



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:00 PM GMT

PDB ID : 4Z91
Title : ELIC cocrystallized with isofluorane in a desensitized state
Authors : Chen, Q.; Kinde, M.N.; Arjunan, P.; Cohen, A.; Xu, Y.; Tang, P.
Deposited on : 2015-04-09
Resolution : 3.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

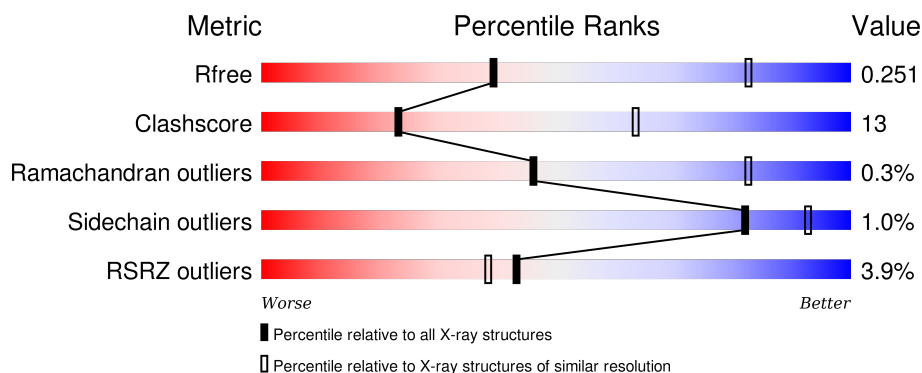
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	<div> <div>4%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	B	322	<div> <div>3%</div> <div>63%</div> <div>31%</div> <div>..</div> </div>
1	C	322	<div> <div>3%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	D	322	<div> <div>3%</div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	E	322	<div> <div>2%</div> <div>63%</div> <div>31%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	

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	4LE	E	401	-	-	-	X
2	4LE	F	401	-	-	-	X
4	4LJ	A	404	-	-	-	X
4	4LJ	B	403	-	-	-	X
4	4LJ	D	402	-	-	-	X
4	4LJ	E	403	-	-	-	X
4	4LJ	G	403	-	-	-	X
4	4LJ	H	403	-	-	-	X
4	4LJ	I	402	-	-	-	X
4	4LJ	J	404	-	-	-	X

2 Entry composition

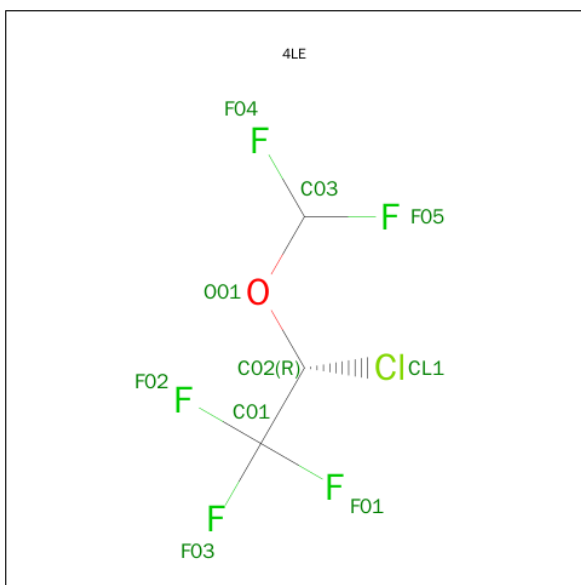
There are 5 unique types of molecules in this entry. The entry contains 25531 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gamma-aminobutyric-acid receptor subunit beta-1.

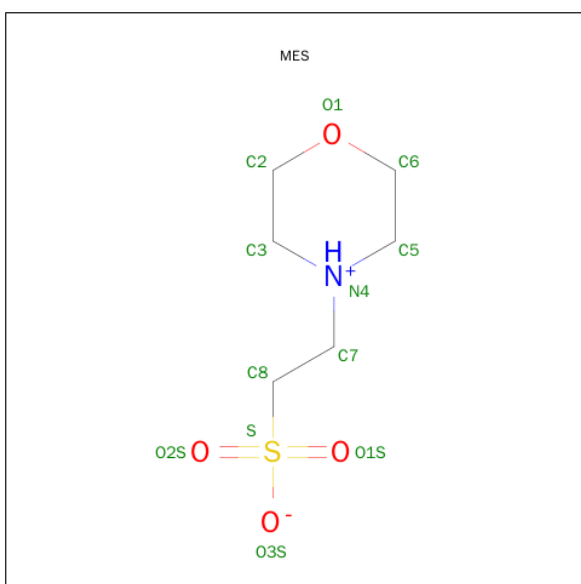
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	B	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	C	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	D	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	E	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	F	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	G	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	H	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	I	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			
1	J	309	Total	C	N	O	S	0	0	0
			2527	1645	424	452	6			

- Molecule 2 is (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (three-letter code: 4LE) (formula: C₃H₂ClF₅O).



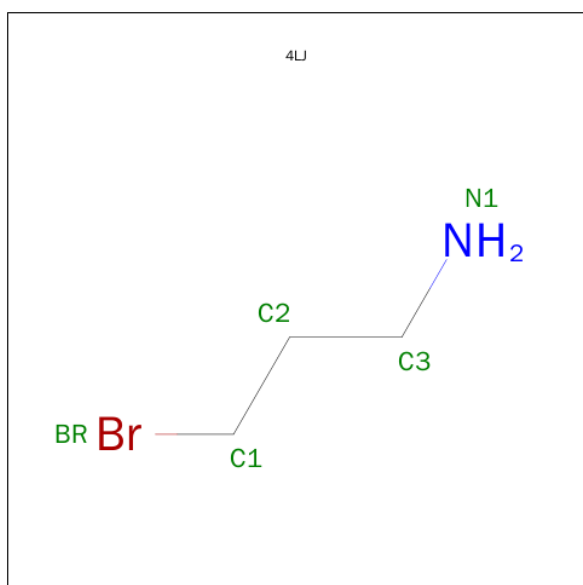
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		
2	E	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		
2	F	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		
2	J	1	Total	C	Cl	F	O	0	0
			10	3	1	5	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is 1.7.6 3-bromanylpropan-1-amine (three-letter code: 4LJ) (formula: C₃H₈BrN).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		
4	A	1	Total	Br	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Br 1	0	0
4	B	1	Total 1	Br 1	0	0
4	C	1	Total 1	Br 1	0	0
4	C	1	Total 1	Br 1	0	0
4	D	1	Total 1	Br 1	0	0
4	E	1	Total 1	Br 1	0	0
4	E	1	Total 1	Br 1	0	0
4	E	1	Total 1	Br 1	0	0
4	F	1	Total 1	Br 1	0	0
4	F	1	Total 1	Br 1	0	0
4	G	1	Total 1	Br 1	0	0
4	G	1	Total 1	Br 1	0	0
4	H	1	Total 1	Br 1	0	0
4	H	1	Total 1	Br 1	0	0
4	I	1	Total 1	Br 1	0	0
4	I	1	Total 1	Br 1	0	0
4	J	1	Total 1	Br 1	0	0
4	J	1	Total 1	Br 1	0	0

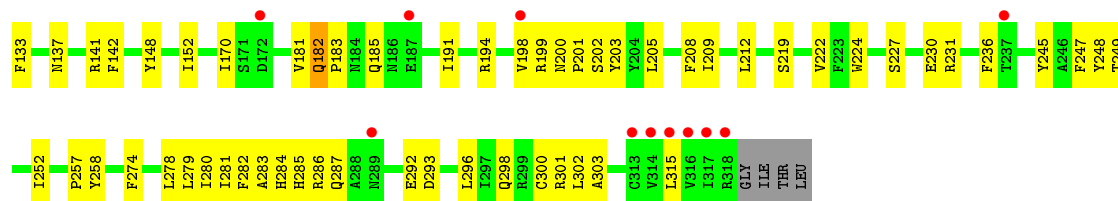
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0

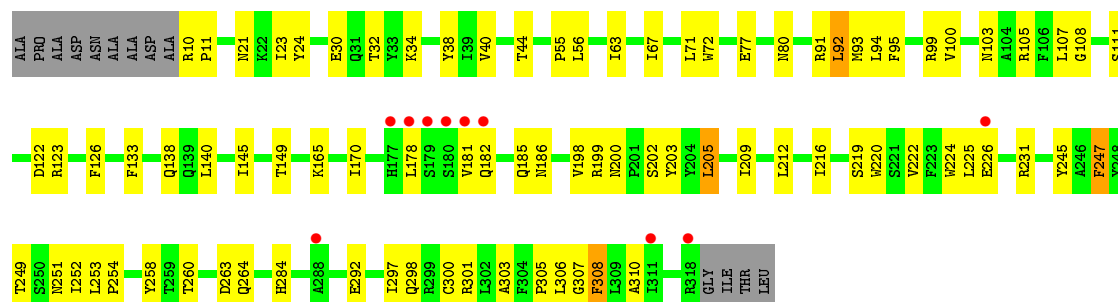
Continued on next page...

Continued from previous page...

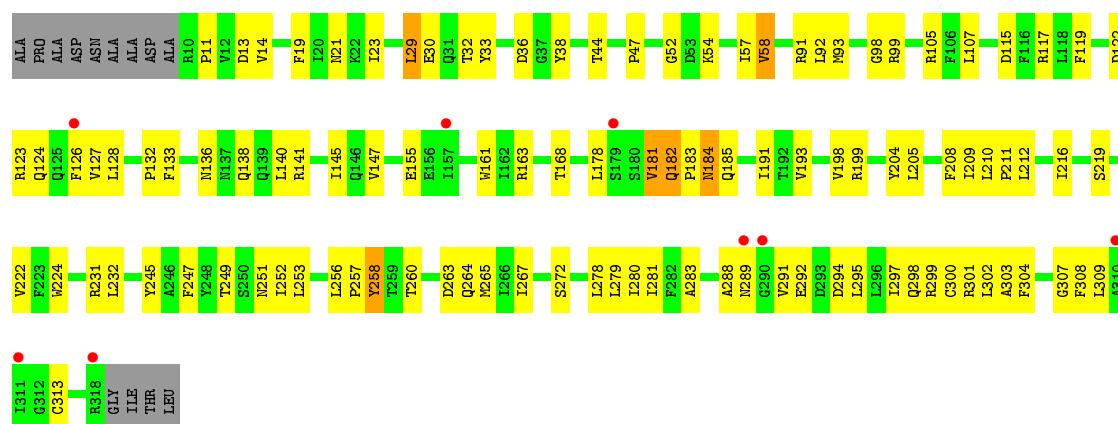
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	8	Total 8	O 8	0	0
5	C	7	Total 7	O 7	0	0
5	D	8	Total 8	O 8	0	0
5	E	11	Total 11	O 11	0	0
5	F	5	Total 5	O 5	0	0
5	G	9	Total 9	O 9	0	0
5	H	7	Total 7	O 7	0	0
5	I	11	Total 11	O 11	0	0
5	J	9	Total 9	O 9	0	0



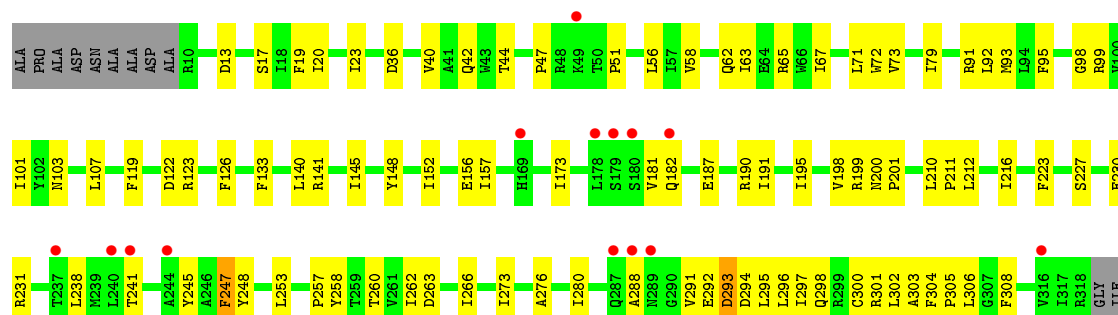
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

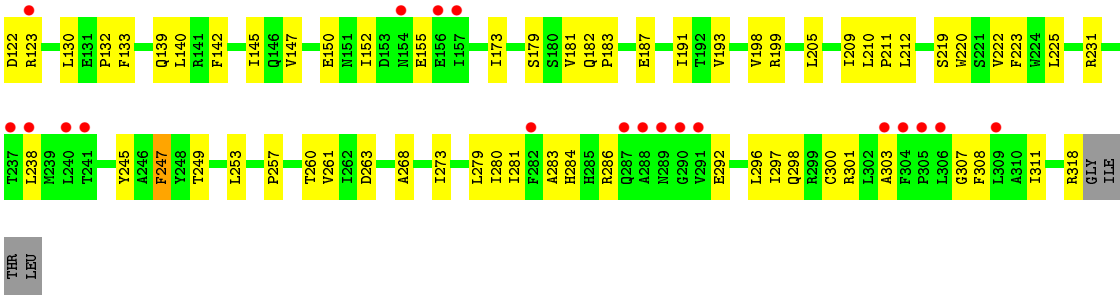


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.76Å 267.60Å 111.37Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	34.89 – 3.39 40.01 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.89-3.39) 97.6 (40.01-3.39)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.192 , 0.247 0.205 , 0.251	Depositor DCC
R_{free} test set	2017 reflections (2.61%)	DCC
Wilson B-factor (Å ²)	110.4	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 79300 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25531	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 4LJ, MES, 4LE

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	0.47	0/2595	0.66	0/3536
1	B	0.52	0/2595	0.74	0/3536
1	C	0.54	0/2595	0.70	0/3536
1	D	0.57	0/2595	0.70	1/3536 (0.0%)
1	E	0.49	0/2595	0.67	0/3536
1	F	0.46	0/2595	0.67	1/3536 (0.0%)
1	G	0.53	0/2595	0.71	1/3536 (0.0%)
1	H	0.51	0/2595	0.68	0/3536
1	I	0.50	0/2595	0.69	0/3536
1	J	0.47	0/2595	0.66	0/3536
All	All	0.51	0/25950	0.69	3/35360 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	240	LEU	CA-CB-CG	5.14	127.11	115.30
1	F	295	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	205	LEU	CA-CB-CG	-5.00	103.79	115.30

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	2527	0	2503	71	0
1	B	2527	0	2503	94	0
1	C	2527	0	2503	69	0
1	D	2527	0	2503	63	0
1	E	2527	0	2503	92	0
1	F	2527	0	2503	69	0
1	G	2527	0	2503	67	0
1	H	2527	0	2503	72	0
1	I	2527	0	2503	70	0
1	J	2527	0	2503	69	0
2	A	10	0	1	0	0
2	E	10	0	1	1	0
2	F	10	0	1	1	0
2	J	10	0	1	1	0
3	A	12	0	12	2	0
3	B	12	0	12	0	0
3	C	12	0	12	1	0
3	D	12	0	12	1	0
3	E	12	0	12	0	0
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	12	0	12	0	0
3	I	12	0	12	0	0
3	J	12	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	1	0
4	E	3	0	0	1	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	2	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
5	A	6	0	0	0	0
5	B	8	0	0	3	0
5	C	7	0	0	0	0
5	D	8	0	0	1	0
5	E	11	0	0	0	0
5	F	5	0	0	0	0
5	G	9	0	0	1	0
5	H	7	0	0	0	0
5	I	11	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	9	0	0	1	0
All	All	25531	0	25154	677	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 13.

The worst 5 of 677 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:HG2	1:A:198:VAL:HG12	1.17	1.15
1:D:123:ARG:HG2	1:D:198:VAL:CG1	1.78	1.14
1:E:183:PRO:O	1:E:185:GLN:HG2	1.45	1.12
1:E:182:GLN:H	1:E:183:PRO:HD2	0.98	1.09
1:I:123:ARG:HG2	1:I:198:VAL:HG12	1.20	1.09

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	307/322 (95%)	284 (92%)	23 (8%)	0	100	100
1	B	307/322 (95%)	279 (91%)	27 (9%)	1 (0%)	46	82
1	C	307/322 (95%)	283 (92%)	23 (8%)	1 (0%)	46	82
1	D	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	46	82
1	E	307/322 (95%)	284 (92%)	20 (6%)	3 (1%)	19	63
1	F	307/322 (95%)	283 (92%)	23 (8%)	1 (0%)	46	82
1	G	307/322 (95%)	283 (92%)	24 (8%)	0	100	100
1	H	307/322 (95%)	281 (92%)	25 (8%)	1 (0%)	46	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	307/322 (95%)	282 (92%)	23 (8%)	2 (1%)	26	70
1	J	307/322 (95%)	284 (92%)	23 (8%)	0	100	100
All	All	3070/3220 (95%)	2825 (92%)	235 (8%)	10 (0%)	46	82

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293	ASP
1	E	184	ASN
1	E	181	VAL
1	E	182	GLN
1	I	182	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/284 (98%)	276 (100%)	1 (0%)	93	97
1	B	277/284 (98%)	274 (99%)	3 (1%)	80	92
1	C	277/284 (98%)	276 (100%)	1 (0%)	93	97
1	D	277/284 (98%)	273 (99%)	4 (1%)	74	90
1	E	277/284 (98%)	272 (98%)	5 (2%)	66	88
1	F	277/284 (98%)	276 (100%)	1 (0%)	93	97
1	G	277/284 (98%)	274 (99%)	3 (1%)	80	92
1	H	277/284 (98%)	271 (98%)	6 (2%)	60	86
1	I	277/284 (98%)	273 (99%)	4 (1%)	74	90
1	J	277/284 (98%)	276 (100%)	1 (0%)	93	97
All	All	2770/2840 (98%)	2741 (99%)	29 (1%)	82	93

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	258	TYR
1	G	247	PHE
1	I	258	TYR
1	F	247	PHE
1	G	258	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	285	HIS
1	E	264	GLN
1	I	169	HIS
1	E	233	GLN
1	E	251	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](#)

Of 34 ligands modelled in this entry, 20 are modelled with single atom - leaving 14 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
2	4LE	A	401	-	7,9,9	0.71	0	10,13,13	1.25	1 (10%)
3	MES	A	402	-	12,12,12	2.13	1 (8%)	15,16,16	3.02	7 (46%)
3	MES	B	401	-	12,12,12	2.03	1 (8%)	15,16,16	2.60	7 (46%)
3	MES	C	401	-	12,12,12	1.96	1 (8%)	15,16,16	3.74	6 (40%)
3	MES	D	401	-	12,12,12	2.00	1 (8%)	15,16,16	3.72	7 (46%)
2	4LE	E	401	-	7,9,9	0.84	0	10,13,13	1.39	2 (20%)
3	MES	E	402	-	12,12,12	2.08	1 (8%)	15,16,16	2.64	4 (26%)
2	4LE	F	401	-	7,9,9	0.81	0	10,13,13	1.56	1 (10%)
3	MES	F	402	-	12,12,12	1.89	1 (8%)	15,16,16	2.90	7 (46%)
3	MES	G	401	-	12,12,12	1.92	1 (8%)	15,16,16	2.47	7 (46%)
3	MES	H	401	-	12,12,12	2.11	1 (8%)	15,16,16	3.14	8 (53%)
3	MES	I	401	-	12,12,12	1.97	1 (8%)	15,16,16	2.61	8 (53%)
2	4LE	J	401	-	7,9,9	0.85	0	10,13,13	1.23	1 (10%)
3	MES	J	402	-	12,12,12	2.14	1 (8%)	15,16,16	2.48	5 (33%)

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	4LE	A	401	-	-	0/6/10/10	0/0/0/0
3	MES	A	402	-	-	0/6/14/14	0/1/1/1
3	MES	B	401	-	-	0/6/14/14	0/1/1/1
3	MES	C	401	-	-	0/6/14/14	0/1/1/1
3	MES	D	401	-	-	0/6/14/14	0/1/1/1
2	4LE	E	401	-	-	0/6/10/10	0/0/0/0
3	MES	E	402	-	-	0/6/14/14	0/1/1/1
2	4LE	F	401	-	-	0/6/10/10	0/0/0/0
3	MES	F	402	-	-	0/6/14/14	0/1/1/1
3	MES	G	401	-	-	0/6/14/14	0/1/1/1
3	MES	H	401	-	-	0/6/14/14	0/1/1/1
3	MES	I	401	-	-	0/6/14/14	0/1/1/1
2	4LE	J	401	-	-	0/6/10/10	0/0/0/0
3	MES	J	402	-	-	0/6/14/14	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	402	MES	C8-S	-7.09	1.66	1.77
3	A	402	MES	C8-S	-7.06	1.66	1.77
3	H	401	MES	C8-S	-6.97	1.67	1.77
3	E	402	MES	C8-S	-6.86	1.67	1.77
3	B	401	MES	C8-S	-6.67	1.67	1.77

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	MES	C2-C3-N4	-3.82	104.27	110.11
3	A	402	MES	C6-C5-N4	-3.45	104.84	110.11
3	H	401	MES	C6-C5-N4	-3.40	104.91	110.11
3	I	401	MES	C6-C5-N4	-2.69	106.00	110.11
3	D	401	MES	O2S-S-O1S	-2.42	107.13	113.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	MES	2	0
3	C	401	MES	1	0
3	D	401	MES	1	0
2	E	401	4LE	1	0
2	F	401	4LE	1	0
2	J	401	4LE	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, 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	309/322 (95%)	0.03	13 (4%)	40	35	77, 115, 164, 199	0
1	B	309/322 (95%)	-0.03	11 (3%)	46	41	70, 102, 176, 211	0
1	C	309/322 (95%)	0.03	11 (3%)	46	41	68, 105, 179, 200	0
1	D	309/322 (95%)	-0.00	10 (3%)	51	47	60, 98, 176, 200	0
1	E	309/322 (95%)	-0.03	8 (2%)	59	54	75, 107, 173, 201	0
1	F	309/322 (95%)	0.07	14 (4%)	37	33	68, 122, 177, 215	0
1	G	309/322 (95%)	-0.06	12 (3%)	43	38	62, 104, 171, 197	0
1	H	309/322 (95%)	0.01	12 (3%)	43	38	68, 111, 181, 210	0
1	I	309/322 (95%)	0.00	12 (3%)	43	38	66, 108, 176, 211	0
1	J	309/322 (95%)	0.11	19 (6%)	25	23	77, 118, 188, 208	0
All	All	3090/3220 (95%)	0.01	122 (3%)	43	38	60, 110, 179, 215	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	SER	9.9
1	D	179	SER	7.4
1	F	287	GLN	6.9
1	F	179	SER	6.0
1	C	314	VAL	5.8

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	4LJ	J	404	1/5	0.72	1.26	22.71	229,229,229,229	0
4	4LJ	E	403	1/5	0.89	1.15	21.74	259,259,259,259	0
4	4LJ	G	403	1/5	0.72	0.70	16.47	205,205,205,205	0
4	4LJ	A	404	1/5	0.18	0.84	10.89	225,225,225,225	0
4	4LJ	H	403	1/5	0.65	0.80	10.32	228,228,228,228	0
4	4LJ	B	403	1/5	0.88	0.32	5.15	206,206,206,206	0
4	4LJ	D	402	1/5	0.88	0.35	5.09	205,205,205,205	0
4	4LJ	I	402	1/5	0.74	0.42	4.14	219,219,219,219	0
4	4LJ	C	403	1/5	0.85	0.30	1.56	224,224,224,224	0
4	4LJ	J	403	1/5	0.82	0.23	1.24	213,213,213,213	0
2	4LE	F	401	10/10	0.95	0.50	0.68	142,147,160,173	0
3	MES	I	401	12/12	0.89	0.23	0.38	147,156,174,183	0
2	4LE	E	401	10/10	0.94	0.43	-0.20	117,149,163,171	0
3	MES	A	402	12/12	0.91	0.24	-0.30	121,138,167,176	0
3	MES	F	402	12/12	0.86	0.18	-0.67	144,157,169,175	0
3	MES	E	402	12/12	0.88	0.14	-1.34	144,162,169,174	0
2	4LE	A	401	10/10	0.96	0.24	-2.97	132,138,150,153	0
2	4LE	J	401	10/10	0.95	0.16	-2.98	147,152,160,165	0
3	MES	B	401	12/12	0.90	0.10	-	133,146,166,183	0
4	4LJ	G	402	1/5	0.77	0.32	-	210,210,210,210	0
4	4LJ	I	403	1/5	0.87	0.20	-	184,184,184,184	0
3	MES	C	401	12/12	0.89	0.14	-	123,138,162,174	0
3	MES	G	401	12/12	0.94	0.15	-	126,140,173,183	0
4	4LJ	H	402	1/5	0.43	0.41	-	236,236,236,236	0
4	4LJ	E	405	1/5	-0.04	0.62	-	272,272,272,272	0
4	4LJ	F	404	1/5	0.60	1.11	-	267,267,267,267	0
3	MES	H	401	12/12	0.88	0.14	-	124,148,161,169	0
4	4LJ	E	404	1/5	0.32	0.74	-	221,221,221,221	0
4	4LJ	C	402	1/5	0.90	0.51	-	203,203,203,203	0
4	4LJ	B	402	1/5	0.67	0.34	-	219,219,219,219	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MES	D	401	12/12	0.83	0.19	-	122,136,158,159	0
4	4LJ	A	403	1/5	0.86	0.24	-	200,200,200,200	0
3	MES	J	402	12/12	0.91	0.19	-	152,164,183,189	0
4	4LJ	F	403	1/5	0.58	0.70	-	206,206,206,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.