



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:41 PM GMT

PDB ID : 3RMT  
Title : Crystal structure of putative 5-enolpyruvoylshikimate-3-phosphate synthase from *Bacillus halodurans* C-125  
Authors : Malashkevich, V.N.; Toro, R.; Seidel, R.; Ramagopal, U.; Zencheck, W.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-04-21  
Resolution : 2.80 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

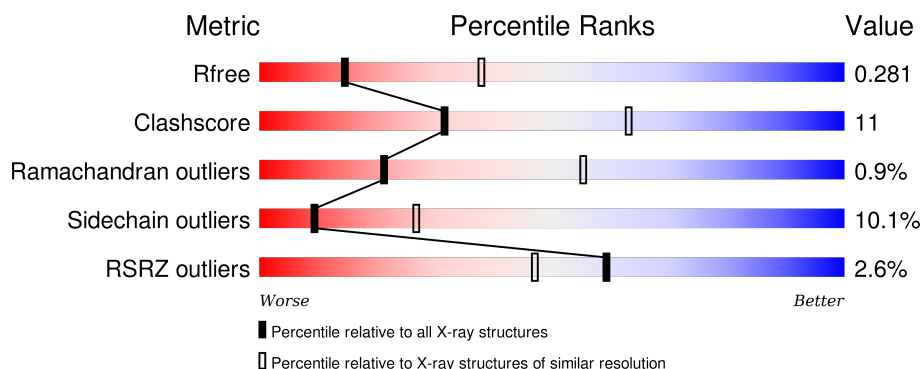
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	455	<div> <div>2%</div> <div>66% 25% 5%</div> </div>
1	B	455	<div> <div>%</div> <div>67% 24% 6%</div> </div>
1	C	455	<div> <div>2%</div> <div>70% 23% . .</div> </div>
1	D	455	<div> <div>4%</div> <div>73% 18% 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
2	SO4	A	503	-	-	-	X
2	SO4	A	504	-	-	-	X
2	SO4	C	503	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13027 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-phosphoshikimate 1-carboxyvinyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3200	2006	559	621	14			
1	B	429	Total	C	N	O	S	0	0	0
			3169	1984	554	617	14			
1	C	436	Total	C	N	O	S	0	0	0
			3231	2026	564	627	14			
1	D	431	Total	C	N	O	S	0	0	0
			3189	1998	557	620	14			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9KCA6
A	2	VAL	-	EXPRESSION TAG	UNP Q9KCA6
A	434	ALA	-	EXPRESSION TAG	UNP Q9KCA6
A	435	GLU	-	EXPRESSION TAG	UNP Q9KCA6
A	436	ASN	-	EXPRESSION TAG	UNP Q9KCA6
A	437	LEU	-	EXPRESSION TAG	UNP Q9KCA6
A	438	TYR	-	EXPRESSION TAG	UNP Q9KCA6
A	439	PHE	-	EXPRESSION TAG	UNP Q9KCA6
A	440	GLN	-	EXPRESSION TAG	UNP Q9KCA6
A	441	SER	-	EXPRESSION TAG	UNP Q9KCA6
A	442	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	443	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	444	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	445	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	446	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	447	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	448	TRP	-	EXPRESSION TAG	UNP Q9KCA6
A	449	SER	-	EXPRESSION TAG	UNP Q9KCA6
A	450	HIS	-	EXPRESSION TAG	UNP Q9KCA6
A	451	PRO	-	EXPRESSION TAG	UNP Q9KCA6
A	452	GLN	-	EXPRESSION TAG	UNP Q9KCA6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	453	PHE	-	EXPRESSION TAG	UNP Q9KCA6
A	454	GLU	-	EXPRESSION TAG	UNP Q9KCA6
A	455	LYS	-	EXPRESSION TAG	UNP Q9KCA6
B	1	MET	-	EXPRESSION TAG	UNP Q9KCA6
B	2	VAL	-	EXPRESSION TAG	UNP Q9KCA6
B	434	ALA	-	EXPRESSION TAG	UNP Q9KCA6
B	435	GLU	-	EXPRESSION TAG	UNP Q9KCA6
B	436	ASN	-	EXPRESSION TAG	UNP Q9KCA6
B	437	LEU	-	EXPRESSION TAG	UNP Q9KCA6
B	438	TYR	-	EXPRESSION TAG	UNP Q9KCA6
B	439	PHE	-	EXPRESSION TAG	UNP Q9KCA6
B	440	GLN	-	EXPRESSION TAG	UNP Q9KCA6
B	441	SER	-	EXPRESSION TAG	UNP Q9KCA6
B	442	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	443	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	444	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	445	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	446	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	447	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	448	TRP	-	EXPRESSION TAG	UNP Q9KCA6
B	449	SER	-	EXPRESSION TAG	UNP Q9KCA6
B	450	HIS	-	EXPRESSION TAG	UNP Q9KCA6
B	451	PRO	-	EXPRESSION TAG	UNP Q9KCA6
B	452	GLN	-	EXPRESSION TAG	UNP Q9KCA6
B	453	PHE	-	EXPRESSION TAG	UNP Q9KCA6
B	454	GLU	-	EXPRESSION TAG	UNP Q9KCA6
B	455	LYS	-	EXPRESSION TAG	UNP Q9KCA6
C	1	MET	-	EXPRESSION TAG	UNP Q9KCA6
C	2	VAL	-	EXPRESSION TAG	UNP Q9KCA6
C	434	ALA	-	EXPRESSION TAG	UNP Q9KCA6
C	435	GLU	-	EXPRESSION TAG	UNP Q9KCA6
C	436	ASN	-	EXPRESSION TAG	UNP Q9KCA6
C	437	LEU	-	EXPRESSION TAG	UNP Q9KCA6
C	438	TYR	-	EXPRESSION TAG	UNP Q9KCA6
C	439	PHE	-	EXPRESSION TAG	UNP Q9KCA6
C	440	GLN	-	EXPRESSION TAG	UNP Q9KCA6
C	441	SER	-	EXPRESSION TAG	UNP Q9KCA6
C	442	HIS	-	EXPRESSION TAG	UNP Q9KCA6
C	443	HIS	-	EXPRESSION TAG	UNP Q9KCA6
C	444	HIS	-	EXPRESSION TAG	UNP Q9KCA6
C	445	HIS	-	EXPRESSION TAG	UNP Q9KCA6
C	446	HIS	-	EXPRESSION TAG	UNP Q9KCA6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	447	HIS	-	EXPRESSION TAG	UNP Q9KCA6
C	448	TRP	-	EXPRESSION TAG	UNP Q9KCA6
C	449	SER	-	EXPRESSION TAG	UNP Q9KCA6
C	450	HIS	-	EXPRESSION TAG	UNP Q9KCA6
C	451	PRO	-	EXPRESSION TAG	UNP Q9KCA6
C	452	GLN	-	EXPRESSION TAG	UNP Q9KCA6
C	453	PHE	-	EXPRESSION TAG	UNP Q9KCA6
C	454	GLU	-	EXPRESSION TAG	UNP Q9KCA6
C	455	LYS	-	EXPRESSION TAG	UNP Q9KCA6
D	1	MET	-	EXPRESSION TAG	UNP Q9KCA6
D	2	VAL	-	EXPRESSION TAG	UNP Q9KCA6
D	434	ALA	-	EXPRESSION TAG	UNP Q9KCA6
D	435	GLU	-	EXPRESSION TAG	UNP Q9KCA6
D	436	ASN	-	EXPRESSION TAG	UNP Q9KCA6
D	437	LEU	-	EXPRESSION TAG	UNP Q9KCA6
D	438	TYR	-	EXPRESSION TAG	UNP Q9KCA6
D	439	PHE	-	EXPRESSION TAG	UNP Q9KCA6
D	440	GLN	-	EXPRESSION TAG	UNP Q9KCA6
D	441	SER	-	EXPRESSION TAG	UNP Q9KCA6
D	442	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	443	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	444	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	445	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	446	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	447	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	448	TRP	-	EXPRESSION TAG	UNP Q9KCA6
D	449	SER	-	EXPRESSION TAG	UNP Q9KCA6
D	450	HIS	-	EXPRESSION TAG	UNP Q9KCA6
D	451	PRO	-	EXPRESSION TAG	UNP Q9KCA6
D	452	GLN	-	EXPRESSION TAG	UNP Q9KCA6
D	453	PHE	-	EXPRESSION TAG	UNP Q9KCA6
D	454	GLU	-	EXPRESSION TAG	UNP Q9KCA6
D	455	LYS	-	EXPRESSION TAG	UNP Q9KCA6

- 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		
2	A	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	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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

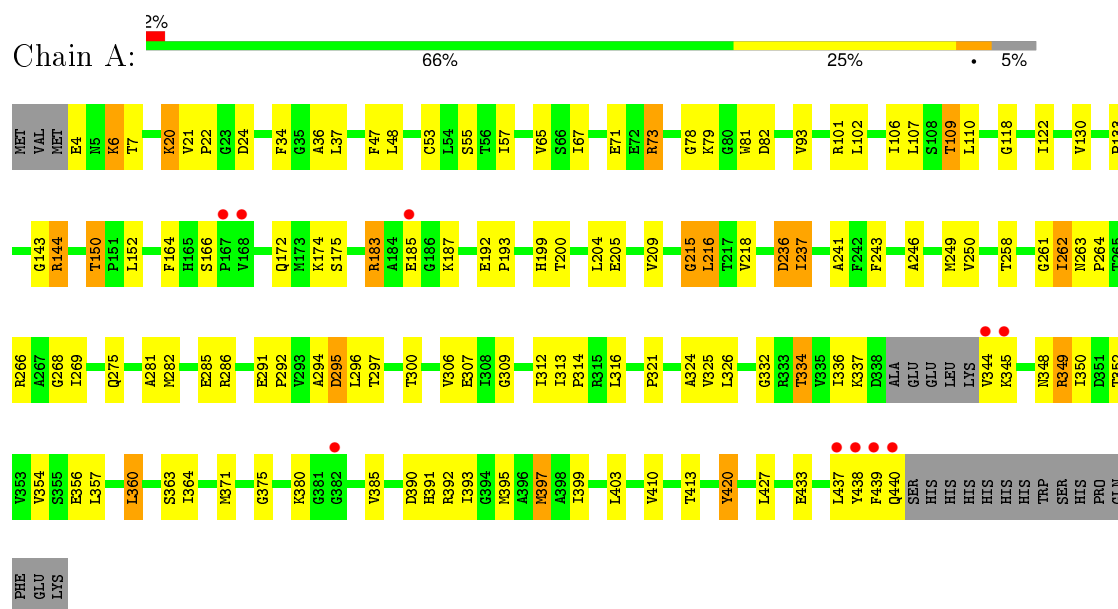
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	38	Total	O	0	0
			38	38		
3	C	15	Total	O	0	0
			15	15		
3	D	19	Total	O	0	0
			19	19		



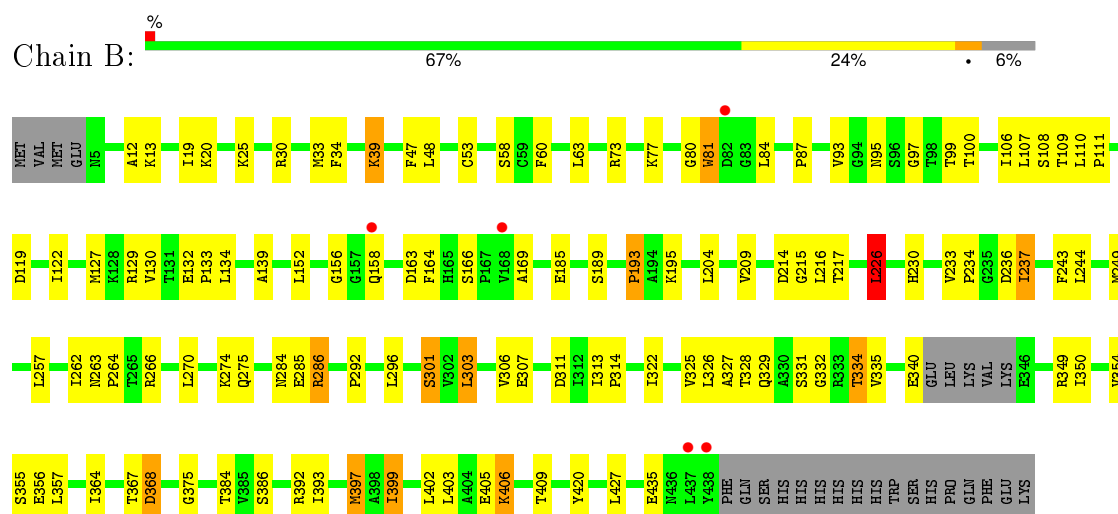
### 3 Residue-property plots

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.

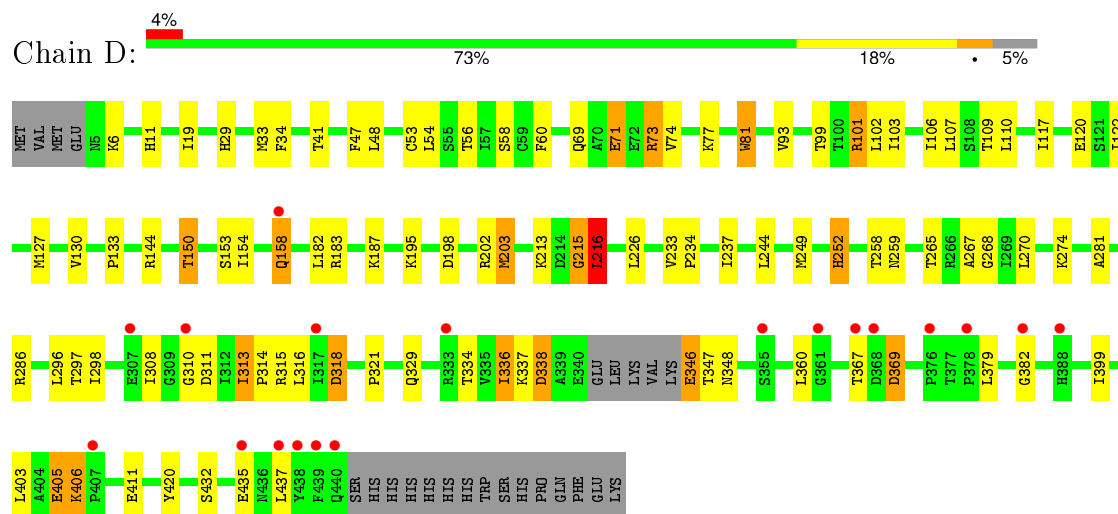
- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase 1



- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase 1



- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.86Å 140.75Å 193.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.80) 99.4 (20.00-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.222 , 0.286 0.222 , 0.281	Depositor DCC
$R_{free}$ test set	2998 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.4	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 59314 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/3245	0.64	0/4390
1	B	0.43	0/3213	0.62	1/4348 (0.0%)
1	C	0.41	0/3277	0.58	1/4434 (0.0%)
1	D	0.39	0/3234	0.59	0/4376
All	All	0.42	0/12969	0.61	2/17548 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	LEU	CA-CB-CG	6.74	130.80	115.30
1	C	226	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3200	0	3287	91	0
1	B	3169	0	3253	67	0
1	C	3231	0	3323	66	0
1	D	3189	0	3270	55	0
2	A	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	40	0	0	3	0
2	C	45	0	0	0	0
2	D	20	0	0	0	0
3	A	21	0	0	0	0
3	B	38	0	0	0	0
3	C	15	0	0	0	0
3	D	19	0	0	0	0
All	All	13027	0	13133	278	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 11.

All (278) 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:D:73:ARG:HG2	1:D:73:ARG:HH11	1.11	1.13
1:A:249:MET:CE	1:A:326:LEU:HA	1.84	1.08
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.25	1.00
1:A:183:ARG:HG2	1:A:183:ARG:HH11	1.29	0.98
1:A:78:GLY:HA3	1:A:79:LYS:HG2	1.48	0.94
1:B:349:ARG:HH22	1:B:392:ARG:HE	1.13	0.94
1:C:259:ASN:ND2	1:C:286:ARG:HH12	1.65	0.93
1:A:249:MET:HE3	1:A:326:LEU:HA	1.51	0.92
1:A:78:GLY:HA3	1:A:79:LYS:CG	2.00	0.91
1:C:81:TRP:HE1	1:C:109:THR:HG21	1.36	0.90
1:D:249:MET:HG2	1:D:329:GLN:HG3	1.56	0.86
1:A:106:ILE:O	1:A:109:THR:HG22	1.73	0.86
1:B:328:THR:HG22	1:B:329:GLN:HE21	1.42	0.84
1:A:281:ALA:HB3	1:A:297:THR:HG22	1.57	0.83
1:D:73:ARG:NH1	1:D:73:ARG:HG2	1.85	0.82
1:C:81:TRP:NE1	1:C:109:THR:HG21	1.95	0.80
1:C:259:ASN:HD22	1:C:286:ARG:HH12	1.31	0.79
1:B:349:ARG:NH2	1:B:392:ARG:HE	1.81	0.79
1:A:81:TRP:HE1	1:A:109:THR:CG2	1.96	0.79
1:A:200:THR:O	1:A:204:LEU:HB2	1.85	0.76
1:A:352:THR:O	1:A:356:GLU:HG2	1.86	0.76
1:A:356:GLU:OE1	1:A:385:VAL:HG13	1.85	0.76
1:A:336:ILE:HD12	1:A:371:MET:HE2	1.67	0.76
1:C:305:GLY:HA2	1:C:334:THR:HG22	1.68	0.75
1:D:346:GLU:HG2	1:D:347:THR:H	1.50	0.75
1:C:349:ARG:O	1:C:353:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HG2	1:A:130:VAL:HG21	1.70	0.74
1:D:308:ILE:HB	1:D:336:ILE:HG22	1.69	0.73
1:A:73:ARG:CG	1:A:73:ARG:HH11	1.99	0.73
1:A:183:ARG:HH11	1:A:183:ARG:CG	2.02	0.73
1:B:262:ILE:HD12	1:B:270:LEU:HD11	1.71	0.72
1:C:144:ARG:NH1	1:C:150:THR:O	2.22	0.71
1:B:243:PHE:HE1	1:B:427:LEU:HD13	1.55	0.71
1:A:306:VAL:H	1:A:334:THR:HB	1.57	0.70
1:A:243:PHE:HE1	1:A:427:LEU:HD12	1.55	0.69
1:A:144:ARG:NH1	1:A:150:THR:O	2.26	0.69
1:D:81:TRP:NE1	1:D:109:THR:HG21	2.08	0.68
1:A:215:GLY:O	1:A:216:LEU:HB2	1.91	0.68
1:C:317:ILE:HD11	1:C:342:LEU:HG	1.76	0.67
1:C:262:ILE:O	1:C:262:ILE:HG22	1.95	0.67
1:B:93:VAL:HG11	1:B:100:THR:OG1	1.94	0.67
1:B:39:LYS:HE2	1:B:80:GLY:HA3	1.77	0.67
1:A:81:TRP:HE1	1:A:109:THR:HG21	1.60	0.67
1:A:258:THR:HA	1:A:295:ASP:HB3	1.78	0.66
1:B:262:ILE:O	1:B:262:ILE:HG22	1.94	0.66
1:B:236:ASP:OD2	1:B:266:ARG:NH2	2.29	0.65
1:A:385:VAL:HG11	1:A:397:MET:HG3	1.80	0.64
1:D:117:ILE:HG13	1:D:150:THR:HG23	1.78	0.64
1:D:215:GLY:O	1:D:216:LEU:HB2	1.97	0.64
1:A:73:ARG:NH1	1:A:73:ARG:HG2	2.03	0.64
1:A:118:GLY:HA3	1:A:122:ILE:HG21	1.80	0.63
1:D:346:GLU:CG	1:D:347:THR:H	2.10	0.63
1:D:281:ALA:HB3	1:D:297:THR:HB	1.82	0.62
1:B:111:PRO:HA	1:B:156:GLY:O	1.99	0.62
1:A:385:VAL:HG11	1:A:397:MET:CG	2.29	0.62
1:D:405:GLU:CD	1:D:406:LYS:H	2.03	0.61
1:C:81:TRP:HE1	1:C:109:THR:CG2	2.10	0.61
1:A:81:TRP:HE1	1:A:109:THR:HG23	1.66	0.61
1:A:249:MET:CE	1:A:326:LEU:CA	2.71	0.61
1:A:183:ARG:HG2	1:A:183:ARG:NH1	2.09	0.60
1:A:7:THR:OG1	1:A:413:THR:HG21	2.01	0.60
1:B:284:ASN:O	1:B:286:ARG:HG3	2.02	0.60
1:A:243:PHE:HE1	1:A:427:LEU:CD1	2.14	0.59
1:B:325:VAL:O	1:B:328:THR:HB	2.01	0.59
1:D:109:THR:HG23	1:D:183:ARG:HB3	1.84	0.59
1:C:262:ILE:HD12	1:C:270:LEU:HD11	1.84	0.59
1:B:95:ASN:ND2	1:B:119:ASP:OD1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ILE:O	1:D:109:THR:HB	2.02	0.58
1:B:195:LYS:HG3	1:B:216:LEU:HD23	1.85	0.58
1:C:81:TRP:NE1	1:C:109:THR:CG2	2.65	0.58
1:B:384:THR:HG23	1:B:409:THR:HB	1.86	0.58
1:D:29:HIS:HD2	1:D:56:THR:OG1	1.86	0.58
1:A:262:ILE:HG22	1:A:292:PRO:HB2	1.84	0.57
1:C:106:ILE:O	1:C:109:THR:HB	2.04	0.57
1:B:332:GLY:H	1:B:375:GLY:HA2	1.69	0.57
1:A:102:LEU:HD22	1:A:175:SER:HB2	1.87	0.57
1:B:357:LEU:HD13	1:B:364:ILE:HD11	1.85	0.57
1:C:83:GLY:HA2	1:C:85:ARG:HH12	1.69	0.57
1:B:107:LEU:HA	1:B:110:LEU:HD12	1.87	0.56
1:D:11:HIS:CD2	1:D:405:GLU:HG2	2.40	0.56
1:C:259:ASN:ND2	1:C:286:ARG:NH1	2.46	0.56
1:A:192:GLU:HB2	1:A:193:PRO:HD2	1.88	0.56
1:C:328:THR:HG22	1:C:329:GLN:NE2	2.20	0.56
1:C:102:LEU:HD22	1:C:175:SER:HB2	1.88	0.55
1:B:97:GLY:HA3	2:B:500:SO4:O1	2.06	0.55
1:D:130:VAL:O	1:D:133:PRO:HD2	2.06	0.55
1:B:262:ILE:HD11	1:B:296:LEU:HD21	1.88	0.55
1:C:313:ILE:HB	1:C:314:PRO:HD3	1.87	0.55
1:B:47:PHE:CZ	1:B:53:CYS:HB3	2.41	0.55
1:C:405:GLU:O	1:C:406:LYS:HB2	2.07	0.55
1:A:281:ALA:HB3	1:A:297:THR:CG2	2.34	0.54
1:B:84:LEU:HD12	1:B:110:LEU:HD21	1.89	0.54
1:B:367:THR:HG22	1:B:368:ASP:H	1.73	0.53
1:C:265:THR:HA	1:C:315:ARG:HD2	1.90	0.53
1:D:130:VAL:C	1:D:133:PRO:HD2	2.29	0.53
1:C:391:HIS:HD2	1:C:395:MET:CE	2.21	0.53
1:C:238:SER:HA	1:C:319:GLU:OE1	2.08	0.53
1:C:331:SER:HA	1:C:376:PRO:HD3	1.91	0.53
1:C:118:GLY:HA3	1:C:122:ILE:HG21	1.90	0.53
1:B:262:ILE:CG2	1:B:262:ILE:O	2.57	0.52
1:C:339:ALA:HA	1:C:342:LEU:HD13	1.92	0.52
1:C:307:GLU:HG3	1:C:335:VAL:HB	1.91	0.52
1:B:209:VAL:CG2	1:B:226:LEU:HD22	2.40	0.52
1:B:349:ARG:HH22	1:B:392:ARG:NE	1.94	0.52
1:A:262:ILE:HD12	1:A:294:ALA:HB3	1.90	0.52
1:A:246:ALA:HB2	1:A:399:ILE:HG23	1.90	0.52
1:A:325:VAL:HG22	1:A:357:LEU:HD21	1.90	0.52
1:A:237:ILE:HG12	1:A:261:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ARG:CG	1:D:73:ARG:HH11	2.01	0.51
1:D:144:ARG:HD3	1:D:150:THR:O	2.10	0.51
1:A:78:GLY:HA3	1:A:79:LYS:HG3	1.87	0.51
1:D:101:ARG:HG3	1:D:130:VAL:HG21	1.92	0.51
1:A:24:ASP:HA	1:A:236:ASP:HB2	1.93	0.51
1:A:324:ALA:HB2	1:A:371:MET:HE1	1.92	0.51
1:B:106:ILE:O	1:B:109:THR:HB	2.10	0.51
1:C:117:ILE:HG13	1:C:150:THR:HG23	1.92	0.51
1:A:199:HIS:HD2	1:A:291:GLU:OE2	1.94	0.50
1:C:249:MET:HE2	1:C:329:GLN:HG2	1.93	0.50
1:A:268:GLY:HA3	1:A:316:LEU:HB3	1.92	0.50
1:D:432:SER:HA	1:D:435:GLU:HG3	1.94	0.50
1:C:37:LEU:O	1:C:80:GLY:HA2	2.11	0.50
1:C:262:ILE:O	1:C:262:ILE:CG2	2.59	0.50
1:A:349:ARG:HH12	1:A:392:ARG:HE	1.59	0.50
1:A:390:ASP:HB3	1:A:393:ILE:HG12	1.94	0.50
1:A:174:LYS:HD2	1:A:218:VAL:HG21	1.94	0.50
1:A:332:GLY:H	1:A:375:GLY:HA2	1.76	0.50
1:C:259:ASN:HD21	1:C:286:ARG:HH12	1.57	0.49
1:A:391:HIS:HD2	1:A:395:MET:CE	2.25	0.49
1:B:329:GLN:HG3	1:B:403:LEU:HD21	1.93	0.49
1:D:346:GLU:HG2	1:D:347:THR:N	2.23	0.49
1:B:356:GLU:OE1	1:B:386:SER:O	2.31	0.49
1:D:337:LYS:HG3	1:D:369:ASP:OD2	2.12	0.49
1:B:63:LEU:HD23	1:B:87:PRO:HG3	1.95	0.49
1:A:36:ALA:HB1	1:A:65:VAL:HG21	1.95	0.49
1:C:44:VAL:HB	1:C:74:VAL:HB	1.94	0.49
1:D:318:ASP:O	1:D:321:PRO:HD2	2.13	0.48
1:D:215:GLY:O	1:D:216:LEU:CB	2.61	0.48
1:B:81:TRP:NE1	1:B:109:THR:HG21	2.28	0.48
1:D:313:ILE:N	1:D:314:PRO:HD2	2.29	0.48
1:C:339:ALA:O	1:C:342:LEU:HB2	2.14	0.48
1:A:344:VAL:HG13	1:A:345:LYS:H	1.79	0.48
1:B:306:VAL:H	1:B:334:THR:HB	1.78	0.48
1:C:288:GLN:NE2	1:C:293:VAL:HG21	2.29	0.48
1:B:392:ARG:NH2	2:B:504:SO4:O3	2.47	0.48
1:A:336:ILE:HD12	1:A:371:MET:CE	2.41	0.48
1:B:237:ILE:HD11	1:B:266:ARG:HB3	1.96	0.47
1:B:132:GLU:HB2	1:B:133:PRO:HD3	1.96	0.47
1:D:99:THR:O	1:D:103:ILE:HG13	2.14	0.47
1:D:360:LEU:HB3	1:D:379:LEU:HD22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ALA:HB2	1:B:193:PRO:HG2	1.97	0.47
1:A:143:GLY:HA3	1:A:152:LEU:HD23	1.95	0.47
1:A:37:LEU:HD11	1:A:106:ILE:HD13	1.97	0.47
1:D:101:ARG:HD2	1:D:127:MET:SD	2.55	0.47
1:D:34:PHE:N	1:D:34:PHE:CD1	2.80	0.47
1:A:439:PHE:O	1:A:440:GLN:HG2	2.15	0.47
1:B:164:PHE:CE2	1:B:166:SER:HB2	2.49	0.47
1:C:249:MET:CE	1:C:329:GLN:HG2	2.46	0.46
1:C:433:GLU:O	1:C:437:LEU:HB2	2.16	0.46
1:B:34:PHE:N	1:B:34:PHE:CD1	2.83	0.46
1:B:275:GLN:HB3	1:B:306:VAL:HG21	1.98	0.46
1:A:263:ASN:HA	1:A:264:PRO:HD3	1.82	0.46
1:A:22:PRO:HD3	1:A:420:TYR:CZ	2.51	0.46
1:B:30:ARG:NH2	2:B:502:SO4:O4	2.45	0.46
1:A:291:GLU:HA	1:A:292:PRO:HD3	1.86	0.46
1:D:313:ILE:HG21	1:D:338:ASP:HB3	1.98	0.45
1:B:93:VAL:HG12	1:B:93:VAL:O	2.16	0.45
1:A:249:MET:HE1	1:A:326:LEU:HA	1.87	0.45
1:B:163:ASP:OD1	1:B:189:SER:HB2	2.16	0.45
1:C:284:ASN:N	1:C:284:ASN:OD1	2.50	0.45
1:A:107:LEU:HA	1:A:110:LEU:HD12	1.99	0.45
1:C:238:SER:OG	1:C:266:ARG:NH2	2.50	0.45
1:D:182:LEU:HD21	1:D:226:LEU:HD21	1.98	0.45
1:C:182:LEU:HD21	1:C:226:LEU:HD21	1.99	0.45
1:B:263:ASN:HA	1:B:292:PRO:HG2	1.98	0.45
1:A:205:GLU:HA	1:A:209:VAL:O	2.16	0.45
1:A:307:GLU:OE2	1:A:337:LYS:HE2	2.17	0.45
1:A:275:GLN:HB3	1:A:306:VAL:HG21	1.99	0.44
1:D:346:GLU:CG	1:D:347:THR:N	2.79	0.44
1:C:317:ILE:HD11	1:C:342:LEU:CG	2.44	0.44
1:A:309:GLY:HA2	1:A:313:ILE:HD11	1.98	0.44
1:B:307:GLU:HG3	1:B:335:VAL:HB	1.99	0.44
1:B:60:PHE:HZ	1:B:106:ILE:HD12	1.82	0.44
1:D:198:ASP:O	1:D:202:ARG:HG3	2.17	0.44
1:A:192:GLU:O	1:A:216:LEU:HD13	2.17	0.44
1:B:34:PHE:N	1:B:34:PHE:HD1	2.15	0.44
1:B:393:ILE:O	1:B:397:MET:HB2	2.18	0.44
1:C:211:ILE:CG2	1:C:212:GLU:N	2.80	0.44
1:C:132:GLU:HB2	1:C:133:PRO:HD3	1.99	0.44
1:C:93:VAL:HG11	1:C:100:THR:OG1	2.17	0.44
1:C:244:LEU:HD11	1:C:296:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:PHE:HD1	1:D:34:PHE:N	2.16	0.44
1:C:211:ILE:HG22	1:C:212:GLU:N	2.33	0.44
1:A:354:VAL:HG22	1:A:364:ILE:HG12	1.99	0.44
1:A:336:ILE:CD1	1:A:371:MET:HE2	2.43	0.43
1:B:327:ALA:HB1	1:B:334:THR:CG2	2.48	0.43
1:D:109:THR:HG23	1:D:183:ARG:CB	2.48	0.43
1:A:249:MET:SD	1:A:403:LEU:HD11	2.58	0.43
1:A:237:ILE:HD12	1:A:266:ARG:HB3	2.00	0.43
1:B:215:GLY:C	1:B:217:THR:H	2.22	0.43
1:D:34:PHE:CE2	1:D:203:MET:HB3	2.52	0.43
1:C:212:GLU:OE2	1:C:212:GLU:HA	2.18	0.43
1:C:352:THR:O	1:C:356:GLU:HG2	2.18	0.43
1:D:267:ALA:HB1	1:D:270:LEU:HD12	2.00	0.43
1:B:127:MET:HG3	1:B:152:LEU:HD11	2.00	0.43
1:B:249:MET:HE3	1:B:326:LEU:HA	2.01	0.43
1:A:360:LEU:HD21	1:A:385:VAL:HG21	1.99	0.43
1:B:244:LEU:HD11	1:B:296:LEU:HD13	2.01	0.43
1:A:57:ILE:HG23	1:A:67:ILE:HG21	2.00	0.43
1:A:34:PHE:N	1:A:34:PHE:CD1	2.86	0.43
1:C:200:THR:O	1:C:204:LEU:CD2	2.67	0.43
1:C:200:THR:O	1:C:204:LEU:HD22	2.19	0.43
1:D:47:PHE:CZ	1:D:53:CYS:HB3	2.54	0.43
1:A:20:LYS:HD2	1:A:21:VAL:O	2.19	0.43
1:B:263:ASN:HA	1:B:264:PRO:HD3	1.82	0.43
1:C:241:ALA:HB1	1:C:269:ILE:HD13	2.01	0.42
1:B:322:ILE:HD11	1:B:399:ILE:HG12	2.02	0.42
1:D:33:MET:HG2	1:D:60:PHE:CE1	2.53	0.42
1:A:321:PRO:O	1:A:324:ALA:HB3	2.19	0.42
1:D:337:LYS:O	1:D:338:ASP:HB2	2.19	0.42
1:A:183:ARG:NH1	1:A:183:ARG:CG	2.70	0.42
1:A:385:VAL:HG11	1:A:397:MET:HG2	2.01	0.42
1:C:245:VAL:HG22	1:C:326:LEU:HD22	2.01	0.42
1:D:103:ILE:HG22	1:D:107:LEU:HG	2.02	0.42
1:D:233:VAL:HA	1:D:234:PRO:HD3	1.86	0.42
1:B:33:MET:HG2	1:B:60:PHE:CE1	2.54	0.42
1:D:268:GLY:HA3	1:D:316:LEU:HB3	2.01	0.42
1:A:133:PRO:HG3	1:A:164:PHE:CZ	2.54	0.42
1:B:301:SER:HB2	1:B:303:LEU:HD13	2.02	0.42
1:A:438:TYR:C	1:A:440:GLN:H	2.22	0.42
1:C:306:VAL:HG12	1:C:308:ILE:HG13	2.02	0.42
1:C:321:PRO:O	1:C:324:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ILE:HD13	1:C:234:PRO:HD2	2.02	0.42
1:B:93:VAL:HG13	1:B:99:THR:HB	2.02	0.42
1:D:244:LEU:HD11	1:D:296:LEU:HD23	2.00	0.42
1:C:29:HIS:HD2	1:C:56:THR:OG1	2.02	0.42
1:B:405:GLU:O	1:B:406:LYS:HB2	2.20	0.42
1:A:101:ARG:HD2	1:A:172:GLN:OE1	2.19	0.42
1:D:308:ILE:HG22	1:D:313:ILE:HG13	2.02	0.42
1:D:107:LEU:HD23	1:D:110:LEU:HD12	2.01	0.42
1:B:350:ILE:O	1:B:354:VAL:HG23	2.19	0.42
1:C:309:GLY:O	1:C:312:ILE:HG12	2.20	0.42
1:C:414:GLU:O	1:C:418:VAL:HG23	2.20	0.42
1:D:6:LYS:HB3	1:D:411:GLU:HG2	2.02	0.42
1:A:350:ILE:O	1:A:354:VAL:HG23	2.20	0.41
1:C:383:VAL:HG12	1:C:384:THR:N	2.34	0.41
1:B:313:ILE:HB	1:B:314:PRO:HD3	2.02	0.41
1:A:250:VAL:O	1:A:300:THR:OG1	2.34	0.41
1:A:73:ARG:NH1	1:A:73:ARG:CG	2.69	0.41
1:A:313:ILE:HB	1:A:314:PRO:CD	2.50	0.41
1:C:262:ILE:HD11	1:C:296:LEU:HD21	2.02	0.41
1:D:244:LEU:HA	1:D:298:ILE:HG21	2.02	0.41
1:B:12:ALA:HB2	1:B:402:LEU:HD22	2.02	0.41
1:D:69:GLN:HG2	1:D:74:VAL:HG22	2.02	0.41
1:B:19:ILE:HB	1:B:257:LEU:CD2	2.51	0.41
1:C:50:GLY:O	1:C:54:LEU:HB2	2.21	0.41
1:B:243:PHE:HE1	1:B:427:LEU:CD1	2.30	0.41
1:D:195:LYS:NZ	1:D:216:LEU:H	2.18	0.41
1:C:350:ILE:O	1:C:354:VAL:HG23	2.20	0.41
1:B:130:VAL:O	1:B:134:LEU:HG	2.20	0.41
1:D:405:GLU:HA	1:D:405:GLU:OE2	2.20	0.41
1:A:164:PHE:CE2	1:A:166:SER:HB2	2.56	0.41
1:A:241:ALA:HB1	1:A:269:ILE:HD13	2.02	0.41
1:D:153:SER:C	1:D:154:ILE:HG13	2.41	0.41
1:D:405:GLU:O	1:D:406:LYS:HB2	2.21	0.41
1:A:410:VAL:O	1:A:413:THR:HG23	2.21	0.41
1:D:69:GLN:CG	1:D:74:VAL:HG22	2.50	0.41
1:B:108:SER:HB3	1:B:139:ALA:HB2	2.03	0.41
1:C:143:GLY:HA3	1:C:152:LEU:HD23	2.03	0.41
1:C:34:PHE:N	1:C:34:PHE:CD1	2.89	0.41
1:A:47:PHE:CZ	1:A:53:CYS:HB3	2.55	0.40
1:C:205:GLU:HA	1:C:209:VAL:O	2.20	0.40
1:A:324:ALA:HB2	1:A:371:MET:CE	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:HA	1:A:6:LYS:HE3	2.02	0.40
1:A:237:ILE:HG13	1:A:237:ILE:H	1.46	0.40
1:B:233:VAL:HA	1:B:234:PRO:HD3	1.92	0.40
1:B:331:SER:HB3	1:C:315:ARG:HH22	1.87	0.40
1:A:349:ARG:NH2	1:A:390:ASP:OD1	2.54	0.40
1:C:289:GLY:HA3	1:C:290:GLY:HA3	1.85	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	428/455 (94%)	403 (94%)	23 (5%)	2 (0%)	34	69
1	B	425/455 (93%)	404 (95%)	19 (4%)	2 (0%)	34	69
1	C	434/455 (95%)	409 (94%)	23 (5%)	2 (0%)	34	69
1	D	427/455 (94%)	396 (93%)	22 (5%)	9 (2%)	9	29
All	All	1714/1820 (94%)	1612 (94%)	87 (5%)	15 (1%)	21	55

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	GLY
1	D	158	GLN
1	D	216	LEU
1	C	197	ARG
1	D	215	GLY
1	A	71	GLU
1	B	193	PRO
1	D	252	HIS
1	D	338	ASP

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Mol	Chain	Res	Type
1	C	49	PRO
1	D	71	GLU
1	D	310	GLY
1	D	382	GLY
1	D	406	LYS
1	B	406	LYS

### 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	349/371 (94%)	316 (90%)	33 (10%)	11	30
1	B	345/371 (93%)	313 (91%)	32 (9%)	11	32
1	C	352/371 (95%)	318 (90%)	34 (10%)	10	29
1	D	347/371 (94%)	305 (88%)	42 (12%)	6	18
All	All	1393/1484 (94%)	1252 (90%)	141 (10%)	9	27

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	20	LYS
1	A	48	LEU
1	A	55	SER
1	A	73	ARG
1	A	82	ASP
1	A	93	VAL
1	A	109	THR
1	A	144	ARG
1	A	150	THR
1	A	183	ARG
1	A	185	GLU
1	A	187	LYS
1	A	216	LEU
1	A	236	ASP

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Mol	Chain	Res	Type
1	A	237	ILE
1	A	262	ILE
1	A	282	MET
1	A	285	GLU
1	A	286	ARG
1	A	295	ASP
1	A	296	LEU
1	A	312	ILE
1	A	334	THR
1	A	348	ASN
1	A	349	ARG
1	A	360	LEU
1	A	363	SER
1	A	380	LYS
1	A	397	MET
1	A	420	TYR
1	A	433	GLU
1	A	437	LEU
1	B	13	LYS
1	B	20	LYS
1	B	25	LYS
1	B	39	LYS
1	B	48	LEU
1	B	58	SER
1	B	73	ARG
1	B	77	LYS
1	B	81	TRP
1	B	122	ILE
1	B	129	ARG
1	B	158	GLN
1	B	185	GLU
1	B	204	LEU
1	B	214	ASP
1	B	226	LEU
1	B	230	HIS
1	B	237	ILE
1	B	274	LYS
1	B	285	GLU
1	B	286	ARG
1	B	301	SER
1	B	303	LEU
1	B	311	ASP

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Mol	Chain	Res	Type
1	B	334	THR
1	B	340	GLU
1	B	355	SER
1	B	368	ASP
1	B	397	MET
1	B	399	ILE
1	B	420	TYR
1	B	435	GLU
1	C	6	LYS
1	C	11	HIS
1	C	13	LYS
1	C	20	LYS
1	C	82	ASP
1	C	93	VAL
1	C	150	THR
1	C	185	GLU
1	C	187	LYS
1	C	197	ARG
1	C	204	LEU
1	C	212	GLU
1	C	217	THR
1	C	226	LEU
1	C	227	THR
1	C	237	ILE
1	C	282	MET
1	C	284	ASN
1	C	286	ARG
1	C	302	VAL
1	C	306	VAL
1	C	307	GLU
1	C	333	ARG
1	C	334	THR
1	C	340	GLU
1	C	347	THR
1	C	359	LYS
1	C	380	LYS
1	C	385	VAL
1	C	397	MET
1	C	399	ILE
1	C	422	SER
1	C	437	LEU
1	C	440	GLN

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Mol	Chain	Res	Type
1	D	19	ILE
1	D	41	THR
1	D	48	LEU
1	D	54	LEU
1	D	58	SER
1	D	71	GLU
1	D	73	ARG
1	D	77	LYS
1	D	81	TRP
1	D	93	VAL
1	D	101	ARG
1	D	102	LEU
1	D	120	GLU
1	D	122	ILE
1	D	150	THR
1	D	158	GLN
1	D	187	LYS
1	D	203	MET
1	D	213	LYS
1	D	216	LEU
1	D	237	ILE
1	D	252	HIS
1	D	258	THR
1	D	259	ASN
1	D	265	THR
1	D	274	LYS
1	D	286	ARG
1	D	311	ASP
1	D	313	ILE
1	D	315	ARG
1	D	318	ASP
1	D	334	THR
1	D	336	ILE
1	D	346	GLU
1	D	348	ASN
1	D	367	THR
1	D	369	ASP
1	D	399	ILE
1	D	403	LEU
1	D	405	GLU
1	D	420	TYR
1	D	437	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	199	HIS
1	A	391	HIS
1	B	158	GLN
1	B	288	GLN
1	B	329	GLN
1	B	391	HIS
1	C	29	HIS
1	C	210	ASN
1	C	224	GLN
1	C	259	ASN
1	C	288	GLN
1	C	329	GLN
1	C	391	HIS
1	C	436	ASN
1	D	11	HIS
1	D	29	HIS
1	D	304	GLN
1	D	440	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

29 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	456	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	A	500	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	A	503	-	4,4,4	0.19	0	6,6,6	0.27	0
2	SO4	A	504	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	A	505	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	A	506	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	A	507	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	B	456	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	B	500	-	4,4,4	0.24	0	6,6,6	0.28	0
2	SO4	B	501	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	B	502	-	4,4,4	0.26	0	6,6,6	0.36	0
2	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.33	0
2	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	B	505	-	4,4,4	0.20	0	6,6,6	0.21	0
2	SO4	B	506	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	C	456	-	4,4,4	0.16	0	6,6,6	0.08	0
2	SO4	C	500	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	C	501	-	4,4,4	0.20	0	6,6,6	0.14	0
2	SO4	C	502	-	4,4,4	0.21	0	6,6,6	0.11	0
2	SO4	C	503	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	C	504	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.28	0
2	SO4	C	506	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	C	507	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	D	501	-	4,4,4	0.22	0	6,6,6	0.34	0
2	SO4	D	502	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	D	503	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.17	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	456	-	-	0/0/0/0	0/0/0/0
2	SO4	A	500	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
2	SO4	A	505	-	-	0/0/0/0	0/0/0/0
2	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	SO4	A	507	-	-	0/0/0/0	0/0/0/0
2	SO4	B	456	-	-	0/0/0/0	0/0/0/0
2	SO4	B	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
2	SO4	B	505	-	-	0/0/0/0	0/0/0/0
2	SO4	B	506	-	-	0/0/0/0	0/0/0/0
2	SO4	C	456	-	-	0/0/0/0	0/0/0/0
2	SO4	C	500	-	-	0/0/0/0	0/0/0/0
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	504	-	-	0/0/0/0	0/0/0/0
2	SO4	C	505	-	-	0/0/0/0	0/0/0/0
2	SO4	C	506	-	-	0/0/0/0	0/0/0/0
2	SO4	C	507	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	D	503	-	-	0/0/0/0	0/0/0/0
2	SO4	D	505	-	-	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	SO4	1	0
2	B	502	SO4	1	0
2	B	504	SO4	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	432/455 (94%)	-0.27	10 (2%) 64 52	35, 64, 97, 115	0
1	B	429/455 (94%)	-0.33	5 (1%) 81 73	31, 59, 88, 111	0
1	C	436/455 (95%)	-0.24	11 (2%) 61 48	46, 72, 107, 140	0
1	D	431/455 (94%)	0.02	19 (4%) 38 26	46, 87, 154, 170	0
All	All	1728/1820 (94%)	-0.20	45 (2%) 59 47	31, 69, 120, 170	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	368	ASP	5.5
1	D	440	GLN	4.5
1	A	344	VAL	4.2
1	C	213	LYS	4.2
1	C	438	TYR	3.6
1	D	438	TYR	3.6
1	C	439	PHE	3.4
1	C	440	GLN	3.4
1	A	439	PHE	3.4
1	D	382	GLY	3.1
1	A	437	LEU	3.1
1	B	438	TYR	3.0
1	D	437	LEU	2.9
1	D	439	PHE	2.9
1	D	407	PRO	2.8
1	B	158	GLN	2.8
1	A	167	PRO	2.7
1	C	185	GLU	2.7
1	C	157	GLY	2.7
1	D	376	PRO	2.7
1	D	388	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	333	ARG	2.7
1	D	310	GLY	2.6
1	A	440	GLN	2.5
1	A	382	GLY	2.5
1	D	378	PRO	2.4
1	A	438	TYR	2.4
1	C	208	GLY	2.4
1	A	345	LYS	2.4
1	A	185	GLU	2.4
1	C	375	GLY	2.4
1	D	435	GLU	2.4
1	C	359	LYS	2.3
1	D	367	THR	2.3
1	C	160	LYS	2.2
1	D	317	ILE	2.1
1	A	168	VAL	2.1
1	B	82	ASP	2.1
1	B	437	LEU	2.1
1	D	361	GLY	2.1
1	D	158	GLN	2.0
1	C	214	ASP	2.0
1	D	307	GLU	2.0
1	B	168	VAL	2.0
1	D	355	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	504	5/5	0.91	0.37	4.64	123,129,130,130	0
2	SO4	A	503	5/5	0.89	0.20	3.27	114,114,116,116	0
2	SO4	C	503	5/5	0.88	0.25	2.08	152,153,154,154	0
2	SO4	A	502	5/5	0.91	0.21	1.21	144,145,149,149	0
2	SO4	D	501	5/5	0.96	0.15	-0.24	86,88,89,91	0
2	SO4	A	507	5/5	0.94	0.14	-0.38	87,88,90,94	0
2	SO4	C	507	5/5	0.96	0.14	-0.70	90,92,94,95	0
2	SO4	D	502	5/5	0.98	0.11	-0.70	68,71,72,73	0
2	SO4	C	505	5/5	0.94	0.13	-0.77	87,87,89,93	0
2	SO4	B	500	5/5	0.98	0.11	-0.77	42,43,44,50	0
2	SO4	A	500	5/5	0.98	0.11	-0.83	65,66,67,74	0
2	SO4	B	506	5/5	0.97	0.15	-0.90	80,84,87,87	0
2	SO4	A	456	5/5	0.93	0.13	-0.96	111,136,136,136	0
2	SO4	B	502	5/5	0.98	0.10	-1.21	66,67,67,68	0
2	SO4	B	501	5/5	0.97	0.10	-2.06	75,75,77,77	0
2	SO4	C	500	5/5	0.98	0.09	-2.45	70,71,71,78	0
2	SO4	C	456	5/5	0.98	0.09	-2.89	73,73,75,80	0
2	SO4	D	505	5/5	0.96	0.17	-	79,80,81,90	0
2	SO4	B	505	5/5	0.91	0.38	-	113,115,116,117	0
2	SO4	C	504	5/5	0.98	0.07	-	86,88,89,96	0
2	SO4	B	456	5/5	0.99	0.10	-	62,62,64,69	0
2	SO4	D	503	5/5	0.96	0.15	-	81,83,85,95	0
2	SO4	A	505	5/5	0.98	0.16	-	80,81,82,83	0
2	SO4	B	504	5/5	0.80	0.29	-	149,150,150,150	0
2	SO4	C	502	5/5	0.84	0.34	-	135,135,135,137	0
2	SO4	B	503	5/5	0.95	0.15	-	63,63,64,78	0
2	SO4	C	501	5/5	0.91	0.11	-	130,131,133,136	0
2	SO4	A	506	5/5	0.93	0.17	-	94,95,96,96	0
2	SO4	C	506	5/5	0.77	0.41	-	167,168,172,173	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.