



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 02:56 PM JST

PDB ID : 5B6P  
Title : Structure of the dodecameric type-II dehydrogenate dehydratase from *Acinetobacter baumannii* at 2.00 Å resolution  
Authors : Kumar, M.; Iqbal, N.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2016-05-31  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

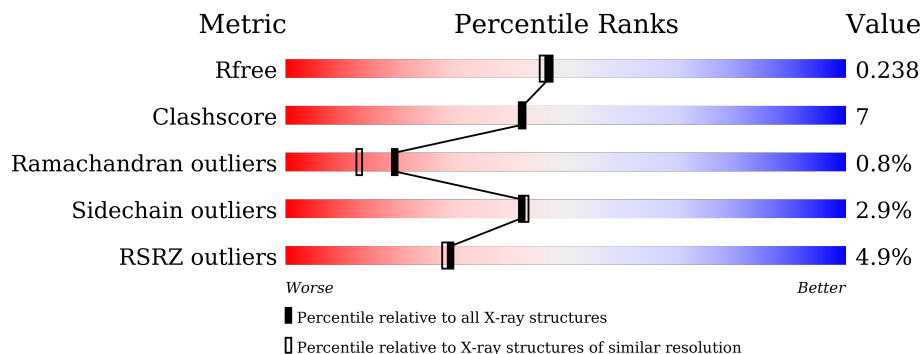
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	151	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: orange; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>11%</span> <span>...</span> </div>
1	B	151	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: orange; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>85%</span> <span>7%</span> <span>..</span> </div>
1	C	151	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: orange; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>83%</span> <span>10%</span> <span>...</span> </div>
1	D	151	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: orange; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>83%</span> <span>9%</span> <span>...</span> </div>
1	E	151	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: orange; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>83%</span> <span>9%</span> <span>..</span> </div>
1	F	151	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: orange; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>82%</span> <span>12%</span> <span>..</span> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	151	 5% 82% 12% . .
1	H	151	 3% 82% 11% . .
1	I	151	 5% 86% 7% . .
1	J	151	 5% 83% 12% . .
1	K	151	 7% 85% 10% . .
1	L	151	 5% 84% 9% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14281 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-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	145	1121	715	199	206	1	0	0	0
1	B	145	1121	715	199	206	1	0	0	0
1	C	145	1121	715	199	206	1	0	0	0
1	D	145	1121	715	199	206	1	0	0	0
1	E	145	1121	715	199	206	1	0	0	0
1	F	145	1121	715	199	206	1	0	0	0
1	G	145	1121	715	199	206	1	0	0	0
1	H	145	1121	715	199	206	1	0	0	0
1	I	145	1121	715	199	206	1	0	0	0
1	J	145	1121	715	199	206	1	0	0	0
1	K	145	1121	715	199	206	1	0	0	0
1	L	145	1121	715	199	206	1	0	0	0

- 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	B	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	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

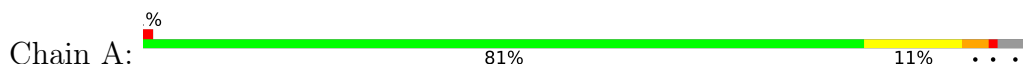
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	85	Total O 85 85	0	0
3	B	86	Total O 86 86	0	0
3	C	94	Total O 94 94	0	0
3	D	70	Total O 70 70	0	0
3	E	69	Total O 69 69	0	0
3	F	51	Total O 51 51	0	0
3	G	55	Total O 55 55	0	0
3	H	51	Total O 51 51	0	0
3	I	56	Total O 56 56	0	0
3	J	56	Total O 56 56	0	0
3	K	40	Total O 40 40	0	0
3	L	56	Total O 56 56	0	0

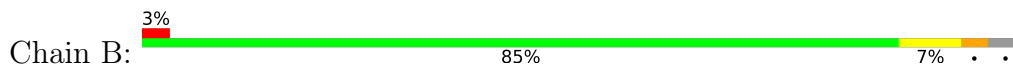
### 3 Residue-property plots [i](#)

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

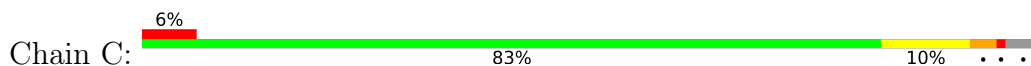
- Molecule 1: 3-dehydroquininate dehydratase



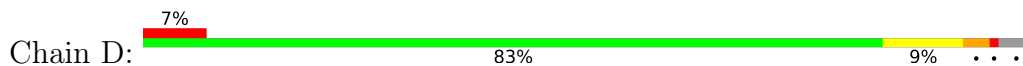
- Molecule 1: 3-dehydroquininate dehydratase



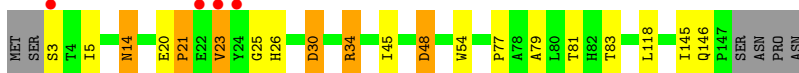
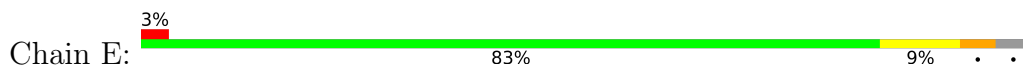
- Molecule 1: 3-dehydroquininate dehydratase



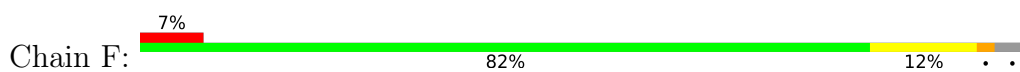
- Molecule 1: 3-dehydroquininate dehydratase



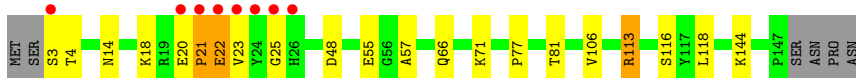
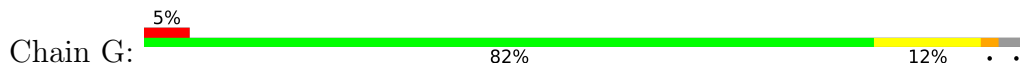
- Molecule 1: 3-dehydroquininate dehydratase



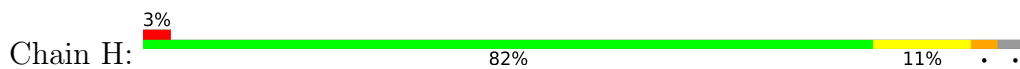
- Molecule 1: 3-dehydroquininate dehydratase



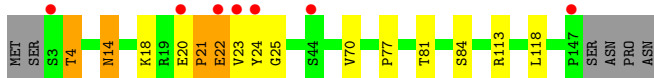
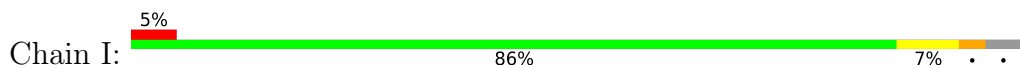
- Molecule 1: 3-dehydroquinatase dehydratase



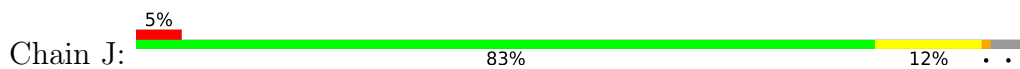
- Molecule 1: 3-dehydroquinatase dehydratase



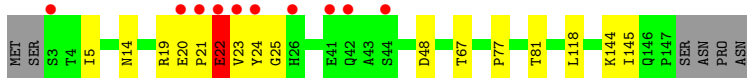
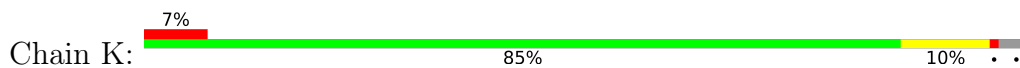
- Molecule 1: 3-dehydroquinatase dehydratase



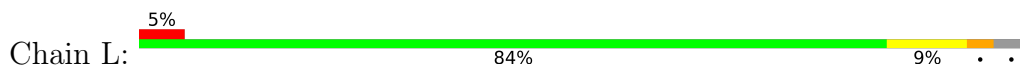
- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase



- Molecule 1: 3-dehydroquinatase dehydratase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.28Å 95.28Å 132.26Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	131.60 – 2.00 46.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (131.60-2.00) 96.2 (46.97-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.36 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.201 , 0.232 0.208 , 0.238	Depositor DCC
$R_{free}$ test set	1603 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.08	1/1143 (0.1%)	1.02	7/1555 (0.5%)
1	B	0.93	0/1143	0.97	3/1555 (0.2%)
1	C	1.13	4/1143 (0.3%)	1.08	8/1555 (0.5%)
1	D	0.94	0/1143	0.99	1/1555 (0.1%)
1	E	1.06	3/1143 (0.3%)	0.99	2/1555 (0.1%)
1	F	0.95	1/1143 (0.1%)	0.95	3/1555 (0.2%)
1	G	0.96	3/1143 (0.3%)	0.97	3/1555 (0.2%)
1	H	0.99	2/1143 (0.2%)	1.00	7/1555 (0.5%)
1	I	0.98	1/1143 (0.1%)	0.97	2/1555 (0.1%)
1	J	0.96	0/1143	0.93	1/1555 (0.1%)
1	K	0.96	1/1143 (0.1%)	0.94	1/1555 (0.1%)
1	L	1.03	1/1143 (0.1%)	1.01	5/1555 (0.3%)
All	All	1.00	17/13716 (0.1%)	0.99	43/18660 (0.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	55	GLU	CD-OE2	-8.29	1.16	1.25
1	L	41	GLU	CD-OE2	6.51	1.32	1.25
1	H	55	GLU	CD-OE2	-6.33	1.18	1.25
1	E	34	ARG	CZ-NH2	6.21	1.41	1.33
1	H	55	GLU	CD-OE1	-6.19	1.18	1.25
1	G	55	GLU	CD-OE1	-6.14	1.18	1.25
1	K	22	GLU	CD-OE2	5.96	1.32	1.25
1	C	68	GLU	CD-OE1	5.87	1.32	1.25
1	I	84	SER	CB-OG	-5.72	1.34	1.42
1	C	55	GLU	CD-OE2	5.50	1.31	1.25
1	G	116	SER	CB-OG	5.44	1.49	1.42
1	E	54	TRP	CE3-CZ3	5.29	1.47	1.38
1	C	71	LYS	CD-CE	5.29	1.64	1.51
1	C	4	THR	C-O	5.28	1.33	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	55	GLU	CG-CD	5.28	1.59	1.51
1	A	81	THR	CB-CG2	-5.06	1.35	1.52
1	E	34	ARG	CZ-NH1	5.02	1.39	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	30	ASP	CB-CG-OD1	9.99	127.29	118.30
1	L	30	ASP	CB-CG-OD1	8.92	126.33	118.30
1	E	30	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C	34	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	H	34	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	E	34	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	C	48	ASP	CB-CG-OD1	6.94	124.55	118.30
1	G	55	GLU	OE1-CD-OE2	-6.82	115.11	123.30
1	L	48	ASP	CB-CG-OD1	6.58	124.23	118.30
1	L	30	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	I	84	SER	N-CA-CB	6.37	120.05	110.50
1	H	55	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	H	61	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	G	48	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	113	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	H	48	ASP	CB-CG-OD1	5.75	123.47	118.30
1	H	30	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	D	25	GLY	C-N-CA	-5.64	107.61	121.70
1	H	113	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	J	48	ASP	CB-CG-OD1	5.57	123.31	118.30
1	I	113	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	113	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	106	VAL	CA-CB-CG1	5.55	119.23	110.90
1	F	48	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	106	VAL	N-CA-CB	-5.49	99.42	111.50
1	B	110	GLU	CG-CD-OE1	-5.43	107.43	118.30
1	G	113	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	30	ASP	CB-CG-OD2	5.37	123.13	118.30
1	F	113	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	L	113	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	K	48	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	48	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	113	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	L	113	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	13	LEU	CB-CG-CD1	5.19	119.83	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	C	20	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	48	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	113	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	47	LEU	CA-CB-CG	-5.09	103.59	115.30
1	C	34	ARG	CG-CD-NE	5.06	122.42	111.80
1	A	85	VAL	CB-CA-C	5.05	121.00	111.40
1	F	85	VAL	CB-CA-C	5.01	120.92	111.40

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	1121	0	1133	15	0
1	B	1121	0	1133	13	0
1	C	1121	0	1133	10	0
1	D	1121	0	1133	27	0
1	E	1121	0	1133	22	0
1	F	1121	0	1133	27	0
1	G	1121	0	1133	18	0
1	H	1121	0	1133	20	0
1	I	1121	0	1133	13	0
1	J	1121	0	1133	12	0
1	K	1121	0	1133	12	0
1	L	1121	0	1133	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	85	0	0	0	0
3	B	86	0	0	1	0
3	C	94	0	0	0	0
3	D	70	0	0	0	0
3	E	69	0	0	2	0
3	F	51	0	0	0	0
3	G	55	0	0	1	0
3	H	51	0	0	0	0
3	I	56	0	0	0	0
3	J	56	0	0	0	0
3	K	40	0	0	0	0
3	L	56	0	0	0	0
All	All	14281	0	13596	188	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 7.

All (188) 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:H:79:ALA:HB1	1:L:85:VAL:HG23	1.14	1.13
1:E:20:GLU:HB3	1:E:23:VAL:HG23	1.29	1.13
1:J:64:GLN:O	1:J:67:THR:HG22	1.49	1.11
1:L:21:PRO:O	1:L:25:GLY:HA2	1.51	1.10
1:E:45:ILE:HD11	1:E:146:GLN:NE2	1.67	1.07
1:G:21:PRO:O	1:G:25:GLY:HA2	1.54	1.06
1:E:21:PRO:O	1:E:25:GLY:HA2	1.58	1.02
1:F:19:ARG:HD3	1:G:66:GLN:NE2	1.74	1.01
1:K:21:PRO:O	1:K:25:GLY:CA	2.08	1.01
1:F:21:PRO:O	1:F:25:GLY:HA2	1.60	1.00
1:G:21:PRO:O	1:G:25:GLY:CA	2.10	0.99
1:L:21:PRO:O	1:L:25:GLY:CA	2.09	0.99
1:C:20:GLU:OE1	1:C:23:VAL:HG21	1.63	0.98
1:K:21:PRO:O	1:K:25:GLY:HA2	1.63	0.98
1:H:79:ALA:HB1	1:L:85:VAL:CG2	1.97	0.94
1:E:3:SER:OG	1:E:48:ASP:OD2	1.88	0.90
1:L:20:GLU:HB2	1:L:23:VAL:CG2	2.01	0.89
1:D:25:GLY:O	1:D:26:HIS:CB	2.12	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:GLU:O	1:L:23:VAL:HG23	1.74	0.87
1:F:21:PRO:O	1:F:25:GLY:CA	2.23	0.86
1:D:17:GLY:HA3	1:D:28:THR:HG22	1.60	0.84
1:E:20:GLU:HB3	1:E:23:VAL:CG2	2.08	0.83
1:E:21:PRO:O	1:E:25:GLY:CA	2.27	0.82
1:D:25:GLY:O	1:D:26:HIS:HB2	1.80	0.82
1:E:79:ALA:HB1	1:F:85:VAL:HG22	1.61	0.82
1:F:19:ARG:CD	1:G:66:GLN:NE2	2.44	0.79
1:F:20:GLU:HB3	1:F:23:VAL:HG23	1.63	0.79
1:F:19:ARG:HD3	1:G:66:GLN:HE22	1.47	0.79
1:E:20:GLU:CB	1:E:23:VAL:HG23	2.11	0.78
1:J:21:PRO:O	1:J:25:GLY:HA2	1.84	0.78
1:D:14:ASN:O	1:D:18:LYS:HD2	1.85	0.77
1:C:23:VAL:HG12	1:C:24:TYR:H	1.51	0.76
1:A:23:VAL:HG12	1:A:24:TYR:N	2.01	0.76
1:H:145:ILE:HG22	1:H:145:ILE:O	1.86	0.75
1:A:85:VAL:HG22	1:C:79:ALA:HB1	1.69	0.74
1:D:21:PRO:HB2	1:H:93:GLY:HA2	1.68	0.74
1:D:21:PRO:HD2	1:D:23:VAL:HG12	1.68	0.74
1:D:85:VAL:HG22	1:L:79:ALA:HB1	1.71	0.73
1:F:20:GLU:CB	1:F:23:VAL:HG23	2.18	0.72
1:I:21:PRO:O	1:I:25:GLY:HA2	1.89	0.72
1:E:45:ILE:CD1	1:E:146:GLN:NE2	2.52	0.71
1:D:20:GLU:O	1:D:20:GLU:HG3	1.90	0.70
1:A:23:VAL:HG12	1:A:24:TYR:H	1.55	0.70
1:E:20:GLU:CB	1:E:23:VAL:CG2	2.69	0.70
1:H:34:ARG:HH11	1:H:34:ARG:HG2	1.55	0.70
1:D:19:ARG:O	1:D:20:GLU:HG3	1.91	0.69
1:D:21:PRO:HA	1:H:93:GLY:O	1.93	0.69
1:G:21:PRO:O	1:G:25:GLY:N	2.25	0.69
1:B:20:GLU:HB2	1:B:23:VAL:HG23	1.74	0.69
1:F:19:ARG:CD	1:G:66:GLN:HE21	2.05	0.68
1:C:20:GLU:O	1:C:22:GLU:N	2.27	0.68
1:J:20:GLU:O	1:J:22:GLU:N	2.26	0.68
1:L:21:PRO:O	1:L:25:GLY:N	2.26	0.67
1:F:20:GLU:OE1	1:F:23:VAL:HG21	1.94	0.66
1:C:23:VAL:HG12	1:C:24:TYR:N	2.10	0.66
1:K:21:PRO:O	1:K:25:GLY:N	2.28	0.66
1:D:19:ARG:O	1:D:20:GLU:CG	2.43	0.66
1:A:143:GLU:HG3	1:D:132:LYS:HE3	1.76	0.66
1:H:30:ASP:O	1:H:34:ARG:HG3	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PRO:O	1:A:25:GLY:HA2	1.96	0.66
1:B:13:LEU:HD21	1:B:78:ALA:HB2	1.78	0.65
1:C:21:PRO:O	1:C:25:GLY:HA2	1.97	0.64
1:I:4:THR:HG23	1:I:70:VAL:HG22	1.78	0.64
1:A:11:PRO:HA	1:A:53:ASN:HD22	1.61	0.64
1:F:20:GLU:OE1	1:F:23:VAL:CG2	2.46	0.64
1:B:21:PRO:O	1:B:25:GLY:HA2	1.98	0.64
1:L:4:THR:HG23	1:L:70:VAL:HG22	1.79	0.63
1:D:25:GLY:O	1:D:26:HIS:HB3	1.99	0.62
1:A:23:VAL:CG1	1:A:24:TYR:N	2.61	0.62
1:A:23:VAL:HG13	1:A:24:TYR:CD2	2.34	0.62
1:J:21:PRO:O	1:J:25:GLY:CA	2.47	0.62
1:L:20:GLU:HB2	1:L:23:VAL:HG23	1.79	0.62
1:H:23:VAL:HG12	1:H:24:TYR:CD2	2.35	0.61
1:I:21:PRO:O	1:I:25:GLY:CA	2.48	0.61
1:J:45:ILE:HD12	1:J:142:ILE:HG12	1.81	0.61
1:E:26:HIS:HD2	3:E:339:HOH:O	1.83	0.61
1:H:20:GLU:CB	1:H:23:VAL:HG23	2.31	0.60
1:D:20:GLU:HB2	1:D:23:VAL:HG13	1.84	0.60
1:L:4:THR:HG22	1:L:70:VAL:HA	1.83	0.60
1:I:20:GLU:O	1:I:22:GLU:N	2.35	0.59
1:H:79:ALA:CB	1:L:85:VAL:HG23	2.09	0.59
1:I:4:THR:HG22	1:I:70:VAL:HA	1.83	0.59
1:L:20:GLU:CB	1:L:23:VAL:CG2	2.78	0.59
1:C:23:VAL:CG1	1:C:24:TYR:N	2.65	0.59
1:L:20:GLU:HB2	1:L:23:VAL:HG21	1.84	0.59
1:D:20:GLU:HA	1:D:23:VAL:CG1	2.34	0.58
1:H:20:GLU:HB2	1:H:23:VAL:HG23	1.85	0.58
1:B:41:GLU:HG3	3:B:365:HOH:O	2.04	0.57
1:D:21:PRO:HG2	1:D:22:GLU:H	1.71	0.56
1:D:20:GLU:HA	1:D:23:VAL:HG12	1.88	0.56
1:E:20:GLU:HB2	1:E:23:VAL:HG21	1.87	0.56
1:F:19:ARG:HD3	1:G:66:GLN:HE21	1.60	0.55
1:E:5:ILE:HD11	1:E:145:ILE:CD1	2.37	0.55
1:L:20:GLU:CB	1:L:23:VAL:HG23	2.37	0.55
1:B:5:ILE:HD11	1:B:145:ILE:CD1	2.37	0.54
1:I:20:GLU:HB2	1:I:23:VAL:HG23	1.88	0.54
1:A:12:ASN:H	1:A:53:ASN:ND2	2.05	0.54
1:K:5:ILE:HD11	1:K:145:ILE:CD1	2.39	0.53
1:J:5:ILE:HD11	1:J:145:ILE:CD1	2.38	0.53
1:F:111:ALA:HA	1:F:114:HIS:HD2	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:PRO:HD2	1:D:23:VAL:CG1	2.38	0.53
1:A:20:GLU:O	1:A:22:GLU:N	2.41	0.53
1:E:5:ILE:HD11	1:E:145:ILE:HD12	1.90	0.53
1:B:20:GLU:CB	1:B:23:VAL:HG23	2.39	0.52
1:E:45:ILE:HD11	1:E:146:GLN:CD	2.28	0.52
1:I:77:PRO:HG3	1:I:118:LEU:HD22	1.92	0.52
1:A:143:GLU:HG3	1:D:132:LYS:CE	2.39	0.51
1:D:24:TYR:HD1	1:D:24:TYR:O	1.92	0.51
1:D:21:PRO:HB2	1:H:93:GLY:CA	2.40	0.51
1:H:20:GLU:HB2	1:H:23:VAL:CG2	2.41	0.51
1:B:20:GLU:O	1:B:22:GLU:N	2.44	0.51
1:H:21:PRO:O	1:H:25:GLY:HA2	2.11	0.51
1:F:106:VAL:CG1	1:F:113:ARG:O	2.59	0.50
1:B:20:GLU:HB2	1:B:23:VAL:CG2	2.42	0.50
1:B:5:ILE:HD11	1:B:145:ILE:HD12	1.93	0.50
1:K:5:ILE:HD11	1:K:145:ILE:HD12	1.95	0.49
1:D:77:PRO:HG2	1:D:81:THR:HB	1.93	0.49
1:B:13:LEU:CD2	1:B:78:ALA:HB2	2.41	0.49
1:G:106:VAL:HG12	1:G:113:ARG:O	2.13	0.49
1:L:30:ASP:O	1:L:34:ARG:HG2	2.13	0.49
1:F:20:GLU:CB	1:F:23:VAL:CG2	2.90	0.49
1:I:14:ASN:HD22	1:I:14:ASN:H	1.60	0.49
1:B:14:ASN:HD22	1:B:14:ASN:H	1.61	0.49
1:E:34:ARG:HD3	3:E:338:HOH:O	2.12	0.49
1:G:20:GLU:HB2	1:G:23:VAL:HG23	1.94	0.49
1:G:20:GLU:O	1:G:22:GLU:N	2.46	0.48
1:J:5:ILE:HD11	1:J:145:ILE:HD12	1.94	0.48
1:I:20:GLU:CB	1:I:23:VAL:HG23	2.43	0.48
1:D:20:GLU:HB2	1:D:23:VAL:CG1	2.44	0.48
1:F:20:GLU:HB2	1:F:23:VAL:HG23	1.95	0.48
1:J:20:GLU:O	1:J:21:PRO:C	2.51	0.48
1:G:77:PRO:HG2	1:G:81:THR:HB	1.96	0.47
1:H:20:GLU:HB3	1:H:23:VAL:HG23	1.96	0.47
1:I:23:VAL:HG12	1:I:24:TYR:CD2	2.49	0.47
1:K:21:PRO:O	1:K:25:GLY:C	2.52	0.47
1:F:111:ALA:HA	1:F:114:HIS:CD2	2.49	0.47
1:E:45:ILE:HD11	1:E:146:GLN:HE21	1.69	0.47
1:G:3:SER:HA	1:G:71:LYS:HG2	1.95	0.47
1:K:20:GLU:O	1:K:22:GLU:N	2.47	0.47
1:E:77:PRO:HG3	1:E:118:LEU:HD12	1.96	0.47
1:J:77:PRO:HG2	1:J:81:THR:HB	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:GLU:HB2	1:F:23:VAL:CG2	2.45	0.47
1:H:106:VAL:HG12	1:H:113:ARG:O	2.15	0.47
1:E:14:ASN:HD22	1:E:14:ASN:H	1.61	0.46
1:H:77:PRO:HG2	1:H:81:THR:HB	1.97	0.46
1:I:77:PRO:HG2	1:I:81:THR:HB	1.98	0.46
1:B:22:GLU:OE2	1:B:22:GLU:HA	2.16	0.46
1:F:54:TRP:CH2	1:G:57:ALA:HB2	2.51	0.45
1:K:77:PRO:HG3	1:K:118:LEU:HD12	1.98	0.45
1:G:77:PRO:HG3	1:G:118:LEU:HD12	1.99	0.45
1:K:23:VAL:CG1	1:K:24:TYR:N	2.80	0.45
1:B:77:PRO:HG3	1:B:118:LEU:HD12	1.98	0.45
1:F:21:PRO:O	1:F:25:GLY:N	2.50	0.45
1:F:77:PRO:HG3	1:F:118:LEU:HD12	1.99	0.44
1:G:144:LYS:HE2	3:G:306:HOH:O	2.17	0.44
1:F:19:ARG:CG	1:G:66:GLN:NE2	2.80	0.44
1:F:35:GLN:HE22	1:F:36:LEU:HD23	1.83	0.44
1:L:77:PRO:HG3	1:L:118:LEU:HD12	1.99	0.44
1:H:77:PRO:HG3	1:H:118:LEU:HD12	2.00	0.44
1:I:4:THR:CG2	1:I:70:VAL:HG22	2.46	0.44
1:E:83:THR:CG2	1:F:85:VAL:HG13	2.48	0.44
1:D:77:PRO:HG3	1:D:118:LEU:HD12	1.99	0.43
1:L:77:PRO:HG2	1:L:81:THR:HB	1.99	0.43
1:I:4:THR:CG2	1:I:70:VAL:HA	2.47	0.43
1:K:77:PRO:HG2	1:K:81:THR:HB	2.00	0.43
1:A:23:VAL:CG1	1:A:24:TYR:CD2	3.00	0.43
1:H:21:PRO:O	1:H:25:GLY:CA	2.67	0.43
1:K:23:VAL:HG13	1:K:24:TYR:N	2.33	0.43
1:A:14:ASN:HD22	1:A:14:ASN:H	1.67	0.42
1:L:20:GLU:O	1:L:22:GLU:N	2.52	0.42
1:C:77:PRO:HG3	1:C:118:LEU:HD12	2.00	0.42
1:K:23:VAL:CG1	1:K:24:TYR:H	2.32	0.42
1:A:77:PRO:HG3	1:A:118:LEU:HD12	2.01	0.42
1:D:23:VAL:HG22	1:D:24:TYR:N	2.35	0.42
1:G:14:ASN:H	1:G:14:ASN:HD22	1.67	0.42
1:C:22:GLU:OE2	1:C:22:GLU:HA	2.20	0.42
1:D:106:VAL:HG12	1:D:113:ARG:O	2.19	0.42
1:E:77:PRO:HG2	1:E:81:THR:HB	2.01	0.41
1:J:77:PRO:HG3	1:J:118:LEU:HD12	2.02	0.41
1:A:57:ALA:HB2	1:C:54:TRP:CH2	2.55	0.41
1:F:14:ASN:HD22	1:F:14:ASN:H	1.67	0.41
1:H:14:ASN:H	1:H:14:ASN:HD22	1.69	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:ILE:O	1:J:98:PHE:HA	2.21	0.41
1:D:20:GLU:CA	1:D:23:VAL:HG12	2.50	0.41
1:J:30:ASP:O	1:J:34:ARG:HG2	2.22	0.40
1:F:77:PRO:HG2	1:F:81:THR:HB	2.02	0.40
1:F:20:GLU:O	1:F:22:GLU:N	2.55	0.40
1:E:30:ASP:O	1:E:34:ARG:HG3	2.22	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	143/151 (95%)	138 (96%)	3 (2%)	2 (1%)	11	5
1	B	143/151 (95%)	138 (96%)	3 (2%)	2 (1%)	11	5
1	C	143/151 (95%)	139 (97%)	2 (1%)	2 (1%)	11	5
1	D	143/151 (95%)	136 (95%)	6 (4%)	1 (1%)	22	16
1	E	143/151 (95%)	138 (96%)	4 (3%)	1 (1%)	22	16
1	F	143/151 (95%)	140 (98%)	3 (2%)	0	100	100
1	G	143/151 (95%)	139 (97%)	3 (2%)	1 (1%)	22	16
1	H	143/151 (95%)	136 (95%)	5 (4%)	2 (1%)	11	5
1	I	143/151 (95%)	139 (97%)	3 (2%)	1 (1%)	22	16
1	J	143/151 (95%)	139 (97%)	3 (2%)	1 (1%)	22	16
1	K	143/151 (95%)	140 (98%)	3 (2%)	0	100	100
1	L	143/151 (95%)	139 (97%)	3 (2%)	1 (1%)	22	16
All	All	1716/1812 (95%)	1661 (97%)	41 (2%)	14 (1%)	19	13

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	PRO
1	B	21	PRO
1	C	21	PRO
1	H	146	GLN
1	D	20	GLU
1	E	23	VAL
1	I	21	PRO
1	J	21	PRO
1	A	23	VAL
1	B	23	VAL
1	G	21	PRO
1	C	23	VAL
1	H	23	VAL
1	L	21	PRO

### 5.3.2 Protein sidechains [i](#)

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	119/125 (95%)	112 (94%)	7 (6%)	19	15
1	B	119/125 (95%)	116 (98%)	3 (2%)	47	49
1	C	119/125 (95%)	115 (97%)	4 (3%)	37	36
1	D	119/125 (95%)	115 (97%)	4 (3%)	37	36
1	E	119/125 (95%)	116 (98%)	3 (2%)	47	49
1	F	119/125 (95%)	117 (98%)	2 (2%)	60	65
1	G	119/125 (95%)	116 (98%)	3 (2%)	47	49
1	H	119/125 (95%)	117 (98%)	2 (2%)	60	65
1	I	119/125 (95%)	115 (97%)	4 (3%)	37	36
1	J	119/125 (95%)	118 (99%)	1 (1%)	81	86
1	K	119/125 (95%)	114 (96%)	5 (4%)	30	27
1	L	119/125 (95%)	116 (98%)	3 (2%)	47	49
All	All	1428/1500 (95%)	1387 (97%)	41 (3%)	42	43

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	18	LYS
1	A	22	GLU
1	A	23	VAL
1	A	45	ILE
1	A	51	GLN
1	A	106	VAL
1	B	18	LYS
1	B	22	GLU
1	B	110	GLU
1	C	18	LYS
1	C	22	GLU
1	C	23	VAL
1	C	47	LEU
1	D	19	ARG
1	D	20	GLU
1	D	24	TYR
1	D	26	HIS
1	E	14	ASN
1	E	21	PRO
1	E	48	ASP
1	F	18	LYS
1	F	22	GLU
1	G	4	THR
1	G	18	LYS
1	G	22	GLU
1	H	18	LYS
1	H	146	GLN
1	I	4	THR
1	I	14	ASN
1	I	18	LYS
1	I	22	GLU
1	J	144	LYS
1	K	14	ASN
1	K	19	ARG
1	K	22	GLU
1	K	67	THR
1	K	144	LYS
1	L	4	THR
1	L	18	LYS
1	L	22	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	31	ASN
1	A	51	GLN
1	A	53	ASN
1	A	146	GLN
1	B	14	ASN
1	B	31	ASN
1	C	35	GLN
1	C	39	GLN
1	C	64	GLN
1	D	14	ASN
1	D	35	GLN
1	D	39	GLN
1	D	115	HIS
1	E	14	ASN
1	E	31	ASN
1	E	39	GLN
1	E	146	GLN
1	F	14	ASN
1	F	35	GLN
1	F	39	GLN
1	F	64	GLN
1	F	146	GLN
1	G	14	ASN
1	G	31	ASN
1	G	66	GLN
1	H	14	ASN
1	H	35	GLN
1	H	39	GLN
1	I	14	ASN
1	I	42	GLN
1	J	14	ASN
1	J	31	ASN
1	K	14	ASN
1	K	31	ASN
1	K	114	HIS
1	K	146	GLN
1	L	31	ASN
1	L	35	GLN
1	L	39	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	L	201	-	4,4,4	0.31	0	6,6,6	0.81	0
2	SO4	B	201	-	4,4,4	0.40	0	6,6,6	0.61	0
2	SO4	A	201	-	4,4,4	0.42	0	6,6,6	0.51	0
2	SO4	G	201	-	4,4,4	0.73	0	6,6,6	0.58	0
2	SO4	J	201	-	4,4,4	0.29	0	6,6,6	0.70	0
2	SO4	H	201	-	4,4,4	0.42	0	6,6,6	0.28	0
2	SO4	D	201	-	4,4,4	0.25	0	6,6,6	0.82	0
2	SO4	F	201	-	4,4,4	0.42	0	6,6,6	1.09	0
2	SO4	C	201	-	4,4,4	0.22	0	6,6,6	0.98	0
2	SO4	I	201	-	4,4,4	0.20	0	6,6,6	0.74	0
2	SO4	E	201	-	4,4,4	0.38	0	6,6,6	0.80	0
2	SO4	K	201	-	4,4,4	0.65	0	6,6,6	1.01	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	K	201	SO4	O4-S-O1	-2.04	98.64	109.31

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	145/151 (96%)	-0.30	2 (1%) 75 74	14, 19, 45, 80	0
1	B	145/151 (96%)	-0.28	5 (3%) 45 44	14, 22, 54, 107	0
1	C	145/151 (96%)	0.00	9 (6%) 20 19	14, 19, 77, 126	0
1	D	145/151 (96%)	-0.00	11 (7%) 13 13	15, 21, 84, 108	0
1	E	145/151 (96%)	-0.24	4 (2%) 53 51	15, 20, 44, 100	0
1	F	145/151 (96%)	-0.07	10 (6%) 16 16	16, 22, 63, 106	0
1	G	145/151 (96%)	0.08	8 (5%) 25 24	18, 27, 71, 117	0
1	H	145/151 (96%)	-0.23	4 (2%) 53 51	15, 22, 59, 104	0
1	I	145/151 (96%)	-0.06	7 (4%) 30 29	18, 26, 59, 111	0
1	J	145/151 (96%)	-0.09	8 (5%) 25 24	19, 26, 68, 113	0
1	K	145/151 (96%)	-0.10	10 (6%) 16 16	18, 25, 63, 105	0
1	L	145/151 (96%)	-0.08	8 (5%) 25 24	17, 24, 56, 105	0
All	All	1740/1812 (96%)	-0.11	86 (4%) 29 28	14, 23, 62, 126	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	PRO	14.1
1	D	23	VAL	12.6
1	C	20	GLU	12.6
1	D	24	TYR	11.4
1	J	24	TYR	10.7
1	G	24	TYR	10.4
1	F	24	TYR	9.9
1	C	25	GLY	9.7
1	C	23	VAL	9.4
1	I	24	TYR	9.4
1	D	25	GLY	9.0

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	26	HIS	8.7
1	E	24	TYR	8.7
1	L	24	TYR	8.7
1	B	24	TYR	8.0
1	H	24	TYR	8.0
1	I	3	SER	7.7
1	A	24	TYR	7.0
1	L	3	SER	6.7
1	H	147	PRO	6.7
1	B	147	PRO	6.6
1	C	24	TYR	6.5
1	G	23	VAL	6.3
1	L	23	VAL	6.3
1	K	24	TYR	6.1
1	E	23	VAL	5.9
1	B	23	VAL	5.8
1	J	3	SER	5.7
1	K	23	VAL	5.6
1	C	22	GLU	5.6
1	D	19	ARG	5.3
1	F	23	VAL	5.1
1	G	3	SER	5.1
1	F	26	HIS	4.8
1	D	26	HIS	4.7
1	D	22	GLU	4.6
1	L	22	GLU	4.4
1	D	17	GLY	4.3
1	G	26	HIS	4.3
1	B	22	GLU	4.1
1	D	18	LYS	4.0
1	F	22	GLU	3.9
1	F	21	PRO	3.8
1	H	22	GLU	3.7
1	G	22	GLU	3.6
1	H	23	VAL	3.5
1	G	20	GLU	3.4
1	K	20	GLU	3.4
1	J	23	VAL	3.4
1	E	22	GLU	3.3
1	G	25	GLY	3.2
1	A	23	VAL	3.2
1	E	3	SER	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	J	22	GLU	3.1
1	K	3	SER	3.0
1	L	20	GLU	2.9
1	J	46	THR	2.9
1	F	41	GLU	2.9
1	I	20	GLU	2.8
1	I	22	GLU	2.7
1	F	25	GLY	2.7
1	I	23	VAL	2.7
1	J	20	GLU	2.7
1	D	21	PRO	2.6
1	G	21	PRO	2.6
1	K	42	GLN	2.6
1	C	19	ARG	2.6
1	F	3	SER	2.5
1	K	22	GLU	2.5
1	I	147	PRO	2.4
1	D	27	LEU	2.3
1	B	26	HIS	2.3
1	F	42	GLN	2.3
1	J	25	GLY	2.3
1	L	147	PRO	2.2
1	C	27	LEU	2.2
1	K	41	GLU	2.2
1	K	26	HIS	2.1
1	D	20	GLU	2.1
1	J	44	SER	2.1
1	K	44	SER	2.1
1	F	19	ARG	2.1
1	K	21	PRO	2.1
1	L	21	PRO	2.1
1	L	25	GLY	2.0
1	I	44	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	K	201	5/5	0.98	0.08	22,29,31,33	0
2	SO4	B	201	5/5	0.99	0.06	21,26,33,34	0
2	SO4	C	201	5/5	0.99	0.10	24,27,30,36	0
2	SO4	D	201	5/5	0.99	0.09	19,21,25,29	0
2	SO4	E	201	5/5	0.99	0.09	26,26,34,36	0
2	SO4	F	201	5/5	0.99	0.07	22,26,34,36	0
2	SO4	G	201	5/5	0.99	0.09	28,28,35,40	0
2	SO4	H	201	5/5	0.99	0.09	21,25,28,28	0
2	SO4	I	201	5/5	0.99	0.09	27,28,36,38	0
2	SO4	J	201	5/5	0.99	0.07	27,27,35,38	0
2	SO4	A	201	5/5	0.99	0.11	19,23,30,32	0
2	SO4	L	201	5/5	0.99	0.08	25,27,34,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.