



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 AM GMT

PDB ID : 2O0T  
Title : The three dimensional structure of diaminopimelate decarboxylase from Mycobacterium tuberculosis reveals a tetrameric enzyme organisation  
Authors : Weyand, S.; Kefala, G.; Weiss, M.S.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2006-11-28  
Resolution : 2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

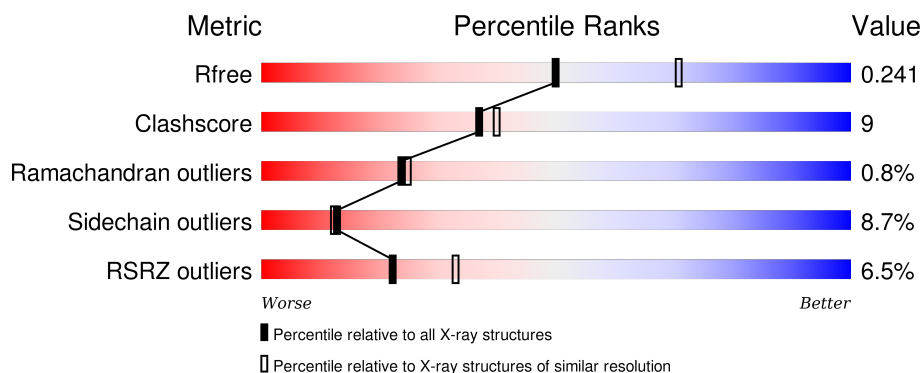
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	467	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	467	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	467	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• • •</div> </div> </div>
1	D	467	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• • •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13753 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 Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3330	2089	591	639	11			
1	B	446	Total	C	N	O	S	0	0	0
			3330	2089	591	639	11			
1	C	446	Total	C	N	O	P	S	0	0
			3345	2097	592	644	1	11		
1	D	446	Total	C	N	O	P	S	0	0
			3345	2097	592	644	1	11		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	INITIATING METHIONINE	UNP P0A5M4
A	0	ALA	-	CLONING ARTIFACT	UNP P0A5M4
A	1	VAL	-	CLONING ARTIFACT	UNP P0A5M4
A	448	GLY	-	CLONING ARTIFACT	UNP P0A5M4
A	449	VAL	-	CLONING ARTIFACT	UNP P0A5M4
A	450	PRO	-	CLONING ARTIFACT	UNP P0A5M4
A	451	ARG	-	CLONING ARTIFACT	UNP P0A5M4
A	452	GLY	-	CLONING ARTIFACT	UNP P0A5M4
A	453	LYS	-	CLONING ARTIFACT	UNP P0A5M4
A	454	LEU	-	CLONING ARTIFACT	UNP P0A5M4
A	455	ALA	-	CLONING ARTIFACT	UNP P0A5M4
A	456	ALA	-	CLONING ARTIFACT	UNP P0A5M4
A	457	ALA	-	CLONING ARTIFACT	UNP P0A5M4
A	458	LEU	-	CLONING ARTIFACT	UNP P0A5M4
A	459	GLU	-	CLONING ARTIFACT	UNP P0A5M4
A	460	HIS	-	EXPRESSION TAG	UNP P0A5M4
A	461	HIS	-	EXPRESSION TAG	UNP P0A5M4
A	462	HIS	-	EXPRESSION TAG	UNP P0A5M4
A	463	HIS	-	EXPRESSION TAG	UNP P0A5M4
A	464	HIS	-	EXPRESSION TAG	UNP P0A5M4
A	465	HIS	-	EXPRESSION TAG	UNP P0A5M4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	INITIATING METHIONINE	UNP P0A5M4
B	0	ALA	-	CLONING ARTIFACT	UNP P0A5M4
B	1	VAL	-	CLONING ARTIFACT	UNP P0A5M4
B	448	GLY	-	CLONING ARTIFACT	UNP P0A5M4
B	449	VAL	-	CLONING ARTIFACT	UNP P0A5M4
B	450	PRO	-	CLONING ARTIFACT	UNP P0A5M4
B	451	ARG	-	CLONING ARTIFACT	UNP P0A5M4
B	452	GLY	-	CLONING ARTIFACT	UNP P0A5M4
B	453	LYS	-	CLONING ARTIFACT	UNP P0A5M4
B	454	LEU	-	CLONING ARTIFACT	UNP P0A5M4
B	455	ALA	-	CLONING ARTIFACT	UNP P0A5M4
B	456	ALA	-	CLONING ARTIFACT	UNP P0A5M4
B	457	ALA	-	CLONING ARTIFACT	UNP P0A5M4
B	458	LEU	-	CLONING ARTIFACT	UNP P0A5M4
B	459	GLU	-	CLONING ARTIFACT	UNP P0A5M4
B	460	HIS	-	EXPRESSION TAG	UNP P0A5M4
B	461	HIS	-	EXPRESSION TAG	UNP P0A5M4
B	462	HIS	-	EXPRESSION TAG	UNP P0A5M4
B	463	HIS	-	EXPRESSION TAG	UNP P0A5M4
B	464	HIS	-	EXPRESSION TAG	UNP P0A5M4
B	465	HIS	-	EXPRESSION TAG	UNP P0A5M4
C	-1	MET	-	INITIATING METHIONINE	UNP P0A5M4
C	0	ALA	-	CLONING ARTIFACT	UNP P0A5M4
C	1	VAL	-	CLONING ARTIFACT	UNP P0A5M4
C	448	GLY	-	CLONING ARTIFACT	UNP P0A5M4
C	449	VAL	-	CLONING ARTIFACT	UNP P0A5M4
C	450	PRO	-	CLONING ARTIFACT	UNP P0A5M4
C	451	ARG	-	CLONING ARTIFACT	UNP P0A5M4
C	452	GLY	-	CLONING ARTIFACT	UNP P0A5M4
C	453	LYS	-	CLONING ARTIFACT	UNP P0A5M4
C	454	LEU	-	CLONING ARTIFACT	UNP P0A5M4
C	455	ALA	-	CLONING ARTIFACT	UNP P0A5M4
C	456	ALA	-	CLONING ARTIFACT	UNP P0A5M4
C	457	ALA	-	CLONING ARTIFACT	UNP P0A5M4
C	458	LEU	-	CLONING ARTIFACT	UNP P0A5M4
C	459	GLU	-	CLONING ARTIFACT	UNP P0A5M4
C	460	HIS	-	EXPRESSION TAG	UNP P0A5M4
C	461	HIS	-	EXPRESSION TAG	UNP P0A5M4
C	462	HIS	-	EXPRESSION TAG	UNP P0A5M4
C	463	HIS	-	EXPRESSION TAG	UNP P0A5M4
C	464	HIS	-	EXPRESSION TAG	UNP P0A5M4
C	465	HIS	-	EXPRESSION TAG	UNP P0A5M4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	INITIATING METHIONINE	UNP P0A5M4
D	0	ALA	-	CLONING ARTIFACT	UNP P0A5M4
D	1	VAL	-	CLONING ARTIFACT	UNP P0A5M4
D	448	GLY	-	CLONING ARTIFACT	UNP P0A5M4
D	449	VAL	-	CLONING ARTIFACT	UNP P0A5M4
D	450	PRO	-	CLONING ARTIFACT	UNP P0A5M4
D	451	ARG	-	CLONING ARTIFACT	UNP P0A5M4
D	452	GLY	-	CLONING ARTIFACT	UNP P0A5M4
D	453	LYS	-	CLONING ARTIFACT	UNP P0A5M4
D	454	LEU	-	CLONING ARTIFACT	UNP P0A5M4
D	455	ALA	-	CLONING ARTIFACT	UNP P0A5M4
D	456	ALA	-	CLONING ARTIFACT	UNP P0A5M4
D	457	ALA	-	CLONING ARTIFACT	UNP P0A5M4
D	458	LEU	-	CLONING ARTIFACT	UNP P0A5M4
D	459	GLU	-	CLONING ARTIFACT	UNP P0A5M4
D	460	HIS	-	EXPRESSION TAG	UNP P0A5M4
D	461	HIS	-	EXPRESSION TAG	UNP P0A5M4
D	462	HIS	-	EXPRESSION TAG	UNP P0A5M4
D	463	HIS	-	EXPRESSION TAG	UNP P0A5M4
D	464	HIS	-	EXPRESSION TAG	UNP P0A5M4
D	465	HIS	-	EXPRESSION TAG	UNP P0A5M4

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



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

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

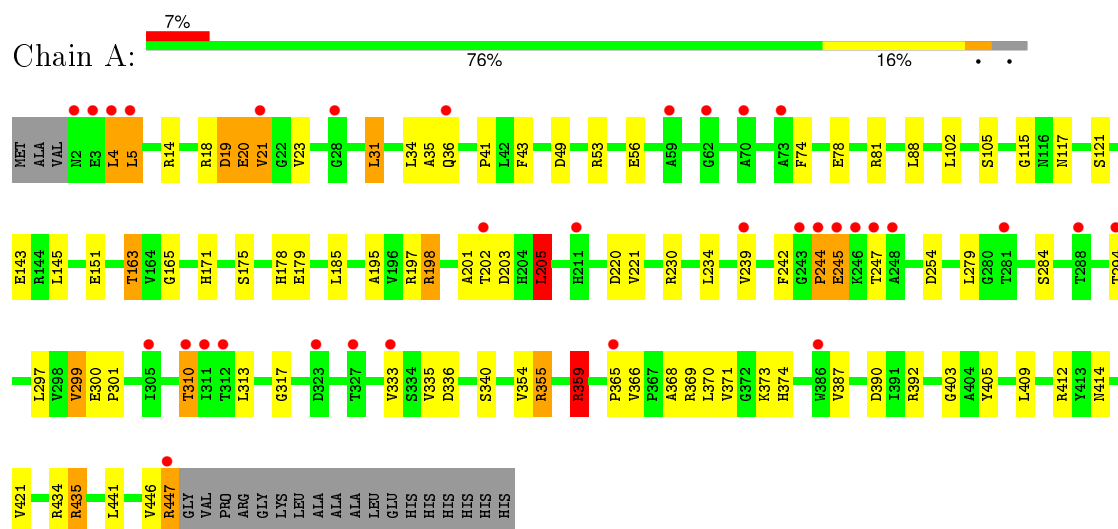
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	87	Total	O		0	0
			87	87			
3	B	123	Total	O		0	0
			123	123			
3	C	90	Total	O		0	0
			90	90			
3	D	93	Total	O		0	0
			93	93			

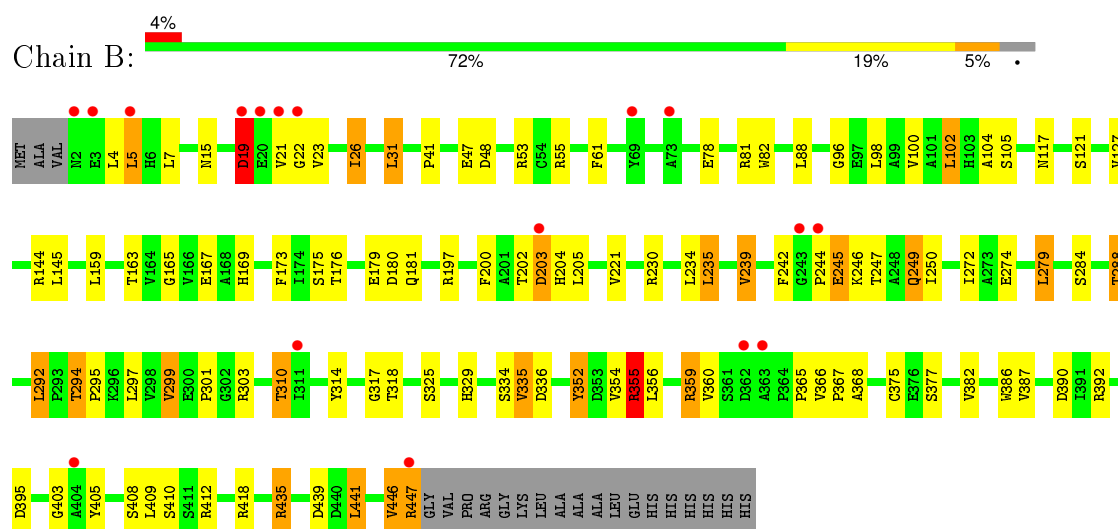
### 3 Residue-property plots [i](#)

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

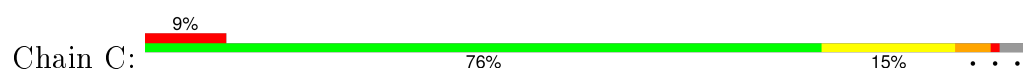
#### • Molecule 1: Diaminopimelate decarboxylase

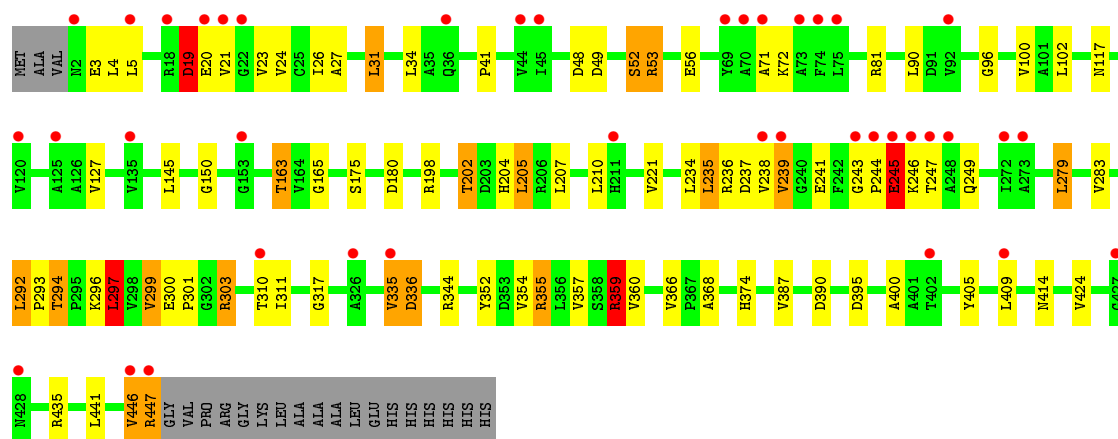


#### • Molecule 1: Diaminopimelate decarboxylase

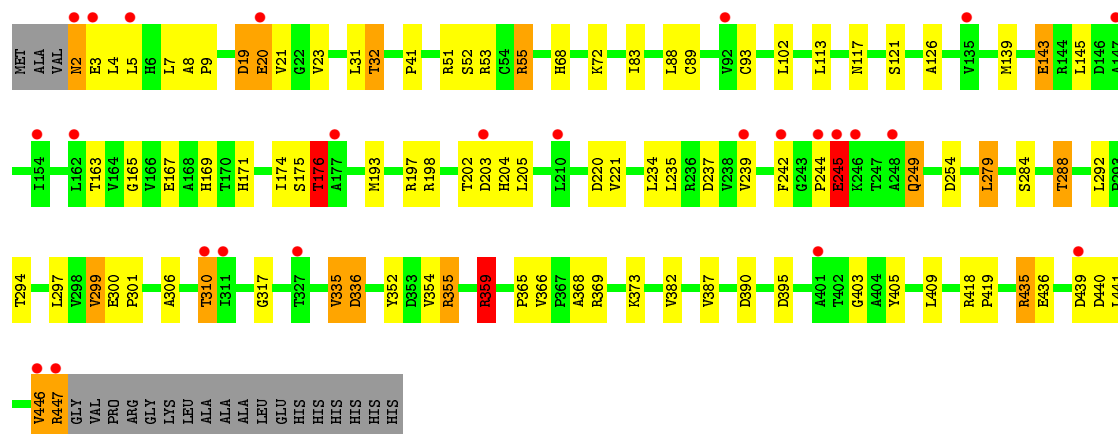
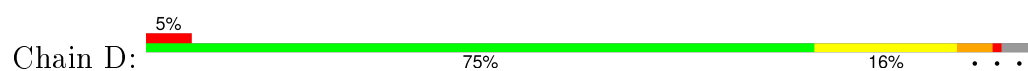


#### • Molecule 1: Diaminopimelate decarboxylase





• Molecule 1: Diaminopimelate decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.78Å 106.88Å 121.93Å 90.00° 104.99° 90.00°	Depositor
Resolution (Å)	30.00 – 2.33 30.88 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.33) 99.9 (30.88-2.33)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.241 0.194 , 0.241	Depositor DCC
$R_{free}$ test set	1597 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 80159 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: LLP, 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	0.93	2/3382 (0.1%)	0.96	11/4612 (0.2%)
1	B	0.98	3/3382 (0.1%)	1.03	18/4612 (0.4%)
1	C	0.87	0/3382	0.94	10/4612 (0.2%)
1	D	0.86	2/3382 (0.1%)	0.93	12/4612 (0.3%)
All	All	0.91	7/13528 (0.1%)	0.96	51/18448 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	93	CYS	CB-SG	-7.34	1.69	1.82
1	B	336	ASP	CB-CG	-7.08	1.36	1.51
1	A	336	ASP	CB-CG	-6.04	1.39	1.51
1	D	336	ASP	CB-CG	-5.40	1.40	1.51
1	B	375	CYS	CB-SG	5.28	1.91	1.82
1	A	435	ARG	CG-CD	5.05	1.64	1.51
1	B	352	TYR	CD1-CE1	5.03	1.46	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	NE-CZ-NH1	-11.28	114.66	120.30
1	B	53	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	A	336	ASP	CB-CG-OD2	-10.88	108.50	118.30
1	D	53	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	C	359	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	D	336	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	B	355	ARG	NE-CZ-NH2	9.12	124.86	120.30
1	C	359	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	D	53	ARG	NE-CZ-NH2	8.81	124.71	120.30
1	B	230	ARG	NE-CZ-NH1	8.80	124.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	C	303	ARG	NE-CZ-NH2	8.15	124.38	120.30
1	A	412	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	C	53	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	A	435	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	D	369	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	B	359	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	434	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	C	336	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	336	ASP	N-CA-CB	-6.71	98.53	110.60
1	C	53	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	B	355	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	D	254	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	230	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	297	LEU	CA-CB-CG	6.39	130.01	115.30
1	B	230	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	144	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	359	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	303	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	5	LEU	CA-CB-CG	5.79	128.60	115.30
1	D	359	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	230	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	435	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	D	435	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	88	LEU	CA-CB-CG	5.53	128.01	115.30
1	C	81	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	B	359	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	180	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	359	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	180	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	435	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	5	LEU	CA-CB-CG	5.27	127.43	115.30
1	D	55	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	392	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	D	53	ARG	CD-NE-CZ	5.20	130.88	123.60
1	B	336	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	176	THR	CB-CA-C	-5.12	97.76	111.60
1	D	336	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	392	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	439	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	205	LEU	CA-CB-CG	5.00	126.81	115.30

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	3330	0	3312	62	0
1	B	3330	0	3312	75	0
1	C	3345	0	3321	66	0
1	D	3345	0	3321	54	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	87	0	0	9	0
3	B	123	0	0	10	0
3	C	90	0	0	8	0
3	D	93	0	0	6	0
All	All	13753	0	13266	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:VAL:HG12	1:B:447:ARG:H	1.22	1.02
1:C:202:THR:HG21	1:C:205:LEU:HB2	1.40	1.00
1:B:446:VAL:O	1:B:447:ARG:HG3	1.69	0.93
1:A:198:ARG:HD3	3:A:560:HOH:O	1.70	0.90
1:C:446:VAL:HG12	1:C:447:ARG:H	1.36	0.90
1:C:41:PRO:O	1:C:435:ARG:NH1	2.06	0.88
1:C:204:HIS:HD2	3:C:479:HOH:O	1.60	0.82
1:A:354:VAL:O	1:A:355:ARG:HD2	1.78	0.82
1:A:78:GLU:OE1	1:A:81:ARG:NH2	2.11	0.82
1:A:447:ARG:NE	1:A:447:ARG:HA	1.96	0.81
1:B:284:SER:O	1:B:288:THR:HG23	1.80	0.81
1:B:19:ASP:HB2	1:B:23:VAL:H	1.46	0.81
1:D:176:THR:HG22	3:D:500:HOH:O	1.81	0.81
1:A:143:GLU:HG2	1:A:198:ARG:HH21	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ARG:HH21	1:C:236:ARG:HG2	1.48	0.79
1:B:446:VAL:HG12	1:B:447:ARG:N	1.98	0.78
1:B:288:THR:HG22	3:B:515:HOH:O	1.82	0.78
1:B:55:ARG:HD2	3:B:543:HOH:O	1.83	0.78
1:A:197:ARG:HG2	1:A:242:PHE:HZ	1.49	0.77
1:C:446:VAL:CG1	1:C:447:ARG:H	1.98	0.76
1:C:5:LEU:HD11	1:C:360:VAL:HG22	1.68	0.74
1:D:19:ASP:HB2	1:D:23:VAL:H	1.50	0.74
1:B:221:VAL:HG23	1:B:279:LEU:HD13	1.68	0.74
1:A:374:HIS:HD2	1:A:414:ASN:HD22	1.35	0.73
1:C:374:HIS:HD2	1:C:414:ASN:HD22	1.35	0.73
1:B:26:ILE:HG13	1:B:31:LEU:HD11	1.70	0.72
1:B:221:VAL:CG2	1:B:279:LEU:HD13	2.20	0.71
1:D:245:GLU:HB2	3:D:513:HOH:O	1.90	0.71
1:B:329:HIS:ND1	3:B:582:HOH:O	2.23	0.71
1:A:19:ASP:HB2	1:A:23:VAL:H	1.54	0.71
1:A:239:VAL:HA	1:A:247:THR:HG21	1.71	0.71
1:C:294:THR:HG22	3:C:543:HOH:O	1.90	0.71
1:B:163:THR:HG23	1:B:179:GLU:OE1	1.91	0.71
1:D:23:VAL:HG11	1:D:32:THR:HG22	1.74	0.70
1:D:41:PRO:O	1:D:435:ARG:NH1	2.24	0.70
1:A:374:HIS:CD2	1:A:414:ASN:HD22	2.10	0.70
1:B:310:THR:HG22	3:B:503:HOH:O	1.90	0.70
1:C:374:HIS:CD2	1:C:414:ASN:HD22	2.11	0.68
1:B:41:PRO:O	1:B:435:ARG:NH1	2.23	0.68
1:B:299:VAL:HG13	1:B:301:PRO:HD3	1.75	0.68
1:B:412:ARG:HD3	1:B:441:LEU:HD12	1.75	0.67
1:A:333:VAL:HG22	1:A:370:LEU:HD12	1.75	0.67
1:C:239:VAL:HG21	1:C:292:LEU:HD11	1.77	0.66
1:D:446:VAL:HG12	1:D:447:ARG:H	1.61	0.66
1:B:274:GLU:OE2	3:B:561:HOH:O	2.15	0.64
1:A:201:ALA:HB3	3:A:560:HOH:O	1.98	0.64
1:D:4:LEU:HD22	1:D:365:PRO:HB3	1.80	0.64
1:A:447:ARG:HA	1:A:447:ARG:HE	1.64	0.63
1:D:284:SER:O	1:D:288:THR:CG2	2.47	0.63
1:A:20:GLU:CD	1:A:20:GLU:H	2.02	0.63
1:C:359:ARG:HH22	1:C:390:ASP:CG	2.02	0.63
1:B:47:GLU:HG3	1:B:82:TRP:CZ2	2.33	0.63
1:B:4:LEU:HD22	1:B:365:PRO:HB3	1.80	0.62
1:B:47:GLU:HG3	1:B:82:TRP:CH2	2.35	0.62
1:C:354:VAL:O	1:C:355:ARG:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASN:HD21	1:B:317:GLY:HA3	1.64	0.62
1:A:202:THR:HB	3:A:557:HOH:O	1.99	0.61
1:C:19:ASP:HB2	1:C:23:VAL:H	1.66	0.61
1:D:72:LLP:H6	1:D:300:GLU:O	2.01	0.61
1:C:236:ARG:HH21	1:C:236:ARG:CG	2.13	0.61
1:C:359:ARG:HD3	1:C:395:ASP:OD1	2.01	0.60
1:C:71:ALA:HB2	1:C:90:LEU:HD11	1.82	0.60
1:C:239:VAL:HA	1:C:247:THR:HG21	1.83	0.60
1:C:241:GLU:HA	3:C:548:HOH:O	2.01	0.60
1:C:294:THR:HG21	3:C:546:HOH:O	2.02	0.60
1:C:303:ARG:HD2	3:C:469:HOH:O	2.01	0.60
1:B:22:GLY:HA3	1:B:360:VAL:HG23	1.82	0.60
1:C:446:VAL:HG12	1:C:447:ARG:N	2.12	0.60
1:B:314:TYR:HB3	1:B:335:VAL:HG22	1.84	0.59
1:A:143:GLU:CG	1:A:198:ARG:HH21	2.15	0.59
1:B:310:THR:HG21	3:B:506:HOH:O	2.01	0.59
1:C:405:TYR:O	1:C:409:LEU:HD12	2.03	0.59
1:A:310:THR:HG23	1:A:403:GLY:HA3	1.85	0.59
1:B:294:THR:HG22	3:B:515:HOH:O	2.01	0.58
1:C:299:VAL:HG13	1:C:301:PRO:HD3	1.85	0.58
1:D:139:MET:O	1:D:143:GLU:HG2	2.03	0.58
1:D:354:VAL:O	1:D:355:ARG:HD2	2.03	0.58
1:C:283:VAL:HG21	1:C:297:LEU:HG	1.86	0.58
1:B:55:ARG:CD	3:B:543:HOH:O	2.47	0.58
1:D:245:GLU:OE2	1:D:245:GLU:HA	2.04	0.58
1:B:203:ASP:OD2	1:B:204:HIS:CE1	2.57	0.57
1:B:354:VAL:O	1:B:355:ARG:HD2	2.04	0.57
1:A:202:THR:OG1	1:A:203:ASP:N	2.35	0.57
1:D:2:ASN:HD22	1:D:3:GLU:H	1.53	0.57
1:A:310:THR:HG21	3:A:544:HOH:O	2.04	0.57
1:D:310:THR:HG21	3:D:478:HOH:O	2.04	0.57
1:C:244:PRO:C	3:C:515:HOH:O	2.43	0.57
1:B:446:VAL:O	1:B:447:ARG:CG	2.49	0.56
1:B:26:ILE:HG13	1:B:31:LEU:CD1	2.34	0.56
1:B:104:ALA:O	1:B:105:SER:HB2	2.05	0.56
1:D:405:TYR:O	1:D:409:LEU:HD12	2.05	0.56
1:D:284:SER:O	1:D:288:THR:HG22	2.06	0.56
1:C:245:GLU:N	3:C:515:HOH:O	2.39	0.56
1:B:239:VAL:HA	1:B:247:THR:HG21	1.86	0.55
1:D:197:ARG:HG2	1:D:242:PHE:HZ	1.72	0.55
1:B:19:ASP:HB2	1:B:23:VAL:N	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:VAL:HG12	1:D:447:ARG:N	2.21	0.55
1:A:299:VAL:HG13	1:A:301:PRO:HD3	1.88	0.55
1:B:359:ARG:HH22	1:B:390:ASP:CG	2.10	0.55
1:C:202:THR:CG2	1:C:205:LEU:HB2	2.26	0.55
1:C:204:HIS:CD2	3:C:479:HOH:O	2.47	0.55
1:B:202:THR:OG1	1:B:203:ASP:N	2.37	0.55
1:B:7:LEU:HD23	1:B:355:ARG:HG2	1.89	0.55
1:D:51:ARG:O	1:D:55:ARG:HG3	2.07	0.54
1:A:19:ASP:HB2	1:A:23:VAL:N	2.21	0.54
1:B:446:VAL:CG1	1:B:447:ARG:H	2.09	0.54
1:A:284:SER:HA	1:A:294:THR:HG22	1.89	0.54
1:A:171:HIS:ND1	1:A:220:ASP:OD2	2.37	0.54
1:B:19:ASP:HB3	1:B:21:VAL:H	1.72	0.54
1:C:20:GLU:H	1:C:20:GLU:CD	2.12	0.54
1:B:446:VAL:CG1	1:B:447:ARG:N	2.71	0.54
1:C:202:THR:HG21	1:C:205:LEU:CB	2.26	0.53
1:D:284:SER:O	1:D:288:THR:HG23	2.07	0.53
1:D:20:GLU:H	1:D:20:GLU:CD	2.11	0.53
1:A:359:ARG:HH22	1:A:390:ASP:CG	2.12	0.53
1:D:359:ARG:NH2	1:D:390:ASP:OD2	2.41	0.53
1:A:294:THR:HG23	3:A:517:HOH:O	2.09	0.53
1:D:359:ARG:HH22	1:D:390:ASP:CG	2.12	0.53
1:C:344:ARG:HD3	1:C:352:TYR:OH	2.09	0.53
1:A:4:LEU:HD22	1:A:365:PRO:HB3	1.91	0.53
1:C:165:GLY:O	1:C:175:SER:HA	2.09	0.52
1:C:317:GLY:HA3	1:D:117:ASN:HD21	1.74	0.52
1:B:359:ARG:NH2	1:B:390:ASP:OD2	2.42	0.52
1:D:193:MET:HE3	1:D:237:ASP:HB3	1.91	0.52
1:C:48:ASP:O	1:C:52:SER:HB2	2.10	0.52
1:D:193:MET:CE	1:D:237:ASP:HB3	2.40	0.52
1:D:19:ASP:HB3	1:D:21:VAL:H	1.75	0.52
1:A:197:ARG:HG2	1:A:242:PHE:CZ	2.38	0.51
1:B:284:SER:O	1:B:288:THR:CG2	2.56	0.51
1:D:299:VAL:HG13	1:D:301:PRO:HD3	1.93	0.51
1:C:72:LLP:H6	1:C:300:GLU:O	2.10	0.51
1:C:31:LEU:HD12	1:C:34:LEU:HD12	1.91	0.51
1:B:200:PHE:HZ	1:B:250:ILE:HD11	1.76	0.51
1:B:249:GLN:H	1:B:249:GLN:NE2	2.09	0.51
1:A:317:GLY:HA3	1:B:117:ASN:HD21	1.76	0.51
1:D:7:LEU:HD23	1:D:355:ARG:HG2	1.93	0.51
1:C:221:VAL:HG23	1:C:279:LEU:HD13	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ARG:NH2	1:C:237:ASP:OD1	2.39	0.50
1:C:446:VAL:CG1	1:C:447:ARG:N	2.71	0.50
1:B:221:VAL:CG2	1:B:279:LEU:CD1	2.89	0.50
1:B:61:PHE:HE1	1:B:272:ILE:HD11	1.77	0.50
1:A:19:ASP:HB3	1:A:21:VAL:H	1.77	0.50
1:D:359:ARG:HD3	1:D:395:ASP:OD1	2.11	0.50
1:B:310:THR:CG2	3:B:503:HOH:O	2.56	0.50
1:B:96:GLY:O	1:B:100:VAL:HG23	2.12	0.49
1:C:19:ASP:HB3	1:C:21:VAL:H	1.78	0.49
1:D:167:GLU:OE2	1:D:169:HIS:HE1	1.95	0.49
1:D:221:VAL:HG23	1:D:279:LEU:HD13	1.94	0.49
1:B:310:THR:HG23	1:B:403:GLY:HA3	1.94	0.49
1:D:368:ALA:HB2	1:D:387:VAL:HG22	1.94	0.49
1:B:15:ASN:ND2	1:B:48:ASP:HB3	2.27	0.49
1:B:197:ARG:HG2	1:B:242:PHE:HZ	1.77	0.49
1:A:359:ARG:NH2	1:A:390:ASP:OD2	2.46	0.49
1:C:49:ASP:O	1:C:53:ARG:HG3	2.13	0.49
1:C:117:ASN:HD21	1:D:317:GLY:HA3	1.78	0.49
1:A:333:VAL:HG22	1:A:370:LEU:CD1	2.41	0.48
1:B:165:GLY:O	1:B:175:SER:HA	2.12	0.48
1:A:43:PHE:HB2	1:A:421:VAL:HG22	1.96	0.48
1:A:221:VAL:HG23	1:A:279:LEU:CD1	2.44	0.48
1:C:335:VAL:HG13	1:C:336:ASP:N	2.29	0.48
1:A:165:GLY:O	1:A:175:SER:HA	2.14	0.47
1:C:21:VAL:HG23	1:C:23:VAL:HG23	1.97	0.47
1:C:49:ASP:OD2	1:C:53:ARG:HD2	2.14	0.47
1:C:296:LYS:HB2	1:C:296:LYS:HE2	1.67	0.47
1:D:171:HIS:HA	1:D:220:ASP:OD1	2.14	0.47
1:B:239:VAL:HG21	1:B:292:LEU:HD11	1.97	0.47
1:D:198:ARG:O	1:D:202:THR:HG23	2.15	0.47
1:D:335:VAL:HG13	1:D:336:ASP:N	2.30	0.47
1:B:359:ARG:HD3	1:B:395:ASP:OD1	2.16	0.46
1:C:311:ILE:HG22	1:C:400:ALA:HA	1.97	0.46
1:A:310:THR:HG22	3:A:558:HOH:O	2.15	0.46
1:C:27:ALA:HB3	1:C:424:VAL:HG23	1.97	0.46
1:C:24:VAL:HB	1:C:357:VAL:HB	1.98	0.46
1:B:167:GLU:OE2	1:B:169:HIS:HE1	1.99	0.46
1:A:405:TYR:O	1:A:409:LEU:HD12	2.16	0.46
1:A:178:HIS:CD2	1:B:325:SER:HA	2.51	0.46
1:A:171:HIS:HD1	1:A:220:ASP:CG	2.19	0.46
1:C:207:LEU:O	1:C:249:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:PHE:CE2	1:D:175:SER:HB3	2.50	0.45
1:B:98:LEU:HG	1:B:102:LEU:HD22	1.98	0.45
1:B:235:LEU:O	1:B:239:VAL:HG13	2.17	0.45
1:B:410:SER:OG	1:B:418:ARG:NE	2.45	0.45
1:B:367:PRO:HD3	1:B:386:TRP:CZ3	2.52	0.45
1:B:78:GLU:OE2	1:B:81:ARG:NH2	2.50	0.45
1:A:31:LEU:HD12	1:A:34:LEU:HD12	1.98	0.44
1:B:405:TYR:O	1:B:409:LEU:HD12	2.17	0.44
1:A:185:LEU:HD13	1:A:195:ALA:HB2	1.99	0.44
1:B:318:THR:HB	1:B:334:SER:HB2	1.99	0.44
1:A:115:GLY:HA2	3:A:568:HOH:O	2.17	0.44
1:D:113:LEU:HD22	1:D:126:ALA:HB2	2.00	0.44
1:A:369:ARG:HG2	1:A:371:VAL:HG13	2.00	0.44
1:B:368:ALA:HB2	1:B:387:VAL:HG22	2.00	0.44
1:C:292:LEU:HD12	1:C:293:PRO:HD2	2.00	0.43
1:D:310:THR:HG22	3:D:511:HOH:O	2.19	0.43
1:C:26:ILE:CD1	1:C:31:LEU:HD11	2.49	0.43
1:A:368:ALA:HB2	1:A:387:VAL:HG22	1.99	0.43
1:A:14:ARG:NH1	1:A:56:GLU:OE1	2.52	0.43
1:D:306:ALA:O	1:D:403:GLY:HA3	2.19	0.43
1:C:210:LEU:HD11	1:C:235:LEU:HD23	2.01	0.43
1:B:356:LEU:HD21	1:B:359:ARG:HG3	1.99	0.43
1:C:198:ARG:HD2	1:C:198:ARG:HA	1.85	0.43
1:A:340:SER:OG	1:A:374:HIS:HE1	2.01	0.43
1:A:239:VAL:HG12	1:A:247:THR:HB	2.00	0.43
1:D:165:GLY:O	1:D:175:SER:HA	2.19	0.43
1:C:52:SER:O	1:C:56:GLU:HG2	2.19	0.43
1:C:96:GLY:O	1:C:100:VAL:HG23	2.19	0.43
1:C:368:ALA:HB2	1:C:387:VAL:HG22	2.01	0.43
1:C:163:THR:O	1:C:163:THR:HG22	2.18	0.43
1:A:446:VAL:HG12	1:A:447:ARG:N	2.34	0.43
1:B:244:PRO:HA	1:B:247:THR:OG1	2.19	0.43
1:D:197:ARG:HG2	1:D:242:PHE:CZ	2.53	0.42
1:A:49:ASP:OD2	1:A:53:ARG:HD2	2.19	0.42
1:D:352:TYR:HB2	1:D:382:VAL:HG22	2.00	0.42
1:D:418:ARG:HA	1:D:419:PRO:HD3	1.88	0.42
1:D:436:GLU:HA	1:D:440:ASP:OD1	2.18	0.42
1:A:374:HIS:HD2	1:A:414:ASN:ND2	2.10	0.42
1:C:359:ARG:NH2	1:C:390:ASP:OD2	2.49	0.42
1:B:294:THR:HA	1:B:295:PRO:HD3	1.53	0.42
1:A:35:ALA:HB2	1:A:313:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ASP:HB2	1:D:23:VAL:N	2.25	0.41
1:C:243:GLY:HA2	1:C:244:PRO:HD3	1.94	0.41
1:C:26:ILE:HG22	1:C:424:VAL:HG21	2.02	0.41
1:B:221:VAL:HG23	1:B:279:LEU:CD1	2.44	0.41
1:C:279:LEU:HB3	1:C:297:LEU:HD11	2.02	0.41
1:A:179:GLU:OE1	3:A:537:HOH:O	2.21	0.41
1:A:254:ASP:OD2	1:A:300:GLU:OE1	2.37	0.41
1:C:4:LEU:HA	1:C:355:ARG:HH11	1.86	0.41
1:A:354:VAL:C	1:A:355:ARG:HD2	2.40	0.41
1:A:244:PRO:HA	1:A:247:THR:OG1	2.19	0.41
1:B:4:LEU:HA	1:B:4:LEU:HD12	1.69	0.41
1:A:117:ASN:HB2	1:B:334:SER:HB3	2.02	0.41
1:B:127:VAL:HG22	3:B:557:HOH:O	2.18	0.41
1:D:68:HIS:CD2	1:D:89:CYS:HB2	2.55	0.41
1:D:245:GLU:CB	3:D:513:HOH:O	2.59	0.41
1:C:150:GLY:HA2	1:C:204:HIS:CD2	2.55	0.41
1:A:163:THR:O	1:A:163:THR:HG22	2.21	0.41
1:B:246:LYS:O	1:B:246:LYS:HG3	2.21	0.41
1:C:202:THR:HG23	1:C:205:LEU:H	1.86	0.41
1:A:202:THR:CG2	1:A:205:LEU:HB2	2.51	0.41
1:B:284:SER:HA	1:B:294:THR:HB	2.03	0.41
1:A:239:VAL:HG12	1:A:247:THR:CB	2.50	0.41
1:D:249:GLN:H	1:D:249:GLN:HG3	1.41	0.41
1:D:83:ILE:HG23	1:D:88:LEU:HB2	2.02	0.41
1:B:352:TYR:HB2	1:B:382:VAL:HG22	2.03	0.40
1:A:4:LEU:HA	1:A:4:LEU:HD12	1.85	0.40
1:A:41:PRO:HA	1:A:313:LEU:O	2.21	0.40
1:A:198:ARG:CD	3:A:560:HOH:O	2.45	0.40
1:D:143:GLU:HG2	1:D:143:GLU:H	1.62	0.40
1:D:8:ALA:HA	1:D:9:PRO:HD2	1.88	0.40
1:D:204:HIS:HD2	3:D:527:HOH:O	2.03	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	443/467 (95%)	426 (96%)	13 (3%)	4 (1%)	21	21
1	B	443/467 (95%)	425 (96%)	15 (3%)	3 (1%)	26	28
1	C	443/467 (95%)	426 (96%)	13 (3%)	4 (1%)	21	21
1	D	443/467 (95%)	427 (96%)	12 (3%)	4 (1%)	21	21
All	All	1772/1868 (95%)	1704 (96%)	53 (3%)	15 (1%)	24	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	ASP
1	B	446	VAL
1	C	19	ASP
1	A	19	ASP
1	B	245	GLU
1	D	19	ASP
1	D	245	GLU
1	D	446	VAL
1	A	245	GLU
1	C	245	GLU
1	A	74	PHE
1	C	446	VAL
1	D	244	PRO
1	A	244	PRO
1	C	238	VAL

### 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	352/367 (96%)	323 (92%)	29 (8%)	14	14
1	B	352/367 (96%)	321 (91%)	31 (9%)	12	11
1	C	352/367 (96%)	325 (92%)	27 (8%)	16	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	352/367 (96%)	317 (90%)	35 (10%)	10	9
All	All	1408/1468 (96%)	1286 (91%)	122 (9%)	13	12

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	18	ARG
1	A	20	GLU
1	A	21	VAL
1	A	31	LEU
1	A	36	GLN
1	A	88	LEU
1	A	102	LEU
1	A	105	SER
1	A	121	SER
1	A	145	LEU
1	A	151	GLU
1	A	163	THR
1	A	198	ARG
1	A	205	LEU
1	A	234	LEU
1	A	245	GLU
1	A	297	LEU
1	A	299	VAL
1	A	310	THR
1	A	335	VAL
1	A	355	ARG
1	A	359	ARG
1	A	366	VAL
1	A	373	LYS
1	A	435	ARG
1	A	441	LEU
1	A	447	ARG
1	B	5	LEU
1	B	19	ASP
1	B	26	ILE
1	B	31	LEU
1	B	102	LEU
1	B	121	SER
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	159	LEU
1	B	176	THR
1	B	181	GLN
1	B	203	ASP
1	B	205	LEU
1	B	234	LEU
1	B	235	LEU
1	B	239	VAL
1	B	245	GLU
1	B	249	GLN
1	B	279	LEU
1	B	288	THR
1	B	292	LEU
1	B	294	THR
1	B	297	LEU
1	B	299	VAL
1	B	310	THR
1	B	335	VAL
1	B	355	ARG
1	B	366	VAL
1	B	377	SER
1	B	408	SER
1	B	441	LEU
1	B	447	ARG
1	C	3	GLU
1	C	19	ASP
1	C	31	LEU
1	C	52	SER
1	C	102	LEU
1	C	127	VAL
1	C	145	LEU
1	C	163	THR
1	C	202	THR
1	C	205	LEU
1	C	234	LEU
1	C	235	LEU
1	C	239	VAL
1	C	245	GLU
1	C	246	LYS
1	C	279	LEU
1	C	292	LEU
1	C	294	THR

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Mol	Chain	Res	Type
1	C	297	LEU
1	C	299	VAL
1	C	310	THR
1	C	335	VAL
1	C	355	ARG
1	C	359	ARG
1	C	366	VAL
1	C	441	LEU
1	C	447	ARG
1	D	2	ASN
1	D	5	LEU
1	D	20	GLU
1	D	31	LEU
1	D	32	THR
1	D	52	SER
1	D	102	LEU
1	D	121	SER
1	D	143	GLU
1	D	145	LEU
1	D	163	THR
1	D	174	ILE
1	D	176	THR
1	D	203	ASP
1	D	205	LEU
1	D	234	LEU
1	D	235	LEU
1	D	239	VAL
1	D	245	GLU
1	D	249	GLN
1	D	279	LEU
1	D	288	THR
1	D	292	LEU
1	D	294	THR
1	D	297	LEU
1	D	299	VAL
1	D	310	THR
1	D	335	VAL
1	D	355	ARG
1	D	359	ARG
1	D	366	VAL
1	D	373	LYS
1	D	439	ASP

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Mol	Chain	Res	Type
1	D	441	LEU
1	D	447	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	117	ASN
1	A	169	HIS
1	A	374	HIS
1	A	414	ASN
1	A	428	ASN
1	B	15	ASN
1	B	66	ASN
1	B	68	HIS
1	B	116	ASN
1	B	117	ASN
1	B	169	HIS
1	B	181	GLN
1	B	249	GLN
1	B	374	HIS
1	B	414	ASN
1	C	36	GLN
1	C	66	ASN
1	C	68	HIS
1	C	116	ASN
1	C	117	ASN
1	C	204	HIS
1	C	374	HIS
1	D	2	ASN
1	D	66	ASN
1	D	68	HIS
1	D	116	ASN
1	D	117	ASN
1	D	169	HIS
1	D	374	HIS

### 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	LLP	A	72	1	7,8,25	0.85	0	6,8,34	0.80	0
1	LLP	B	72	1	7,8,25	0.80	0	6,8,34	1.03	1 (16%)
1	LLP	C	72	1	23,24,25	1.68	6 (26%)	28,32,34	2.22	6 (21%)
1	LLP	D	72	1	23,24,25	1.84	8 (34%)	28,32,34	2.35	8 (28%)

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	LLP	A	72	1	-	0/5/7/19	0/0/0/1
1	LLP	B	72	1	-	0/5/7/19	0/0/0/1
1	LLP	C	72	1	-	0/15/17/19	0/1/1/1
1	LLP	D	72	1	-	1/15/17/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	LLP	O3-C3	-5.02	1.25	1.37
1	C	72	LLP	O3-C3	-4.62	1.26	1.37
1	C	72	LLP	P-OP2	-2.28	1.46	1.54
1	D	72	LLP	P-OP3	-2.14	1.47	1.54
1	D	72	LLP	P-OP2	-2.07	1.47	1.54
1	D	72	LLP	C3-C2	2.01	1.42	1.40
1	D	72	LLP	C6-N1	2.04	1.38	1.34
1	C	72	LLP	C4-C4'	2.22	1.50	1.46
1	D	72	LLP	CE-NZ	2.22	1.51	1.46
1	C	72	LLP	C6-N1	2.44	1.39	1.34
1	C	72	LLP	C2-N1	2.68	1.39	1.34
1	D	72	LLP	C4'-NZ	2.98	1.36	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	LLP	C4'-NZ	3.06	1.36	1.27
1	D	72	LLP	C4-C4'	3.20	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	LLP	C4-C4'-NZ	-4.57	99.61	125.06
1	D	72	LLP	CE-NZ-C4'	-3.40	109.16	118.97
1	D	72	LLP	C4-C4'-NZ	-3.26	106.93	125.06
1	C	72	LLP	C3-C4-C4'	-3.13	116.11	120.16
1	D	72	LLP	C3-C4-C4'	-2.58	116.82	120.16
1	C	72	LLP	O-C-CA	-2.50	118.97	125.49
1	D	72	LLP	O-C-CA	-2.41	119.22	125.49
1	B	72	LLP	O-C-CA	-2.37	119.31	125.49
1	C	72	LLP	C5-C6-N1	-2.07	120.27	123.86
1	D	72	LLP	O3-C3-C2	2.08	121.28	117.66
1	D	72	LLP	C3-C4-C5	2.76	120.17	118.11
1	D	72	LLP	C5'-C5-C4	2.84	126.25	121.47
1	C	72	LLP	C3-C4-C5	4.66	121.60	118.11
1	C	72	LLP	OP4-C5'-C5	7.81	121.89	108.99
1	D	72	LLP	OP4-C5'-C5	8.77	123.48	108.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	72	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	72	LLP	1	0
1	D	72	LLP	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.56	0
2	SO4	B	502	-	4,4,4	0.26	0	6,6,6	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	445/467 (95%)	0.65	33 (7%)	17 26	38, 45, 55, 74	0
1	B	445/467 (95%)	0.44	17 (3%)	44 56	39, 45, 55, 74	0
1	C	445/467 (95%)	0.61	40 (8%)	12 18	38, 45, 55, 74	0
1	D	445/467 (95%)	0.54	25 (5%)	28 40	38, 45, 55, 74	0
All	All	1780/1868 (95%)	0.56	115 (6%)	22 33	38, 45, 55, 74	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ASN	8.7
1	A	248	ALA	7.0
1	B	2	ASN	7.0
1	B	244	PRO	6.7
1	A	244	PRO	6.5
1	A	245	GLU	6.5
1	C	447	ARG	6.1
1	B	21	VAL	6.1
1	A	2	ASN	5.6
1	C	248	ALA	5.4
1	C	2	ASN	5.2
1	D	447	ARG	5.2
1	B	22	GLY	5.1
1	C	5	LEU	4.8
1	A	3	GLU	4.6
1	A	5	LEU	4.5
1	D	244	PRO	4.4
1	C	239	VAL	4.2
1	A	239	VAL	4.1
1	C	20	GLU	4.0
1	D	203	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	73	ALA	3.9
1	C	244	PRO	3.8
1	A	243	GLY	3.7
1	D	327	THR	3.6
1	A	327	THR	3.5
1	C	245	GLU	3.4
1	A	62	GLY	3.4
1	B	203	ASP	3.4
1	B	3	GLU	3.4
1	B	5	LEU	3.3
1	A	28	GLY	3.3
1	C	70	ALA	3.3
1	D	135	VAL	3.2
1	A	447	ARG	3.2
1	A	246	LYS	3.2
1	C	243	GLY	3.2
1	A	247	THR	3.2
1	A	323	ASP	3.2
1	A	21	VAL	3.1
1	B	20	GLU	3.1
1	D	3	GLU	3.1
1	A	202	THR	3.1
1	C	21	VAL	3.0
1	A	305	ILE	2.9
1	C	247	THR	2.9
1	B	362	ASP	2.9
1	B	447	ARG	2.8
1	D	239	VAL	2.8
1	D	245	GLU	2.8
1	D	246	LYS	2.8
1	D	154	ILE	2.8
1	B	311	ILE	2.8
1	D	5	LEU	2.7
1	D	242	PHE	2.7
1	A	294	THR	2.7
1	C	69	TYR	2.7
1	A	311	ILE	2.6
1	D	310	THR	2.6
1	C	310	THR	2.6
1	A	365	PRO	2.5
1	B	404	ALA	2.5
1	B	19	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	326	ALA	2.5
1	C	92	VAL	2.5
1	D	20	GLU	2.5
1	B	243	GLY	2.4
1	D	210	LEU	2.4
1	A	70	ALA	2.4
1	C	71	ALA	2.4
1	C	246	LYS	2.4
1	D	248	ALA	2.4
1	A	386	TRP	2.4
1	C	402	THR	2.3
1	C	36	GLN	2.3
1	B	363	ALA	2.3
1	C	273	ALA	2.3
1	C	428	ASN	2.2
1	A	59	ALA	2.2
1	B	73	ALA	2.2
1	C	153	GLY	2.2
1	A	288	THR	2.2
1	D	446	VAL	2.2
1	C	18	ARG	2.2
1	D	162	LEU	2.2
1	A	36	GLN	2.2
1	C	272	ILE	2.2
1	D	311	ILE	2.2
1	C	446	VAL	2.2
1	C	427	GLY	2.2
1	B	69	TYR	2.2
1	A	211	HIS	2.2
1	A	73	ALA	2.2
1	D	401	ALA	2.2
1	C	45	ILE	2.1
1	C	135	VAL	2.1
1	C	335	VAL	2.1
1	C	75	LEU	2.1
1	D	177	ALA	2.1
1	C	22	GLY	2.1
1	C	74	PHE	2.1
1	A	4	LEU	2.1
1	A	312	THR	2.1
1	D	439	ASP	2.1
1	A	333	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	44	VAL	2.1
1	C	211	HIS	2.1
1	C	120	VAL	2.0
1	C	238	VAL	2.0
1	D	92	VAL	2.0
1	A	281	THR	2.0
1	A	310	THR	2.0
1	C	125	ALA	2.0
1	C	409	LEU	2.0
1	D	147	ALA	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	LLP	D	72	24/25	0.95	0.16	-	43,53,71,72	0
1	LLP	C	72	24/25	0.95	0.23	-	41,52,76,77	0
1	LLP	B	72	9/25	0.93	0.25	-	44,44,55,66	0
1	LLP	A	72	9/25	0.92	0.25	-	43,44,53,56	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
2	SO4	B	502	5/5	0.99	0.07	-2.53	29,36,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	501	5/5	0.99	0.08	-2.64	39,42,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.