



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:09 pm GMT

PDB ID : 4RLH  
Title : Crystal structure of enoyl ACP reductase from Burkholderia pseudomallei in complex with AFN-1252  
Authors : Rao, K.N.; Sarah, J.; Anirudha, L.; Subramanya, H.S.  
Deposited on : 2014-10-17  
Resolution : 2.26 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

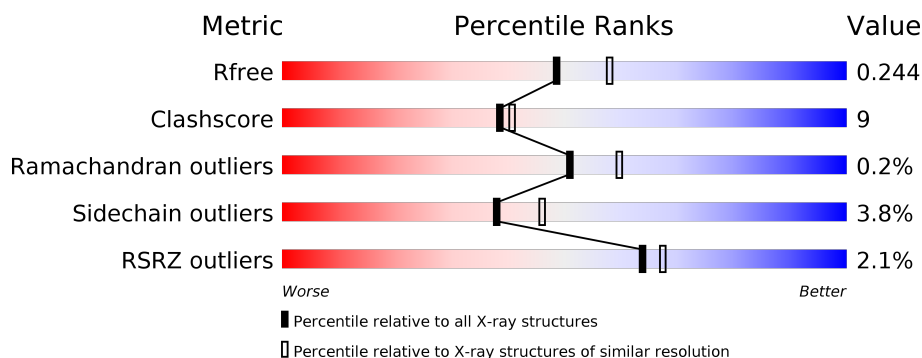
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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))
$R_{free}$	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	272	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	B	272	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	C	272	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	D	272	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 7%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0WE	A	500	-	-	-	X
2	0WE	C	500	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8214 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	253	Total	C	N	O	S	0	0	0
			1877	1196	317	358	6			
1	B	258	Total	C	N	O	S	0	0	0
			1904	1212	322	364	6			
1	D	253	Total	C	N	O	S	0	0	0
			1877	1196	317	358	6			
1	C	258	Total	C	N	O	S	0	0	0
			1903	1212	322	363	6			

There are 36 discrepancies between the modelled and reference sequences:

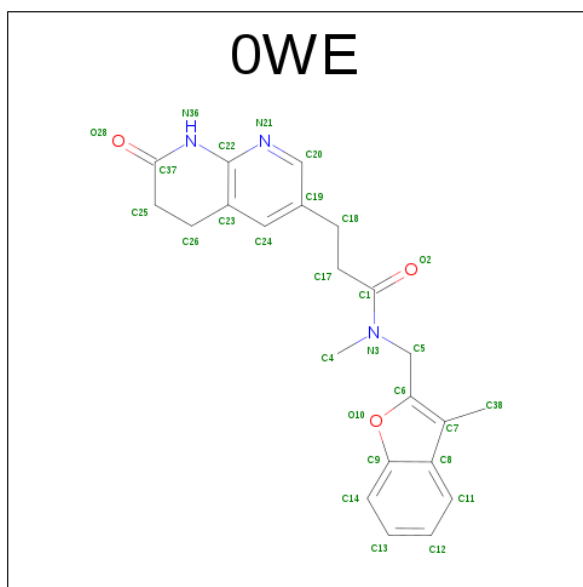
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q63SW7
A	-7	MET	-	EXPRESSION TAG	UNP Q63SW7
A	-6	ALA	-	EXPRESSION TAG	UNP Q63SW7
A	-5	HIS	-	EXPRESSION TAG	UNP Q63SW7
A	-4	HIS	-	EXPRESSION TAG	UNP Q63SW7
A	-3	HIS	-	EXPRESSION TAG	UNP Q63SW7
A	-2	HIS	-	EXPRESSION TAG	UNP Q63SW7
A	-1	HIS	-	EXPRESSION TAG	UNP Q63SW7
A	0	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	-8	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	-7	MET	-	EXPRESSION TAG	UNP Q63SW7
B	-6	ALA	-	EXPRESSION TAG	UNP Q63SW7
B	-5	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	-4	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	-3	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	-2	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	-1	HIS	-	EXPRESSION TAG	UNP Q63SW7
B	0	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	-8	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	-7	MET	-	EXPRESSION TAG	UNP Q63SW7
D	-6	ALA	-	EXPRESSION TAG	UNP Q63SW7

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	-4	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	-3	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	-2	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	-1	HIS	-	EXPRESSION TAG	UNP Q63SW7
D	0	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	-8	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	-7	MET	-	EXPRESSION TAG	UNP Q63SW7
C	-6	ALA	-	EXPRESSION TAG	UNP Q63SW7
C	-5	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	-4	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	-3	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	-2	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	-1	HIS	-	EXPRESSION TAG	UNP Q63SW7
C	0	HIS	-	EXPRESSION TAG	UNP Q63SW7

- Molecule 2 is N-METHYL-N-[(3-METHYL-1-BENZOFURAN-2-YL)METHYL]-3-(7-OXO-5,6,7,8-TETRAHYDRO-1,8-NAPHTHYRIDIN-3-YL)PROPANAMIDE (three-letter code: OWE) (formula: C<sub>22</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	22	3	3		
2	B	1	Total	C	N	O	0	0
			28	22	3	3		
2	D	1	Total	C	N	O	0	0
			28	22	3	3		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			28	22	3	3		

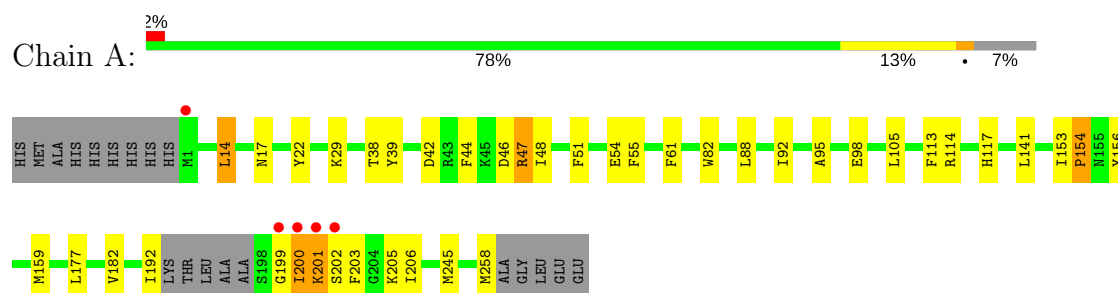
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		
3	B	142	Total	O	0	0
			142	142		
3	D	114	Total	O	0	0
			114	114		
3	C	159	Total	O	0	0
			159	159		

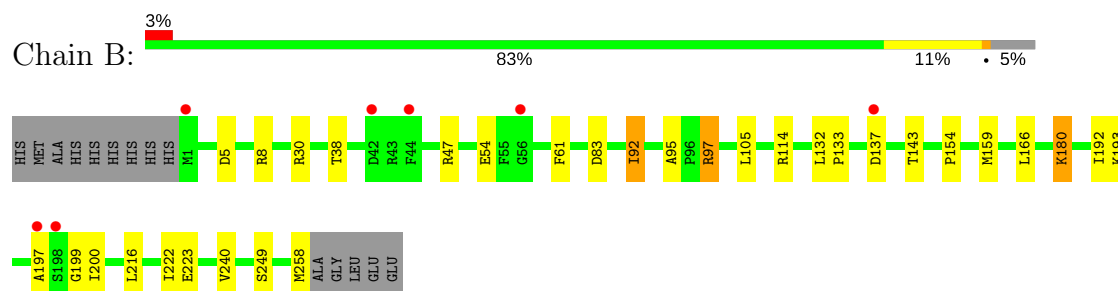
### 3 Residue-property plots [i](#)

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

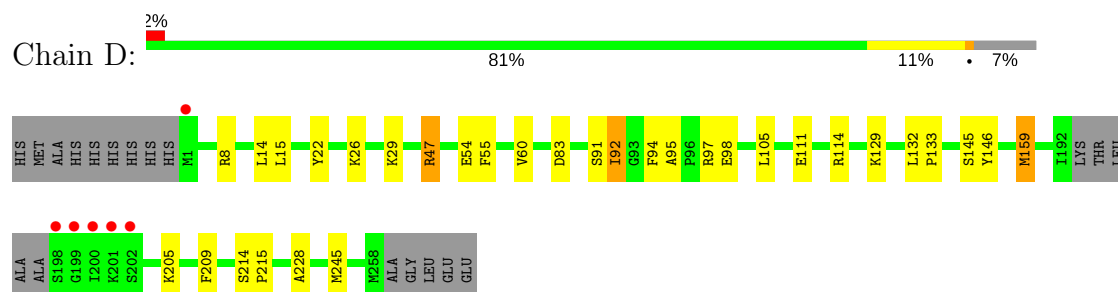
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



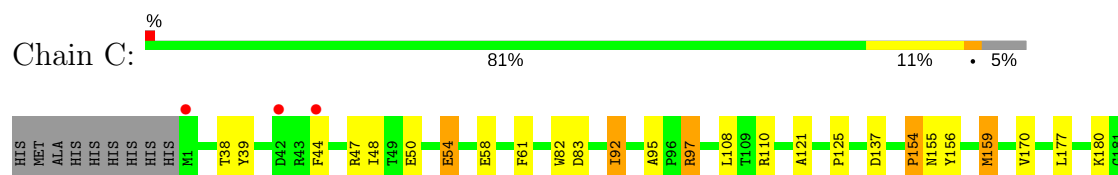
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



Y182	A186	P191	A197	I200	K201	S202	I206	F209	L216	E223	S249	K258	ALA	GLY	LEU	GLU	GLU
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.79Å 63.45Å 121.85Å 90.00° 107.08° 90.00°	Depositor
Resolution (Å)	36.59 – 2.26 36.59 – 2.26	Depositor EDS
% Data completeness (in resolution range)	92.5 (36.59-2.26) 92.5 (36.59-2.26)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.167 , 0.250 0.177 , 0.244	Depositor DCC
$R_{free}$ test set	2171 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0WE

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	0.86	2/1909 (0.1%)	0.86	3/2582 (0.1%)
1	B	0.87	0/1937	0.88	4/2623 (0.2%)
1	C	0.85	3/1936 (0.2%)	0.89	4/2622 (0.2%)
1	D	0.88	2/1909 (0.1%)	0.91	4/2582 (0.2%)
All	All	0.87	7/7691 (0.1%)	0.89	15/10409 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	TRP	CD2-CE2	5.78	1.48	1.41
1	D	94	PHE	CD2-CE2	-5.60	1.28	1.39
1	A	156	TYR	CD2-CE2	-5.58	1.30	1.39
1	A	82	TRP	CD2-CE2	5.32	1.47	1.41
1	D	91	SER	CB-OG	-5.25	1.35	1.42
1	C	54	GLU	CD-OE2	5.18	1.31	1.25
1	C	156	TYR	CD2-CE2	-5.04	1.31	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ASN	N-CA-CB	-10.03	92.55	110.60
1	A	114	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	D	114	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	D	159	MET	CG-SD-CE	-6.88	89.19	100.20
1	C	154	PRO	N-CA-C	6.83	129.85	112.10
1	D	92	ILE	CG1-CB-CG2	-6.31	97.53	111.40
1	D	8	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	154	PRO	C-N-CA	-6.19	106.22	121.70
1	C	110	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	114	ARG	NE-CZ-NH1	5.85	123.22	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	MET	CG-SD-CE	-5.63	91.18	100.20
1	B	154	PRO	C-N-CA	-5.51	107.93	121.70
1	A	199	GLY	N-CA-C	5.37	126.53	113.10
1	B	83	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	B	92	ILE	CG1-CB-CG2	-5.24	99.87	111.40

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	1877	0	1871	44	0
1	B	1904	0	1893	29	1
1	C	1903	0	1890	31	1
1	D	1877	0	1871	28	1
2	A	28	0	23	6	0
2	B	28	0	23	1	0
2	C	28	0	23	5	0
2	D	28	0	23	2	0
3	A	126	0	0	5	0
3	B	142	0	0	3	0
3	C	159	0	0	6	1
3	D	114	0	0	2	1
All	All	8214	0	7617	132	3

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

All (132) 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:A:42:ASP:HB2	3:A:617:HOH:O	1.59	1.02
1:B:95:ALA:CB	1:B:159:MET:HE1	1.93	0.99
1:C:97:ARG:HH11	1:C:97:ARG:HG3	1.27	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ALA:CB	1:C:159:MET:HE1	1.99	0.93
1:B:97:ARG:HG2	3:B:627:HOH:O	1.69	0.93
1:B:95:ALA:CB	1:B:159:MET:CE	2.50	0.89
1:B:95:ALA:HB2	1:B:159:MET:HE1	1.56	0.88
1:C:95:ALA:HB2	1:C:159:MET:CE	2.06	0.86
1:B:180:LYS:HD3	3:B:624:HOH:O	1.76	0.85
1:A:159:MET:CE	2:A:500:OWE:H10	2.06	0.85
1:C:95:ALA:CB	1:C:159:MET:CE	2.54	0.85
1:C:97:ARG:NH1	2:C:500:OWE:H9	1.93	0.84
1:D:95:ALA:HB2	1:D:159:MET:CE	2.08	0.84
1:B:95:ALA:HB2	1:B:159:MET:CE	2.06	0.83
1:A:95:ALA:HB2	1:A:159:MET:HE2	1.60	0.82
1:D:95:ALA:CB	1:D:159:MET:CE	2.58	0.81
1:A:95:ALA:CB	1:A:159:MET:HE2	2.11	0.81
1:B:197:ALA:O	1:B:199:GLY:HA2	1.79	0.81
1:D:22:TYR:OH	1:D:54:GLU:OE2	1.99	0.80
1:C:97:ARG:CZ	2:C:500:OWE:H9	2.12	0.79
1:D:95:ALA:HB2	1:D:159:MET:HE2	1.66	0.77
1:B:197:ALA:O	1:B:200:ILE:HB	1.86	0.76
1:D:95:ALA:CB	1:D:159:MET:HE2	2.16	0.76
1:A:200:ILE:CD1	1:A:200:ILE:N	2.51	0.74
1:A:159:MET:HE1	2:A:500:OWE:H10	1.71	0.73
1:A:14:LEU:HD21	1:A:22:TYR:HB2	1.71	0.72
1:D:95:ALA:CB	1:D:159:MET:HE1	2.18	0.72
1:C:95:ALA:HB2	1:C:159:MET:HE1	1.64	0.72
1:C:92:ILE:HG22	3:C:659:HOH:O	1.90	0.71
1:A:200:ILE:H	1:A:200:ILE:HD13	1.57	0.70
1:B:95:ALA:HB3	1:B:159:MET:CE	2.19	0.70
1:C:223:GLU:HG2	3:C:724:HOH:O	1.91	0.70
1:B:97:ARG:HH11	1:B:97:ARG:CG	2.06	0.68
1:C:206:ILE:HD11	3:C:729:HOH:O	1.92	0.68
1:D:95:ALA:N	1:D:159:MET:HE1	2.09	0.68
1:A:159:MET:HE3	2:A:500:OWE:H10	1.75	0.67
1:C:95:ALA:HB3	1:C:159:MET:CE	2.24	0.66
1:C:95:ALA:HB2	1:C:159:MET:HE2	1.77	0.66
1:A:44:PHE:HA	1:A:47:ARG:HH12	1.59	0.66
1:A:200:ILE:H	1:A:200:ILE:CD1	2.10	0.64
1:A:95:ALA:N	1:A:159:MET:HE1	2.13	0.64
1:A:98:GLU:HG2	3:A:618:HOH:O	1.97	0.63
1:A:46:ASP:HB2	1:A:47:ARG:HH21	1.64	0.63
1:D:47:ARG:H	1:D:47:ARG:HE	1.47	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HB	1:A:203:PHE:HB2	1.81	0.62
1:C:95:ALA:N	1:C:159:MET:HE1	2.14	0.62
1:D:95:ALA:HB3	1:D:159:MET:CE	2.30	0.62
1:A:29:LYS:HD2	3:A:664:HOH:O	2.00	0.61
1:B:95:ALA:N	1:B:159:MET:HE1	2.16	0.60
1:D:228:ALA:HB1	1:D:245:MET:CE	2.31	0.60
1:C:95:ALA:CB	1:C:159:MET:HE2	2.30	0.60
1:B:180:LYS:O	1:B:180:LYS:HG2	2.02	0.60
1:B:97:ARG:NH1	1:B:97:ARG:CG	2.64	0.59
1:B:95:ALA:HB2	1:B:159:MET:HE2	1.83	0.58
1:D:97:ARG:HG2	1:D:97:ARG:HH11	1.69	0.57
1:C:200:ILE:HD11	2:C:500:OWE:H5	1.85	0.57
1:C:97:ARG:HH11	1:C:97:ARG:CG	2.10	0.57
2:C:500:OWE:O10	2:C:500:OWE:H4	2.05	0.57
1:A:105:LEU:HD22	1:D:129:LYS:HB2	1.87	0.56
1:A:201:LYS:HE3	1:A:205:LYS:HE2	1.88	0.56
1:A:42:ASP:CB	3:A:617:HOH:O	2.32	0.56
2:D:500:OWE:O10	2:D:500:OWE:H4	2.05	0.56
1:D:95:ALA:HB2	1:D:159:MET:HE1	1.80	0.55
1:A:95:ALA:CB	1:A:159:MET:CE	2.84	0.55
1:A:95:ALA:HB3	1:A:159:MET:HE2	1.89	0.54
2:B:500:OWE:O10	2:B:500:OWE:H2	2.07	0.54
1:C:39:TYR:CD2	1:C:48:ILE:HG21	2.43	0.54
2:A:500:OWE:H2	2:A:500:OWE:O10	2.07	0.54
1:B:97:ARG:HG3	1:B:97:ARG:NH1	2.22	0.54
1:D:97:ARG:NH1	1:D:97:ARG:HG2	2.23	0.53
1:A:202:SER:O	1:A:206:ILE:HG12	2.09	0.53
1:B:95:ALA:CB	1:B:159:MET:HE2	2.38	0.53
1:D:98:GLU:HB3	3:D:622:HOH:O	2.08	0.53
1:D:228:ALA:HB1	1:D:245:MET:HE1	1.92	0.52
1:A:153:ILE:HG23	1:A:154:PRO:HD2	1.90	0.52
1:C:197:ALA:HA	1:C:200:ILE:HD12	1.90	0.52
1:A:177:LEU:HD21	1:D:105:LEU:HD12	1.92	0.51
1:A:200:ILE:HD12	1:A:200:ILE:N	2.24	0.51
1:A:88:LEU:HB3	1:A:141:LEU:HD22	1.91	0.51
1:D:228:ALA:HB1	1:D:245:MET:HE2	1.93	0.51
1:B:197:ALA:C	1:B:199:GLY:HA2	2.32	0.50
1:A:245:MET:CE	1:B:240:VAL:HG21	2.41	0.49
1:D:132:LEU:HB3	1:D:133:PRO:HD3	1.94	0.49
1:C:170:VAL:HG21	1:C:186:ALA:HB2	1.93	0.49
1:C:47:ARG:HA	1:C:50:GLU:OE1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:H	1:A:47:ARG:CZ	2.25	0.48
1:A:29:LYS:HE3	1:A:55:PHE:O	2.14	0.48
1:D:29:LYS:HE3	1:D:55:PHE:O	2.14	0.47
1:A:51:PHE:O	1:A:54:GLU:HB3	2.15	0.47
1:A:47:ARG:NH2	3:A:629:HOH:O	2.47	0.47
1:D:14:LEU:C	1:D:14:LEU:HD23	2.34	0.47
1:B:192:ILE:HD13	1:B:222:ILE:HG22	1.96	0.47
1:C:177:LEU:HB3	1:C:182:VAL:HB	1.97	0.47
1:A:200:ILE:CG2	1:A:202:SER:OG	2.63	0.47
1:A:95:ALA:HB2	1:A:159:MET:CE	2.37	0.46
1:C:38:THR:HA	1:C:61:PHE:O	2.16	0.46
1:A:177:LEU:HB3	1:A:182:VAL:HB	1.97	0.45
1:C:191:PRO:HD2	3:C:613:HOH:O	2.16	0.45
1:D:97:ARG:HG3	3:D:670:HOH:O	2.17	0.44
1:A:245:MET:HE3	1:B:240:VAL:HG21	2.00	0.44
1:D:26:LYS:HB2	1:D:26:LYS:HE3	1.90	0.44
1:A:39:TYR:CD2	1:A:48:ILE:HG21	2.53	0.44
1:B:143:THR:OG1	1:B:166:LEU:HD21	2.18	0.44
1:C:97:ARG:HG3	1:C:97:ARG:NH1	2.07	0.44
1:C:108:LEU:HA	3:C:618:HOH:O	2.17	0.43
2:C:500:OWE:H3	2:C:500:OWE:H15	1.99	0.43
1:A:159:MET:HE1	2:A:500:OWE:C20	2.44	0.43
1:C:177:LEU:HD23	3:C:657:HOH:O	2.19	0.43
1:C:202:SER:O	1:C:206:ILE:HG12	2.18	0.43
1:B:258:MET:HG2	1:D:209:PHE:CG	2.54	0.43
1:A:200:ILE:HG22	1:A:202:SER:N	2.34	0.42
1:B:216:LEU:HD12	1:B:249:SER:HA	2.00	0.42
2:D:500:OWE:H3	2:D:500:OWE:H15	1.99	0.42
1:C:216:LEU:HD12	1:C:249:SER:HA	2.02	0.42
1:B:95:ALA:CA	1:B:159:MET:HE1	2.46	0.42
1:C:95:ALA:CA	1:C:159:MET:HE1	2.50	0.42
1:D:14:LEU:HD23	1:D:15:LEU:N	2.35	0.42
1:A:113:PHE:CE1	1:A:117:HIS:CE1	3.07	0.42
1:B:200:ILE:HD12	1:B:200:ILE:HG23	1.72	0.42
1:B:30:ARG:HA	3:B:739:HOH:O	2.18	0.42
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.90	0.42
1:A:38:THR:HA	1:A:61:PHE:O	2.19	0.42
1:A:200:ILE:HG22	1:A:202:SER:H	1.85	0.41
1:A:113:PHE:CD2	1:A:113:PHE:C	2.93	0.41
1:C:121:ALA:O	1:C:125:PRO:HD2	2.20	0.41
1:B:132:LEU:HB3	1:B:133:PRO:HD3	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:HG2	1:C:209:PHE:CG	2.56	0.41
1:D:214:SER:O	1:D:215:PRO:C	2.58	0.41
1:D:95:ALA:HB3	1:D:159:MET:HE2	1.94	0.41
1:D:145:SER:OG	1:D:146:TYR:N	2.54	0.41
1:A:159:MET:CE	2:A:500:OWE:C20	2.89	0.41
1:B:38:THR:HA	1:B:61:PHE:O	2.21	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLU:OE1	3:C:724:HOH:O[4_554]	1.97	0.23
1:B:54:GLU:OE2	1:B:137:ASP:OD2[4_555]	2.11	0.09
1:C:223:GLU:OE1	3:D:697:HOH:O[4_544]	2.12	0.08

## 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	249/272 (92%)	238 (96%)	10 (4%)	1 (0%)	38	42
1	B	256/272 (94%)	246 (96%)	10 (4%)	0	100	100
1	C	256/272 (94%)	245 (96%)	10 (4%)	1 (0%)	38	42
1	D	249/272 (92%)	235 (94%)	14 (6%)	0	100	100
All	All	1010/1088 (93%)	964 (95%)	44 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	C	154	PRO

### 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	191/207 (92%)	185 (97%)	6 (3%)	45	55
1	B	192/207 (93%)	184 (96%)	8 (4%)	34	40
1	C	191/207 (92%)	182 (95%)	9 (5%)	30	34
1	D	191/207 (92%)	185 (97%)	6 (3%)	45	55
All	All	765/828 (92%)	736 (96%)	29 (4%)	38	46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	47	ARG
1	A	92	ILE
1	A	192	ILE
1	A	200	ILE
1	A	201	LYS
1	B	5	ASP
1	B	8	ARG
1	B	47	ARG
1	B	92	ILE
1	B	97	ARG
1	B	180	LYS
1	B	193	LYS
1	B	223	GLU
1	D	47	ARG
1	D	60	VAL
1	D	83	ASP
1	D	92	ILE
1	D	111	GLU
1	D	205	LYS
1	C	44	PHE
1	C	54	GLU
1	C	58	GLU
1	C	83	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	92	ILE
1	C	97	ARG
1	C	137	ASP
1	C	180	LYS
1	C	223	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	155	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	0WE	A	500	-	26,31,31	1.87	6 (23%)	31,44,44	2.10	7 (22%)
2	0WE	B	500	-	26,31,31	1.87	5 (19%)	31,44,44	2.11	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	0WE	C	500	-	26,31,31	1.88	7 (26%)	31,44,44	3.34	12 (38%)
2	0WE	D	500	-	26,31,31	1.89	7 (26%)	31,44,44	3.34	12 (38%)

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	0WE	A	500	-	-	0/11/22/22	0/3/4/4
2	0WE	B	500	-	-	0/11/22/22	0/3/4/4
2	0WE	C	500	-	-	0/11/22/22	0/3/4/4
2	0WE	D	500	-	-	0/11/22/22	0/3/4/4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	0WE	C26-C25	-6.17	1.35	1.51
2	D	500	0WE	C26-C25	-6.16	1.36	1.51
2	B	500	0WE	C26-C25	-6.08	1.36	1.51
2	A	500	0WE	C26-C25	-6.07	1.36	1.51
2	C	500	0WE	C18-C17	-3.56	1.34	1.52
2	B	500	0WE	C18-C17	-3.54	1.35	1.52
2	D	500	0WE	C18-C17	-3.54	1.35	1.52
2	A	500	0WE	C18-C17	-3.53	1.35	1.52
2	A	500	0WE	C17-C1	-2.15	1.46	1.51
2	C	500	0WE	C26-C23	-2.15	1.47	1.51
2	D	500	0WE	C26-C23	-2.13	1.47	1.51
2	B	500	0WE	C17-C1	-2.13	1.46	1.51
2	D	500	0WE	C17-C1	-2.07	1.46	1.51
2	C	500	0WE	C17-C1	-2.02	1.46	1.51
2	D	500	0WE	C13-C14	2.00	1.41	1.36
2	A	500	0WE	C13-C14	2.02	1.41	1.36
2	C	500	0WE	C13-C14	2.02	1.41	1.36
2	A	500	0WE	C22-N36	2.02	1.40	1.38
2	C	500	0WE	C22-N36	2.02	1.40	1.38
2	B	500	0WE	C13-C14	2.04	1.41	1.36
2	D	500	0WE	C22-N36	2.06	1.40	1.38
2	C	500	0WE	C7-C8	2.26	1.43	1.40
2	D	500	0WE	C7-C8	2.32	1.43	1.40
2	A	500	0WE	C7-C8	2.38	1.43	1.40
2	B	500	0WE	C7-C8	2.41	1.43	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	0WE	C11-C8-C9	-4.16	117.75	120.38
2	A	500	0WE	C11-C8-C9	-4.11	117.78	120.38
2	C	500	0WE	C11-C8-C9	-4.05	117.82	120.38
2	D	500	0WE	C11-C8-C9	-3.95	117.89	120.38
2	D	500	0WE	O2-C1-C17	-2.37	116.82	121.37
2	C	500	0WE	O2-C1-C17	-2.35	116.85	121.37
2	C	500	0WE	C4-N3-C1	-2.21	116.13	121.95
2	D	500	0WE	C4-N3-C1	-2.17	116.23	121.95
2	D	500	0WE	O2-C1-N3	-2.12	119.03	122.18
2	C	500	0WE	O2-C1-N3	-2.09	119.06	122.18
2	A	500	0WE	C18-C19-C20	-2.07	118.44	121.82
2	B	500	0WE	C18-C19-C20	-2.04	118.49	121.82
2	B	500	0WE	C6-C5-N3	-2.00	109.58	113.86
2	A	500	0WE	C18-C19-C24	2.01	123.85	120.56
2	D	500	0WE	C38-C7-C6	2.24	129.16	124.94
2	C	500	0WE	C38-C7-C6	2.26	129.20	124.94
2	C	500	0WE	N36-C22-N21	2.48	119.69	116.89
2	D	500	0WE	N36-C22-N21	2.48	119.69	116.89
2	C	500	0WE	C17-C1-N3	3.10	124.08	118.19
2	D	500	0WE	C17-C1-N3	3.13	124.15	118.19
2	C	500	0WE	C26-C25-C37	3.26	121.20	113.90
2	D	500	0WE	C26-C25-C37	3.27	121.23	113.90
2	A	500	0WE	C26-C25-C37	3.32	121.33	113.90
2	B	500	0WE	C26-C25-C37	3.34	121.39	113.90
2	C	500	0WE	C17-C18-C19	3.54	125.48	112.76
2	D	500	0WE	C17-C18-C19	3.55	125.49	112.76
2	A	500	0WE	C17-C18-C19	3.58	125.60	112.76
2	D	500	0WE	C5-N3-C1	3.58	131.28	120.64
2	B	500	0WE	C17-C18-C19	3.60	125.67	112.76
2	C	500	0WE	C5-N3-C1	3.61	131.35	120.64
2	D	500	0WE	C25-C26-C23	3.61	119.83	112.03
2	C	500	0WE	C25-C26-C23	3.62	119.86	112.03
2	B	500	0WE	C25-C26-C23	3.71	120.05	112.03
2	A	500	0WE	C25-C26-C23	3.71	120.05	112.03
2	A	500	0WE	C18-C17-C1	6.26	120.03	112.42
2	B	500	0WE	C18-C17-C1	6.29	120.06	112.42
2	C	500	0WE	C18-C17-C1	14.82	130.42	112.42
2	D	500	0WE	C18-C17-C1	14.82	130.42	112.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	0WE	6	0
2	B	500	0WE	1	0
2	C	500	0WE	5	0
2	D	500	0WE	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	253/272 (93%)	-0.25	5 (1%) 65 69	9, 15, 29, 88	0
1	B	258/272 (94%)	-0.25	7 (2%) 55 58	10, 15, 36, 54	0
1	C	258/272 (94%)	-0.31	3 (1%) 79 81	9, 15, 33, 57	0
1	D	253/272 (93%)	-0.30	6 (2%) 59 63	9, 14, 32, 88	0
All	All	1022/1088 (93%)	-0.28	21 (2%) 64 67	9, 15, 33, 88	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	ILE	9.2
1	D	200	ILE	8.9
1	D	199	GLY	7.4
1	D	198	SER	5.3
1	D	201	LYS	5.1
1	A	201	LYS	4.6
1	C	1	MET	3.8
1	C	42	ASP	3.5
1	B	198	SER	3.2
1	B	44	PHE	3.1
1	A	199	GLY	3.0
1	D	1	MET	2.7
1	B	1	MET	2.6
1	A	1	MET	2.5
1	A	202	SER	2.5
1	C	44	PHE	2.3
1	B	42	ASP	2.3
1	B	56	GLY	2.2
1	D	202	SER	2.1
1	B	137	ASP	2.1
1	B	197	ALA	2.1

## 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( $\text{\AA}^2$ )	Q<0.9
2	0WE	A	500	28/28	0.90	0.23	2.99	37,39,40,40	0
2	0WE	C	500	28/28	0.82	0.23	2.01	32,32,33,34	0
2	0WE	D	500	28/28	0.83	0.23	1.87	32,32,33,34	0
2	0WE	B	500	28/28	0.87	0.20	1.28	37,39,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.