



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:12 PM GMT

PDB ID : 6CSC  
Title : CHICKEN CITRATE SYNTHASE COMPLEX WITH TRIFLUOROACET  
ONYL-COAAND CITRATE  
Authors : Usher, K.C.; Remington, S.J.  
Deposited on : 1997-06-19  
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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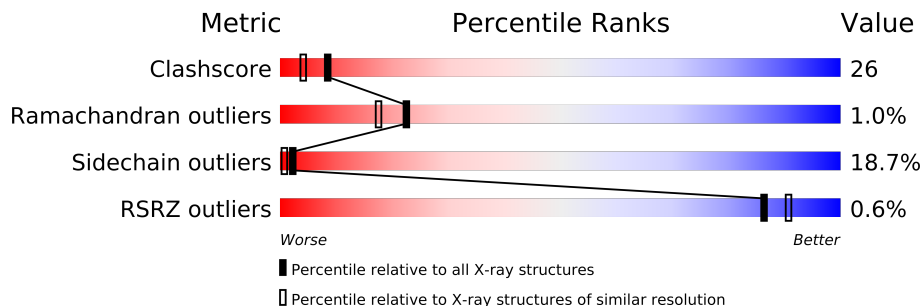
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	437	
1	B	437	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7101 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3402	2173	585	628	16			
1	B	434	Total	C	N	O	S	0	0	0
			3385	2164	582	623	16			

There are 52 discrepancies between the modelled and reference sequences:

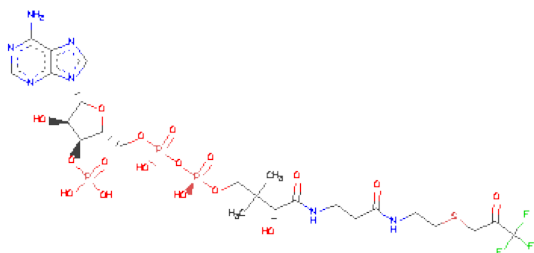
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	ALA	CONFLICT	UNP P23007
A	30	ASN	GLY	CONFLICT	UNP P23007
A	33	VAL	LEU	CONFLICT	UNP P23007
A	52	ILE	VAL	CONFLICT	UNP P23007
A	81	ALA	-	INSERTION	UNP P23007
A	85	GLU	GLY	CONFLICT	UNP P23007
A	104	PRO	GLY	CONFLICT	UNP P23007
A	105	GLU	ALA	CONFLICT	UNP P23007
A	110	VAL	LEU	CONFLICT	UNP P23007
A	163	ASN	LEU	CONFLICT	UNP P23007
A	170	PHE	MET	CONFLICT	UNP P23007
A	174	ASP	SER	CONFLICT	UNP P23007
A	222	PRO	ALA	CONFLICT	UNP P23007
A	283	LEU	GLY	CONFLICT	UNP P23007
A	286	SER	ALA	CONFLICT	UNP P23007
A	291	ASP	ALA	CONFLICT	UNP P23007
A	292	LEU	ALA	CONFLICT	UNP P23007
A	298	ASP	-	INSERTION	UNP P23007
A	299	GLU	-	INSERTION	UNP P23007
A	300	LYS	-	INSERTION	UNP P23007
A	343	SER	GLY	CONFLICT	UNP P23007
A	366	LYS	ALA	CONFLICT	UNP P23007
A	368	LYS	ALA	CONFLICT	UNP P23007
A	428	ALA	ASP	CONFLICT	UNP P23007
A	431	GLU	ILE	CONFLICT	UNP P23007

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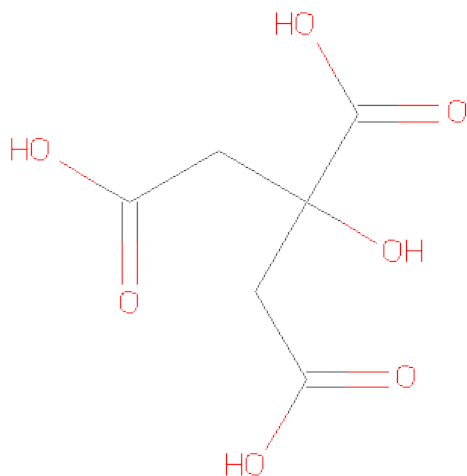
Chain	Residue	Modelled	Actual	Comment	Reference
A	432	LYS	ALA	CONFLICT	UNP P23007
B	12	SER	ALA	CONFLICT	UNP P23007
B	30	ASN	GLY	CONFLICT	UNP P23007
B	33	VAL	LEU	CONFLICT	UNP P23007
B	52	ILE	VAL	CONFLICT	UNP P23007
B	81	ALA	-	INSERTION	UNP P23007
B	85	GLU	GLY	CONFLICT	UNP P23007
B	104	PRO	GLY	CONFLICT	UNP P23007
B	105	GLU	ALA	CONFLICT	UNP P23007
B	110	VAL	LEU	CONFLICT	UNP P23007
B	163	ASN	LEU	CONFLICT	UNP P23007
B	170	PHE	MET	CONFLICT	UNP P23007
B	174	ASP	SER	CONFLICT	UNP P23007
B	222	PRO	ALA	CONFLICT	UNP P23007
B	283	LEU	GLY	CONFLICT	UNP P23007
B	286	SER	ALA	CONFLICT	UNP P23007
B	291	ASP	ALA	CONFLICT	UNP P23007
B	292	LEU	ALA	CONFLICT	UNP P23007
B	298	ASP	-	INSERTION	UNP P23007
B	299	GLU	-	INSERTION	UNP P23007
B	300	LYS	-	INSERTION	UNP P23007
B	343	SER	GLY	CONFLICT	UNP P23007
B	366	LYS	ALA	CONFLICT	UNP P23007
B	368	LYS	ALA	CONFLICT	UNP P23007
B	428	ALA	ASP	CONFLICT	UNP P23007
B	431	GLU	ILE	CONFLICT	UNP P23007
B	432	LYS	ALA	CONFLICT	UNP P23007

- Molecule 2 is TRIFLUOROACETONYL COENZYME A (three-letter code: COF) (formula:  $C_{24}H_{37}F_3N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	S	0	1
			71	32	6	9	19	3	2		
2	B	1	Total	C	F	N	O	P	S	0	1
			71	32	6	9	19	3	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

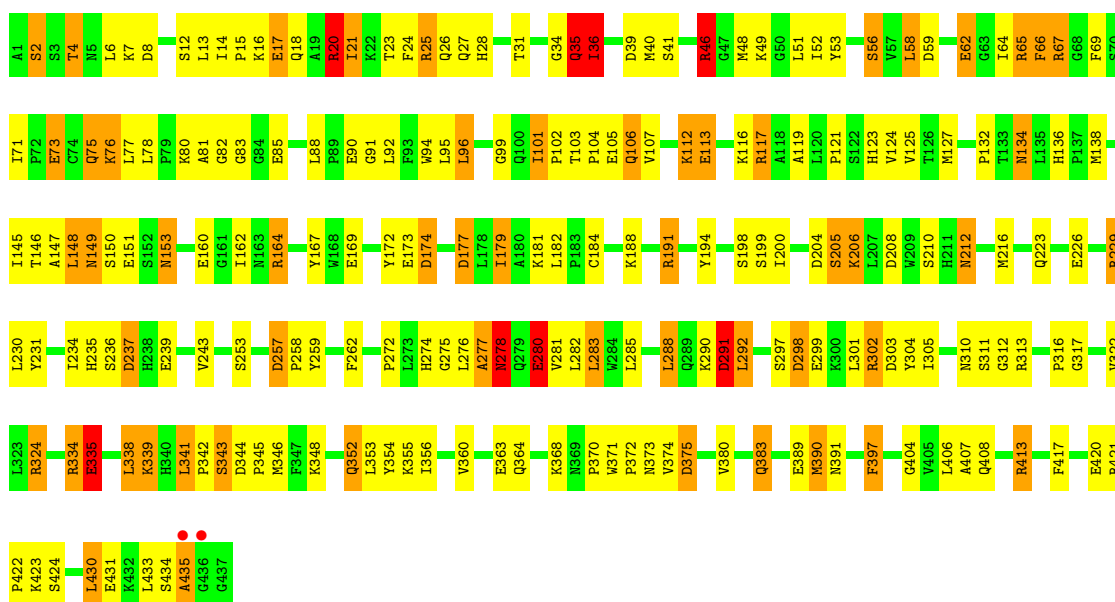
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	74	Total 74	O 74	0	0

### 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.

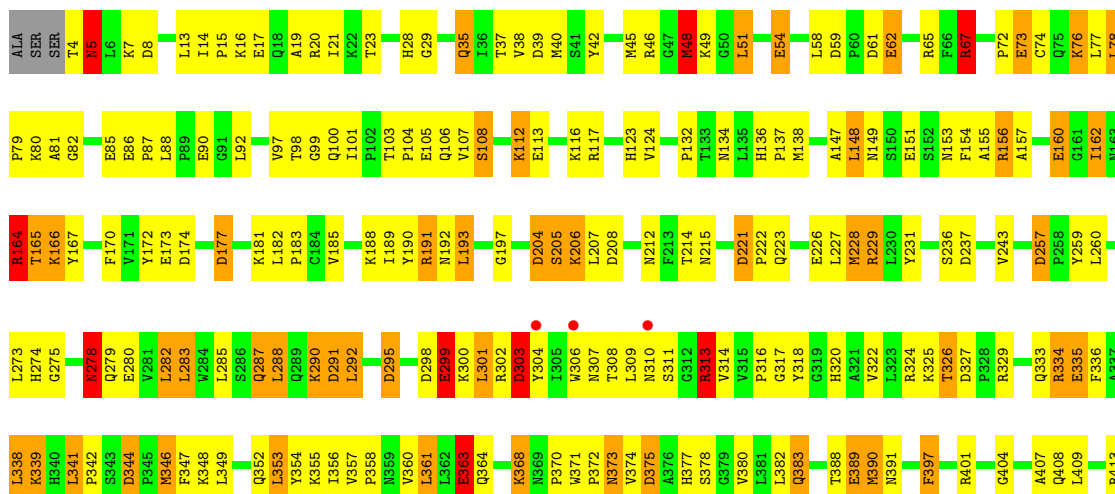
#### • Molecule 1: CITRATE SYNTHASE

Chain A:



#### • Molecule 1: CITRATE SYNTHASE

Chain B:



F417	E420	L430
R421	R421	E431
		K432
		L433
		S434
		A435
		G436
		G437

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.37Å 100.21Å 87.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 34.54 – 2.23	Depositor EDS
% Data completeness (in resolution range)	86.0 (25.00-2.25) 84.1 (34.54-2.23)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.22Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, $R_{free}$	0.158 , (Not available) 0.148 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	14.2	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 86.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 40588 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COF, CIT

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	1.01	21/3487 (0.6%)	1.36	46/4736 (1.0%)
1	B	0.97	18/3470 (0.5%)	1.41	49/4713 (1.0%)
All	All	0.99	39/6957 (0.6%)	1.39	95/9449 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	0
All	All	2	0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLU	CD-OE1	8.07	1.34	1.25
1	A	90	GLU	CD-OE2	7.66	1.34	1.25
1	B	335	GLU	CD-OE1	7.18	1.33	1.25
1	B	90	GLU	CD-OE2	6.86	1.33	1.25
1	A	151	GLU	CD-OE2	6.80	1.33	1.25
1	B	113	GLU	CD-OE2	6.80	1.33	1.25
1	A	105	GLU	CD-OE2	6.75	1.33	1.25
1	A	173	GLU	CD-OE1	6.70	1.33	1.25
1	A	85	GLU	CD-OE1	6.67	1.32	1.25
1	B	173	GLU	CD-OE1	6.61	1.32	1.25
1	A	113	GLU	CD-OE2	6.45	1.32	1.25
1	B	363	GLU	CD-OE1	6.41	1.32	1.25
1	B	105	GLU	CD-OE2	6.37	1.32	1.25
1	B	299	GLU	CD-OE2	6.35	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLU	CD-OE2	6.35	1.32	1.25
1	A	17	GLU	CD-OE2	6.24	1.32	1.25
1	A	226	GLU	CD-OE2	6.16	1.32	1.25
1	B	160	GLU	CD-OE2	6.16	1.32	1.25
1	B	226	GLU	CD-OE2	6.10	1.32	1.25
1	B	151	GLU	CD-OE2	6.05	1.32	1.25
1	A	299	GLU	CD-OE2	6.00	1.32	1.25
1	A	363	GLU	CD-OE1	5.86	1.32	1.25
1	A	160	GLU	CD-OE2	5.86	1.32	1.25
1	B	420	GLU	CD-OE1	5.85	1.32	1.25
1	A	280	GLU	CD-OE2	5.81	1.32	1.25
1	A	335	GLU	CD-OE1	5.68	1.31	1.25
1	B	280	GLU	CD-OE2	5.65	1.31	1.25
1	B	85	GLU	CD-OE1	5.64	1.31	1.25
1	B	62	GLU	CD-OE2	5.58	1.31	1.25
1	B	17	GLU	CD-OE2	5.51	1.31	1.25
1	B	431	GLU	CD-OE2	5.42	1.31	1.25
1	A	90	GLU	CD-OE1	-5.36	1.19	1.25
1	A	431	GLU	CD-OE2	5.34	1.31	1.25
1	B	73	GLU	CD-OE1	5.27	1.31	1.25
1	B	54	GLU	CD-OE2	5.23	1.31	1.25
1	A	420	GLU	CD-OE1	5.20	1.31	1.25
1	A	239	GLU	CD-OE1	5.17	1.31	1.25
1	A	239	GLU	CD-OE2	-5.17	1.20	1.25
1	A	73	GLU	CD-OE2	5.16	1.31	1.25

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	NE-CZ-NH1	16.28	128.44	120.30
1	B	229	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	B	117	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	B	174	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	B	401	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	B	257	ASP	CB-CG-OD2	-9.65	109.61	118.30
1	B	174	ASP	CB-CG-OD1	8.86	126.27	118.30
1	B	61	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	A	257	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	B	295	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	257	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	20	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	B	59	ASP	CB-CG-OD2	-7.83	111.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	SER	N-CA-CB	-7.76	98.85	110.50
1	B	65	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	67	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	A	291	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	298	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	B	5	ASN	N-CA-CB	7.51	124.13	110.60
1	A	229	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	295	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	8	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	4	THR	N-CA-C	7.13	130.25	111.00
1	A	208	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	A	237	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	375	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	237	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	303	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	375	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	A	36	ILE	N-CA-CB	6.85	126.55	110.80
1	A	46	ARG	CD-NE-CZ	-6.85	114.01	123.60
1	B	61	ASP	CB-CG-OD2	6.84	124.46	118.30
1	A	35	GLN	N-CA-CB	-6.80	98.35	110.60
1	A	8	ASP	CB-CG-OD2	6.72	124.34	118.30
1	B	401	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	164	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	208	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	35	GLN	CB-CA-C	-6.62	97.16	110.40
1	A	298	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	303	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	39	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	B	191	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	174	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	65	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	229	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	327	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	B	59	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	59	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	39	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	324	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	303	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	39	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	59	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	34	GLY	C-N-CA	6.14	137.06	121.70
1	A	277	ALA	CB-CA-C	6.09	119.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	343	SER	N-CA-CB	5.92	119.37	110.50
1	B	48	MET	N-CA-CB	5.87	121.16	110.60
1	A	117	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	8	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	B	51	LEU	CB-CA-C	-5.82	99.15	110.20
1	A	67	ARG	N-CA-CB	5.80	121.04	110.60
1	B	344	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	2	SER	C-N-CA	5.69	135.93	121.70
1	A	177	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	257	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	278	ASN	CB-CA-C	-5.64	99.13	110.40
1	B	67	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	291	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	46	ARG	N-CA-CB	5.52	120.54	110.60
1	A	208	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	324	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	155	ALA	N-CA-CB	5.45	117.73	110.10
1	A	39	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	375	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	278	ASN	CB-CA-C	-5.34	99.72	110.40
1	A	407	ALA	CB-CA-C	5.33	118.10	110.10
1	B	164	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	208	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	302	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	221	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	313	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	67	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	204	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	324	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	2	SER	N-CA-C	5.16	124.92	111.00
1	B	48	MET	CG-SD-CE	-5.14	91.97	100.20
1	B	344	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	B	221	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	67	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	344	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	A	375	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	A	65	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	278	ASN	N-CA-CB	-5.01	101.58	110.60
1	B	177	ASP	CB-CG-OD1	-5.00	113.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	THR	CA
1	B	5	ASN	CA

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3402	0	3383	162	0
1	B	3385	0	3365	194	0
2	A	71	0	24	9	0
2	B	71	0	24	17	0
3	A	13	0	5	2	0
3	B	13	0	5	2	0
4	A	72	0	0	4	0
4	B	74	0	0	5	0
All	All	7101	0	6806	359	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (359) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:314:VAL:HG21	2:B:700[A]:COF:H72	1.34	1.09
1:B:124:VAL:HG21	1:B:148:LEU:HD13	1.40	1.02
1:A:124:VAL:HG21	1:A:148:LEU:HD13	1.40	1.02
1:A:24:PHE:HA	1:B:437:GLY:HA3	1.44	0.99
1:B:136:HIS:HD2	1:B:138:MET:H	1.10	0.98
1:B:314:VAL:HG21	2:B:700[B]:COF:H72	1.46	0.96
2:B:700[A]:COF:HI12	3:B:701:CIT:O3	1.62	0.95
1:A:67:ARG:HD3	1:A:99:GLY:HA2	1.49	0.95
1:A:373:ASN:HD21	2:A:700[A]:COF:H32	1.31	0.95
1:A:20:ARG:HH11	1:A:20:ARG:HG2	1.32	0.94
1:B:164:ARG:HH11	1:B:164:ARG:HG3	1.32	0.94
1:B:228:MET:HE2	1:B:228:MET:HA	1.50	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:204:ASP:H	1:A:212:ASN:HD21	0.94	0.93
1:A:136:HIS:HD2	1:A:138:MET:H	1.09	0.93
1:B:306:TRP:HH2	1:B:363:GLU:HG2	1.35	0.91
1:B:103:THR:H	1:B:106:GLN:HE21	1.16	0.90
1:B:282:LEU:HD23	1:B:390:MET:HE3	1.53	0.89
1:B:88:LEU:HD23	1:B:229:ARG:HD2	1.56	0.88
1:A:346:MET:HG2	1:A:380:VAL:HG12	1.53	0.87
1:B:156:ARG:HH11	1:B:156:ARG:HG3	1.37	0.87
1:A:56:SER:HB2	1:A:64:ILE:HD11	1.54	0.87
1:B:292:LEU:HD21	1:B:304:TYR:CD2	2.09	0.86
1:B:288:LEU:HD13	1:B:292:LEU:HD23	1.58	0.85
1:B:165:THR:HB	1:B:166:LYS:HZ2	1.38	0.85
1:A:136:HIS:CD2	1:A:138:MET:H	1.93	0.85
1:B:306:TRP:CH2	1:B:363:GLU:HG2	2.12	0.85
1:B:165:THR:HB	1:B:166:LYS:NZ	1.90	0.85
1:B:103:THR:H	1:B:106:GLN:NE2	1.76	0.83
1:B:204:ASP:H	1:B:212:ASN:HD21	1.22	0.83
1:A:204:ASP:H	1:A:212:ASN:ND2	1.75	0.82
1:B:228:MET:CE	1:B:228:MET:HA	2.09	0.81
1:B:136:HIS:CD2	1:B:138:MET:H	1.99	0.81
1:B:282:LEU:HD23	1:B:390:MET:CE	2.11	0.80
1:A:373:ASN:HD21	2:A:700[A]:COF:C3P	1.94	0.80
1:B:302:ARG:NH1	1:B:306:TRP:NE1	2.29	0.80
1:A:346:MET:HG2	1:A:380:VAL:CG1	2.11	0.80
1:B:302:ARG:HH11	1:B:306:TRP:HE1	1.30	0.79
1:A:204:ASP:N	1:A:212:ASN:HD21	1.79	0.78
1:B:166:LYS:N	1:B:166:LYS:HE3	1.97	0.78
2:B:700[A]:COF:HI12	3:B:701:CIT:C5	2.14	0.77
1:A:17:GLU:O	1:A:21:ILE:HD13	1.84	0.77
1:A:14:ILE:O	1:A:18:GLN:HG3	1.85	0.76
1:B:112:LYS:N	1:B:112:LYS:HD2	1.98	0.76
1:A:301:LEU:HD22	1:A:352:GLN:OE1	1.84	0.76
1:B:329:ARG:O	1:B:333:GLN:HG3	1.85	0.75
1:A:352:GLN:HG2	1:A:355:LYS:NZ	2.02	0.74
1:A:88:LEU:HD23	1:A:229:ARG:CD	2.19	0.73
1:B:204:ASP:OD1	1:B:206:LYS:HE3	1.90	0.72
1:B:326:THR:HG21	1:B:354:TYR:OH	1.91	0.71
1:A:132:PRO:HB2	1:A:134:ASN:ND2	2.06	0.71
1:B:19:ALA:O	1:B:23:THR:HG23	1.90	0.71
1:B:316:PRO:HA	2:B:700[B]:COF:O5P	1.91	0.71
1:A:352:GLN:HG2	1:A:355:LYS:HZ1	1.55	0.71
1:B:166:LYS:CA	1:B:166:LYS:HE3	2.21	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:37:THR:OG1	1:B:40:MET:HG3	1.92	0.70
1:B:45:MET:HB3	1:B:48:MET:HG3	1.73	0.70
1:A:67:ARG:HD3	1:A:99:GLY:CA	2.22	0.70
1:B:371:TRP:HB3	1:B:372:PRO:HD2	1.73	0.70
1:A:103:THR:H	1:A:106:GLN:HE21	1.39	0.70
1:A:134:ASN:HD22	1:A:134:ASN:H	1.40	0.69
1:A:334:ARG:HG2	1:A:338:LEU:CD2	2.23	0.69
1:A:14:ILE:HG22	1:A:15:PRO:HD3	1.76	0.69
1:B:72:PRO:O	1:B:76:LYS:HG2	1.94	0.68
1:A:35:GLN:O	1:A:36:ILE:HG13	1.93	0.68
1:B:342:PRO:O	1:B:348:LYS:HE2	1.92	0.68
1:B:40:MET:HE3	1:B:48:MET:HG2	1.75	0.68
1:A:181:LYS:O	1:A:184:CYS:HB2	1.94	0.67
1:B:292:LEU:HD21	1:B:304:TYR:HD2	1.58	0.67
1:B:325:LYS:HE3	1:B:326:THR:H	1.60	0.67
1:B:228:MET:HE2	1:B:231:TYR:HB3	1.75	0.67
1:A:88:LEU:HD23	1:A:229:ARG:HD2	1.76	0.66
1:A:334:ARG:HG2	1:A:338:LEU:HD22	1.77	0.66
1:B:413:ARG:NH2	4:B:716:HOH:O	2.28	0.66
1:B:314:VAL:CG2	2:B:700[A]:COF:H72	2.20	0.65
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.08	0.65
1:A:231:TYR:O	1:A:234:ILE:HG22	1.97	0.65
1:A:46:ARG:HG2	1:A:46:ARG:NH1	2.13	0.64
1:B:204:ASP:H	1:B:212:ASN:ND2	1.93	0.64
1:B:112:LYS:H	1:B:112:LYS:HD2	1.62	0.63
1:A:430:LEU:HD12	1:A:430:LEU:O	1.98	0.63
1:A:20:ARG:NH1	1:A:20:ARG:HG2	2.02	0.63
1:A:277:ALA:HB1	2:A:700[A]:COF:HN4	1.65	0.62
1:B:67:ARG:HG2	1:B:99:GLY:HA2	1.81	0.62
1:B:40:MET:HE3	1:B:48:MET:CG	2.29	0.62
1:A:153:ASN:ND2	1:A:174:ASP:OD1	2.29	0.62
1:A:88:LEU:HD23	1:A:229:ARG:HD3	1.81	0.62
1:B:336:PHE:HA	1:B:339:LYS:HD2	1.80	0.62
2:B:700[A]:COF:H62	2:B:700[A]:COF:S1P	2.40	0.62
1:B:92:LEU:HD21	1:B:236:SER:OG	2.00	0.61
1:B:165:THR:C	1:B:166:LYS:HE3	2.21	0.61
1:A:206:LYS:HB2	1:A:206:LYS:NZ	2.15	0.61
1:A:257:ASP:HB2	1:A:258:PRO:HD2	1.83	0.61
1:A:162:ILE:HD12	1:A:167:TYR:HD1	1.65	0.61
1:A:316:PRO:HA	2:A:700[B]:COF:O5P	2.01	0.61
1:A:311:SER:OG	1:A:313:ARG:HD3	2.00	0.61
1:B:353:LEU:O	1:B:357:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:SER:HB3	1:A:106:GLN:OE1	2.00	0.61
1:A:283:LEU:HD13	1:A:390:MET:SD	2.41	0.60
1:A:288:LEU:O	1:A:288:LEU:HD12	2.01	0.60
1:B:103:THR:N	1:B:106:GLN:HE21	1.95	0.60
2:A:700[A]:COF:HI12	3:A:701:CIT:O4	2.02	0.59
1:A:136:HIS:HD2	1:A:138:MET:N	1.91	0.59
1:A:257:ASP:OD1	1:A:259:TYR:HB2	2.01	0.59
1:A:153:ASN:H	1:A:153:ASN:HD22	1.49	0.59
1:A:24:PHE:HA	1:B:437:GLY:CA	2.28	0.59
1:A:413:ARG:NH1	1:A:417:PHE:O	2.29	0.59
1:B:132:PRO:HB2	1:B:134:ASN:OD1	2.03	0.59
1:B:177:ASP:O	1:B:181:LYS:HG3	2.03	0.58
1:A:413:ARG:NH2	4:A:709:HOH:O	2.28	0.58
1:B:298:ASP:HB3	1:B:356:ILE:HD11	1.85	0.58
1:B:136:HIS:HD2	1:B:138:MET:N	1.92	0.58
1:A:121:PRO:HD2	1:A:148:LEU:HD11	1.85	0.58
1:B:35:GLN:OE1	1:B:35:GLN:N	2.30	0.58
1:B:40:MET:HE1	1:B:48:MET:HB3	1.86	0.58
1:B:341:LEU:N	1:B:342:PRO:HD3	2.19	0.57
1:B:137:PRO:HG2	1:B:391:ASN:O	2.03	0.57
1:B:162:ILE:HD13	1:B:167:TYR:CE1	2.39	0.57
1:A:234:ILE:HG23	1:A:235:HIS:ND1	2.19	0.57
1:B:157:ALA:O	1:B:160:GLU:HB2	2.05	0.57
1:A:162:ILE:CD1	1:A:167:TYR:HD1	2.17	0.57
1:B:185:VAL:O	1:B:189:ILE:HG13	2.05	0.57
1:B:77:LEU:HB3	1:B:101:ILE:HD12	1.86	0.57
1:B:317:GLY:H	2:B:700[A]:COF:HN4	1.49	0.57
1:A:51:LEU:HD23	1:A:52:ILE:N	2.20	0.57
1:B:81:ALA:HB2	1:B:88:LEU:HD21	1.86	0.56
1:B:308:THR:O	1:B:313:ARG:HG3	2.04	0.56
1:B:316:PRO:HG3	2:B:700[B]:COF:HI11	1.87	0.56
1:B:162:ILE:HD13	1:B:167:TYR:HE1	1.71	0.56
1:B:164:ARG:HG3	1:B:164:ARG:NH1	2.08	0.56
1:B:124:VAL:HG21	1:B:148:LEU:CD1	2.26	0.56
1:B:166:LYS:HA	1:B:166:LYS:HE3	1.87	0.56
1:B:314:VAL:HG21	2:B:700[A]:COF:C7P	2.24	0.55
1:A:179:ILE:CD1	1:A:406:LEU:HD12	2.36	0.55
1:A:65:ARG:NH1	1:A:73:GLU:OE1	2.39	0.55
1:B:54:GLU:H	1:B:408:GLN:HE22	1.54	0.55
1:B:373:ASN:C	1:B:373:ASN:HD22	2.09	0.55
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.72	0.54
1:A:81:ALA:O	1:A:83:GLY:N	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:73:GLU:HA	1:B:76:LYS:HE3	1.88	0.54
1:A:23:THR:O	1:A:26:GLN:HB3	2.08	0.54
1:A:66:PHE:N	1:A:69:PHE:O	2.38	0.54
1:B:335:GLU:O	1:B:339:LYS:HG3	2.08	0.54
1:A:288:LEU:HD12	1:A:288:LEU:C	2.27	0.54
1:A:288:LEU:HD22	1:A:304:TYR:CE2	2.42	0.54
1:B:4:THR:O	1:B:4:THR:HG23	2.08	0.54
1:B:300:LYS:HA	1:B:303:ASP:OD1	2.09	0.53
1:B:88:LEU:HD23	1:B:229:ARG:CD	2.36	0.53
1:A:132:PRO:HB2	1:A:134:ASN:HD22	1.73	0.53
1:A:146:THR:O	1:A:149:ASN:HB3	2.07	0.53
1:B:16:LYS:N	1:B:16:LYS:HD2	2.22	0.53
1:B:283:LEU:N	1:B:283:LEU:HD13	2.24	0.53
1:B:282:LEU:CD2	1:B:390:MET:HE3	2.31	0.53
1:B:278:ASN:ND2	4:B:768:HOH:O	2.42	0.53
1:B:333:GLN:HE22	1:B:378:SER:HB3	1.74	0.53
1:B:292:LEU:H	1:B:292:LEU:HD22	1.74	0.53
1:A:53:TYR:CD1	1:A:408:GLN:HG2	2.44	0.53
1:A:430:LEU:HD12	1:A:430:LEU:C	2.29	0.52
1:B:357:VAL:HB	1:B:358:PRO:HD3	1.91	0.52
1:A:383:GLN:HG2	4:A:757:HOH:O	2.07	0.52
1:B:192:ASN:HD22	1:B:197:GLY:HA2	1.74	0.52
1:A:276:LEU:O	1:A:280:GLU:HG2	2.08	0.52
1:B:371:TRP:HB3	1:B:372:PRO:CD	2.39	0.52
1:A:145:ILE:HD13	1:A:262:PHE:CE2	2.43	0.52
1:B:7:LYS:HD3	1:B:172:TYR:CE1	2.44	0.52
1:A:75:GLN:O	1:A:80:LYS:NZ	2.37	0.52
1:B:40:MET:CE	1:B:48:MET:HB3	2.40	0.52
1:A:194:TYR:CD2	1:A:389:GLU:HG3	2.45	0.52
1:A:101:ILE:HG12	1:A:102:PRO:HD2	1.92	0.52
1:B:391:ASN:HD22	1:B:391:ASN:N	2.06	0.52
1:A:14:ILE:CG2	1:A:15:PRO:HD3	2.39	0.51
1:A:335:GLU:O	1:A:339:LYS:HD3	2.09	0.51
1:A:20:ARG:CG	1:A:20:ARG:HH11	2.13	0.51
1:A:113:GLU:O	1:A:117:ARG:HG3	2.10	0.51
1:B:28:HIS:O	1:B:29:GLY:C	2.48	0.51
1:B:275:GLY:O	1:B:278:ASN:HB2	2.10	0.51
1:A:277:ALA:HB1	2:A:700[A]:COF:N4P	2.25	0.51
1:A:177:ASP:HB3	1:A:181:LYS:HE3	1.93	0.51
1:B:74:CYS:HB3	1:B:78:LEU:HD12	1.93	0.51
1:A:28:HIS:O	1:B:38:VAL:HB	2.11	0.51
1:B:301:LEU:HD23	1:B:352:GLN:HG2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:347:PHE:HA	1:B:380:VAL:HG21	1.93	0.51
1:A:67:ARG:HD2	1:A:96:LEU:O	2.11	0.50
1:B:204:ASP:HB3	1:B:207:LEU:HG	1.93	0.50
1:B:299:GLU:O	1:B:303:ASP:OD1	2.29	0.50
1:B:98:THR:OG1	1:B:100:GLN:HG2	2.11	0.50
1:B:302:ARG:NH1	1:B:306:TRP:HE1	1.92	0.50
1:A:124:VAL:HG21	1:A:148:LEU:CD1	2.28	0.50
1:A:145:ILE:HD13	1:A:262:PHE:CD2	2.46	0.50
1:B:377:HIS:ND1	1:B:377:HIS:O	2.40	0.50
1:B:285:LEU:HD22	1:B:349:LEU:CD2	2.41	0.50
1:A:21:ILE:O	1:A:25:ARG:HB2	2.12	0.50
1:B:104:PRO:O	1:B:108:SER:OG	2.29	0.50
1:B:374:VAL:HG13	1:B:375:ASP:N	2.25	0.50
1:A:56:SER:OG	1:A:237:ASP:OD2	2.29	0.49
1:A:24:PHE:CA	1:B:437:GLY:HA3	2.29	0.49
1:A:14:ILE:CB	1:A:15:PRO:HD3	2.42	0.49
1:A:352:GLN:O	1:A:356:ILE:HG12	2.11	0.49
1:B:344:ASP:O	1:B:348:LYS:HG3	2.12	0.49
1:A:123:HIS:HE1	1:A:147:ALA:O	1.94	0.49
1:B:192:ASN:HA	1:B:197:GLY:HA2	1.93	0.49
1:A:305:ILE:HG22	1:A:360:VAL:HG11	1.94	0.49
1:B:214:THR:HG22	1:B:228:MET:HG3	1.95	0.49
1:B:123:HIS:HE1	1:B:147:ALA:O	1.96	0.49
1:A:46:ARG:CG	1:A:46:ARG:HH11	2.23	0.49
1:A:237:ASP:OD1	1:A:404:GLY:HA3	2.13	0.48
1:A:272:PRO:HA	1:A:276:LEU:HB3	1.95	0.48
1:A:28:HIS:HB3	1:A:31:THR:HB	1.96	0.48
1:A:95:LEU:O	1:A:99:GLY:N	2.42	0.48
1:A:112:LYS:O	1:A:116:LYS:HG3	2.13	0.48
1:A:364:GLN:HG2	1:A:364:GLN:O	2.11	0.48
1:A:257:ASP:HB2	1:A:258:PRO:CD	2.43	0.48
1:A:374:VAL:HG13	1:A:375:ASP:N	2.28	0.48
1:B:54:GLU:H	1:B:408:GLN:NE2	2.11	0.48
1:B:302:ARG:NH1	1:B:306:TRP:CD1	2.81	0.48
1:A:162:ILE:HD12	1:A:167:TYR:CD1	2.48	0.48
1:A:281:VAL:HG22	1:A:316:PRO:HB2	1.96	0.47
1:B:334:ARG:HG3	1:B:335:GLU:N	2.25	0.47
1:B:58:LEU:HD23	1:B:322:VAL:HG11	1.95	0.47
1:B:78:LEU:HB3	4:B:720:HOH:O	2.15	0.47
1:B:236:SER:O	1:B:404:GLY:HA3	2.15	0.47
1:A:164:ARG:HH11	1:A:164:ARG:CG	2.28	0.46
1:A:164:ARG:HH11	1:A:164:ARG:CB	2.28	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:ASN:C	1:A:312:GLY:H	2.19	0.46
1:B:112:LYS:HE3	1:B:205:SER:O	2.16	0.46
1:A:153:ASN:ND2	1:A:153:ASN:N	2.63	0.46
1:A:292:LEU:N	1:A:292:LEU:CD2	2.79	0.46
1:B:190:TYR:CE1	1:B:389:GLU:HG3	2.50	0.46
1:B:257:ASP:OD1	1:B:259:TYR:HB2	2.15	0.46
1:B:74:CYS:HB3	1:B:78:LEU:CD1	2.44	0.46
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.68	0.46
1:B:346:MET:HE3	1:B:346:MET:HB2	1.86	0.46
1:B:341:LEU:N	1:B:342:PRO:CD	2.78	0.46
1:B:283:LEU:HD11	1:B:390:MET:CG	2.46	0.46
1:B:329:ARG:HB3	1:B:374:VAL:HG23	1.97	0.46
1:B:316:PRO:HB3	2:B:700[B]:COF:H21	1.97	0.46
1:B:285:LEU:O	1:B:288:LEU:HB3	2.16	0.45
1:A:53:TYR:CE1	1:A:408:GLN:HG2	2.51	0.45
1:B:80:LYS:HD3	1:B:87:PRO:HA	1.98	0.45
1:B:370:PRO:HD2	1:B:371:TRP:CD1	2.51	0.45
1:A:35:GLN:HG3	1:A:40:MET:SD	2.56	0.45
1:B:413:ARG:NH1	1:B:417:PHE:O	2.29	0.45
1:A:234:ILE:HG23	1:A:235:HIS:HD1	1.82	0.45
1:A:162:ILE:CD1	1:A:167:TYR:CD1	2.99	0.45
1:A:119:ALA:HB2	4:A:738:HOH:O	2.15	0.45
1:A:21:ILE:N	1:A:21:ILE:CD1	2.79	0.45
1:A:341:LEU:N	1:A:342:PRO:CD	2.79	0.45
1:B:292:LEU:N	1:B:292:LEU:HD22	2.31	0.45
1:A:46:ARG:HD3	1:A:46:ARG:HA	1.46	0.45
1:A:297:SER:O	1:A:298:ASP:C	2.54	0.45
1:A:200:ILE:HB	1:A:216:MET:HB3	1.99	0.45
1:A:334:ARG:O	1:A:338:LEU:HD22	2.17	0.45
1:A:305:ILE:CG2	1:A:360:VAL:HG11	2.47	0.45
1:A:243:VAL:HB	1:A:274:HIS:CD2	2.51	0.45
1:B:260:LEU:N	1:B:260:LEU:HD23	2.32	0.45
1:B:79:PRO:HG2	1:B:107:VAL:HG21	1.98	0.45
1:A:14:ILE:HG22	1:A:15:PRO:CD	2.45	0.45
1:B:338:LEU:CD1	1:B:347:PHE:CZ	3.00	0.44
1:B:154:PHE:HA	1:B:170:PHE:HB3	1.97	0.44
1:A:103:THR:HB	1:A:104:PRO:HD2	2.00	0.44
1:B:279:GLN:O	1:B:283:LEU:HD22	2.16	0.44
1:B:357:VAL:N	1:B:358:PRO:CD	2.80	0.44
1:B:189:ILE:O	1:B:193:LEU:HB2	2.17	0.44
1:B:338:LEU:HA	1:B:338:LEU:HD12	1.68	0.44
1:A:35:GLN:HG3	1:A:40:MET:CE	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:354:TYR:CD1	1:A:372:PRO:HG3	2.53	0.44
1:B:283:LEU:CD1	1:B:390:MET:HG3	2.48	0.44
1:B:76:LYS:HG2	1:B:76:LYS:H	1.66	0.44
1:B:14:ILE:HB	1:B:15:PRO:HD3	1.98	0.44
1:B:214:THR:CG2	1:B:228:MET:HG3	2.48	0.44
1:A:25:ARG:HE	1:B:42:TYR:CB	2.30	0.44
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.46	0.44
1:B:215:ASN:HA	1:B:215:ASN:HD22	1.59	0.44
1:A:121:PRO:O	1:A:125:VAL:HG23	2.17	0.44
1:A:21:ILE:H	1:A:21:ILE:CD1	2.31	0.43
1:B:326:THR:HB	1:B:372:PRO:HD2	1.99	0.43
1:A:413:ARG:HA	1:A:413:ARG:HD3	1.75	0.43
1:B:279:GLN:HB2	1:B:390:MET:O	2.17	0.43
1:B:97:VAL:HG23	1:B:407:ALA:HB1	2.00	0.43
1:A:191:ARG:HG3	1:A:198:SER:O	2.18	0.43
1:B:283:LEU:HD13	1:B:390:MET:HG3	1.99	0.43
1:B:35:GLN:CD	1:B:35:GLN:H	2.19	0.43
1:A:434:SER:O	1:A:435:ALA:HB2	2.18	0.43
1:A:149:ASN:ND2	1:A:257:ASP:OD2	2.49	0.43
1:A:281:VAL:O	1:A:285:LEU:HG	2.18	0.43
1:A:397:PHE:O	1:A:397:PHE:HD1	2.01	0.43
1:B:16:LYS:N	1:B:16:LYS:CD	2.80	0.43
1:B:86:GLU:HA	1:B:86:GLU:OE1	2.19	0.43
1:B:40:MET:CE	1:B:48:MET:CG	2.96	0.43
1:A:71:ILE:O	1:A:75:GLN:HB2	2.19	0.43
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.75	0.43
1:B:314:VAL:HG13	2:B:700[B]:COF:H22	2.00	0.43
1:A:153:ASN:ND2	1:A:153:ASN:H	2.15	0.43
1:A:345:PRO:HA	1:A:348:LYS:HD3	2.01	0.43
1:A:24:PHE:HD1	1:B:437:GLY:HA3	1.84	0.43
1:B:221:ASP:OD1	1:B:222:PRO:HD2	2.19	0.43
1:A:206:LYS:HB2	1:A:206:LYS:HZ3	1.83	0.42
1:A:317:GLY:HA2	2:A:700[A]:COF:H32	2.00	0.42
1:B:88:LEU:CD2	1:B:229:ARG:HD2	2.37	0.42
1:A:76:LYS:HG3	1:A:77:LEU:HD13	2.01	0.42
1:A:311:SER:CB	1:A:313:ARG:HH11	2.29	0.42
1:B:298:ASP:CB	1:B:356:ILE:HD11	2.48	0.42
1:A:7:LYS:HD2	1:A:172:TYR:CE1	2.54	0.42
1:A:324:ARG:HD3	1:A:324:ARG:HA	1.70	0.42
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.81	0.42
1:A:253:SER:HA	1:A:413:ARG:NH2	2.35	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:243:VAL:HB	1:B:274:HIS:CD2	2.55	0.42
1:B:164:ARG:HA	1:B:167:TYR:CE1	2.54	0.42
1:A:91:GLY:HA3	4:A:713:HOH:O	2.19	0.42
1:B:320:HIS:HA	2:B:700[A]:COF:F2I	2.10	0.42
1:B:357:VAL:O	1:B:361:LEU:HB2	2.19	0.42
1:A:127:MET:HB3	1:A:127:MET:HE3	1.77	0.42
1:B:40:MET:CE	1:B:48:MET:SD	3.08	0.42
1:B:215:ASN:ND2	4:B:759:HOH:O	2.52	0.42
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.82	0.42
1:B:288:LEU:HD22	1:B:304:TYR:CE1	2.55	0.42
1:A:421:ARG:HD3	1:A:422:PRO:O	2.20	0.41
1:A:275:GLY:O	1:A:278:ASN:HB2	2.20	0.41
1:A:352:GLN:HG2	1:A:355:LYS:HZ2	1.84	0.41
1:A:234:ILE:HD13	1:A:234:ILE:HG21	1.36	0.41
1:B:153:ASN:ND2	4:B:749:HOH:O	2.28	0.41
1:A:301:LEU:HD22	1:A:352:GLN:CD	2.40	0.41
1:B:374:VAL:CG1	1:B:375:ASP:N	2.83	0.41
1:B:373:ASN:HD21	1:B:375:ASP:HB2	1.86	0.41
1:A:112:LYS:HE2	1:A:112:LYS:HB3	1.68	0.41
1:A:58:LEU:HD13	1:A:322:VAL:CG1	2.50	0.41
1:A:370:PRO:HD2	1:A:371:TRP:CD1	2.56	0.41
1:B:182:LEU:HB2	1:B:183:PRO:HD3	2.03	0.41
1:A:103:THR:HG23	1:A:106:GLN:NE2	2.36	0.41
1:B:287:GLN:HA	1:B:290:LYS:HG3	2.01	0.41
1:A:92:LEU:HD21	1:A:236:SER:CB	2.50	0.41
1:B:306:TRP:CE2	1:B:360:VAL:HG22	2.56	0.41
1:B:40:MET:CE	1:B:48:MET:CB	2.99	0.41
1:B:7:LYS:HD3	1:B:172:TYR:CD1	2.56	0.41
1:A:91:GLY:HA2	1:A:107:VAL:HG22	2.03	0.41
1:B:397:PHE:O	1:B:397:PHE:HD1	2.03	0.41
1:A:274:HIS:CE1	3:A:701:CIT:H22	2.56	0.41
1:B:124:VAL:CG2	1:B:148:LEU:HD13	2.30	0.40
1:B:156:ARG:HA	1:B:156:ARG:HD2	1.73	0.40
1:B:156:ARG:NH1	1:B:156:ARG:CG	2.80	0.40
1:B:40:MET:HE2	1:B:48:MET:SD	2.62	0.40
1:B:380:VAL:O	1:B:383:GLN:NE2	2.54	0.40
1:B:382:LEU:HA	1:B:382:LEU:HD23	1.88	0.40
1:A:230:LEU:O	1:A:234:ILE:HG22	2.22	0.40
1:A:291:ASP:HB3	1:A:292:LEU:HD22	2.03	0.40
1:B:273:LEU:O	2:B:700[A]:COF:S1P	2.79	0.40
1:B:338:LEU:CD1	1:B:347:PHE:HZ	2.34	0.40
1:A:283:LEU:CD1	1:A:390:MET:SD	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:TRP:HB3	1:A:102:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	435/437 (100%)	411 (94%)	19 (4%)	5 (1%)	21	15
1	B	432/437 (99%)	410 (95%)	18 (4%)	4 (1%)	25	20
All	All	867/874 (99%)	821 (95%)	37 (4%)	9 (1%)	22	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	36	ILE
1	A	435	ALA
1	B	311	SER
1	B	435	ALA
1	A	66	PHE
1	B	5	ASN
1	B	82	GLY
1	A	82	GLY

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/362 (100%)	295 (82%)	67 (18%)	2	1
1	B	360/362 (99%)	292 (81%)	68 (19%)	2	1
All	All	722/724 (100%)	587 (81%)	135 (19%)	2	1

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	6	LEU
1	A	12	SER
1	A	13	LEU
1	A	16	LYS
1	A	20	ARG
1	A	21	ILE
1	A	25	ARG
1	A	27	GLN
1	A	35	GLN
1	A	41	SER
1	A	46	ARG
1	A	48	MET
1	A	49	LYS
1	A	56	SER
1	A	58	LEU
1	A	62	GLU
1	A	75	GLN
1	A	76	LYS
1	A	78	LEU
1	A	96	LEU
1	A	101	ILE
1	A	106	GLN
1	A	112	LYS
1	A	134	ASN
1	A	148	LEU
1	A	149	ASN
1	A	150	SER
1	A	153	ASN
1	A	164	ARG
1	A	179	ILE
1	A	182	LEU

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Mol	Chain	Res	Type
1	A	188	LYS
1	A	191	ARG
1	A	199	SER
1	A	205	SER
1	A	206	LYS
1	A	210	SER
1	A	212	ASN
1	A	223	GLN
1	A	278	ASN
1	A	280	GLU
1	A	282	LEU
1	A	283	LEU
1	A	288	LEU
1	A	290	LYS
1	A	291	ASP
1	A	292	LEU
1	A	302	ARG
1	A	334	ARG
1	A	335	GLU
1	A	338	LEU
1	A	339	LYS
1	A	341	LEU
1	A	343	SER
1	A	352	GLN
1	A	353	LEU
1	A	368	LYS
1	A	383	GLN
1	A	390	MET
1	A	391	ASN
1	A	397	PHE
1	A	413	ARG
1	A	423	LYS
1	A	424	SER
1	A	430	LEU
1	A	433	LEU
1	B	5	ASN
1	B	13	LEU
1	B	20	ARG
1	B	21	ILE
1	B	35	GLN
1	B	46	ARG
1	B	48	MET

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Mol	Chain	Res	Type
1	B	49	LYS
1	B	51	LEU
1	B	62	GLU
1	B	67	ARG
1	B	76	LYS
1	B	78	LEU
1	B	108	SER
1	B	112	LYS
1	B	116	LYS
1	B	148	LEU
1	B	149	ASN
1	B	156	ARG
1	B	162	ILE
1	B	164	ARG
1	B	165	THR
1	B	166	LYS
1	B	188	LYS
1	B	191	ARG
1	B	193	LEU
1	B	205	SER
1	B	206	LYS
1	B	223	GLN
1	B	227	LEU
1	B	228	MET
1	B	278	ASN
1	B	282	LEU
1	B	283	LEU
1	B	287	GLN
1	B	288	LEU
1	B	290	LYS
1	B	291	ASP
1	B	292	LEU
1	B	295	ASP
1	B	299	GLU
1	B	301	LEU
1	B	303	ASP
1	B	307	ASN
1	B	310	ASN
1	B	313	ARG
1	B	326	THR
1	B	334	ARG
1	B	338	LEU

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Mol	Chain	Res	Type
1	B	339	LYS
1	B	341	LEU
1	B	346	MET
1	B	353	LEU
1	B	355	LYS
1	B	361	LEU
1	B	363	GLU
1	B	364	GLN
1	B	368	LYS
1	B	373	ASN
1	B	383	GLN
1	B	388	THR
1	B	389	GLU
1	B	390	MET
1	B	397	PHE
1	B	421	ARG
1	B	430	LEU
1	B	432	LYS
1	B	433	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	35	GLN
1	A	106	GLN
1	A	123	HIS
1	A	134	ASN
1	A	136	HIS
1	A	140	GLN
1	A	192	ASN
1	A	211	HIS
1	A	212	ASN
1	A	267	ASN
1	A	289	GLN
1	A	359	ASN
1	A	373	ASN
1	A	383	GLN
1	A	391	ASN
1	A	408	GLN
1	B	5	ASN
1	B	18	GLN

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	75	GLN
1	B	100	GLN
1	B	106	GLN
1	B	123	HIS
1	B	136	HIS
1	B	140	GLN
1	B	192	ASN
1	B	211	HIS
1	B	212	ASN
1	B	215	ASN
1	B	267	ASN
1	B	287	GLN
1	B	289	GLN
1	B	333	GLN
1	B	340	HIS
1	B	373	ASN
1	B	383	GLN
1	B	391	ASN
1	B	408	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	COF	A	700[A]	-	14,15,57	1.55	2 (14%)	18,19,86	1.93	2 (11%)
2	COF	A	700[B]	-	14,15,57	0.97	0	18,19,86	1.21	2 (11%)
3	CIT	A	701	-	12,12,12	0.87	0	17,17,17	2.54	6 (35%)
2	COF	B	700[A]	-	14,15,57	1.51	3 (21%)	18,19,86	1.33	2 (11%)
2	COF	B	700[B]	-	14,15,57	1.19	1 (7%)	18,19,86	1.14	2 (11%)
3	CIT	B	701	-	12,12,12	0.80	0	17,17,17	2.33	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COF	A	700[A]	-	-	0/17/17/74	0/0/0/3
2	COF	A	700[B]	-	-	0/17/17/74	0/0/0/3
3	CIT	A	701	-	-	0/16/16/16	0/0/0/0
2	COF	B	700[A]	-	-	0/17/17/74	0/0/0/3
2	COF	B	700[B]	-	-	0/17/17/74	0/0/0/3
3	CIT	B	701	-	-	0/16/16/16	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700[A]	COF	O1I-C2I	3.77	1.28	1.21
2	B	700[A]	COF	C1I-C2I	3.21	1.56	1.51
2	A	700[A]	COF	C1I-C2I	2.88	1.56	1.51
2	B	700[A]	COF	O1I-C2I	2.62	1.26	1.21
2	B	700[B]	COF	O1I-C2I	2.08	1.25	1.21
2	B	700[A]	COF	C1I-S1P	2.01	1.85	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700[A]	COF	O1I-C2I-C1I	7.11	129.51	121.65
3	A	701	CIT	O5-C6-C3	-5.93	114.03	122.20
3	B	701	CIT	O5-C6-C3	-5.84	114.15	122.20
3	A	701	CIT	O6-C6-C3	5.55	120.97	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	CIT	O6-C6-C3	5.12	120.33	112.89
3	B	701	CIT	O7-C3-C6	3.92	114.60	108.95
3	A	701	CIT	O7-C3-C6	3.66	114.22	108.95
2	B	700[A]	COF	C2P-S1P-C1I	-3.24	96.95	102.00
2	B	700[B]	COF	C2P-S1P-C1I	-3.14	97.11	102.00
2	A	700[B]	COF	C1I-C2I-C3I	2.84	121.24	115.67
3	A	701	CIT	O3-C5-C4	-2.74	114.07	122.74
2	B	700[A]	COF	O1I-C2I-C3I	2.51	123.75	115.98
3	A	701	CIT	C4-C3-C6	-2.47	104.41	110.12
2	B	700[B]	COF	O1I-C2I-C3I	2.33	123.21	115.98
2	A	700[A]	COF	C1I-C2I-C3I	2.32	120.22	115.67
2	A	700[B]	COF	O1I-C2I-C1I	-2.21	119.21	121.65
3	A	701	CIT	O1-C1-C2	-2.17	115.88	122.74
3	B	701	CIT	C3-C4-C5	-2.07	108.75	113.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	437/437 (100%)	-0.81	2 (0%) 88 92	1, 13, 51, 95	0
1	B	434/437 (99%)	-0.76	3 (0%) 84 89	2, 14, 53, 74	0
All	All	871/874 (99%)	-0.78	5 (0%) 86 91	1, 14, 53, 95	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	TRP	5.0
1	A	436	GLY	3.4
1	A	435	ALA	3.1
1	B	310	ASN	2.2
1	B	304	TYR	2.1

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

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

### 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	COF	B	700[A]	16/55	0.11	1.27	1,55,100,100	16
2	COF	A	700[A]	16/55	0.09	1.03	1,15,100,100	16
2	COF	A	700[B]	16/55	0.09	1.03	1,13,100,100	16
2	COF	B	700[B]	16/55	0.11	0.24	1,26,100,100	16
3	CIT	B	701	13/13	0.09	-0.38	1,5,26,29	0
3	CIT	A	701	13/13	0.07	-0.51	1,4,29,46	0

## 6.5 Other polymers

There are no such residues in this entry.