



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2022 – 10:16 AM EDT

PDB ID : 8DOP  
Title : Crystal structure of 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase from *Klebsiella aerogenes* (P1 Form)  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2022-07-14  
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>.

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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  
Xtrriage (Phenix) : 1.13  
EDS : 2.29  
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) : 2.29

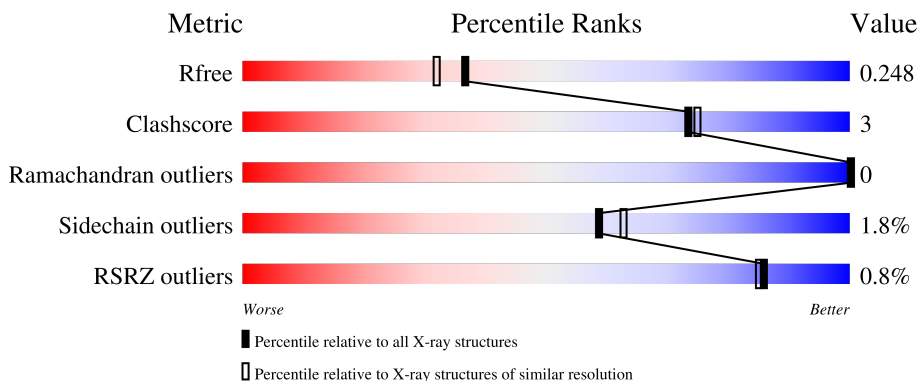
# 1 Overall quality at a glance i

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	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	

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Mol	Chain	Length	Quality of chain
1	F	253	 83% 6% 10%
1	G	253	 84% 5% 11%
1	H	253	 % 78% 9% 13%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	E	302	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13210 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 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1595	1010	276	298	11	0	0	0
1	B	214	1568	994	275	289	10	0	0	0
1	C	215	1569	996	271	292	10	0	0	0
1	D	215	1595	1009	276	299	11	0	0	0
1	E	221	1588	1007	275	296	10	0	0	0
1	F	227	1676	1058	296	311	11	0	0	0
1	G	224	1632	1034	281	306	11	0	0	0
1	H	221	1579	1006	274	288	11	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A0M3H420
A	-17	ALA	-	expression tag	UNP A0A0M3H420
A	-16	HIS	-	expression tag	UNP A0A0M3H420
A	-15	HIS	-	expression tag	UNP A0A0M3H420
A	-14	HIS	-	expression tag	UNP A0A0M3H420
A	-13	HIS	-	expression tag	UNP A0A0M3H420
A	-12	HIS	-	expression tag	UNP A0A0M3H420
A	-11	HIS	-	expression tag	UNP A0A0M3H420
A	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
A	133	MET	THR	engineered mutation	UNP A0A0M3H420
A	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
A	220	VAL	ALA	engineered mutation	UNP A0A0M3H420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	231	ASN	-	expression tag	UNP A0A0M3H420
A	232	LYS	-	expression tag	UNP A0A0M3H420
A	233	GLY	-	expression tag	UNP A0A0M3H420
A	234	VAL	-	expression tag	UNP A0A0M3H420
B	-18	MET	-	initiating methionine	UNP A0A0M3H420
B	-17	ALA	-	expression tag	UNP A0A0M3H420
B	-16	HIS	-	expression tag	UNP A0A0M3H420
B	-15	HIS	-	expression tag	UNP A0A0M3H420
B	-14	HIS	-	expression tag	UNP A0A0M3H420
B	-13	HIS	-	expression tag	UNP A0A0M3H420
B	-12	HIS	-	expression tag	UNP A0A0M3H420
B	-11	HIS	-	expression tag	UNP A0A0M3H420
B	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
B	133	MET	THR	engineered mutation	UNP A0A0M3H420
B	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
B	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
B	231	ASN	-	expression tag	UNP A0A0M3H420
B	232	LYS	-	expression tag	UNP A0A0M3H420
B	233	GLY	-	expression tag	UNP A0A0M3H420
B	234	VAL	-	expression tag	UNP A0A0M3H420
C	-18	MET	-	initiating methionine	UNP A0A0M3H420
C	-17	ALA	-	expression tag	UNP A0A0M3H420
C	-16	HIS	-	expression tag	UNP A0A0M3H420
C	-15	HIS	-	expression tag	UNP A0A0M3H420
C	-14	HIS	-	expression tag	UNP A0A0M3H420
C	-13	HIS	-	expression tag	UNP A0A0M3H420
C	-12	HIS	-	expression tag	UNP A0A0M3H420
C	-11	HIS	-	expression tag	UNP A0A0M3H420
C	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
C	133	MET	THR	engineered mutation	UNP A0A0M3H420
C	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
C	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
C	231	ASN	-	expression tag	UNP A0A0M3H420
C	232	LYS	-	expression tag	UNP A0A0M3H420
C	233	GLY	-	expression tag	UNP A0A0M3H420
C	234	VAL	-	expression tag	UNP A0A0M3H420
D	-18	MET	-	initiating methionine	UNP A0A0M3H420
D	-17	ALA	-	expression tag	UNP A0A0M3H420
D	-16	HIS	-	expression tag	UNP A0A0M3H420
D	-15	HIS	-	expression tag	UNP A0A0M3H420
D	-14	HIS	-	expression tag	UNP A0A0M3H420
D	-13	HIS	-	expression tag	UNP A0A0M3H420

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP A0A0M3H420
D	-11	HIS	-	expression tag	UNP A0A0M3H420
D	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
D	133	MET	THR	engineered mutation	UNP A0A0M3H420
D	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
D	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
D	231	ASN	-	expression tag	UNP A0A0M3H420
D	232	LYS	-	expression tag	UNP A0A0M3H420
D	233	GLY	-	expression tag	UNP A0A0M3H420
D	234	VAL	-	expression tag	UNP A0A0M3H420
E	-18	MET	-	initiating methionine	UNP A0A0M3H420
E	-17	ALA	-	expression tag	UNP A0A0M3H420
E	-16	HIS	-	expression tag	UNP A0A0M3H420
E	-15	HIS	-	expression tag	UNP A0A0M3H420
E	-14	HIS	-	expression tag	UNP A0A0M3H420
E	-13	HIS	-	expression tag	UNP A0A0M3H420
E	-12	HIS	-	expression tag	UNP A0A0M3H420
E	-11	HIS	-	expression tag	UNP A0A0M3H420
E	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
E	133	MET	THR	engineered mutation	UNP A0A0M3H420
E	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
E	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
E	231	ASN	-	expression tag	UNP A0A0M3H420
E	232	LYS	-	expression tag	UNP A0A0M3H420
E	233	GLY	-	expression tag	UNP A0A0M3H420
E	234	VAL	-	expression tag	UNP A0A0M3H420
F	-18	MET	-	initiating methionine	UNP A0A0M3H420
F	-17	ALA	-	expression tag	UNP A0A0M3H420
F	-16	HIS	-	expression tag	UNP A0A0M3H420
F	-15	HIS	-	expression tag	UNP A0A0M3H420
F	-14	HIS	-	expression tag	UNP A0A0M3H420
F	-13	HIS	-	expression tag	UNP A0A0M3H420
F	-12	HIS	-	expression tag	UNP A0A0M3H420
F	-11	HIS	-	expression tag	UNP A0A0M3H420
F	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
F	133	MET	THR	engineered mutation	UNP A0A0M3H420
F	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
F	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
F	231	ASN	-	expression tag	UNP A0A0M3H420
F	232	LYS	-	expression tag	UNP A0A0M3H420
F	233	GLY	-	expression tag	UNP A0A0M3H420
F	234	VAL	-	expression tag	UNP A0A0M3H420

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	MET	-	initiating methionine	UNP A0A0M3H420
G	-17	ALA	-	expression tag	UNP A0A0M3H420
G	-16	HIS	-	expression tag	UNP A0A0M3H420
G	-15	HIS	-	expression tag	UNP A0A0M3H420
G	-14	HIS	-	expression tag	UNP A0A0M3H420
G	-13	HIS	-	expression tag	UNP A0A0M3H420
G	-12	HIS	-	expression tag	UNP A0A0M3H420
G	-11	HIS	-	expression tag	UNP A0A0M3H420
G	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
G	133	MET	THR	engineered mutation	UNP A0A0M3H420
G	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
G	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
G	231	ASN	-	expression tag	UNP A0A0M3H420
G	232	LYS	-	expression tag	UNP A0A0M3H420
G	233	GLY	-	expression tag	UNP A0A0M3H420
G	234	VAL	-	expression tag	UNP A0A0M3H420
H	-18	MET	-	initiating methionine	UNP A0A0M3H420
H	-17	ALA	-	expression tag	UNP A0A0M3H420
H	-16	HIS	-	expression tag	UNP A0A0M3H420
H	-15	HIS	-	expression tag	UNP A0A0M3H420
H	-14	HIS	-	expression tag	UNP A0A0M3H420
H	-13	HIS	-	expression tag	UNP A0A0M3H420
H	-12	HIS	-	expression tag	UNP A0A0M3H420
H	-11	HIS	-	expression tag	UNP A0A0M3H420
H	23	GLU	ASP	engineered mutation	UNP A0A0M3H420
H	133	MET	THR	engineered mutation	UNP A0A0M3H420
H	163	VAL	ALA	engineered mutation	UNP A0A0M3H420
H	220	VAL	ALA	engineered mutation	UNP A0A0M3H420
H	231	ASN	-	expression tag	UNP A0A0M3H420
H	232	LYS	-	expression tag	UNP A0A0M3H420
H	233	GLY	-	expression tag	UNP A0A0M3H420
H	234	VAL	-	expression tag	UNP A0A0M3H420

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total I 2 2	0	0
2	B	1	Total I 1 1	0	0
2	C	2	Total I 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total I 1 1	0	0
2	E	2	Total I 2 2	0	0
2	F	1	Total I 1 1	0	0
2	G	1	Total I 1 1	0	0
2	H	2	Total I 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	36	Total O 36 36	0	0
4	C	51	Total O 51 51	0	0
4	D	72	Total O 72 72	0	0
4	E	30	Total O 30 30	0	0
4	F	58	Total O 58 58	0	0

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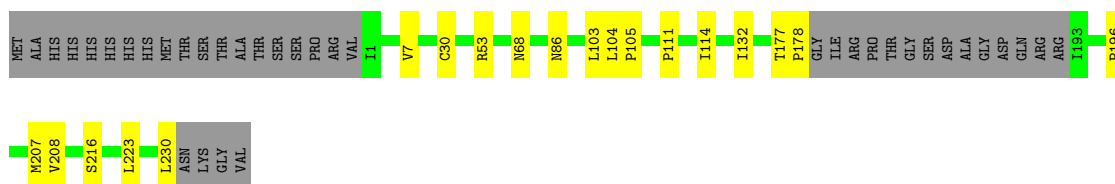
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	G	56	Total	O	0	0
			56	56		
4	H	22	Total	O	0	0
			22	22		

### 3 Residue-property plots


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: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase

Chain A: 



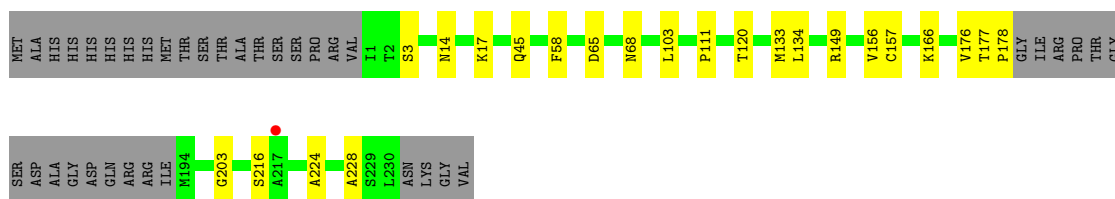
- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase

Chain B: 




- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase

Chain C: 



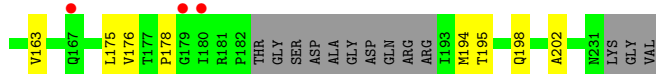
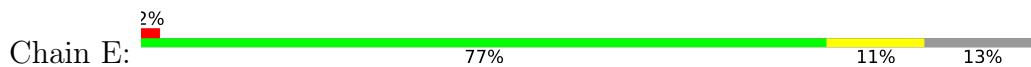
- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase

Chain D: 

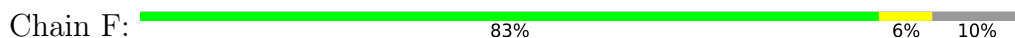




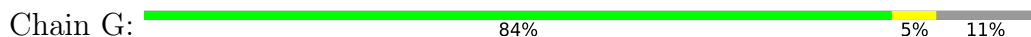
- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase



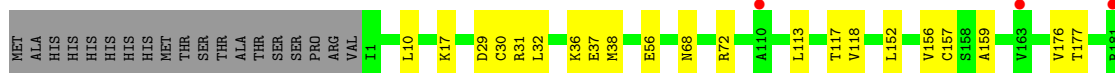
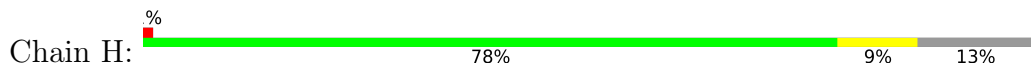
- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase



- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase



- Molecule 1: 2,3-diketo-5-methylthiopentyl-1-phosphate enolase-phosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.02Å 71.16Å 93.18Å 108.39° 102.23° 89.99°	Depositor
Resolution (Å)	49.41 – 2.00 49.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.41-2.00) 97.6 (49.41-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.188 , 0.246 0.194 , 0.248	Depositor DCC
$R_{free}$ test set	5279 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtrriage
Anisotropy	0.518	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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: NA, IOD

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	0.43	0/1621	0.63	0/2203
1	B	0.42	0/1594	0.60	0/2168
1	C	0.41	0/1595	0.61	0/2171
1	D	0.43	0/1621	0.62	0/2203
1	E	0.41	0/1615	0.59	0/2203
1	F	0.41	0/1703	0.62	0/2315
1	G	0.41	0/1659	0.59	0/2257
1	H	0.36	0/1606	0.58	0/2190
All	All	0.41	0/13014	0.60	0/17710

There are no bond length outliers.

There are no bond angle outliers.

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	1595	0	1597	11	0
1	B	1568	0	1563	11	0
1	C	1569	0	1563	12	0
1	D	1595	0	1599	9	0
1	E	1588	0	1555	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1676	0	1684	8	0
1	G	1632	0	1628	6	0
1	H	1579	0	1560	15	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	2	0
2	F	1	0	0	0	0
2	G	1	0	0	1	0
2	H	2	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
4	A	65	0	0	1	0
4	B	36	0	0	1	0
4	C	51	0	0	2	0
4	D	72	0	0	2	0
4	E	30	0	0	1	0
4	F	58	0	0	2	0
4	G	56	0	0	1	0
4	H	22	0	0	3	0
All	All	13210	0	12749	85	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 3.

All (85) 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)
2:H:302:IOD:I	4:H:422:HOH:O	2.78	0.71
1:B:18:ALA:O	1:B:22:VAL:HG23	1.92	0.68
1:E:16:ASP:OD1	1:G:53:ARG:NH2	2.31	0.64
2:E:302:IOD:I	4:E:424:HOH:O	2.85	0.64
1:H:177:THR:HG21	1:H:204:VAL:HG22	1.81	0.62
1:D:207:MET:HE1	1:D:230:LEU:HD11	1.82	0.62
1:A:177:THR:HG23	4:A:401:HOH:O	1.98	0.62
1:E:74:VAL:HG12	1:E:103:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HD11	1:B:132:ILE:HD11	1.82	0.61
1:H:36:LYS:NZ	4:H:401:HOH:O	2.32	0.60
1:C:149:ARG:NH2	4:C:404:HOH:O	2.37	0.56
1:G:106:PHE:HB2	1:G:110:ALA:HB2	1.86	0.56
1:H:159:ALA:HB1	1:H:194:MET:SD	2.45	0.56
1:E:49:ASP:O	1:E:53:ARG:NH1	2.36	0.55
1:D:177:THR:HG22	1:D:207:MET:HA	1.89	0.55
1:D:120:THR:HG21	1:D:178:PRO:HG2	1.87	0.54
1:A:196:PRO:HB3	1:A:207:MET:HE1	1.89	0.54
1:D:196:PRO:HB3	1:D:207:MET:HE1	1.90	0.54
1:B:120:THR:HG21	1:B:178:PRO:HG2	1.89	0.54
1:H:31:ARG:NE	1:H:56:GLU:OE1	2.30	0.53
1:E:93:ALA:HB2	1:E:146:LEU:HD11	1.91	0.53
1:E:163:VAL:HG22	1:E:202:ALA:HB1	1.90	0.53
1:E:14:ASN:OD1	1:E:17:LYS:N	2.32	0.53
1:F:106:PHE:HB2	1:F:110:ALA:HB2	1.90	0.53
1:G:33:LYS:HE2	2:G:301:IOD:I	2.79	0.53
1:E:178:PRO:HB3	2:E:302:IOD:I	2.79	0.52
1:A:178:PRO:HA	1:A:208:VAL:HB	1.91	0.52
1:G:159:ALA:HB1	1:G:194:MET:SD	2.50	0.52
1:C:157:CYS:O	1:C:177:THR:HG22	2.10	0.51
1:C:17:LYS:NZ	4:C:401:HOH:O	2.26	0.50
1:B:177:THR:HG23	4:B:402:HOH:O	2.11	0.50
1:H:177:THR:HG21	1:H:204:VAL:CG2	2.42	0.50
1:C:120:THR:HG21	1:C:178:PRO:HG2	1.94	0.49
1:B:178:PRO:HA	1:B:208:VAL:HB	1.93	0.49
1:G:149:ARG:NH2	4:G:403:HOH:O	2.46	0.49
1:H:29:ASP:CB	1:H:223:LEU:HD23	2.43	0.49
1:D:163:VAL:HG13	4:D:405:HOH:O	2.13	0.48
1:C:65:ASP:HB2	1:D:36:LYS:HE3	1.96	0.48
1:B:31:ARG:NE	1:B:56:GLU:OE1	2.41	0.48
1:E:75:ALA:O	1:E:79:GLU:HG3	2.14	0.48
1:E:157:CYS:SG	1:E:175:LEU:HD13	2.54	0.47
1:F:166:LYS:HD2	1:F:171:GLN:HA	1.97	0.47
1:D:86:ASN:HA	1:D:114:ILE:O	2.15	0.47
1:H:117:THR:OG1	1:H:118:VAL:N	2.47	0.47
1:E:195:THR:OG1	1:E:198:GLN:HG3	2.16	0.46
1:A:103:LEU:HD22	1:A:111:PRO:HD2	1.98	0.46
1:F:37:GLU:O	1:F:41:LEU:HD13	2.16	0.46
1:E:156:VAL:HA	1:E:176:VAL:O	2.16	0.45
1:B:177:THR:HG22	1:B:207:MET:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:NH2	1:C:45:GLN:HG3	2.31	0.45
1:B:7:VAL:O	1:B:208:VAL:HA	2.15	0.45
1:F:28:ARG:NH2	4:F:401:HOH:O	2.32	0.45
1:D:177:THR:HG23	4:D:408:HOH:O	2.16	0.45
1:B:31:ARG:NH2	1:B:56:GLU:OE1	2.48	0.45
1:C:166:LYS:HE3	1:C:203:GLY:O	2.18	0.44
1:E:79:GLU:HG2	1:E:106:PHE:CE1	2.51	0.44
1:A:30:CYS:SG	1:A:223:LEU:HD11	2.56	0.44
1:H:68:ASN:O	1:H:72:ARG:HG2	2.18	0.44
1:F:161:GLU:CG	4:F:412:HOH:O	2.66	0.44
1:E:117:THR:OG1	1:E:118:VAL:N	2.50	0.44
1:F:103:LEU:HD22	1:F:111:PRO:HD2	2.00	0.44
1:F:159:ALA:HB1	1:F:194:MET:SD	2.58	0.44
1:A:104:LEU:N	1:A:105:PRO:CD	2.81	0.44
1:H:156:VAL:HA	1:H:176:VAL:O	2.18	0.43
1:H:17:LYS:NZ	4:H:402:HOH:O	2.51	0.43
1:H:113:LEU:HD23	1:H:152:LEU:HG	2.01	0.43
1:G:86:ASN:HA	1:G:114:ILE:O	2.18	0.43
1:C:133:MET:C	1:C:134:LEU:HD12	2.39	0.42
1:A:207:MET:HE1	1:A:230:LEU:HD11	2.01	0.42
1:C:120:THR:HG21	1:C:178:PRO:CG	2.49	0.42
1:C:103:LEU:HD22	1:C:111:PRO:HD2	2.00	0.42
1:H:30:CYS:SG	1:H:223:LEU:HD21	2.60	0.42
1:H:157:CYS:O	1:H:177:THR:HG22	2.20	0.42
1:A:86:ASN:HA	1:A:114:ILE:O	2.19	0.42
1:H:29:ASP:HB2	1:H:223:LEU:HD23	2.02	0.42
1:E:79:GLU:HG2	1:E:106:PHE:CZ	2.55	0.42
1:D:156:VAL:HA	1:D:176:VAL:O	2.19	0.41
1:F:48:ARG:O	1:F:52:GLN:HG2	2.19	0.41
1:H:10:LEU:HD21	1:H:32:LEU:HD22	2.02	0.41
1:B:154:GLY:HA3	1:B:174:LYS:O	2.21	0.41
1:A:7:VAL:O	1:A:208:VAL:HA	2.21	0.41
1:B:166:LYS:HE2	1:B:175:LEU:HG	2.01	0.41
1:C:156:VAL:HA	1:C:176:VAL:O	2.21	0.41
1:C:224:ALA:O	1:C:228:ALA:N	2.52	0.40
1:E:113:LEU:HD23	1:E:152:LEU:HG	2.04	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	212/253 (84%)	208 (98%)	4 (2%)	0	100	100
1	B	210/253 (83%)	201 (96%)	9 (4%)	0	100	100
1	C	211/253 (83%)	207 (98%)	4 (2%)	0	100	100
1	D	211/253 (83%)	207 (98%)	4 (2%)	0	100	100
1	E	217/253 (86%)	213 (98%)	4 (2%)	0	100	100
1	F	223/253 (88%)	217 (97%)	6 (3%)	0	100	100
1	G	220/253 (87%)	215 (98%)	5 (2%)	0	100	100
1	H	217/253 (86%)	210 (97%)	7 (3%)	0	100	100
All	All	1721/2024 (85%)	1678 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	164/203 (81%)	162 (99%)	2 (1%)	71	76
1	B	158/203 (78%)	154 (98%)	4 (2%)	47	49
1	C	159/203 (78%)	154 (97%)	5 (3%)	40	40
1	D	166/203 (82%)	163 (98%)	3 (2%)	59	63
1	E	157/203 (77%)	155 (99%)	2 (1%)	69	74
1	F	173/203 (85%)	170 (98%)	3 (2%)	60	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	167/203 (82%)	164 (98%)	3 (2%)	59	63
1	H	155/203 (76%)	153 (99%)	2 (1%)	69	74
All	All	1299/1624 (80%)	1275 (98%)	24 (2%)	59	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	216	SER
1	B	14	ASN
1	B	58	PHE
1	B	135	SER
1	B	194	MET
1	C	3	SER
1	C	14	ASN
1	C	58	PHE
1	C	68	ASN
1	C	216	SER
1	D	52	GLN
1	D	58	PHE
1	D	216	SER
1	E	36	LYS
1	E	194	MET
1	F	37	GLU
1	F	167	GLN
1	F	186	ASP
1	G	26	ASP
1	G	58	PHE
1	G	172	GLU
1	H	37	GLU
1	H	38	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	51	HIS

### 5.3.3 RNA

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](#)

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

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	216/253 (85%)	-0.35	0 <b>100</b> <b>100</b>	23, 34, 50, 73	0
1	B	214/253 (84%)	-0.15	2 (0%) <b>84</b> <b>83</b>	25, 44, 68, 77	0
1	C	215/253 (84%)	-0.30	1 (0%) <b>91</b> <b>90</b>	26, 40, 63, 69	0
1	D	215/253 (84%)	-0.39	0 <b>100</b> <b>100</b>	24, 34, 52, 69	0
1	E	221/253 (87%)	-0.21	6 (2%) <b>54</b> <b>53</b>	25, 42, 66, 78	0
1	F	227/253 (89%)	-0.34	1 (0%) <b>92</b> <b>92</b>	24, 38, 57, 73	0
1	G	224/253 (88%)	-0.43	1 (0%) <b>92</b> <b>92</b>	26, 37, 53, 62	0
1	H	221/253 (87%)	-0.08	3 (1%) <b>75</b> <b>74</b>	29, 48, 69, 80	0
All	All	1753/2024 (86%)	-0.28	14 (0%) <b>86</b> <b>85</b>	23, 40, 64, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	163	VAL	3.5
1	E	159	ALA	3.0
1	E	133	MET	3.0
1	E	180	ILE	2.6
1	G	193	ILE	2.6
1	B	197	GLU	2.5
1	E	179	GLY	2.5
1	F	186	ASP	2.4
1	H	181	ARG	2.2
1	E	167	GLN	2.2
1	B	217	ALA	2.2
1	E	109	GLU	2.2
1	C	217	ALA	2.1
1	H	110	ALA	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(Å <sup>2</sup> )	Q<0.9
2	IOD	C	302	1/1	0.56	0.11	118,118,118,118	1
2	IOD	A	302	1/1	0.87	0.09	86,86,86,86	1
2	IOD	E	301	1/1	0.88	0.06	71,71,71,71	0
2	IOD	D	301	1/1	0.91	0.08	81,81,81,81	1
3	NA	H	303	1/1	0.91	0.17	51,51,51,51	0
2	IOD	H	301	1/1	0.93	0.07	84,84,84,84	0
2	IOD	H	302	1/1	0.93	0.08	62,62,62,62	1
2	IOD	B	301	1/1	0.93	0.05	69,69,69,69	1
3	NA	B	302	1/1	0.94	0.35	47,47,47,47	0
2	IOD	C	301	1/1	0.94	0.11	69,69,69,69	0
3	NA	D	302	1/1	0.95	0.27	42,42,42,42	0
3	NA	E	303	1/1	0.95	0.18	47,47,47,47	0
2	IOD	A	301	1/1	0.95	0.09	62,62,62,62	0
2	IOD	E	302	1/1	0.96	0.09	48,48,48,48	1
3	NA	C	303	1/1	0.97	0.14	39,39,39,39	0
3	NA	A	303	1/1	0.97	0.21	38,38,38,38	0
2	IOD	F	301	1/1	0.98	0.11	35,35,35,35	1
2	IOD	G	301	1/1	0.99	0.13	32,32,32,32	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.