



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:04 AM UTC

PDB ID : 7PZF / pdb_00007pzf
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)

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A user guide is available at

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

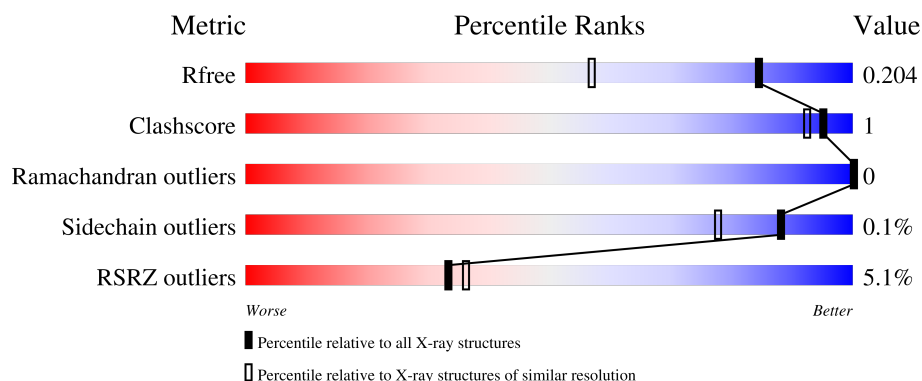
1 Overall quality at a glance

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 ≥ 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	5% 99%
1	B	347	5% 96%
1	C	347	4% 98%
1	D	347	5% 97%
1	E	347	5% 97%

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Mol	Chain	Length	Quality of chain
1	F	347	5% 95% 5%

2 Entry composition

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

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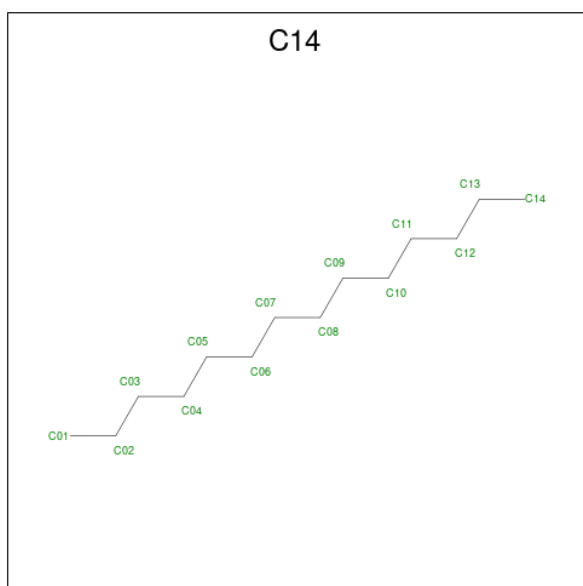
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Chain	Residue	Modelled	Actual	Comment	Reference
F	116	ASP	-	insertion	UNP D6QLY0

- Molecule 2 is LITHIUM ION (CCD ID: 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 (CCD ID: C14) (formula: C₁₄H₃₀).



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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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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.

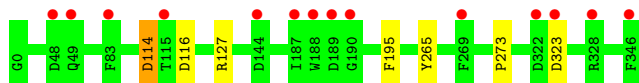
- Molecule 1: OmpK36



- Molecule 1: OmpK36



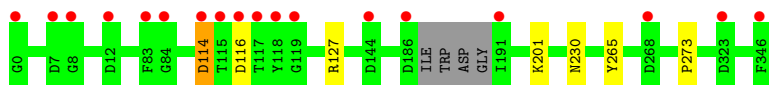
- Molecule 1: OmpK36



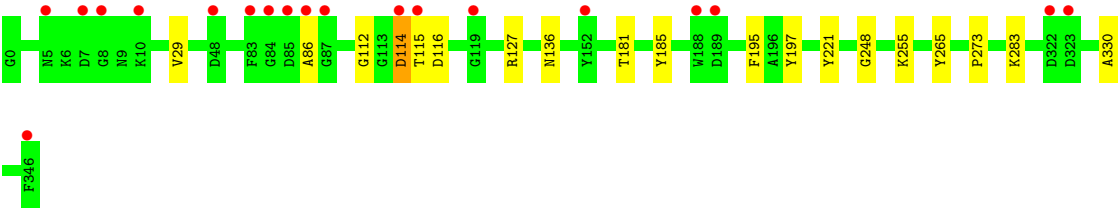
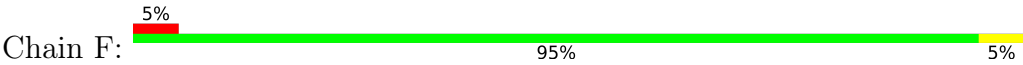
- Molecule 1: OmpK36



- Molecule 1: OmpK36



- Molecule 1: OmpK36



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 95.7 (54.25-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	18389 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: LI, C14

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	0.66	1/2810 (0.0%)	0.88	2/3806 (0.1%)
1	B	0.68	1/2817 (0.0%)	0.88	1/3813 (0.0%)
1	C	0.63	1/2798 (0.0%)	0.87	2/3790 (0.1%)
1	D	0.64	1/2796 (0.0%)	0.88	3/3787 (0.1%)
1	E	0.66	1/2764 (0.0%)	0.88	2/3740 (0.1%)
1	F	0.67	1/2791 (0.0%)	0.88	3/3780 (0.1%)
All	All	0.66	6/16776 (0.0%)	0.88	13/22716 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	116	ASP	CA-C	9.02	1.56	1.52
1	B	116	ASP	CA-C	8.85	1.56	1.52
1	A	116	ASP	CA-C	7.48	1.55	1.52
1	C	116	ASP	CA-C	6.33	1.55	1.52
1	D	116	ASP	CA-C	6.30	1.55	1.52
1	F	116	ASP	CA-C	5.61	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	ASP	CA-C-O	-6.03	116.33	119.77
1	D	346	PHE	CA-CB-CG	5.97	119.77	113.80
1	C	114	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	116	ASP	CA-C-O	-5.80	116.47	119.77
1	D	29	VAL	N-CA-CB	-5.79	103.97	111.90
1	A	116	ASP	CA-C-O	-5.75	116.49	119.77
1	E	114	ASP	CA-CB-CG	5.50	118.10	112.60
1	F	116	ASP	CA-C-O	-5.37	116.71	119.77
1	A	114	ASP	CA-CB-CG	5.30	117.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASP	CA-C-O	-5.21	116.80	119.77
1	F	114	ASP	CA-CB-CG	5.21	117.81	112.60
1	E	116	ASP	CA-C-O	-5.18	116.82	119.77
1	F	29	VAL	N-CA-CB	-5.14	103.23	111.82

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
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	1.57	0.70
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: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:B:201:LYS:HZ2	3:B:402:C14:H082	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	283 (100%)	0	100	100
1	B	284/278 (102%)	284 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	282/278 (101%)	281 (100%)	1 (0%)	84	71
1	D	281/278 (101%)	281 (100%)	0	100	100
1	E	280/278 (101%)	280 (100%)	0	100	100
1	F	281/278 (101%)	281 (100%)	0	100	100
All	All	1691/1668 (101%)	1690 (100%)	1 (0%)	88	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	323	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	71	GLN
1	A	230	ASN
1	B	9	ASN
1	B	55	GLN
1	B	71	GLN
1	B	199	HIS
1	B	230	ASN
1	B	329	ASN
1	C	9	ASN
1	C	71	GLN
1	C	230	ASN
1	D	55	GLN
1	D	71	GLN
1	D	125	GLN
1	D	230	ASN
1	E	9	ASN
1	E	55	GLN
1	E	71	GLN
1	E	230	ASN
1	F	9	ASN
1	F	71	GLN
1	F	230	ASN
1	F	240	GLN
1	F	257	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	405	-	9,9,13	0.24	0	8,8,12	0.45	0
3	C14	D	404	-	8,8,13	0.23	0	7,7,12	0.69	0
3	C14	B	406	-	10,10,13	0.22	0	9,9,12	0.69	0
3	C14	E	407	-	8,8,13	0.31	0	7,7,12	0.43	0
3	C14	E	406	-	10,10,13	0.25	0	9,9,12	0.47	0
3	C14	D	403	-	10,10,13	0.23	0	9,9,12	0.49	0
3	C14	B	407	-	10,10,13	0.24	0	9,9,12	0.60	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	D	405	-	13,13,13	0.20	0	12,12,12	0.58	0
3	C14	E	404	-	11,11,13	0.30	0	10,10,12	0.59	0
3	C14	A	404	-	9,9,13	0.30	0	8,8,12	0.48	0
3	C14	B	402	-	13,13,13	0.19	0	12,12,12	0.67	0
3	C14	E	403	-	9,9,13	0.28	0	8,8,12	0.67	0
3	C14	A	403	-	7,7,13	0.21	0	6,6,12	0.69	0
3	C14	D	402	-	13,13,13	0.24	0	12,12,12	0.65	0
3	C14	B	409	-	12,12,13	0.17	0	11,11,12	1.03	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C14	B	403	-	10,10,13	0.18	0	9,9,12	0.72	0
3	C14	F	404	-	12,12,13	0.35	0	11,11,12	0.81	0
3	C14	B	408	-	11,11,13	0.27	0	10,10,12	0.43	0
3	C14	E	405	-	12,12,13	0.31	0	11,11,12	0.55	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	B	405	-	-	5/7/7/11	-
3	C14	D	404	-	-	1/6/6/11	-
3	C14	B	406	-	-	2/8/8/11	-
3	C14	E	407	-	-	5/6/6/11	-
3	C14	E	406	-	-	5/8/8/11	-
3	C14	D	403	-	-	4/8/8/11	-
3	C14	B	407	-	-	5/8/8/11	-
3	C14	B	404	-	-	1/7/7/11	-
3	C14	C	401	-	-	2/11/11/11	-
3	C14	D	405	-	-	3/11/11/11	-
3	C14	E	404	-	-	4/9/9/11	-
3	C14	A	404	-	-	1/7/7/11	-
3	C14	B	402	-	-	2/11/11/11	-
3	C14	E	403	-	-	2/7/7/11	-
3	C14	A	403	-	-	0/5/5/11	-
3	C14	D	402	-	-	3/11/11/11	-
3	C14	B	409	-	-	4/10/10/11	-
3	C14	B	403	-	-	1/8/8/11	-
3	C14	F	404	-	-	4/10/10/11	-
3	C14	B	408	-	-	6/9/9/11	-
3	C14	E	405	-	-	2/10/10/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	409	C14	C09-C08-C07	-2.19	103.31	114.37

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	B	408	C14	C05-C06-C07-C08
3	E	404	C14	C06-C07-C08-C09
3	E	406	C14	C02-C03-C04-C05
3	D	402	C14	C05-C06-C07-C08
3	E	403	C14	C07-C08-C09-C10
3	A	404	C14	C05-C06-C07-C08
3	B	407	C14	C02-C03-C04-C05
3	F	404	C14	C03-C04-C05-C06
3	D	405	C14	C05-C06-C07-C08
3	D	403	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	B	408	C14	C03-C04-C05-C06
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	E	406	C14	C06-C07-C08-C09
3	B	409	C14	C04-C05-C06-C07
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	E	407	C14	C06-C07-C08-C09
3	B	408	C14	C01-C02-C03-C04
3	B	403	C14	C02-C03-C04-C05
3	B	405	C14	C05-C06-C07-C08
3	E	404	C14	C11-C12-C13-C14
3	E	406	C14	C08-C09-C10-C11
3	E	405	C14	C10-C11-C12-C13
3	B	405	C14	C07-C08-C09-C10
3	B	408	C14	C06-C07-C08-C09
3	B	407	C14	C06-C07-C08-C09
3	B	405	C14	C06-C07-C08-C09
3	D	403	C14	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
3	D	405	C14	C09-C10-C11-C12
3	B	405	C14	C01-C02-C03-C04
3	E	407	C14	C01-C02-C03-C04
3	D	405	C14	C03-C04-C05-C06
3	B	405	C14	C02-C03-C04-C05
3	B	406	C14	C05-C06-C07-C08
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	B	402	C14	C07-C08-C09-C10
3	D	403	C14	C02-C03-C04-C05
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	B	406	C14	1	0
3	E	406	C14	1	0
3	C	401	C14	2	0
3	E	404	C14	1	0
3	B	402	C14	4	0
3	E	403	C14	1	0
3	A	403	C14	1	0
3	B	409	C14	1	0
3	F	404	C14	4	0
3	E	405	C14	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	347/347 (100%)	-0.06	19 (5%)	30	33	9, 15, 26, 37	5 (1%)
1	B	347/347 (100%)	0.12	19 (5%)	30	33	8, 16, 29, 45	6 (1%)
1	C	347/347 (100%)	0.07	14 (4%)	42	46	9, 16, 27, 43	4 (1%)
1	D	347/347 (100%)	0.08	17 (4%)	35	38	9, 16, 28, 44	3 (0%)
1	E	343/347 (98%)	0.02	18 (5%)	33	35	7, 15, 27, 36	5 (1%)
1	F	347/347 (100%)	0.07	19 (5%)	30	33	9, 16, 29, 42	3 (0%)
All	All	2078/2082 (99%)	0.05	106 (5%)	33	36	7, 15, 28, 45	26 (1%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	188	TRP	7.2
1	C	188	TRP	7.0
1	B	188	TRP	6.5
1	B	115	THR	5.9
1	B	8	GLY	5.8
1	F	86	ALA	5.4
1	C	187	ILE	5.1
1	E	118	TYR	4.9
1	F	8	GLY	4.7
1	B	118	TYR	4.5
1	B	119	GLY	4.4
1	F	115	THR	4.3
1	B	7	ASP	4.3
1	D	187	ILE	4.2
1	F	85	ASP	4.1
1	F	84	GLY	4.1
1	E	115	THR	4.0
1	F	83	PHE	3.9
1	C	346	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	114	ASP	3.8
1	D	346	PHE	3.8
1	A	189	ASP	3.7
1	E	83	PHE	3.7
1	B	114	ASP	3.6
1	F	188	TRP	3.5
1	E	323	ASP	3.4
1	A	115	THR	3.3
1	E	116	ASP	3.3
1	F	10	LYS	3.3
1	E	119	GLY	3.2
1	B	0	GLY	3.1
1	D	189	ASP	3.1
1	D	114	ASP	3.1
1	D	152	TYR	3.0
1	B	48	ASP	3.0
1	E	84	GLY	3.0
1	D	195[A]	PHE	3.0
1	E	191	ILE	3.0
1	D	83	PHE	2.9
1	B	346	PHE	2.9
1	C	189	ASP	2.9
1	A	152	TYR	2.8
1	D	118	TYR	2.8
1	A	114	ASP	2.8
1	A	116	ASP	2.8
1	A	119	GLY	2.8
1	F	346	PHE	2.8
1	B	191	ILE	2.8
1	B	189	ASP	2.7
1	B	323	ASP	2.7
1	A	83	PHE	2.7
1	E	346	PHE	2.7
1	E	186	ASP	2.7
1	E	268	ASP	2.7
1	F	48	ASP	2.7
1	B	116	ASP	2.7
1	A	6	LYS	2.6
1	E	7	ASP	2.6
1	B	84	GLY	2.6
1	F	87	GLY	2.6
1	A	12	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	323	ASP	2.6
1	A	191	ILE	2.5
1	A	269	PHE	2.5
1	D	48	ASP	2.5
1	D	115	THR	2.5
1	F	7	ASP	2.5
1	A	118	TYR	2.5
1	F	152	TYR	2.5
1	C	323	ASP	2.5
1	A	7	ASP	2.5
1	F	322	ASP	2.5
1	F	114	ASP	2.4
1	B	187	ILE	2.4
1	C	190	GLY	2.4
1	C	322	ASP	2.3
1	D	116	ASP	2.3
1	D	120	SER	2.3
1	E	117	THR	2.3
1	F	119	GLY	2.3
1	C	48	ASP	2.3
1	B	29	VAL	2.3
1	C	115	THR	2.3
1	C	144	ASP	2.3
1	A	195[A]	PHE	2.3
1	D	190	GLY	2.3
1	A	188	TRP	2.3
1	B	6	LYS	2.3
1	F	5	ASN	2.2
1	A	322	ASP	2.2
1	A	323	ASP	2.2
1	E	0	GLY	2.2
1	F	189	ASP	2.2
1	E	144	ASP	2.1
1	C	269	PHE	2.1
1	B	120[A]	SER	2.1
1	D	119	GLY	2.1
1	D	117	THR	2.1
1	D	191	ILE	2.1
1	C	328	ARG	2.1
1	A	120	SER	2.1
1	E	8	GLY	2.1
1	A	8	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	49	GLN	2.0
1	E	12	ASP	2.0
1	C	83	PHE	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
3	C14	B	408	12/14	0.78	0.23	41,42,42,42	0
3	C14	C	401	14/14	0.79	0.22	35,36,36,37	0
3	C14	D	403	11/14	0.80	0.22	35,37,39,39	0
3	C14	E	404	12/14	0.80	0.23	33,34,34,34	0
3	C14	D	405	14/14	0.81	0.22	37,38,41,41	0
3	C14	A	404	10/14	0.81	0.18	29,30,32,33	0
3	C14	D	402	14/14	0.82	0.22	26,30,32,33	0
3	C14	B	409	13/14	0.82	0.22	44,45,47,47	0
3	C14	B	406	11/14	0.83	0.21	40,40,42,42	0
3	C14	F	404	13/14	0.83	0.17	20,21,26,27	0
3	C14	B	403	11/14	0.84	0.18	27,28,33,34	0
3	C14	B	405	10/14	0.84	0.22	31,34,35,35	0
3	C14	E	403	10/14	0.84	0.18	27,28,31,31	0
3	C14	B	402	14/14	0.84	0.19	26,29,31,31	0
3	C14	B	407	11/14	0.84	0.20	42,43,44,44	0
3	C14	E	407	9/14	0.85	0.20	39,39,39,40	0
3	C14	E	405	13/14	0.85	0.17	34,35,38,38	0
3	C14	B	404	10/14	0.87	0.16	32,33,34,34	0
3	C14	E	406	11/14	0.87	0.18	39,41,42,42	0
3	C14	D	404	9/14	0.88	0.19	31,32,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C14	A	403	8/14	0.89	0.16	32,32,33,33	0
2	LI	D	401	1/1	0.93	0.45	3,3,3,3	0
2	LI	F	402	1/1	0.94	0.45	3,3,3,3	0
2	LI	B	401	1/1	0.96	0.47	3,3,3,3	0
2	LI	E	401	1/1	0.97	0.46	3,3,3,3	0
2	LI	A	401	1/1	0.97	0.32	3,3,3,3	0
2	LI	F	403	1/1	0.97	0.25	6,6,6,6	0
2	LI	F	401	1/1	0.98	0.42	3,3,3,3	0
2	LI	A	402	1/1	0.98	0.47	3,3,3,3	0
2	LI	E	402	1/1	0.99	0.28	3,3,3,3	0

6.5 Other polymers [i](#)

There are no such residues in this entry.