



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:09 PM GMT

PDB ID : 4BO2  
Title : Crystal structure of 3-oxoacyl-(acyl-carrier-protein) reductase (FabG) from *Pseudomonas aeruginosa* in complex with 1-(1-ethylbenzimidazol-2-yl)-3-(2-methoxyphenyl)urea at 1.9Å resolution  
Authors : Cukier, C.D.; Schnell, R.; Lindqvist, Y.; Schneider, G.  
Deposited on : 2013-05-18  
Resolution : 1.90 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

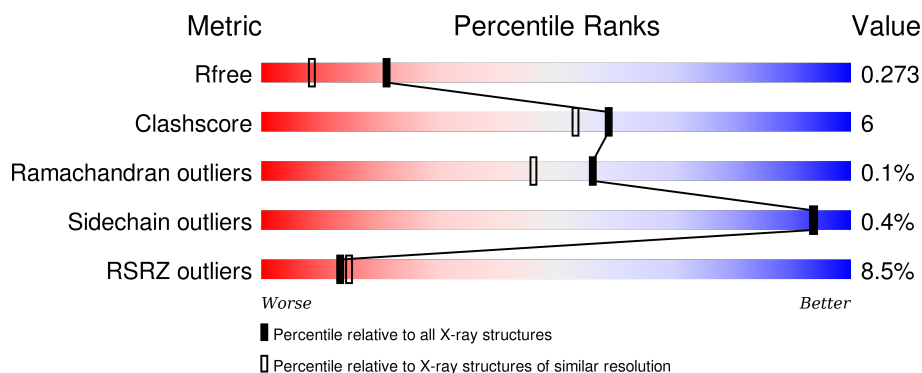
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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>8%</div> <div>78%10%12%</div> </div>
1	B	269	<div> <div>8%</div> <div>78%9%13%</div> </div>
1	C	269	<div> <div>9%</div> <div>83%6%11%</div> </div>
1	D	269	<div> <div>6%</div> <div>86%.9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	36K	A	1248[A]	-	-	X	X
2	36K	A	1248[B]	-	-	X	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7250 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] REDUCTASE FABG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	3	0
			1740	1089	308	337	6			
1	B	235	Total	C	N	O	S	0	2	0
			1704	1066	304	329	5			
1	C	240	Total	C	N	O	S	0	1	0
			1745	1092	310	337	6			
1	D	245	Total	C	N	O	S	0	1	0
			1789	1117	319	346	7			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP O54438
A	-20	HIS	-	EXPRESSION TAG	UNP O54438
A	-19	HIS	-	EXPRESSION TAG	UNP O54438
A	-18	HIS	-	EXPRESSION TAG	UNP O54438
A	-17	HIS	-	EXPRESSION TAG	UNP O54438
A	-16	HIS	-	EXPRESSION TAG	UNP O54438
A	-15	HIS	-	EXPRESSION TAG	UNP O54438
A	-14	SER	-	EXPRESSION TAG	UNP O54438
A	-13	SER	-	EXPRESSION TAG	UNP O54438
A	-12	GLY	-	EXPRESSION TAG	UNP O54438
A	-11	VAL	-	EXPRESSION TAG	UNP O54438
A	-10	ASP	-	EXPRESSION TAG	UNP O54438
A	-9	LEU	-	EXPRESSION TAG	UNP O54438
A	-8	GLY	-	EXPRESSION TAG	UNP O54438
A	-7	THR	-	EXPRESSION TAG	UNP O54438
A	-6	GLU	-	EXPRESSION TAG	UNP O54438
A	-5	ASN	-	EXPRESSION TAG	UNP O54438
A	-4	LEU	-	EXPRESSION TAG	UNP O54438
A	-3	TYR	-	EXPRESSION TAG	UNP O54438
A	-2	PHE	-	EXPRESSION TAG	UNP O54438

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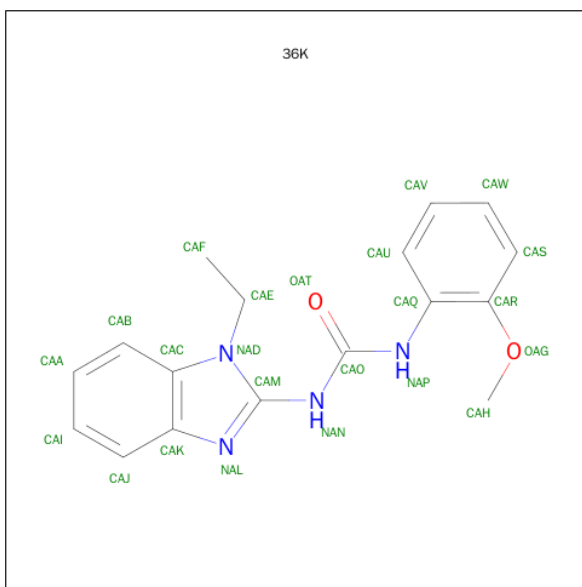
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	EXPRESSION TAG	UNP O54438
A	0	SER	-	EXPRESSION TAG	UNP O54438
B	-21	MET	-	EXPRESSION TAG	UNP O54438
B	-20	HIS	-	EXPRESSION TAG	UNP O54438
B	-19	HIS	-	EXPRESSION TAG	UNP O54438
B	-18	HIS	-	EXPRESSION TAG	UNP O54438
B	-17	HIS	-	EXPRESSION TAG	UNP O54438
B	-16	HIS	-	EXPRESSION TAG	UNP O54438
B	-15	HIS	-	EXPRESSION TAG	UNP O54438
B	-14	SER	-	EXPRESSION TAG	UNP O54438
B	-13	SER	-	EXPRESSION TAG	UNP O54438
B	-12	GLY	-	EXPRESSION TAG	UNP O54438
B	-11	VAL	-	EXPRESSION TAG	UNP O54438
B	-10	ASP	-	EXPRESSION TAG	UNP O54438
B	-9	LEU	-	EXPRESSION TAG	UNP O54438
B	-8	GLY	-	EXPRESSION TAG	UNP O54438
B	-7	THR	-	EXPRESSION TAG	UNP O54438
B	-6	GLU	-	EXPRESSION TAG	UNP O54438
B	-5	ASN	-	EXPRESSION TAG	UNP O54438
B	-4	LEU	-	EXPRESSION TAG	UNP O54438
B	-3	TYR	-	EXPRESSION TAG	UNP O54438
B	-2	PHE	-	EXPRESSION TAG	UNP O54438
B	-1	GLN	-	EXPRESSION TAG	UNP O54438
B	0	SER	-	EXPRESSION TAG	UNP O54438
C	-21	MET	-	EXPRESSION TAG	UNP O54438
C	-20	HIS	-	EXPRESSION TAG	UNP O54438
C	-19	HIS	-	EXPRESSION TAG	UNP O54438
C	-18	HIS	-	EXPRESSION TAG	UNP O54438
C	-17	HIS	-	EXPRESSION TAG	UNP O54438
C	-16	HIS	-	EXPRESSION TAG	UNP O54438
C	-15	HIS	-	EXPRESSION TAG	UNP O54438
C	-14	SER	-	EXPRESSION TAG	UNP O54438
C	-13	SER	-	EXPRESSION TAG	UNP O54438
C	-12	GLY	-	EXPRESSION TAG	UNP O54438
C	-11	VAL	-	EXPRESSION TAG	UNP O54438
C	-10	ASP	-	EXPRESSION TAG	UNP O54438
C	-9	LEU	-	EXPRESSION TAG	UNP O54438
C	-8	GLY	-	EXPRESSION TAG	UNP O54438
C	-7	THR	-	EXPRESSION TAG	UNP O54438
C	-6	GLU	-	EXPRESSION TAG	UNP O54438
C	-5	ASN	-	EXPRESSION TAG	UNP O54438
C	-4	LEU	-	EXPRESSION TAG	UNP O54438

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	TYR	-	EXPRESSION TAG	UNP O54438
C	-2	PHE	-	EXPRESSION TAG	UNP O54438
C	-1	GLN	-	EXPRESSION TAG	UNP O54438
C	0	SER	-	EXPRESSION TAG	UNP O54438
D	-21	MET	-	EXPRESSION TAG	UNP O54438
D	-20	HIS	-	EXPRESSION TAG	UNP O54438
D	-19	HIS	-	EXPRESSION TAG	UNP O54438
D	-18	HIS	-	EXPRESSION TAG	UNP O54438
D	-17	HIS	-	EXPRESSION TAG	UNP O54438
D	-16	HIS	-	EXPRESSION TAG	UNP O54438
D	-15	HIS	-	EXPRESSION TAG	UNP O54438
D	-14	SER	-	EXPRESSION TAG	UNP O54438
D	-13	SER	-	EXPRESSION TAG	UNP O54438
D	-12	GLY	-	EXPRESSION TAG	UNP O54438
D	-11	VAL	-	EXPRESSION TAG	UNP O54438
D	-10	ASP	-	EXPRESSION TAG	UNP O54438
D	-9	LEU	-	EXPRESSION TAG	UNP O54438
D	-8	GLY	-	EXPRESSION TAG	UNP O54438
D	-7	THR	-	EXPRESSION TAG	UNP O54438
D	-6	GLU	-	EXPRESSION TAG	UNP O54438
D	-5	ASN	-	EXPRESSION TAG	UNP O54438
D	-4	LEU	-	EXPRESSION TAG	UNP O54438
D	-3	TYR	-	EXPRESSION TAG	UNP O54438
D	-2	PHE	-	EXPRESSION TAG	UNP O54438
D	-1	GLN	-	EXPRESSION TAG	UNP O54438
D	0	SER	-	EXPRESSION TAG	UNP O54438

- Molecule 2 is 1-(1-ETHYLBENZIMIDAZOL-2-YL)-3-(2-METHOXYPHENYL)UREA (three-letter code: 36K) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			46	34	8	4		
2	C	1	Total	C	N	O	0	0
			23	17	4	2		

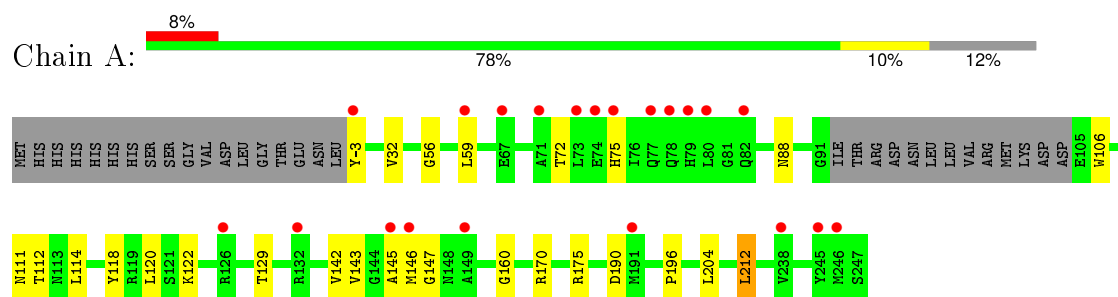
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	48	Total	O	0	0
			48	48		
3	C	43	Total	O	0	0
			43	43		
3	D	57	Total	O	0	0
			57	57		

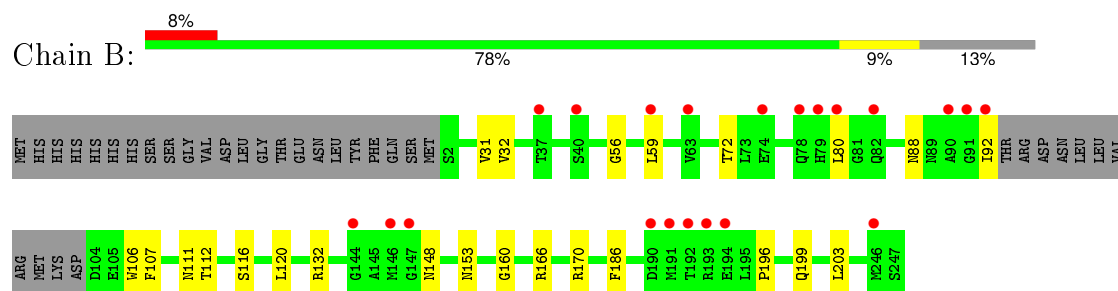
### 3 Residue-property plots [i](#)

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.

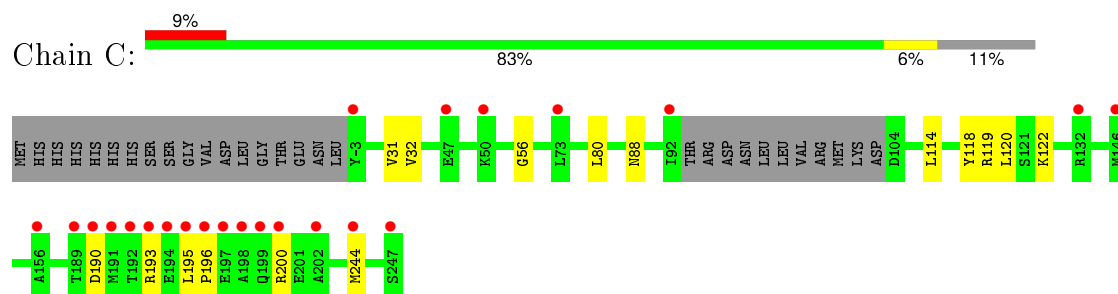
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



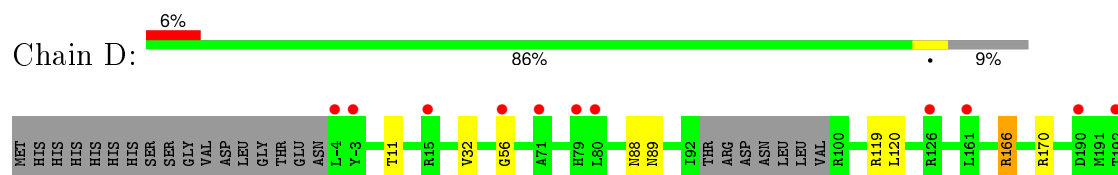
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



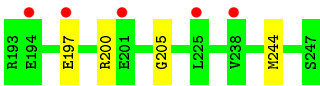
#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG



#### • Molecule 1: 3-OXOACYL-[ACYL-CARRIER-PROTEIN] REDUCTASE FABG







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.55Å 108.92Å 149.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.56 – 1.90 38.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.3 (38.56-1.90) 87.3 (38.53-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.235 , 0.269 0.240 , 0.273	Depositor DCC
$R_{free}$ test set	3401 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	18 of 66563 reflections (0.027%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 36K

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	0.80	0/1768	0.84	2/2392 (0.1%)
1	B	0.85	0/1727	0.87	2/2338 (0.1%)
1	C	0.82	0/1767	0.82	2/2391 (0.1%)
1	D	0.82	0/1811	0.87	4/2448 (0.2%)
All	All	0.82	0/7073	0.85	10/9569 (0.1%)

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	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	244	MET	CG-SD-CE	5.88	109.61	100.20
1	A	170	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	D	244	MET	CG-SD-CE	5.60	109.16	100.20
1	D	170	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	212	LEU	CB-CG-CD2	5.44	120.25	111.00
1	C	119	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	132	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	170	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	170	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	GLY	Peptide

## 5.2 Too-close contacts

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	1740	0	1775	22	0
1	B	1704	0	1748	19	0
1	C	1745	0	1780	11	0
1	D	1789	0	1823	6	0
2	A	46	0	36	31	0
2	C	23	0	18	5	0
3	A	55	0	0	3	0
3	B	48	0	0	1	0
3	C	43	0	0	0	0
3	D	57	0	0	0	0
All	All	7250	0	7180	82	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 6.

All (82) 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)
2:A:1248[B]:36K:HAP	2:A:1248[B]:36K:CAH	1.29	1.43
2:A:1248[B]:36K:HAB	2:A:1248[B]:36K:CAF	1.64	1.27
2:A:1248[B]:36K:CAU	2:A:1248[B]:36K:HAN	1.34	1.21
2:A:1248[A]:36K:HAN	2:A:1248[A]:36K:CAU	1.43	1.14
1:A:59[B]:LEU:HD21	1:A:72:THR:HG23	1.24	1.10
2:A:1248[B]:36K:HAU	2:A:1248[B]:36K:NAN	1.37	1.08
1:B:59[B]:LEU:HD21	1:B:72:THR:CG2	1.83	1.06
2:A:1248[B]:36K:HAB	2:A:1248[B]:36K:HAF2	1.35	1.06
2:A:1248[B]:36K:HAF3	2:A:1248[B]:36K:HAB	1.36	1.06
2:A:1248[B]:36K:HAH2	2:A:1248[B]:36K:HAP	0.92	1.04
2:A:1248[B]:36K:HAH2	2:A:1248[B]:36K:NAP	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59[B]:LEU:CD2	1:B:72:THR:HG23	1.88	1.02
2:A:1248[A]:36K:NAN	2:A:1248[A]:36K:HAU	1.51	1.02
2:A:1248[B]:36K:HAP	2:A:1248[B]:36K:HAH3	1.25	1.00
2:A:1248[A]:36K:HAF2	2:A:1248[A]:36K:OAT	1.62	1.00
2:A:1248[B]:36K:NAP	2:A:1248[B]:36K:CAH	2.00	0.99
1:A:59[B]:LEU:CD2	1:A:72:THR:HG23	1.92	0.99
2:A:1248[B]:36K:CAB	2:A:1248[B]:36K:CAF	2.35	0.90
1:B:59[B]:LEU:HD21	1:B:72:THR:HG23	0.93	0.88
2:A:1248[A]:36K:HAU	2:A:1248[A]:36K:HAN	0.66	0.83
2:A:1248[B]:36K:HAF2	2:A:1248[B]:36K:CAB	2.05	0.81
2:A:1248[A]:36K:CAF	2:A:1248[A]:36K:OAT	2.30	0.80
2:A:1248[B]:36K:NAP	2:A:1248[B]:36K:HAH3	1.87	0.78
2:A:1248[B]:36K:HAF3	2:A:1248[B]:36K:CAB	2.06	0.77
1:D:197:GLU:OE2	1:D:200:ARG:NH1	2.19	0.76
2:A:1248[B]:36K:HAN	2:A:1248[B]:36K:HAU	0.59	0.75
2:A:1248[A]:36K:CAE	2:A:1248[A]:36K:OAT	2.43	0.67
2:A:1248[A]:36K:HAH1	1:B:107:PHE:CE1	2.34	0.63
2:A:1248[B]:36K:CAU	2:A:1248[B]:36K:NAN	2.08	0.62
1:A:160:GLY:HA2	2:A:1248[B]:36K:HAE2	1.82	0.62
1:C:193:ARG:O	1:C:200:ARG:NH2	2.33	0.61
1:A:-3:TYR:CD2	3:A:2001:HOH:O	2.52	0.60
1:A:204:LEU:HD21	1:A:212:LEU:HD12	1.84	0.59
1:B:92:ILE:HG13	1:B:112:THR:HG22	1.82	0.59
2:A:1248[B]:36K:NAL	2:A:1248[B]:36K:OAT	2.26	0.58
1:A:118:TYR:OH	1:A:122:LYS:HE3	2.05	0.57
1:C:195:LEU:HG	1:C:196:PRO:HD2	1.85	0.57
1:B:148:ASN:ND2	1:D:205:GLY:O	2.26	0.55
2:A:1248[B]:36K:HAE1	1:B:160:GLY:HA2	1.90	0.54
1:A:114:LEU:HD13	2:A:1248[A]:36K:HAH2	1.90	0.52
1:A:112:THR:HG23	3:A:2018:HOH:O	2.09	0.52
1:A:190:ASP:OD1	1:A:190:ASP:N	2.43	0.52
1:A:204:LEU:HD21	1:A:212:LEU:CD1	2.40	0.52
1:A:112:THR:HA	3:A:2018:HOH:O	2.10	0.52
1:C:118:TYR:OH	1:C:122:LYS:HE2	2.10	0.51
1:B:106:TRP:HB3	1:B:153:ASN:HD22	1.74	0.51
1:C:190:ASP:OD1	1:C:190:ASP:N	2.44	0.50
1:C:114:LEU:HD12	2:C:1248:36K:NAN	2.27	0.49
1:A:32:VAL:O	1:A:56:GLY:HA3	2.13	0.49
1:D:32:VAL:O	1:D:56:GLY:HA3	2.11	0.49
2:A:1248[B]:36K:HAH1	1:B:111:ASN:HB2	1.96	0.48
1:B:31:VAL:HG11	1:B:80:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PRO:HD2	1:B:199:GLN:HG3	1.94	0.48
1:A:106:TRP:CZ3	2:A:1248[B]:36K:HAI	2.50	0.47
1:C:32:VAL:O	1:C:56:GLY:HA3	2.14	0.47
1:A:160:GLY:CA	2:A:1248[B]:36K:HAE2	2.43	0.46
1:A:88:ASN:OD1	1:A:120:LEU:HD23	2.15	0.46
1:B:116:SER:HB2	3:B:2015:HOH:O	2.15	0.46
1:A:111:ASN:OD1	1:B:111:ASN:ND2	2.48	0.46
1:B:59[B]:LEU:CD2	1:B:72:THR:CG2	2.69	0.46
1:C:88:ASN:OD1	1:C:120:LEU:HD23	2.16	0.45
1:B:92:ILE:HG13	1:B:112:THR:CG2	2.47	0.45
2:C:1248:36K:NAL	2:C:1248:36K:NAP	2.61	0.45
1:B:88:ASN:OD1	1:B:120:LEU:HD23	2.17	0.44
1:D:88:ASN:OD1	1:D:120:LEU:HD23	2.18	0.43
1:B:32:VAL:O	1:B:56:GLY:HA3	2.19	0.43
1:B:186:PHE:CD2	1:B:203:LEU:HD11	2.53	0.43
1:D:11:THR:O	1:D:89:ASN:HB3	2.19	0.43
1:A:142:VAL:HG12	1:A:143:VAL:O	2.19	0.43
2:C:1248:36K:OAT	2:C:1248:36K:HAU	2.18	0.42
1:A:59[B]:LEU:HD23	1:A:72:THR:HG23	1.92	0.42
1:A:118:TYR:CZ	1:A:122:LYS:HE3	2.54	0.42
1:C:31:VAL:HG11	1:C:80:LEU:HD22	2.01	0.42
1:B:106:TRP:HB3	1:B:153:ASN:ND2	2.34	0.42
1:C:114:LEU:HD12	2:C:1248:36K:CAO	2.50	0.41
2:A:1248[A]:36K:HAE1	2:A:1248[A]:36K:OAT	2.19	0.41
1:C:114:LEU:CD1	2:C:1248:36K:CAM	2.99	0.41
1:A:129:THR:HG23	1:A:175:ARG:HD3	2.02	0.41
1:A:122:LYS:HA	1:A:122:LYS:HD3	1.76	0.41
1:A:146:MET:HE1	1:A:196:PRO:HD2	2.02	0.41
1:D:166:ARG:HD2	1:D:166:ARG:HH11	1.73	0.40
1:C:118:TYR:CZ	1:C:122:LYS:HE2	2.56	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	237/269 (88%)	232 (98%)	4 (2%)	1 (0%)	39	27
1	B	233/269 (87%)	230 (99%)	3 (1%)	0	100	100
1	C	237/269 (88%)	235 (99%)	2 (1%)	0	100	100
1	D	242/269 (90%)	239 (99%)	3 (1%)	0	100	100
All	All	949/1076 (88%)	936 (99%)	12 (1%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ALA

### 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	175/201 (87%)	174 (99%)	1 (1%)	90	90
1	B	171/201 (85%)	170 (99%)	1 (1%)	90	90
1	C	175/201 (87%)	175 (100%)	0	100	100
1	D	180/201 (90%)	179 (99%)	1 (1%)	90	90
All	All	701/804 (87%)	698 (100%)	3 (0%)	93	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	B	166	ARG
1	D	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	214	GLN
1	B	153	ASN
1	B	214	GLN
1	C	19	GLN
1	C	206	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](#)

3 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	36K	A	1248[A]	-	21,25,25	2.26	5 (23%)	27,34,34	2.90	6 (22%)
2	36K	A	1248[B]	-	21,25,25	2.16	6 (28%)	27,34,34	2.92	4 (14%)
2	36K	C	1248	-	21,25,25	2.00	6 (28%)	27,34,34	2.68	8 (29%)

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	36K	A	1248[A]	-	-	0/10/12/12	0/3/3/3
2	36K	A	1248[B]	-	-	3/10/12/12	0/3/3/3
2	36K	C	1248	-	-	0/10/12/12	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1248[B]	36K	CAJ-CAK	-6.13	1.30	1.41
2	A	1248[A]	36K	CAJ-CAK	-5.94	1.31	1.41
2	C	1248	36K	CAJ-CAK	-5.60	1.31	1.41
2	A	1248[A]	36K	CAB-CAC	-4.97	1.30	1.41
2	A	1248[B]	36K	CAB-CAC	-4.19	1.32	1.41
2	A	1248[A]	36K	CAQ-NAP	-4.14	1.33	1.41
2	A	1248[B]	36K	CAQ-NAP	-3.77	1.34	1.41
2	C	1248	36K	CAQ-NAP	-3.73	1.34	1.41
2	A	1248[B]	36K	CAC-CAK	-2.99	1.34	1.40
2	A	1248[A]	36K	CAC-CAK	-2.96	1.34	1.40
2	A	1248[A]	36K	CAK-NAL	-2.80	1.29	1.39
2	A	1248[B]	36K	CAO-NAP	-2.56	1.32	1.37
2	C	1248	36K	CAC-CAK	-2.38	1.35	1.40
2	A	1248[B]	36K	CAK-NAL	-2.04	1.32	1.39
2	C	1248	36K	CAB-CAC	-2.03	1.36	1.41
2	C	1248	36K	CAI-CAJ	2.88	1.43	1.36
2	C	1248	36K	CAO-NAP	3.03	1.42	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1248[B]	36K	CAM-NAN-CAO	-11.24	115.94	130.19
2	A	1248[A]	36K	CAM-NAN-CAO	-6.66	121.74	130.19
2	A	1248[A]	36K	CAH-OAG-CAR	-6.61	107.51	117.54
2	C	1248	36K	CAM-NAN-CAO	-6.47	121.99	130.19
2	C	1248	36K	OAT-CAO-NAN	-5.61	115.07	123.58
2	A	1248[B]	36K	CAQ-NAP-CAO	-5.03	115.01	125.57
2	A	1248[A]	36K	CAQ-NAP-CAO	-3.56	118.09	125.57
2	A	1248[B]	36K	CAH-OAG-CAR	-3.50	112.24	117.54
2	A	1248[A]	36K	CAA-CAI-CAJ	-2.63	116.62	120.45
2	C	1248	36K	CAI-CAA-CAB	-2.62	116.64	120.45
2	C	1248	36K	CAF-CAE-NAD	-2.51	106.49	111.80
2	A	1248[A]	36K	CAS-CAR-CAQ	2.12	122.65	120.43
2	C	1248	36K	CAB-CAC-CAK	2.28	125.20	121.36
2	C	1248	36K	CAH-OAG-CAR	3.49	122.83	117.54
2	C	1248	36K	NAP-CAO-NAN	4.44	119.51	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1248[B]	36K	CAE-NAD-CAM	7.06	133.70	127.06
2	C	1248	36K	CAE-NAD-CAM	7.73	134.33	127.06
2	A	1248[A]	36K	CAE-NAD-CAM	10.06	136.52	127.06

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1248[B]	36K	CAF-CAE-NAD-CAC
2	A	1248[B]	36K	CAF-CAE-NAD-CAM
2	A	1248[B]	36K	CAH-OAG-CAR-CAQ

There are no ring outliers.

3 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1248[A]	36K	9	0
2	A	1248[B]	36K	22	0
2	C	1248	36K	5	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	238/269 (88%)	0.69	21 (8%)	12 14	20, 36, 69, 91	0
1	B	235/269 (87%)	0.70	21 (8%)	12 13	20, 34, 72, 105	0
1	C	240/269 (89%)	0.66	23 (9%)	10 11	18, 33, 78, 114	0
1	D	245/269 (91%)	0.58	16 (6%)	22 25	19, 34, 66, 92	0
All	All	958/1076 (89%)	0.66	81 (8%)	13 15	18, 34, 71, 114	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	ILE	9.6
1	C	191	MET	7.4
1	C	195	LEU	7.2
1	B	191	MET	7.1
1	A	80	LEU	5.8
1	C	192	THR	5.7
1	C	92	ILE	5.6
1	C	193	ARG	5.4
1	A	146	MET	5.4
1	C	-3	TYR	5.3
1	B	144	GLY	4.9
1	C	190	ASP	4.9
1	B	59[A]	LEU	4.6
1	A	149	ALA	4.5
1	A	75	HIS	3.9
1	C	146	MET	3.8
1	B	192	THR	3.7
1	D	192	THR	3.7
1	C	198	ALA	3.6
1	D	-3	TYR	3.6
1	B	147	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	67	GLU	3.5
1	C	189	THR	3.5
1	D	56	GLY	3.5
1	A	77	GLN	3.5
1	B	80	LEU	3.3
1	D	201	GLU	3.3
1	A	-3	TYR	3.3
1	D	190	ASP	3.2
1	D	80	LEU	3.2
1	D	-4	LEU	3.2
1	C	73[A]	LEU	3.0
1	B	90	ALA	3.0
1	C	194	GLU	3.0
1	C	199	GLN	3.0
1	D	197	GLU	2.9
1	A	59[A]	LEU	2.9
1	B	146	MET	2.9
1	A	78	GLN	2.9
1	C	50	LYS	2.8
1	D	126	ARG	2.8
1	A	73	LEU	2.7
1	A	82	GLN	2.6
1	B	63	VAL	2.6
1	C	202	ALA	2.6
1	D	15	ARG	2.6
1	B	79	HIS	2.6
1	A	245	TYR	2.5
1	C	196	PRO	2.5
1	D	194	GLU	2.4
1	B	78	GLN	2.4
1	A	74	GLU	2.4
1	B	246	MET	2.4
1	C	47	GLU	2.4
1	B	194	GLU	2.4
1	D	79	HIS	2.3
1	A	71	ALA	2.3
1	A	246	MET	2.3
1	C	132	ARG	2.3
1	D	225	LEU	2.3
1	B	193	ARG	2.3
1	B	91	GLY	2.2
1	B	37	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	40	SER	2.2
1	B	190	ASP	2.2
1	D	238	VAL	2.2
1	A	238	VAL	2.2
1	C	200	ARG	2.2
1	A	126	ARG	2.2
1	A	145	ALA	2.1
1	B	74	GLU	2.1
1	C	197	GLU	2.1
1	C	156	ALA	2.1
1	A	79	HIS	2.1
1	A	132	ARG	2.1
1	C	244	MET	2.1
1	A	191	MET	2.1
1	C	247	SER	2.0
1	D	161	LEU	2.0
1	B	82	GLN	2.0
1	D	71	ALA	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	36K	A	1248[A]	23/23	0.90	0.18	2.59	22,34,44,44	23
2	36K	A	1248[B]	23/23	0.90	0.18	2.56	37,42,50,53	23
2	36K	C	1248	23/23	0.93	0.13	-0.37	19,26,31,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.