



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:02 am BST

PDB ID : 2IMJ  
Title : X-ray Crystal Structure of Protein PFL\_3262 from *Pseudomonas fluorescens*.  
Northeast Structural Genomics Consortium Target PIR14.  
Authors : Zhou, W.; Forouhar, F.; Seetharaman, J.; Chen, C.X.; Fang, Y.; Cunningham,  
K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Montelione, G.T.;  
Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-10-04  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

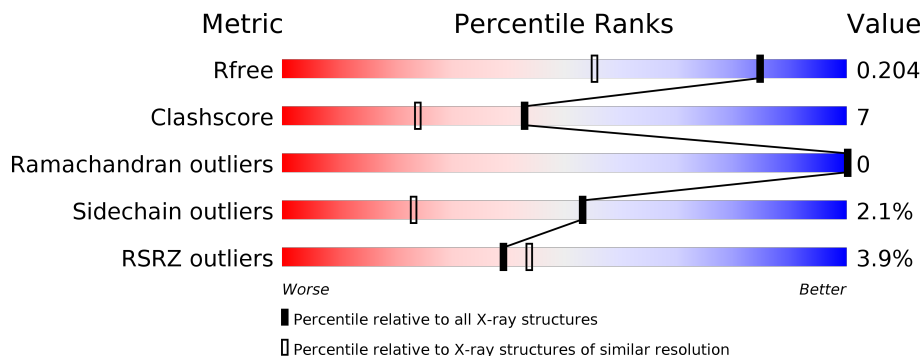
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	166	<p>4% 80% 14% • 5%</p>
1	B	166	<p>5% 70% 23% • 6%</p>
1	C	166	<p>2% 79% 14% 7%</p>
1	D	166	<p>2% 79% 13% 8%</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 6227 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 Hypothetical protein DUF1348.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	158	1345	851	251	240	1	2	0	0	0
1	B	156	1325	839	245	238	1	2	0	0	0
1	C	155	1316	834	244	235	1	2	0	0	0
1	D	153	1304	824	243	234	1	2	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

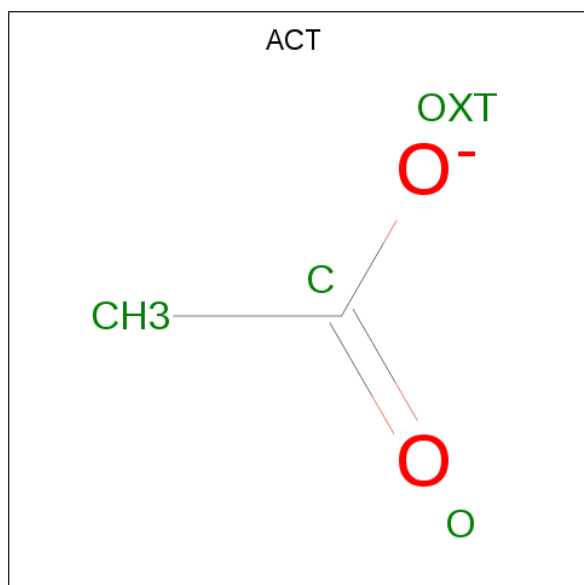
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
A	121	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
A	131	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
A	159	LEU	-	CLONING ARTIFACT	UNP Q4KBL6
A	160	GLU	-	CLONING ARTIFACT	UNP Q4KBL6
A	161	HIS	-	EXPRESSION TAG	UNP Q4KBL6
A	162	HIS	-	EXPRESSION TAG	UNP Q4KBL6
A	163	HIS	-	EXPRESSION TAG	UNP Q4KBL6
A	164	HIS	-	EXPRESSION TAG	UNP Q4KBL6
A	165	HIS	-	EXPRESSION TAG	UNP Q4KBL6
A	166	HIS	-	EXPRESSION TAG	UNP Q4KBL6
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
B	121	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
B	131	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
B	159	LEU	-	CLONING ARTIFACT	UNP Q4KBL6
B	160	GLU	-	CLONING ARTIFACT	UNP Q4KBL6
B	161	HIS	-	EXPRESSION TAG	UNP Q4KBL6
B	162	HIS	-	EXPRESSION TAG	UNP Q4KBL6
B	163	HIS	-	EXPRESSION TAG	UNP Q4KBL6
B	164	HIS	-	EXPRESSION TAG	UNP Q4KBL6
B	165	HIS	-	EXPRESSION TAG	UNP Q4KBL6

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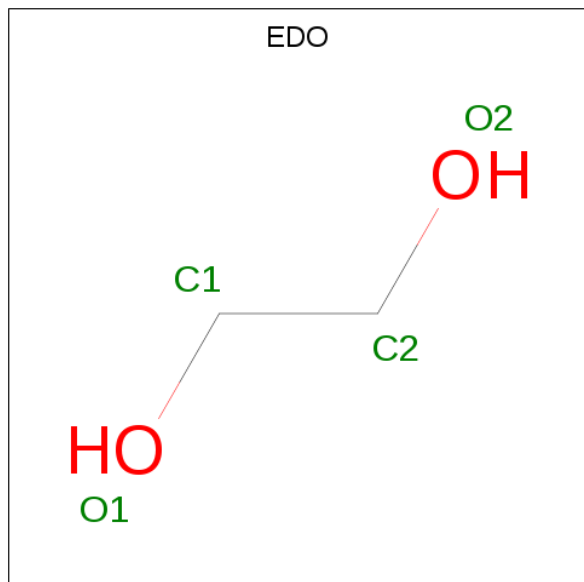
Chain	Residue	Modelled	Actual	Comment	Reference
B	166	HIS	-	EXPRESSION TAG	UNP Q4KBL6
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
C	121	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
C	131	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
C	159	LEU	-	CLONING ARTIFACT	UNP Q4KBL6
C	160	GLU	-	CLONING ARTIFACT	UNP Q4KBL6
C	161	HIS	-	EXPRESSION TAG	UNP Q4KBL6
C	162	HIS	-	EXPRESSION TAG	UNP Q4KBL6
C	163	HIS	-	EXPRESSION TAG	UNP Q4KBL6
C	164	HIS	-	EXPRESSION TAG	UNP Q4KBL6
C	165	HIS	-	EXPRESSION TAG	UNP Q4KBL6
C	166	HIS	-	EXPRESSION TAG	UNP Q4KBL6
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
D	121	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
D	131	MSE	MET	MODIFIED RESIDUE	UNP Q4KBL6
D	159	LEU	-	CLONING ARTIFACT	UNP Q4KBL6
D	160	GLU	-	CLONING ARTIFACT	UNP Q4KBL6
D	161	HIS	-	EXPRESSION TAG	UNP Q4KBL6
D	162	HIS	-	EXPRESSION TAG	UNP Q4KBL6
D	163	HIS	-	EXPRESSION TAG	UNP Q4KBL6
D	164	HIS	-	EXPRESSION TAG	UNP Q4KBL6
D	165	HIS	-	EXPRESSION TAG	UNP Q4KBL6
D	166	HIS	-	EXPRESSION TAG	UNP Q4KBL6

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	240	Total O 240 240	0	0
4	B	197	Total O 197 197	0	0

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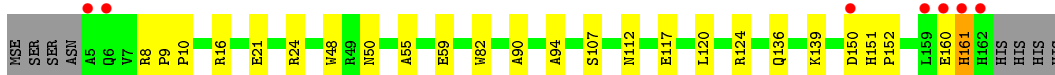
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	233	Total 233	O 233	0	0
4	D	235	Total 235	O 235	0	0

### 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.

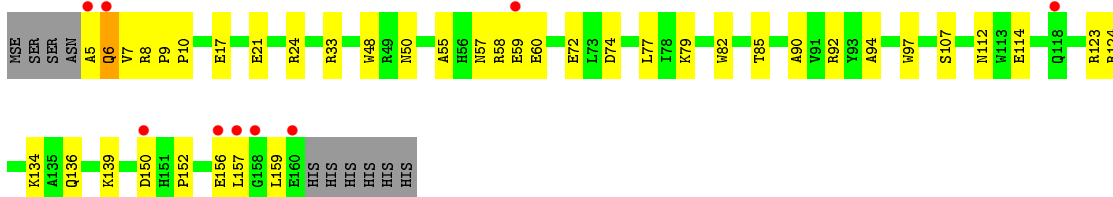
- Molecule 1: Hypothetical protein DUF1348

Chain A: 




- Molecule 1: Hypothetical protein DUF1348

Chain B: 




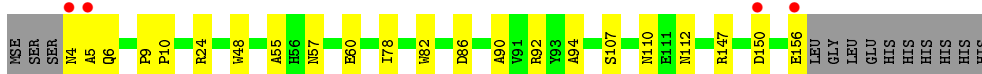
- Molecule 1: Hypothetical protein DUF1348

Chain C: 



- Molecule 1: Hypothetical protein DUF1348

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.86Å 88.76Å 74.70Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	33.35 – 1.50 33.35 – 1.50	Depositor EDS
% Data completeness (in resolution range)	81.5 (33.35-1.50) 93.0 (33.35-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.50Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.169 , 0.193 0.181 , 0.204	Depositor DCC
$R_{free}$ test set	18845 reflections (9.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.9	Xtrriage
Anisotropy	0.538	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6227	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/1386	0.64	0/1874
1	B	0.31	0/1364	0.61	0/1844
1	C	0.32	0/1355	0.65	0/1832
1	D	0.32	0/1343	0.62	0/1816
All	All	0.32	0/5448	0.63	0/7366

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	1345	0	1266	18	0
1	B	1325	0	1252	25	0
1	C	1316	0	1246	17	0
1	D	1304	0	1227	14	0
2	A	12	0	9	1	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	240	0	0	6	0
4	B	197	0	0	5	0
4	C	233	0	0	2	0
4	D	235	0	0	2	0
All	All	6227	0	5021	70	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 (70) 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:C:50:ASN:HD22	1:C:124:ARG:HH12	1.23	0.85
1:A:50:ASN:HD22	1:A:124:ARG:HH12	1.31	0.79
1:A:21:GLU:HG3	4:A:514:HOH:O	1.83	0.77
1:B:50:ASN:HD22	1:B:124:ARG:HH12	1.33	0.73
1:B:6:GLN:HG2	1:B:7:VAL:N	2.03	0.72
1:B:48:TRP:HB2	1:B:55:ALA:HB3	1.71	0.72
1:A:139:LYS:NZ	1:A:160:GLU:HG2	2.10	0.66
1:B:156:GLU:HG3	4:B:753:HOH:O	1.96	0.65
1:D:150:ASP:HB3	4:D:430:HOH:O	1.95	0.65
1:D:82:TRP:CE3	1:D:92:ARG:HD3	2.33	0.63
1:A:139:LYS:HZ2	1:A:160:GLU:HG2	1.62	0.62
1:D:48:TRP:HB2	1:D:55:ALA:HB3	1.81	0.62
1:A:151:HIS:HE1	4:A:414:HOH:O	1.83	0.62
1:B:5:ALA:N	1:B:58:ARG:HH12	1.98	0.61
1:B:152:PRO:HG2	1:B:157:LEU:HD21	1.87	0.56
1:C:48:TRP:HB2	1:C:55:ALA:HB3	1.88	0.56
2:A:202:ACT:H3	1:B:92:ARG:HH22	1.73	0.53
1:C:82:TRP:CE3	1:C:92:ARG:HD3	2.43	0.53
1:D:57:ASN:OD1	1:D:60:GLU:HG3	2.10	0.52
1:A:90:ALA:HA	1:A:112:ASN:HD22	1.74	0.52
1:B:8:ARG:HG2	4:B:428:HOH:O	2.10	0.52
1:C:6:GLN:OE1	1:C:8:ARG:HD2	2.09	0.52
1:A:117:GLU:CD	1:A:117:GLU:H	2.11	0.51
1:C:8:ARG:HD3	1:C:120:LEU:CD2	2.40	0.51
1:B:17:GLU:O	1:B:21:GLU:HG3	2.11	0.51
1:B:114:GLU:OE2	1:B:123:ARG:HD3	2.11	0.51
1:C:134:LYS:HE3	1:C:136:GLN:NE2	2.26	0.51
1:C:8:ARG:HD3	1:C:120:LEU:HD23	1.93	0.51
1:B:150:ASP:HB3	4:B:834:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TRP:HB2	1:A:55:ALA:HB3	1.93	0.49
1:A:139:LYS:HZ2	1:A:160:GLU:HA	1.78	0.48
1:C:9:PRO:HA	1:C:10:PRO:C	2.33	0.48
1:A:82:TRP:CE2	1:B:112:ASN:HB3	2.48	0.48
1:A:112:ASN:HB3	1:B:82:TRP:CE2	2.48	0.48
1:D:92:ARG:HG2	1:D:110:ASN:ND2	2.30	0.47
1:A:9:PRO:HA	1:A:10:PRO:C	2.35	0.46
1:A:16:ARG:NH2	4:A:541:HOH:O	2.49	0.46
1:B:59:GLU:HG3	4:B:811:HOH:O	2.14	0.46
1:B:6:GLN:CG	1:B:7:VAL:N	2.74	0.46
1:C:38:VAL:HG13	4:C:331:HOH:O	2.16	0.46
1:A:151:HIS:HD2	1:A:152:PRO:O	1.99	0.45
1:C:90:ALA:HA	1:C:112:ASN:HD22	1.80	0.45
1:D:86:ASP:HB3	4:D:405:HOH:O	2.16	0.45
1:D:94:ALA:HA	1:D:107:SER:O	2.17	0.45
1:D:90:ALA:HA	1:D:112:ASN:HD22	1.82	0.45
1:D:92:ARG:HG2	1:D:110:ASN:HD21	1.82	0.44
1:A:59:GLU:HG3	4:A:425:HOH:O	2.16	0.44
1:D:4:ASN:OD1	1:D:5:ALA:N	2.51	0.44
1:C:112:ASN:HB3	1:D:82:TRP:CE2	2.53	0.44
1:B:57:ASN:OD1	1:B:60:GLU:HG3	2.18	0.43
1:B:94:ALA:HA	1:B:107:SER:O	2.18	0.43
1:A:94:ALA:HA	1:A:107:SER:O	2.18	0.43
1:B:74:ASP:HB3	4:B:749:HOH:O	2.18	0.42
1:C:92:ARG:HG2	1:C:110:ASN:HD21	1.85	0.42
1:B:72:GLU:HA	1:B:97:TRP:CE3	2.55	0.42
1:C:143:PRO:O	1:C:144:LEU:C	2.57	0.42
1:C:151:HIS:HA	1:C:152:PRO:HD3	1.90	0.42
1:A:161:HIS:HB2	4:A:381:HOH:O	2.18	0.42
1:C:82:TRP:CE2	1:D:112:ASN:HB3	2.54	0.42
1:C:92:ARG:HG2	4:C:208:HOH:O	2.19	0.41
1:A:8:ARG:HD3	1:A:120:LEU:HD23	2.02	0.41
1:B:77:LEU:HD21	1:B:79:LYS:HE2	2.03	0.41
1:B:90:ALA:HA	1:B:112:ASN:HD22	1.86	0.40
1:B:139:LYS:HD2	1:B:159:LEU:HD21	2.03	0.40
1:D:9:PRO:HA	1:D:10:PRO:C	2.42	0.40
1:C:94:ALA:HA	1:C:107:SER:O	2.20	0.40
1:B:9:PRO:HA	1:B:10:PRO:C	2.42	0.40
1:B:134:LYS:HE3	1:B:136:GLN:NE2	2.36	0.40
4:A:541:HOH:O	1:B:85:THR:HG21	2.21	0.40
1:D:78:ILE:HG12	1:D:147:ARG:HD3	2.03	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	156/166 (94%)	152 (97%)	4 (3%)	0	100	100
1	B	154/166 (93%)	148 (96%)	6 (4%)	0	100	100
1	C	153/166 (92%)	149 (97%)	4 (3%)	0	100	100
1	D	151/166 (91%)	146 (97%)	5 (3%)	0	100	100
All	All	614/664 (92%)	595 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/141 (96%)	132 (97%)	4 (3%)	42	13
1	B	134/141 (95%)	131 (98%)	3 (2%)	52	22
1	C	133/141 (94%)	132 (99%)	1 (1%)	81	66
1	D	132/141 (94%)	129 (98%)	3 (2%)	50	20
All	All	535/564 (95%)	524 (98%)	11 (2%)	53	23

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	136	GLN
1	A	150	ASP
1	A	161	HIS
1	B	6	GLN
1	B	24	ARG
1	B	33	ARG
1	C	24	ARG
1	D	6	GLN
1	D	24	ARG
1	D	156	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	110	ASN
1	A	112	ASN
1	A	151	HIS
1	B	50	ASN
1	B	110	ASN
1	B	112	ASN
1	C	47	GLN
1	C	50	ASN
1	C	56	HIS
1	C	103	ASN
1	C	110	ASN
1	C	112	ASN
1	D	110	ASN
1	D	112	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](#)

8 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	ACT	B	201	-	1,3,3	3.81	1 (100%)	0,3,3	0.00	-
2	ACT	D	201	-	1,3,3	3.35	1 (100%)	0,3,3	0.00	-
2	ACT	A	202	-	1,3,3	3.27	1 (100%)	0,3,3	0.00	-
2	ACT	A	201	-	1,3,3	4.02	1 (100%)	0,3,3	0.00	-
2	ACT	A	203	-	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
3	EDO	A	302	-	3,3,3	0.57	0	2,2,2	0.65	0
3	EDO	A	301	-	3,3,3	0.54	0	2,2,2	0.64	0
2	ACT	C	201	-	1,3,3	4.02	1 (100%)	0,3,3	0.00	-

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
3	EDO	A	301	-	-	1/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	ACT	CH3-C	4.02	1.53	1.48
2	A	201	ACT	CH3-C	4.02	1.53	1.48
2	B	201	ACT	CH3-C	3.81	1.53	1.48
2	D	201	ACT	CH3-C	3.35	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	ACT	CH3-C	3.27	1.52	1.48
2	A	203	ACT	CH3-C	2.78	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	EDO	O1-C1-C2-O2
3	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	202	ACT	1	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	156/166 (93%)	0.17	7 (4%) 33 36	8, 12, 26, 36	0
1	B	154/166 (92%)	0.37	9 (5%) 23 25	8, 16, 27, 38	0
1	C	153/166 (92%)	0.04	4 (2%) 56 61	8, 11, 25, 32	0
1	D	151/166 (90%)	0.10	4 (2%) 56 61	8, 13, 27, 33	0
All	All	614/664 (92%)	0.17	24 (3%) 39 44	8, 13, 27, 38	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ALA	8.9
1	D	4	ASN	7.0
1	A	5	ALA	6.7
1	D	5	ALA	6.2
1	C	159	LEU	6.0
1	B	158	GLY	5.0
1	C	158	GLY	4.7
1	A	161	HIS	4.5
1	A	159	LEU	4.2
1	B	156	GLU	3.3
1	B	160	GLU	3.3
1	B	150	ASP	3.0
1	B	6	GLN	3.0
1	A	162	HIS	2.8
1	D	150	ASP	2.8
1	D	156	GLU	2.7
1	B	157	LEU	2.7
1	A	150	ASP	2.5
1	A	160	GLU	2.3
1	C	156	GLU	2.3
1	A	6	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	5	ALA	2.1
1	B	118	GLN	2.0
1	B	59	GLU	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	302	4/4	0.62	0.22	40,41,42,43	0
3	EDO	A	301	4/4	0.76	0.24	42,43,43,45	0
2	ACT	A	202	4/4	0.78	0.22	18,20,20,23	0
2	ACT	A	203	4/4	0.85	0.18	35,36,36,37	0
2	ACT	C	201	4/4	0.93	0.14	9,9,10,10	0
2	ACT	A	201	4/4	0.94	0.16	9,10,11,11	0
2	ACT	B	201	4/4	0.95	0.10	10,12,14,15	0
2	ACT	D	201	4/4	0.95	0.12	10,11,11,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.