



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2023 – 05:30 AM EDT

PDB ID : 3Q6N  
Title : Crystal Structure of Human MC-HSP90 in P21 space group  
Authors : Lee, C.C.; Lin, T.W.; Ko, T.P.; Wang, A.H.-J.  
Deposited on : 2011-01-03  
Resolution : 3.05 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 : 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

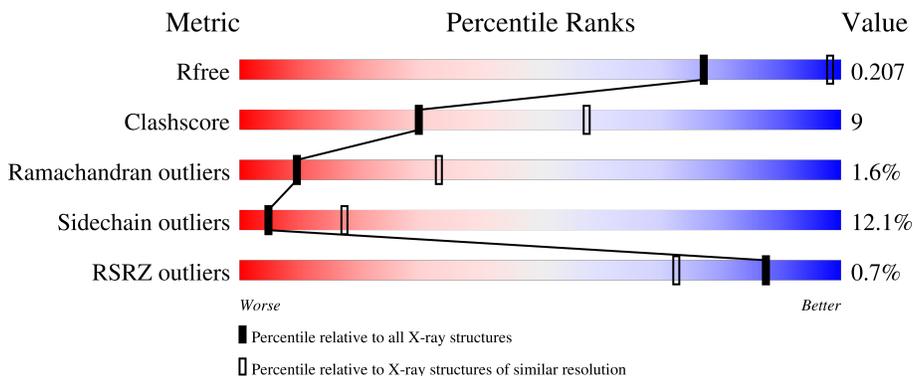
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	

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Mol	Chain	Length	Quality of chain
1	F	448	 63% 15% 19%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18134 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2974	1894	499	567	14	0	0	0
1	B	362	2990	1904	502	570	14	0	0	0
1	C	354	2927	1867	493	553	14	0	0	0
1	D	360	2971	1895	501	561	14	0	0	0
1	E	360	2971	1889	500	568	14	0	0	0
1	F	363	2994	1910	506	563	15	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

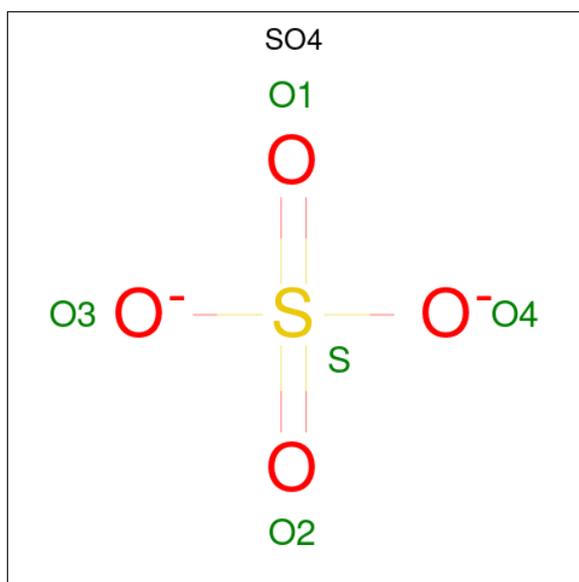
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	-	expression tag	UNP P07900
A	292	ALA	-	expression tag	UNP P07900
A	733	HIS	-	expression tag	UNP P07900
A	734	HIS	-	expression tag	UNP P07900
A	735	HIS	-	expression tag	UNP P07900
A	736	HIS	-	expression tag	UNP P07900
A	737	HIS	-	expression tag	UNP P07900
A	738	HIS	-	expression tag	UNP P07900
B	291	ALA	-	expression tag	UNP P07900
B	292	ALA	-	expression tag	UNP P07900
B	733	HIS	-	expression tag	UNP P07900
B	734	HIS	-	expression tag	UNP P07900
B	735	HIS	-	expression tag	UNP P07900
B	736	HIS	-	expression tag	UNP P07900
B	737	HIS	-	expression tag	UNP P07900
B	738	HIS	-	expression tag	UNP P07900
C	291	ALA	-	expression tag	UNP P07900

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Chain	Residue	Modelled	Actual	Comment	Reference
C	292	ALA	-	expression tag	UNP P07900
C	733	HIS	-	expression tag	UNP P07900
C	734	HIS	-	expression tag	UNP P07900
C	735	HIS	-	expression tag	UNP P07900
C	736	HIS	-	expression tag	UNP P07900
C	737	HIS	-	expression tag	UNP P07900
C	738	HIS	-	expression tag	UNP P07900
D	291	ALA	-	expression tag	UNP P07900
D	292	ALA	-	expression tag	UNP P07900
D	733	HIS	-	expression tag	UNP P07900
D	734	HIS	-	expression tag	UNP P07900
D	735	HIS	-	expression tag	UNP P07900
D	736	HIS	-	expression tag	UNP P07900
D	737	HIS	-	expression tag	UNP P07900
D	738	HIS	-	expression tag	UNP P07900
E	291	ALA	-	expression tag	UNP P07900
E	292	ALA	-	expression tag	UNP P07900
E	733	HIS	-	expression tag	UNP P07900
E	734	HIS	-	expression tag	UNP P07900
E	735	HIS	-	expression tag	UNP P07900
E	736	HIS	-	expression tag	UNP P07900
E	737	HIS	-	expression tag	UNP P07900
E	738	HIS	-	expression tag	UNP P07900
F	291	ALA	-	expression tag	UNP P07900
F	292	ALA	-	expression tag	UNP P07900
F	733	HIS	-	expression tag	UNP P07900
F	734	HIS	-	expression tag	UNP P07900
F	735	HIS	-	expression tag	UNP P07900
F	736	HIS	-	expression tag	UNP P07900
F	737	HIS	-	expression tag	UNP P07900
F	738	HIS	-	expression tag	UNP P07900

- 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		

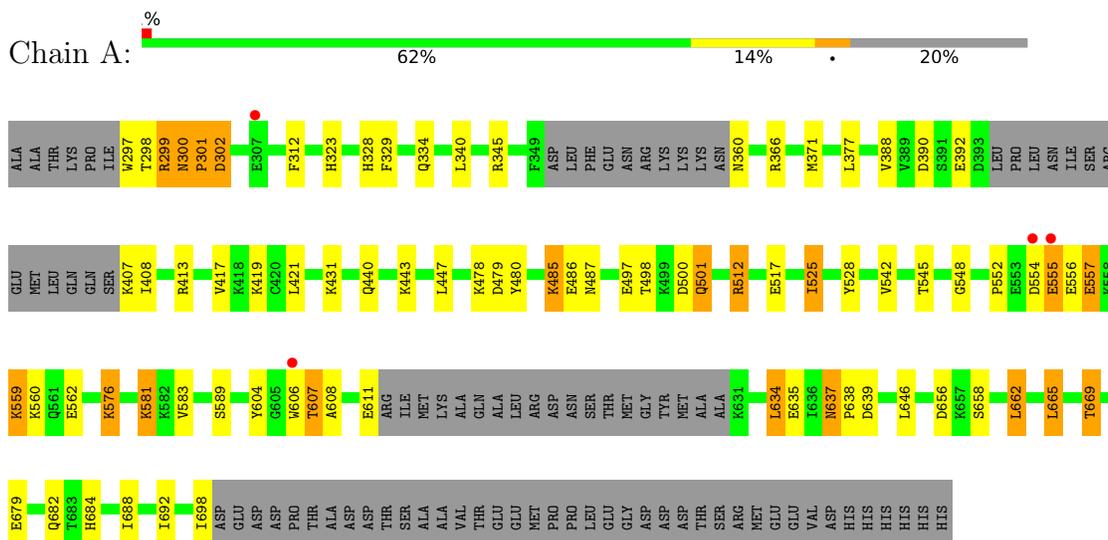
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	57	Total	O	0	0
			57	57		
3	C	45	Total	O	0	0
			45	45		
3	D	46	Total	O	0	0
			46	46		
3	E	46	Total	O	0	0
			46	46		
3	F	50	Total	O	0	0
			50	50		

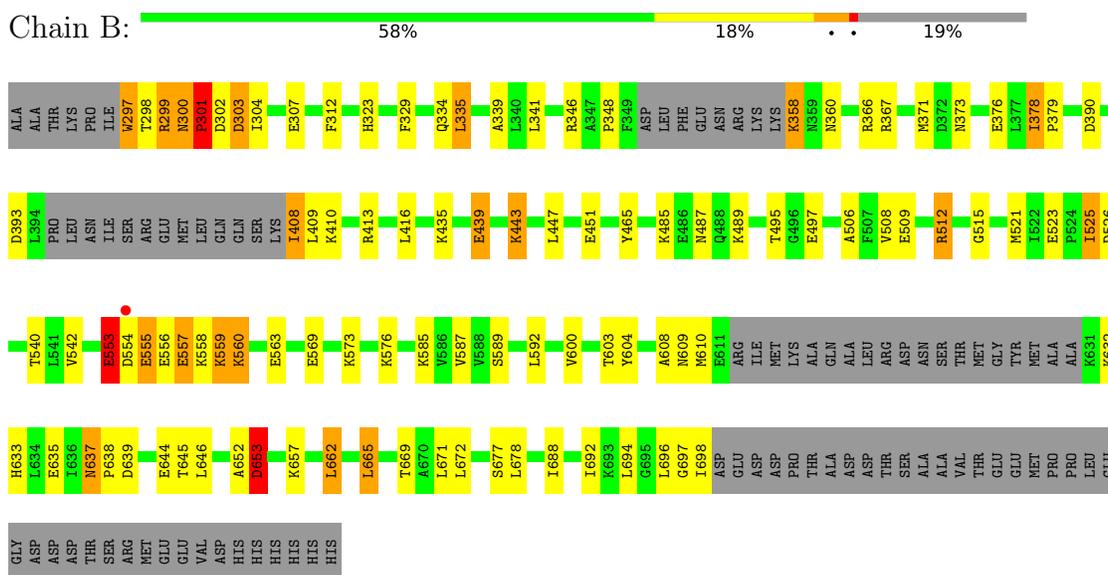
### 3 Residue-property plots [i](#)

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.

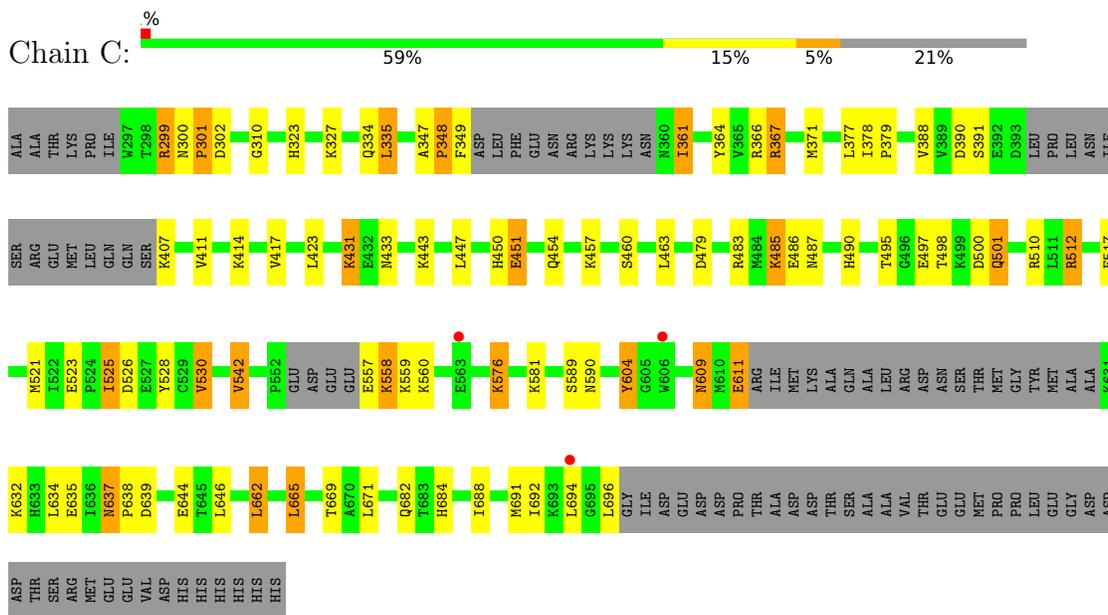
- Molecule 1: Heat shock protein HSP 90-alpha



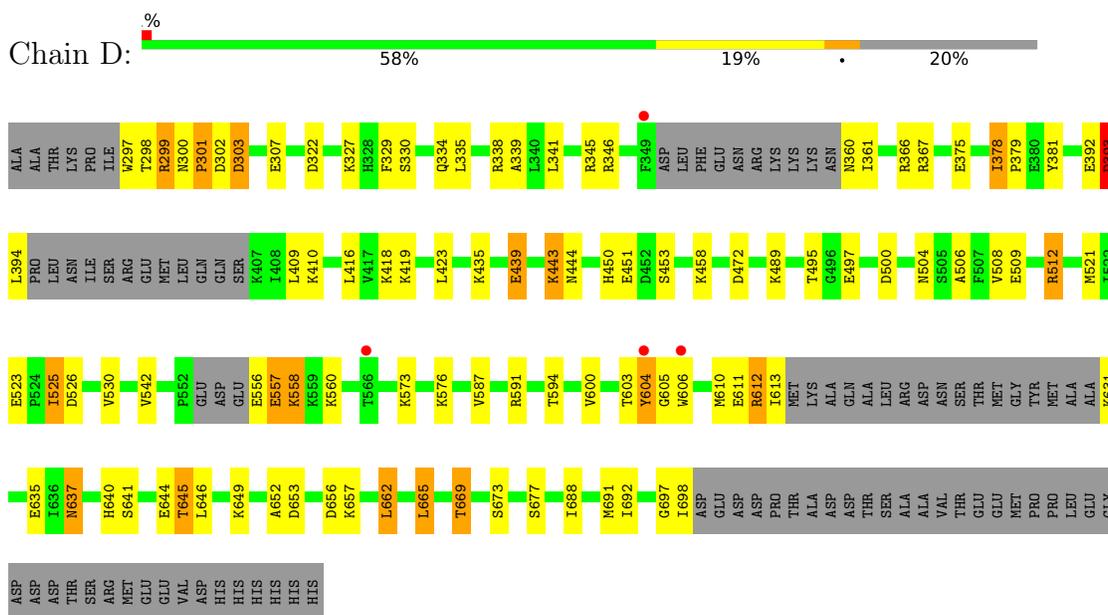
- Molecule 1: Heat shock protein HSP 90-alpha



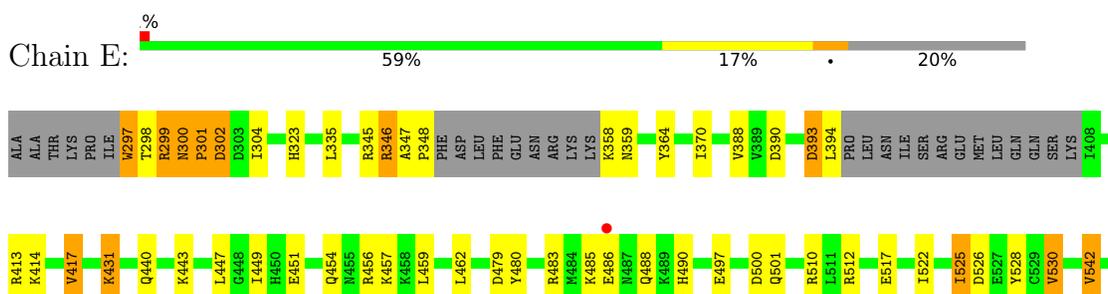
- Molecule 1: Heat shock protein HSP 90-alpha

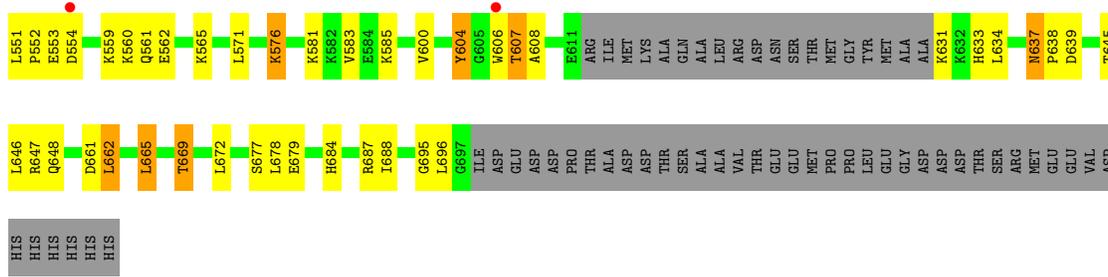


• Molecule 1: Heat shock protein HSP 90-alpha

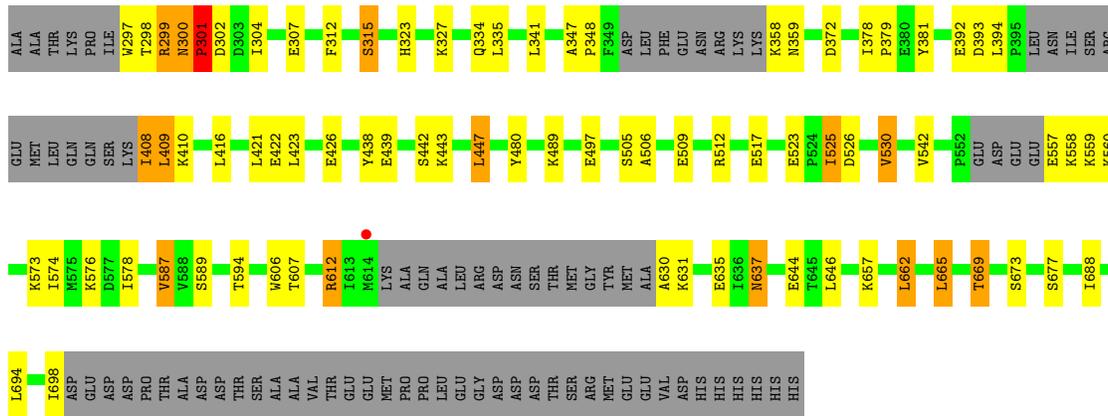


• Molecule 1: Heat shock protein HSP 90-alpha





• Molecule 1: Heat shock protein HSP 90-alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.90Å 90.87Å 167.09Å 90.00° 115.85° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 29.75 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-3.05) 94.4 (29.75-3.02)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.21 (at 3.00Å)	Xtrriage
Refinement program	CNS 1.2, REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.204 , 0.259 0.206 , 0.207	Depositor DCC
$R_{free}$ test set	4051 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.3	Xtrriage
Anisotropy	0.348	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	0.63	0/3023	0.68	0/4058
1	B	0.64	0/3039	0.70	1/4080 (0.0%)
1	C	0.64	0/2975	0.68	0/3992
1	D	0.62	0/3019	0.70	0/4052
1	E	0.62	0/3019	0.70	1/4053 (0.0%)
1	F	0.61	0/3043	0.70	0/4084
All	All	0.63	0/18118	0.69	2/24319 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	302	ASP	N-CA-C	5.21	125.07	111.00
1	B	304	ILE	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	301	PRO	Peptide
1	D	303	ASP	Peptide
1	F	301	PRO	Peptide

## 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	2974	0	3000	52	0
1	B	2990	0	3017	64	0
1	C	2927	0	2963	66	0
1	D	2971	0	3007	62	0
1	E	2971	0	2997	63	0
1	F	2994	0	3039	44	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
3	A	33	0	0	1	0
3	B	57	0	0	3	0
3	C	45	0	0	2	0
3	D	46	0	0	5	0
3	E	46	0	0	1	0
3	F	50	0	0	1	0
All	All	18134	0	18023	337	0

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

The worst 5 of 337 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:525:ILE:HD13	1:B:525:ILE:H	1.00	1.14
1:C:512:ARG:HH11	1:C:512:ARG:HG2	1.11	1.10
1:F:299:ARG:HB3	1:F:299:ARG:HH11	1.10	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ILE:HD13	1:A:525:ILE:H	1.17	1.09
1:D:525:ILE:HD13	1:D:525:ILE:H	1.16	1.06

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	352/448 (79%)	327 (93%)	17 (5%)	8 (2%)	6	24
1	B	354/448 (79%)	331 (94%)	14 (4%)	9 (2%)	5	22
1	C	344/448 (77%)	315 (92%)	25 (7%)	4 (1%)	13	40
1	D	350/448 (78%)	327 (93%)	18 (5%)	5 (1%)	11	36
1	E	352/448 (79%)	328 (93%)	21 (6%)	3 (1%)	17	47
1	F	353/448 (79%)	327 (93%)	22 (6%)	4 (1%)	14	42
All	All	2105/2688 (78%)	1955 (93%)	117 (6%)	33 (2%)	9	33

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	609	ASN
1	C	334	GLN
1	D	393	ASP
1	F	334	GLN
1	F	394	LEU

### 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	335/412 (81%)	297 (89%)	38 (11%)	6	21
1	B	337/412 (82%)	296 (88%)	41 (12%)	5	17
1	C	330/412 (80%)	294 (89%)	36 (11%)	6	22
1	D	334/412 (81%)	292 (87%)	42 (13%)	4	16
1	E	335/412 (81%)	292 (87%)	43 (13%)	4	16
1	F	337/412 (82%)	294 (87%)	43 (13%)	4	16
All	All	2008/2472 (81%)	1765 (88%)	243 (12%)	5	17

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	299	ARG
1	F	525	ILE
1	D	603	THR
1	F	505	SER
1	F	657	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	637	ASN
1	E	637	ASN
1	D	686	ASN
1	E	373	ASN
1	E	686	ASN

### 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](#)

6 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	F	1	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	C	5	-	4,4,4	0.15	0	6,6,6	0.35	0
2	SO4	E	6	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	3	-	4,4,4	0.16	0	6,6,6	0.32	0
2	SO4	A	2	-	4,4,4	0.18	0	6,6,6	0.34	0
2	SO4	D	4	-	4,4,4	0.14	0	6,6,6	0.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	360/448 (80%)	-0.25	4 (1%) 80 60	61, 83, 117, 142	1 (0%)
1	B	362/448 (80%)	-0.28	1 (0%) 94 85	59, 77, 117, 138	1 (0%)
1	C	354/448 (79%)	-0.22	3 (0%) 86 70	62, 86, 125, 150	1 (0%)
1	D	360/448 (80%)	-0.27	4 (1%) 80 60	60, 84, 127, 138	1 (0%)
1	E	360/448 (80%)	-0.19	3 (0%) 86 70	60, 82, 120, 158	1 (0%)
1	F	363/448 (81%)	-0.29	1 (0%) 94 85	58, 78, 118, 138	1 (0%)
All	All	2159/2688 (80%)	-0.25	16 (0%) 87 72	58, 82, 122, 158	6 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	TRP	4.2
1	E	606	TRP	3.9
1	C	606	TRP	3.5
1	D	604	TYR	3.1
1	B	554	ASP	2.9

### 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	D	4	5/5	0.85	0.27	127,128,128,128	0
2	SO4	E	6	5/5	0.87	0.15	139,139,140,140	0
2	SO4	B	3	5/5	0.90	0.23	125,126,126,126	0
2	SO4	A	2	5/5	0.92	0.17	112,113,113,113	0
2	SO4	F	1	5/5	0.92	0.14	120,120,120,121	0
2	SO4	C	5	5/5	0.94	0.17	116,116,117,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.