



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 06:12 PM EST

PDB ID : 3JTY  
Title : Crystal structure of a BenF-like porin from *Pseudomonas fluorescens* Pf-5  
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Deposited on : 2009-09-14  
Resolution : 2.58 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	:	2.16
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)	:	2.16

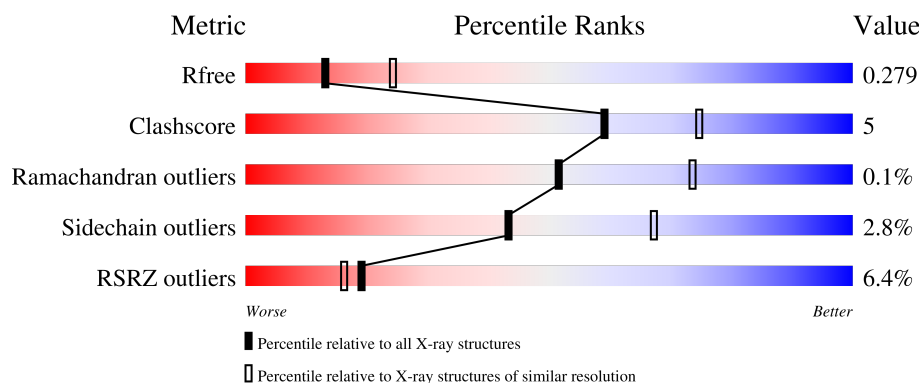
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	402	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div> </div>
1	B	402	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	C	402	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	402	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	2	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11916 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 BenF-like porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2978	1876	517	576	9			
1	B	383	Total	C	N	O	S	0	0	0
			2958	1864	515	570	9			
1	C	384	Total	C	N	O	S	0	0	0
			2967	1870	518	570	9			
1	D	384	Total	C	N	O	S	0	0	0
			2956	1864	512	571	9			

There are 44 discrepancies between the modelled and reference sequences:

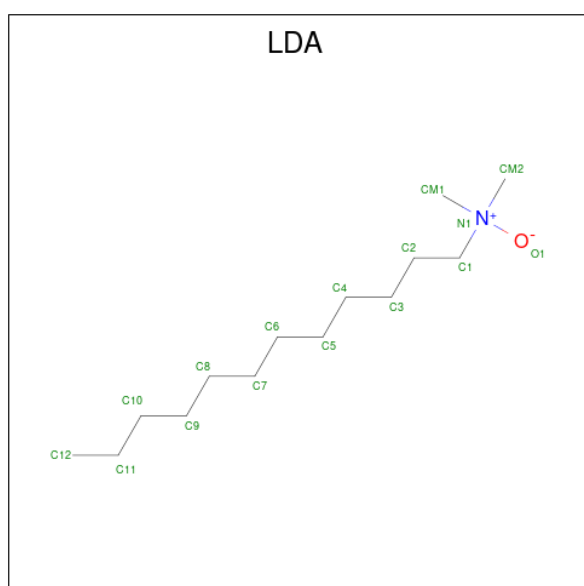
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q4KH25
A	28	SER	-	expression tag	UNP Q4KH25
A	29	LEU	-	expression tag	UNP Q4KH25
A	421	GLU	-	expression tag	UNP Q4KH25
A	422	GLY	-	expression tag	UNP Q4KH25
A	423	HIS	-	expression tag	UNP Q4KH25
A	424	HIS	-	expression tag	UNP Q4KH25
A	425	HIS	-	expression tag	UNP Q4KH25
A	426	HIS	-	expression tag	UNP Q4KH25
A	427	HIS	-	expression tag	UNP Q4KH25
A	428	HIS	-	expression tag	UNP Q4KH25
B	27	MET	-	expression tag	UNP Q4KH25
B	28	SER	-	expression tag	UNP Q4KH25
B	29	LEU	-	expression tag	UNP Q4KH25
B	421	GLU	-	expression tag	UNP Q4KH25
B	422	GLY	-	expression tag	UNP Q4KH25
B	423	HIS	-	expression tag	UNP Q4KH25
B	424	HIS	-	expression tag	UNP Q4KH25
B	425	HIS	-	expression tag	UNP Q4KH25
B	426	HIS	-	expression tag	UNP Q4KH25
B	427	HIS	-	expression tag	UNP Q4KH25

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Chain	Residue	Modelled	Actual	Comment	Reference
B	428	HIS	-	expression tag	UNP Q4KH25
C	27	MET	-	expression tag	UNP Q4KH25
C	28	SER	-	expression tag	UNP Q4KH25
C	29	LEU	-	expression tag	UNP Q4KH25
C	421	GLU	-	expression tag	UNP Q4KH25
C	422	GLY	-	expression tag	UNP Q4KH25
C	423	HIS	-	expression tag	UNP Q4KH25
C	424	HIS	-	expression tag	UNP Q4KH25
C	425	HIS	-	expression tag	UNP Q4KH25
C	426	HIS	-	expression tag	UNP Q4KH25
C	427	HIS	-	expression tag	UNP Q4KH25
C	428	HIS	-	expression tag	UNP Q4KH25
D	27	MET	-	expression tag	UNP Q4KH25
D	28	SER	-	expression tag	UNP Q4KH25
D	29	LEU	-	expression tag	UNP Q4KH25
D	421	GLU	-	expression tag	UNP Q4KH25
D	422	GLY	-	expression tag	UNP Q4KH25
D	423	HIS	-	expression tag	UNP Q4KH25
D	424	HIS	-	expression tag	UNP Q4KH25
D	425	HIS	-	expression tag	UNP Q4KH25
D	426	HIS	-	expression tag	UNP Q4KH25
D	427	HIS	-	expression tag	UNP Q4KH25
D	428	HIS	-	expression tag	UNP Q4KH25

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		

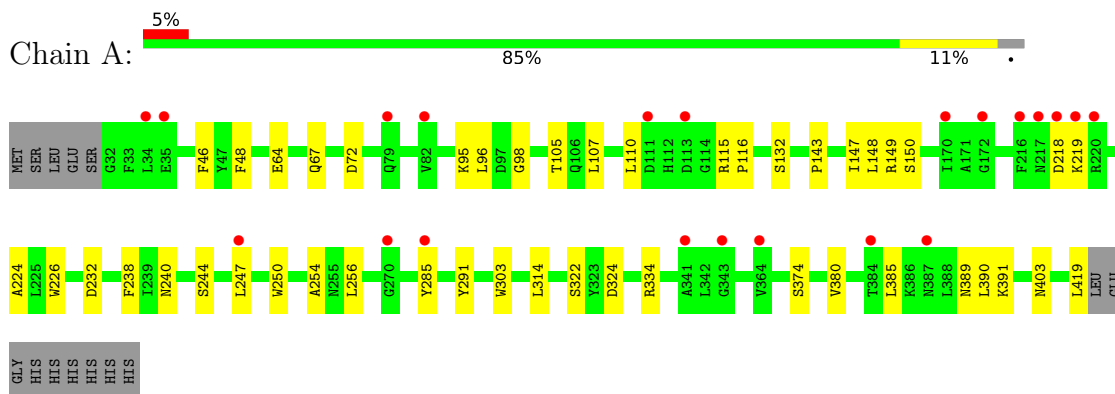
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	7	Total	O	0	0
			7	7		
3	C	2	Total	O	0	0
			2	2		
3	D	5	Total	O	0	0
			5	5		

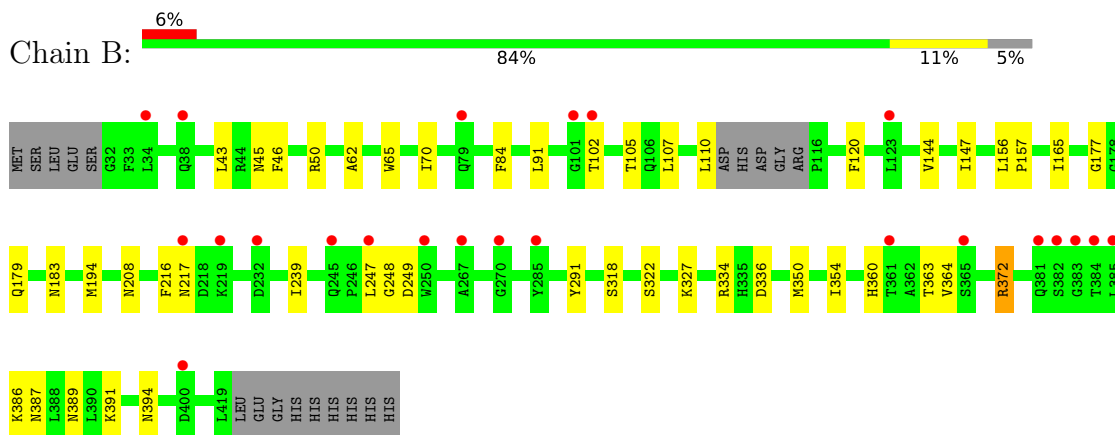
### 3 Residue-property plots [i](#)

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.

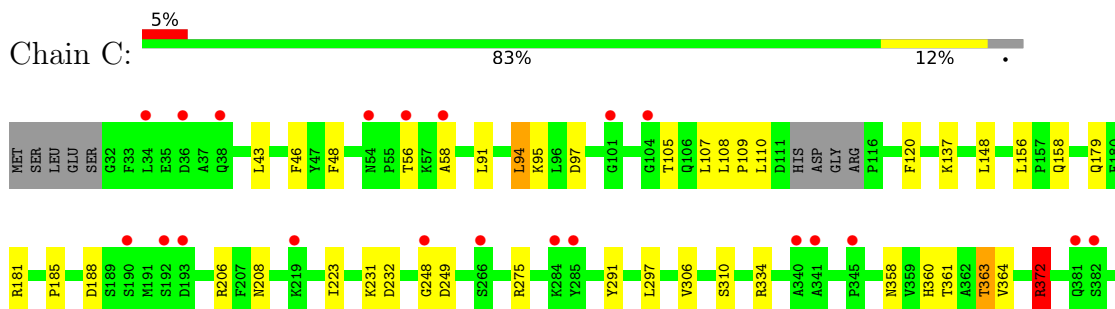
#### • Molecule 1: BenF-like porin

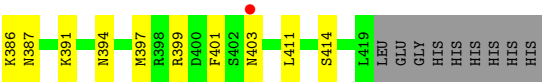


#### • Molecule 1: BenF-like porin

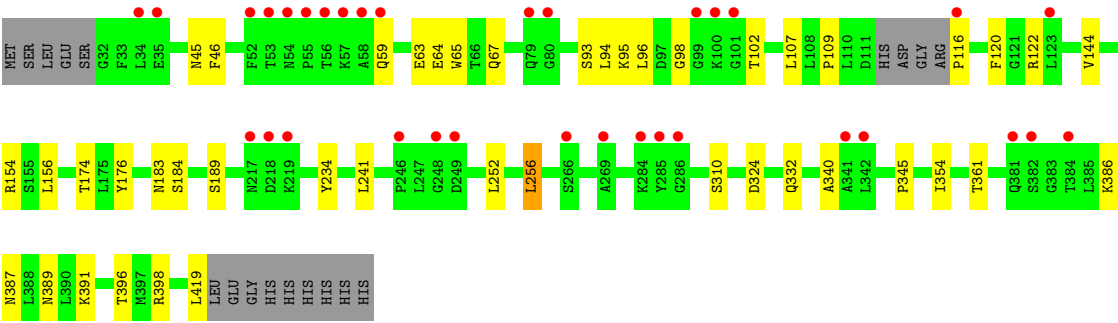
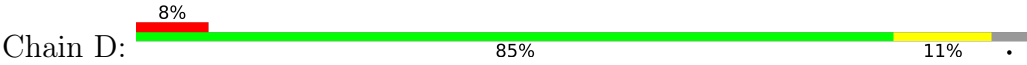


#### • Molecule 1: BenF-like porin





● Molecule 1: BenF-like porin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.10Å 210.62Å 84.07Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	35.11 – 2.58 35.10 – 2.58	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.11-2.58) 100.0 (35.10-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220 , 0.275 0.231 , 0.279	Depositor DCC
$R_{free}$ test set	3390 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8629e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: LDA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.80	0/3046	0.80	3/4122 (0.1%)
1	B	0.81	0/3025	0.81	1/4091 (0.0%)
1	C	0.81	0/3034	0.85	7/4100 (0.2%)
1	D	0.81	0/3023	0.79	0/4088
All	All	0.81	0/12128	0.81	11/16401 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	C	372	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	C	94	LEU	CA-CB-CG	7.44	132.40	115.30
1	A	72	ASP	CB-CG-OD1	7.31	124.88	118.30
1	C	97	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	149	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	403	ASN	CB-CA-C	-5.49	99.42	110.40
1	C	399	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	188	ASP	CB-CG-OD1	5.43	123.18	118.30
1	C	372	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	372	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	2978	0	2802	21	0
1	B	2958	0	2800	29	0
1	C	2967	0	2812	32	0
1	D	2956	0	2789	23	0
2	A	16	0	31	1	0
2	D	16	0	31	4	0
3	A	11	0	0	0	0
3	B	7	0	0	0	0
3	C	2	0	0	0	0
3	D	5	0	0	0	0
All	All	11916	0	11265	109	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 5.

All (109) 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:56:THR:HB	1:C:403:ASN:HD21	1.34	0.91
1:B:45:ASN:HD21	1:B:65:TRP:HE1	1.19	0.87
1:B:45:ASN:ND2	1:B:65:TRP:HE1	1.80	0.80
1:C:109:PRO:O	1:C:110:LEU:HD12	1.89	0.72
1:B:102:THR:O	1:B:102:THR:HG22	1.89	0.71
1:D:45:ASN:HD21	1:D:65:TRP:HE1	1.38	0.69
1:A:291:TYR:HB2	1:A:334:ARG:HB3	1.76	0.66
1:D:59:GLN:HE21	1:D:102:THR:HA	1.64	0.63
1:B:102:THR:CG2	1:B:102:THR:O	2.48	0.62
1:C:56:THR:HB	1:C:403:ASN:ND2	2.11	0.62
1:A:389:ASN:HD21	1:A:391:LYS:HE3	1.65	0.62
1:B:105:THR:HG21	1:B:107:LEU:HG	1.81	0.62
1:D:396:THR:HG23	1:D:398:ARG:NH1	2.15	0.61
1:C:56:THR:CB	1:C:403:ASN:HD21	2.12	0.60
1:C:291:TYR:HB2	1:C:334:ARG:HB3	1.83	0.59
1:C:372:ARG:HH22	1:C:394:ASN:HD22	1.51	0.58
2:D:1:LDA:C4	2:D:1:LDA:HM11	2.34	0.57
1:C:109:PRO:C	1:C:110:LEU:HD12	2.25	0.56
1:B:70:ILE:HG23	1:B:91:LEU:CD2	2.35	0.56
1:B:389:ASN:HD21	1:B:391:LYS:HE2	1.71	0.55
1:C:43:LEU:N	1:C:43:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLN:HE21	1:B:208:ASN:HD21	1.55	0.55
1:B:179:GLN:HE21	1:B:208:ASN:ND2	2.05	0.54
1:B:327:LYS:HD2	1:B:360:HIS:CD2	2.43	0.54
1:B:372:ARG:HH22	1:B:394:ASN:ND2	2.06	0.54
1:B:291:TYR:HB2	1:B:334:ARG:HB3	1.89	0.54
1:C:361:THR:HG22	1:C:363:THR:H	1.73	0.54
1:C:179:GLN:NE2	1:C:206:ARG:HD2	2.24	0.53
1:D:389:ASN:HD21	1:D:391:LYS:HE3	1.74	0.53
1:B:105:THR:CG2	1:B:107:LEU:HG	2.39	0.53
1:B:363:THR:HG22	1:B:363:THR:O	2.09	0.53
1:D:95:LYS:HD2	1:D:98:GLY:O	2.09	0.53
1:B:70:ILE:HG23	1:B:91:LEU:HD23	1.91	0.52
1:C:105:THR:HG21	1:C:107:LEU:HG	1.92	0.51
1:D:63:GLU:O	1:D:64:GLU:HG3	2.10	0.51
1:B:120:PHE:CE1	1:B:156:LEU:HD12	2.46	0.51
1:A:64:GLU:OE1	1:A:105:THR:HB	2.12	0.50
1:C:120:PHE:CZ	1:C:156:LEU:HD12	2.47	0.50
1:A:48:PHE:CG	1:A:105:THR:HG23	2.46	0.49
1:C:95:LYS:HD3	1:C:108:LEU:HD13	1.94	0.49
1:D:45:ASN:ND2	1:D:65:TRP:HE1	2.08	0.49
1:D:174:THR:HG22	1:D:176:TYR:CE2	2.47	0.49
1:A:105:THR:CG2	1:A:107:LEU:HG	2.44	0.48
1:B:50:ARG:HB3	1:B:62:ALA:HB3	1.96	0.47
1:D:386:LYS:O	1:D:387:ASN:HB2	2.14	0.47
1:B:363:THR:CG2	1:B:363:THR:O	2.62	0.47
1:D:109:PRO:O	1:D:116:PRO:HA	2.14	0.47
1:D:332:GLN:HG3	1:D:354:ILE:HG12	1.95	0.47
1:A:224:ALA:HB3	1:A:240:ASN:HB3	1.95	0.47
1:A:303:TRP:CE3	1:A:314:LEU:HD11	2.49	0.47
1:A:48:PHE:CD2	1:A:105:THR:HG23	2.50	0.47
1:D:340:ALA:HB2	1:D:345:PRO:HA	1.97	0.47
1:B:179:GLN:HB3	1:B:208:ASN:HD22	1.79	0.47
1:D:234:TYR:CD1	1:D:234:TYR:C	2.87	0.46
1:A:147:ILE:HD12	1:A:148:LEU:N	2.30	0.46
1:B:183:ASN:HB2	1:B:194:MET:HG2	1.98	0.46
1:B:336:ASP:OD1	1:B:350:MET:HG2	2.15	0.46
1:C:148:LEU:CD1	1:C:306:VAL:HG21	2.46	0.46
1:C:248:GLY:O	1:C:249:ASP:CB	2.64	0.45
1:A:95:LYS:HD2	1:A:98:GLY:O	2.15	0.45
1:A:143:PRO:HD2	1:A:150:SER:OG	2.15	0.45
1:C:275:ARG:O	1:C:297:LEU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:LYS:O	1:C:387:ASN:HB2	2.17	0.45
1:B:147:ILE:HD12	1:B:147:ILE:C	2.37	0.45
1:D:183:ASN:OD1	1:D:184:SER:N	2.50	0.45
1:C:43:LEU:N	1:C:43:LEU:CD1	2.80	0.44
1:C:91:LEU:HB3	1:C:156:LEU:HD22	1.99	0.44
1:D:120:PHE:CZ	1:D:156:LEU:HD12	2.52	0.44
1:D:67:GLN:HB2	1:D:96:LEU:HD11	2.00	0.44
1:C:391:LYS:O	1:C:411:LEU:HD12	2.18	0.44
1:B:386:LYS:O	1:B:387:ASN:HB2	2.17	0.44
1:D:107:LEU:HD23	1:D:154:ARG:HB3	1.98	0.44
1:B:318:SER:HB3	1:B:354:ILE:CD1	2.47	0.44
1:C:364:VAL:HG21	1:C:401:PHE:HB2	1.99	0.44
1:D:120:PHE:CE1	1:D:156:LEU:HD12	2.52	0.44
1:B:248:GLY:O	1:B:249:ASP:HB2	2.17	0.43
1:B:327:LYS:HD2	1:B:360:HIS:CG	2.52	0.43
1:C:120:PHE:CE1	1:C:156:LEU:HD12	2.52	0.43
1:A:247:LEU:HD23	1:A:247:LEU:O	2.18	0.43
1:B:91:LEU:HD22	1:B:157:PRO:HD2	2.01	0.43
1:C:179:GLN:HE21	1:C:208:ASN:HD21	1.66	0.43
1:D:93:SER:HB3	1:D:120:PHE:CE2	2.53	0.43
1:D:144:VAL:HG23	1:D:144:VAL:O	2.19	0.43
1:B:120:PHE:CZ	1:B:156:LEU:HD12	2.54	0.43
2:A:2:LDA:H42	2:A:2:LDA:HM11	2.00	0.43
1:C:105:THR:CG2	1:C:107:LEU:HG	2.49	0.43
1:C:372:ARG:HH11	1:C:372:ARG:HG3	1.84	0.42
1:A:324:ASP:N	1:A:324:ASP:OD1	2.49	0.42
1:D:122:ARG:NH1	1:D:189:SER:O	2.44	0.42
1:C:231:LYS:O	1:C:232:ASP:HB2	2.19	0.42
1:A:218:ASP:O	1:A:219:LYS:CB	2.68	0.42
1:A:105:THR:HG21	1:A:107:LEU:HG	2.02	0.42
1:A:67:GLN:HB2	1:A:96:LEU:HD11	2.01	0.42
1:C:181:ARG:HG2	1:C:206:ARG:NH1	2.35	0.41
1:C:358:ASN:O	1:C:360:HIS:HD2	2.02	0.41
2:D:1:LDA:HM11	2:D:1:LDA:C3	2.49	0.41
2:D:1:LDA:H42	2:D:1:LDA:HM11	2.01	0.41
1:A:226:TRP:HB2	1:A:238:PHE:HB3	2.01	0.41
1:D:256:LEU:HG	2:D:1:LDA:H62	2.03	0.41
1:C:158:GLN:HG3	1:C:185:PRO:HA	2.03	0.41
1:D:324:ASP:N	1:D:324:ASP:OD1	2.46	0.41
1:A:250:TRP:CE3	1:A:285:TYR:HB2	2.56	0.40
1:C:48:PHE:CG	1:C:105:THR:CG2	3.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:MET:HB2	1:C:397:MET:HE2	1.98	0.40
1:A:254:ALA:HB1	1:A:256:LEU:HD13	2.04	0.40
1:B:165:ILE:HG22	1:B:177:GLY:O	2.22	0.40
1:A:115:ARG:HA	1:A:116:PRO:HD3	1.93	0.40
1:C:43:LEU:O	1:C:414:SER:HA	2.21	0.40
1:A:380:VAL:HG11	1:A:385:LEU:O	2.21	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	386/402 (96%)	370 (96%)	15 (4%)	1 (0%)	41	62
1	B	379/402 (94%)	359 (95%)	20 (5%)	0	100	100
1	C	380/402 (94%)	359 (94%)	20 (5%)	1 (0%)	41	62
1	D	380/402 (94%)	360 (95%)	20 (5%)	0	100	100
All	All	1525/1608 (95%)	1448 (95%)	75 (5%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	C	58	ALA

### 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	302/329 (92%)	294 (97%)	8 (3%)	46	69
1	B	303/329 (92%)	292 (96%)	11 (4%)	35	59
1	C	303/329 (92%)	296 (98%)	7 (2%)	50	73
1	D	301/329 (92%)	293 (97%)	8 (3%)	44	68
All	All	1209/1316 (92%)	1175 (97%)	34 (3%)	43	67

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	PHE
1	A	110	LEU
1	A	232	ASP
1	A	244	SER
1	A	322	SER
1	A	374	SER
1	A	390	LEU
1	A	419	LEU
1	B	43	LEU
1	B	46	PHE
1	B	84	PHE
1	B	110	LEU
1	B	144	VAL
1	B	216	PHE
1	B	217	ASN
1	B	239	ILE
1	B	247	LEU
1	B	322	SER
1	B	364	VAL
1	C	46	PHE
1	C	94	LEU
1	C	137	LYS
1	C	223	ILE
1	C	310	SER
1	C	363	THR
1	C	372	ARG
1	D	46	PHE
1	D	94	LEU
1	D	241	LEU
1	D	252	LEU

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Mol	Chain	Res	Type
1	D	256	LEU
1	D	310	SER
1	D	361	THR
1	D	419	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	67	GLN
1	A	179	GLN
1	A	229	GLN
1	A	236	GLN
1	A	389	ASN
1	A	394	ASN
1	B	45	ASN
1	B	67	GLN
1	B	208	ASN
1	B	217	ASN
1	B	229	GLN
1	B	389	ASN
1	B	394	ASN
1	C	59	GLN
1	C	67	GLN
1	C	208	ASN
1	C	229	GLN
1	C	245	GLN
1	C	274	ASN
1	C	320	ASN
1	C	332	GLN
1	C	360	HIS
1	C	381	GLN
1	C	394	ASN
1	C	403	ASN
1	D	45	ASN
1	D	59	GLN
1	D	79	GLN
1	D	179	GLN
1	D	288	ASN
1	D	358	ASN
1	D	389	ASN
1	D	394	ASN



### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	LDA	A	2	-	12,15,15	2.00	1 (8%)	14,17,17	0.60	0
2	LDA	D	1	-	12,15,15	1.96	1 (8%)	14,17,17	0.49	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
2	LDA	A	2	-	-	8/13/13/13	-
2	LDA	D	1	-	-	9/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	LDA	O1-N1	-6.83	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	LDA	O1-N1	-6.69	1.26	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	LDA	N1-C1-C2-C3
2	D	1	LDA	N1-C1-C2-C3
2	D	1	LDA	C3-C4-C5-C6
2	A	2	LDA	C6-C7-C8-C9
2	D	1	LDA	C7-C8-C9-C10
2	A	2	LDA	C4-C5-C6-C7
2	A	2	LDA	C1-C2-C3-C4
2	A	2	LDA	C3-C4-C5-C6
2	D	1	LDA	C1-C2-C3-C4
2	D	1	LDA	C11-C10-C9-C8
2	A	2	LDA	C2-C3-C4-C5
2	D	1	LDA	C9-C10-C11-C12
2	A	2	LDA	C7-C8-C9-C10
2	D	1	LDA	C2-C3-C4-C5
2	D	1	LDA	C6-C7-C8-C9
2	A	2	LDA	C2-C1-N1-O1
2	D	1	LDA	C2-C1-N1-O1

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	LDA	1	0
2	D	1	LDA	4	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	388/402 (96%)	0.50	21 (5%)	25 22	29, 41, 56, 63	0
1	B	383/402 (95%)	0.46	23 (6%)	21 18	30, 41, 54, 63	0
1	C	384/402 (95%)	0.49	22 (5%)	23 20	30, 41, 55, 64	0
1	D	384/402 (95%)	0.53	33 (8%)	10 8	30, 41, 55, 63	0
All	All	1539/1608 (95%)	0.49	99 (6%)	19 16	29, 41, 56, 64	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	VAL	5.0
1	D	58	ALA	4.7
1	B	382	SER	4.6
1	B	384	THR	4.4
1	D	218	ASP	4.3
1	D	382	SER	4.2
1	D	101	GLY	4.1
1	D	248	GLY	4.0
1	B	247	LEU	3.8
1	B	385	LEU	3.8
1	A	35	GLU	3.7
1	D	53	THR	3.5
1	A	341	ALA	3.4
1	C	382	SER	3.4
1	A	34	LEU	3.4
1	C	219	LYS	3.4
1	D	54	ASN	3.4
1	D	55	PRO	3.2
1	D	249	ASP	3.2
1	D	285	TYR	3.2
1	D	219	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	285	TYR	3.1
1	B	381	GLN	3.1
1	D	384	THR	3.1
1	B	267	ALA	3.1
1	A	384	THR	3.1
1	B	383	GLY	3.0
1	D	341	ALA	3.0
1	A	219	LYS	3.0
1	C	266	SER	3.0
1	C	58	ALA	3.0
1	D	52	PHE	3.0
1	B	270	GLY	3.0
1	C	248	GLY	3.0
1	A	218	ASP	2.9
1	D	59	GLN	2.9
1	D	286	GLY	2.8
1	D	246	PRO	2.8
1	B	102	THR	2.8
1	A	387	ASN	2.8
1	D	56	THR	2.7
1	C	345	PRO	2.7
1	A	217	ASN	2.7
1	B	217	ASN	2.7
1	B	38	GLN	2.7
1	A	285	TYR	2.6
1	D	284	LYS	2.6
1	D	342	LEU	2.6
1	B	219	LYS	2.6
1	C	190	SER	2.5
1	B	232	ASP	2.5
1	A	247	LEU	2.5
1	C	341	ALA	2.5
1	C	284	LYS	2.4
1	B	361	THR	2.4
1	D	34	LEU	2.4
1	C	34	LEU	2.4
1	A	270	GLY	2.4
1	C	101	GLY	2.4
1	D	217	ASN	2.4
1	C	56	THR	2.4
1	A	343	GLY	2.4
1	A	79	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	365	SER	2.3
1	D	99	GLY	2.3
1	D	266	SER	2.3
1	B	123	LEU	2.3
1	B	245	GLN	2.3
1	D	269	ALA	2.3
1	A	172	GLY	2.2
1	B	285	TYR	2.2
1	A	113	ASP	2.2
1	C	192	SER	2.2
1	A	82	VAL	2.2
1	A	216	PHE	2.2
1	C	193	ASP	2.2
1	C	104	GLY	2.2
1	A	170	ILE	2.1
1	D	116	PRO	2.1
1	A	111	ASP	2.1
1	A	220	ARG	2.1
1	C	54	ASN	2.1
1	B	250	TRP	2.1
1	D	80	GLY	2.1
1	C	381	GLN	2.1
1	D	57	LYS	2.1
1	C	38	GLN	2.1
1	B	400	ASP	2.1
1	D	100	LYS	2.1
1	C	403	ASN	2.1
1	B	34	LEU	2.1
1	D	123	LEU	2.1
1	B	101	GLY	2.0
1	D	35	GLU	2.0
1	B	79	GLN	2.0
1	C	340	ALA	2.0
1	D	79	GLN	2.0
1	D	381	GLN	2.0
1	C	36	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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( $\text{\AA}^2$ )	Q<0.9
2	LDA	A	2	16/16	0.76	0.47	68,73,77,78	0
2	LDA	D	1	16/16	0.81	0.39	67,77,84,85	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.