



# Full wwPDB X-ray Structure Validation Report i

Sep 26, 2023 – 11:51 PM EDT

PDB ID : 6CON  
Title : Crystal structure of Mycobacterium tuberculosis IpdB  
Authors : Crowe, A.M.; Workman, S.D.; Watanabe, N.; Worrall, L.J.; Strynadka, N.C.J.; Eltis, L.D.  
Deposited on : 2018-03-12  
Resolution : 2.10 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

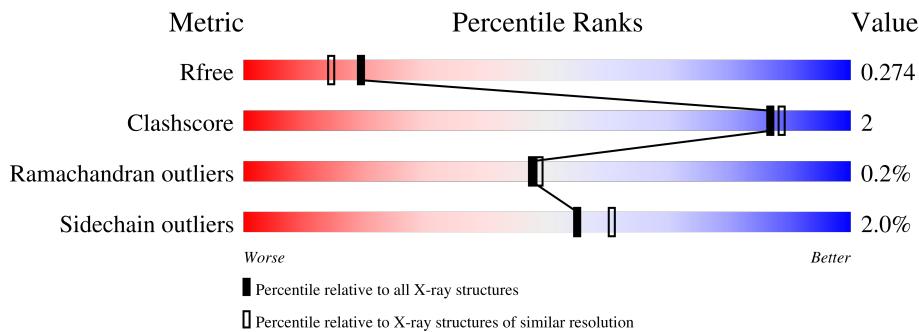
## 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

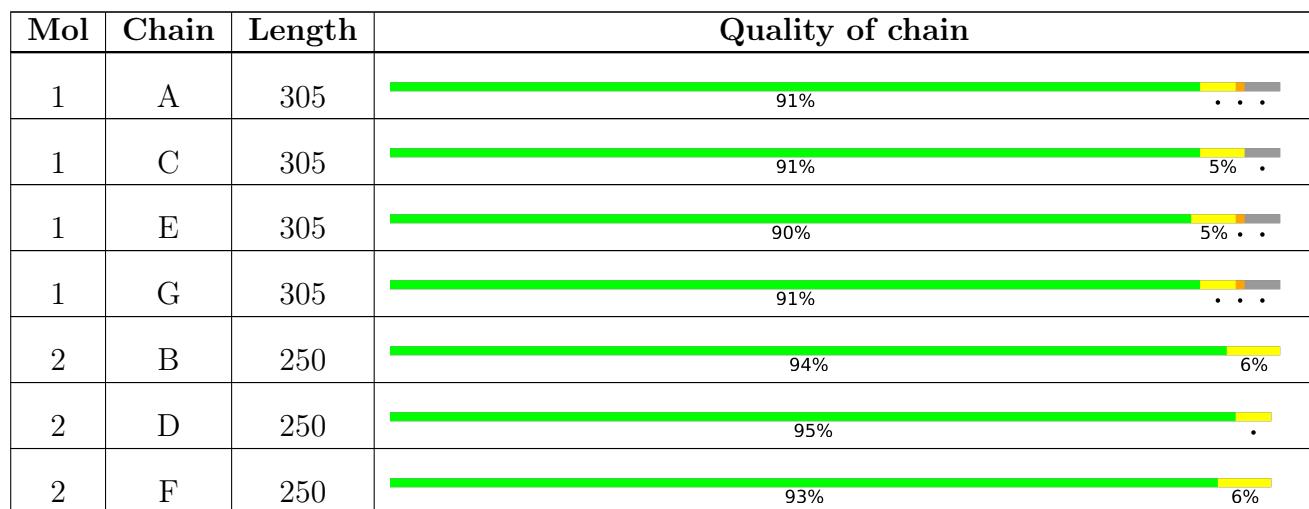
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $>=3$ , 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  $\leq 5\%$ .



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Mol	Chain	Length	Quality of chain
2	H	250	<div style="width: 96%;">96%</div> .

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17593 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 CoA-transferase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2236	1420	391	414	11			
1	C	292	Total	C	N	O	S	0	0	0
			2236	1420	391	414	11			
1	E	292	Total	C	N	O	S	0	0	0
			2236	1420	391	414	11			
1	G	292	Total	C	N	O	S	0	0	0
			2236	1420	391	414	11			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP A0A045J8X5
A	-11	HIS	-	expression tag	UNP A0A045J8X5
A	-10	HIS	-	expression tag	UNP A0A045J8X5
A	-9	HIS	-	expression tag	UNP A0A045J8X5
A	-8	HIS	-	expression tag	UNP A0A045J8X5
A	-7	HIS	-	expression tag	UNP A0A045J8X5
A	-6	HIS	-	expression tag	UNP A0A045J8X5
A	-5	LEU	-	expression tag	UNP A0A045J8X5
A	-4	VAL	-	expression tag	UNP A0A045J8X5
A	-3	PRO	-	expression tag	UNP A0A045J8X5
A	-2	ARG	-	expression tag	UNP A0A045J8X5
A	-1	GLY	-	expression tag	UNP A0A045J8X5
A	0	SER	-	expression tag	UNP A0A045J8X5
C	-12	MET	-	initiating methionine	UNP A0A045J8X5
C	-11	HIS	-	expression tag	UNP A0A045J8X5
C	-10	HIS	-	expression tag	UNP A0A045J8X5
C	-9	HIS	-	expression tag	UNP A0A045J8X5
C	-8	HIS	-	expression tag	UNP A0A045J8X5
C	-7	HIS	-	expression tag	UNP A0A045J8X5
C	-6	HIS	-	expression tag	UNP A0A045J8X5
C	-5	LEU	-	expression tag	UNP A0A045J8X5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	VAL	-	expression tag	UNP A0A045J8X5
C	-3	PRO	-	expression tag	UNP A0A045J8X5
C	-2	ARG	-	expression tag	UNP A0A045J8X5
C	-1	GLY	-	expression tag	UNP A0A045J8X5
C	0	SER	-	expression tag	UNP A0A045J8X5
E	-12	MET	-	initiating methionine	UNP A0A045J8X5
E	-11	HIS	-	expression tag	UNP A0A045J8X5
E	-10	HIS	-	expression tag	UNP A0A045J8X5
E	-9	HIS	-	expression tag	UNP A0A045J8X5
E	-8	HIS	-	expression tag	UNP A0A045J8X5
E	-7	HIS	-	expression tag	UNP A0A045J8X5
E	-6	HIS	-	expression tag	UNP A0A045J8X5
E	-5	LEU	-	expression tag	UNP A0A045J8X5
E	-4	VAL	-	expression tag	UNP A0A045J8X5
E	-3	PRO	-	expression tag	UNP A0A045J8X5
E	-2	ARG	-	expression tag	UNP A0A045J8X5
E	-1	GLY	-	expression tag	UNP A0A045J8X5
E	0	SER	-	expression tag	UNP A0A045J8X5
G	-12	MET	-	initiating methionine	UNP A0A045J8X5
G	-11	HIS	-	expression tag	UNP A0A045J8X5
G	-10	HIS	-	expression tag	UNP A0A045J8X5
G	-9	HIS	-	expression tag	UNP A0A045J8X5
G	-8	HIS	-	expression tag	UNP A0A045J8X5
G	-7	HIS	-	expression tag	UNP A0A045J8X5
G	-6	HIS	-	expression tag	UNP A0A045J8X5
G	-5	LEU	-	expression tag	UNP A0A045J8X5
G	-4	VAL	-	expression tag	UNP A0A045J8X5
G	-3	PRO	-	expression tag	UNP A0A045J8X5
G	-2	ARG	-	expression tag	UNP A0A045J8X5
G	-1	GLY	-	expression tag	UNP A0A045J8X5
G	0	SER	-	expression tag	UNP A0A045J8X5

- Molecule 2 is a protein called CoA-transferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S			
			1917	1197	353	357	10	0	0	0
2	D	249	Total	C	N	O	S			
			1917	1197	353	357	10	0	0	0
2	F	249	Total	C	N	O	S			
			1917	1197	353	357	10	0	0	0
2	H	249	Total	C	N	O	S			
			1917	1197	353	357	10	0	0	0

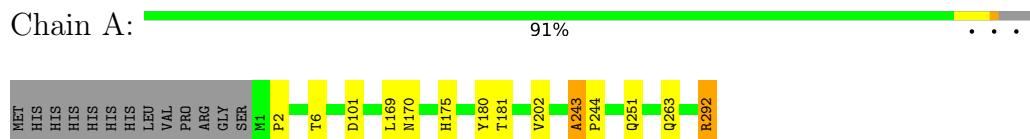
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	123	Total O 123 123	0	0
3	B	116	Total O 116 116	0	0
3	C	149	Total O 149 149	0	0
3	D	128	Total O 128 128	0	0
3	E	158	Total O 158 158	0	0
3	F	100	Total O 100 100	0	0
3	G	68	Total O 68 68	0	0
3	H	139	Total O 139 139	0	0

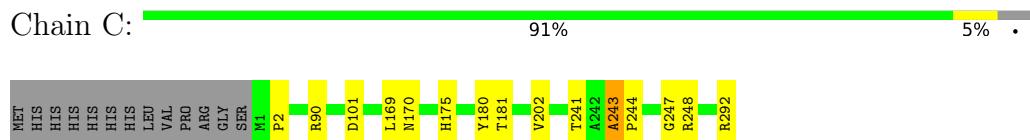
### 3 Residue-property plots [\(i\)](#)

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. 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. 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.

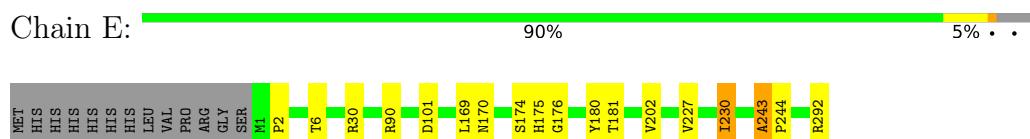
- Molecule 1: CoA-transferase subunit alpha



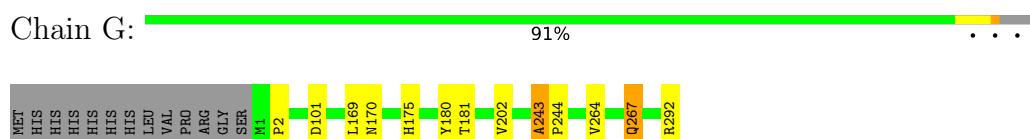
- Molecule 1: CoA-transferase subunit alpha



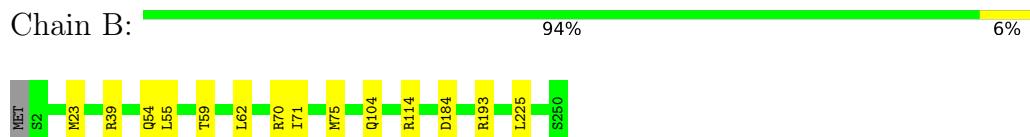
- Molecule 1: CoA-transferase subunit alpha



- Molecule 1: CoA-transferase subunit alpha



- Molecule 2: CoA-transferase subunit beta



- Molecule 2: CoA-transferase subunit beta





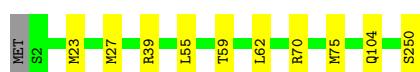
- Molecule 2: CoA-transferase subunit beta

Chain F: 93% 6%



- Molecule 2: CoA-transferase subunit beta

Chain H: 96% .



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.88Å 133.82Å 118.84Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	88.86 – 2.10 88.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (88.86-2.10) 97.6 (88.86-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	4.56 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
$R$ , $R_{free}$	0.251 , 0.274 0.251 , 0.274	Depositor DCC
$R_{free}$ test set	5983 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 19.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.388 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

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	0.67	0/2294	0.74	0/3121
1	C	0.69	0/2294	0.75	0/3121
1	E	0.70	0/2294	0.74	0/3121
1	G	0.65	0/2294	0.74	0/3121
2	B	0.64	0/1960	0.81	0/2664
2	D	0.66	0/1960	0.81	0/2664
2	F	0.65	0/1960	0.81	0/2664
2	H	0.65	0/1960	0.81	0/2664
All	All	0.67	0/17016	0.77	0/23140

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	2236	0	2175	10	0
1	C	2236	0	2175	13	0
1	E	2236	0	2175	16	0
1	G	2236	0	2175	10	0
2	B	1917	0	1870	6	0
2	D	1917	0	1870	6	0
2	F	1917	0	1870	6	0
2	H	1917	0	1870	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	123	0	0	0	0
3	B	116	0	0	1	0
3	C	149	0	0	1	0
3	D	128	0	0	2	0
3	E	158	0	0	1	0
3	F	100	0	0	1	0
3	G	68	0	0	0	0
3	H	139	0	0	0	0
All	All	17593	0	16180	69	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 2.

All (69) 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:E:243:ALA:HB1	1:E:244:PRO:HD3	1.55	0.89
1:G:243:ALA:HB1	1:G:244:PRO:HD3	1.54	0.88
1:C:243:ALA:HB1	1:C:244:PRO:HD3	1.55	0.88
1:C:243:ALA:CB	1:C:244:PRO:CD	2.53	0.86
1:E:243:ALA:CB	1:E:244:PRO:CD	2.53	0.86
1:G:243:ALA:CB	1:G:244:PRO:CD	2.53	0.86
1:A:243:ALA:HB1	1:A:244:PRO:HD3	1.58	0.85
1:A:243:ALA:CB	1:A:244:PRO:CD	2.54	0.85
1:E:243:ALA:HB1	1:E:244:PRO:CD	2.11	0.79
1:G:243:ALA:HB1	1:G:244:PRO:CD	2.11	0.79
1:C:243:ALA:HB1	1:C:244:PRO:CD	2.12	0.77
1:A:243:ALA:HB1	1:A:244:PRO:CD	2.16	0.75
1:C:241:THR:HG23	1:C:247:GLY:HA2	1.73	0.71
1:C:243:ALA:HB3	1:C:244:PRO:HD2	1.73	0.70
1:E:243:ALA:HB3	1:E:244:PRO:HD2	1.74	0.70
1:G:243:ALA:HB3	1:G:244:PRO:HD2	1.74	0.69
1:C:243:ALA:HB2	3:C:426:HOH:O	1.94	0.68
1:A:243:ALA:HB3	1:A:244:PRO:HD2	1.75	0.68
1:E:230:ILE:HB	3:E:425:HOH:O	1.96	0.66
1:E:174:SER:O	1:E:230:ILE:HD11	1.95	0.66
1:E:176:GLY:HA2	1:E:230:ILE:HG21	1.82	0.61
1:A:243:ALA:HB3	1:A:244:PRO:CD	2.29	0.61
2:D:23:MET:CE	2:D:55:LEU:HD21	2.31	0.61
1:E:243:ALA:CB	1:E:244:PRO:HD2	2.30	0.61
2:B:184:ASP:OD1	2:B:193:ARG:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:MET:CE	2:H:55:LEU:HD21	2.32	0.60
1:G:243:ALA:CB	1:G:244:PRO:HD2	2.29	0.60
2:F:250:SER:N	3:F:301:HOH:O	2.31	0.59
2:B:23:MET:CE	2:B:55:LEU:HD21	2.32	0.59
1:E:227:VAL:HG11	1:E:230:ILE:HG23	1.86	0.57
2:F:23:MET:CE	2:F:55:LEU:HD21	2.34	0.57
1:G:264:VAL:O	1:G:267:GLN:HG3	2.05	0.57
2:H:23:MET:HE1	2:H:75:MET:HG2	1.91	0.52
1:E:90:ARG:O	2:F:115:PRO:HD2	2.10	0.52
1:E:174:SER:O	1:E:230:ILE:CD1	2.58	0.50
2:D:23:MET:HE1	2:D:75:MET:HG2	1.93	0.50
1:E:227:VAL:HG11	1:E:230:ILE:CG2	2.41	0.50
1:C:170:ASN:HD22	1:C:180:TYR:HA	1.77	0.49
1:A:170:ASN:HD22	1:A:180:TYR:HA	1.76	0.49
1:G:170:ASN:HD22	1:G:180:TYR:HA	1.78	0.49
1:E:170:ASN:HD22	1:E:180:TYR:HA	1.77	0.48
2:B:39:ARG:HD3	2:B:59:THR:OG1	2.14	0.47
2:B:114:ARG:NH1	3:B:304:HOH:O	2.45	0.47
2:F:23:MET:HE1	2:F:75:MET:HG2	1.96	0.47
2:D:39:ARG:HD3	2:D:59:THR:OG1	2.14	0.47
2:B:23:MET:HE1	2:B:75:MET:HG2	1.96	0.47
2:H:39:ARG:HD3	2:H:59:THR:OG1	2.15	0.46
1:A:2:PRO:O	1:A:175:HIS:HD2	1.98	0.46
1:G:2:PRO:O	1:G:175:HIS:HD2	1.98	0.46
1:E:169:LEU:O	1:E:202:VAL:HA	2.16	0.46
1:A:251:GLN:HE22	1:A:292:ARG:HG2	1.81	0.45
2:F:39:ARG:HD3	2:F:59:THR:OG1	2.16	0.45
1:A:169:LEU:O	1:A:202:VAL:HA	2.17	0.45
1:E:170:ASN:ND2	1:E:181:THR:H	2.16	0.44
1:C:241:THR:HG22	1:C:243:ALA:H	1.82	0.44
1:C:2:PRO:O	1:C:175:HIS:HD2	2.00	0.44
1:A:170:ASN:ND2	1:A:181:THR:H	2.16	0.43
1:G:170:ASN:ND2	1:G:181:THR:H	2.15	0.43
1:G:169:LEU:O	1:G:202:VAL:HA	2.17	0.43
1:C:170:ASN:ND2	1:C:181:THR:H	2.16	0.43
1:C:90:ARG:O	2:D:115:PRO:HD2	2.18	0.43
2:D:36:ARG:NH2	3:D:311:HOH:O	2.52	0.43
1:E:2:PRO:O	1:E:175:HIS:HD2	2.01	0.43
1:C:169:LEU:O	1:C:202:VAL:HA	2.18	0.43
2:B:54:GLN:NE2	2:B:71:ILE:HD13	2.34	0.42
2:D:39:ARG:NH2	3:D:312:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:THR:OG1	1:C:248:ARG:HB2	2.21	0.41
2:H:23:MET:HE1	2:H:55:LEU:HD21	2.03	0.40
2:F:138:VAL:O	2:F:178:SER:HA	2.21	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	290/305 (95%)	281 (97%)	8 (3%)	1 (0%)	41 41
1	C	290/305 (95%)	281 (97%)	8 (3%)	1 (0%)	41 41
1	E	290/305 (95%)	281 (97%)	8 (3%)	1 (0%)	41 41
1	G	290/305 (95%)	282 (97%)	7 (2%)	1 (0%)	41 41
2	B	247/250 (99%)	238 (96%)	9 (4%)	0	100 100
2	D	247/250 (99%)	238 (96%)	9 (4%)	0	100 100
2	F	247/250 (99%)	236 (96%)	11 (4%)	0	100 100
2	H	247/250 (99%)	238 (96%)	9 (4%)	0	100 100
All	All	2148/2220 (97%)	2075 (97%)	69 (3%)	4 (0%)	47 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	C	243	ALA
1	E	243	ALA
1	G	243	ALA

### 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	225/237 (95%)	221 (98%)	4 (2%)	59 65
1	C	225/237 (95%)	223 (99%)	2 (1%)	78 84
1	E	225/237 (95%)	220 (98%)	5 (2%)	52 57
1	G	225/237 (95%)	222 (99%)	3 (1%)	69 75
2	B	203/204 (100%)	199 (98%)	4 (2%)	55 60
2	D	203/204 (100%)	199 (98%)	4 (2%)	55 60
2	F	203/204 (100%)	196 (97%)	7 (3%)	37 39
2	H	203/204 (100%)	198 (98%)	5 (2%)	47 52
All	All	1712/1764 (97%)	1678 (98%)	34 (2%)	55 60

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	101	ASP
1	A	263	GLN
1	A	292	ARG
2	B	62	LEU
2	B	70	ARG
2	B	104	GLN
2	B	225	LEU
1	C	101	ASP
1	C	292	ARG
2	D	62	LEU
2	D	70	ARG
2	D	100	ARG
2	D	225	LEU
1	E	6	THR
1	E	30	ARG
1	E	101	ASP
1	E	230	ILE
1	E	292	ARG

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Mol	Chain	Res	Type
2	F	17	ARG
2	F	62	LEU
2	F	70	ARG
2	F	104	GLN
2	F	225	LEU
2	F	248	ILE
2	F	249	ARG
1	G	101	ASP
1	G	267	GLN
1	G	292	ARG
2	H	27	MET
2	H	62	LEU
2	H	70	ARG
2	H	104	GLN
2	H	250	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	168	HIS
1	A	170	ASN
1	A	175	HIS
1	A	251	GLN
1	A	253	GLN
2	B	54	GLN
2	B	103	ASN
1	C	168	HIS
1	C	170	ASN
1	C	175	HIS
1	C	253	GLN
1	C	263	GLN
1	C	282	GLN
2	D	54	GLN
2	D	103	ASN
1	E	168	HIS
1	E	170	ASN
1	E	175	HIS
1	E	253	GLN
1	E	282	GLN
2	F	54	GLN
2	F	103	ASN

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Mol	Chain	Res	Type
1	G	114	GLN
1	G	168	HIS
1	G	170	ASN
1	G	175	HIS
1	G	253	GLN
1	G	267	GLN
1	G	282	GLN
2	H	103	ASN
2	H	104	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 [\(i\)](#)

There are no ligands in this entry.

### 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 [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.