



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:29 PM GMT

PDB ID : 4EWP  
Title : Crystal structure of FabH from *Micrococcus luteus*  
Authors : Pereira, J.H.; Goh, E.-B.; Keasling, J.D.; Beller, H.R.; Adams, P.D.  
Deposited on : 2012-04-27  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

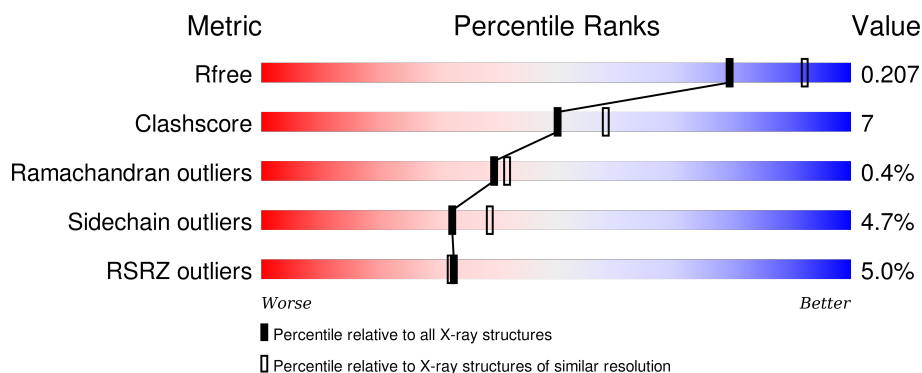
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	350	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	350	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	350	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	350	<div> <div>9%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	E	350	<div> <div>5%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	350	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '5%', a green segment in the middle labeled '83%', and a yellow segment at the end labeled '15%'. A small black dot is located at the far right end of the bar.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16333 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2576	1608	460	500	8			
1	B	349	Total	C	N	O	S	0	0	0
			2576	1608	460	500	8			
1	C	349	Total	C	N	O	S	0	0	0
			2576	1608	460	500	8			
1	D	349	Total	C	N	O	S	0	0	0
			2576	1608	460	500	8			
1	E	349	Total	C	N	O	S	0	0	0
			2576	1608	460	500	8			
1	F	349	Total	C	N	O	S	0	0	0
			2576	1608	460	500	8			

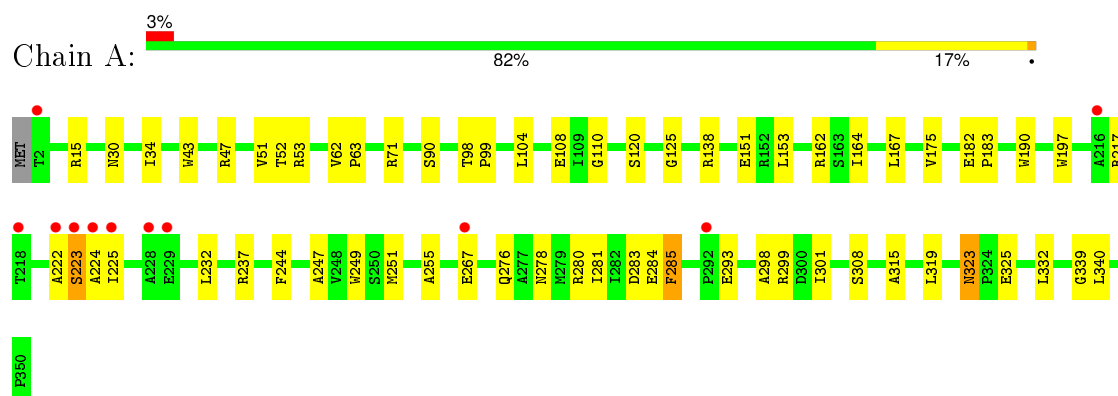
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	176	Total	O	0	0
			176	176		
2	C	164	Total	O	0	0
			164	164		
2	D	99	Total	O	0	0
			99	99		
2	E	125	Total	O	0	0
			125	125		
2	F	153	Total	O	0	0
			153	153		

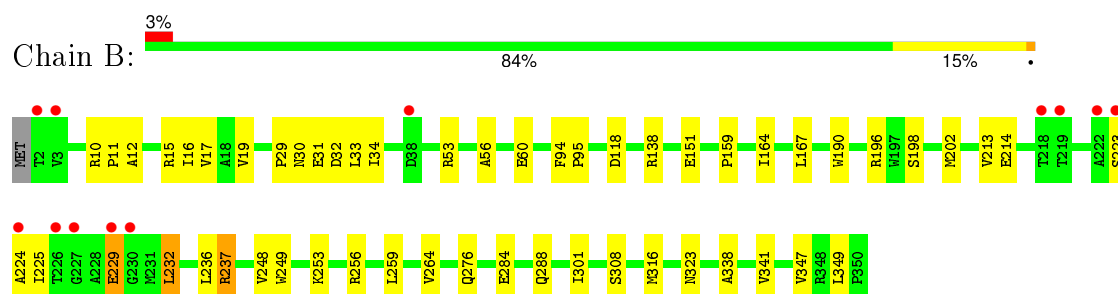
### 3 Residue-property plots [i](#)

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

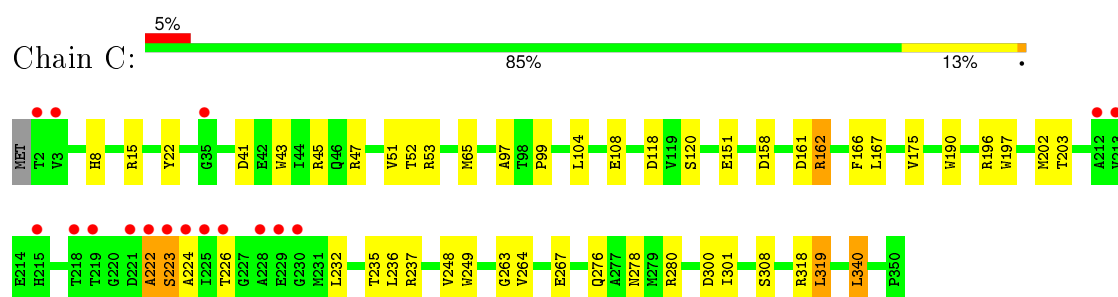
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3



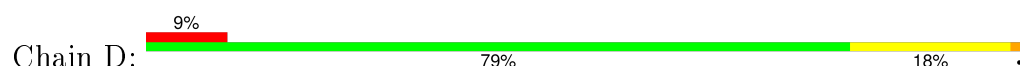
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

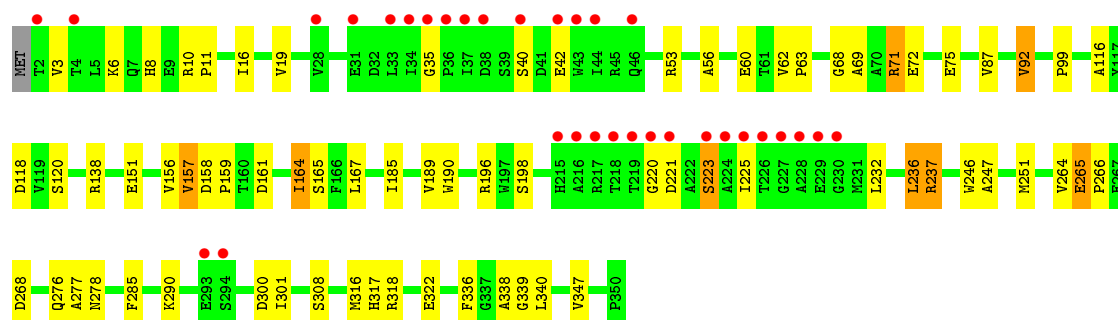


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

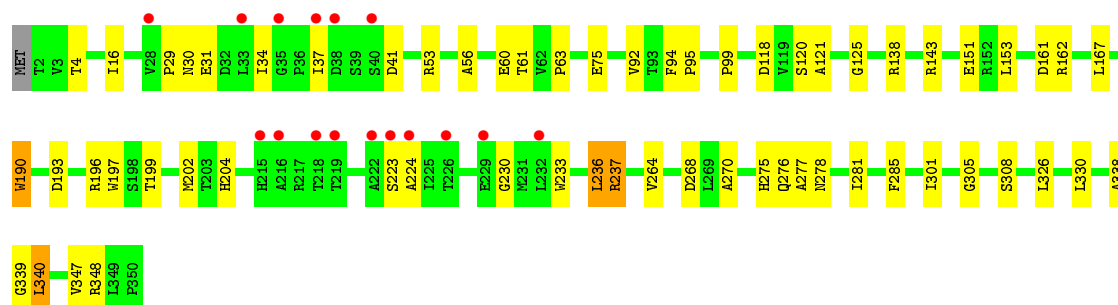
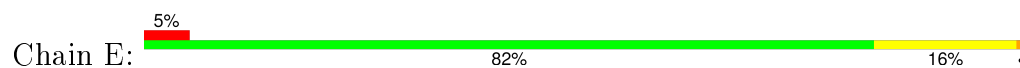


- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

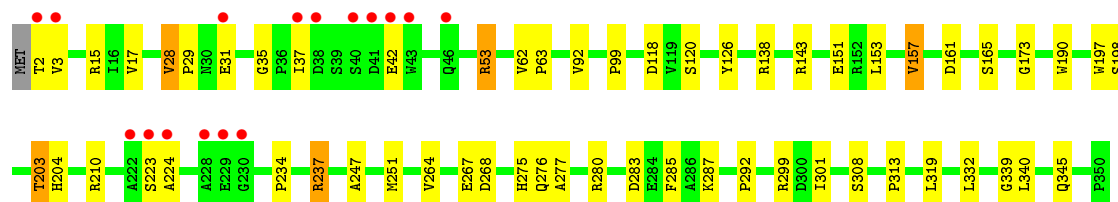
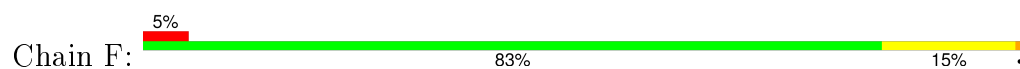




- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.14Å 85.03Å 96.92Å 69.82° 71.37° 85.66°	Depositor
Resolution (Å)	49.80 – 2.20 49.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.80-2.20) 85.9 (49.79-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_718)	Depositor
R, $R_{free}$	0.169 , 0.210 0.168 , 0.207	Depositor DCC
$R_{free}$ test set	5574 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 111257 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/2626	0.55	0/3588
1	B	0.39	0/2626	0.56	0/3588
1	C	0.39	0/2626	0.55	0/3588
1	D	0.35	0/2626	0.53	0/3588
1	E	0.36	0/2626	0.52	0/3588
1	F	0.38	0/2626	0.54	1/3588 (0.0%)
All	All	0.38	0/15756	0.54	1/21528 (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	F	319	LEU	CA-CB-CG	5.26	127.39	115.30

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	2576	0	2549	38	0
1	B	2576	0	2549	36	0
1	C	2576	0	2549	38	0
1	D	2576	0	2549	47	0
1	E	2576	0	2549	41	0
1	F	2576	0	2549	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	160	0	0	6	0
2	B	176	0	0	7	0
2	C	164	0	0	5	0
2	D	99	0	0	8	0
2	E	125	0	0	4	0
2	F	153	0	0	2	0
All	All	16333	0	15294	216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (216) 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:D:8:HIS:ND1	2:D:448:HOH:O	2.07	0.84
1:B:256:ARG:HD3	2:B:414:HOH:O	1.79	0.81
1:C:45:ARG:NH1	2:C:490:HOH:O	2.09	0.81
1:A:283:ASP:OD1	1:A:299:ARG:NH1	2.15	0.79
1:B:138:ARG:NH1	2:B:417:HOH:O	2.13	0.75
1:A:104:LEU:O	1:A:108:GLU:HG2	1.86	0.74
1:A:280:ARG:NH1	2:A:549:HOH:O	2.21	0.74
1:E:199:THR:OG1	2:E:498:HOH:O	2.06	0.73
1:D:68:GLY:O	2:D:445:HOH:O	2.07	0.70
1:B:16:ILE:HD12	1:B:347:VAL:HG11	1.74	0.69
1:D:278:ASN:HA	1:D:301:ILE:CD1	2.22	0.69
1:D:198:SER:O	1:D:237:ARG:NH2	2.26	0.69
1:D:71:ARG:N	2:D:445:HOH:O	2.25	0.68
1:B:12:ALA:O	2:B:504:HOH:O	2.12	0.67
1:E:16:ILE:HD12	1:E:347:VAL:HG11	1.76	0.67
1:A:280:ARG:NH2	2:A:554:HOH:O	2.27	0.67
1:F:173:GLY:HA3	1:F:313:PRO:HB2	1.78	0.64
1:B:19:VAL:HB	1:B:316:MET:HE2	1.79	0.63
1:F:151:GLU:HG3	1:F:308:SER:HB3	1.82	0.62
1:C:97:ALA:O	1:D:92:VAL:HG22	2.00	0.61
1:A:151:GLU:HG3	1:A:308:SER:HB3	1.82	0.61
1:F:283:ASP:OD1	1:F:299:ARG:NH1	2.34	0.60
1:D:264:VAL:HG13	1:D:268:ASP:HB2	1.82	0.60
1:A:223:SER:C	1:A:225:ILE:H	2.04	0.60
1:A:280:ARG:NH1	1:A:284:GLU:HB2	2.16	0.60
1:A:267:GLU:OE1	1:A:267:GLU:N	2.34	0.59
1:B:253:LYS:N	1:B:253:LYS:HD2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:SER:O	1:A:225:ILE:N	2.34	0.59
1:D:276:GLN:HB3	1:D:301:ILE:HB	1.84	0.58
1:C:237:ARG:HH11	1:C:237:ARG:HG3	1.68	0.58
1:F:223:SER:O	1:F:224:ALA:HB3	2.03	0.58
1:E:237:ARG:HH11	1:E:237:ARG:CG	2.17	0.58
1:A:244:PHE:HE1	1:A:280:ARG:HG3	1.68	0.57
1:E:118:ASP:HB2	1:F:120:SER:HB3	1.85	0.57
1:B:19:VAL:HB	1:B:316:MET:CE	2.34	0.57
1:F:264:VAL:HG13	1:F:268:ASP:HB2	1.86	0.57
1:C:235:THR:HG22	2:C:526:HOH:O	2.04	0.57
1:E:301:ILE:HD12	1:E:305:GLY:C	2.25	0.57
1:E:223:SER:O	1:E:224:ALA:HB3	2.05	0.57
1:F:203:THR:HG23	1:F:204:HIS:ND1	2.20	0.56
1:C:158:ASP:HB2	1:C:235:THR:HG21	1.88	0.56
1:E:138:ARG:NH1	2:E:476:HOH:O	2.18	0.56
1:B:196:ARG:NE	2:B:506:HOH:O	2.39	0.56
1:E:233:TRP:CG	1:F:210:ARG:HG3	2.41	0.56
1:D:300:ASP:HA	1:D:318:ARG:HH11	1.70	0.55
1:C:118:ASP:HB2	1:D:120:SER:HB3	1.87	0.55
1:F:126:TYR:CD2	1:F:313:PRO:HG3	2.42	0.55
1:B:248:VAL:HG12	1:B:284:GLU:HG2	1.87	0.55
1:D:221:ASP:OD1	1:D:223:SER:HB3	2.06	0.55
1:E:151:GLU:HG3	1:E:308:SER:HB3	1.88	0.55
1:C:99:PRO:HG3	1:D:338:ALA:HB1	1.89	0.55
1:E:338:ALA:HB1	1:F:99:PRO:HG3	1.89	0.55
1:D:62:VAL:HB	1:D:63:PRO:HD3	1.88	0.55
1:B:253:LYS:NZ	1:B:288:GLN:NE2	2.56	0.54
1:B:31:GLU:OE1	1:B:31:GLU:N	2.32	0.54
1:D:225:ILE:HA	1:D:232:LEU:HD11	1.89	0.54
1:D:265:GLU:HG3	1:D:266:PRO:HD2	1.90	0.53
1:A:71:ARG:NH1	2:A:475:HOH:O	2.39	0.53
1:D:19:VAL:HB	1:D:316:MET:HE1	1.91	0.53
1:C:235:THR:HG23	1:C:237:ARG:NH1	2.24	0.53
1:F:339:GLY:N	1:F:340:LEU:HA	2.23	0.53
1:A:278:ASN:OD1	1:A:280:ARG:HB3	2.09	0.52
1:D:247:ALA:O	1:D:251:MET:HB2	2.09	0.52
1:D:196:ARG:NH1	2:D:455:HOH:O	2.39	0.52
1:A:244:PHE:CE1	1:A:280:ARG:HG3	2.45	0.51
1:D:278:ASN:HA	1:D:301:ILE:HD13	1.92	0.51
1:C:166:PHE:CE2	1:C:167:LEU:HD12	2.45	0.51
1:C:202:MET:SD	1:C:236:LEU:HD13	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:HIS:CE1	1:E:277:ALA:HB2	2.46	0.51
1:B:253:LYS:HZ2	1:B:288:GLN:NE2	2.09	0.51
1:A:247:ALA:O	1:A:251:MET:HB2	2.11	0.50
1:C:120:SER:HB3	1:D:118:ASP:HB2	1.93	0.50
1:D:138:ARG:NH1	2:D:450:HOH:O	2.34	0.50
1:C:224:ALA:N	2:C:522:HOH:O	2.40	0.50
1:B:223:SER:O	1:B:224:ALA:HB3	2.11	0.50
1:C:197:TRP:CZ2	1:D:99:PRO:HD2	2.47	0.50
1:D:339:GLY:N	1:D:340:LEU:HA	2.27	0.49
1:C:43:TRP:CE2	1:C:47:ARG:HG3	2.47	0.49
1:E:270:ALA:HB1	1:E:326:LEU:HD22	1.95	0.49
1:D:151:GLU:HG3	1:D:308:SER:HB3	1.93	0.49
1:C:237:ARG:HG3	1:C:237:ARG:NH1	2.28	0.49
1:D:71:ARG:O	1:D:75:GLU:HG3	2.11	0.49
1:F:35:GLY:O	1:F:37:ILE:O	2.30	0.49
1:D:318:ARG:O	1:D:322:GLU:HG2	2.13	0.49
1:B:56:ALA:HB1	1:B:60:GLU:HB2	1.94	0.49
1:C:41:ASP:OD2	1:C:45:ARG:NH2	2.46	0.49
1:C:45:ARG:NH1	2:C:546:HOH:O	2.33	0.49
1:C:203:THR:HG22	1:C:237:ARG:HD2	1.94	0.49
1:F:157:VAL:HG13	1:F:165:SER:HB2	1.94	0.49
1:F:276:GLN:HB3	1:F:301:ILE:HB	1.95	0.49
1:B:16:ILE:HD12	1:B:347:VAL:CG1	2.43	0.48
1:E:99:PRO:HD2	1:F:197:TRP:CZ2	2.48	0.48
1:D:290:LYS:NZ	2:D:446:HOH:O	2.36	0.48
1:E:120:SER:HB3	1:F:118:ASP:HB2	1.96	0.48
1:E:276:GLN:O	1:E:301:ILE:HD13	2.14	0.48
1:A:120:SER:HB3	1:B:118:ASP:HB2	1.96	0.48
1:D:157:VAL:HG22	1:D:165:SER:HA	1.96	0.47
1:A:323:ASN:HB3	1:A:325:GLU:OE2	2.14	0.47
1:D:16:ILE:HD12	1:D:347:VAL:HG11	1.95	0.47
1:F:153:LEU:HD11	1:F:308:SER:HB2	1.96	0.47
1:F:203:THR:HG22	1:F:234:PRO:HA	1.96	0.47
1:B:213:VAL:HG13	1:B:214:GLU:N	2.30	0.47
1:D:19:VAL:HB	1:D:316:MET:CE	2.45	0.47
1:A:90:SER:OG	1:A:125:GLY:HA3	2.15	0.46
1:C:300:ASP:HA	1:C:318:ARG:HH11	1.78	0.46
1:F:283:ASP:O	1:F:287:LYS:HG3	2.14	0.46
1:F:138:ARG:NH1	2:F:407:HOH:O	2.36	0.46
1:A:138:ARG:NH1	2:A:454:HOH:O	2.36	0.46
1:A:339:GLY:N	1:A:340:LEU:HA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:GLY:N	1:E:340:LEU:HA	2.29	0.46
1:F:42:GLU:H	1:F:42:GLU:CD	2.19	0.46
1:F:28:VAL:HA	1:F:29:PRO:HD3	1.74	0.46
1:E:202:MET:SD	1:E:236:LEU:HD13	2.55	0.46
1:A:110:GLY:HA2	2:A:526:HOH:O	2.16	0.46
1:E:190:TRP:CD1	1:E:190:TRP:N	2.84	0.46
1:E:237:ARG:HG2	1:E:237:ARG:NH1	2.30	0.46
1:F:62:VAL:HB	1:F:63:PRO:HD3	1.97	0.46
1:B:276:GLN:HB3	1:B:301:ILE:HB	1.98	0.45
1:E:30:ASN:HB2	1:E:41:ASP:OD2	2.16	0.45
1:F:42:GLU:CD	1:F:42:GLU:N	2.70	0.45
1:D:156:VAL:HG23	1:D:236:LEU:CD2	2.46	0.45
1:A:62:VAL:HB	1:A:63:PRO:HD3	1.97	0.45
1:A:223:SER:C	1:A:225:ILE:N	2.70	0.45
1:E:348:ARG:NH2	1:F:3:VAL:O	2.50	0.45
1:C:222:ALA:O	1:C:223:SER:C	2.54	0.45
1:E:276:GLN:HB3	1:E:301:ILE:HB	1.99	0.45
1:B:30:ASN:O	1:B:34:ILE:HG23	2.17	0.45
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.78	0.45
1:A:249:TRP:CE2	1:C:52:THR:HG21	2.52	0.45
1:E:61:THR:HB	1:E:63:PRO:HD2	1.98	0.45
1:E:92:VAL:CG1	1:E:92:VAL:O	2.65	0.45
1:C:196:ARG:HB2	1:C:340:LEU:HD22	1.99	0.44
1:B:253:LYS:N	1:B:253:LYS:CD	2.81	0.44
1:F:157:VAL:HG22	1:F:165:SER:HA	1.99	0.44
1:C:22:TYR:CE1	1:C:65:MET:HG2	2.52	0.44
1:D:164:ILE:O	1:D:167:LEU:HB2	2.17	0.44
1:B:151:GLU:HG3	1:B:308:SER:HB3	1.98	0.44
1:E:278:ASN:HB3	1:E:281:ILE:HG13	1.99	0.44
1:A:153:LEU:HD11	1:A:308:SER:HB2	2.00	0.44
1:A:43:TRP:CE2	1:A:47:ARG:HG3	2.53	0.44
1:D:72:GLU:OE1	1:D:317:HIS:NE2	2.49	0.44
1:B:196:ARG:CZ	2:B:506:HOH:O	2.65	0.44
1:F:267:GLU:HA	1:F:292:PRO:HG2	2.00	0.44
1:A:138:ARG:HD2	2:A:454:HOH:O	2.18	0.44
1:B:248:VAL:CG1	1:B:284:GLU:HG2	2.47	0.43
1:E:37:ILE:O	1:E:37:ILE:HG13	2.18	0.43
1:C:236:LEU:HA	1:C:236:LEU:HD12	1.81	0.43
1:D:156:VAL:HG23	1:D:236:LEU:HD23	2.00	0.43
1:D:246:TRP:CH2	1:D:336:PHE:HB2	2.53	0.43
1:F:15:ARG:NH2	2:F:495:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:VAL:HG22	1:D:3:VAL:HG21	1.99	0.43
1:C:43:TRP:CZ2	1:C:47:ARG:HG3	2.54	0.43
1:C:248:VAL:HG23	1:C:249:TRP:HD1	1.83	0.43
1:C:278:ASN:OD1	1:C:280:ARG:HB2	2.19	0.43
1:B:248:VAL:HG23	1:B:249:TRP:HD1	1.84	0.43
1:C:278:ASN:OD1	1:C:280:ARG:N	2.52	0.43
1:A:281:ILE:O	1:A:285:PHE:HB2	2.19	0.43
1:A:222:ALA:C	1:A:223:SER:O	2.53	0.43
1:D:69:ALA:C	2:D:445:HOH:O	2.57	0.43
1:D:277:ALA:O	1:D:278:ASN:HB3	2.18	0.43
1:E:264:VAL:HG13	1:E:268:ASP:HB2	2.01	0.43
1:A:197:TRP:HA	1:A:339:GLY:O	2.19	0.43
1:F:53:ARG:H	1:F:53:ARG:HD2	1.84	0.43
1:E:56:ALA:HB1	1:E:60:GLU:HB2	2.00	0.43
1:C:151:GLU:HG3	1:C:308:SER:HB3	2.01	0.43
1:E:94:PHE:HA	1:E:95:PRO:HD3	1.71	0.42
1:B:94:PHE:CD2	1:B:95:PRO:HD2	2.54	0.42
1:E:61:THR:CB	1:E:63:PRO:HD2	2.49	0.42
1:B:229:GLU:H	1:B:229:GLU:HG2	1.48	0.42
1:A:298:ALA:HB1	1:A:315:ALA:HB1	2.01	0.42
1:E:230:GLY:N	2:E:465:HOH:O	2.49	0.42
1:B:10:ARG:HA	1:B:11:PRO:HD3	1.87	0.42
1:F:247:ALA:O	1:F:251:MET:HB2	2.19	0.42
1:E:153:LEU:HD11	1:E:308:SER:HB2	2.01	0.42
1:B:29:PRO:HD2	1:B:32:ASP:OD2	2.20	0.42
1:E:121:ALA:HB3	1:E:125:GLY:HA2	2.01	0.42
1:E:34:ILE:O	1:E:37:ILE:O	2.37	0.42
1:A:51:VAL:HG12	1:A:52:THR:HG23	2.02	0.42
1:B:15:ARG:NE	2:B:526:HOH:O	2.15	0.42
1:E:29:PRO:HB2	1:E:31:GLU:HG2	2.01	0.41
1:D:308:SER:OG	2:D:436:HOH:O	2.08	0.41
1:E:330:LEU:HD11	1:F:3:VAL:CG2	2.50	0.41
1:C:263:GLY:HA3	1:D:6:LYS:HE3	2.01	0.41
1:E:193:ASP:OD2	1:E:196:ARG:NH1	2.50	0.41
1:A:255:ALA:HB1	1:A:332:LEU:HD21	2.02	0.41
1:C:104:LEU:O	1:C:108:GLU:HG2	2.20	0.41
1:D:56:ALA:HB1	1:D:60:GLU:HB3	2.01	0.41
1:A:30:ASN:O	1:A:34:ILE:HG23	2.21	0.41
1:B:202:MET:SD	1:B:236:LEU:HD13	2.60	0.41
1:B:259:LEU:HD22	1:B:264:VAL:HG12	2.02	0.41
1:D:185:ILE:HG12	1:D:347:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ILE:HA	1:D:167:LEU:HD23	2.02	0.41
1:F:198:SER:O	1:F:237:ARG:NH2	2.54	0.41
1:B:198:SER:O	1:B:237:ARG:NH2	2.53	0.41
1:E:197:TRP:HA	1:E:339:GLY:O	2.20	0.41
1:C:162:ARG:HG2	1:C:162:ARG:H	1.72	0.41
1:C:276:GLN:HB3	1:C:301:ILE:HB	2.02	0.41
1:A:217:ARG:HG3	1:B:225:ILE:O	2.20	0.41
1:F:203:THR:HG23	1:F:204:HIS:CE1	2.56	0.41
1:C:51:VAL:HG12	1:C:52:THR:HG23	2.03	0.41
1:C:319:LEU:HD12	1:C:319:LEU:HA	1.78	0.41
1:B:225:ILE:HA	1:B:232:LEU:HD21	2.03	0.41
1:C:226:THR:HG22	1:D:220:GLY:HA2	2.02	0.41
1:E:223:SER:O	1:E:224:ALA:CB	2.69	0.40
1:D:10:ARG:HA	1:D:11:PRO:HD3	1.88	0.40
1:B:338:ALA:O	1:B:341:VAL:HG22	2.21	0.40
1:B:159:PRO:HD2	2:B:450:HOH:O	2.21	0.40
1:C:45:ARG:NH2	2:C:546:HOH:O	2.48	0.40
1:E:30:ASN:O	1:E:34:ILE:HG23	2.21	0.40
1:D:158:ASP:HA	1:D:159:PRO:HD3	1.90	0.40
1:A:276:GLN:HB3	1:A:301:ILE:HB	2.02	0.40
1:F:275:HIS:CD2	1:F:277:ALA:HB2	2.55	0.40
1:D:87:VAL:O	1:D:116:ALA:HA	2.21	0.40
1:A:98:THR:OG1	1:A:99:PRO:HA	2.21	0.40
1:E:143:ARG:NH1	2:E:462:HOH:O	2.53	0.40
1:A:182:GLU:HA	1:A:183:PRO:HD3	1.93	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	347/350 (99%)	333 (96%)	11 (3%)	3 (1%)	21 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	347/350 (99%)	332 (96%)	14 (4%)	1 (0%)	46	50
1	C	347/350 (99%)	331 (95%)	14 (4%)	2 (1%)	30	29
1	D	347/350 (99%)	332 (96%)	13 (4%)	2 (1%)	30	29
1	E	347/350 (99%)	331 (95%)	16 (5%)	0	100	100
1	F	347/350 (99%)	330 (95%)	17 (5%)	0	100	100
All	All	2082/2100 (99%)	1989 (96%)	85 (4%)	8 (0%)	39	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	C	222	ALA
1	A	224	ALA
1	C	223	SER
1	B	164	ILE
1	D	35	GLY
1	A	164	ILE
1	D	164	ILE

### 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	264/265 (100%)	253 (96%)	11 (4%)	36	44
1	B	264/265 (100%)	254 (96%)	10 (4%)	40	49
1	C	264/265 (100%)	253 (96%)	11 (4%)	36	44
1	D	264/265 (100%)	250 (95%)	14 (5%)	28	32
1	E	264/265 (100%)	252 (96%)	12 (4%)	34	41
1	F	264/265 (100%)	248 (94%)	16 (6%)	23	26
All	All	1584/1590 (100%)	1510 (95%)	74 (5%)	32	39

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	53	ARG
1	A	162	ARG
1	A	167	LEU
1	A	175	VAL
1	A	190	TRP
1	A	232	LEU
1	A	237	ARG
1	A	285	PHE
1	A	293	GLU
1	A	323	ASN
1	B	17	VAL
1	B	33	LEU
1	B	53	ARG
1	B	167	LEU
1	B	190	TRP
1	B	229	GLU
1	B	232	LEU
1	B	237	ARG
1	B	323	ASN
1	B	349	LEU
1	C	8	HIS
1	C	15	ARG
1	C	53	ARG
1	C	161	ASP
1	C	162	ARG
1	C	175	VAL
1	C	190	TRP
1	C	232	LEU
1	C	267	GLU
1	C	319	LEU
1	C	340	LEU
1	D	40	SER
1	D	42	GLU
1	D	53	ARG
1	D	71	ARG
1	D	92	VAL
1	D	157	VAL
1	D	161	ASP
1	D	189	VAL
1	D	190	TRP
1	D	223	SER
1	D	236	LEU

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Mol	Chain	Res	Type
1	D	237	ARG
1	D	265	GLU
1	D	285	PHE
1	E	4	THR
1	E	53	ARG
1	E	75	GLU
1	E	161	ASP
1	E	162	ARG
1	E	167	LEU
1	E	190	TRP
1	E	204	HIS
1	E	236	LEU
1	E	237	ARG
1	E	285	PHE
1	E	340	LEU
1	F	2	THR
1	F	17	VAL
1	F	28	VAL
1	F	31	GLU
1	F	53	ARG
1	F	92	VAL
1	F	143	ARG
1	F	157	VAL
1	F	161	ASP
1	F	190	TRP
1	F	203	THR
1	F	237	ARG
1	F	280	ARG
1	F	285	PHE
1	F	332	LEU
1	F	345	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	B	288	GLN
1	C	96	HIS
1	E	288	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 carbohydrates 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 ⓘ

### 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	349/350 (99%)	0.12	11 (3%)	51	50	15, 27, 55, 84	0
1	B	349/350 (99%)	0.20	12 (3%)	49	47	13, 25, 53, 88	0
1	C	349/350 (99%)	0.12	17 (4%)	33	33	14, 26, 62, 98	0
1	D	349/350 (99%)	0.55	32 (9%)	11	10	16, 42, 77, 91	0
1	E	349/350 (99%)	0.08	16 (4%)	36	35	17, 34, 65, 87	0
1	F	349/350 (99%)	0.14	16 (4%)	36	35	16, 29, 61, 80	0
All	All	2094/2100 (99%)	0.20	104 (4%)	32	32	13, 30, 64, 98	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	THR	6.2
1	C	2	THR	6.1
1	C	223	SER	5.6
1	C	224	ALA	5.6
1	D	2	THR	5.4
1	D	227	GLY	4.7
1	D	229	GLU	4.7
1	E	224	ALA	4.6
1	F	228	ALA	4.5
1	C	212	ALA	4.3
1	D	38	ASP	4.1
1	C	222	ALA	4.1
1	F	229	GLU	3.9
1	F	230	GLY	3.9
1	D	34	ILE	3.9
1	B	222	ALA	3.9
1	C	229	GLU	3.9
1	B	224	ALA	3.7
1	D	44	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	37	ILE	3.7
1	F	3	VAL	3.6
1	D	228	ALA	3.6
1	A	2	THR	3.5
1	E	218	THR	3.5
1	B	218	THR	3.5
1	D	46	GLN	3.5
1	D	42	GLU	3.5
1	B	223	SER	3.4
1	E	229	GLU	3.4
1	F	222	ALA	3.4
1	D	37	ILE	3.3
1	F	40	SER	3.2
1	D	43	TRP	3.2
1	C	226	THR	3.2
1	D	33	LEU	3.2
1	C	230	GLY	3.1
1	D	223	SER	3.1
1	F	223	SER	3.1
1	F	43	TRP	3.1
1	B	226	THR	3.1
1	D	4	THR	3.0
1	C	3	VAL	3.0
1	D	293	GLU	3.0
1	C	218	THR	3.0
1	E	219	THR	3.0
1	E	223	SER	3.0
1	B	3	VAL	2.9
1	E	215	HIS	2.9
1	D	216	ALA	2.9
1	B	219	THR	2.9
1	D	294	SER	2.8
1	D	215	HIS	2.8
1	B	227	GLY	2.8
1	B	230	GLY	2.8
1	B	229	GLU	2.8
1	D	226	THR	2.7
1	F	38	ASP	2.7
1	D	35	GLY	2.7
1	C	35	GLY	2.7
1	A	267	GLU	2.6
1	B	38	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	226	THR	2.6
1	C	213	VAL	2.6
1	C	228	ALA	2.5
1	C	215	HIS	2.5
1	E	216	ALA	2.5
1	A	224	ALA	2.5
1	E	38	ASP	2.5
1	D	218	THR	2.5
1	F	46	GLN	2.5
1	C	221	ASP	2.4
1	E	232	LEU	2.4
1	F	224	ALA	2.4
1	A	229	GLU	2.4
1	E	33	LEU	2.4
1	A	223	SER	2.4
1	E	37	ILE	2.3
1	A	218	THR	2.3
1	E	222	ALA	2.3
1	D	225	ILE	2.3
1	C	219	THR	2.3
1	D	40	SER	2.2
1	D	220	GLY	2.2
1	F	2	THR	2.2
1	F	31	GLU	2.2
1	A	216	ALA	2.2
1	A	222	ALA	2.2
1	D	217	ARG	2.2
1	F	42	GLU	2.2
1	D	230	GLY	2.2
1	A	228	ALA	2.2
1	C	225	ILE	2.2
1	D	36	PRO	2.2
1	D	28	VAL	2.1
1	D	224	ALA	2.1
1	D	219	THR	2.1
1	E	40	SER	2.1
1	A	292	PRO	2.1
1	E	35	GLY	2.1
1	F	41	ASP	2.0
1	A	225	ILE	2.0
1	E	28	VAL	2.0
1	D	31	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	221	ASP	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.