



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:35 AM GMT

PDB ID : 3PGS  
Title : Phe3Gly mutant of EcFadL  
Authors : van den Berg, B.; Lepore, B.W.  
Deposited on : 2010-11-02  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

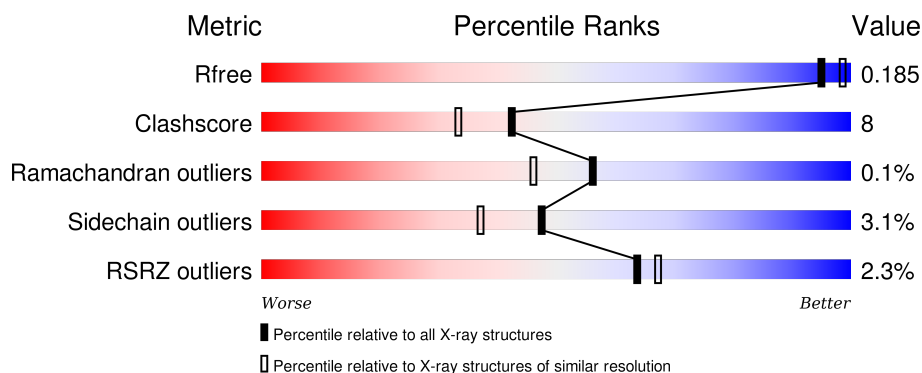
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	427	
1	B	427	

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
3	C8E	A	430	-	-	-	X
3	C8E	A	438	-	-	-	X
3	C8E	A	439	-	-	-	X
3	C8E	A	440	-	-	-	X
3	C8E	A	441	-	-	-	X
3	C8E	A	442	-	-	-	X
3	C8E	A	443	-	-	-	X
3	C8E	B	431	-	-	-	X
3	C8E	B	433	-	-	-	X
3	C8E	B	434	-	-	-	X
3	C8E	B	435	-	-	-	X
4	LDA	A	431	-	-	-	X
4	LDA	A	432	-	-	-	X
4	LDA	A	433	-	-	-	X
4	LDA	A	434	-	-	-	X
4	LDA	A	437	-	-	-	X
4	LDA	B	429	-	-	-	X
4	LDA	B	430	-	-	-	X
5	ACT	A	1428	-	-	-	X
6	2PE	B	436	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8014 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 Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	3	23	0
			3459	2194	592	666	7			
1	B	426	Total	C	N	O	S	5	19	0
			3411	2167	583	654	7			

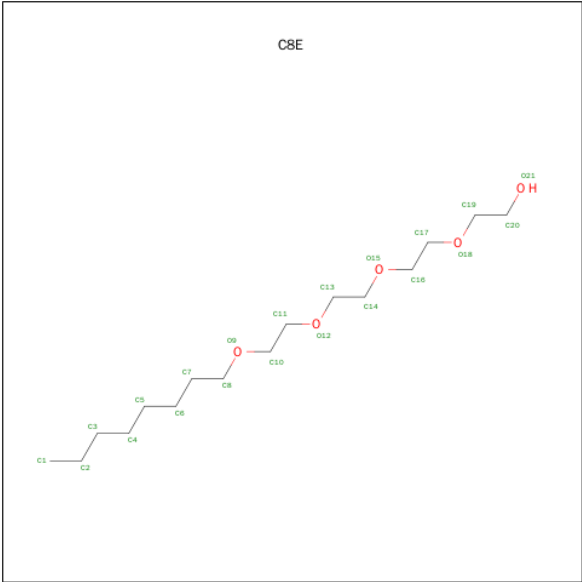
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	PHE	ENGINEERED MUTATION	UNP P10384
A	422	HIS	-	EXPRESSION TAG	UNP P10384
A	423	HIS	-	EXPRESSION TAG	UNP P10384
A	424	HIS	-	EXPRESSION TAG	UNP P10384
A	425	HIS	-	EXPRESSION TAG	UNP P10384
A	426	HIS	-	EXPRESSION TAG	UNP P10384
A	427	HIS	-	EXPRESSION TAG	UNP P10384
B	3	GLY	PHE	ENGINEERED MUTATION	UNP P10384
B	422	HIS	-	EXPRESSION TAG	UNP P10384
B	423	HIS	-	EXPRESSION TAG	UNP P10384
B	424	HIS	-	EXPRESSION TAG	UNP P10384
B	425	HIS	-	EXPRESSION TAG	UNP P10384
B	426	HIS	-	EXPRESSION TAG	UNP P10384
B	427	HIS	-	EXPRESSION TAG	UNP P10384

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

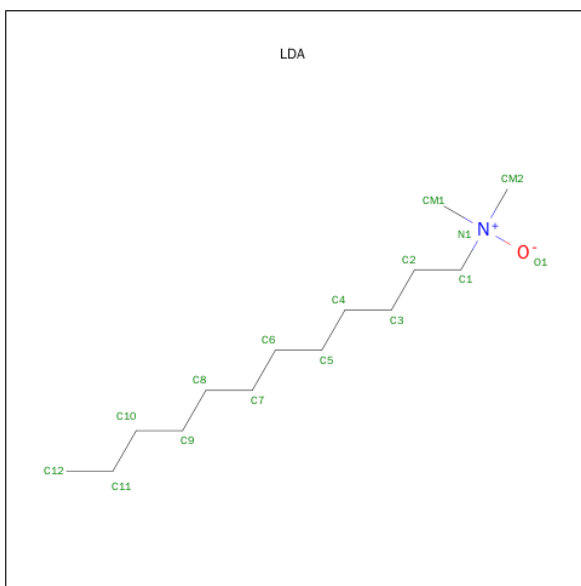
- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			14	12	2		
3	A	1	Total	C	O	0	0
			20	15	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			13	11	2		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			15	10	5		
3	B	1	Total	C	O	0	0
			21	16	5		

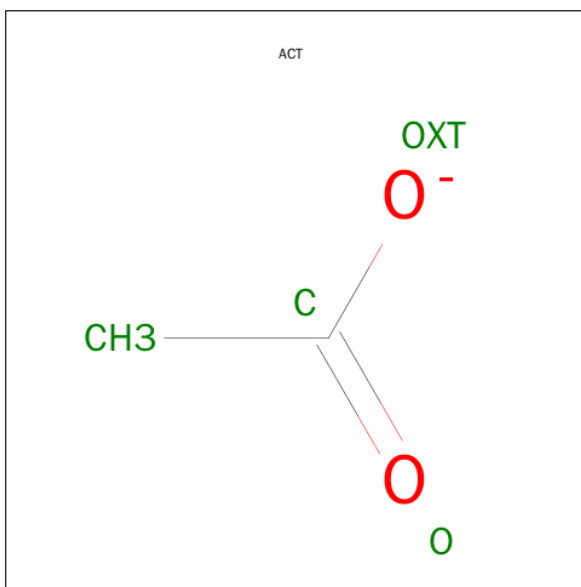
- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



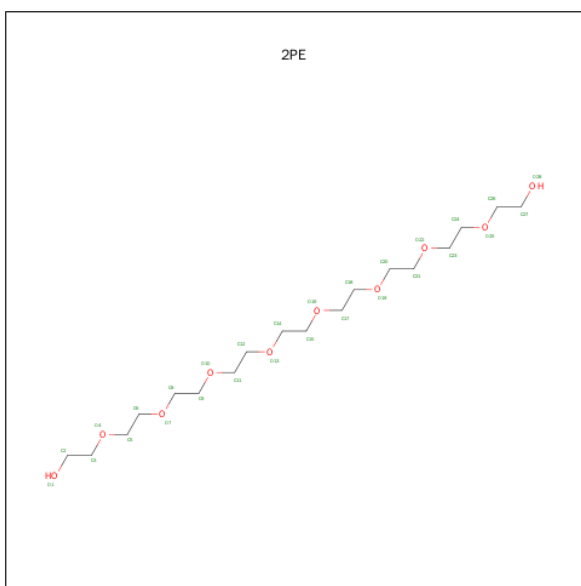
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 11 11	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C<sub>18</sub>H<sub>38</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			28	18	10		

- Molecule 7 is water.

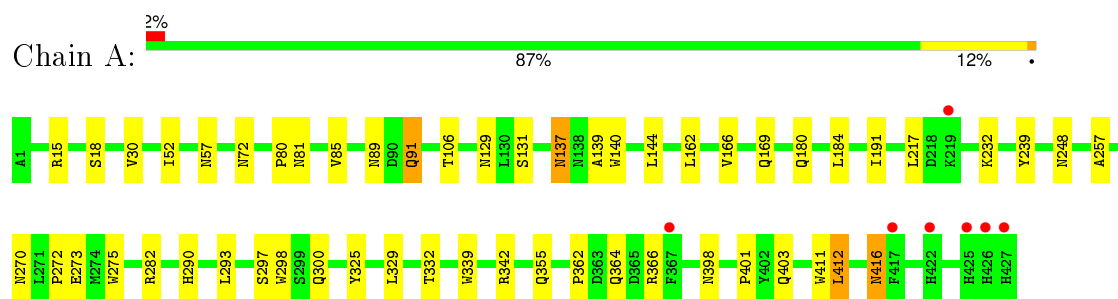
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	394	Total 394	O 394	0	0
7	B	383	Total 383	O 383	0	0



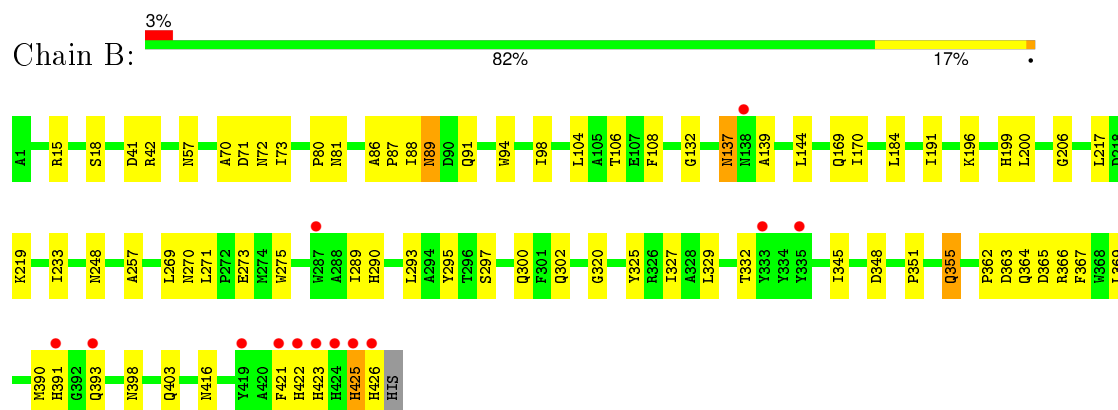
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Long-chain fatty acid transport protein



- Molecule 1: Long-chain fatty acid transport protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.07Å 147.51Å 151.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 – 1.90 38.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.78-1.90) 93.9 (38.78-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_704)	Depositor
R, $R_{free}$	0.167 , 0.192 0.165 , 0.185	Depositor DCC
$R_{free}$ test set	1834 reflections (1.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.5	EDS
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 119844 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.17% 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, 0.375 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: LDA, ACT, 2PE, CA, C8E

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	0.39	0/3607	0.55	0/4903
1	B	0.37	0/3553	0.54	0/4834
All	All	0.38	0/7160	0.54	0/9737

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	3459	0	3266	44	0
1	B	3411	0	3220	59	0
2	A	1	0	0	0	0
3	A	144	0	226	22	0
3	B	99	0	155	17	0
4	A	67	0	124	5	0
4	B	20	0	38	3	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	B	28	0	38	2	0
7	A	394	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	383	0	0	5	0
All	All	8014	0	7073	118	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 8.

All (118) 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:191:ILE:HG21	3:B:434:C8E:H202	1.40	1.02
3:A:443:C8E:H32	1:B:169:GLN:HE22	1.26	0.98
1:B:248:ASN:HD21	1:B:257:ALA:H	1.10	0.97
1:A:248:ASN:HD21	1:A:257:ALA:H	1.15	0.94
1:B:355:GLN:HE21	1:B:355:GLN:H	1.07	0.93
4:A:433:LDA:H111	1:B:170:ILE:HG12	1.52	0.90
1:A:169[A]:GLN:HE22	3:A:442:C8E:H112	1.40	0.85
1:A:166:VAL:HG11	3:A:442:C8E:H191	1.58	0.84
1:A:169[A]:GLN:NE2	3:A:442:C8E:H112	1.97	0.80
1:A:30:VAL:HG21	1:A:85[B]:VAL:HG11	1.63	0.78
3:A:443:C8E:H32	1:B:169:GLN:NE2	2.00	0.76
1:B:365:ASP:H	1:B:393:GLN:HE21	1.31	0.75
1:B:355:GLN:NE2	1:B:355:GLN:H	1.83	0.74
1:B:200:LEU:HB3	3:B:431:C8E:H161	1.69	0.73
1:B:355:GLN:HE21	1:B:355:GLN:N	1.87	0.71
1:A:162:LEU:HD22	3:A:440:C8E:H111	1.73	0.69
1:A:81:ASN:HD21	1:A:416:ASN:HD21	1.40	0.68
1:B:132:GLY:HA3	3:B:433:C8E:H81	1.78	0.66
1:A:57:ASN:ND2	1:A:72:ASN:H	1.96	0.63
5:A:1428:ACT:H2	7:A:772:HOH:O	1.97	0.63
1:A:401:PRO:HA	3:A:442:C8E:H22	1.80	0.63
1:B:41:ASP:O	1:B:425:HIS:HE1	1.82	0.63
1:B:81:ASN:HD21	1:B:416:ASN:HD21	1.48	0.61
1:B:364:GLN:HB2	1:B:393:GLN:HG3	1.82	0.61
1:B:57:ASN:ND2	1:B:72:ASN:H	1.99	0.60
1:B:89:ASN:ND2	1:B:91:GLN:H	2.00	0.60
1:A:239:TYR:HB2	3:A:438:C8E:C2	2.33	0.59
1:B:270:ASN:O	3:B:431:C8E:H11	2.01	0.59
1:A:57:ASN:HD22	1:A:72:ASN:H	1.51	0.58
1:A:137:ASN:ND2	1:A:140:TRP:H	2.01	0.58
1:B:57:ASN:HD22	1:B:72:ASN:H	1.50	0.58
1:A:275:TRP:CH2	4:A:432:LDA:H71	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:HIS:HE1	1:B:332:THR:OG1	1.87	0.57
1:B:269:LEU:HD11	3:B:431:C8E:H13	1.87	0.57
1:B:89:ASN:HD22	1:B:89:ASN:C	2.08	0.56
4:A:433:LDA:H81	3:B:435:C8E:H11	1.88	0.55
1:B:365:ASP:H	1:B:393:GLN:NE2	2.01	0.54
3:B:434:C8E:H111	7:B:488:HOH:O	2.08	0.54
1:B:271:LEU:HD23	3:B:431:C8E:H22	1.89	0.54
1:B:422:HIS:C	1:B:423:HIS:HD1	2.10	0.54
1:A:273:GLU:H	1:A:300:GLN:HE22	1.55	0.53
3:A:440:C8E:O15	3:A:440:C8E:H191	2.08	0.53
1:B:73[B]:ILE:HG21	1:B:108:PHE:CZ	2.44	0.52
1:A:137:ASN:C	1:A:137:ASN:HD22	2.13	0.52
1:B:137[A]:ASN:HD22	1:B:139[A]:ALA:H	1.57	0.51
1:A:30:VAL:CG2	1:A:85[B]:VAL:HG11	2.38	0.51
1:A:18:SER:OG	1:A:290:HIS:HD2	1.95	0.50
1:B:73[B]:ILE:HG21	1:B:108:PHE:CE1	2.46	0.50
1:A:290:HIS:HE1	1:A:332:THR:OG1	1.95	0.50
1:A:411:TRP:CZ3	3:A:430:C8E:H82	2.46	0.50
1:B:289:ILE:HD11	6:B:436:2PE:H181	1.94	0.50
1:A:339:TRP:CD1	3:A:441:C8E:H171	2.46	0.49
1:B:366:ARG:HD3	1:B:390:MET:CE	2.43	0.49
1:B:89:ASN:HD22	1:B:91:GLN:H	1.59	0.48
1:A:52:ILE:HG23	1:A:412[A]:LEU:HD13	1.94	0.48
1:B:367[A]:PHE:HD2	1:B:391[A]:HIS:CE1	2.31	0.48
1:A:293:LEU:HD11	1:A:325[B]:TYR:HD2	1.78	0.48
1:B:275:TRP:HH2	4:B:430:LDA:H82	1.79	0.48
1:B:351:PRO:HD2	1:B:363:ASP:OD2	2.13	0.48
3:B:435:C8E:H192	7:B:734:HOH:O	2.13	0.48
3:A:439:C8E:H61	7:A:583:HOH:O	2.14	0.47
1:A:80:PRO:HB2	4:A:434:LDA:H41	1.96	0.47
1:A:52:ILE:HG12	1:A:412[A]:LEU:CD1	2.44	0.47
1:A:298:TRP:CZ3	3:A:438:C8E:H202	2.49	0.47
1:A:180:GLN:HE21	4:A:433:LDA:C1	2.28	0.46
3:B:433:C8E:H111	7:B:599:HOH:O	2.14	0.46
1:B:137[A]:ASN:HD22	1:B:137[A]:ASN:C	2.19	0.46
1:B:273:GLU:H	1:B:300:GLN:HE22	1.63	0.46
1:A:137:ASN:ND2	1:A:139:ALA:H	2.14	0.46
1:B:273:GLU:HG2	1:B:297:SER:HB2	1.96	0.46
1:B:295:TYR:HD1	1:B:325[B]:TYR:CE1	2.34	0.46
1:B:18:SER:OG	1:B:290:HIS:HD2	1.99	0.46
1:B:196:LYS:HD3	1:B:199:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:441:C8E:H13	3:A:441:C8E:H42	1.53	0.45
1:B:42:ARG:HD2	1:B:421:PHE:O	2.16	0.45
1:A:411:TRP:CH2	3:A:430:C8E:H82	2.52	0.45
1:A:272:PRO:HA	1:A:300:GLN:HE21	1.80	0.45
1:B:275:TRP:CH2	4:B:430:LDA:H82	2.52	0.45
1:A:293:LEU:HD11	1:A:325[B]:TYR:CD2	2.52	0.45
1:B:70:ALA:HB1	1:B:73[B]:ILE:HD11	1.98	0.44
1:A:89:ASN:HB3	1:A:91:GLN:H	1.83	0.44
1:A:30:VAL:HG21	1:A:85[A]:VAL:HG21	1.98	0.44
1:B:106[A]:THR:HG21	1:B:362:PRO:CD	2.47	0.44
1:A:298:TRP:HZ3	3:A:438:C8E:H202	1.83	0.44
3:A:443:C8E:H81	3:B:435:C8E:H41	1.99	0.44
1:B:398:ASN:OD1	1:B:403:GLN:HG2	2.18	0.44
1:A:52:ILE:HG23	1:A:412[A]:LEU:CD1	2.48	0.43
1:B:302:GLN:NE2	1:B:320:GLY:HA2	2.32	0.43
3:A:440:C8E:H202	3:A:442:C8E:H12	2.00	0.43
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.83	0.43
1:A:273:GLU:HG2	1:A:297:SER:HB2	1.99	0.43
1:A:364:GLN:HE21	1:A:366:ARG:HE	1.66	0.43
3:A:440:C8E:H41	3:A:440:C8E:H71	1.63	0.43
1:B:345:ILE:HG22	1:B:369:LEU:HD13	2.00	0.43
1:B:88:ILE:O	1:B:426:HIS:NE2	2.51	0.42
1:A:232:LYS:HG2	1:A:270:ASN:HD22	1.83	0.42
1:B:206:GLY:HA3	1:B:233:ILE:HD13	2.01	0.42
1:A:191:ILE:HG13	3:A:440:C8E:H21	2.01	0.42
3:A:443:C8E:C8	3:B:435:C8E:H41	2.50	0.42
3:B:431:C8E:H13	3:B:431:C8E:H42	1.61	0.42
1:B:293:LEU:HD11	1:B:325[B]:TYR:CD1	2.55	0.42
1:A:15[B]:ARG:HG3	1:A:342:ARG:HD3	2.01	0.42
1:B:80:PRO:HD2	3:B:432:C8E:H202	2.02	0.41
3:B:434:C8E:H81	7:B:624:HOH:O	2.21	0.41
1:A:191:ILE:HG21	3:A:440:C8E:H21	2.03	0.41
1:A:272:PRO:HA	1:A:300:GLN:NE2	2.36	0.41
1:B:98:ILE:HG13	4:B:429:LDA:H91	2.01	0.41
3:B:432:C8E:H142	7:B:619:HOH:O	2.21	0.41
1:B:137[A]:ASN:ND2	1:B:139[A]:ALA:H	2.18	0.41
1:A:106[B]:THR:HG21	1:A:362:PRO:HD3	2.03	0.41
1:A:398:ASN:OD1	1:A:403:GLN:HG2	2.20	0.41
1:B:86:ALA:HA	1:B:87:PRO:HD3	1.94	0.41
1:B:327:ILE:HD11	6:B:436:2PE:H92	2.03	0.40
1:B:94:TRP:HB3	3:B:433:C8E:H101	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:HD21	1:A:131:SER:HG	1.66	0.40
1:B:422:HIS:C	1:B:423:HIS:ND1	2.75	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	449/427 (105%)	444 (99%)	5 (1%)	0	100	100
1	B	443/427 (104%)	437 (99%)	5 (1%)	1 (0%)	52	42
All	All	892/854 (104%)	881 (99%)	10 (1%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	425	HIS

### 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	360/336 (107%)	349 (97%)	11 (3%)	47	37
1	B	353/336 (105%)	341 (97%)	12 (3%)	44	33
All	All	713/672 (106%)	690 (97%)	23 (3%)	47	35

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	137	ASN
1	A	144	LEU
1	A	184	LEU
1	A	217	LEU
1	A	282	ARG
1	A	329	LEU
1	A	355	GLN
1	A	412[A]	LEU
1	A	412[B]	LEU
1	A	416	ASN
1	B	15	ARG
1	B	89	ASN
1	B	104	LEU
1	B	137[A]	ASN
1	B	137[B]	ASN
1	B	144	LEU
1	B	184	LEU
1	B	217	LEU
1	B	219	LYS
1	B	329	LEU
1	B	348	ASP
1	B	355	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	57	ASN
1	A	83	HIS
1	A	127	ASN
1	A	129	ASN
1	A	137	ASN
1	A	138	ASN
1	A	180	GLN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	300	GLN
1	A	302	GLN

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Mol	Chain	Res	Type
1	A	303	GLN
1	A	316	GLN
1	A	356	ASN
1	A	364	GLN
1	A	416	ASN
1	A	418	ASN
1	B	57	ASN
1	B	83	HIS
1	B	89	ASN
1	B	127	ASN
1	B	129	ASN
1	B	169	GLN
1	B	180	GLN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS
1	B	300	GLN
1	B	302	GLN
1	B	303	GLN
1	B	316	GLN
1	B	355	GLN
1	B	356	ASN
1	B	393	GLN
1	B	416	ASN
1	B	418	ASN
1	B	425	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\# Z  > 2$
5	ACT	A	1428	-	1,3,3	0.76	0	0,3,3	0.00	-
3	C8E	A	429	-	12,12,20	0.40	0	11,11,19	0.48	0
3	C8E	A	430	-	13,13,20	0.39	0	12,12,19	0.42	0
4	LDA	A	431	-	10,10,15	0.27	0	9,9,17	0.52	0
4	LDA	A	432	-	9,9,15	0.27	0	8,8,17	0.52	0
4	LDA	A	433	-	11,11,15	0.28	0	10,10,17	0.50	0
4	LDA	A	434	-	9,9,15	0.24	0	8,8,17	0.57	0
4	LDA	A	435	-	6,6,15	0.26	0	5,5,17	0.41	0
4	LDA	A	436	-	6,6,15	0.27	0	5,5,17	0.46	0
4	LDA	A	437	-	9,9,15	0.27	0	8,8,17	0.50	0
3	C8E	A	438	-	19,19,20	0.40	0	18,18,19	0.54	0
3	C8E	A	439	-	20,20,20	0.37	0	19,19,19	0.41	0
3	C8E	A	440	-	20,20,20	0.35	0	19,19,19	0.55	0
3	C8E	A	441	-	20,20,20	0.38	0	19,19,19	0.50	0
3	C8E	A	442	-	20,20,20	0.39	0	19,19,19	0.47	0
3	C8E	A	443	-	12,12,20	0.33	0	11,11,19	0.39	0
5	ACT	B	1428	-	1,3,3	1.67	0	0,3,3	0.00	-
4	LDA	B	429	-	9,9,15	0.26	0	8,8,17	0.56	0
4	LDA	B	430	-	9,9,15	0.27	0	8,8,17	0.54	0
3	C8E	B	431	-	20,20,20	0.39	0	19,19,19	0.63	0
3	C8E	B	432	-	20,20,20	0.39	0	19,19,19	0.34	0
3	C8E	B	433	-	20,20,20	0.37	0	19,19,19	0.40	0
3	C8E	B	434	-	14,14,20	0.43	0	13,13,19	0.46	0
3	C8E	B	435	-	20,20,20	0.35	0	19,19,19	0.56	0
6	2PE	B	436	-	27,27,27	0.71	0	26,26,26	1.54	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
5	ACT	A	1428	-	-	0/0/0/0	0/0/0/0
3	C8E	A	429	-	-	0/10/10/18	0/0/0/0
3	C8E	A	430	-	-	0/11/11/18	0/0/0/0
4	LDA	A	431	-	-	0/8/8/13	0/0/0/0
4	LDA	A	432	-	-	0/7/7/13	0/0/0/0
4	LDA	A	433	-	-	0/9/9/13	0/0/0/0
4	LDA	A	434	-	-	0/7/7/13	0/0/0/0
4	LDA	A	435	-	-	0/4/4/13	0/0/0/0
4	LDA	A	436	-	-	0/4/4/13	0/0/0/0
4	LDA	A	437	-	-	0/7/7/13	0/0/0/0
3	C8E	A	438	-	-	0/17/17/18	0/0/0/0
3	C8E	A	439	-	-	0/18/18/18	0/0/0/0
3	C8E	A	440	-	-	0/18/18/18	0/0/0/0
3	C8E	A	441	-	-	0/18/18/18	0/0/0/0
3	C8E	A	442	-	-	0/18/18/18	0/0/0/0
3	C8E	A	443	-	-	0/10/10/18	0/0/0/0
5	ACT	B	1428	-	-	0/0/0/0	0/0/0/0
4	LDA	B	429	-	-	0/7/7/13	0/0/0/0
4	LDA	B	430	-	-	0/7/7/13	0/0/0/0
3	C8E	B	431	-	-	0/18/18/18	0/0/0/0
3	C8E	B	432	-	-	0/18/18/18	0/0/0/0
3	C8E	B	433	-	-	0/18/18/18	0/0/0/0
3	C8E	B	434	-	-	0/12/12/18	0/0/0/0
3	C8E	B	435	-	-	0/18/18/18	0/0/0/0
6	2PE	B	436	-	-	0/25/25/25	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1428	ACT	1	0
3	A	430	C8E	2	0
4	A	432	LDA	1	0
4	A	433	LDA	3	0
4	A	434	LDA	1	0
3	A	438	C8E	3	0
3	A	439	C8E	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	440	C8E	6	0
3	A	441	C8E	2	0
3	A	442	C8E	5	0
3	A	443	C8E	4	0
4	B	429	LDA	1	0
4	B	430	LDA	2	0
3	B	431	C8E	5	0
3	B	432	C8E	2	0
3	B	433	C8E	3	0
3	B	434	C8E	3	0
3	B	435	C8E	4	0
6	B	436	2PE	2	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	427/427 (100%)	-0.38	7 (1%) 74 78	17, 28, 47, 67	0
1	B	426/427 (99%)	-0.25	13 (3%) 52 56	17, 29, 49, 110	1 (0%)
All	All	853/854 (99%)	-0.32	20 (2%) 64 67	17, 29, 49, 110	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	HIS	10.3
1	B	423	HIS	7.6
1	B	424	HIS	4.4
1	B	419	TYR	4.4
1	B	422	HIS	4.0
1	B	425	HIS	3.7
1	B	335	TYR	3.5
1	B	421	PHE	2.9
1	A	417[A]	PHE	2.8
1	A	425	HIS	2.8
1	A	426	HIS	2.7
1	A	427	HIS	2.6
1	B	287	TRP	2.6
1	B	393	GLN	2.6
1	B	391[A]	HIS	2.5
1	A	367[A]	PHE	2.5
1	B	138[A]	ASN	2.4
1	A	422	HIS	2.3
1	B	333	TYR	2.2
1	A	219	LYS	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LDA	A	432	10/16	0.82	0.23	14.51	44,60,63,66	0
4	LDA	B	430	10/16	0.87	0.13	7.73	36,53,70,70	0
4	LDA	A	434	10/16	0.86	0.27	7.66	58,65,72,74	0
4	LDA	B	429	10/16	0.85	0.28	7.11	40,49,53,54	0
6	2PE	B	436	28/28	0.75	0.28	6.14	75,88,96,97	0
3	C8E	B	435	21/21	0.91	0.20	5.22	22,45,93,94	0
4	LDA	A	433	12/16	0.82	0.17	5.06	41,49,53,54	0
3	C8E	B	431	21/21	0.89	0.19	4.75	37,50,57,59	0
3	C8E	A	442	21/21	0.79	0.25	4.71	37,69,78,79	0
3	C8E	A	439	21/21	0.85	0.22	4.56	56,67,74,77	0
3	C8E	B	434	15/21	0.85	0.21	4.25	39,48,73,76	0
3	C8E	A	440	21/21	0.92	0.24	3.98	35,53,96,102	0
3	C8E	A	443	13/21	0.76	0.23	3.96	32,49,57,59	0
4	LDA	A	437	10/16	0.75	0.18	3.96	50,57,58,59	0
3	C8E	A	441	21/21	0.76	0.23	3.80	54,77,89,95	0
3	C8E	B	433	21/21	0.86	0.19	3.80	38,52,62,78	0
3	C8E	A	438	20/21	0.91	0.14	2.95	27,44,62,62	0
3	C8E	A	430	14/21	0.67	0.24	2.47	64,72,88,89	0
4	LDA	A	431	11/16	0.88	0.18	2.39	36,47,52,54	0
5	ACT	A	1428	4/4	0.93	0.15	2.04	45,47,48,49	0
3	C8E	B	432	21/21	0.77	0.22	1.90	51,72,83,86	0
5	ACT	B	1428	4/4	0.84	0.14	1.83	39,42,45,48	0
3	C8E	A	429	13/21	0.90	0.12	1.46	31,42,51,64	0
2	CA	A	428	1/1	0.98	0.04	-1.19	30,30,30,30	0
4	LDA	A	436	7/16	0.93	0.15	-	43,49,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LDA	A	435	7/16	0.94	0.18	-	50,56,60,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.