2.15	0.46
1:A:247[A]:ILE:HG13	1:A:248[A]:ILE:N	2.30	0.46
1:A:184:ASP:HB2	1:A:201[C]:SER:HA	1.97	0.46
1:B:247[B]:ILE:HB	5:B:2671:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ALA:HA	1:D:277:TYR:CE2	2.51	0.45
1:A:232[B]:PHE:N	1:A:232[B]:PHE:CD1	2.84	0.45
1:A:236[B]:PHE:CE1	1:A:239[B]:MET:HB2	2.51	0.45
1:C:245[B]:GLU:CD	1:C:248[B]:ILE:HD11	2.36	0.45
1:C:232[C]:PHE:HA	1:C:281:LEU:HD13	1.98	0.45
1:B:232[B]:PHE:CD1	1:B:232[B]:PHE:N	2.84	0.45
1:B:365:VAL:CG1	1:B:373:TYR:OH	2.65	0.45
1:A:232[A]:PHE:N	1:A:232[A]:PHE:CD1	2.85	0.45
1:A:240[C]:GLY:O	1:A:243:ALA:N	2.49	0.45
1:B:79:GLU:OE2	1:B:111[A]:SCY:HE2	2.17	0.45
1:B:245[A]:GLU:CD	1:B:248[A]:ILE:HD11	2.36	0.45
1:B:38:GLY:HA3	1:B:237[A]:THR:OG1	2.16	0.45
1:B:294:LEU:CB	1:B:318:LEU:HD11	2.47	0.45
1:A:236[A]:PHE:CE1	1:A:239[A]:MET:HB2	2.52	0.45
3:A:1401[B]:HMG:N8P	3:A:1401[B]:HMG:H131	2.30	0.45
1:D:232[C]:PHE:HB3	1:D:303:PHE:HB3	1.99	0.45
1:A:38:GLY:HA3	1:A:237[B]:THR:OG1	2.17	0.45
1:A:184:ASP:HB2	1:A:201[B]:SER:HA	1.99	0.45
1:C:197[B]:ASP:OD1	1:C:200[B]:LEU:HB2	2.17	0.45
3:A:1401[B]:HMG:H8	3:A:1401[B]:HMG:CDP	2.30	0.45
1:D:232[C]:PHE:HA	1:D:281:LEU:HD13	1.98	0.45
1:B:232[A]:PHE:CD1	1:B:232[A]:PHE:N	2.85	0.45
1:A:184:ASP:HB2	1:A:201[A]:SER:HA	1.99	0.44
1:C:245[A]:GLU:CD	1:C:248[A]:ILE:HD11	2.36	0.44
1:A:343:VAL:O	1:A:347:GLU:HG3	2.17	0.44
1:A:232[C]:PHE:HB3	1:A:303:PHE:HB3	1.98	0.44
1:B:290:GLU:OE2	1:B:331:HIS:ND1	2.50	0.44
1:A:307:SER:OG	3:A:1401[B]:HMG:H21	2.18	0.44
1:B:38:GLY:HA3	1:B:237[C]:THR:OG1	2.17	0.44
1:D:237[B]:THR:HG22	1:D:267:VAL:HB	2.00	0.44
1:D:237[A]:THR:HG22	1:D:267:VAL:HB	2.00	0.44
1:C:197[A]:ASP:OD1	1:C:200[A]:LEU:HB2	2.18	0.44
1:D:307:SER:OG	3:D:4401[B]:HMG:H21	2.18	0.44
1:B:235[B]:PRO:HG3	1:B:239[B]:MET:HG2	1.99	0.44
1:D:245[B]:GLU:OE2	1:D:248[B]:ILE:HD11	2.18	0.44
1:A:245[B]:GLU:OE2	1:A:248[B]:ILE:HD11	2.18	0.44
1:A:67:ASP:O	1:A:71:ILE:HG13	2.18	0.44
1:B:307:SER:OG	3:B:2401[B]:HMG:H21	2.18	0.44
3:C:3401[B]:HMG:H131	3:C:3401[B]:HMG:N8P	2.23	0.44
1:B:235[A]:PRO:HG3	1:B:239[A]:MET:HG2	1.99	0.44
1:B:205[C]:TYR:CE1	1:B:239[C]:MET:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245[A]:GLU:OE2	1:A:248[A]:ILE:HD11	2.18	0.44
1:C:38:GLY:HA3	1:C:237[B]:THR:OG1	2.18	0.43
1:B:150:GLU:HB3	1:B:151:PRO:HD3	2.00	0.43
1:D:240[C]:GLY:O	1:D:243:ALA:N	2.51	0.43
1:A:238[B]:LYS:HD3	5:A:1633:HOH:O	2.18	0.43
1:D:245[A]:GLU:OE2	1:D:248[A]:ILE:HD11	2.18	0.43
1:C:386[B]:ARG:HD3	5:C:3773:HOH:O	2.17	0.43
1:A:237[B]:THR:HG21	1:A:271:ARG:HG2	1.99	0.43
1:A:237[A]:THR:HG22	1:A:267:VAL:HB	2.00	0.43
1:A:38:GLY:HA3	1:A:237[A]:THR:OG1	2.17	0.43
1:A:376:ASN:HB3	5:A:1740:HOH:O	2.18	0.43
1:C:343:VAL:O	1:C:347:GLU:HG3	2.18	0.43
1:C:177:ALA:O	1:D:101:PHE:HA	2.17	0.43
1:A:238[A]:LYS:HD3	5:A:1633:HOH:O	2.18	0.43
1:C:386[A]:ARG:HD3	5:C:3773:HOH:O	2.17	0.43
1:C:366:HIS:HE1	1:C:369:ARG:NH2	2.17	0.43
1:A:239[C]:MET:O	1:A:239[C]:MET:HE2	2.18	0.43
1:B:141:ALA:HA	1:B:277:TYR:CE2	2.54	0.43
1:A:237[A]:THR:HG21	1:A:271:ARG:HG2	1.99	0.43
1:D:185:PHE:C	1:D:185:PHE:CD1	2.92	0.43
1:B:185:PHE:C	1:B:185:PHE:CD1	2.91	0.43
1:A:185:PHE:C	1:A:185:PHE:CD1	2.92	0.43
1:B:232[C]:PHE:HA	1:B:281:LEU:HD13	2.01	0.42
1:A:232[C]:PHE:HA	1:A:281:LEU:HD13	2.00	0.42
1:D:376:ASN:CG	1:D:377:ILE:N	2.72	0.42
1:C:118:ILE:CG2	1:C:160[C]:MET:HE2	2.35	0.42
1:C:38:GLY:HA3	1:C:237[A]:THR:OG1	2.19	0.42
1:B:245[B]:GLU:OE2	1:B:248[B]:ILE:HD11	2.20	0.42
1:C:201[A]:SER:HB2	4:C:3402[A]:CAA:H31	2.01	0.42
1:A:101:PHE:HA	1:B:177:ALA:O	2.19	0.42
1:C:37:ILE:HG23	1:C:236[C]:PHE:CD1	2.55	0.42
1:A:237[B]:THR:HG22	1:A:267:VAL:HB	2.00	0.42
1:D:150:GLU:HB3	1:D:151:PRO:HD3	2.02	0.42
1:A:239[C]:MET:HE3	1:A:242:LYS:HB2	2.02	0.42
1:C:236[C]:PHE:CE1	1:C:239[C]:MET:HB2	2.55	0.41
1:B:245[A]:GLU:OE2	1:B:248[A]:ILE:HD11	2.20	0.41
1:D:108[C]:LYS:HE2	5:D:4717:HOH:O	2.20	0.41
1:B:326:LEU:HA	5:B:2759:HOH:O	2.19	0.41
1:D:118:ILE:HD13	1:D:160[C]:MET:HE1	2.02	0.41
1:D:236[C]:PHE:CE2	1:D:239[C]:MET:HB2	2.55	0.41
1:B:248[B]:ILE:O	1:B:251[B]:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PHE:HA	1:D:177:ALA:O	2.21	0.41
1:A:177:ALA:O	1:B:101:PHE:HA	2.21	0.41
1:A:308:GLY:N	1:A:309:SER:HA	2.36	0.41
1:B:248[A]:ILE:O	1:B:251[A]:ALA:HB3	2.20	0.41
1:D:236[A]:PHE:HE1	4:D:4402[A]:CAA:H31	1.86	0.41
1:B:232[C]:PHE:HB3	1:B:303:PHE:HB3	2.01	0.41
1:A:150:GLU:HB3	1:A:151:PRO:HD3	2.03	0.41
1:D:236[B]:PHE:CE1	1:D:239[B]:MET:HB2	2.55	0.41
1:D:5:ILE:HD13	1:D:160[C]:MET:HE3	2.02	0.41
1:B:376:ASN:CG	1:B:377:ILE:N	2.74	0.41
1:A:141:ALA:HA	1:A:277:TYR:CE2	2.56	0.41
1:C:5:ILE:CG1	1:C:160[C]:MET:HE3	2.50	0.40
1:C:294:LEU:CB	1:C:318:LEU:HD11	2.51	0.40
1:C:200[C]:LEU:HD23	1:C:200[C]:LEU:HA	1.96	0.40
3:C:3401[B]:HMG:CDP	3:C:3401[B]:HMG:N8P	2.80	0.40
1:C:108:LYS:HE2	5:D:4705:HOH:O	2.21	0.40
1:A:290:GLU:HG2	1:A:326:LEU:HD13	2.03	0.40
1:C:5:ILE:CD1	1:C:160[C]:MET:HE3	2.52	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	A	450/397 (113%)	413 (92%)	33 (7%)	4 (1%)	21	5
1	B	448/397 (113%)	411 (92%)	36 (8%)	1 (0%)	52	28
1	C	448/397 (113%)	414 (92%)	27 (6%)	7 (2%)	12	2
1	D	449/397 (113%)	410 (91%)	35 (8%)	4 (1%)	21	5
All	All	1795/1588 (113%)	1648 (92%)	131 (7%)	16 (1%)	34	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	109	GLU
1	C	109	GLU
1	C	199[A]	ALA
1	C	199[B]	ALA
1	C	199[C]	ALA
1	D	237[A]	THR
1	D	237[B]	THR
1	D	237[C]	THR
1	A	109	GLU
1	C	198[A]	GLY
1	C	198[B]	GLY
1	C	198[C]	GLY
1	D	109	GLU
1	A	237[A]	THR
1	A	237[B]	THR
1	A	237[C]	THR

### 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	356/326 (109%)	344 (97%)	12 (3%)	44	16
1	B	345/326 (106%)	337 (98%)	8 (2%)	58	29
1	C	345/326 (106%)	337 (98%)	8 (2%)	58	29
1	D	352/326 (108%)	346 (98%)	6 (2%)	68	44
All	All	1398/1304 (107%)	1364 (98%)	34 (2%)	72	27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	185	PHE
1	A	200[A]	LEU
1	A	200[B]	LEU
1	A	200[C]	LEU
1	A	232[A]	PHE

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Mol	Chain	Res	Type
1	A	232[B]	PHE
1	A	232[C]	PHE
1	A	249[A]	ASP
1	A	249[B]	ASP
1	A	249[C]	ASP
1	A	346	TYR
1	B	109	GLU
1	B	200[A]	LEU
1	B	200[B]	LEU
1	B	200[C]	LEU
1	B	232[A]	PHE
1	B	232[B]	PHE
1	B	232[C]	PHE
1	B	346	TYR
1	C	109	GLU
1	C	200[A]	LEU
1	C	200[B]	LEU
1	C	200[C]	LEU
1	C	232[A]	PHE
1	C	232[B]	PHE
1	C	232[C]	PHE
1	C	346	TYR
1	D	109	GLU
1	D	185	PHE
1	D	232[A]	PHE
1	D	232[B]	PHE
1	D	232[C]	PHE
1	D	346	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	HIS
1	A	336	ASN
1	B	325	HIS
1	C	146	ASN
1	D	325	HIS
1	D	336	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SCY	A	111[A]	1	7,8,9	0.64	0	4,9,11	1.11	0
1	SCY	B	111[A]	1	7,8,9	0.62	0	4,9,11	1.11	0
1	SCY	C	111[A]	1	7,8,9	0.61	0	4,9,11	1.11	1 (25%)
1	SCY	D	111[A]	1	7,8,9	0.62	0	4,9,11	1.10	0

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
1	SCY	A	111[A]	1	-	0/5/7/9	0/0/0/0
1	SCY	B	111[A]	1	-	0/5/7/9	0/0/0/0
1	SCY	C	111[A]	1	-	0/5/7/9	0/0/0/0
1	SCY	D	111[A]	1	-	0/5/7/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111[A]	SCY	O-C-CA	-2.02	120.24	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	111[A]	SCY	3	0
1	B	111[A]	SCY	3	0
1	C	111[A]	SCY	3	0
1	D	111[A]	SCY	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	HMG	A	1401[B]	-	47,60,60	0.98	1 (2%)	58,90,90	1.69	6 (10%)
4	CAA	A	1402[A]	-	45,56,56	0.73	0	58,83,83	1.63	5 (8%)
2	SO4	A	1501	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	A	1502	-	4,4,4	0.20	0	6,6,6	0.09	0
3	HMG	B	2401[B]	-	47,60,60	0.98	1 (2%)	58,90,90	1.72	6 (10%)
4	CAA	B	2402[A]	-	45,56,56	0.73	0	58,83,83	1.63	4 (6%)
2	SO4	B	2501	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	2502	-	4,4,4	0.20	0	6,6,6	0.09	0
3	HMG	C	3401[B]	-	47,60,60	0.98	2 (4%)	58,90,90	1.68	5 (8%)
4	CAA	C	3402[A]	-	45,56,56	0.71	0	58,83,83	1.62	5 (8%)
2	SO4	C	3501	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	C	3502	-	4,4,4	0.21	0	6,6,6	0.10	0
3	HMG	D	4401[B]	-	47,60,60	1.00	2 (4%)	58,90,90	1.37	3 (5%)
4	CAA	D	4402[A]	-	45,56,56	0.71	0	58,83,83	1.56	3 (5%)
2	SO4	D	4501	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	D	4502	-	4,4,4	0.20	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HMG	A	1401[B]	-	-	0/54/77/77	0/3/3/3
4	CAA	A	1402[A]	-	-	0/50/71/71	0/3/3/3
2	SO4	A	1501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1502	-	-	0/0/0/0	0/0/0/0
3	HMG	B	2401[B]	-	-	0/54/77/77	0/3/3/3
4	CAA	B	2402[A]	-	-	0/50/71/71	0/3/3/3
2	SO4	B	2501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2502	-	-	0/0/0/0	0/0/0/0
3	HMG	C	3401[B]	-	-	0/54/77/77	0/3/3/3
4	CAA	C	3402[A]	-	-	1/50/71/71	0/3/3/3
2	SO4	C	3501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3502	-	-	0/0/0/0	0/0/0/0
3	HMG	D	4401[B]	-	-	0/54/77/77	0/3/3/3
4	CAA	D	4402[A]	-	-	0/50/71/71	0/3/3/3
2	SO4	D	4501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4502	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3401[B]	HMG	C1-S1P	2.11	1.80	1.76
3	D	4401[B]	HMG	C1-S1P	2.41	1.81	1.76
3	D	4401[B]	HMG	P3B-O9A	4.43	1.59	1.51
3	A	1401[B]	HMG	P3B-O9A	4.46	1.59	1.51
3	B	2401[B]	HMG	P3B-O9A	4.50	1.59	1.51
3	C	3401[B]	HMG	P3B-O9A	4.52	1.59	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2402[A]	CAA	P2A-O3A-P1A	-7.79	110.85	132.73
3	B	2401[B]	HMG	P1A-O3A-P2A	-7.78	110.89	132.73
4	A	1402[A]	CAA	P2A-O3A-P1A	-7.77	110.92	132.73
4	C	3402[A]	CAA	P2A-O3A-P1A	-7.71	111.08	132.73
3	C	3401[B]	HMG	P1A-O3A-P2A	-7.64	111.28	132.73
3	A	1401[B]	HMG	P1A-O3A-P2A	-7.55	111.53	132.73
4	D	4402[A]	CAA	P2A-O3A-P1A	-7.38	112.01	132.73
3	B	2401[B]	HMG	C2-C1-S1P	-7.24	106.84	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401[B]	HMG	C2-C1-S1P	-7.15	106.92	113.36
3	C	3401[B]	HMG	C2-C1-S1P	-7.08	106.99	113.36
4	B	2402[A]	CAA	C2-C1-S1P	-6.75	106.76	113.50
4	C	3402[A]	CAA	C2-C1-S1P	-6.73	106.79	113.50
4	A	1402[A]	CAA	C2-C1-S1P	-6.69	106.83	113.50
4	D	4402[A]	CAA	C2-C1-S1P	-6.57	106.94	113.50
3	D	4401[B]	HMG	P1A-O3A-P2A	-5.99	115.91	132.73
3	D	4401[B]	HMG	C2-C1-S1P	-5.57	108.34	113.36
4	C	3402[A]	CAA	C2P-S1P-C1	-2.15	94.43	102.09
3	B	2401[B]	HMG	C2P-S1P-C1	-2.12	94.53	102.09
3	C	3401[B]	HMG	C2P-S1P-C1	-2.09	94.64	102.09
3	A	1401[B]	HMG	O3A-P1A-O5B	2.07	108.42	102.94
4	A	1402[A]	CAA	O3A-P1A-O5B	2.14	108.61	102.94
4	A	1402[A]	CAA	O3A-P2A-O6A	2.37	109.22	102.94
4	C	3402[A]	CAA	O3A-P2A-O6A	2.38	109.25	102.94
3	B	2401[B]	HMG	O3A-P2A-O6A	2.41	109.34	102.94
4	B	2402[A]	CAA	O3A-P2A-O6A	2.42	109.37	102.94
3	A	1401[B]	HMG	O3A-P2A-O6A	2.43	109.39	102.94
3	C	3401[B]	HMG	O2-C1-C2	2.97	126.60	123.70
3	B	2401[B]	HMG	O2-C1-C2	3.07	126.70	123.70
3	A	1401[B]	HMG	O2-C1-C2	3.11	126.74	123.70
3	D	4401[B]	HMG	O2-C1-S1P	4.03	126.03	122.83
3	A	1401[B]	HMG	O2-C1-S1P	4.41	126.34	122.83
4	D	4402[A]	CAA	O1-C1-S1P	4.48	126.39	122.83
3	C	3401[B]	HMG	O2-C1-S1P	4.51	126.41	122.83
3	B	2401[B]	HMG	O2-C1-S1P	4.56	126.45	122.83
4	A	1402[A]	CAA	O1-C1-S1P	4.59	126.48	122.83
4	C	3402[A]	CAA	O1-C1-S1P	4.62	126.50	122.83
4	B	2402[A]	CAA	O1-C1-S1P	4.67	126.54	122.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3402[A]	CAA	C6P-C5P-N4P-C3P

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1401[B]	HMG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2401[B]	HMG	1	0
3	C	3401[B]	HMG	4	0
4	C	3402[A]	CAA	4	0
3	D	4401[B]	HMG	2	0
4	D	4402[A]	CAA	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 ⓘ

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	A	388/397 (97%)	-0.14	12 (3%) 52 50	11, 19, 32, 43	2 (0%)
1	B	388/397 (97%)	-0.15	9 (2%) 64 62	11, 18, 31, 42	2 (0%)
1	C	388/397 (97%)	-0.14	10 (2%) 59 57	11, 18, 31, 42	3 (0%)
1	D	388/397 (97%)	-0.12	10 (2%) 59 57	11, 19, 32, 45	3 (0%)
All	All	1552/1588 (97%)	-0.13	41 (2%) 59 57	11, 19, 32, 45	10 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	199[A]	ALA	8.7
1	B	199[A]	ALA	7.1
1	A	199[A]	ALA	7.0
1	D	199[A]	ALA	6.4
1	C	247[A]	ILE	5.3
1	C	198[A]	GLY	5.1
1	B	389	LEU	4.7
1	A	389	LEU	4.6
1	D	389	LEU	4.4
1	B	247[A]	ILE	4.2
1	D	247[A]	ILE	4.0
1	B	390	GLU	3.8
1	C	390	GLU	3.7
1	D	390	GLU	3.6
1	C	389	LEU	3.6
1	B	198[A]	GLY	3.4
1	C	200[A]	LEU	3.3
1	A	247[A]	ILE	3.2
1	C	249[A]	ASP	2.9
1	A	198[A]	GLY	2.9
1	A	390	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	249[A]	ASP	2.8
1	D	249[A]	ASP	2.7
1	D	248[A]	ILE	2.7
1	B	232[A]	PHE	2.7
1	C	234[A]	VAL	2.5
1	D	239[A]	MET	2.5
1	C	248[A]	ILE	2.5
1	D	198[A]	GLY	2.5
1	B	63	ILE	2.4
1	A	238[A]	LYS	2.4
1	B	197[A]	ASP	2.4
1	D	251[A]	ALA	2.4
1	C	197[A]	ASP	2.3
1	A	248[A]	ILE	2.3
1	B	249[A]	ASP	2.2
1	A	240[A]	GLY	2.2
1	A	239[A]	MET	2.2
1	D	236[A]	PHE	2.1
1	A	236[A]	PHE	2.1
1	A	232[A]	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	SCY	C	111[A]	9/10	0.96	0.08	-	12,14,21,22	9
1	SCY	B	111[A]	9/10	0.95	0.10	-	12,14,22,22	9
1	SCY	D	111[A]	9/10	0.97	0.07	-	13,14,23,24	9
1	SCY	A	111[A]	9/10	0.97	0.07	-	13,14,22,23	9

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

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(Å <sup>2</sup> )	Q<0.9
4	CAA	C	3402[A]	54/54	0.82	0.19	0.99	20,30,35,35	54
3	HMG	D	4401[B]	58/58	0.84	0.17	0.98	17,27,33,34	58
3	HMG	B	2401[B]	58/58	0.85	0.17	0.97	18,28,34,35	58
4	CAA	B	2402[A]	54/54	0.85	0.17	0.86	17,29,34,35	54
3	HMG	A	1401[B]	58/58	0.88	0.16	0.59	13,27,33,34	58
4	CAA	D	4402[A]	54/54	0.83	0.17	0.58	24,29,38,39	54
4	CAA	A	1402[A]	54/54	0.88	0.16	0.51	19,28,35,36	54
3	HMG	C	3401[B]	58/58	0.82	0.18	0.50	18,28,35,35	58
2	SO4	D	4502	5/5	0.92	0.14	-	73,73,73,74	0
2	SO4	A	1502	5/5	0.92	0.14	-	75,75,75,75	0
2	SO4	C	3501	5/5	0.90	0.15	-	34,35,37,38	0
2	SO4	D	4501	5/5	0.93	0.11	-	38,38,39,40	0
2	SO4	B	2501	5/5	0.90	0.16	-	36,37,40,40	0
2	SO4	B	2502	5/5	0.94	0.16	-	80,81,81,81	0
2	SO4	A	1501	5/5	0.94	0.12	-	36,37,38,39	0
2	SO4	C	3502	5/5	0.94	0.20	-	78,78,79,79	0

## 6.5 Other polymers

There are no such residues in this entry.