



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:44 PM GMT

PDB ID : 1QFL  
Title : BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COMPLEX 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 (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

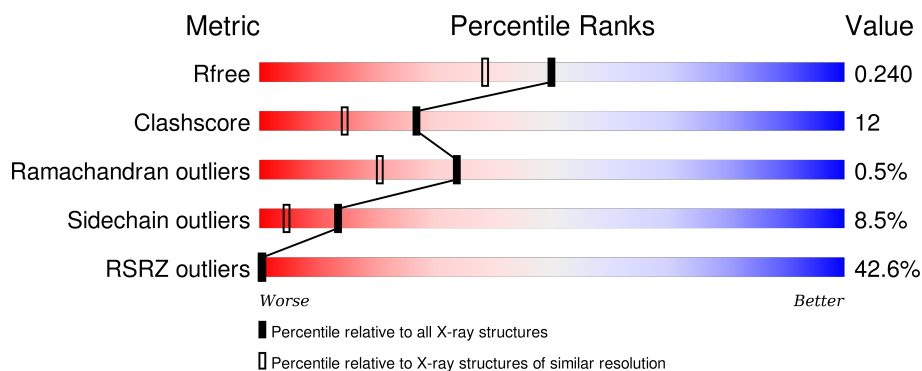
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (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>20%</div> <div>67%</div> <div>27%</div> <div>6%</div> <div>.</div> </div>
1	B	389	<div> <div>21%</div> <div>72%</div> <div>21%</div> <div>.</div> <div>.</div> </div>
1	C	389	<div> <div>58%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	D	389	<div> <div>72%</div> <div>67%</div> <div>27%</div> <div>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:

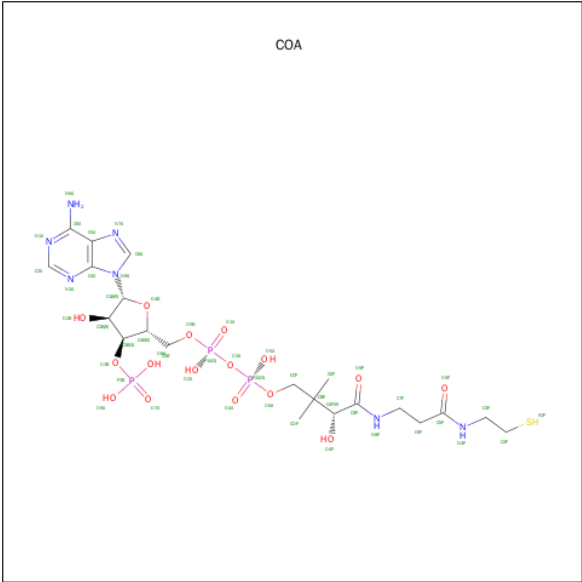
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	INSERTION	UNP P07097
A	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	11	ALA	-	INSERTION	UNP P07097
B	89	SCY	CYS	MODIFIED RESIDUE	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	11	ALA	-	INSERTION	UNP P07097
C	89	SCY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

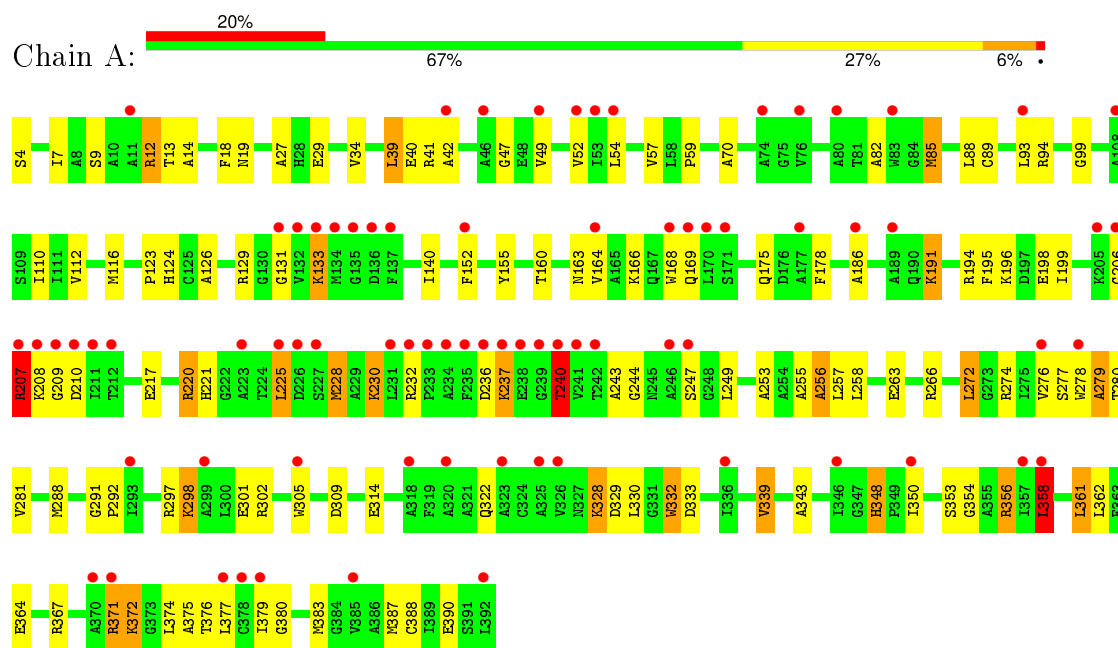
- Molecule 4 is water.

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		

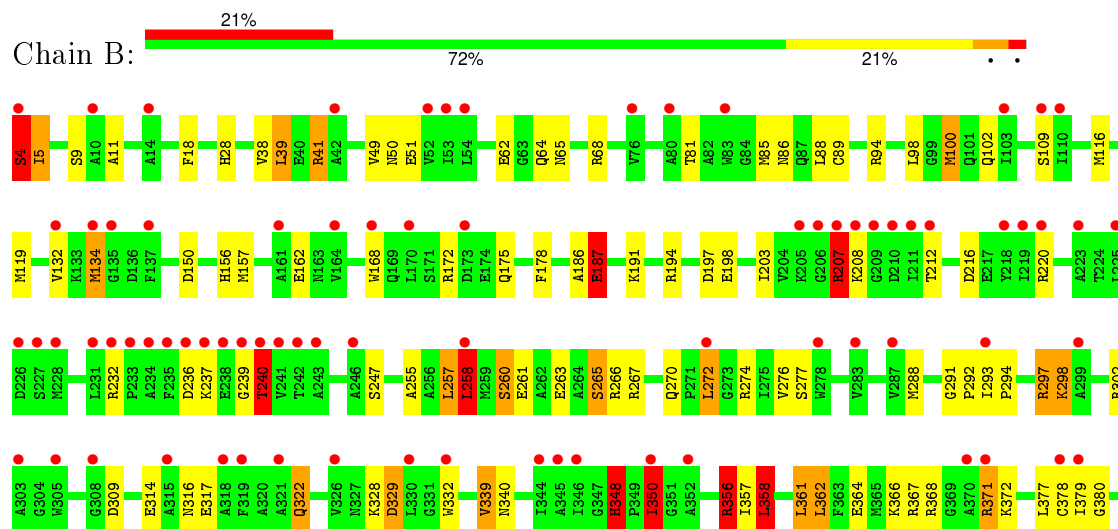
### 3 Residue-property plots

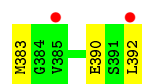
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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

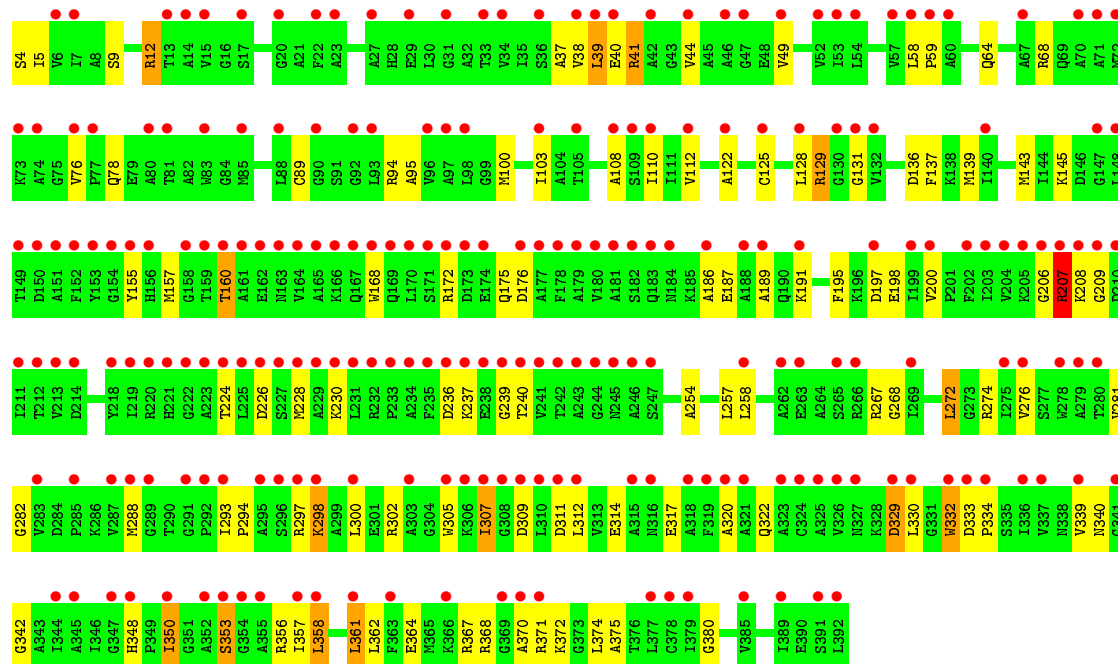


#### • Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

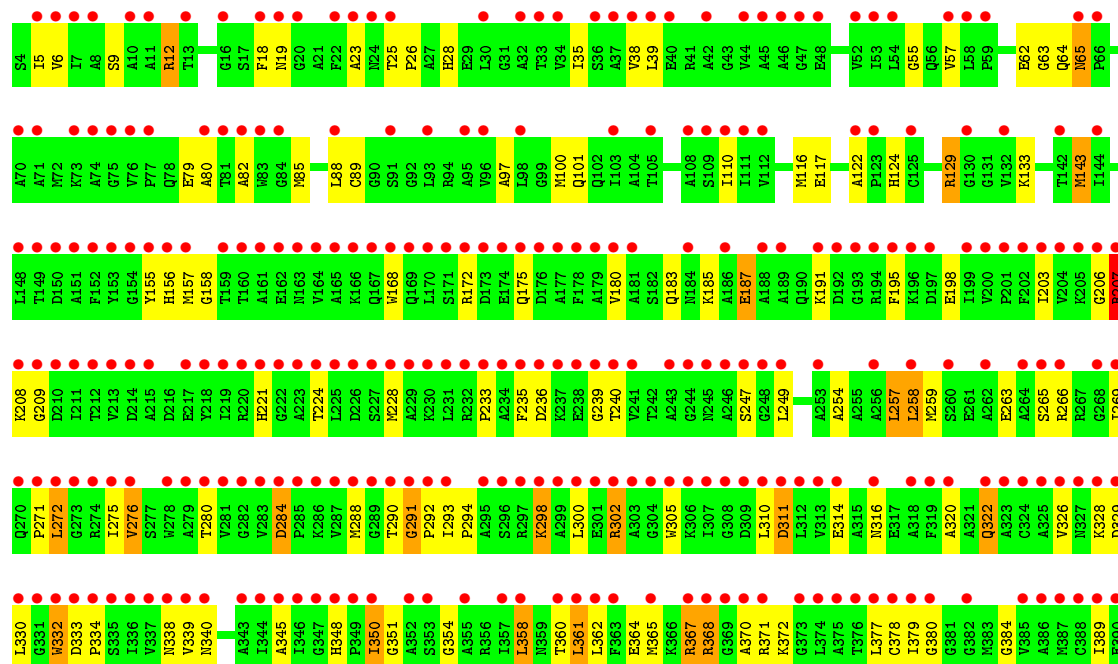
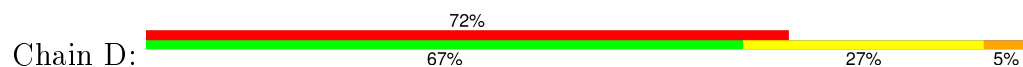




● Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)



● 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, $\alpha$ , $\beta$ , $\gamma$	84.46 Å   78.86 Å   149.75 Å 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) 94.5 (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 1.92 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209   ,   0.256 0.235   ,   0.240	Depositor DCC
$R_{free}$ test set	7058 reflections (5.29%)	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 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 140523 reflections	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, 0.375 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: 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:C:5:ILE:HG13	1:C:100:MET:HG2	1.58	0.84
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.39	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:D:89:SCY:HE1	1:D:380:GLY:N	1.97	0.79
1:C:89:SCY:CE	1:C:380:GLY:H	1.96	0.79
1:B:390:GLU:OE2	4:B:961:HOH:O	2.01	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:392:LEU:HB2	4:B:854:HOH:O	1.96	0.65
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.61	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:C:175:GLN:HE22	1:C:240:THR:CG2	2.11	0.64
1:B:5:ILE:HG13	1:B:100:MET:HG2	1.79	0.64
1:A:358:LEU:HD21	1:A:387:MET:HE3	1.78	0.63
1:D:322:GLN:O	1:D:326:VAL:HG23	1.99	0.63
1:B:4:SER:CA	4:B:999:HOH:O	2.46	0.63
1:A:225:LEU:HG	4:A:926:HOH:O	1.98	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:D:97:ALA:O	1:D:101:GLN:HG3	2.04	0.58
1:C:236:ASP:HB3	1:C:239:GLY:HA3	1.86	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:B:348:HIS:HB2	4:B:840:HOH:O	2.05	0.56
1:A:40:GLU:HG3	4:A:1010:HOH:O	2.05	0.56
1:C:41:ARG:NH1	1:C:197:ASP:O	2.39	0.56
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.87	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:D:275:ILE:HA	1:D:389:ILE:HD13	1.90	0.54
1:A:9:SER:HA	1:A:272:LEU:HD22	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:C:168:TRP:CH2	1:C:329:ASP:HB2	2.43	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:B:132:VAL:O	1:D:129:ARG:HA	2.08	0.53
1:D:314:GLU:OE2	1:D:338:ASN:HA	2.09	0.53
1:C:374:LEU:HD23	1:C:374:LEU:C	2.29	0.53
1:A:34:VAL:HG12	1:A:255:ALA:HB3	1.90	0.53
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.91	0.52
1:D:258:LEU:N	1:D:258:LEU:HD22	2.24	0.52
1:D:187:GLU:HG3	1:D:221:HIS:HA	1.91	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:D:330:LEU:HD13	1:D:332:TRP:CH2	2.45	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: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:4:SER:N	4:B:862:HOH:O	2.43	0.51
1:B:236:ASP:O	1:B:239:GLY:N	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:D:18:PHE:O	1:D:19:ASN:HB2	2.12	0.50
1:A:305:TRP:CZ3	1:A:388:CYS:HB3	2.47	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:D:293:ILE:HB	1:D:294:PRO:HD3	1.95	0.49
1:D:195:PHE:O	1:D:198:GLU:HG2	2.12	0.49
1:C:305:TRP:CE2	1:C:372:LYS:HD3	2.47	0.49
1:C:258:LEU:N	1:C:258:LEU:HD22	2.26	0.49
1:D:272:LEU:HD21	4:D:430:HOH:O	2.12	0.48
4:B:899:HOH:O	1:C:145:LYS:HB2	2.12	0.48
1:B:257:LEU:C	1:B:257:LEU:CD2	2.82	0.48
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.47	0.48
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.48	0.48
1:A:371:ARG:HG3	4:A:932:HOH:O	2.12	0.48
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.75	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:B:9:SER:HA	1:B:272:LEU:HD22	1.95	0.47
1:A:257:LEU:C	1:A:257:LEU:HD23	2.35	0.47
1:B:260:SER:OG	2:B:721:SO4:O2	2.24	0.47
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.30	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:D:240:THR:HA	4:D:436:HOH:O	2.14	0.47
1:B:298:LYS:HE2	2:B:719:SO4:O1	2.13	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: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
1:C:189:ALA:CB	1:C:340:ASN:HB3	2.46	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:C:49:VAL:HB	1:C:76:VAL:HG13	1.99	0.45
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.69	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:D:293:ILE:N	1:D:294:PRO:HD2	2.32	0.44
1:C:268:GLY:HA2	4:C:486:HOH:O	2.17	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:293:ILE:HG21	1:D:329:ASP:OD2	2.17	0.44
1:D:117:GLU:OE2	1:D:351:GLY:N	2.50	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:C:282:GLY:N	1:D:79:GLU:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ASP:HA	1:D:334:PRO:HD2	1.83	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: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:A:124:HIS:HA	1:A:140:ILE:O	2.17	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:D:89:SCY:O	1:D:377:LEU:HD22	2.20	0.42
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.53	0.42
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.51	0.42
1:A:291:GLY:N	1:A:292:PRO:CD	2.82	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:371:ARG:HH11	1:B:371:ARG:HD2	1.55	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:12:ARG:HA	1:D:254:ALA:HA	2.01	0.42
1:D:183:GLN:HA	1:D:345:ALA:HB2	2.02	0.42
1:B:187:GLU:O	1:B:191:LYS:HG3	2.20	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:64:GLN:HE22	1:D:157:MET:CE	2.32	0.41
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.84	0.41
1:C:293:ILE:CB	1:C:294:PRO:CD	2.98	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:D:143:MET:HE1	1:D:249:LEU:HD13	2.03	0.41
1:B:156:HIS:ND1	1:B:157:MET:N	2.69	0.41
1:A:7:ILE:HG23	1:A:256:ALA:HB1	2.03	0.41
1:B:5:ILE:CG1	1:B:100:MET:HG2	2.48	0.41
1:B:236:ASP:O	1:B:237:LYS:C	2.59	0.41
1:D:156:HIS:ND1	1:D:157:MET:N	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PHE:O	1:C:198:GLU:HG2	2.21	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:D:280:THR:HA	1:D:384:GLY:O	2.21	0.40
1:C:314:GLU:O	1:C:375:ALA:HA	2.21	0.40
1:D:89:SCY:HE1	1:D:380:GLY:CA	2.51	0.40
1:C:350:ILE:HD13	1:C:350:ILE:HG21	1.86	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%)	46	34
1	B	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	46	34
1	C	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	46	34
1	D	386/389 (99%)	366 (95%)	15 (4%)	5 (1%)	15	4
All	All	1544/1556 (99%)	1480 (96%)	56 (4%)	8 (0%)	34	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%)	10	3
1	B	275/275 (100%)	249 (90%)	26 (10%)	11	3
1	C	275/275 (100%)	255 (93%)	20 (7%)	17	7
1	D	275/275 (100%)	255 (93%)	20 (7%)	17	7
All	All	1100/1100 (100%)	1007 (92%)	93 (8%)	13	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	7,8,9	1.23	1 (14%)	4,9,11	1.29	1 (25%)
1	SCY	B	89	1	7,8,9	1.21	1 (14%)	4,9,11	1.66	1 (25%)
1	SCY	C	89	1	7,8,9	1.50	1 (14%)	4,9,11	1.64	1 (25%)
1	SCY	D	89	1	7,8,9	0.58	0	4,9,11	1.10	1 (25%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	89	SCY	CB-SG	-3.44	1.77	1.81
1	B	89	SCY	CB-CA	2.01	1.58	1.53
1	A	89	SCY	CB-CA	2.36	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	SCY	O-C-CA	-3.19	117.17	125.49
1	B	89	SCY	O-C-CA	-2.98	117.72	125.49
1	A	89	SCY	O-C-CA	-2.29	119.52	125.49
1	D	89	SCY	O-C-CA	-2.13	119.94	125.49

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	-	40,50,50	1.97	15 (37%)	50,75,75	2.99	21 (42%)
2	SO4	A	720	-	4,4,4	0.87	0	6,6,6	0.15	0
2	SO4	A	722	-	4,4,4	0.87	0	6,6,6	0.37	0
2	SO4	A	723	-	4,4,4	1.24	0	6,6,6	0.55	0
3	COA	B	393	-	40,50,50	1.70	8 (20%)	50,75,75	2.76	17 (34%)
2	SO4	B	719	-	4,4,4	0.98	0	6,6,6	0.16	0
2	SO4	B	721	-	4,4,4	0.92	0	6,6,6	0.44	0
2	SO4	B	724	-	4,4,4	1.17	0	6,6,6	0.40	0
3	COA	C	393	-	40,50,50	1.92	10 (25%)	50,75,75	2.14	18 (36%)
3	COA	D	393	-	40,50,50	1.92	10 (25%)	50,75,75	2.18	9 (18%)

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 (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	393	COA	C9P-N8P	-3.07	1.27	1.33
3	A	393	COA	C7P-C6P	-2.42	1.43	1.51
3	D	393	COA	C7P-N8P	-2.32	1.40	1.46
3	A	393	COA	O3B-C3B	-2.26	1.37	1.44
3	D	393	COA	C9P-N8P	-2.25	1.28	1.33
3	C	393	COA	C9P-N8P	-2.24	1.28	1.33
3	B	393	COA	O3B-C3B	-2.08	1.37	1.44
3	C	393	COA	O3B-C3B	-2.06	1.37	1.44
3	A	393	COA	C4A-N3A	-2.02	1.32	1.35
3	A	393	COA	O4B-C1B	2.03	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	393	COA	CDP-CBP	2.07	1.58	1.53
3	C	393	COA	O4B-C4B	2.11	1.49	1.45
3	B	393	COA	O4B-C4B	2.14	1.50	1.45
3	A	393	COA	CDP-CBP	2.17	1.58	1.53
3	A	393	COA	O5P-C5P	2.30	1.28	1.23
3	A	393	COA	O4B-C4B	2.32	1.50	1.45
3	C	393	COA	C2A-N1A	2.39	1.38	1.33
3	A	393	COA	C2A-N3A	2.40	1.36	1.32
3	D	393	COA	C2A-N1A	2.40	1.38	1.33
3	B	393	COA	P3B-O3B	2.41	1.67	1.60
3	A	393	COA	C2A-N1A	2.43	1.38	1.33
3	D	393	COA	O4B-C4B	2.43	1.50	1.45
3	B	393	COA	C3P-N4P	2.44	1.51	1.46
3	C	393	COA	P3B-O3B	2.45	1.67	1.60
3	B	393	COA	P3B-O7A	2.52	1.59	1.51
3	A	393	COA	P2A-O6A	2.53	1.70	1.59
3	A	393	COA	P3B-O3B	2.57	1.67	1.60
3	A	393	COA	OAP-CAP	2.66	1.47	1.42
3	D	393	COA	P3B-O7A	2.73	1.60	1.51
3	D	393	COA	P3B-O3B	2.74	1.68	1.60
3	C	393	COA	P3B-O7A	2.76	1.60	1.51
3	A	393	COA	C3P-N4P	3.08	1.53	1.46
3	D	393	COA	O5P-C5P	3.10	1.29	1.23
3	A	393	COA	P3B-O7A	3.20	1.61	1.51
3	D	393	COA	C3P-N4P	3.28	1.53	1.46
3	C	393	COA	O4B-C1B	3.32	1.45	1.41
3	C	393	COA	O5P-C5P	3.49	1.30	1.23
3	C	393	COA	C3P-N4P	3.69	1.54	1.46
3	D	393	COA	O4B-C1B	4.30	1.46	1.41
3	B	393	COA	O9P-C9P	5.38	1.34	1.23
3	D	393	COA	O9P-C9P	6.43	1.36	1.23
3	A	393	COA	O9P-C9P	6.55	1.36	1.23
3	C	393	COA	O9P-C9P	6.70	1.36	1.23

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393	COA	C2P-C3P-N4P	-11.13	90.40	112.37
3	B	393	COA	C6P-C5P-N4P	-7.98	102.59	116.46
3	B	393	COA	C2P-C3P-N4P	-6.27	99.99	112.37
3	D	393	COA	P3B-O3B-C3B	-6.09	106.96	121.56
3	D	393	COA	CEP-CBP-CCP	-5.81	100.96	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	393	COA	C4B-O4B-C1B	-5.80	103.35	109.72
3	A	393	COA	O6A-CCP-CBP	-5.75	101.31	110.55
3	A	393	COA	C7P-N8P-C9P	-5.57	111.51	122.53
3	A	393	COA	O3A-P2A-O6A	-5.32	88.81	102.94
3	C	393	COA	C2P-C3P-N4P	-4.97	102.55	112.37
3	A	393	COA	C2B-C3B-C4B	-4.50	94.84	103.29
3	C	393	COA	CEP-CBP-CCP	-4.21	103.05	108.50
3	A	393	COA	C6P-C5P-N4P	-4.09	109.35	116.46
3	B	393	COA	N3A-C2A-N1A	-4.04	125.80	128.89
3	B	393	COA	O6A-CCP-CBP	-4.00	104.11	110.55
3	A	393	COA	O4B-C4B-C5B	-3.99	95.07	109.32
3	C	393	COA	C4B-O4B-C1B	-3.87	105.47	109.72
3	B	393	COA	P3B-O3B-C3B	-3.62	112.88	121.56
3	B	393	COA	O3A-P2A-O6A	-3.40	93.92	102.94
3	A	393	COA	P3B-O3B-C3B	-3.26	113.76	121.56
3	A	393	COA	C4B-O4B-C1B	-3.11	106.31	109.72
3	C	393	COA	O3A-P2A-O6A	-2.90	95.24	102.94
3	A	393	COA	O5B-C5B-C4B	-2.88	98.49	109.12
3	C	393	COA	O6A-CCP-CBP	-2.85	105.97	110.55
3	C	393	COA	N3A-C2A-N1A	-2.72	126.81	128.89
3	C	393	COA	P3B-O3B-C3B	-2.65	115.20	121.56
3	B	393	COA	OAP-CAP-C9P	-2.49	104.67	110.38
3	B	393	COA	C4B-O4B-C1B	-2.40	107.08	109.72
3	B	393	COA	C2B-C3B-C4B	-2.34	98.89	103.29
3	C	393	COA	C2B-C1B-N9A	-2.32	110.75	114.29
3	A	393	COA	C2B-C1B-N9A	-2.23	110.88	114.29
3	A	393	COA	OAP-CAP-C9P	-2.11	105.54	110.38
3	D	393	COA	C2P-C3P-N4P	-2.11	108.21	112.37
3	C	393	COA	CAP-C9P-N8P	-2.11	111.80	116.47
3	C	393	COA	O5P-C5P-C6P	-2.11	118.35	121.98
3	A	393	COA	CEP-CBP-CCP	-2.10	105.78	108.50
3	D	393	COA	O9A-P3B-O8A	2.01	115.05	107.38
3	C	393	COA	O9A-P3B-O8A	2.03	115.11	107.38
3	C	393	COA	C5B-C4B-C3B	2.05	121.69	114.31
3	B	393	COA	O3B-C3B-C4B	2.15	118.44	109.99
3	C	393	COA	O4B-C1B-N9A	2.18	112.67	108.10
3	A	393	COA	CEP-CBP-CDP	2.27	113.83	109.28
3	A	393	COA	CEP-CBP-CAP	2.37	113.67	109.34
3	A	393	COA	O9A-P3B-O8A	2.40	116.53	107.38
3	C	393	COA	C4A-C5A-N7A	2.48	111.76	109.48
3	C	393	COA	CEP-CBP-CAP	2.51	113.92	109.34
3	B	393	COA	C2A-N1A-C6A	2.71	123.61	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393	COA	P2A-O3A-P1A	2.72	140.36	132.73
3	D	393	COA	C4A-C5A-N7A	2.73	111.99	109.48
3	A	393	COA	C4A-C5A-N7A	2.89	112.14	109.48
3	C	393	COA	C6P-C5P-N4P	2.92	121.53	116.46
3	C	393	COA	CDP-CBP-CCP	2.99	112.37	108.50
3	A	393	COA	N6A-C6A-N1A	3.02	125.68	119.20
3	B	393	COA	C5B-C4B-C3B	3.03	125.23	114.31
3	B	393	COA	O9P-C9P-N8P	3.07	129.24	123.08
3	A	393	COA	CAP-C9P-N8P	3.34	123.86	116.47
3	B	393	COA	C4A-C5A-N7A	3.95	113.11	109.48
3	D	393	COA	CDP-CBP-CCP	3.98	113.67	108.50
3	D	393	COA	C6P-C7P-N8P	4.23	121.16	111.88
3	B	393	COA	C7P-N8P-C9P	5.38	133.17	122.53
3	B	393	COA	O5P-C5P-C6P	6.08	132.46	121.98
3	D	393	COA	C7P-N8P-C9P	6.25	134.90	122.53
3	A	393	COA	C6P-C7P-N8P	6.95	127.13	111.88
3	C	393	COA	C7P-N8P-C9P	7.03	136.44	122.53
3	B	393	COA	C7P-C6P-C5P	7.69	124.98	112.31

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	1.51	77 (19%) 1 1	12, 21, 44, 87	0
1	B	388/389 (99%)	1.47	80 (20%) 1 1	11, 20, 42, 97	0
1	C	388/389 (99%)	2.69	225 (57%) 0 0	25, 45, 77, 119	0
1	D	388/389 (99%)	3.19	279 (71%) 0 0	22, 52, 115, 138	0
All	All	1552/1556 (99%)	2.22	661 (42%) 0 0	11, 36, 84, 138	0

All (661) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	239	GLY	13.4
1	C	224	THR	13.1
1	D	224	THR	11.4
1	C	206	GLY	11.4
1	C	237	LYS	11.4
1	D	227	SER	11.3
1	C	207	ARG	10.5
1	C	233	PRO	10.0
1	C	239	GLY	10.0
1	D	207	ARG	9.7
1	C	227	SER	9.6
1	C	208	LYS	9.4
1	D	206	GLY	9.3
1	D	208	LYS	9.1
1	D	226	ASP	9.1
1	D	229	ALA	9.0
1	B	206	GLY	8.5
1	D	237	LYS	8.5
1	D	238	GLU	8.4
1	D	330	LEU	8.4
1	B	392	LEU	8.1

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Mol	Chain	Res	Type	RSRZ
1	B	208	LYS	8.0
1	C	226	ASP	7.7
1	A	233	PRO	7.7
1	A	208	LYS	7.6
1	D	308	GLY	7.6
1	D	219	ILE	7.6
1	D	235	PHE	7.5
1	A	237	LYS	7.5
1	D	170	LEU	7.4
1	D	392	LEU	7.4
1	C	243	ALA	7.1
1	C	229	ALA	7.1
1	C	235	PHE	7.1
1	D	240	THR	7.1
1	C	209	GLY	7.0
1	A	206	GLY	7.0
1	C	232	ARG	7.0
1	D	228	MET	7.0
1	D	230	LYS	7.0
1	B	237	LYS	6.9
1	D	164	VAL	6.9
1	D	236	ASP	6.9
1	C	240	THR	6.8
1	C	236	ASP	6.8
1	D	223	ALA	6.8
1	D	232	ARG	6.8
1	D	203	ILE	6.8
1	D	234	ALA	6.7
1	D	233	PRO	6.7
1	B	239	GLY	6.6
1	D	326	VAL	6.6
1	B	207	ARG	6.5
1	C	234	ALA	6.5
1	C	238	GLU	6.4
1	D	171	SER	6.4
1	A	236	ASP	6.3
1	D	370	ALA	6.3
1	C	169	GLN	6.3
1	D	209	GLY	6.3
1	A	207	ARG	6.2
1	D	310	LEU	6.1
1	C	211	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	336	ILE	6.1
1	D	222	GLY	6.0
1	D	225	LEU	5.9
1	D	173	ASP	5.9
1	C	231	LEU	5.9
1	D	231	LEU	5.9
1	C	379	ILE	5.9
1	D	221	HIS	5.8
1	B	235	PHE	5.8
1	C	371	ARG	5.8
1	B	238	GLU	5.8
1	C	225	LEU	5.8
1	D	371	ARG	5.8
1	D	247	SER	5.8
1	A	209	GLY	5.8
1	B	134	MET	5.7
1	A	239	GLY	5.7
1	D	156	HIS	5.6
1	D	191	LYS	5.6
1	D	379	ILE	5.6
1	C	242	THR	5.5
1	D	153	TYR	5.5
1	A	235	PHE	5.5
1	D	181	ALA	5.5
1	C	305	TRP	5.5
1	C	161	ALA	5.4
1	D	305	TRP	5.4
1	D	211	ILE	5.4
1	D	188	ALA	5.4
1	D	169	GLN	5.4
1	C	180	VAL	5.4
1	C	170	LEU	5.3
1	B	233	PRO	5.3
1	C	228	MET	5.3
1	C	205	LYS	5.3
1	C	392	LEU	5.2
1	B	232	ARG	5.2
1	A	392	LEU	5.2
1	C	156	HIS	5.1
1	C	153	TYR	5.1
1	D	179	ALA	5.1
1	D	285	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	334	PRO	5.1
1	C	241	VAL	5.1
1	D	189	ALA	5.0
1	C	297	ARG	5.0
1	D	320	ALA	5.0
1	C	165	ALA	5.0
1	D	385	VAL	5.0
1	B	226	ASP	5.0
1	A	238	GLU	4.9
1	D	339	VAL	4.9
1	C	246	ALA	4.9
1	C	378	CYS	4.9
1	D	375	ALA	4.9
1	C	223	ALA	4.9
1	D	37	ALA	4.9
1	D	325	ALA	4.9
1	D	166	LYS	4.9
1	D	168	TRP	4.9
1	A	240	THR	4.8
1	C	173	ASP	4.8
1	B	227	SER	4.8
1	D	204	VAL	4.7
1	B	236	ASP	4.7
1	D	350	ILE	4.7
1	D	328	LYS	4.7
1	C	287	VAL	4.6
1	C	230	LYS	4.6
1	D	349	PRO	4.6
1	B	240	THR	4.6
1	D	210	ASP	4.6
1	D	352	ALA	4.6
1	C	310	LEU	4.6
1	D	218	TYR	4.6
1	D	306	LYS	4.6
1	D	289	GLY	4.6
1	D	241	VAL	4.5
1	D	265	SER	4.5
1	A	133	LYS	4.5
1	D	318	ALA	4.5
1	C	221	HIS	4.5
1	D	152	PHE	4.5
1	C	148	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	167	GLN	4.5
1	D	283	VAL	4.5
1	C	296	SER	4.5
1	D	157	MET	4.5
1	C	204	VAL	4.5
1	D	22	PHE	4.4
1	D	176	ASP	4.4
1	D	192	ASP	4.4
1	C	330	LEU	4.4
1	A	234	ALA	4.4
1	D	374	LEU	4.4
1	D	388	CYS	4.4
1	C	306	LYS	4.3
1	A	232	ARG	4.3
1	D	200	VAL	4.3
1	C	155	TYR	4.3
1	C	53	ILE	4.3
1	C	177	ALA	4.3
1	C	171	SER	4.3
1	D	327	ASN	4.3
1	D	193	GLY	4.3
1	A	226	ASP	4.2
1	D	18	PHE	4.2
1	C	213	VAL	4.2
1	D	178	PHE	4.2
1	D	391	SER	4.2
1	C	179	ALA	4.2
1	D	264	ALA	4.1
1	D	299	ALA	4.1
1	D	196	LYS	4.1
1	D	165	ALA	4.1
1	C	159	THR	4.1
1	D	286	LYS	4.1
1	D	95	ALA	4.1
1	C	178	PHE	4.1
1	C	333	ASP	4.0
1	D	295	ALA	4.0
1	D	159	THR	4.0
1	D	331	GLY	4.0
1	D	160	THR	4.0
1	D	45	ALA	4.0
1	D	332	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	262	ALA	4.0
1	D	269	ILE	3.9
1	D	180	VAL	3.9
1	B	209	GLY	3.9
1	C	361	LEU	3.9
1	D	319	PHE	3.9
1	D	39	LEU	3.9
1	D	163	ASN	3.9
1	C	222	GLY	3.9
1	D	329	ASP	3.9
1	D	151	ALA	3.8
1	D	309	ASP	3.8
1	C	219	ILE	3.8
1	D	161	ALA	3.8
1	C	293	ILE	3.8
1	C	311	ASP	3.8
1	D	175	GLN	3.8
1	A	227	SER	3.8
1	D	13	THR	3.8
1	D	172	ARG	3.8
1	C	176	ASP	3.7
1	D	270	GLN	3.7
1	D	246	ALA	3.7
1	D	249	LEU	3.7
1	D	300	LEU	3.7
1	D	363	PHE	3.7
1	C	220	ARG	3.7
1	D	148	LEU	3.7
1	D	19	ASN	3.7
1	C	355	ALA	3.7
1	C	218	TYR	3.7
1	A	132	VAL	3.6
1	D	194	ARG	3.6
1	C	168	TRP	3.6
1	C	54	LEU	3.6
1	D	167	GLN	3.6
1	C	203	ILE	3.6
1	C	151	ALA	3.6
1	D	8	ALA	3.6
1	D	323	ALA	3.6
1	A	169	GLN	3.6
1	C	128	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	52	VAL	3.6
1	C	160	THR	3.6
1	C	57	VAL	3.6
1	D	287	VAL	3.6
1	D	343	ALA	3.6
1	D	47	GLY	3.6
1	C	166	LYS	3.6
1	C	83	TRP	3.6
1	C	262	ALA	3.6
1	C	325	ALA	3.6
1	D	201	PRO	3.5
1	D	215	ALA	3.5
1	D	202	PHE	3.5
1	D	362	LEU	3.5
1	D	377	LEU	3.5
1	D	365	MET	3.5
1	C	46	ALA	3.5
1	C	34	VAL	3.5
1	C	344	ILE	3.5
1	C	210	ASP	3.5
1	C	323	ALA	3.5
1	C	38	VAL	3.5
1	C	326	VAL	3.5
1	D	96	VAL	3.5
1	D	186	ALA	3.5
1	B	132	VAL	3.5
1	C	332	TRP	3.5
1	D	212	THR	3.5
1	D	243	ALA	3.5
1	C	172	ARG	3.4
1	D	378	CYS	3.4
1	C	174	GLU	3.4
1	D	313	VAL	3.4
1	B	234	ALA	3.4
1	D	177	ALA	3.4
1	D	368	ARG	3.4
1	C	191	LYS	3.4
1	C	212	THR	3.4
1	D	382	GLY	3.4
1	C	324	CYS	3.4
1	D	93	LEU	3.4
1	D	44	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	320	ALA	3.3
1	D	367	ARG	3.3
1	D	98	LEU	3.3
1	B	4	SER	3.3
1	C	132	VAL	3.3
1	C	337	VAL	3.3
1	D	337	VAL	3.3
1	C	77	PRO	3.3
1	D	268	GLY	3.3
1	D	340	ASN	3.3
1	D	278	TRP	3.3
1	C	152	PHE	3.3
1	C	309	ASP	3.3
1	D	76	VAL	3.3
1	D	271	PRO	3.2
1	D	324	CYS	3.2
1	C	308	GLY	3.2
1	D	293	ILE	3.2
1	C	162	GLU	3.2
1	C	14	ALA	3.2
1	D	272	LEU	3.2
1	C	163	ASN	3.2
1	D	83	TRP	3.2
1	D	108	ALA	3.2
1	D	205	LYS	3.2
1	D	155	TYR	3.2
1	C	76	VAL	3.2
1	D	348	HIS	3.2
1	C	318	ALA	3.2
1	D	162	GLU	3.2
1	D	258	LEU	3.2
1	B	164	VAL	3.2
1	D	38	VAL	3.2
1	A	131	GLY	3.2
1	D	125	CYS	3.2
1	C	98	LEU	3.1
1	C	345	ALA	3.1
1	C	307	ILE	3.1
1	D	389	ILE	3.1
1	D	312	LEU	3.1
1	C	276	VAL	3.1
1	C	366	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	297	ARG	3.1
1	D	361	LEU	3.1
1	C	47	GLY	3.1
1	D	75	GLY	3.1
1	C	202	PHE	3.1
1	C	303	ALA	3.1
1	C	334	PRO	3.1
1	D	301	GLU	3.1
1	C	130	GLY	3.1
1	C	369	GLY	3.1
1	D	291	GLY	3.1
1	C	27	ALA	3.1
1	C	370	ALA	3.1
1	C	49	VAL	3.1
1	D	174	GLU	3.1
1	D	217	GLU	3.0
1	A	370	ALA	3.0
1	B	210	ASP	3.0
1	D	70	ALA	3.0
1	C	319	PHE	3.0
1	C	357	ILE	3.0
1	C	377	LEU	3.0
1	D	380	GLY	3.0
1	D	213	VAL	3.0
1	A	242	THR	3.0
1	B	212	THR	3.0
1	D	122	ALA	3.0
1	C	292	PRO	3.0
1	C	125	CYS	3.0
1	C	278	TRP	3.0
1	B	330	LEU	3.0
1	C	93	LEU	3.0
1	C	181	ALA	2.9
1	D	288	MET	2.9
1	D	91	SER	2.9
1	C	312	LEU	2.9
1	A	350	ILE	2.9
1	C	103	ILE	2.9
1	C	275	ILE	2.9
1	B	52	VAL	2.9
1	C	6	VAL	2.9
1	D	298	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	296	SER	2.9
1	D	353	SER	2.9
1	D	311	ASP	2.9
1	C	72	MET	2.9
1	C	182	SER	2.9
1	C	15	VAL	2.9
1	B	218	TYR	2.9
1	D	80	ALA	2.9
1	D	333	ASP	2.9
1	B	379	ILE	2.9
1	C	350	ILE	2.9
1	C	158	GLY	2.9
1	C	154	GLY	2.8
1	D	373	GLY	2.8
1	D	23	ALA	2.8
1	C	200	VAL	2.8
1	D	274	ARG	2.8
1	D	16	GLY	2.8
1	D	11	ALA	2.8
1	D	346	ILE	2.8
1	D	132	VAL	2.8
1	C	263	GLU	2.8
1	C	122	ALA	2.8
1	D	292	PRO	2.8
1	D	5	ILE	2.8
1	D	103	ILE	2.8
1	D	307	ILE	2.8
1	D	81	THR	2.8
1	D	387	MET	2.8
1	D	302	ARG	2.8
1	B	53	ILE	2.8
1	C	389	ILE	2.8
1	A	326	VAL	2.8
1	C	266	ARG	2.8
1	B	318	ALA	2.7
1	D	184	ASN	2.7
1	D	33	THR	2.7
1	D	142	THR	2.7
1	D	256	ALA	2.7
1	A	231	LEU	2.7
1	A	53	ILE	2.7
1	C	199	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	385	VAL	2.7
1	D	36	SER	2.7
1	A	205	LYS	2.7
1	A	212	THR	2.7
1	C	131	GLY	2.7
1	B	54	LEU	2.7
1	C	58	LEU	2.7
1	C	36	SER	2.7
1	D	53	ILE	2.7
1	A	164	VAL	2.7
1	D	57	VAL	2.7
1	D	112	VAL	2.7
1	C	81	THR	2.7
1	D	32	ALA	2.7
1	B	326	VAL	2.7
1	D	281	VAL	2.7
1	C	289	GLY	2.7
1	C	149	THR	2.7
1	B	223	ALA	2.7
1	D	338	ASN	2.7
1	C	90	GLY	2.7
1	C	247	SER	2.6
1	D	77	PRO	2.6
1	A	134	MET	2.6
1	C	385	VAL	2.6
1	B	378	CYS	2.6
1	C	80	ALA	2.6
1	D	82	ALA	2.6
1	D	195	PHE	2.6
1	C	39	LEU	2.6
1	C	358	LEU	2.6
1	A	46	ALA	2.6
1	A	379	ILE	2.6
1	D	84	GLY	2.6
1	C	13	THR	2.6
1	D	42	ALA	2.6
1	D	71	ALA	2.6
1	C	339	VAL	2.6
1	D	20	GLY	2.6
1	D	275	ILE	2.6
1	C	288	MET	2.6
1	D	344	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	109	SER	2.6
1	D	24	ASN	2.5
1	D	245	ASN	2.5
1	C	189	ALA	2.5
1	A	385	VAL	2.5
1	B	205	LYS	2.5
1	C	33	THR	2.5
1	A	168	TRP	2.5
1	C	108	ALA	2.5
1	D	279	ALA	2.5
1	A	54	LEU	2.5
1	A	225	LEU	2.5
1	D	335	SER	2.5
1	A	241	VAL	2.5
1	C	44	VAL	2.5
1	C	164	VAL	2.5
1	A	293	ILE	2.5
1	D	357	ILE	2.5
1	D	154	GLY	2.5
1	C	279	ALA	2.5
1	C	321	ALA	2.5
1	B	168	TRP	2.5
1	A	211	ILE	2.5
1	B	219	ILE	2.5
1	D	260	SER	2.5
1	A	299	ALA	2.5
1	C	188	ALA	2.5
1	B	242	THR	2.5
1	D	54	LEU	2.5
1	D	88	LEU	2.5
1	D	290	THR	2.5
1	D	390	GLU	2.4
1	C	336	ILE	2.4
1	A	93	LEU	2.4
1	C	183	GLN	2.4
1	D	150	ASP	2.4
1	B	243	ALA	2.4
1	C	20	GLY	2.4
1	C	110	ILE	2.4
1	D	7	ILE	2.4
1	D	40	GLU	2.4
1	D	110	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	253	ALA	2.4
1	D	123	PRO	2.4
1	D	360	THR	2.4
1	D	220	ARG	2.4
1	B	76	VAL	2.4
1	D	6	VAL	2.4
1	C	327	ASN	2.4
1	C	354	GLY	2.4
1	D	304	GLY	2.4
1	B	246	ALA	2.4
1	D	345	ALA	2.4
1	D	199	ILE	2.4
1	D	197	ASP	2.4
1	B	231	LEU	2.4
1	D	358	LEU	2.4
1	C	291	GLY	2.4
1	A	186	ALA	2.4
1	A	318	ALA	2.4
1	D	10	ALA	2.4
1	D	355	ALA	2.4
1	C	59	PRO	2.4
1	A	336	ILE	2.4
1	D	369	GLY	2.4
1	A	358	LEU	2.4
1	A	108	ALA	2.4
1	B	42	ALA	2.4
1	D	34	VAL	2.4
1	A	152	PHE	2.4
1	B	135	GLY	2.3
1	C	60	ALA	2.3
1	C	67	ALA	2.3
1	C	315	ALA	2.3
1	C	112	VAL	2.3
1	A	278	TRP	2.3
1	B	225	LEU	2.3
1	C	391	SER	2.3
1	A	42	ALA	2.3
1	B	321	ALA	2.3
1	C	73	LYS	2.3
1	C	283	VAL	2.3
1	D	284	ASP	2.3
1	A	137	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	66	PRO	2.3
1	B	161	ALA	2.3
1	C	258	LEU	2.3
1	D	58	LEU	2.3
1	D	322	GLN	2.3
1	B	346	ILE	2.3
1	A	80	ALA	2.3
1	A	323	ALA	2.3
1	C	105	THR	2.3
1	D	244	GLY	2.3
1	D	30	LEU	2.3
1	B	287	VAL	2.3
1	C	184	ASN	2.3
1	C	353	SER	2.3
1	B	319	PHE	2.3
1	C	7	ILE	2.3
1	C	347	GLY	2.3
1	D	105	THR	2.3
1	A	223	ALA	2.3
1	B	14	ALA	2.3
1	B	272	LEU	2.2
1	A	83	TRP	2.2
1	B	332	TRP	2.2
1	C	298	LYS	2.2
1	C	92	GLY	2.2
1	D	280	THR	2.2
1	B	293	ILE	2.2
1	C	70	ALA	2.2
1	C	348	HIS	2.2
1	D	144	ILE	2.2
1	A	377	LEU	2.2
1	C	88	LEU	2.2
1	C	300	LEU	2.2
1	A	305	TRP	2.2
1	C	244	GLY	2.2
1	C	316	ASN	2.2
1	B	137	PHE	2.2
1	A	246	ALA	2.2
1	D	74	ALA	2.2
1	C	269	ILE	2.2
1	C	341	GLY	2.2
1	D	347	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	283	VAL	2.2
1	C	96	VAL	2.2
1	C	150	ASP	2.2
1	C	197	ASP	2.2
1	B	345	ALA	2.2
1	C	295	ALA	2.2
1	C	22	PHE	2.2
1	C	147	GLY	2.2
1	C	214	ASP	2.2
1	C	329	ASP	2.2
1	C	280	THR	2.2
1	D	276	VAL	2.2
1	C	17	SER	2.2
1	D	59	PRO	2.2
1	D	282	GLY	2.2
1	B	170	LEU	2.2
1	A	52	VAL	2.2
1	C	52	VAL	2.2
1	D	109	SER	2.2
1	C	245	ASN	2.1
1	D	376	THR	2.1
1	B	228	MET	2.1
1	A	49	VAL	2.1
1	B	308	GLY	2.1
1	C	97	ALA	2.1
1	D	386	ALA	2.1
1	B	371	ARG	2.1
1	C	29	GLU	2.1
1	C	363	PHE	2.1
1	A	171	SER	2.1
1	A	247	SER	2.1
1	C	140	ILE	2.1
1	D	149	THR	2.1
1	D	316	ASN	2.1
1	D	273	GLY	2.1
1	A	177	ALA	2.1
1	C	74	ALA	2.1
1	D	303	ALA	2.1
1	B	109	SER	2.1
1	D	65	ASN	2.1
1	D	25	THR	2.1
1	B	211	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	220	ARG	2.1
1	B	305	TRP	2.1
1	B	344	ILE	2.1
1	D	111	ILE	2.1
1	D	248	GLY	2.1
1	D	266	ARG	2.1
1	A	378	CYS	2.1
1	B	299	ALA	2.1
1	B	315	ALA	2.1
1	B	352	ALA	2.1
1	C	23	ALA	2.1
1	D	46	ALA	2.1
1	A	276	VAL	2.1
1	A	210	ASP	2.1
1	D	314	GLU	2.1
1	D	130	GLY	2.1
1	B	103	ILE	2.1
1	A	170	LEU	2.1
1	A	189	ALA	2.1
1	A	325	ALA	2.1
1	B	10	ALA	2.1
1	B	173	ASP	2.1
1	C	186	ALA	2.1
1	D	214	ASP	2.1
1	D	48	GLU	2.0
1	A	11	ALA	2.0
1	B	370	ALA	2.0
1	C	42	ALA	2.0
1	B	83	TRP	2.0
1	A	76	VAL	2.0
1	A	135	GLY	2.0
1	B	241	VAL	2.0
1	A	136	ASP	2.0
1	C	285	PRO	2.0
1	A	371	ARG	2.0
1	B	80	ALA	2.0
1	C	71	ALA	2.0
1	C	352	ALA	2.0
1	B	258	LEU	2.0
1	C	31	GLY	2.0
1	C	40	GLU	2.0
1	D	73	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	278	TRP	2.0
1	C	85	MET	2.0
1	C	265	SER	2.0
1	A	74	ALA	2.0
1	A	320	ALA	2.0
1	B	303	ALA	2.0
1	A	346	ILE	2.0
1	A	357	ILE	2.0
1	B	110	ILE	2.0
1	B	350	ILE	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	D	89	9/10	0.79	0.24	-	35,39,63,69	0
1	SCY	C	89	9/10	0.66	0.31	-	33,40,55,57	0
1	SCY	B	89	9/10	0.82	0.22	-	13,16,28,31	0
1	SCY	A	89	9/10	0.77	0.23	-	14,18,31,34	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	COA	B	393	48/48	0.62	0.43	4.11	26,36,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	COA	D	393	48/48	0.10	0.79	4.02	88,117,126,126	0
2	SO4	B	724	5/5	0.76	0.24	3.02	45,48,50,52	0
3	COA	C	393	48/48	0.22	0.57	2.51	68,82,96,97	0
3	COA	A	393	48/48	0.65	0.46	1.96	25,37,51,55	0
2	SO4	A	722	5/5	0.94	0.21	1.10	50,51,56,58	0
2	SO4	A	723	5/5	0.83	0.27	-	44,46,52,53	0
2	SO4	A	720	5/5	0.89	0.21	-	60,60,62,63	0
2	SO4	B	719	5/5	0.94	0.24	-	58,58,59,60	0
2	SO4	B	721	5/5	0.90	0.23	-	53,56,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.