



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:21 am BST

PDB ID : 6NS4  
Title : Crystal structure of fungal lipoxygenase from *Fusarium graminearum*. C2 crystal form.  
Authors : Pakhomova, S.; Boeglin, W.E.; Neau, D.B.; Bartlett, S.G.; Brash, A.R.; Newcomer, M.E.  
Deposited on : 2019-01-24  
Resolution : 2.40 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 : 2.11  
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) : 2.11

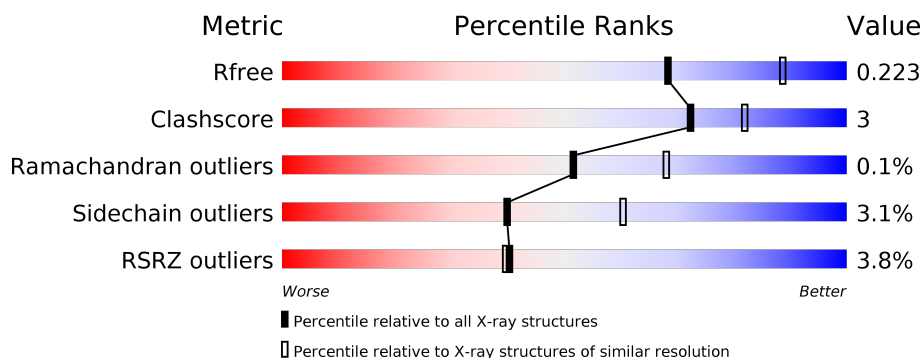
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	769	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	769	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11121 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 lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	5	0
			5470	3502	910	1047	11			
1	B	670	Total	C	N	O	S	0	0	0
			5321	3410	884	1017	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP I1REW2
A	-22	GLY	-	expression tag	UNP I1REW2
A	-21	ARG	-	expression tag	UNP I1REW2
A	-20	ASP	-	expression tag	UNP I1REW2
A	-19	PRO	-	expression tag	UNP I1REW2
A	-18	ASN	-	expression tag	UNP I1REW2
A	-17	SER	-	expression tag	UNP I1REW2
A	-16	SER	-	expression tag	UNP I1REW2
A	-15	SER	-	expression tag	UNP I1REW2
A	-14	VAL	-	expression tag	UNP I1REW2
A	-13	ASP	-	expression tag	UNP I1REW2
A	-12	LYS	-	expression tag	UNP I1REW2
A	-11	LEU	-	expression tag	UNP I1REW2
A	-10	ALA	-	expression tag	UNP I1REW2
A	-9	ALA	-	expression tag	UNP I1REW2
A	-8	ALA	-	expression tag	UNP I1REW2
A	-7	LEU	-	expression tag	UNP I1REW2
A	-6	GLU	-	expression tag	UNP I1REW2
A	-5	HIS	-	expression tag	UNP I1REW2
A	-4	HIS	-	expression tag	UNP I1REW2
A	-3	HIS	-	expression tag	UNP I1REW2
A	-2	HIS	-	expression tag	UNP I1REW2
A	-1	HIS	-	expression tag	UNP I1REW2
A	0	HIS	-	expression tag	UNP I1REW2
B	-23	MET	-	expression tag	UNP I1REW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP I1REW2
B	-21	ARG	-	expression tag	UNP I1REW2
B	-20	ASP	-	expression tag	UNP I1REW2
B	-19	PRO	-	expression tag	UNP I1REW2
B	-18	ASN	-	expression tag	UNP I1REW2
B	-17	SER	-	expression tag	UNP I1REW2
B	-16	SER	-	expression tag	UNP I1REW2
B	-15	SER	-	expression tag	UNP I1REW2
B	-14	VAL	-	expression tag	UNP I1REW2
B	-13	ASP	-	expression tag	UNP I1REW2
B	-12	LYS	-	expression tag	UNP I1REW2
B	-11	LEU	-	expression tag	UNP I1REW2
B	-10	ALA	-	expression tag	UNP I1REW2
B	-9	ALA	-	expression tag	UNP I1REW2
B	-8	ALA	-	expression tag	UNP I1REW2
B	-7	LEU	-	expression tag	UNP I1REW2
B	-6	GLU	-	expression tag	UNP I1REW2
B	-5	HIS	-	expression tag	UNP I1REW2
B	-4	HIS	-	expression tag	UNP I1REW2
B	-3	HIS	-	expression tag	UNP I1REW2
B	-2	HIS	-	expression tag	UNP I1REW2
B	-1	HIS	-	expression tag	UNP I1REW2
B	0	HIS	-	expression tag	UNP I1REW2

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

- Molecule 3 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
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	153	Total	O	0	0
			153	153		
5	B	147	Total	O	0	0
			147	147		

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

Chain A:

Category	Amino Acids
3%	MET
80%	GLY, ASN, ARG, ASP, PRO, ASN, SER, SER, VAL, ASP, LYS, LEU, ALA, ALA, LEU, GLU, HIS, HIS, HIS, HIS, HIS, MET, SER, ALA, VAL, ALA, SER, HIS
8%	V8, I27, D28, H29, D30, H54, E55, H56, S57, T58, E62, K75, R78, L79, Y85, S86, E102, D112, R116
11%	D134, GLY, ASP, GLU, ALA, ASN, LEU, PRO, ALA, ASP, GLU, ARG, GLN, SER, LYS, PRO, GLY, SER, ALA, ARG, GLY, VAL, GLY, Q160, I161, Q165, GLU, THR, ALA, PHE, VAL, S171, K172, I173, V177, F209, K210, T211, ASP, GLY, ASP, ALA, SER, ASN, GLN, ASP, ASN, LEU, ASN, LYS, A225, D226, T227, Y228, K229, S271, K280, K289, E308, L318, T321, K326, A333, L354, R370, L371, S372, P373, D375, T376, C377, D378, W385, P386, E403, T411, E415, I419, L432, W440, F441, R442, L446, L453, L454, V455, P456, P470, S471, L472, Y510

Chain B:

Sequence logo for Chain B. The y-axis represents information content in bits, ranging from 0 to 3. The x-axis lists amino acids. The logo shows high conservation at the N-terminus (positions 1-10) and C-terminus (positions 90-100), with a large gap of low conservation in the middle (positions 11-89).

Position	Amino Acid	Information Content (bits)
1	Q623	~2.8
2	D226	~2.8
3	K634	~2.8
4	I227	~2.8
5	K652	~2.8
6	K229	~2.8
7	D264	~2.8
8	K319	~2.8
9	G320	~2.8
10	T321	~2.8
11	A333	~2.8
12	L354	~2.8
13	D361	~2.8
14	R370	~2.8
15	P373	~2.8
16	D378	~2.8
17	W385	~2.8
18	P386	~2.8
19	E403	~2.8
20	E415	~2.8
21	I419	~2.8
22	W440	~2.8
23	L446	~2.8
24	S471	~2.8
25	L472	~2.8
26	D473	~2.8
27	F474	~2.8
28	K475	~2.8
29	Y496	~2.8
30	I497	~2.8
31	Y519	~2.8
32	D583	~2.8
33	S593	~2.8
34	P594	~2.8
35	A598	~2.8
36	Q603	~2.8
37	D604	~2.8
38	V610	~2.8
39	P611	~2.8
40	Q623	~2.8
41	D226	~2.8
42	K634	~2.8
43	I227	~2.8
44	K652	~2.8
45	K229	~2.8
46	D264	~2.8
47	K319	~2.8
48	G320	~2.8
49	T321	~2.8
50	A333	~2.8
51	L354	~2.8
52	D361	~2.8
53	R370	~2.8
54	P373	~2.8
55	D378	~2.8
56	W385	~2.8
57	P386	~2.8
58	E403	~2.8
59	E415	~2.8
60	I419	~2.8
61	W440	~2.8
62	L446	~2.8
63	S471	~2.8
64	L472	~2.8
65	D473	~2.8
66	F474	~2.8
67	K475	~2.8
68	Y496	~2.8
69	I497	~2.8
70	Y519	~2.8
71	D583	~2.8
72	S593	~2.8
73	P594	~2.8
74	A598	~2.8
75	Q603	~2.8
76	D604	~2.8
77	V610	~2.8
78	P611	~2.8
79	Q623	~2.8
80	D226	~2.8
81	K634	~2.8
82	I227	~2.8
83	K652	~2.8
84	K229	~2.8
85	D264	~2.8
86	K319	~2.8
87	G320	~2.8
88	T321	~2.8
89	A333	~2.8
90	L354	~2.8
91	D361	~2.8
92	R370	~2.8
93	P373	~2.8
94	D378	~2.8
95	W385	~2.8
96	P386	~2.8
97	E403	~2.8
98	E415	~2.8
99	I419	~2.8
100	W440	~2.8

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.96Å 121.12Å 102.12Å 90.00° 95.13° 90.00°	Depositor
Resolution (Å)	35.40 – 2.40 35.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.40-2.40) 99.7 (35.38-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.190 , 0.221 0.195 , 0.223	Depositor DCC
$R_{free}$ test set	1139 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.9	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	0.94	EDS
Total number of atoms	11121	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 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FE2, ACT

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	0.63	0/5616	0.73	0/7628
1	B	0.63	0/5451	0.72	0/7407
All	All	0.63	0/11067	0.73	0/15035

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	5470	0	5358	43	0
1	B	5321	0	5215	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	9	0	0
3	B	4	0	3	0	0
4	A	12	0	16	0	0
5	A	153	0	0	1	0
5	B	147	0	0	0	0
All	All	11121	0	10601	72	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 3.

All (72) 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:78[B]:ARG:CB	1:A:78[B]:ARG:HH11	0.90	1.52
1:A:78[B]:ARG:HB2	1:A:78[B]:ARG:NH1	0.92	1.24
1:A:78[B]:ARG:HH11	1:A:78[B]:ARG:CG	1.80	0.94
1:A:78[B]:ARG:HB2	1:A:78[B]:ARG:CZ	2.00	0.92
1:B:403:GLU:OE2	1:B:603:GLN:NE2	2.06	0.89
1:A:403:GLU:OE2	1:A:603:GLN:NE2	2.07	0.88
1:A:78[B]:ARG:NH1	1:A:78[B]:ARG:CG	2.43	0.78
1:B:9:VAL:HG23	1:B:14:LYS:HE3	1.65	0.78
1:A:161:ILE:HD11	1:A:173:ILE:HG12	1.72	0.72
1:A:78[B]:ARG:NH1	1:A:78[B]:ARG:CA	2.55	0.70
1:A:78[B]:ARG:CB	1:A:78[B]:ARG:NH1	1.75	0.66
1:A:593:SER:HB3	1:A:594:PRO:CD	2.28	0.63
1:A:62:GLU:HA	1:A:172:LYS:HE2	1.82	0.62
1:B:593:SER:HB3	1:B:594:PRO:CD	2.29	0.62
1:A:403:GLU:CD	1:A:603:GLN:HE22	2.07	0.58
1:B:403:GLU:CD	1:B:603:GLN:HE22	2.06	0.57
1:A:603:GLN:HG2	1:A:659:PRO:HA	1.87	0.57
1:B:598:ALA:HA	1:B:733:VAL:HG11	1.87	0.57
1:B:593:SER:HB3	1:B:594:PRO:HD3	1.88	0.55
1:A:318:LEU:HD11	1:A:470:PRO:HG3	1.88	0.55
1:A:593:SER:HB3	1:A:594:PRO:HD3	1.89	0.54
1:A:735:GLN:O	1:A:738:THR:N	2.41	0.54
1:B:603:GLN:HG2	1:B:659:PRO:HA	1.89	0.54
1:B:735:GLN:O	1:B:738:THR:N	2.41	0.54
1:B:107:VAL:HG13	1:B:109:ARG:HD2	1.91	0.53
1:A:85:TYR:HD1	1:A:453:LEU:HD23	1.76	0.51
1:A:419:ILE:HG12	1:A:440:TRP:CD2	2.47	0.50
1:B:419:ILE:HG12	1:B:440:TRP:CD2	2.47	0.50
1:A:442:ARG:O	1:A:446:LEU:HG	2.14	0.47
1:B:370:ARG:NH2	1:B:373:PRO:O	2.48	0.47
1:A:568:GLN:NE2	5:A:902:HOH:O	2.37	0.47
1:A:603:GLN:HG3	1:A:659:PRO:HB3	1.97	0.46
1:A:78[B]:ARG:NH1	1:A:78[B]:ARG:HA	2.30	0.46
1:A:415[B]:GLU:OE1	1:A:592:ALA:HA	2.15	0.46
1:A:658:LEU:N	1:A:659:PRO:HD2	2.32	0.45
1:B:603:GLN:HG3	1:B:659:PRO:HB3	1.98	0.44
1:B:658:LEU:N	1:B:659:PRO:HD2	2.32	0.44
1:A:78[B]:ARG:HH21	1:A:656:ALA:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370[B]:ARG:NH2	1:A:373:PRO:O	2.48	0.44
1:A:385:TRP:N	1:A:386:PRO:CD	2.81	0.43
1:A:610:VAL:N	1:A:611:PRO:CD	2.81	0.43
1:B:385:TRP:N	1:B:386:PRO:CD	2.81	0.43
1:A:280:LYS:HB3	1:A:371:LEU:CD2	2.49	0.43
1:A:56:ASN:ND2	1:A:58:THR:OG1	2.52	0.43
1:B:610:VAL:N	1:B:611:PRO:CD	2.82	0.43
1:A:177:VAL:HG21	1:A:453:LEU:CD1	2.49	0.42
1:B:67:GLU:OE2	1:B:319:LYS:HE2	2.19	0.42
1:B:611:PRO:HD3	1:B:652:TRP:CH2	2.54	0.42
1:A:112:ASP:OD2	1:A:116:ARG:NH1	2.50	0.42
1:A:455:VAL:HB	1:A:456:PRO:HD3	2.01	0.42
1:B:61:GLY:O	1:B:172:LYS:HG3	2.19	0.42
1:B:75:LYS:H	1:B:75:LYS:HD3	1.85	0.42
1:A:411:THR:O	1:A:415[A]:GLU:HB2	2.20	0.42
1:B:472:LEU:HD12	1:B:473:ASP:HB2	2.02	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.94	0.42
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.93	0.42
1:B:623:GLN:NE2	1:B:623:GLN:HA	2.35	0.42
1:A:27:ILE:HD11	1:B:677:LYS:HA	2.02	0.41
1:B:361:ASP:N	1:B:361:ASP:OD1	2.52	0.41
1:B:496:TYR:CE2	1:B:583:ASP:HB3	2.55	0.41
1:A:333:ALA:HB1	1:A:354:LEU:O	2.21	0.41
1:A:611:PRO:HD3	1:A:652:TRP:CH2	2.55	0.41
1:B:497:ILE:HA	1:B:497:ILE:HD13	1.98	0.41
1:B:9:VAL:HG23	1:B:14:LYS:CE	2.42	0.41
1:B:333:ALA:HB1	1:B:354:LEU:O	2.21	0.41
1:B:84:ILE:HA	1:B:84:ILE:HD12	1.92	0.41
1:A:102[A]:GLU:OE1	1:A:442:ARG:HA	2.22	0.40
1:A:454:LEU:HD13	1:A:662:LEU:HD21	2.02	0.40
1:B:415:GLU:O	1:B:419:ILE:HG13	2.22	0.40
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.95	0.40
1:A:30:ASP:O	1:B:677:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	680/769 (88%)	658 (97%)	21 (3%)	1 (0%)	51	68
1	B	660/769 (86%)	642 (97%)	17 (3%)	1 (0%)	47	62
All	All	1340/1538 (87%)	1300 (97%)	38 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	SER
1	B	593	SER

### 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	588/660 (89%)	569 (97%)	19 (3%)	39	59
1	B	572/660 (87%)	555 (97%)	17 (3%)	41	61
All	All	1160/1320 (88%)	1124 (97%)	36 (3%)	40	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	75	LYS
1	A	86	SER
1	A	172	LYS

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Mol	Chain	Res	Type
1	A	228	MET
1	A	229	LYS
1	A	271	SER
1	A	289	LYS
1	A	321	THR
1	A	326	LYS
1	A	375	ASP
1	A	376	THR
1	A	471	SER
1	A	519	TYR
1	A	527	LEU
1	A	604	ASP
1	A	681	ASN
1	A	686	ARG
1	A	688	ILE
1	B	12	ARG
1	B	56	ASN
1	B	71	LYS
1	B	75	LYS
1	B	86	SER
1	B	98	LYS
1	B	321	THR
1	B	361	ASP
1	B	378	ASP
1	B	446	LEU
1	B	471	SER
1	B	474	PHE
1	B	519	TYR
1	B	604	ASP
1	B	634	LYS
1	B	681	ASN
1	B	739	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	189	ASN
1	A	294	GLN
1	A	307	ASN
1	A	543	GLN
1	A	595	GLN

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Mol	Chain	Res	Type
1	A	603	GLN
1	A	623	GLN
1	A	629	GLN
1	A	719	ASN
1	B	189	ASN
1	B	294	GLN
1	B	307	ASN
1	B	478	ASN
1	B	568	GLN
1	B	595	GLN
1	B	600	ASN
1	B	603	GLN
1	B	623	GLN
1	B	629	GLN
1	B	719	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	ACT	A	803	-	1,3,3	3.80	1 (100%)	0,3,3	0.00	-
3	ACT	A	804	-	1,3,3	3.83	1 (100%)	0,3,3	0.00	-
3	ACT	B	802	-	1,3,3	3.21	1 (100%)	0,3,3	0.00	-
3	ACT	A	802	-	1,3,3	3.87	1 (100%)	0,3,3	0.00	-
4	GOL	A	806	-	5,5,5	0.13	0	5,5,5	0.32	0
4	GOL	A	805	-	5,5,5	0.10	0	5,5,5	0.27	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
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	A	806	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ACT	CH3-C	3.87	1.53	1.48
3	A	804	ACT	CH3-C	3.83	1.53	1.48
3	A	803	ACT	CH3-C	3.80	1.53	1.48
3	B	802	ACT	CH3-C	3.21	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	A	806	GOL	O2-C2-C3-O3
4	A	805	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	685/769 (89%)	-0.07	25 (3%)	42 42	16, 32, 63, 88	0
1	B	670/769 (87%)	-0.12	26 (3%)	39 38	18, 32, 59, 90	0
All	All	1355/1538 (88%)	-0.09	51 (3%)	40 39	16, 32, 61, 90	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	THR	6.3
1	B	664	TYR	5.0
1	B	739	THR	4.7
1	A	664	TYR	4.6
1	B	695	ASN	4.5
1	A	472	LEU	4.4
1	A	688	ILE	4.4
1	B	474	PHE	4.4
1	A	227	ILE	4.3
1	A	689	THR	4.3
1	B	9	VAL	3.9
1	A	55	GLU	3.9
1	A	739	THR	3.8
1	A	209	PRO	3.6
1	A	738	THR	3.4
1	B	694	PHE	3.4
1	B	685	ASN	3.4
1	A	226	ASP	3.3
1	A	8	VAL	3.3
1	B	737	GLU	3.2
1	B	473	ASP	3.1
1	A	56	ASN	3.1
1	B	378	ASP	3.1
1	B	227	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	691	ASN	3.0
1	A	58	THR	3.0
1	A	29	HIS	3.0
1	A	210	LYS	2.9
1	B	736	PRO	2.8
1	B	210	LYS	2.8
1	A	687	THR	2.8
1	B	472	LEU	2.8
1	A	669	ASP	2.8
1	A	225	ALA	2.8
1	B	56	ASN	2.8
1	A	692	THR	2.7
1	A	308	GLU	2.7
1	B	475	LYS	2.7
1	B	229	LYS	2.7
1	B	226	ASP	2.6
1	A	378	ASP	2.6
1	B	171	SER	2.6
1	B	8	VAL	2.5
1	B	33	GLU	2.4
1	A	54	ASN	2.3
1	A	737	GLU	2.3
1	B	225	ALA	2.2
1	B	264	ASP	2.2
1	B	670	TYR	2.1
1	B	669	ASP	2.0
1	B	58	THR	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 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. 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
4	GOL	A	806	6/6	0.81	0.16	47,50,51,51	0
4	GOL	A	805	6/6	0.83	0.27	48,50,51,52	0
3	ACT	A	804	4/4	0.84	0.17	47,49,50,52	0
3	ACT	A	802	4/4	0.92	0.25	39,42,42,42	0
3	ACT	A	803	4/4	0.95	0.23	43,44,44,44	0
2	FE2	A	801	1/1	0.97	0.04	29,29,29,29	0
3	ACT	B	802	4/4	0.97	0.09	38,38,38,38	0
2	FE2	B	801	1/1	0.97	0.04	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.