



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:05 PM GMT

PDB ID : 4BGE  
Title : Crystal structure of InhA(S94A) mutant in complex with pyridomycin  
Authors : Pojer, F.; Hartkoorn, R.C.; Cole, S.T.  
Deposited on : 2013-03-26  
Resolution : 2.25 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

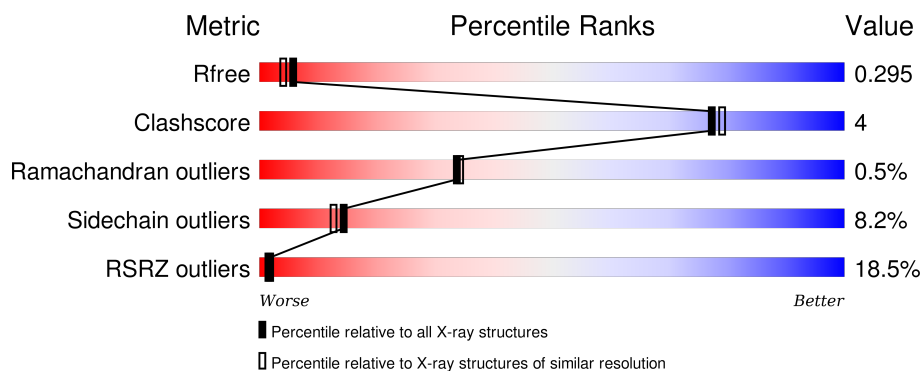
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	269	<div> <div>10%</div> <div>84%</div> <div>13%</div> <div>••</div> </div>
1	B	269	<div> <div>13%</div> <div>84%</div> <div>14%</div> <div>••</div> </div>
1	C	269	<div> <div>22%</div> <div>83%</div> <div>11%</div> <div>• 6%</div> </div>
1	D	269	<div> <div>16%</div> <div>82%</div> <div>10%</div> <div>• 6%</div> </div>
1	E	269	<div> <div>20%</div> <div>80%</div> <div>12%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	269	<div><div></div><div>26%</div><div></div><div>82%</div><div></div><div>15%</div><div>..</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12612 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.

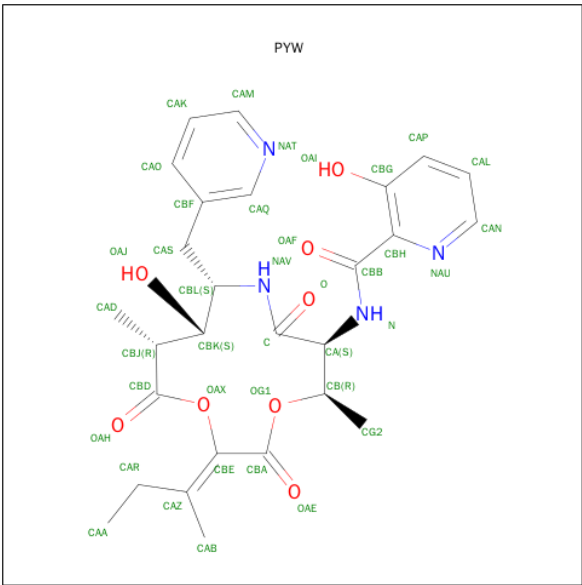
- Molecule 1 is a protein called ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			
1	B	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			
1	C	254	Total	C	N	O	S	0	0	0
			1909	1210	334	356	9			
1	D	252	Total	C	N	O	S	0	0	0
			1889	1199	329	352	9			
1	E	251	Total	C	N	O	S	0	0	0
			1889	1199	331	350	9			
1	F	267	Total	C	N	O	S	0	0	0
			1988	1260	347	371	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
B	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
C	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
D	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
E	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6
F	94	ALA	SER	ENGINEERED MUTATION	UNP P0A5Y6

- Molecule 2 is PYRIDOMYCIN (three-letter code: PYW) (formula: C<sub>27</sub>H<sub>32</sub>N<sub>4</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	27	4	8		
2	B	1	Total	C	N	O	0	0
			39	27	4	8		
2	C	1	Total	C	N	O	0	0
			39	27	4	8		
2	D	1	Total	C	N	O	0	0
			39	27	4	8		
2	E	1	Total	C	N	O	0	0
			39	27	4	8		
2	F	1	Total	C	N	O	0	0
			39	27	4	8		

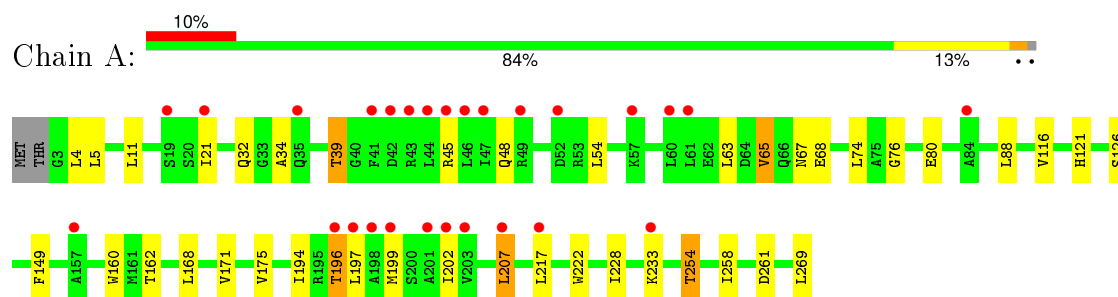
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total	O	0	0
			154	154		
3	B	114	Total	O	0	0
			114	114		
3	C	76	Total	O	0	0
			76	76		
3	D	109	Total	O	0	0
			109	109		
3	E	86	Total	O	0	0
			86	86		
3	F	188	Total	O	0	0
			188	188		

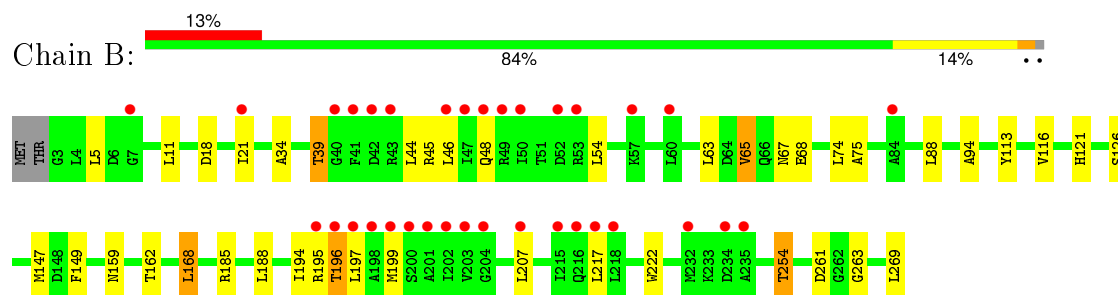
### 3 Residue-property plots [i](#)

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.

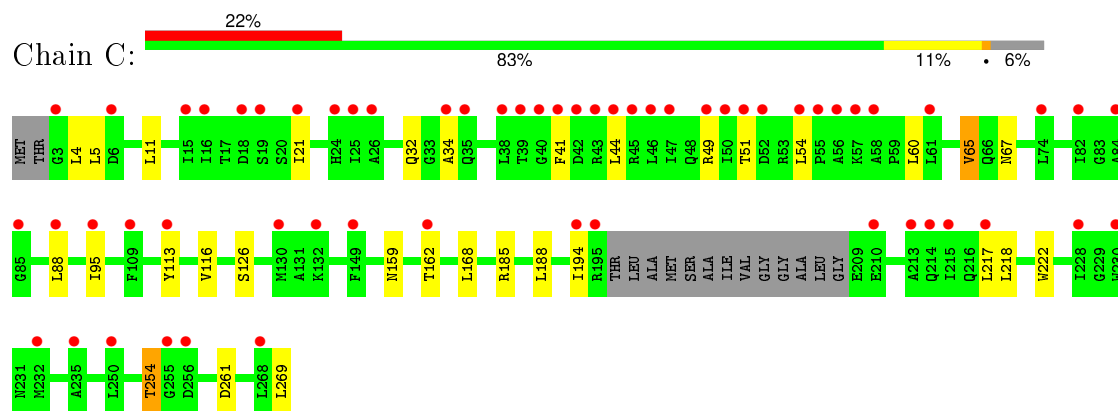
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



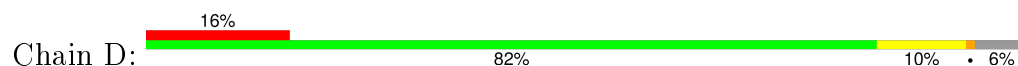
#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

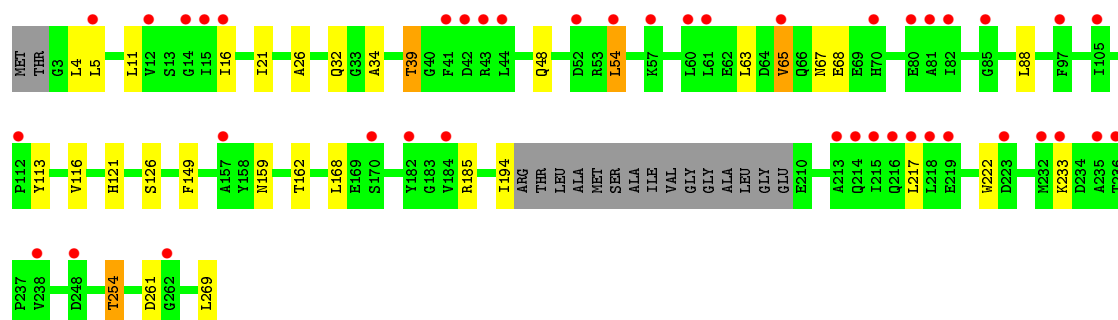


#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

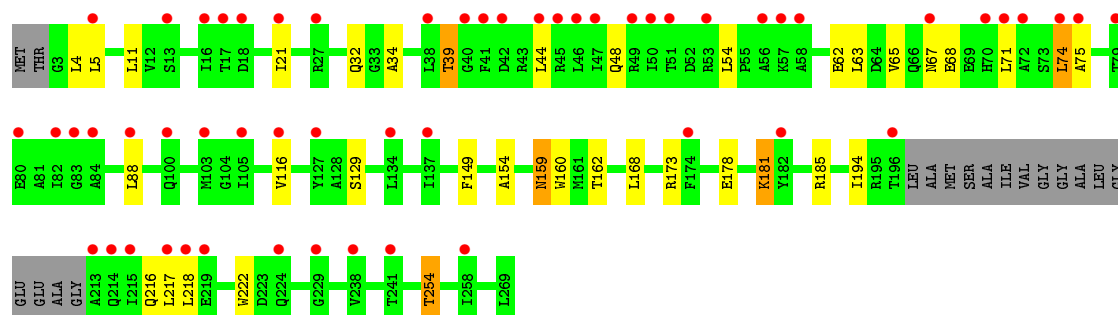
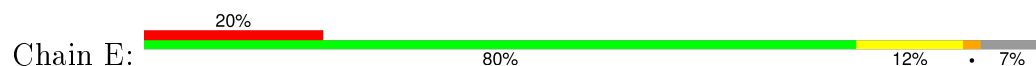


#### • Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]

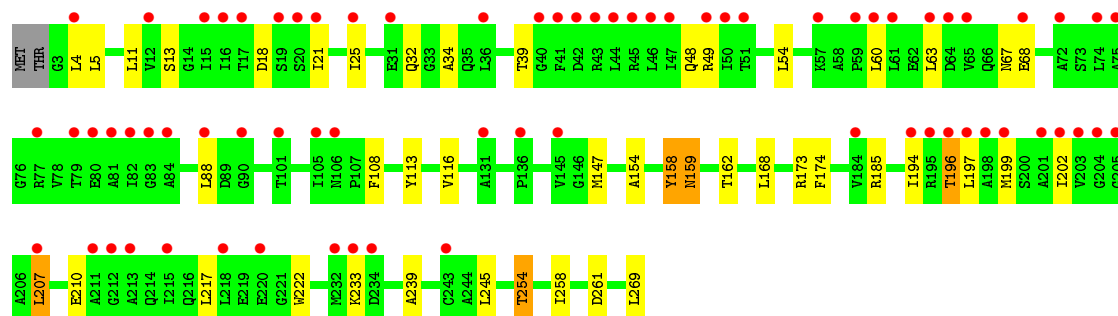
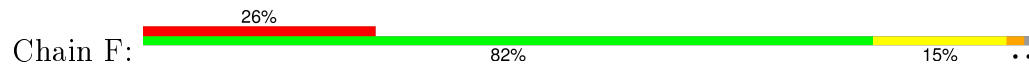




- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADH]



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.60Å 83.05Å 190.68Å 90.00° 94.84° 90.00°	Depositor
Resolution (Å)	47.50 – 2.25 46.26 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.50-2.25) 77.6 (46.26-2.25)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.240 , 0.278 0.266 , 0.295	Depositor DCC
$R_{free}$ test set	3722 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	1 of 73988 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	12612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYW

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	0.42	0/2026	0.63	0/2750
1	B	0.42	0/2026	0.64	0/2750
1	C	0.41	0/1946	0.62	0/2640
1	D	0.41	0/1926	0.62	0/2614
1	E	0.42	0/1926	0.64	0/2614
1	F	0.42	0/2026	0.62	0/2750
All	All	0.42	0/11876	0.63	0/16118

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	1988	0	2006	16	0
1	B	1988	0	2006	15	0
1	C	1909	0	1918	10	0
1	D	1889	0	1899	13	0
1	E	1889	0	1905	16	0
1	F	1988	0	2006	22	0
2	A	39	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	31	3	0
2	C	39	0	31	0	0
2	D	39	0	31	1	0
2	E	39	0	31	1	0
2	F	39	0	31	2	0
3	A	154	0	0	1	0
3	B	114	0	0	2	0
3	C	76	0	0	0	0
3	D	109	0	0	1	0
3	E	86	0	0	0	0
3	F	188	0	0	0	0
All	All	12612	0	11926	88	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 4.

All (88) 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:21:ILE:HD11	1:D:194:ILE:HD13	1.37	1.06
1:B:254:THR:HG21	3:B:2082:HOH:O	1.80	0.82
1:E:71:LEU:HD21	1:E:129:SER:HB3	1.66	0.75
1:D:149:PHE:HB2	2:D:1270:PYW:HAQ	1.67	0.75
1:A:254:THR:HG22	1:B:263:GLY:HA3	1.70	0.73
1:D:254:THR:HG21	3:D:2081:HOH:O	1.89	0.72
1:A:149:PHE:HB2	2:A:1270:PYW:HAQ	1.73	0.70
1:D:21:ILE:CD1	1:D:194:ILE:HD13	2.22	0.67
1:E:4:LEU:H	1:E:32:GLN:HE21	1.45	0.65
1:A:4:LEU:H	1:A:32:GLN:HE21	1.46	0.64
1:C:4:LEU:H	1:C:32:GLN:HE21	1.46	0.62
1:D:4:LEU:H	1:D:32:GLN:HE21	1.46	0.62
1:E:44:LEU:HD11	1:E:62:GLU:HG3	1.81	0.61
1:F:147:MET:HB3	2:F:1270:PYW:HAM	1.83	0.61
1:A:116:VAL:HG11	1:A:160:TRP:CE3	2.36	0.60
1:F:25:ILE:HD13	1:F:239:ALA:HA	1.83	0.60
1:E:178:GLU:O	1:E:181:LYS:HG2	2.06	0.56
1:E:149:PHE:HB2	2:E:1270:PYW:HAQ	1.88	0.56
1:F:11:LEU:HB2	1:F:88:LEU:HD21	1.91	0.53
1:D:11:LEU:HB2	1:D:88:LEU:HD21	1.90	0.53
1:B:11:LEU:HB2	1:B:88:LEU:HD21	1.91	0.53
1:F:5:LEU:HB3	1:F:34:ALA:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ILE:O	1:F:25:ILE:HG12	2.08	0.53
1:C:11:LEU:HB2	1:C:88:LEU:HD21	1.91	0.52
1:E:11:LEU:HB2	1:E:88:LEU:HD21	1.91	0.51
1:A:11:LEU:HB2	1:A:88:LEU:HD21	1.91	0.51
1:E:159:ASN:HA	1:F:174:PHE:CE2	2.46	0.51
1:C:21:ILE:HD11	1:C:194:ILE:HG13	1.94	0.50
1:C:51:THR:HA	1:C:54:LEU:HD13	1.92	0.50
1:E:21:ILE:HD11	1:E:194:ILE:HG13	1.94	0.50
1:A:5:LEU:HB3	1:A:34:ALA:HB2	1.93	0.50
1:B:5:LEU:HB3	1:B:34:ALA:HB2	1.93	0.50
1:F:25:ILE:CD1	1:F:239:ALA:HA	2.43	0.49
1:D:5:LEU:HB3	1:D:34:ALA:HB2	1.94	0.49
1:E:5:LEU:HB3	1:E:34:ALA:HB2	1.94	0.49
1:B:39:THR:HG23	1:B:63:LEU:HB3	1.96	0.48
1:C:5:LEU:HB3	1:C:34:ALA:HB2	1.95	0.48
1:B:21:ILE:HD11	1:B:194:ILE:HG13	1.96	0.48
1:A:171:VAL:O	1:A:175:VAL:HG23	2.14	0.48
1:A:21:ILE:HD11	1:A:194:ILE:HG13	1.95	0.47
1:E:116:VAL:HG11	1:E:160:TRP:CE3	2.48	0.47
1:F:21:ILE:HD11	1:F:194:ILE:HG13	1.96	0.47
1:C:168:LEU:HG	1:C:188:LEU:HD21	1.96	0.47
1:E:173:ARG:HB3	1:F:154:ALA:HB2	1.96	0.47
1:F:222:TRP:HE1	1:F:261:ASP:HB2	1.80	0.47
1:B:168:LEU:HD22	1:B:188:LEU:HD11	1.97	0.46
1:B:149:PHE:HB2	2:B:1270:PYW:HAQ	1.96	0.46
1:F:4:LEU:H	1:F:32:GLN:HE21	1.62	0.46
1:E:154:ALA:HB2	1:F:173:ARG:HB3	1.98	0.45
1:E:39:THR:HG23	1:E:63:LEU:HB3	1.98	0.45
1:C:113:TYR:HA	1:C:116:VAL:HG22	1.99	0.45
1:C:65:VAL:HG21	1:C:126:SER:HB2	1.99	0.45
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.82	0.45
1:D:222:TRP:HE1	1:D:261:ASP:HB2	1.82	0.45
1:F:108:PHE:HD1	1:F:159:ASN:HB3	1.82	0.45
1:D:113:TYR:HA	1:D:116:VAL:HG22	1.99	0.45
1:C:222:TRP:HE1	1:C:261:ASP:HB2	1.82	0.45
1:A:202:ILE:HG22	1:A:207:LEU:HB2	1.99	0.45
1:F:39:THR:HG23	1:F:63:LEU:HB3	1.98	0.44
1:B:196:THR:H	1:B:199:MET:HB2	1.83	0.44
1:B:113:TYR:HA	1:B:116:VAL:HG22	1.99	0.44
1:F:185:ARG:HA	1:F:254:THR:HG23	1.99	0.44
1:D:39:THR:HG23	1:D:63:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:TYR:HA	1:F:116:VAL:HG22	1.99	0.44
1:F:196:THR:H	1:F:199:MET:HB2	1.83	0.44
1:B:222:TRP:HE1	1:B:261:ASP:HB2	1.82	0.44
1:A:39:THR:HG23	1:A:63:LEU:HB3	2.00	0.43
1:B:147:MET:HB3	2:B:1270:PYW:HAM	2.00	0.43
1:A:196:THR:H	1:A:199:MET:HB2	1.84	0.43
1:C:185:ARG:HA	1:C:254:THR:HG23	2.00	0.43
1:B:65:VAL:HG21	1:B:126:SER:HB2	2.00	0.43
1:D:65:VAL:HG21	1:D:126:SER:HB2	2.00	0.43
1:B:185:ARG:HA	1:B:254:THR:HG23	2.01	0.43
1:F:13:SER:HA	1:F:39:THR:HB	2.00	0.43
1:E:185:ARG:HA	1:E:254:THR:HG23	2.01	0.43
1:B:94:ALA:HA	2:B:1270:PYW:HAL	2.01	0.42
1:E:63:LEU:HD13	1:E:74:LEU:HG	2.01	0.42
1:A:258:ILE:HA	3:A:2150:HOH:O	2.17	0.42
1:D:185:ARG:HA	1:D:254:THR:HG23	2.01	0.42
1:A:228:ILE:HG23	3:B:2082:HOH:O	2.21	0.41
1:F:158:TYR:HD1	2:F:1270:PYW:HAA2	1.84	0.41
1:D:26:ALA:HB1	1:D:54:LEU:HD21	2.03	0.41
1:F:245:LEU:HD11	1:F:258:ILE:HG13	2.03	0.41
1:A:65:VAL:HG21	1:A:126:SER:HB2	2.03	0.41
1:F:21:ILE:HG22	1:F:25:ILE:HD11	2.03	0.40
1:A:76:GLY:O	1:A:80:GLU:HG2	2.21	0.40
1:E:216:GLN:HB3	1:E:216:GLN:HE21	1.75	0.40
1:F:202:ILE:HG22	1:F:207:LEU:HB2	2.02	0.40

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	265/269 (98%)	250 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	265/269 (98%)	250 (94%)	13 (5%)	2 (1%)	24	21
1	C	250/269 (93%)	237 (95%)	12 (5%)	1 (0%)	39	43
1	D	248/269 (92%)	234 (94%)	13 (5%)	1 (0%)	39	43
1	E	247/269 (92%)	231 (94%)	14 (6%)	2 (1%)	24	21
1	F	265/269 (98%)	250 (94%)	14 (5%)	1 (0%)	39	43
All	All	1540/1614 (95%)	1452 (94%)	81 (5%)	7 (0%)	34	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	ALA
1	C	159	ASN
1	D	159	ASN
1	E	75	ALA
1	E	159	ASN
1	F	159	ASN
1	B	159	ASN

### 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	202/204 (99%)	184 (91%)	18 (9%)	12	10
1	B	202/204 (99%)	181 (90%)	21 (10%)	9	6
1	C	195/204 (96%)	183 (94%)	12 (6%)	23	22
1	D	193/204 (95%)	179 (93%)	14 (7%)	17	16
1	E	194/204 (95%)	180 (93%)	14 (7%)	18	16
1	F	202/204 (99%)	184 (91%)	18 (9%)	12	10
All	All	1188/1224 (97%)	1091 (92%)	97 (8%)	14	13

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	45	ARG
1	A	48	GLN
1	A	54	LEU
1	A	65	VAL
1	A	67	ASN
1	A	68	GLU
1	A	74	LEU
1	A	121	HIS
1	A	162	THR
1	A	168	LEU
1	A	196	THR
1	A	197	LEU
1	A	207	LEU
1	A	217	LEU
1	A	233	LYS
1	A	254	THR
1	A	269	LEU
1	B	18	ASP
1	B	39	THR
1	B	44	LEU
1	B	45	ARG
1	B	46	LEU
1	B	48	GLN
1	B	54	LEU
1	B	65	VAL
1	B	67	ASN
1	B	68	GLU
1	B	74	LEU
1	B	121	HIS
1	B	162	THR
1	B	168	LEU
1	B	195	ARG
1	B	196	THR
1	B	197	LEU
1	B	207	LEU
1	B	217	LEU
1	B	254	THR
1	B	269	LEU
1	C	41	PHE
1	C	44	LEU
1	C	49	ARG
1	C	60	LEU

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Mol	Chain	Res	Type
1	C	65	VAL
1	C	67	ASN
1	C	95	ILE
1	C	162	THR
1	C	217	LEU
1	C	218	LEU
1	C	254	THR
1	C	269	LEU
1	D	16	ILE
1	D	39	THR
1	D	48	GLN
1	D	54	LEU
1	D	65	VAL
1	D	67	ASN
1	D	68	GLU
1	D	121	HIS
1	D	162	THR
1	D	168	LEU
1	D	217	LEU
1	D	233	LYS
1	D	254	THR
1	D	269	LEU
1	E	39	THR
1	E	48	GLN
1	E	54	LEU
1	E	65	VAL
1	E	67	ASN
1	E	68	GLU
1	E	74	LEU
1	E	162	THR
1	E	168	LEU
1	E	181	LYS
1	E	217	LEU
1	E	218	LEU
1	E	222	TRP
1	E	254	THR
1	F	18	ASP
1	F	48	GLN
1	F	49	ARG
1	F	54	LEU
1	F	60	LEU
1	F	67	ASN

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Mol	Chain	Res	Type
1	F	68	GLU
1	F	158	TYR
1	F	162	THR
1	F	168	LEU
1	F	196	THR
1	F	197	LEU
1	F	207	LEU
1	F	210	GLU
1	F	217	LEU
1	F	233	LYS
1	F	254	THR
1	F	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	48	GLN
1	A	67	ASN
1	A	187	ASN
1	A	216	GLN
1	B	67	ASN
1	B	187	ASN
1	C	32	GLN
1	C	67	ASN
1	C	187	ASN
1	D	32	GLN
1	D	67	ASN
1	D	121	HIS
1	D	187	ASN
1	E	32	GLN
1	E	67	ASN
1	E	121	HIS
1	E	187	ASN
1	E	216	GLN
1	F	24	HIS
1	F	32	GLN
1	F	35	GLN
1	F	187	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	PYW	A	1270	-	39,41,41	1.61	4 (10%)	47,57,57	1.36	7 (14%)
2	PYW	B	1270	-	39,41,41	1.58	5 (12%)	47,57,57	1.30	5 (10%)
2	PYW	C	1270	-	39,41,41	1.59	7 (17%)	47,57,57	1.35	3 (6%)
2	PYW	D	1270	-	39,41,41	1.56	4 (10%)	47,57,57	1.27	4 (8%)
2	PYW	E	1270	-	39,41,41	1.51	5 (12%)	47,57,57	1.35	6 (12%)
2	PYW	F	1270	-	39,41,41	1.60	6 (15%)	47,57,57	1.20	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PYW	A	1270	-	-	2/52/54/54	0/2/3/3
2	PYW	B	1270	-	-	2/52/54/54	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PYW	C	1270	-	-	1/52/54/54	0/2/3/3
2	PYW	D	1270	-	-	4/52/54/54	0/2/3/3
2	PYW	E	1270	-	-	0/52/54/54	0/2/3/3
2	PYW	F	1270	-	-	4/52/54/54	0/2/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1270	PYW	CAQ-NAT	2.03	1.38	1.34
2	E	1270	PYW	CBG-CBH	2.06	1.43	1.40
2	C	1270	PYW	CBG-CBH	2.19	1.43	1.40
2	F	1270	PYW	CAQ-CBF	2.22	1.42	1.38
2	C	1270	PYW	CBH-NAU	2.23	1.38	1.34
2	B	1270	PYW	CBB-N	2.27	1.39	1.34
2	A	1270	PYW	CAQ-CBF	2.28	1.42	1.38
2	B	1270	PYW	CBG-CBH	2.30	1.43	1.40
2	A	1270	PYW	C-NAV	2.34	1.39	1.34
2	C	1270	PYW	C-NAV	2.41	1.39	1.34
2	F	1270	PYW	CBH-NAU	2.49	1.39	1.34
2	F	1270	PYW	CBB-N	2.51	1.39	1.34
2	F	1270	PYW	CBG-CBH	2.51	1.44	1.40
2	D	1270	PYW	CBB-N	2.52	1.39	1.34
2	C	1270	PYW	CBB-N	2.63	1.40	1.34
2	E	1270	PYW	CBB-N	2.66	1.40	1.34
2	D	1270	PYW	CBG-CBH	2.68	1.44	1.40
2	B	1270	PYW	C-NAV	2.75	1.40	1.34
2	B	1270	PYW	CAQ-CBF	2.75	1.43	1.38
2	D	1270	PYW	CAQ-CBF	2.77	1.43	1.38
2	F	1270	PYW	C-NAV	2.90	1.40	1.34
2	A	1270	PYW	CBG-CBH	3.00	1.44	1.40
2	E	1270	PYW	CAQ-CBF	3.02	1.43	1.38
2	E	1270	PYW	C-NAV	3.09	1.41	1.34
2	C	1270	PYW	CAQ-CBF	3.22	1.43	1.38
2	E	1270	PYW	CAZ-CBE	5.37	1.39	1.33
2	D	1270	PYW	CAZ-CBE	6.01	1.39	1.33
2	C	1270	PYW	CAZ-CBE	6.26	1.40	1.33
2	B	1270	PYW	CAZ-CBE	6.34	1.40	1.33
2	F	1270	PYW	CAZ-CBE	6.62	1.40	1.33
2	A	1270	PYW	CAZ-CBE	7.24	1.41	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1270	PYW	OG1-CBA-CBE	-2.08	108.80	111.45
2	E	1270	PYW	C-CA-N	-2.07	104.96	110.59
2	A	1270	PYW	C-CA-N	-2.03	105.08	110.59
2	F	1270	PYW	CBK-CBJ-CBD	2.02	114.42	109.95
2	D	1270	PYW	OAE-CBA-CBE	2.03	128.37	123.37
2	B	1270	PYW	CBK-CBJ-CBD	2.09	114.58	109.95
2	A	1270	PYW	CB-CA-C	2.11	114.81	110.44
2	C	1270	PYW	OAE-CBA-CBE	2.12	128.59	123.37
2	D	1270	PYW	CB-CA-C	2.14	114.87	110.44
2	B	1270	PYW	CBD-OAX-CBE	2.16	121.82	117.71
2	A	1270	PYW	OAF-CBB-CBH	2.23	124.03	121.00
2	E	1270	PYW	CBK-CBJ-CBD	2.24	114.92	109.95
2	B	1270	PYW	CBJ-CBK-CBL	2.32	116.95	113.52
2	F	1270	PYW	CB-CA-C	2.36	115.33	110.44
2	B	1270	PYW	CAZ-CBE-CBA	2.37	126.31	124.25
2	A	1270	PYW	CBK-CBJ-CBD	2.38	115.23	109.95
2	E	1270	PYW	CA-N-CBB	2.62	126.84	121.43
2	A	1270	PYW	CBD-OAX-CBE	3.04	123.49	117.71
2	F	1270	PYW	CAZ-CBE-CBA	3.31	127.13	124.25
2	A	1270	PYW	CAZ-CBE-CBA	3.57	127.35	124.25
2	D	1270	PYW	CAZ-CBE-CBA	3.71	127.47	124.25
2	E	1270	PYW	CAZ-CBE-CBA	3.88	127.62	124.25
2	C	1270	PYW	CAZ-CBE-CBA	4.47	128.13	124.25
2	F	1270	PYW	CB-OG1-CBA	4.49	122.75	117.44
2	D	1270	PYW	CB-OG1-CBA	4.85	123.17	117.44
2	A	1270	PYW	CB-OG1-CBA	4.92	123.25	117.44
2	E	1270	PYW	CB-OG1-CBA	5.35	123.75	117.44
2	C	1270	PYW	CB-OG1-CBA	5.41	123.83	117.44
2	B	1270	PYW	CB-OG1-CBA	5.46	123.89	117.44

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1270	PYW	NAU-CBH-CBB-N
2	B	1270	PYW	NAU-CBH-CBB-N
2	F	1270	PYW	OAF-CBB-CBH-NAU
2	A	1270	PYW	NAU-CBH-CBB-N
2	F	1270	PYW	OAF-CBB-CBH-CBG
2	D	1270	PYW	OAF-CBB-CBH-CBG
2	D	1270	PYW	OAF-CBB-CBH-NAU
2	B	1270	PYW	CBG-CBH-CBB-N
2	A	1270	PYW	CBG-CBH-CBB-N

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Mol	Chain	Res	Type	Atoms
2	F	1270	PYW	CBG-CBH-CBB-N
2	F	1270	PYW	NAU-CBH-CBB-N
2	D	1270	PYW	NAU-CBH-CBB-N
2	D	1270	PYW	CBG-CBH-CBB-N

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1270	PYW	1	0
2	B	1270	PYW	3	0
2	D	1270	PYW	1	0
2	E	1270	PYW	1	0
2	F	1270	PYW	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 ⓘ

### 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	267/269 (99%)	0.88	27 (10%) 9 10	6, 22, 50, 66	0
1	B	267/269 (99%)	0.86	34 (12%) 5 5	5, 20, 54, 76	0
1	C	254/269 (94%)	1.32	59 (23%) 1 1	14, 36, 59, 77	0
1	D	252/269 (93%)	1.28	42 (16%) 2 2	17, 35, 58, 76	0
1	E	251/269 (93%)	1.48	55 (21%) 1 1	16, 36, 63, 75	0
1	F	267/269 (99%)	1.49	71 (26%) 1 1	17, 38, 63, 74	0
All	All	1558/1614 (96%)	1.21	288 (18%) 2 1	5, 32, 60, 77	0

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	214	GLN	7.1
1	E	217	LEU	6.8
1	E	196	THR	6.6
1	F	203	VAL	6.4
1	A	198	ALA	6.2
1	F	82	ILE	6.2
1	A	46	LEU	6.0
1	C	3	GLY	5.8
1	B	50	ILE	5.7
1	C	45	ARG	5.6
1	D	15	ILE	5.5
1	E	74	LEU	5.5
1	A	202	ILE	5.1
1	A	207	LEU	5.0
1	D	215	ILE	5.0
1	F	50	ILE	5.0
1	F	197	LEU	5.0
1	C	41	PHE	4.9
1	F	16	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	202	ILE	4.8
1	A	47	ILE	4.7
1	B	41	PHE	4.7
1	F	47	ILE	4.7
1	E	213	ALA	4.6
1	E	219	GLU	4.6
1	C	50	ILE	4.6
1	B	197	LEU	4.6
1	F	211	ALA	4.5
1	D	41	PHE	4.5
1	B	43	ARG	4.4
1	F	198	ALA	4.4
1	B	46	LEU	4.3
1	A	41	PHE	4.3
1	A	203	VAL	4.3
1	E	57	LYS	4.3
1	C	16	ILE	4.2
1	D	236	THR	4.2
1	D	44	LEU	4.2
1	D	105	ILE	4.1
1	C	40	GLY	3.9
1	E	46	LEU	3.9
1	E	40	GLY	3.9
1	E	82	ILE	3.9
1	D	214	GLN	3.8
1	F	81	ALA	3.8
1	E	72	ALA	3.8
1	F	212	GLY	3.8
1	B	202	ILE	3.8
1	D	43	ARG	3.8
1	F	204	GLY	3.8
1	C	15	ILE	3.8
1	F	12	VAL	3.8
1	C	57	LYS	3.8
1	E	218	LEU	3.8
1	F	84	ALA	3.8
1	F	57	LYS	3.7
1	C	195	ARG	3.7
1	E	42	ASP	3.7
1	E	49	ARG	3.6
1	B	196	THR	3.6
1	E	84	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	44	LEU	3.6
1	C	235	ALA	3.5
1	D	233	LYS	3.5
1	F	43	ARG	3.4
1	D	218	LEU	3.4
1	F	61	LEU	3.4
1	F	65	VAL	3.4
1	B	201	ALA	3.4
1	F	105	ILE	3.4
1	C	58	ALA	3.4
1	B	42	ASP	3.4
1	C	42	ASP	3.4
1	B	47	ILE	3.3
1	E	67	ASN	3.3
1	A	42	ASP	3.3
1	D	217	LEU	3.3
1	E	238	VAL	3.3
1	C	54	LEU	3.3
1	F	20	SER	3.2
1	B	207	LEU	3.2
1	C	232	MET	3.2
1	D	82	ILE	3.2
1	B	7	GLY	3.2
1	E	51	THR	3.2
1	F	21	ILE	3.1
1	C	82	ILE	3.1
1	C	194	ILE	3.1
1	E	50	ILE	3.1
1	C	149	PHE	3.1
1	C	21	ILE	3.1
1	E	5	LEU	3.1
1	D	232	MET	3.0
1	D	81	ALA	3.0
1	C	85	GLY	3.0
1	C	39	THR	3.0
1	F	19	SER	3.0
1	E	116	VAL	3.0
1	F	44	LEU	3.0
1	F	199	MET	3.0
1	A	49	ARG	3.0
1	E	79	THR	3.0
1	E	224	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	218	LEU	2.9
1	A	57	LYS	2.9
1	C	213	ALA	2.9
1	E	75	ALA	2.9
1	F	207	LEU	2.9
1	A	157	ALA	2.9
1	C	84	ALA	2.9
1	B	195	ARG	2.9
1	D	112	PRO	2.9
1	E	17	THR	2.8
1	F	196	THR	2.8
1	B	48	GLN	2.8
1	C	46	LEU	2.8
1	D	57	LYS	2.8
1	F	83	GLY	2.8
1	C	6	ASP	2.8
1	C	52	ASP	2.8
1	A	44	LEU	2.8
1	F	80	GLU	2.8
1	F	233	LYS	2.8
1	F	201	ALA	2.8
1	F	101	THR	2.8
1	E	27	ARG	2.8
1	D	16	ILE	2.8
1	D	97	PHE	2.8
1	E	44	LEU	2.8
1	B	204	GLY	2.8
1	D	213	ALA	2.8
1	A	19	SER	2.8
1	E	137	ILE	2.8
1	C	25	ILE	2.8
1	C	130	MET	2.8
1	D	5	LEU	2.8
1	F	63	LEU	2.8
1	A	43	ARG	2.7
1	E	229	GLY	2.7
1	C	51	THR	2.7
1	A	197	LEU	2.7
1	F	49	ARG	2.7
1	D	238	VAL	2.7
1	C	47	ILE	2.7
1	E	134	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	41	PHE	2.7
1	A	196	THR	2.7
1	E	258	ILE	2.7
1	A	199	MET	2.7
1	D	235	ALA	2.7
1	C	38	LEU	2.6
1	F	60	LEU	2.6
1	D	216	GLN	2.6
1	D	85	GLY	2.6
1	F	41	PHE	2.6
1	D	184	VAL	2.6
1	A	84	ALA	2.6
1	F	74	LEU	2.6
1	F	184	VAL	2.6
1	E	70	HIS	2.6
1	B	84	ALA	2.6
1	B	203	VAL	2.6
1	B	217	LEU	2.6
1	E	88	LEU	2.6
1	F	90	GLY	2.5
1	B	218	LEU	2.5
1	C	74	LEU	2.5
1	C	250	LEU	2.5
1	F	75	ALA	2.5
1	C	215	ILE	2.5
1	A	21	ILE	2.5
1	E	21	ILE	2.5
1	A	35	GLN	2.5
1	C	88	LEU	2.5
1	E	80	GLU	2.5
1	F	46	LEU	2.5
1	C	113	TYR	2.4
1	E	47	ILE	2.4
1	E	105	ILE	2.4
1	E	58	ALA	2.4
1	E	241	THR	2.4
1	F	234	ASP	2.4
1	C	132	LYS	2.4
1	C	228	ILE	2.4
1	C	19	SER	2.4
1	A	201	ALA	2.4
1	F	243	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	14	GLY	2.4
1	E	56	ALA	2.4
1	A	52	ASP	2.4
1	B	200	SER	2.4
1	F	213	ALA	2.4
1	C	214	GLN	2.4
1	B	40	GLY	2.3
1	F	145	VAL	2.3
1	D	157	ALA	2.3
1	E	83	GLY	2.3
1	B	232	MET	2.3
1	D	54	LEU	2.3
1	F	88	LEU	2.3
1	E	53	ARG	2.3
1	F	31	GLU	2.3
1	F	59	PRO	2.3
1	C	217	LEU	2.3
1	E	38	LEU	2.3
1	C	95	ILE	2.3
1	C	256	ASP	2.3
1	E	215	ILE	2.3
1	B	235	ALA	2.3
1	C	61	LEU	2.3
1	C	43	ARG	2.3
1	E	71	LEU	2.3
1	B	215	ILE	2.2
1	C	34	ALA	2.2
1	C	162	THR	2.2
1	E	103	MET	2.2
1	D	182	TYR	2.2
1	F	106	ASN	2.2
1	B	234	ASP	2.2
1	F	79	THR	2.2
1	E	13	SER	2.2
1	F	194	ILE	2.2
1	B	216	GLN	2.2
1	C	109	PHE	2.2
1	F	40	GLY	2.2
1	D	52	ASP	2.2
1	F	25	ILE	2.2
1	E	174	PHE	2.2
1	D	42	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	205	GLY	2.2
1	B	198	ALA	2.2
1	F	45	ARG	2.2
1	C	268	LEU	2.2
1	F	17	THR	2.2
1	D	223	ASP	2.1
1	C	255	GLY	2.1
1	D	60	LEU	2.1
1	C	56	ALA	2.1
1	F	64	ASP	2.1
1	B	21	ILE	2.1
1	E	100	GLN	2.1
1	A	217	LEU	2.1
1	B	199	MET	2.1
1	F	36	LEU	2.1
1	F	232	MET	2.1
1	E	18	ASP	2.1
1	D	219	GLU	2.1
1	D	65	VAL	2.1
1	F	136	PRO	2.1
1	B	52	ASP	2.1
1	C	230	TRP	2.1
1	A	60	LEU	2.1
1	C	35	GLN	2.1
1	F	4	LEU	2.1
1	F	51	THR	2.1
1	D	262	GLY	2.1
1	B	53	ARG	2.1
1	F	42	ASP	2.1
1	E	127	TYR	2.1
1	A	233	LYS	2.1
1	C	26	ALA	2.1
1	F	220	GLU	2.1
1	C	55	PRO	2.1
1	F	215	ILE	2.1
1	D	248	ASP	2.1
1	D	70	HIS	2.1
1	D	170	SER	2.1
1	C	210	GLU	2.0
1	F	77	ARG	2.0
1	B	60	LEU	2.0
1	E	182	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	16	ILE	2.0
1	D	12	VAL	2.0
1	C	18	ASP	2.0
1	D	61	LEU	2.0
1	F	72	ALA	2.0
1	F	131	ALA	2.0
1	D	80	GLU	2.0
1	A	45	ARG	2.0
1	B	49	ARG	2.0
1	F	195	ARG	2.0
1	F	15	ILE	2.0
1	B	57	LYS	2.0
1	F	68	GLU	2.0
1	A	61	LEU	2.0
1	C	24	HIS	2.0
1	C	49	ARG	2.0
1	E	45	ARG	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PYW	F	1270	39/39	0.81	0.24	0.18	30,36,45,46	0
2	PYW	C	1270	39/39	0.84	0.20	0.03	20,30,36,37	0
2	PYW	E	1270	39/39	0.79	0.21	-0.18	26,32,40,42	0
2	PYW	B	1270	39/39	0.86	0.18	-0.18	7,15,28,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PYW	D	1270	39/39	0.86	0.17	-0.37	15,22,29,30	0
2	PYW	A	1270	39/39	0.86	0.17	-0.39	8,16,22,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.