



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 09:19 AM EDT

PDB ID : 2I6E  
Title : Crystal structure of protein DR0370 from *Deinococcus radiodurans*, Pfam DUF178  
Authors : Tyagi, R.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2006-08-28  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

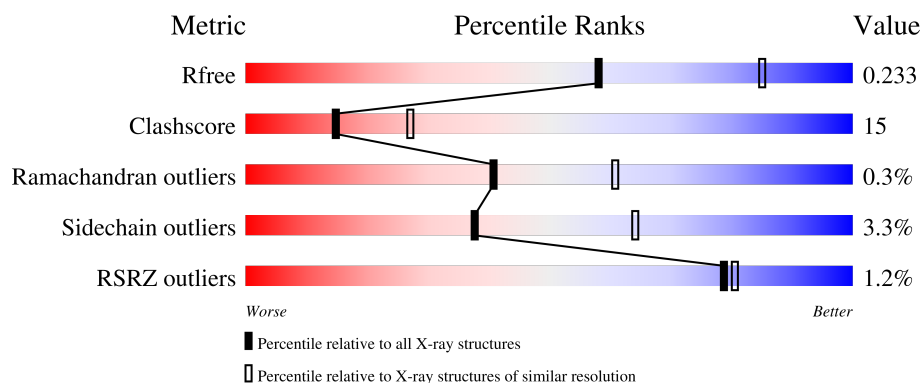
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	301	
1	B	301	
1	C	301	
1	D	301	
1	E	301	

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Mol	Chain	Length	Quality of chain
1	F	301	
1	G	301	
1	H	301	

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	SO4	B	717	-	-	X	-
2	SO4	F	718	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17623 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 Hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	B	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	C	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	D	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	E	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	F	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	G	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			
1	H	272	Total	C	N	O	S	Se	0	0	0
			2110	1351	373	381	1	4			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9RXE3
A	2	SER	-	expression tag	UNP Q9RXE3
A	3	LEU	-	expression tag	UNP Q9RXE3
A	50	MSE	MET	modified residue	UNP Q9RXE3
A	115	MSE	MET	modified residue	UNP Q9RXE3
A	175	MSE	MET	modified residue	UNP Q9RXE3
A	223	MSE	MET	modified residue	UNP Q9RXE3
A	294	GLU	-	expression tag	UNP Q9RXE3
A	295	GLY	-	expression tag	UNP Q9RXE3
A	296	HIS	-	expression tag	UNP Q9RXE3
A	297	HIS	-	expression tag	UNP Q9RXE3
A	298	HIS	-	expression tag	UNP Q9RXE3
A	299	HIS	-	expression tag	UNP Q9RXE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	300	HIS	-	expression tag	UNP Q9RXE3
A	301	HIS	-	expression tag	UNP Q9RXE3
B	1	MSE	-	expression tag	UNP Q9RXE3
B	2	SER	-	expression tag	UNP Q9RXE3
B	3	LEU	-	expression tag	UNP Q9RXE3
B	50	MSE	MET	modified residue	UNP Q9RXE3
B	115	MSE	MET	modified residue	UNP Q9RXE3
B	175	MSE	MET	modified residue	UNP Q9RXE3
B	223	MSE	MET	modified residue	UNP Q9RXE3
B	294	GLU	-	expression tag	UNP Q9RXE3
B	295	GLY	-	expression tag	UNP Q9RXE3
B	296	HIS	-	expression tag	UNP Q9RXE3
B	297	HIS	-	expression tag	UNP Q9RXE3
B	298	HIS	-	expression tag	UNP Q9RXE3
B	299	HIS	-	expression tag	UNP Q9RXE3
B	300	HIS	-	expression tag	UNP Q9RXE3
B	301	HIS	-	expression tag	UNP Q9RXE3
C	1	MSE	-	expression tag	UNP Q9RXE3
C	2	SER	-	expression tag	UNP Q9RXE3
C	3	LEU	-	expression tag	UNP Q9RXE3
C	50	MSE	MET	modified residue	UNP Q9RXE3
C	115	MSE	MET	modified residue	UNP Q9RXE3
C	175	MSE	MET	modified residue	UNP Q9RXE3
C	223	MSE	MET	modified residue	UNP Q9RXE3
C	294	GLU	-	expression tag	UNP Q9RXE3
C	295	GLY	-	expression tag	UNP Q9RXE3
C	296	HIS	-	expression tag	UNP Q9RXE3
C	297	HIS	-	expression tag	UNP Q9RXE3
C	298	HIS	-	expression tag	UNP Q9RXE3
C	299	HIS	-	expression tag	UNP Q9RXE3
C	300	HIS	-	expression tag	UNP Q9RXE3
C	301	HIS	-	expression tag	UNP Q9RXE3
D	1	MSE	-	expression tag	UNP Q9RXE3
D	2	SER	-	expression tag	UNP Q9RXE3
D	3	LEU	-	expression tag	UNP Q9RXE3
D	50	MSE	MET	modified residue	UNP Q9RXE3
D	115	MSE	MET	modified residue	UNP Q9RXE3
D	175	MSE	MET	modified residue	UNP Q9RXE3
D	223	MSE	MET	modified residue	UNP Q9RXE3
D	294	GLU	-	expression tag	UNP Q9RXE3
D	295	GLY	-	expression tag	UNP Q9RXE3
D	296	HIS	-	expression tag	UNP Q9RXE3

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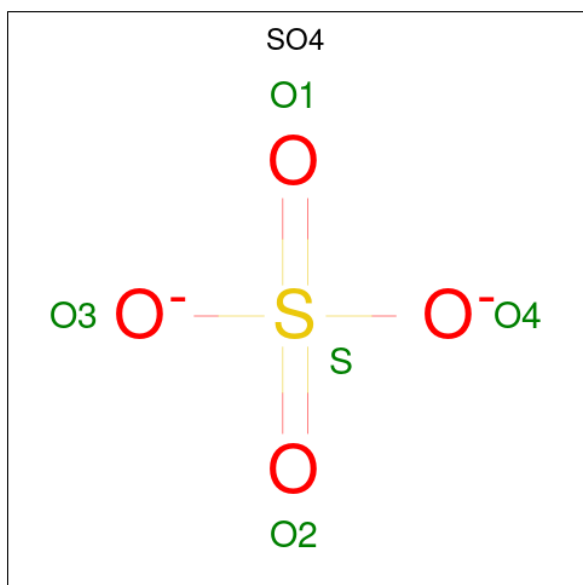
Chain	Residue	Modelled	Actual	Comment	Reference
D	297	HIS	-	expression tag	UNP Q9RXE3
D	298	HIS	-	expression tag	UNP Q9RXE3
D	299	HIS	-	expression tag	UNP Q9RXE3
D	300	HIS	-	expression tag	UNP Q9RXE3
D	301	HIS	-	expression tag	UNP Q9RXE3
E	1	MSE	-	expression tag	UNP Q9RXE3
E	2	SER	-	expression tag	UNP Q9RXE3
E	3	LEU	-	expression tag	UNP Q9RXE3
E	50	MSE	MET	modified residue	UNP Q9RXE3
E	115	MSE	MET	modified residue	UNP Q9RXE3
E	175	MSE	MET	modified residue	UNP Q9RXE3
E	223	MSE	MET	modified residue	UNP Q9RXE3
E	294	GLU	-	expression tag	UNP Q9RXE3
E	295	GLY	-	expression tag	UNP Q9RXE3
E	296	HIS	-	expression tag	UNP Q9RXE3
E	297	HIS	-	expression tag	UNP Q9RXE3
E	298	HIS	-	expression tag	UNP Q9RXE3
E	299	HIS	-	expression tag	UNP Q9RXE3
E	300	HIS	-	expression tag	UNP Q9RXE3
E	301	HIS	-	expression tag	UNP Q9RXE3
F	1	MSE	-	expression tag	UNP Q9RXE3
F	2	SER	-	expression tag	UNP Q9RXE3
F	3	LEU	-	expression tag	UNP Q9RXE3
F	50	MSE	MET	modified residue	UNP Q9RXE3
F	115	MSE	MET	modified residue	UNP Q9RXE3
F	175	MSE	MET	modified residue	UNP Q9RXE3
F	223	MSE	MET	modified residue	UNP Q9RXE3
F	294	GLU	-	expression tag	UNP Q9RXE3
F	295	GLY	-	expression tag	UNP Q9RXE3
F	296	HIS	-	expression tag	UNP Q9RXE3
F	297	HIS	-	expression tag	UNP Q9RXE3
F	298	HIS	-	expression tag	UNP Q9RXE3
F	299	HIS	-	expression tag	UNP Q9RXE3
F	300	HIS	-	expression tag	UNP Q9RXE3
F	301	HIS	-	expression tag	UNP Q9RXE3
G	1	MSE	-	expression tag	UNP Q9RXE3
G	2	SER	-	expression tag	UNP Q9RXE3
G	3	LEU	-	expression tag	UNP Q9RXE3
G	50	MSE	MET	modified residue	UNP Q9RXE3
G	115	MSE	MET	modified residue	UNP Q9RXE3
G	175	MSE	MET	modified residue	UNP Q9RXE3
G	223	MSE	MET	modified residue	UNP Q9RXE3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	294	GLU	-	expression tag	UNP Q9RXE3
G	295	GLY	-	expression tag	UNP Q9RXE3
G	296	HIS	-	expression tag	UNP Q9RXE3
G	297	HIS	-	expression tag	UNP Q9RXE3
G	298	HIS	-	expression tag	UNP Q9RXE3
G	299	HIS	-	expression tag	UNP Q9RXE3
G	300	HIS	-	expression tag	UNP Q9RXE3
G	301	HIS	-	expression tag	UNP Q9RXE3
H	1	MSE	-	expression tag	UNP Q9RXE3
H	2	SER	-	expression tag	UNP Q9RXE3
H	3	LEU	-	expression tag	UNP Q9RXE3
H	50	MSE	MET	modified residue	UNP Q9RXE3
H	115	MSE	MET	modified residue	UNP Q9RXE3
H	175	MSE	MET	modified residue	UNP Q9RXE3
H	223	MSE	MET	modified residue	UNP Q9RXE3
H	294	GLU	-	expression tag	UNP Q9RXE3
H	295	GLY	-	expression tag	UNP Q9RXE3
H	296	HIS	-	expression tag	UNP Q9RXE3
H	297	HIS	-	expression tag	UNP Q9RXE3
H	298	HIS	-	expression tag	UNP Q9RXE3
H	299	HIS	-	expression tag	UNP Q9RXE3
H	300	HIS	-	expression tag	UNP Q9RXE3
H	301	HIS	-	expression tag	UNP Q9RXE3

- 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 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	56	Total O 56 56	0	0
3	B	77	Total O 77 77	0	0

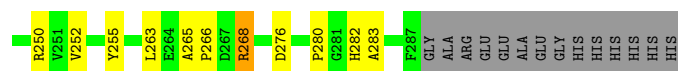
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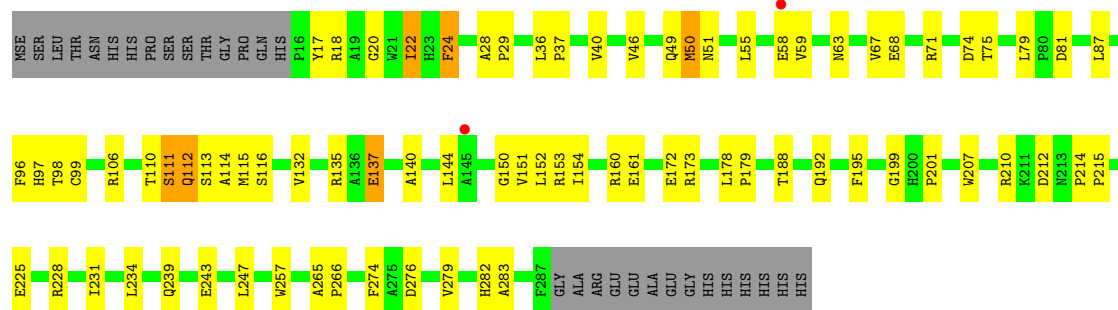
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	77	Total 77	O 77	0	0
3	D	67	Total 67	O 67	0	0
3	E	65	Total 65	O 65	0	0
3	F	121	Total 121	O 121	0	0
3	G	105	Total 105	O 105	0	0
3	H	85	Total 85	O 85	0	0

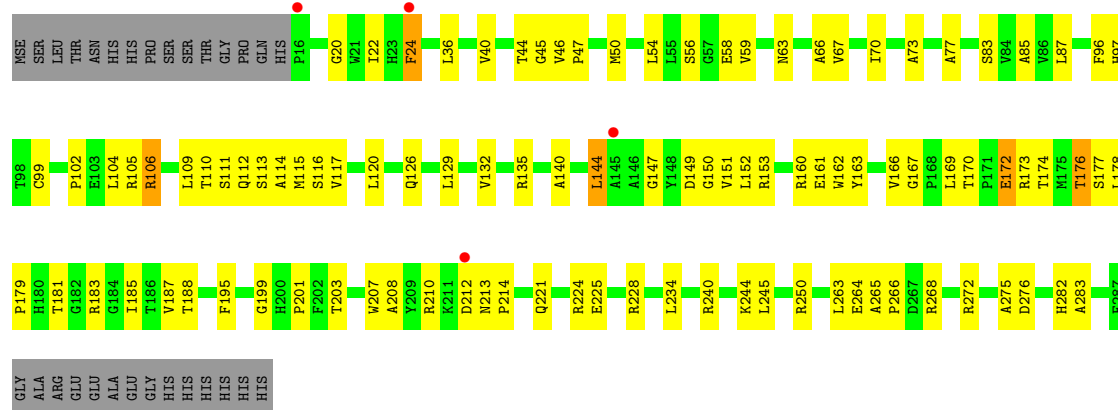




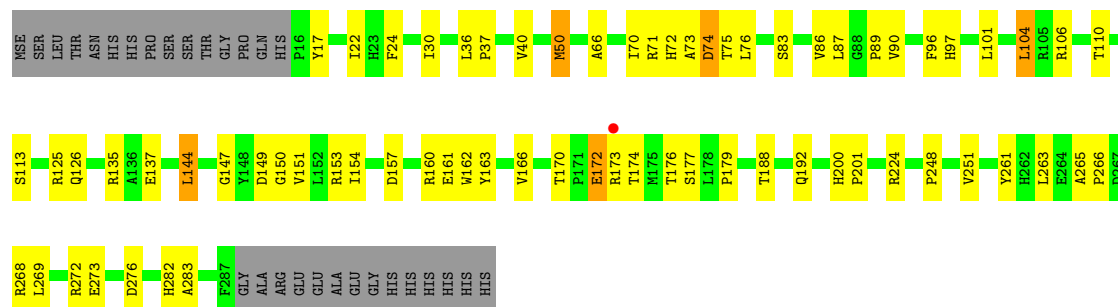
• Molecule 1: Hypothetical protein



• Molecule 1: Hypothetical protein



• Molecule 1: Hypothetical protein



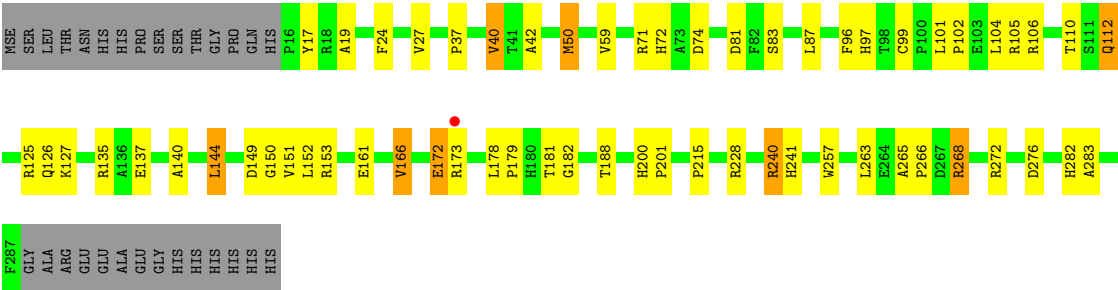
• Molecule 1: Hypothetical protein

Chain G: 

70%

18%

10%



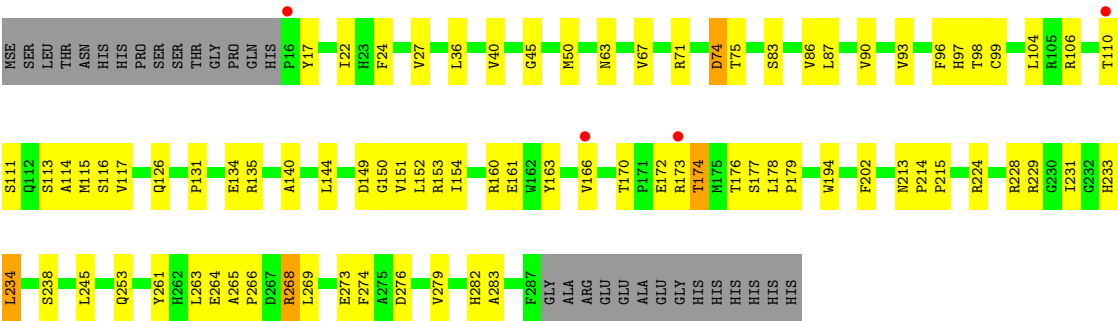
• Molecule 1: Hypothetical protein

Chain H: 

63%

26%

10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.31Å 139.37Å 153.62Å 90.00° 92.79° 90.00°	Depositor
Resolution (Å)	48.03 – 2.50 49.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.03-2.50) 95.2 (49.09-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.235 0.202 , 0.233	Depositor DCC
$R_{free}$ test set	3150 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.06% 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	0.34	0/2162	0.61	0/2949
1	B	0.35	0/2162	0.61	0/2949
1	C	0.36	0/2162	0.62	0/2949
1	D	0.35	0/2162	0.63	1/2949 (0.0%)
1	E	0.35	0/2162	0.64	0/2949
1	F	0.36	0/2162	0.63	0/2949
1	G	0.36	0/2162	0.62	0/2949
1	H	0.36	0/2162	0.63	0/2949
All	All	0.35	0/17296	0.62	1/23592 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	ILE	N-CA-C	-5.17	97.03	111.00

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	2110	0	2102	61	0
1	B	2110	0	2102	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2110	0	2102	59	0
1	D	2110	0	2102	66	0
1	E	2110	0	2102	82	0
1	F	2110	0	2102	59	0
1	G	2110	0	2102	60	0
1	H	2110	0	2102	72	0
2	A	10	0	0	0	0
2	B	15	0	0	3	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	15	0	0	2	0
2	G	15	0	0	0	0
2	H	5	0	0	0	0
3	A	56	0	0	8	0
3	B	77	0	0	9	0
3	C	77	0	0	9	0
3	D	67	0	0	5	0
3	E	65	0	0	10	0
3	F	121	0	0	16	0
3	G	105	0	0	7	0
3	H	85	0	0	14	0
All	All	17623	0	16816	512	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 15.

The worst 5 of 512 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ARG:HB3	3:B:794:HOH:O	1.56	1.05
1:D:113:SER:HB3	3:D:778:HOH:O	1.63	0.97
1:H:229:ARG:HD2	3:H:800:HOH:O	1.71	0.90
1:H:113:SER:HB2	3:H:760:HOH:O	1.71	0.90
1:C:169:LEU:HD13	1:C:178:LEU:HD21	1.51	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/301 (90%)	243 (90%)	23 (8%)	4 (2%)	10	18
1	B	270/301 (90%)	256 (95%)	13 (5%)	1 (0%)	34	54
1	C	270/301 (90%)	257 (95%)	12 (4%)	1 (0%)	34	54
1	D	270/301 (90%)	256 (95%)	14 (5%)	0	100	100
1	E	270/301 (90%)	253 (94%)	17 (6%)	0	100	100
1	F	270/301 (90%)	253 (94%)	17 (6%)	0	100	100
1	G	270/301 (90%)	259 (96%)	11 (4%)	0	100	100
1	H	270/301 (90%)	259 (96%)	11 (4%)	0	100	100
All	All	2160/2408 (90%)	2036 (94%)	118 (6%)	6 (0%)	41	61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	THR
1	A	173	ARG
1	B	23	HIS
1	C	243	GLU
1	A	23	HIS

### 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	220/239 (92%)	214 (97%)	6 (3%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	220/239 (92%)	213 (97%)	7 (3%)	39	65
1	C	220/239 (92%)	209 (95%)	11 (5%)	24	46
1	D	220/239 (92%)	215 (98%)	5 (2%)	50	76
1	E	220/239 (92%)	211 (96%)	9 (4%)	30	55
1	F	220/239 (92%)	214 (97%)	6 (3%)	44	71
1	G	220/239 (92%)	211 (96%)	9 (4%)	30	55
1	H	220/239 (92%)	215 (98%)	5 (2%)	50	76
All	All	1760/1912 (92%)	1702 (97%)	58 (3%)	38	64

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	137	GLU
1	H	174	THR
1	E	172	GLU
1	H	74	ASP
1	G	166	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	282	HIS
1	G	49	GLN
1	F	72	HIS
1	F	239	GLN
1	G	94	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

18 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	G	707	-	4,4,4	0.35	0	6,6,6	0.14	0
2	SO4	A	709	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	E	713	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	F	718	-	4,4,4	0.15	0	6,6,6	0.40	0
2	SO4	B	702	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	C	703	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	C	711	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	D	712	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	E	705	-	4,4,4	0.35	0	6,6,6	0.13	0
2	SO4	G	715	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	G	708	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	H	716	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	F	706	-	4,4,4	0.33	0	6,6,6	0.06	0
2	SO4	F	714	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	B	710	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	B	717	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	D	704	-	4,4,4	0.35	0	6,6,6	0.16	0
2	SO4	A	701	-	4,4,4	0.38	0	6,6,6	0.07	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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	713	SO4	1	0
2	F	718	SO4	2	0
2	B	710	SO4	1	0
2	B	717	SO4	2	0

## 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	268/301 (89%)	0.14	9 (3%) 45 48	20, 38, 63, 76	0
1	B	268/301 (89%)	-0.25	2 (0%) 87 89	15, 30, 50, 71	0
1	C	268/301 (89%)	-0.22	2 (0%) 87 89	14, 30, 47, 64	0
1	D	268/301 (89%)	-0.10	2 (0%) 87 89	14, 31, 54, 71	0
1	E	268/301 (89%)	-0.06	4 (1%) 73 75	15, 33, 58, 74	0
1	F	268/301 (89%)	-0.32	1 (0%) 92 93	13, 25, 43, 70	0
1	G	268/301 (89%)	-0.29	1 (0%) 92 93	14, 25, 44, 68	0
1	H	268/301 (89%)	-0.20	4 (1%) 73 75	12, 26, 49, 69	0
All	All	2144/2408 (89%)	-0.16	25 (1%) 79 80	12, 30, 54, 76	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	173	ARG	4.4
1	G	173	ARG	4.1
1	A	16	PRO	3.5
1	D	58	GLU	3.0
1	B	173	ARG	3.0

### 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	SO4	B	717	5/5	0.92	0.17	71,72,73,73	0
2	SO4	H	716	5/5	0.94	0.20	66,67,68,68	0
2	SO4	D	712	5/5	0.96	0.17	71,72,72,73	0
2	SO4	F	718	5/5	0.96	0.19	70,70,70,71	0
2	SO4	G	715	5/5	0.96	0.19	53,54,57,57	0
2	SO4	C	711	5/5	0.96	0.15	45,45,47,48	0
2	SO4	E	713	5/5	0.97	0.15	62,62,62,63	0
2	SO4	A	709	5/5	0.97	0.15	65,66,67,67	0
2	SO4	A	701	5/5	0.97	0.13	49,49,51,52	0
2	SO4	E	705	5/5	0.97	0.17	50,50,52,53	0
2	SO4	B	710	5/5	0.98	0.23	63,65,66,67	0
2	SO4	G	708	5/5	0.98	0.15	46,46,48,49	0
2	SO4	C	703	5/5	0.98	0.13	35,36,39,40	0
2	SO4	F	714	5/5	0.98	0.16	35,36,39,40	0
2	SO4	G	707	5/5	0.99	0.12	35,35,36,37	0
2	SO4	F	706	5/5	0.99	0.16	39,42,43,43	0
2	SO4	D	704	5/5	0.99	0.13	37,38,39,39	0
2	SO4	B	702	5/5	0.99	0.12	42,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.