



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 29, 2022 – 01:18 pm BST

PDB ID : 7PZF  
Title : Crystal structure of the OmpK36 TD insertion chimera from Klebsiella pneumonia  
Authors : Kwong, H.; Beis, K.  
Deposited on : 2021-10-12  
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)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

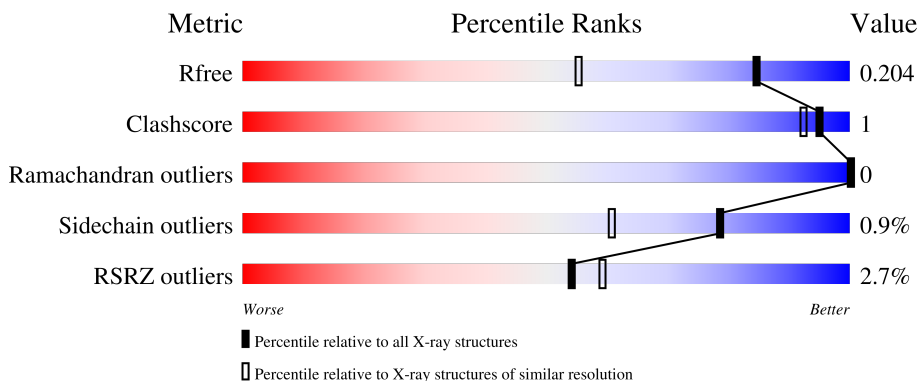
# 1 Overall quality at a glance

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.



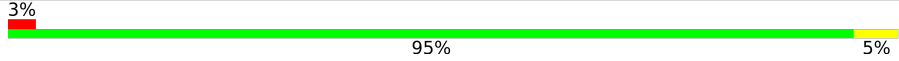
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 of 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	347	98%
1	B	347	96%
1	C	347	98%
1	D	347	97%
1	E	347	96%

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Mol	Chain	Length	Quality of chain
1	F	347	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '95%', and a small yellow segment on the right labeled '5%'.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17802 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 OmpK36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	Total 2734	C 1718	N 454	O 560	S 2	0	5	0
1	B	347	Total 2741	C 1721	N 456	O 562	S 2	0	6	0
1	C	347	Total 2726	C 1711	N 454	O 559	S 2	0	4	0
1	D	347	Total 2726	C 1712	N 454	O 558	S 2	0	3	0
1	E	343	Total 2698	C 1687	N 451	O 558	S 2	0	5	0
1	F	347	Total 2722	C 1707	N 454	O 559	S 2	0	3	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	insertion	UNP D6QLY0
A	115	THR	-	insertion	UNP D6QLY0
A	116	ASP	-	insertion	UNP D6QLY0
B	0	GLY	-	insertion	UNP D6QLY0
B	115	THR	-	insertion	UNP D6QLY0
B	116	ASP	-	insertion	UNP D6QLY0
C	0	GLY	-	insertion	UNP D6QLY0
C	115	THR	-	insertion	UNP D6QLY0
C	116	ASP	-	insertion	UNP D6QLY0
D	0	GLY	-	insertion	UNP D6QLY0
D	115	THR	-	insertion	UNP D6QLY0
D	116	ASP	-	insertion	UNP D6QLY0
E	0	GLY	-	insertion	UNP D6QLY0
E	115	THR	-	insertion	UNP D6QLY0
E	116	ASP	-	insertion	UNP D6QLY0
F	0	GLY	-	insertion	UNP D6QLY0
F	115	THR	-	insertion	UNP D6QLY0

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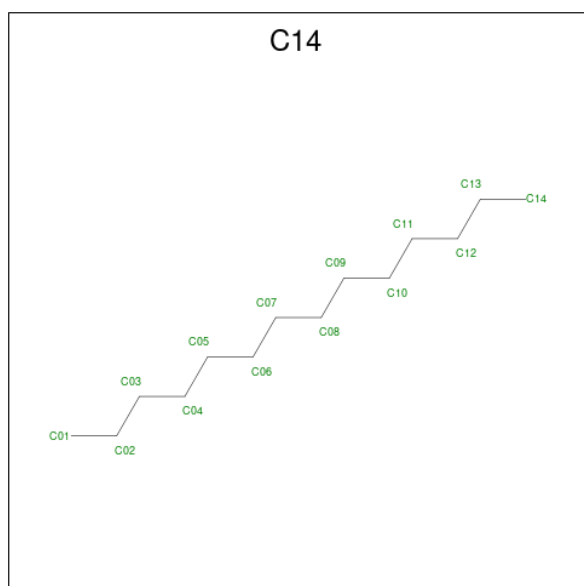
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Chain	Residue	Modelled	Actual	Comment	Reference
F	116	ASP	-	insertion	UNP D6QLY0

- Molecule 2 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Li 2 2	0	0
2	B	1	Total Li 1 1	0	0
2	D	1	Total Li 1 1	0	0
2	E	2	Total Li 2 2	0	0
2	F	3	Total Li 3 3	0	0

- Molecule 3 is TETRADECANE (three-letter code: C14) (formula: C<sub>14</sub>H<sub>30</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 8 8	0	0
3	A	1	Total C 10 10	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 13 13	0	0
3	C	1	Total C 14 14	0	0
3	D	1	Total C 14 14	0	0
3	D	1	Total C 11 11	0	0
3	D	1	Total C 9 9	0	0
3	D	1	Total C 14 14	0	0
3	E	1	Total C 10 10	0	0
3	E	1	Total C 12 12	0	0
3	E	1	Total C 13 13	0	0
3	E	1	Total C 11 11	0	0
3	E	1	Total C 9 9	0	0
3	F	1	Total C 13 13	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	232	Total O 232 232	0	0
4	B	176	Total O 176 176	0	0

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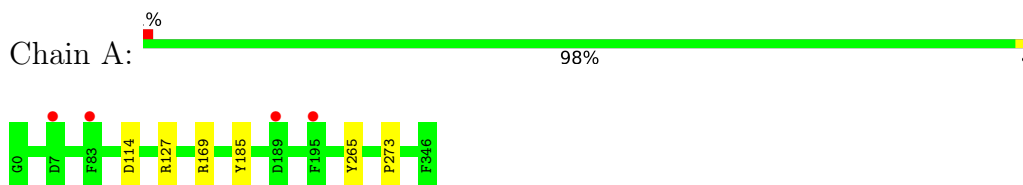
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	183	Total 183	O 183	0	0
4	D	197	Total 197	O 197	0	0
4	E	214	Total 214	O 214	0	0
4	F	204	Total 204	O 204	0	0

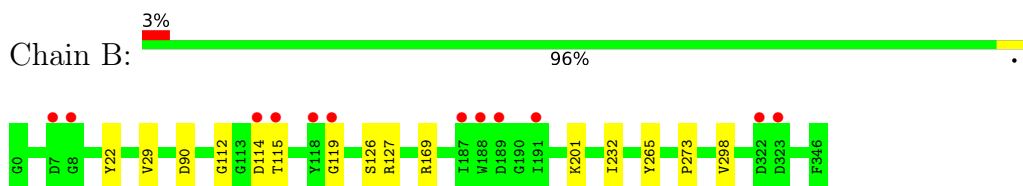
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

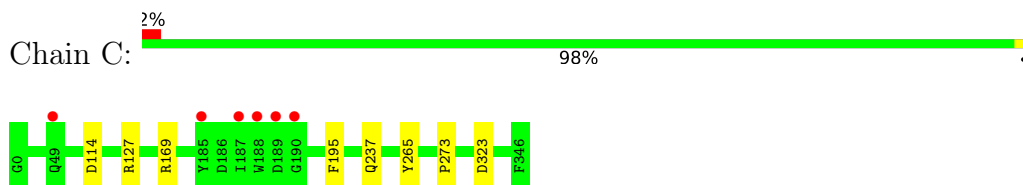
- Molecule 1: OmpK36



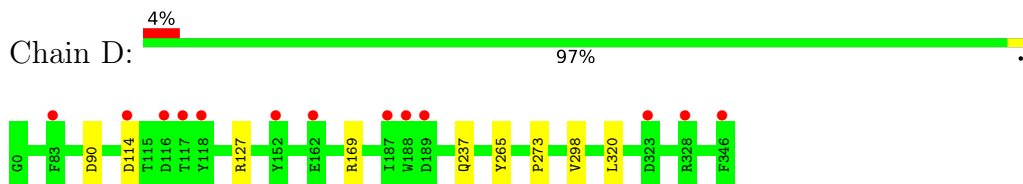
- Molecule 1: OmpK36



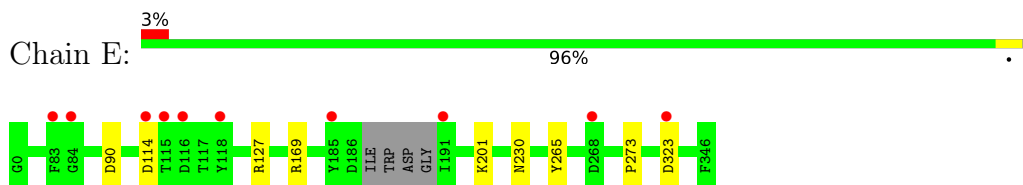
- Molecule 1: OmpK36



- Molecule 1: OmpK36

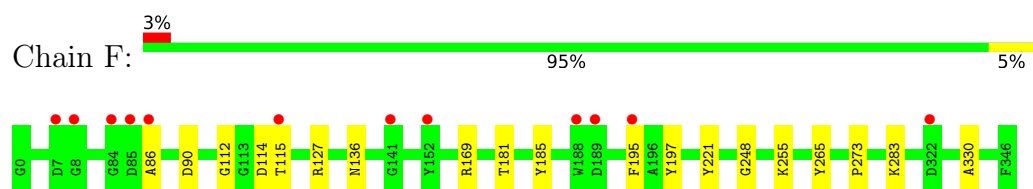


- Molecule 1: OmpK36



- Molecule 1: OmpK36





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.11Å 73.43Å 158.84Å 91.12° 97.17° 103.09°	Depositor
Resolution (Å)	54.25 – 1.50 54.25 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (54.25-1.50) 95.8 (54.25-1.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 1.50Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, $R_{free}$	0.190 , 0.205 0.189 , 0.204	Depositor DCC
$R_{free}$ test set	18383 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17802	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 5.84% 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: C14, LI

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	0.43	0/2810	0.63	0/3806
1	B	0.44	0/2817	0.63	0/3813
1	C	0.41	0/2798	0.62	0/3790
1	D	0.42	0/2796	0.63	0/3787
1	E	0.42	0/2764	0.62	0/3740
1	F	0.43	0/2791	0.63	0/3780
All	All	0.42	0/16776	0.63	0/22716

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

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	2734	0	2529	3	0
1	B	2741	0	2535	12	0
1	C	2726	0	2522	3	0
1	D	2726	0	2515	3	0
1	E	2698	0	2486	5	0
1	F	2722	0	2513	11	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	18	0	34	1	0
3	B	92	0	176	6	0
3	C	14	0	30	2	0
3	D	48	0	98	0	0
3	E	55	0	105	4	0
3	F	13	0	25	4	0
4	A	232	0	0	0	0
4	B	176	0	0	0	0
4	C	183	0	0	0	0
4	D	197	0	0	0	0
4	E	214	0	0	0	0
4	F	204	0	0	0	0
All	All	17802	0	15568	38	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 1.

All (38) 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:B:232:ILE:HD11	3:B:409:C14:H091	1.44	0.98
1:F:221:TYR:HB3	3:F:404:C14:H032	1.68	0.75
1:B:201:LYS:HZ1	3:B:402:C14:H112	1.58	0.69
1:B:22:TYR:HD2	1:B:29:VAL:HG22	1.61	0.64
1:B:201:LYS:NZ	3:B:402:C14:H082	2.13	0.64
1:A:273:PRO:HB2	3:A:403:C14:H142	1.83	0.61
1:B:114:ASP:OD2	1:B:127:ARG:NH1	2.35	0.59
1:B:22:TYR:CD2	1:B:29:VAL:HG22	2.36	0.59
1:F:181:THR:OG1	3:F:404:C14:H112	2.06	0.56
3:C:401:C14:H082	1:F:185:TYR:CE2	2.41	0.56
1:F:112:GLY:O	1:F:115:THR:HG22	2.06	0.56
1:E:114:ASP:OD2	1:E:127:ARG:NH1	2.39	0.56
1:D:114:ASP:OD2	1:D:127:ARG:NH1	2.39	0.55
1:F:195:PHE:HB3	3:F:404:C14:H082	1.89	0.55
1:B:112:GLY:O	1:B:115:THR:HG22	2.08	0.53
1:A:114:ASP:OD1	1:A:127:ARG:NH1	2.42	0.52
1:B:201:LYS:HZ2	3:B:402:C14:H082	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:VAL:HG11	3:B:406:C14:H061	1.90	0.52
1:F:114:ASP:OD1	1:F:127:ARG:NH1	2.44	0.50
1:F:197:TYR:HB2	3:F:404:C14:H081	1.94	0.49
1:C:114:ASP:OD1	1:C:127:ARG:NH1	2.47	0.47
1:E:201:LYS:HE3	3:E:403:C14:H092	1.96	0.46
1:C:265:TYR:O	1:C:273:PRO:HD2	2.17	0.45
1:B:201:LYS:NZ	3:B:402:C14:H112	2.31	0.45
1:D:265:TYR:O	1:D:273:PRO:HD2	2.16	0.45
1:D:298:VAL:HG23	1:D:320:LEU:HD11	1.99	0.44
1:E:230:ASN:HB3	3:E:405:C14:H111	1.98	0.44
1:F:265:TYR:O	1:F:273:PRO:HD2	2.18	0.43
1:A:265:TYR:O	1:A:273:PRO:HD2	2.19	0.43
1:B:265:TYR:O	1:B:273:PRO:HD2	2.17	0.43
1:E:265:TYR:O	1:E:273:PRO:HD2	2.18	0.43
1:F:248:GLY:HA3	1:F:330:ALA:HB1	2.01	0.43
1:C:195:PHE:HB3	3:C:401:C14:H071	2.01	0.43
1:F:86:ALA:O	1:F:136:ASN:HA	2.20	0.42
1:F:255:LYS:HB3	1:F:283:LYS:HB2	2.01	0.41
1:B:119:GLY:O	1:B:126:SER:HB3	2.21	0.40
1:E:273:PRO:HB2	3:E:406:C14:H052	2.03	0.40
3:E:404:C14:H132	3:E:404:C14:H102	1.89	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	350/347 (101%)	331 (95%)	19 (5%)	0	100	100
1	B	351/347 (101%)	332 (95%)	19 (5%)	0	100	100
1	C	349/347 (101%)	332 (95%)	17 (5%)	0	100	100
1	D	348/347 (100%)	329 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	344/347 (99%)	327 (95%)	17 (5%)	0	100	100
1	F	348/347 (100%)	332 (95%)	16 (5%)	0	100	100
All	All	2090/2082 (100%)	1983 (95%)	107 (5%)	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	283/278 (102%)	281 (99%)	2 (1%)	84	69
1	B	284/278 (102%)	282 (99%)	2 (1%)	84	69
1	C	282/278 (101%)	279 (99%)	3 (1%)	73	53
1	D	281/278 (101%)	278 (99%)	3 (1%)	73	53
1	E	280/278 (101%)	277 (99%)	3 (1%)	73	53
1	F	281/278 (101%)	279 (99%)	2 (1%)	84	69
All	All	1691/1668 (101%)	1676 (99%)	15 (1%)	78	61

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	185	TYR
1	B	90	ASP
1	B	169	ARG
1	C	169	ARG
1	C	237	GLN
1	C	323	ASP
1	D	90	ASP
1	D	169	ARG
1	D	237	GLN
1	E	90	ASP
1	E	169	ARG

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Mol	Chain	Res	Type
1	E	323	ASP
1	F	90	ASP
1	F	169	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 9 are monoatomic - leaving 21 for Mogul analysis.

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	$\# Z  > 2$
3	C14	E	405	-	12,12,13	0.30	0	11,11,12	0.55	0
3	C14	E	404	-	11,11,13	0.29	0	10,10,12	0.59	0
3	C14	B	404	-	9,9,13	0.26	0	8,8,12	0.44	0
3	C14	C	401	-	13,13,13	0.25	0	12,12,12	0.65	0
3	C14	B	405	-	9,9,13	0.24	0	8,8,12	0.45	0
3	C14	B	406	-	10,10,13	0.22	0	9,9,12	0.69	0
3	C14	A	404	-	9,9,13	0.29	0	8,8,12	0.48	0
3	C14	E	407	-	8,8,13	0.30	0	7,7,12	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	C14	E	406	-	10,10,13	0.26	0	9,9,12	0.48	0
3	C14	B	408	-	11,11,13	0.27	0	10,10,12	0.43	0
3	C14	B	407	-	10,10,13	0.24	0	9,9,12	0.59	0
3	C14	B	402	-	13,13,13	0.19	0	12,12,12	0.67	0
3	C14	A	403	-	7,7,13	0.21	0	6,6,12	0.68	0
3	C14	F	404	-	12,12,13	0.33	0	11,11,12	0.80	0
3	C14	B	409	-	12,12,13	0.18	0	11,11,12	1.03	1 (9%)
3	C14	D	403	-	10,10,13	0.23	0	9,9,12	0.49	0
3	C14	B	403	-	10,10,13	0.19	0	9,9,12	0.72	0
3	C14	D	405	-	13,13,13	0.20	0	12,12,12	0.59	0
3	C14	D	402	-	13,13,13	0.24	0	12,12,12	0.65	0
3	C14	E	403	-	9,9,13	0.28	0	8,8,12	0.66	0
3	C14	D	404	-	8,8,13	0.23	0	7,7,12	0.68	0

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	C14	E	405	-	-	2/10/10/11	-
3	C14	E	404	-	-	4/9/9/11	-
3	C14	B	404	-	-	1/7/7/11	-
3	C14	C	401	-	-	2/11/11/11	-
3	C14	B	405	-	-	5/7/7/11	-
3	C14	B	406	-	-	2/8/8/11	-
3	C14	A	404	-	-	1/7/7/11	-
3	C14	E	407	-	-	5/6/6/11	-
3	C14	E	406	-	-	5/8/8/11	-
3	C14	B	408	-	-	6/9/9/11	-
3	C14	B	407	-	-	5/8/8/11	-
3	C14	B	402	-	-	2/11/11/11	-
3	C14	A	403	-	-	0/5/5/11	-
3	C14	F	404	-	-	4/10/10/11	-
3	C14	B	409	-	-	4/10/10/11	-
3	C14	D	403	-	-	4/8/8/11	-
3	C14	B	403	-	-	1/8/8/11	-
3	C14	D	405	-	-	3/11/11/11	-
3	C14	D	402	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C14	E	403	-	-	2/7/7/11	-
3	C14	D	404	-	-	1/6/6/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	B	409	C14	C09-C08-C07	-2.19	103.31	114.42

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	407	C14	C05-C06-C07-C08
3	B	407	C14	C04-C05-C06-C07
3	F	404	C14	C09-C10-C11-C12
3	E	404	C14	C06-C07-C08-C09
3	B	407	C14	C02-C03-C04-C05
3	B	408	C14	C05-C06-C07-C08
3	A	404	C14	C05-C06-C07-C08
3	F	404	C14	C03-C04-C05-C06
3	E	406	C14	C02-C03-C04-C05
3	D	405	C14	C05-C06-C07-C08
3	E	403	C14	C07-C08-C09-C10
3	D	403	C14	C05-C06-C07-C08
3	D	402	C14	C05-C06-C07-C08
3	E	406	C14	C07-C08-C09-C10
3	B	409	C14	C02-C03-C04-C05
3	E	403	C14	C06-C07-C08-C09
3	B	404	C14	C06-C07-C08-C09
3	B	408	C14	C04-C05-C06-C07
3	C	401	C14	C06-C07-C08-C09
3	F	404	C14	C04-C05-C06-C07
3	D	402	C14	C09-C10-C11-C12
3	B	402	C14	C03-C04-C05-C06
3	B	408	C14	C03-C04-C05-C06
3	E	406	C14	C06-C07-C08-C09
3	B	408	C14	C07-C08-C09-C10
3	E	405	C14	C09-C10-C11-C12
3	B	409	C14	C09-C10-C11-C12
3	B	408	C14	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
3	E	407	C14	C06-C07-C08-C09
3	B	403	C14	C02-C03-C04-C05
3	B	409	C14	C04-C05-C06-C07
3	E	406	C14	C08-C09-C10-C11
3	E	404	C14	C11-C12-C13-C14
3	B	405	C14	C05-C06-C07-C08
3	E	405	C14	C10-C11-C12-C13
3	B	408	C14	C06-C07-C08-C09
3	B	405	C14	C07-C08-C09-C10
3	B	407	C14	C06-C07-C08-C09
3	D	403	C14	C01-C02-C03-C04
3	B	405	C14	C06-C07-C08-C09
3	B	405	C14	C01-C02-C03-C04
3	E	407	C14	C01-C02-C03-C04
3	D	405	C14	C09-C10-C11-C12
3	D	405	C14	C03-C04-C05-C06
3	B	406	C14	C05-C06-C07-C08
3	B	405	C14	C02-C03-C04-C05
3	E	407	C14	C02-C03-C04-C05
3	E	404	C14	C08-C09-C10-C11
3	D	402	C14	C10-C11-C12-C13
3	E	404	C14	C10-C11-C12-C13
3	E	407	C14	C04-C05-C06-C07
3	B	407	C14	C05-C06-C07-C08
3	F	404	C14	C08-C09-C10-C11
3	B	406	C14	C04-C05-C06-C07
3	D	403	C14	C04-C05-C06-C07
3	D	404	C14	C02-C03-C04-C05
3	C	401	C14	C10-C11-C12-C13
3	D	403	C14	C02-C03-C04-C05
3	B	402	C14	C07-C08-C09-C10
3	E	406	C14	C04-C05-C06-C07
3	B	407	C14	C01-C02-C03-C04
3	B	409	C14	C07-C08-C09-C10

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	405	C14	1	0
3	E	404	C14	1	0
3	C	401	C14	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	C14	1	0
3	E	406	C14	1	0
3	B	402	C14	4	0
3	A	403	C14	1	0
3	F	404	C14	4	0
3	B	409	C14	1	0
3	E	403	C14	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	347/347 (100%)	-0.24	4 (1%) 79 82	10, 15, 26, 37	0
1	B	347/347 (100%)	-0.07	12 (3%) 44 48	11, 16, 29, 45	0
1	C	347/347 (100%)	-0.09	6 (1%) 70 75	10, 16, 27, 43	0
1	D	347/347 (100%)	-0.15	13 (3%) 41 46	11, 16, 28, 44	0
1	E	343/347 (98%)	-0.12	10 (2%) 51 56	10, 15, 27, 36	0
1	F	347/347 (100%)	-0.05	12 (3%) 44 48	11, 16, 29, 42	0
All	All	2078/2082 (99%)	-0.12	57 (2%) 54 59	10, 16, 28, 45	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	188	TRP	9.9
1	D	188	TRP	9.5
1	C	188	TRP	8.6
1	F	188	TRP	6.0
1	D	187	ILE	4.9
1	C	187	ILE	4.8
1	B	118	TYR	4.8
1	F	85	ASP	4.2
1	B	8	GLY	4.2
1	B	189	ASP	4.2
1	F	86	ALA	4.1
1	E	118	TYR	4.0
1	B	115	THR	3.8
1	A	83	PHE	3.6
1	E	83	PHE	3.5
1	E	191	ILE	3.3
1	C	189	ASP	3.3
1	B	7	ASP	3.2
1	F	8	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	3.0
1	A	189	ASP	2.9
1	F	84	GLY	2.8
1	E	185	TYR	2.7
1	D	346	PHE	2.7
1	E	114	ASP	2.6
1	D	118	TYR	2.5
1	D	189	ASP	2.5
1	F	189	ASP	2.5
1	E	116	ASP	2.5
1	B	191	ILE	2.5
1	F	141	GLY	2.4
1	F	115	THR	2.4
1	F	152	TYR	2.4
1	B	119	GLY	2.3
1	B	114	ASP	2.3
1	D	328	ARG	2.3
1	F	322	ASP	2.3
1	D	114	ASP	2.3
1	D	117	THR	2.3
1	E	115	THR	2.2
1	C	49	GLN	2.2
1	B	323	ASP	2.2
1	B	187	ILE	2.2
1	D	323	ASP	2.2
1	F	7	ASP	2.2
1	A	7	ASP	2.2
1	C	185	TYR	2.1
1	E	84	GLY	2.1
1	A	195[A]	PHE	2.1
1	F	195	PHE	2.1
1	D	162	GLU	2.1
1	D	116	ASP	2.1
1	E	323	ASP	2.1
1	D	152	TYR	2.0
1	C	190	GLY	2.0
1	B	322	ASP	2.0
1	E	268	ASP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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	C14	D	403	11/14	0.76	0.14	35,37,39,39	0
3	C14	E	404	12/14	0.76	0.20	33,34,34,34	0
3	C14	A	404	10/14	0.77	0.14	29,30,32,33	0
3	C14	B	408	12/14	0.78	0.15	41,42,42,42	0
3	C14	D	402	14/14	0.79	0.18	26,30,32,33	0
3	C14	B	409	13/14	0.79	0.17	44,45,47,47	0
3	C14	C	401	14/14	0.79	0.15	35,36,36,37	0
3	C14	F	404	13/14	0.81	0.14	20,21,26,27	0
3	C14	B	405	10/14	0.82	0.14	31,34,35,35	0
3	C14	B	403	11/14	0.83	0.16	27,28,33,34	0
3	C14	D	405	14/14	0.83	0.13	37,38,41,41	0
3	C14	E	403	10/14	0.84	0.14	27,28,31,31	0
3	C14	B	402	14/14	0.84	0.17	26,29,31,31	0
3	C14	E	406	11/14	0.84	0.14	39,41,42,42	0
3	C14	B	407	11/14	0.84	0.16	42,43,44,44	0
3	C14	D	404	9/14	0.86	0.11	31,32,33,33	0
3	C14	E	405	13/14	0.86	0.14	34,35,38,38	0
3	C14	B	406	11/14	0.87	0.13	40,40,42,42	0
3	C14	A	403	8/14	0.88	0.13	32,32,33,33	0
3	C14	E	407	9/14	0.89	0.11	39,39,39,40	0
3	C14	B	404	10/14	0.91	0.11	32,33,34,34	0
2	LI	D	401	1/1	0.95	0.52	3,3,3,3	0
2	LI	B	401	1/1	0.95	0.44	3,3,3,3	0
2	LI	F	403	1/1	0.97	0.26	6,6,6,6	0
2	LI	E	401	1/1	0.98	0.51	3,3,3,3	0
2	LI	F	401	1/1	0.98	0.43	3,3,3,3	0
2	LI	F	402	1/1	0.98	0.47	3,3,3,3	0
2	LI	A	401	1/1	0.98	0.31	3,3,3,3	0
2	LI	A	402	1/1	0.98	0.52	3,3,3,3	0
2	LI	E	402	1/1	0.99	0.27	3,3,3,3	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.