



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:07 am GMT

PDB ID : 1QFL  
Title : BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COM-  
PLEX WITH A REACTION INTERMEDIATE.  
Authors : Modis, Y.; Wierenga, R.K.  
Deposited on : 1999-04-12  
Resolution : 1.92 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

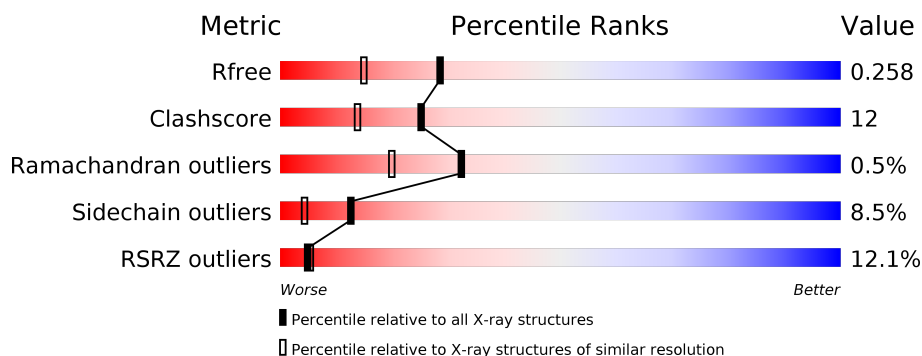
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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	389	<div> <div>4%</div> <div>67% 27% 6%</div> </div>
1	B	389	<div> <div>5%</div> <div>72% 21%</div> </div>
1	C	389	<div> <div>14%</div> <div>71% 25%</div> </div>
1	D	389	<div> <div>25%</div> <div>67% 27% 5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SCY	A	89	-	-	X	-
1	SCY	B	89	-	-	X	-
1	SCY	C	89	-	-	X	-
1	SCY	D	89	-	-	X	-
2	SO4	B	724	-	-	-	X
3	COA	A	393	-	-	-	X
3	COA	B	393	-	-	-	X
3	COA	C	393	-	-	-	X
3	COA	D	393	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12204 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 PROTEIN (ACETOACETYL-COA THIOLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			
1	B	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			
1	C	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			
1	D	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			

There are 12 discrepancies between the modelled and reference sequences:

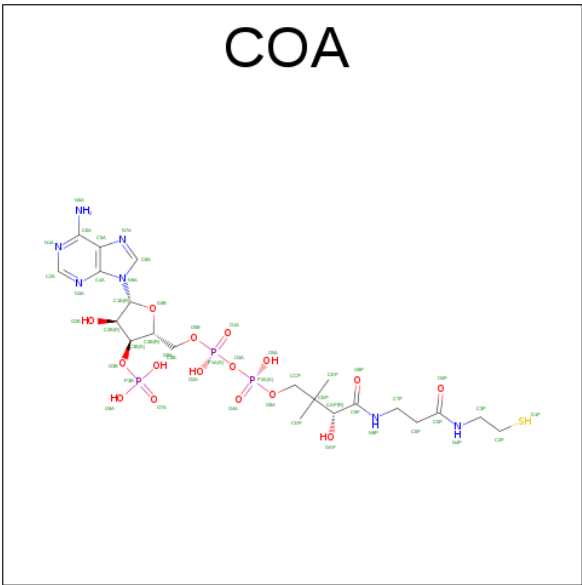
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	11	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	11	ALA	-	INSERTION	UNP P07097
C	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	11	ALA	-	INSERTION	UNP P07097
D	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

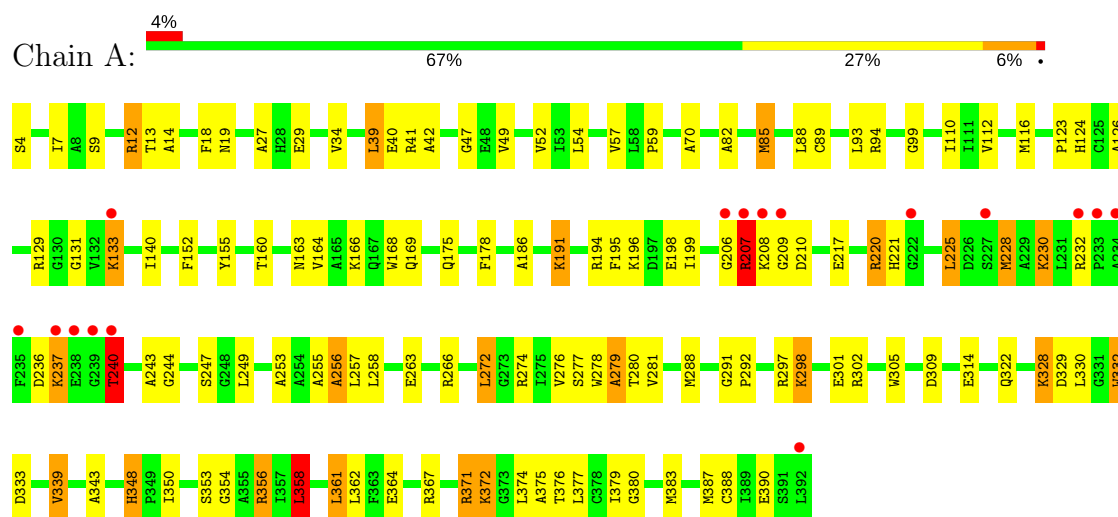
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	0	0
			287	287		
4	B	275	Total	O	0	0
			275	275		
4	C	94	Total	O	0	0
			94	94		
4	D	62	Total	O	0	0
			62	62		

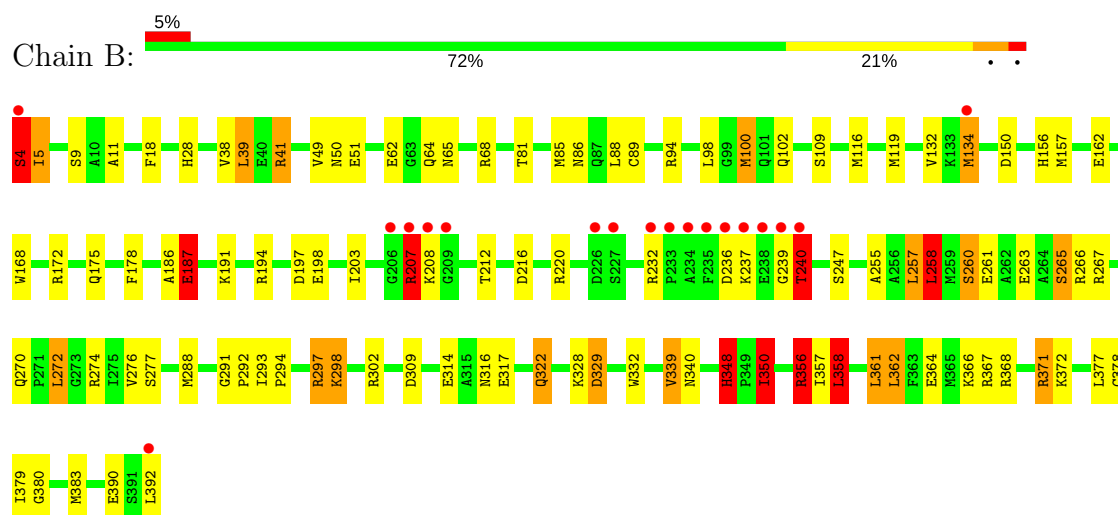
### 3 Residue-property plots

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

#### • Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

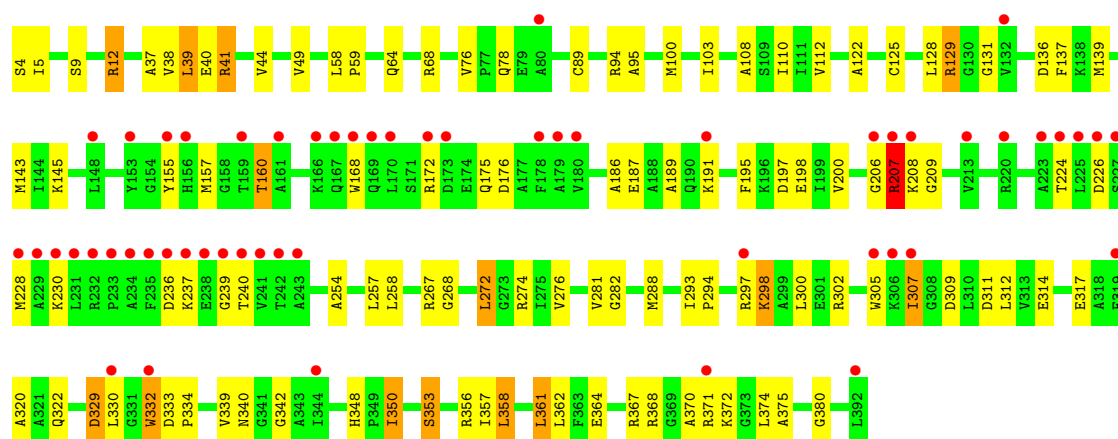


#### • Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

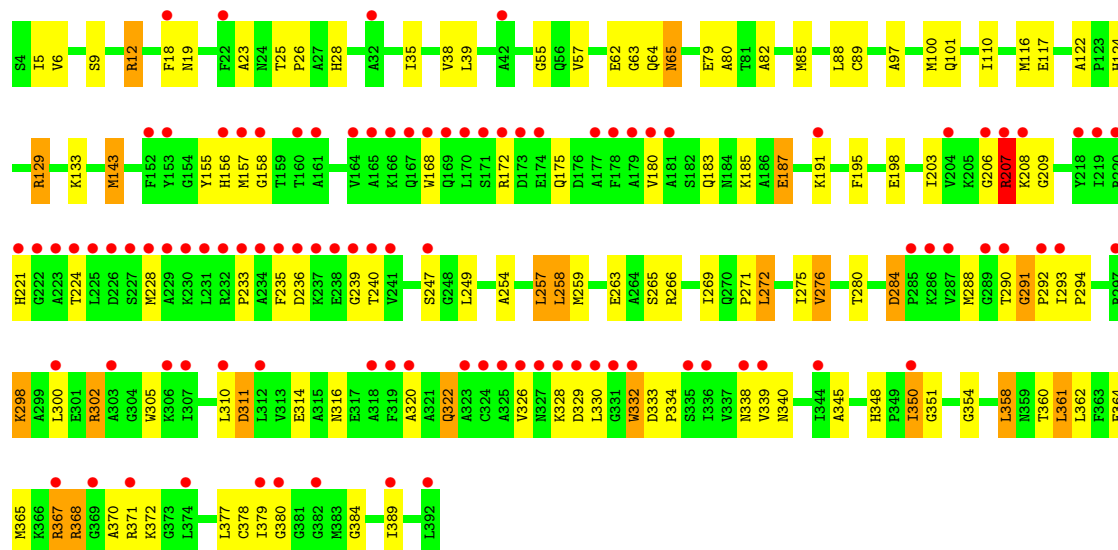


#### • Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)





• Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.46Å 78.86Å 149.75Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 49.83 – 1.93	Depositor EDS
% Data completeness (in resolution range)	85.5 (50.00-1.92) 79.2 (49.83-1.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	8.40	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209 , 0.256 0.255 , 0.258	Depositor DCC
$R_{free}$ test set	7053 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, 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	1.10	0/2847	2.12	89/3842 (2.3%)
1	B	1.11	1/2847 (0.0%)	2.05	81/3842 (2.1%)
1	C	0.59	0/2847	1.50	26/3842 (0.7%)
1	D	0.53	0/2847	1.35	17/3842 (0.4%)
All	All	0.88	1/11388 (0.0%)	1.79	213/15368 (1.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	SER	CA-CB	5.12	1.60	1.52

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	CD-NE-CZ	23.58	156.61	123.60
1	B	367	ARG	NE-CZ-NH2	-19.56	110.52	120.30
1	A	12	ARG	NE-CZ-NH1	18.50	129.55	120.30
1	A	302	ARG	NE-CZ-NH2	-15.98	112.31	120.30
1	C	41	ARG	NE-CZ-NH2	-14.46	113.07	120.30
1	A	228	MET	CA-CB-CG	14.45	137.86	113.30
1	B	297	ARG	NE-CZ-NH1	14.13	127.36	120.30
1	A	129	ARG	NE-CZ-NH2	-14.12	113.24	120.30
1	B	41	ARG	NE-CZ-NH2	-14.09	113.25	120.30
1	B	302	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	B	216	ASP	CB-CG-OD1	12.63	129.67	118.30
1	A	220	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	B	367	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	216	ASP	CB-CG-OD2	-11.69	107.78	118.30
1	A	302	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	A	41	ARG	NE-CZ-NH2	-11.25	114.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH1	11.09	125.85	120.30
1	A	367	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	B	41	ARG	NH1-CZ-NH2	10.98	131.48	119.40
1	A	356	ARG	NE-CZ-NH2	10.93	125.76	120.30
1	C	129	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	178	PHE	CB-CG-CD1	10.51	128.16	120.80
1	B	41	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	B	4	SER	CA-C-O	-10.38	98.31	120.10
1	A	195	PHE	CB-CG-CD2	-10.25	113.62	120.80
1	A	339	VAL	CA-CB-CG2	10.16	126.15	110.90
1	A	266	ARG	CD-NE-CZ	10.11	137.75	123.60
1	B	187	GLU	OE1-CD-OE2	10.01	135.32	123.30
1	A	297	ARG	CD-NE-CZ	9.87	137.41	123.60
1	C	207	ARG	CD-NE-CZ	9.83	137.37	123.60
1	B	361	LEU	CA-CB-CG	9.79	137.81	115.30
1	A	207	ARG	CD-NE-CZ	9.78	137.29	123.60
1	B	371	ARG	CG-CD-NE	9.78	132.34	111.80
1	A	129	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	B	150	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	D	207	ARG	CD-NE-CZ	9.53	136.94	123.60
1	A	195	PHE	CB-CG-CD1	9.41	127.39	120.80
1	A	371	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	266	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	C	329	ASP	CB-CG-OD1	-9.16	110.06	118.30
1	C	302	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	A	228	MET	CG-SD-CE	-8.84	86.05	100.20
1	A	240	THR	N-CA-CB	-8.49	94.17	110.30
1	B	350	ILE	CA-CB-CG1	8.39	126.95	111.00
1	A	371	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	220	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	94	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	B	368	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	C	41	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	18	PHE	CB-CG-CD1	8.08	126.45	120.80
1	A	198	GLU	O-C-N	-8.04	109.84	122.70
1	B	207	ARG	CD-NE-CZ	8.03	134.84	123.60
1	A	94	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	100	MET	CG-SD-CE	-7.91	87.55	100.20
1	C	172	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	D	367	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	C	94	ARG	CD-NE-CZ	7.60	134.24	123.60
1	D	367	ARG	CD-NE-CZ	7.53	134.14	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	PHE	CB-CG-CD2	-7.47	115.57	120.80
1	C	136	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	B	68	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	B	339	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	B	98	LEU	CB-CG-CD2	-7.39	98.44	111.00
1	B	240	THR	N-CA-CB	-7.34	96.36	110.30
1	B	261	GLU	OE1-CD-OE2	-7.30	114.54	123.30
1	B	367	ARG	CD-NE-CZ	7.30	133.82	123.60
1	B	361	LEU	CB-CG-CD2	7.28	123.38	111.00
1	A	358	LEU	CA-CB-CG	7.27	132.03	115.30
1	B	4	SER	CA-C-N	7.27	133.19	117.20
1	A	129	ARG	CG-CD-NE	-7.24	96.59	111.80
1	C	12	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	356	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	207	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	297	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	D	172	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	D	129	ARG	CG-CD-NE	-7.09	96.92	111.80
1	D	172	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	4	SER	N-CA-CB	6.92	120.88	110.50
1	A	274	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	B	356	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	B	364	GLU	OE1-CD-OE2	-6.81	115.13	123.30
1	A	12	ARG	CD-NE-CZ	6.79	133.11	123.60
1	A	358	LEU	CB-CG-CD2	6.79	122.54	111.00
1	C	68	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	390	GLU	OE1-CD-OE2	6.77	131.43	123.30
1	B	317	GLU	OE1-CD-OE2	6.76	131.41	123.30
1	B	197	ASP	CB-CG-OD2	6.76	124.38	118.30
1	A	266	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	367	ARG	CD-NE-CZ	-6.70	114.22	123.60
1	A	281	VAL	CG1-CB-CG2	-6.69	100.19	110.90
1	B	49	VAL	CG1-CB-CG2	-6.69	100.20	110.90
1	A	13	THR	CA-CB-OG1	6.68	123.03	109.00
1	A	12	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	358	LEU	CA-CB-CG	6.67	130.64	115.30
1	B	274	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	256	ALA	N-CA-CB	6.65	119.41	110.10
1	C	356	ARG	NE-CZ-NH2	6.63	123.62	120.30
1	A	41	ARG	NH1-CZ-NH2	6.56	126.62	119.40
1	D	284	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	217	GLU	OE1-CD-OE2	-6.54	115.46	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ILE	O-C-N	-6.51	112.28	122.70
1	B	302	ARG	CD-NE-CZ	6.50	132.70	123.60
1	D	12	ARG	CG-CD-NE	6.46	125.36	111.80
1	B	11	ALA	O-C-N	6.45	133.02	122.70
1	B	339	VAL	CA-CB-CG2	6.45	120.58	110.90
1	A	196	LYS	O-C-N	-6.45	112.38	122.70
1	B	11	ALA	N-CA-CB	6.44	119.12	110.10
1	A	19	ASN	C-N-CA	6.44	135.83	122.30
1	B	49	VAL	CA-CB-CG1	6.37	120.45	110.90
1	B	4	SER	N-CA-CB	6.31	119.97	110.50
1	A	49	VAL	CG1-CB-CG2	-6.26	100.89	110.90
1	A	57	VAL	O-C-N	6.25	132.71	122.70
1	A	309	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	14	ALA	CB-CA-C	-6.25	100.73	110.10
1	A	178	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	B	116	MET	O-C-N	6.23	132.66	122.70
1	B	266	ARG	CD-NE-CZ	6.20	132.28	123.60
1	D	284	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	302	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	C	348	HIS	N-CA-CB	-6.18	99.47	110.60
1	B	302	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	253	ALA	CB-CA-C	6.17	119.36	110.10
1	D	82	ALA	CB-CA-C	6.17	119.35	110.10
1	A	367	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	210	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	70	ALA	O-C-N	-6.08	112.97	122.70
1	B	267	ARG	CD-NE-CZ	-6.05	115.13	123.60
1	A	279	ALA	CB-CA-C	-6.02	101.07	110.10
1	A	57	VAL	CA-CB-CG2	-5.99	101.92	110.90
1	B	339	VAL	N-CA-CB	-5.95	98.40	111.50
1	A	39	LEU	CA-CB-CG	5.92	128.93	115.30
1	C	356	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	B	378	CYS	O-C-N	-5.88	113.29	122.70
1	C	267	ARG	CD-NE-CZ	5.88	131.83	123.60
1	B	194	ARG	CD-NE-CZ	5.85	131.78	123.60
1	C	172	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	47	GLY	O-C-N	-5.83	113.36	122.70
1	A	230	LYS	N-CA-CB	-5.83	100.11	110.60
1	B	172	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	C	298	LYS	CA-CB-CG	5.77	126.09	113.40
1	A	39	LEU	CB-CG-CD1	5.76	120.80	111.00
1	A	152	PHE	CB-CG-CD1	-5.75	116.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	LEU	CB-CG-CD2	5.75	120.77	111.00
1	B	51	GLU	O-C-N	-5.74	113.52	122.70
1	B	162	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	B	258	LEU	CB-CG-CD2	5.74	120.75	111.00
1	B	362	LEU	CB-CG-CD2	-5.73	101.25	111.00
1	A	12	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	B	119	MET	CA-CB-CG	-5.72	103.58	113.30
1	B	187	GLU	CG-CD-OE1	-5.71	106.87	118.30
1	D	368	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	247	SER	N-CA-CB	5.71	119.06	110.50
1	A	42	ALA	N-CA-CB	-5.68	102.14	110.10
1	B	364	GLU	CG-CD-OE1	5.67	129.64	118.30
1	D	311	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	371	ARG	CD-NE-CZ	5.64	131.49	123.60
1	B	5	ILE	CB-CA-C	-5.63	100.34	111.60
1	A	4	SER	CA-C-N	5.62	129.57	117.20
1	B	102	GLN	CG-CD-OE1	-5.62	110.35	121.60
1	B	357	ILE	CA-C-N	5.61	129.53	117.20
1	A	364	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	C	59	PRO	CB-CA-C	-5.60	98.00	112.00
1	B	368	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	C	139	MET	N-CA-C	-5.58	95.93	111.00
1	A	333	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	187	GLU	CB-CG-CD	-5.58	99.15	114.20
1	A	339	VAL	CB-CA-C	5.55	121.94	111.40
1	B	314	GLU	OE1-CD-OE2	-5.54	116.64	123.30
1	A	99	GLY	CA-C-O	5.47	130.45	120.60
1	B	258	LEU	CB-CA-C	-5.46	99.82	110.20
1	B	198	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	B	276	VAL	CA-CB-CG2	5.42	119.03	110.90
1	A	186	ALA	O-C-N	5.40	131.34	122.70
1	C	367	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	329	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	C	58	LEU	N-CA-CB	-5.37	99.65	110.40
1	A	277	SER	O-C-N	5.37	131.29	122.70
1	A	364	GLU	CG-CD-OE1	5.34	128.99	118.30
1	A	4	SER	CA-C-O	-5.34	108.88	120.10
1	A	112	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	A	220	ARG	N-CA-CB	5.32	120.18	110.60
1	B	86	ASN	CB-CG-ND2	5.30	129.41	116.70
1	B	348	HIS	N-CA-CB	-5.29	101.08	110.60
1	B	322	GLN	CA-CB-CG	5.26	124.97	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	ARG	CD-NE-CZ	5.26	130.96	123.60
1	A	372	LYS	CD-CE-NZ	-5.24	99.65	111.70
1	A	278	TRP	CB-CG-CD2	-5.21	119.83	126.60
1	B	255	ALA	O-C-N	5.21	131.03	122.70
1	B	94	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	178	PHE	CB-CG-CD2	5.20	124.44	120.80
1	A	27	ALA	N-CA-CB	-5.20	102.83	110.10
1	B	297	ARG	CD-NE-CZ	5.17	130.84	123.60
1	D	143	MET	CG-SD-CE	5.17	108.47	100.20
1	B	260	SER	N-CA-CB	5.16	118.23	110.50
1	C	139	MET	N-CA-CB	5.13	119.83	110.60
1	A	54	LEU	CA-C-O	5.12	130.85	120.10
1	A	116	MET	CG-SD-CE	5.11	108.38	100.20
1	B	377	LEU	O-C-N	5.11	130.88	122.70
1	A	228	MET	N-CA-CB	-5.10	101.42	110.60
1	A	343	ALA	CA-C-N	5.10	128.42	117.20
1	D	129	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	309	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	54	LEU	CA-CB-CG	-5.09	103.59	115.30
1	B	39	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	29	GLU	O-C-N	-5.06	114.60	122.70
1	A	126	ALA	N-CA-CB	5.06	117.18	110.10
1	A	278	TRP	CB-CG-CD1	5.06	133.57	127.00
1	B	265	SER	CB-CA-C	5.05	119.69	110.10
1	B	277	SER	O-C-N	5.04	130.76	122.70
1	C	95	ALA	CB-CA-C	-5.04	102.54	110.10
1	C	129	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	143	MET	CA-CB-CG	5.02	121.83	113.30
1	A	361	LEU	CB-CG-CD2	5.01	119.51	111.00

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	2816	0	2821	69	0
1	B	2816	0	2821	61	0
1	C	2816	0	2821	70	0
1	D	2816	0	2821	88	0
2	A	15	0	0	0	0
2	B	15	0	0	2	0
3	A	48	0	32	4	0
3	B	48	0	31	0	0
3	C	48	0	31	1	0
3	D	48	0	31	1	0
4	A	287	0	0	10	0
4	B	275	0	0	19	0
4	C	94	0	0	6	0
4	D	62	0	0	7	0
All	All	12204	0	11409	277	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 12.

All (277) 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:A:258:LEU:HG	4:A:770:HOH:O	1.45	1.12
1:B:258:LEU:HG	4:B:939:HOH:O	1.53	1.07
1:D:88:LEU:HB3	1:D:89:SCY:HE2	1.39	1.03
1:D:89:SCY:HE1	1:D:380:GLY:H	1.24	1.03
1:D:258:LEU:HG	4:D:421:HOH:O	1.62	0.98
1:C:89:SCY:HE1	1:C:380:GLY:H	1.31	0.92
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.30	0.92
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.11	0.85
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.39	0.84
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.58	0.84
1:B:247:SER:HB2	4:B:840:HOH:O	1.77	0.83
1:D:89:SCY:CE	1:D:380:GLY:H	1.94	0.79
1:B:390:GLU:OE2	4:B:961:HOH:O	2.01	0.79
1:C:89:SCY:CE	1:C:380:GLY:H	1.96	0.79
1:D:89:SCY:HE1	1:D:380:GLY:N	1.97	0.79
1:B:134:MET:HG3	4:C:401:HOH:O	1.81	0.78
1:A:89:SCY:HE1	1:A:380:GLY:H	1.47	0.78
1:A:175:GLN:HE22	1:A:240:THR:CG2	1.95	0.77
1:B:372:LYS:HE3	4:B:928:HOH:O	1.84	0.77
1:A:387:MET:SD	4:A:887:HOH:O	2.43	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:CB	1:D:89:SCY:HE2	2.15	0.75
1:D:300:LEU:HD21	1:D:310:LEU:HD11	1.67	0.74
1:B:89:SCY:HE1	1:B:380:GLY:H	1.52	0.74
1:D:88:LEU:HB3	1:D:89:SCY:CE	2.14	0.73
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.71	0.72
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.54	0.72
1:C:89:SCY:HE1	1:C:380:GLY:N	2.04	0.72
1:D:298:LYS:HE2	1:D:302:ARG:HG3	1.72	0.72
1:A:88:LEU:HB3	1:A:89:SCY:HE2	1.73	0.70
1:A:298:LYS:HA	1:A:298:LYS:NZ	2.07	0.70
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.57	0.70
1:B:356:ARG:HD2	1:B:356:ARG:C	2.13	0.69
1:A:279:ALA:HB1	1:A:298:LYS:HG3	1.75	0.69
1:D:290:THR:HA	4:D:444:HOH:O	1.92	0.68
1:A:247:SER:HB2	4:A:951:HOH:O	1.93	0.67
1:B:392:LEU:HD12	4:B:854:HOH:O	1.95	0.67
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.76	0.67
1:A:279:ALA:CB	1:A:298:LYS:HG3	2.25	0.66
1:D:326:VAL:HG22	4:D:444:HOH:O	1.95	0.66
1:D:203:ILE:HB	4:D:448:HOH:O	1.95	0.66
1:D:89:SCY:H	1:D:89:SCY:HE2	1.61	0.65
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.61	0.65
1:B:392:LEU:HB2	4:B:854:HOH:O	1.96	0.65
1:A:163:ASN:HA	1:A:166:LYS:NZ	2.12	0.65
1:A:12:ARG:HD2	1:A:356:ARG:HG2	1.79	0.65
1:B:41:ARG:HD2	4:B:907:HOH:O	1.96	0.65
1:B:257:LEU:HD23	1:B:258:LEU:N	2.11	0.64
1:B:5:ILE:HG13	1:B:100:MET:HG2	1.79	0.64
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.11	0.64
1:A:225:LEU:HG	4:A:926:HOH:O	1.98	0.63
1:A:358:LEU:HD21	1:A:387:MET:HE3	1.78	0.63
1:B:4:SER:CA	4:B:999:HOH:O	2.46	0.63
1:D:322:GLN:O	1:D:326:VAL:HG23	1.99	0.63
1:B:88:LEU:HB3	1:B:89:SCY:HE2	1.82	0.62
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.62	0.62
1:D:88:LEU:HB2	1:D:379:ILE:HG23	1.80	0.62
1:A:89:SCY:CE	1:A:380:GLY:H	2.12	0.61
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.13	0.61
1:B:186:ALA:HA	1:B:340:ASN:O	2.00	0.61
1:A:247:SER:HB2	1:A:348:HIS:HB2	1.83	0.60
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SCY:HE1	1:A:380:GLY:N	2.16	0.60
1:D:55:GLY:HA2	1:D:85:MET:O	2.01	0.60
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.37	0.60
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.14	0.59
1:C:207:ARG:HH11	1:C:207:ARG:HG2	1.68	0.59
1:A:52:VAL:O	1:A:82:ALA:HA	2.03	0.58
1:B:41:ARG:HB2	4:B:907:HOH:O	2.02	0.58
1:A:191:LYS:NZ	4:A:736:HOH:O	2.36	0.58
1:C:236:ASP:HB3	1:C:239:GLY:HA3	1.86	0.58
1:D:97:ALA:O	1:D:101:GLN:HG3	2.04	0.58
1:C:37:ALA:HB2	1:C:200:VAL:HG21	1.86	0.57
1:A:163:ASN:HA	1:A:166:LYS:HZ1	1.70	0.57
1:C:89:SCY:SG	1:C:350:ILE:HG23	2.44	0.57
1:A:133:LYS:HA	4:C:464:HOH:O	2.04	0.57
1:C:129:ARG:NH2	1:D:122:ALA:O	2.35	0.56
1:B:257:LEU:C	1:B:257:LEU:HD23	2.26	0.56
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.87	0.56
1:A:40:GLU:HG3	4:A:1010:HOH:O	2.05	0.56
1:B:348:HIS:HB2	4:B:840:HOH:O	2.05	0.56
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.87	0.56
1:C:41:ARG:NH1	1:C:197:ASP:O	2.39	0.56
1:B:41:ARG:CD	4:B:907:HOH:O	2.53	0.56
1:D:358:LEU:HD22	1:D:362:LEU:HG	1.88	0.56
1:B:4:SER:N	4:B:999:HOH:O	2.38	0.56
1:B:89:SCY:HE1	1:B:380:GLY:N	2.21	0.55
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.88	0.55
1:D:9:SER:HA	1:D:272:LEU:CD2	2.36	0.55
1:A:228:MET:HE3	1:A:244:GLY:HA3	1.87	0.55
1:A:12:ARG:O	1:A:199:ILE:HA	2.07	0.54
1:B:4:SER:CB	4:B:999:HOH:O	2.55	0.54
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.71	0.54
1:B:356:ARG:HD2	1:B:356:ARG:O	2.06	0.54
1:A:9:SER:HA	1:A:272:LEU:HD22	1.90	0.54
1:D:275:ILE:HA	1:D:389:ILE:HD13	1.90	0.54
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.56	0.54
1:A:206:GLY:HA3	1:A:209:GLY:O	2.08	0.54
1:A:298:LYS:HA	1:A:298:LYS:HZ3	1.70	0.54
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.73	0.54
1:C:129:ARG:HD3	1:D:18:PHE:CZ	2.43	0.53
1:D:311:ASP:HB2	1:D:370:ALA:HB1	1.89	0.53
1:D:291:GLY:O	1:D:294:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LYS:HD3	4:D:426:HOH:O	2.08	0.53
1:B:132:VAL:O	1:D:129:ARG:HA	2.08	0.53
1:B:50:ASN:HB3	4:B:953:HOH:O	2.08	0.53
1:C:103:ILE:HA	1:C:108:ALA:O	2.07	0.53
1:C:168:TRP:CH2	1:C:329:ASP:HB2	2.43	0.53
1:D:314:GLU:OE2	1:D:338:ASN:HA	2.09	0.53
1:A:34:VAL:HG12	1:A:255:ALA:HB3	1.90	0.53
1:C:374:LEU:C	1:C:374:LEU:HD23	2.29	0.53
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.91	0.52
1:D:187:GLU:HG3	1:D:221:HIS:HA	1.91	0.52
1:D:258:LEU:N	1:D:258:LEU:HD22	2.24	0.52
1:D:180:VAL:HG22	1:D:228:MET:HE3	1.90	0.52
1:A:372:LYS:HE3	4:A:922:HOH:O	2.08	0.52
1:C:300:LEU:HD13	1:C:307:ILE:HG12	1.90	0.52
1:B:316:ASN:HB3	4:B:744:HOH:O	2.09	0.52
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.45	0.52
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.45	0.52
1:D:263:GLU:OE1	1:D:266:ARG:NH1	2.43	0.52
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.91	0.52
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.30	0.51
1:B:237:LYS:HB2	4:B:855:HOH:O	2.09	0.51
1:B:293:ILE:HB	1:B:294:PRO:HD3	1.91	0.51
1:C:272:LEU:HG	4:C:430:HOH:O	2.10	0.51
1:A:207:ARG:HG2	1:A:208:LYS:H	1.75	0.51
1:B:89:SCY:CE	1:B:380:GLY:H	2.21	0.51
1:C:293:ILE:HB	1:C:294:PRO:HD3	1.93	0.51
1:B:88:LEU:HB2	1:B:379:ILE:HG23	1.93	0.51
1:D:206:GLY:HA3	1:D:209:GLY:O	2.10	0.51
1:A:258:LEU:HD22	1:A:258:LEU:N	2.26	0.51
1:C:12:ARG:HA	1:C:254:ALA:HA	1.93	0.51
1:B:236:ASP:O	1:B:239:GLY:N	2.43	0.51
1:B:4:SER:N	4:B:862:HOH:O	2.43	0.51
1:D:35:ILE:O	1:D:38:VAL:HG22	2.11	0.51
1:B:89:SCY:H	1:B:89:SCY:HE2	1.75	0.50
1:C:207:ARG:HG2	1:C:208:LYS:H	1.77	0.50
1:C:39:LEU:HD12	1:C:44:VAL:O	2.12	0.50
1:B:293:ILE:HB	1:B:294:PRO:CD	2.41	0.50
1:C:293:ILE:HB	1:C:294:PRO:CD	2.41	0.50
1:A:298:LYS:HA	1:A:298:LYS:HZ2	1.77	0.50
1:B:207:ARG:HG2	1:B:208:LYS:H	1.75	0.50
1:C:122:ALA:O	1:D:129:ARG:NH2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ARG:HG2	1:D:208:LYS:H	1.77	0.50
1:B:134:MET:O	1:B:134:MET:HG2	2.11	0.50
1:A:305:TRP:CZ3	1:A:388:CYS:HB3	2.47	0.50
1:D:18:PHE:O	1:D:19:ASN:HB2	2.12	0.50
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.47	0.50
1:C:187:GLU:OE1	1:C:191:LYS:HE2	2.11	0.50
1:A:85:MET:HA	1:B:85:MET:HA	1.94	0.49
1:C:145:LYS:O	1:D:63:GLY:HA2	2.12	0.49
1:A:93:LEU:HD11	1:A:387:MET:CE	2.43	0.49
1:B:89:SCY:SG	1:B:350:ILE:HG23	2.53	0.49
1:A:258:LEU:CG	4:A:770:HOH:O	2.27	0.49
1:C:353:SER:O	1:C:357:ILE:HG23	2.13	0.49
1:C:305:TRP:CE2	1:C:372:LYS:HD3	2.47	0.49
1:D:195:PHE:O	1:D:198:GLU:HG2	2.12	0.49
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.95	0.49
1:C:258:LEU:N	1:C:258:LEU:HD22	2.26	0.49
4:B:899:HOH:O	1:C:145:LYS:HB2	2.12	0.48
1:D:272:LEU:HD21	4:D:430:HOH:O	2.12	0.48
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.47	0.48
1:B:257:LEU:C	1:B:257:LEU:CD2	2.82	0.48
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.48	0.48
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.75	0.48
1:A:371:ARG:HG3	4:A:932:HOH:O	2.12	0.48
1:C:176:ASP:CG	1:C:228:MET:HG3	2.34	0.48
1:D:276:VAL:HG11	1:D:305:TRP:CZ2	2.49	0.48
1:C:312:LEU:HD21	1:C:364:GLU:HB3	1.95	0.47
1:A:257:LEU:C	1:A:257:LEU:HD23	2.35	0.47
1:B:9:SER:HA	1:B:272:LEU:HD22	1.95	0.47
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.30	0.47
1:B:260:SER:OG	2:B:721:SO4:O2	2.24	0.47
1:C:143:MET:CG	4:C:421:HOH:O	2.61	0.47
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.50	0.47
1:A:314:GLU:O	1:A:375:ALA:HA	2.15	0.47
1:B:298:LYS:HE2	2:B:719:SO4:O1	2.13	0.47
1:D:240:THR:HA	4:D:436:HOH:O	2.14	0.47
1:D:64:GLN:O	1:D:65:ASN:C	2.53	0.47
1:A:280:THR:HG23	1:B:81:THR:HG21	1.97	0.47
1:A:374:LEU:HD21	1:A:376:THR:HB	1.97	0.46
1:C:189:ALA:CB	1:C:340:ASN:HB3	2.46	0.46
1:C:89:SCY:OCD	3:C:393:COA:S1P	2.72	0.46
1:D:292:PRO:HD3	1:D:378:CYS:CA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:393:COA:H2B	3:A:393:COA:H52A	1.54	0.46
1:C:305:TRP:CZ3	1:C:372:LYS:HB3	2.51	0.46
1:C:311:ASP:HB2	1:C:370:ALA:HB1	1.97	0.46
1:C:312:LEU:HD23	1:C:361:LEU:CD2	2.46	0.46
1:D:175:GLN:HB3	1:D:320:ALA:HB3	1.96	0.46
1:B:350:ILE:HG21	1:B:350:ILE:HD13	1.69	0.45
1:C:175:GLN:HB3	1:C:320:ALA:HB3	1.97	0.45
1:C:206:GLY:HA3	1:C:209:GLY:O	2.16	0.45
1:A:243:ALA:CB	3:A:393:COA:H51A	2.46	0.45
1:C:186:ALA:HA	1:C:340:ASN:O	2.17	0.45
1:D:110:ILE:HG23	1:D:257:LEU:HD21	1.98	0.45
1:A:88:LEU:HB2	1:A:379:ILE:HG23	1.98	0.45
1:C:38:VAL:HG21	1:C:112:VAL:HG13	1.98	0.45
1:D:361:LEU:HD22	1:D:365:MET:SD	2.57	0.45
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.69	0.45
1:C:49:VAL:HB	1:C:76:VAL:HG13	1.99	0.45
1:C:125:CYS:HA	1:D:124:HIS:O	2.16	0.45
1:A:168:TRP:O	1:A:169:GLN:HB2	2.16	0.45
1:C:297:ARG:NH1	1:C:297:ARG:HG2	2.30	0.45
1:C:364:GLU:O	1:C:368:ARG:HG2	2.17	0.45
1:D:207:ARG:HD3	1:D:207:ARG:N	2.32	0.45
1:C:309:ASP:HB3	1:C:372:LYS:HD2	1.99	0.45
1:D:354:GLY:HA2	1:D:377:LEU:HD21	1.99	0.45
1:A:160:THR:O	1:A:164:VAL:HG23	2.16	0.45
1:A:379:ILE:HB	1:A:383:MET:HB2	2.00	0.44
1:C:268:GLY:HA2	4:C:486:HOH:O	2.17	0.44
1:D:293:ILE:N	1:D:294:PRO:HD2	2.32	0.44
1:D:28:HIS:ND1	1:D:62:GLU:OE2	2.42	0.44
1:C:281:VAL:HG12	1:C:282:GLY:N	2.32	0.44
1:C:143:MET:HB2	4:C:421:HOH:O	2.16	0.44
1:C:78:GLN:NE2	1:D:284:ASP:HA	2.32	0.44
1:D:117:GLU:OE2	1:D:351:GLY:N	2.50	0.44
1:D:293:ILE:HG21	1:D:329:ASP:OD2	2.17	0.44
1:C:330:LEU:HD13	1:C:332:TRP:CH2	2.52	0.44
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.53	0.44
1:B:358:LEU:O	1:B:362:LEU:HG	2.17	0.44
1:C:110:ILE:HG23	1:C:257:LEU:HD21	2.00	0.44
1:A:247:SER:OG	3:A:393:COA:H61	2.18	0.43
1:C:226:ASP:O	1:C:230:LYS:HG3	2.18	0.43
1:D:28:HIS:HA	1:D:116:MET:SD	2.58	0.43
1:D:333:ASP:HA	1:D:334:PRO:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:GLY:N	1:D:79:GLU:O	2.47	0.43
1:A:133:LYS:H	1:A:133:LYS:HG2	1.67	0.43
1:D:233:PRO:HB2	1:D:236:ASP:O	2.18	0.43
1:A:131:GLY:HA2	1:C:131:GLY:HA2	2.00	0.43
1:C:157:MET:HA	1:C:160:THR:HG23	2.00	0.43
1:B:38:VAL:HA	4:B:907:HOH:O	2.18	0.43
1:D:364:GLU:O	1:D:368:ARG:HG2	2.19	0.43
1:A:124:HIS:HA	1:A:140:ILE:O	2.17	0.42
1:A:358:LEU:O	1:A:362:LEU:HG	2.18	0.42
1:B:28:HIS:ND1	1:B:62:GLU:OE2	2.40	0.42
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.37	0.42
1:D:157:MET:HG3	3:D:393:COA:S1P	2.59	0.42
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.81	0.42
1:B:379:ILE:HB	1:B:383:MET:HB2	2.00	0.42
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.51	0.42
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.53	0.42
1:D:89:SCY:O	1:D:377:LEU:HD22	2.20	0.42
1:A:291:GLY:N	1:A:292:PRO:CD	2.82	0.42
1:B:371:ARG:HH11	1:B:371:ARG:HD2	1.55	0.42
1:C:333:ASP:O	1:C:334:PRO:C	2.57	0.42
1:D:339:VAL:HG12	1:D:340:ASN:OD1	2.20	0.42
1:B:291:GLY:N	1:B:292:PRO:CD	2.83	0.42
1:A:236:ASP:O	1:A:237:LYS:C	2.57	0.42
1:A:18:PHE:HB2	1:A:249:LEU:O	2.20	0.42
1:D:183:GLN:HA	1:D:345:ALA:HB2	2.02	0.42
1:D:12:ARG:HA	1:D:254:ALA:HA	2.01	0.42
1:B:187:GLU:O	1:B:191:LYS:HG3	2.20	0.41
1:C:64:GLN:HE22	1:D:157:MET:CE	2.32	0.41
1:C:89:SCY:HE2	1:C:89:SCY:H	1.85	0.41
1:C:9:SER:HA	1:C:272:LEU:HD22	2.02	0.41
1:C:293:ILE:CB	1:C:294:PRO:CD	2.98	0.41
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.84	0.41
1:D:185:LYS:HD2	1:D:339:VAL:O	2.19	0.41
1:D:269:ILE:O	1:D:271:PRO:HD3	2.21	0.41
1:A:243:ALA:HB3	3:A:393:COA:H51A	2.01	0.41
1:B:156:HIS:ND1	1:B:157:MET:N	2.69	0.41
1:D:143:MET:HE1	1:D:249:LEU:HD13	2.03	0.41
1:A:7:ILE:HG23	1:A:256:ALA:HB1	2.03	0.41
1:B:236:ASP:O	1:B:237:LYS:C	2.59	0.41
1:C:195:PHE:O	1:C:198:GLU:HG2	2.21	0.41
1:B:5:ILE:CG1	1:B:100:MET:HG2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:HIS:ND1	1:D:157:MET:N	2.69	0.41
1:D:25:THR:HA	1:D:26:PRO:HD3	1.86	0.41
1:D:187:GLU:OE1	1:D:191:LYS:HG3	2.21	0.40
1:D:6:VAL:HG22	1:D:259:MET:O	2.21	0.40
1:A:191:LYS:HE2	1:A:191:LYS:HB3	1.86	0.40
1:A:225:LEU:CG	4:A:926:HOH:O	2.64	0.40
1:B:64:GLN:O	1:B:65:ASN:C	2.60	0.40
1:C:314:GLU:O	1:C:375:ALA:HA	2.21	0.40
1:D:280:THR:HA	1:D:384:GLY:O	2.21	0.40
1:C:350:ILE:HD13	1:C:350:ILE:HG21	1.86	0.40
1:D:89:SCY:HE1	1:D:380:GLY:CA	2.51	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	386/389 (99%)	374 (97%)	11 (3%)	1 (0%)	44	33
1	B	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	44	33
1	C	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	44	33
1	D	386/389 (99%)	366 (95%)	15 (4%)	5 (1%)	14	4
All	All	1544/1556 (99%)	1480 (96%)	56 (4%)	8 (0%)	32	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	B	350	ILE
1	D	23	ALA

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Mol	Chain	Res	Type
1	D	80	ALA
1	A	350	ILE
1	D	291	GLY
1	D	65	ASN

### 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	275/275 (100%)	248 (90%)	27 (10%)	9	3
1	B	275/275 (100%)	249 (90%)	26 (10%)	10	3
1	C	275/275 (100%)	255 (93%)	20 (7%)	16	6
1	D	275/275 (100%)	255 (93%)	20 (7%)	16	6
All	All	1100/1100 (100%)	1007 (92%)	93 (8%)	12	4

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	59	PRO
1	A	85	MET
1	A	123	PRO
1	A	133	LYS
1	A	155	TYR
1	A	191	LYS
1	A	207	ARG
1	A	220	ARG
1	A	221	HIS
1	A	225	LEU
1	A	230	LYS
1	A	232	ARG
1	A	237	LYS
1	A	240	THR
1	A	263	GLU
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	339	VAL
1	A	348	HIS
1	A	353	SER
1	A	358	LEU
1	A	361	LEU
1	B	4	SER
1	B	39	LEU
1	B	134	MET
1	B	187	GLU
1	B	207	ARG
1	B	220	ARG
1	B	232	ARG
1	B	240	THR
1	B	257	LEU
1	B	258	LEU
1	B	263	GLU
1	B	265	SER
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	297	ARG
1	B	298	LYS
1	B	322	GLN
1	B	328	LYS
1	B	332	TRP
1	B	339	VAL
1	B	348	HIS
1	B	356	ARG
1	B	358	LEU
1	B	361	LEU
1	B	366	LYS
1	C	4	SER
1	C	39	LEU
1	C	40	GLU
1	C	155	TYR
1	C	160	THR
1	C	207	ARG

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Mol	Chain	Res	Type
1	C	224	THR
1	C	237	LYS
1	C	272	LEU
1	C	276	VAL
1	C	288	MET
1	C	298	LYS
1	C	307	ILE
1	C	322	GLN
1	C	332	TRP
1	C	339	VAL
1	C	353	SER
1	C	358	LEU
1	C	361	LEU
1	C	371	ARG
1	D	39	LEU
1	D	155	TYR
1	D	187	GLU
1	D	207	ARG
1	D	224	THR
1	D	257	LEU
1	D	258	LEU
1	D	265	SER
1	D	272	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	328	LYS
1	D	332	TRP
1	D	358	LEU
1	D	360	THR
1	D	361	LEU
1	D	367	ARG
1	D	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	B	175	GLN
1	B	184	ASN

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Mol	Chain	Res	Type
1	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	D	78	GLN
1	D	175	GLN
1	D	316	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	89	1	8,8,9	1.17	1 (12%)	4,9,11	1.19	0
1	SCY	B	89	1	8,8,9	1.42	2 (25%)	4,9,11	1.54	1 (25%)
1	SCY	C	89	1	8,8,9	1.44	1 (12%)	4,9,11	1.48	1 (25%)
1	SCY	D	89	1	8,8,9	1.13	1 (12%)	4,9,11	0.97	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	89	1	-	0/5/7/9	0/0/0/0
1	SCY	B	89	1	-	0/5/7/9	0/0/0/0
1	SCY	C	89	1	-	0/5/7/9	0/0/0/0
1	SCY	D	89	1	-	0/5/7/9	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	SCY	CB-SG	-3.43	1.77	1.81
1	B	89	SCY	CA-C	-2.29	1.47	1.50
1	B	89	SCY	CB-CA	2.08	1.58	1.53
1	A	89	SCY	CB-CA	2.45	1.59	1.53
1	D	89	SCY	CA-C	2.79	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	SCY	O-C-CA	-2.84	117.17	125.02
1	B	89	SCY	O-C-CA	-2.64	117.72	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	89	SCY	4	0
1	B	89	SCY	6	0
1	C	89	SCY	6	0
1	D	89	SCY	9	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	COA	A	393	-	43,50,50	2.06	14 (32%)	48,75,75	2.89	17 (35%)
2	SO4	A	720	-	4,4,4	0.60	0	6,6,6	0.11	0
2	SO4	A	722	-	4,4,4	0.72	0	6,6,6	0.36	0
2	SO4	A	723	-	4,4,4	0.95	0	6,6,6	0.62	0
3	COA	B	393	-	43,50,50	1.73	6 (13%)	48,75,75	2.70	16 (33%)
2	SO4	B	719	-	4,4,4	0.78	0	6,6,6	0.22	0
2	SO4	B	721	-	4,4,4	0.68	0	6,6,6	0.61	0
2	SO4	B	724	-	4,4,4	0.68	0	6,6,6	0.42	0
3	COA	C	393	-	43,50,50	1.96	10 (23%)	48,75,75	2.07	12 (25%)
3	COA	D	393	-	43,50,50	1.98	11 (25%)	48,75,75	2.02	8 (16%)

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	COA	A	393	-	-	0/44/64/64	0/3/3/3
2	SO4	A	720	-	-	0/0/0/0	0/0/0/0
2	SO4	A	722	-	-	0/0/0/0	0/0/0/0
2	SO4	A	723	-	-	0/0/0/0	0/0/0/0
3	COA	B	393	-	-	0/44/64/64	0/3/3/3
2	SO4	B	719	-	-	0/0/0/0	0/0/0/0
2	SO4	B	721	-	-	0/0/0/0	0/0/0/0
2	SO4	B	724	-	-	0/0/0/0	0/0/0/0
3	COA	C	393	-	-	0/44/64/64	0/3/3/3
3	COA	D	393	-	-	0/44/64/64	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	393	COA	C9P-N8P	-3.17	1.27	1.33
3	D	393	COA	C7P-N8P	-2.35	1.40	1.46
3	D	393	COA	C9P-N8P	-2.33	1.28	1.33
3	C	393	COA	C9P-N8P	-2.31	1.28	1.33
3	A	393	COA	C7P-C6P	-2.30	1.43	1.51
3	A	393	COA	C4A-N3A	-2.03	1.32	1.35
3	A	393	COA	CDP-CBP	2.03	1.58	1.53
3	C	393	COA	O4B-C4B	2.16	1.49	1.45
3	B	393	COA	O4B-C4B	2.18	1.50	1.45
3	A	393	COA	O5P-C5P	2.32	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	393	COA	O4B-C4B	2.37	1.50	1.45
3	C	393	COA	C2A-N1A	2.42	1.38	1.33
3	D	393	COA	C2A-N1A	2.43	1.38	1.33
3	A	393	COA	C2A-N1A	2.46	1.38	1.33
3	B	393	COA	C3P-N4P	2.46	1.51	1.46
3	D	393	COA	O4B-C4B	2.48	1.50	1.45
3	D	393	COA	CCP-CBP	2.49	1.56	1.52
3	A	393	COA	C2A-N3A	2.55	1.36	1.32
3	B	393	COA	P3B-O7A	2.56	1.59	1.50
3	C	393	COA	CCP-CBP	2.62	1.56	1.52
3	A	393	COA	P2A-O6A	2.68	1.70	1.59
3	A	393	COA	OAP-CAP	2.69	1.47	1.42
3	D	393	COA	P3B-O7A	2.76	1.60	1.50
3	C	393	COA	P3B-O7A	2.79	1.60	1.50
3	C	393	COA	O4B-C1B	3.00	1.45	1.41
3	A	393	COA	C3P-N4P	3.10	1.53	1.46
3	D	393	COA	O5P-C5P	3.12	1.29	1.23
3	A	393	COA	P3B-O7A	3.21	1.61	1.50
3	D	393	COA	C3P-N4P	3.31	1.53	1.46
3	C	393	COA	O5P-C5P	3.52	1.30	1.23
3	A	393	COA	CCP-CBP	3.55	1.57	1.52
3	C	393	COA	C3P-N4P	3.72	1.54	1.46
3	D	393	COA	O4B-C1B	3.89	1.46	1.41
3	B	393	COA	P3B-O3B	4.44	1.67	1.59
3	C	393	COA	P3B-O3B	4.51	1.67	1.59
3	A	393	COA	P3B-O3B	4.72	1.67	1.59
3	D	393	COA	P3B-O3B	5.01	1.68	1.59
3	B	393	COA	O9P-C9P	5.39	1.34	1.23
3	D	393	COA	O9P-C9P	6.44	1.36	1.23
3	A	393	COA	O9P-C9P	6.55	1.36	1.23
3	C	393	COA	O9P-C9P	6.71	1.36	1.23

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393	COA	C2P-C3P-N4P	-10.16	90.40	112.50
3	B	393	COA	C6P-C5P-N4P	-8.06	102.59	116.49
3	D	393	COA	C4B-O4B-C1B	-6.03	103.35	109.77
3	A	393	COA	C7P-N8P-C9P	-5.94	111.51	122.59
3	B	393	COA	C2P-C3P-N4P	-5.75	99.99	112.50
3	A	393	COA	O6A-CCP-CBP	-5.75	101.31	110.55
3	D	393	COA	CEP-CBP-CCP	-5.04	100.96	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393	COA	C2B-C3B-C4B	-4.69	94.84	103.23
3	C	393	COA	C2P-C3P-N4P	-4.57	102.55	112.50
3	A	393	COA	O4B-C4B-C5B	-4.25	95.07	109.40
3	A	393	COA	C6P-C5P-N4P	-4.14	109.35	116.49
3	C	393	COA	C4B-O4B-C1B	-4.04	105.47	109.77
3	B	393	COA	O6A-CCP-CBP	-4.00	104.11	110.55
3	C	393	COA	CEP-CBP-CCP	-3.62	103.05	108.37
3	B	393	COA	N3A-C2A-N1A	-3.51	125.80	128.86
3	A	393	COA	C4B-O4B-C1B	-3.25	106.31	109.77
3	A	393	COA	O5B-C5B-C4B	-2.96	98.49	109.00
3	C	393	COA	O6A-CCP-CBP	-2.85	105.97	110.55
3	B	393	COA	C4B-O4B-C1B	-2.52	107.08	109.77
3	B	393	COA	C2B-C3B-C4B	-2.43	98.89	103.23
3	C	393	COA	N3A-C2A-N1A	-2.35	126.81	128.86
3	C	393	COA	CAP-C9P-N8P	-2.30	111.80	116.58
3	A	393	COA	C5B-C4B-C3B	-2.08	107.23	114.30
3	D	393	COA	CAP-C9P-N8P	-2.02	112.39	116.58
3	D	393	COA	CEP-CBP-CAP	2.03	112.34	108.82
3	C	393	COA	C5B-C4B-C3B	2.18	121.69	114.30
3	A	393	COA	OAP-CAP-CBP	2.18	115.39	110.25
3	A	393	COA	CEP-CBP-CDP	2.19	113.83	109.19
3	A	393	COA	O9A-P3B-O8A	2.21	116.53	107.61
3	B	393	COA	O3B-C3B-C4B	2.24	118.44	110.04
3	B	393	COA	N6A-C6A-N1A	2.33	123.38	118.77
3	B	393	COA	OAP-CAP-CBP	2.41	115.92	110.25
3	C	393	COA	C4A-C5A-N7A	2.43	111.76	109.41
3	D	393	COA	C4A-C5A-N7A	2.67	111.99	109.41
3	C	393	COA	CDP-CBP-CCP	2.73	112.37	108.37
3	B	393	COA	C2A-N1A-C6A	2.77	123.61	118.77
3	A	393	COA	CEP-CBP-CAP	2.79	113.67	108.82
3	A	393	COA	C4A-C5A-N7A	2.82	112.14	109.41
3	C	393	COA	C6P-C5P-N4P	2.92	121.53	116.49
3	C	393	COA	CEP-CBP-CAP	2.94	113.92	108.82
3	B	393	COA	O9P-C9P-N8P	3.20	129.24	123.07
3	B	393	COA	C5B-C4B-C3B	3.23	125.23	114.30
3	A	393	COA	N6A-C6A-N1A	3.49	125.68	118.77
3	A	393	COA	CAP-C9P-N8P	3.50	123.86	116.58
3	D	393	COA	CDP-CBP-CCP	3.61	113.67	108.37
3	B	393	COA	C4A-C5A-N7A	3.83	113.11	109.41
3	D	393	COA	C6P-C7P-N8P	4.49	121.16	111.87
3	B	393	COA	O5P-C5P-C6P	5.56	132.46	122.01
3	B	393	COA	C7P-N8P-C9P	5.68	133.17	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	393	COA	C7P-N8P-C9P	6.61	134.90	122.59
3	A	393	COA	C6P-C7P-N8P	7.37	127.13	111.87
3	C	393	COA	C7P-N8P-C9P	7.43	136.44	122.59
3	B	393	COA	C7P-C6P-C5P	7.93	124.98	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	393	COA	4	0
2	B	719	SO4	1	0
2	B	721	SO4	1	0
3	C	393	COA	1	0
3	D	393	COA	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	388/389 (99%)	0.14	16 (4%) 38 42	12, 21, 44, 87	0
1	B	388/389 (99%)	0.21	18 (4%) 33 37	11, 20, 42, 97	0
1	C	388/389 (99%)	1.04	55 (14%) 3 3	25, 45, 77, 119	0
1	D	388/389 (99%)	1.52	99 (25%) 1 0	22, 52, 115, 138	0
All	All	1552/1556 (99%)	0.73	188 (12%) 5 5	11, 36, 84, 138	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	227	SER	9.9
1	D	237	LYS	9.8
1	B	206	GLY	8.2
1	C	237	LYS	7.9
1	D	226	ASP	7.4
1	D	229	ALA	7.3
1	C	224	THR	7.2
1	D	164	VAL	7.1
1	D	224	THR	6.7
1	D	230	LYS	6.6
1	C	227	SER	6.4
1	D	234	ALA	6.4
1	D	239	GLY	6.3
1	D	392	LEU	6.3
1	C	207	ARG	6.1
1	D	235	PHE	6.1
1	D	231	LEU	6.0
1	C	234	ALA	5.9
1	D	168	TRP	5.8
1	B	235	PHE	5.7
1	A	237	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	330	LEU	5.7
1	C	239	GLY	5.6
1	D	240	THR	5.6
1	D	225	LEU	5.6
1	D	238	GLU	5.5
1	C	232	ARG	5.5
1	C	235	PHE	5.5
1	D	208	LYS	5.5
1	D	207	ARG	5.4
1	C	233	PRO	5.2
1	D	170	LEU	5.2
1	D	228	MET	5.2
1	B	237	LYS	5.0
1	B	207	ARG	4.8
1	C	225	LEU	4.7
1	C	208	LYS	4.7
1	D	371	ARG	4.7
1	D	233	PRO	4.6
1	D	232	ARG	4.5
1	C	231	LEU	4.5
1	A	207	ARG	4.5
1	C	243	ALA	4.4
1	A	233	PRO	4.4
1	D	236	ASP	4.4
1	D	287	VAL	4.3
1	B	208	LYS	4.3
1	D	153	TYR	4.2
1	D	156	HIS	4.2
1	D	223	ALA	4.2
1	D	221	HIS	4.1
1	A	235	PHE	4.1
1	B	238	GLU	4.1
1	C	240	THR	4.1
1	D	181	ALA	4.1
1	C	229	ALA	4.0
1	D	219	ILE	4.0
1	D	165	ALA	4.0
1	D	323	ALA	3.9
1	C	228	MET	3.9
1	A	209	GLY	3.9
1	A	239	GLY	3.9
1	C	156	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	166	LYS	3.9
1	D	326	VAL	3.8
1	D	179	ALA	3.8
1	D	319	PHE	3.7
1	C	242	THR	3.6
1	D	178	PHE	3.6
1	C	223	ALA	3.6
1	A	234	ALA	3.5
1	D	325	ALA	3.5
1	C	180	VAL	3.5
1	A	206	GLY	3.5
1	C	238	GLU	3.5
1	B	227	SER	3.4
1	D	332	TRP	3.4
1	B	232	ARG	3.4
1	C	306	LYS	3.4
1	D	247	SER	3.3
1	D	382	GLY	3.3
1	C	392	LEU	3.3
1	C	230	LYS	3.3
1	C	173	ASP	3.3
1	D	174	GLU	3.2
1	A	238	GLU	3.2
1	B	239	GLY	3.2
1	B	134	MET	3.2
1	D	222	GLY	3.2
1	D	306	LYS	3.2
1	D	161	ALA	3.2
1	C	319	PHE	3.2
1	D	241	VAL	3.1
1	D	158	GLY	3.1
1	D	367	ARG	3.1
1	D	180	VAL	3.1
1	D	177	ALA	3.1
1	C	297	ARG	3.1
1	B	226	ASP	3.1
1	A	232	ARG	3.0
1	D	169	GLN	3.0
1	B	233	PRO	3.0
1	D	339	VAL	3.0
1	D	318	ALA	2.9
1	D	206	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	290	THR	2.9
1	A	208	LYS	2.9
1	C	236	ASP	2.9
1	D	369	GLY	2.9
1	C	179	ALA	2.9
1	D	336	ILE	2.8
1	C	178	PHE	2.8
1	C	148	LEU	2.8
1	D	173	ASP	2.8
1	D	307	ILE	2.8
1	A	133	LYS	2.8
1	D	389	ILE	2.8
1	C	371	ARG	2.7
1	C	167	GLN	2.7
1	D	300	LEU	2.7
1	D	324	CYS	2.7
1	A	227	SER	2.7
1	D	312	LEU	2.7
1	B	240	THR	2.6
1	C	80	ALA	2.6
1	D	220	ARG	2.6
1	C	226	ASP	2.6
1	D	218	TYR	2.6
1	C	305	TRP	2.6
1	D	327	ASN	2.6
1	D	331	GLY	2.5
1	A	392	LEU	2.5
1	C	206	GLY	2.5
1	D	293	ILE	2.5
1	D	18	PHE	2.5
1	D	338	ASN	2.5
1	D	310	LEU	2.5
1	D	160	THR	2.4
1	C	168	TRP	2.4
1	D	329	ASP	2.4
1	C	132	VAL	2.4
1	D	152	PHE	2.4
1	D	328	LYS	2.4
1	D	320	ALA	2.4
1	C	241	VAL	2.4
1	C	153	TYR	2.4
1	D	157	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	170	LEU	2.3
1	D	172	ARG	2.3
1	B	236	ASP	2.3
1	D	292	PRO	2.3
1	D	191	LYS	2.3
1	B	209	GLY	2.3
1	B	4	SER	2.3
1	D	350	ILE	2.3
1	A	240	THR	2.3
1	C	159	THR	2.3
1	D	42	ALA	2.2
1	D	379	ILE	2.2
1	B	234	ALA	2.2
1	B	392	LEU	2.2
1	C	191	LYS	2.2
1	D	171	SER	2.2
1	C	166	LYS	2.2
1	C	172	ARG	2.2
1	D	167	GLN	2.2
1	C	213	VAL	2.2
1	C	220	ARG	2.2
1	C	169	GLN	2.2
1	D	335	SER	2.2
1	C	330	LEU	2.2
1	D	289	GLY	2.2
1	A	222	GLY	2.1
1	D	32	ALA	2.1
1	D	303	ALA	2.1
1	D	285	PRO	2.1
1	C	344	ILE	2.1
1	D	374	LEU	2.1
1	D	286	LYS	2.1
1	D	380	GLY	2.1
1	C	155	TYR	2.1
1	C	161	ALA	2.1
1	C	307	ILE	2.1
1	D	344	ILE	2.1
1	C	332	TRP	2.0
1	D	297	ARG	2.0
1	D	204	VAL	2.0
1	D	22	PHE	2.0

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

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	D	89	9/10	0.82	0.21	-	35,39,63,69	0
1	SCY	C	89	9/10	0.68	0.27	-	33,40,55,57	0
1	SCY	B	89	9/10	0.77	0.20	-	13,16,28,31	0
1	SCY	A	89	9/10	0.70	0.21	-	14,18,31,34	0

## 6.3 Carbohydrates ⓘ

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
2	SO4	B	724	5/5	0.76	0.23	9.50	45,48,50,52	0
3	COA	B	393	48/48	0.65	0.39	3.68	26,36,62,64	0
3	COA	D	393	48/48	0.18	0.68	3.56	88,117,126,126	0
3	COA	C	393	48/48	0.32	0.51	3.22	68,82,96,97	0
3	COA	A	393	48/48	0.74	0.37	2.70	25,37,51,55	0
2	SO4	A	722	5/5	0.96	0.16	1.40	50,51,56,58	0
2	SO4	A	723	5/5	0.77	0.22	-	44,46,52,53	0
2	SO4	A	720	5/5	0.90	0.20	-	60,60,62,63	0
2	SO4	B	719	5/5	0.94	0.17	-	58,58,59,60	0
2	SO4	B	721	5/5	0.89	0.18	-	53,56,61,62	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.