



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:18 AM BST

PDB ID : 3ET0  
Title : Structure of PPARgamma with 3-(5-Methoxy-1H-indol-3-yl)-propionic acid  
Authors : Zhang, K.Y.J.; Wang, W.  
Deposited on : 2008-10-06  
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.

---

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 : 2.13.1  
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) : 2.13.1

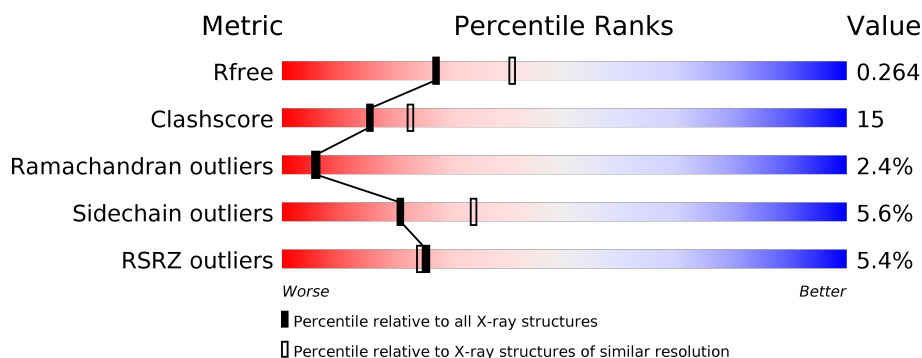
# 1 Overall quality at a glance

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	292	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	292	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4289 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 Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2088	1347	338	391	12			
1	B	259	Total	C	N	O	S	0	0	0
			2075	1338	337	388	12			

There are 42 discrepancies between the modelled and reference sequences:

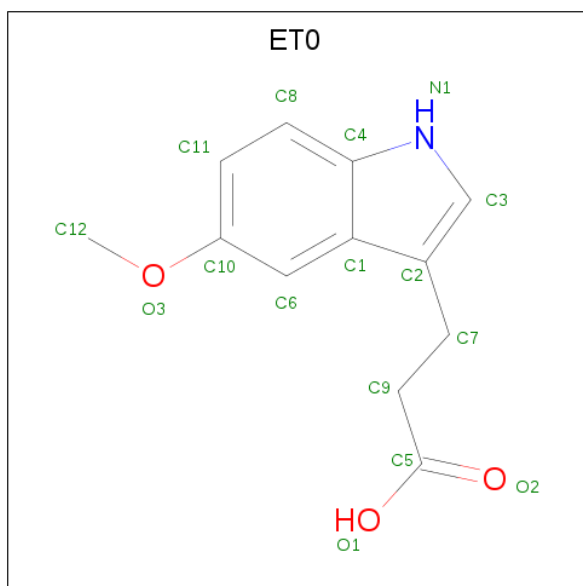
Chain	Residue	Modelled	Actual	Comment	Reference
A	186	MET	-	expression tag	UNP P37231
A	187	GLY	-	expression tag	UNP P37231
A	188	SER	-	expression tag	UNP P37231
A	189	SER	-	expression tag	UNP P37231
A	190	HIS	-	expression tag	UNP P37231
A	191	HIS	-	expression tag	UNP P37231
A	192	HIS	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	HIS	-	expression tag	UNP P37231
A	195	HIS	-	expression tag	UNP P37231
A	196	SER	-	expression tag	UNP P37231
A	197	SER	-	expression tag	UNP P37231
A	198	GLY	-	expression tag	UNP P37231
A	199	LEU	-	expression tag	UNP P37231
A	200	VAL	-	expression tag	UNP P37231
A	201	PRO	-	expression tag	UNP P37231
A	202	ARG	-	expression tag	UNP P37231
A	203	GLY	-	expression tag	UNP P37231
A	204	SER	-	expression tag	UNP P37231
A	205	HIS	-	expression tag	UNP P37231
A	206	MET	-	expression tag	UNP P37231
B	186	MET	-	expression tag	UNP P37231
B	187	GLY	-	expression tag	UNP P37231
B	188	SER	-	expression tag	UNP P37231
B	189	SER	-	expression tag	UNP P37231

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	HIS	-	expression tag	UNP P37231
B	191	HIS	-	expression tag	UNP P37231
B	192	HIS	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	HIS	-	expression tag	UNP P37231
B	195	HIS	-	expression tag	UNP P37231
B	196	SER	-	expression tag	UNP P37231
B	197	SER	-	expression tag	UNP P37231
B	198	GLY	-	expression tag	UNP P37231
B	199	LEU	-	expression tag	UNP P37231
B	200	VAL	-	expression tag	UNP P37231
B	201	PRO	-	expression tag	UNP P37231
B	202	ARG	-	expression tag	UNP P37231
B	203	GLY	-	expression tag	UNP P37231
B	204	SER	-	expression tag	UNP P37231
B	205	HIS	-	expression tag	UNP P37231
B	206	MET	-	expression tag	UNP P37231

- Molecule 2 is 3-(5-methoxy-1H-indol-3-yl)propanoic acid (three-letter code: ET0) (formula:  $C_{12}H_{13}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	12	1	3		

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	46	Total	O	0	0
			46	46		



- Molecule 1: Peroxisome proliferator-activated receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.35Å 62.45Å 119.24Å 90.00° 101.73° 90.00°	Depositor
Resolution (Å)	29.19 – 2.40 29.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.19-2.40) 94.4 (29.48-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.200 , 0.255 0.214 , 0.264	Depositor DCC
$R_{free}$ test set	1622 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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: CME, GLC, ET0

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	0.36	0/2111	0.53	0/2840
1	B	0.36	0/2097	0.52	0/2822
All	All	0.36	0/4208	0.53	0/5662

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	2088	0	2148	51	0
1	B	2075	0	2139	76	0
2	A	16	0	12	1	0
3	B	12	0	12	2	0
4	A	52	0	0	3	0
4	B	46	0	0	1	0
All	All	4289	0	4311	126	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 15.

All (126) 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:285:CME:SG	1:B:285:CME:SD	2.33	1.25
1:A:285:CME:SD	1:A:285:CME:SG	2.34	1.24
1:A:319:LYS:HE3	1:A:476:LEU:HD23	1.45	0.97
1:B:460:GLU:HB2	1:B:463:MET:HA	1.49	0.95
1:B:459:THR:HG22	1:B:460:GLU:H	1.33	0.93
1:B:341:ILE:HG22	3:B:2:GLC:H5	1.58	0.86
1:B:476:LEU:H	1:B:476:LEU:HD23	1.41	0.86
1:B:325:ILE:HD13	1:B:388:ILE:HG23	1.58	0.85
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.65	0.78
1:B:459:THR:HG22	1:B:460:GLU:N	1.97	0.77
1:A:358:LYS:HB3	1:A:359:PRO:CD	2.16	0.76
1:B:279:ILE:O	1:B:283:GLN:HG2	1.88	0.73
1:A:325:ILE:HD12	1:A:388:ILE:HG23	1.71	0.72
1:B:363:PHE:HE2	1:B:449:HIS:CE1	2.06	0.72
1:B:475:ASP:HB3	1:B:476:LEU:HD23	1.70	0.71
1:B:466:HIS:HE1	1:B:468:LEU:HD13	1.55	0.71
1:B:455:VAL:C	1:B:457:LYS:H	1.94	0.70
1:A:321:GLY:O	1:A:325:ILE:HG12	1.93	0.68
1:B:402:ASN:O	1:B:405:PRO:HD2	1.95	0.66
1:B:357:ARG:HH12	1:B:458:LYS:HE2	1.62	0.65
1:A:241:THR:HB	1:A:243:ASP:HB2	1.79	0.65
1:B:471:GLU:O	1:B:474:LYS:HB2	1.98	0.64
1:A:440:THR:HG21	1:B:443:ARG:HD2	1.82	0.61
1:A:358:LYS:HB3	1:A:359:PRO:HD3	1.83	0.61
1:B:319:LYS:HE3	1:B:320:TYR:CZ	2.36	0.61
1:B:285:CME:HZ3	1:B:288:ARG:HG3	1.83	0.60
1:A:364:MET:SD	2:A:1:ET0:H8	2.42	0.60
1:B:454:GLN:C	1:B:456:ILE:H	2.04	0.60
1:B:474:LYS:NZ	1:B:475:ASP:HB2	2.16	0.60
1:A:418:GLU:HG2	1:A:422:LYS:HE3	1.84	0.59
1:B:459:THR:CG2	1:B:460:GLU:H	2.09	0.59
1:A:455:VAL:O	1:A:459:THR:HG22	2.02	0.59
1:B:283:GLN:O	1:B:286:GLN:HG2	2.05	0.57
1:A:459:THR:HG23	1:A:460:GLU:HG2	1.86	0.56
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.87	0.56
1:B:322:VAL:HG21	1:B:476:LEU:HD12	1.86	0.56
1:B:370:PHE:CB	1:B:445:ILE:HD11	2.35	0.56
1:B:466:HIS:CE1	1:B:468:LEU:HD13	2.38	0.56
1:B:322:VAL:O	1:B:326:ILE:HG13	2.06	0.56
1:B:474:LYS:HZ3	1:B:475:ASP:HB2	1.70	0.56
1:B:363:PHE:HE2	1:B:449:HIS:HE1	1.54	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:VAL:C	1:B:457:LYS:N	2.57	0.55
1:A:241:THR:CB	1:A:243:ASP:HB2	2.37	0.55
1:B:283:GLN:HA	1:B:286:GLN:HG2	1.88	0.55
1:A:392:ILE:HG22	1:A:393:LEU:HD22	1.89	0.55
1:A:323:HIS:CE1	1:A:473:TYR:CZ	2.95	0.54
1:B:327:TYR:CZ	1:B:367:LYS:HE3	2.42	0.54
1:B:454:GLN:OE1	1:B:454:GLN:HA	2.07	0.54
1:B:260:ASP:HB2	1:B:261:LYS:NZ	2.23	0.53
1:A:241:THR:CG2	1:A:243:ASP:HB2	2.38	0.53
1:A:243:ASP:HA	4:A:510:HOH:O	2.09	0.53
1:B:285:CME:HB3	3:B:2:GLC:H2	1.90	0.53
1:B:260:ASP:HB2	1:B:261:LYS:HZ3	1.74	0.53
1:A:229:THR:OG1	1:A:232:LYS:HD2	2.09	0.53
1:B:260:ASP:O	1:B:261:LYS:HB3	2.08	0.53
1:A:242:THR:O	1:A:244:LYS:N	2.42	0.53
1:B:370:PHE:HB2	1:B:445:ILE:HD11	1.90	0.52
1:A:279:ILE:O	1:A:283:GLN:HG2	2.09	0.52
1:A:236:ILE:HG23	4:A:514:HOH:O	2.09	0.52
1:B:359:PRO:HG2	1:B:458:LYS:HE2	1.90	0.52
1:B:460:GLU:HB2	1:B:463:MET:CA	2.32	0.52
1:A:323:HIS:CE1	1:A:473:TYR:HH	2.28	0.51
1:B:319:LYS:HE3	1:B:320:TYR:CE1	2.46	0.51
1:B:461:THR:HG21	1:B:470:GLN:HB2	1.92	0.51
1:B:435:LEU:O	1:B:438:LYS:HB2	2.11	0.51
1:B:329:MET:O	1:B:332:SER:HB2	2.10	0.51
1:A:456:ILE:HA	1:A:459:THR:HG22	1.94	0.50
1:A:341:ILE:HD13	1:A:348:MET:CE	2.42	0.50
1:B:261:LYS:HB3	1:B:261:LYS:HZ2	1.77	0.50
1:A:402:ASN:O	1:A:405:PRO:HD2	2.11	0.50
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.93	0.49
1:A:286:GLN:OE1	1:A:465:LEU:HD12	2.12	0.49
1:B:428:SER:HB3	1:B:431:LEU:HB2	1.94	0.48
1:A:241:THR:HB	1:A:243:ASP:N	2.28	0.48
1:B:348:MET:SD	1:B:353:LEU:HD21	2.52	0.48
1:B:476:LEU:H	1:B:476:LEU:CD2	2.19	0.48
1:B:282:PHE:CE1	1:B:363:PHE:CZ	3.02	0.48
1:B:474:LYS:NZ	1:B:474:LYS:HB3	2.29	0.48
1:A:245:SER:HB3	1:A:246:PRO:HD2	1.95	0.48
1:A:258:GLY:C	1:A:260:ASP:H	2.16	0.48
1:B:357:ARG:HH12	1:B:458:LYS:CE	2.25	0.48
1:B:405:PRO:O	1:B:409:ILE:HG13	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:MET:O	1:B:464:SER:HB3	2.13	0.47
1:A:276:GLU:O	1:A:280:ARG:HG3	2.14	0.47
1:B:276:GLU:HG2	1:B:279:ILE:HD12	1.96	0.47
1:A:220:ASP:O	1:A:224:LYS:HG3	2.15	0.47
1:A:207:GLU:HG2	1:A:210:ASP:OD2	2.16	0.46
1:B:474:LYS:HZ3	1:B:474:LYS:HB3	1.80	0.46
1:A:243:ASP:O	1:A:244:LYS:C	2.54	0.46
1:A:242:THR:HA	4:A:505:HOH:O	2.15	0.46
1:B:475:ASP:HB3	1:B:476:LEU:H	1.58	0.46
1:A:282:PHE:CE2	1:A:463:MET:HE1	2.50	0.46
1:B:275:LYS:HE3	1:B:464:SER:HB3	1.98	0.46
1:A:476:LEU:HD13	1:A:477:TYR:CD1	2.51	0.46
1:B:260:ASP:C	1:B:261:LYS:HZ2	2.19	0.46
1:A:441:ASP:O	1:A:445:ILE:HG13	2.17	0.45
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.82	0.45
1:A:241:THR:HG21	1:A:243:ASP:HB2	1.98	0.44
1:A:354:LYS:HE3	1:A:354:LYS:HB3	1.79	0.44
1:B:325:ILE:O	1:B:329:MET:HG3	2.18	0.43
1:B:335:ASN:HB2	4:B:543:HOH:O	2.16	0.43
1:A:456:ILE:HA	1:A:459:THR:CG2	2.48	0.43
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.82	0.43
1:B:466:HIS:ND1	1:B:467:PRO:HD2	2.34	0.43
1:B:327:TYR:CE2	1:B:367:LYS:HE3	2.53	0.43
1:B:469:LEU:HA	1:B:469:LEU:HD23	1.79	0.43
1:A:329:MET:O	1:A:332:SER:HB2	2.19	0.43
1:A:363:PHE:CD2	1:A:452:LEU:HD13	2.54	0.43
1:B:208:SER:O	1:B:212:ARG:HG2	2.18	0.42
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.19	0.42
1:B:287:PHE:C	1:B:287:PHE:CD1	2.92	0.42
1:B:454:GLN:C	1:B:456:ILE:N	2.71	0.42
1:A:351:GLU:O	1:A:355:SER:HB3	2.19	0.42
1:B:418:GLU:O	1:B:422:LYS:HG3	2.20	0.41
1:B:458:LYS:HB2	1:B:463:MET:SD	2.61	0.41
1:B:283:GLN:H	1:B:283:GLN:HG2	1.52	0.41
1:A:275:LYS:HB3	1:A:276:GLU:H	1.70	0.41
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.44	0.41
1:A:237:LEU:HA	1:A:237:LEU:HD12	1.91	0.40
1:A:323:HIS:CE1	1:A:473:TYR:OH	2.75	0.40
1:B:321:GLY:O	1:B:325:ILE:HG13	2.21	0.40
1:A:241:THR:HB	1:A:243:ASP:H	1.86	0.40
1:A:357:ARG:NH1	1:A:359:PRO:HD2	2.36	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TYR:CE2	1:A:367:LYS:HE3	2.56	0.40
1:A:275:LYS:HE2	1:A:462:ASP:OD2	2.22	0.40
1:A:356:LEU:HA	1:A:356:LEU:HD23	1.91	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	255/292 (87%)	240 (94%)	10 (4%)	5 (2%)	7	9
1	B	254/292 (87%)	236 (93%)	11 (4%)	7 (3%)	5	4
All	All	509/584 (87%)	476 (94%)	21 (4%)	12 (2%)	6	6

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	261	LYS
1	A	358	LYS
1	B	261	LYS
1	B	358	LYS
1	B	455	VAL
1	B	464	SER
1	B	461	THR
1	A	259	GLU
1	A	240	LYS
1	B	459	THR
1	B	456	ILE

### 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	232/261 (89%)	218 (94%)	14 (6%)	19	31
1	B	231/261 (88%)	219 (95%)	12 (5%)	23	38
All	All	463/522 (89%)	437 (94%)	26 (6%)	21	34

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	220	ASP
1	A	221	SER
1	A	232	LYS
1	A	237	LEU
1	A	261	LYS
1	A	262	ILE
1	A	277	VAL
1	A	393	LEU
1	A	453	LEU
1	A	454	GLN
1	A	464	SER
1	A	465	LEU
1	A	476	LEU
1	B	234	ARG
1	B	237	LEU
1	B	241	THR
1	B	260	ASP
1	B	261	LYS
1	B	277	VAL
1	B	283	GLN
1	B	363	PHE
1	B	441	ASP
1	B	452	LEU
1	B	474	LYS
1	B	476	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	GLN
1	B	283	GLN
1	B	308	ASN
1	B	437	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	A	285	1	8,9,10	1.46	1 (12%)	5,9,11	1.12	0
1	CME	B	285	1	8,9,10	1.44	1 (12%)	5,9,11	1.41	1 (20%)

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
1	CME	A	285	1	-	3/5/8/10	-
1	CME	B	285	1	-	3/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	CME	SD-SG	4.02	2.34	2.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	CME	SD-SG	3.94	2.33	2.03

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	CME	CB-SG-SD	2.81	111.09	103.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	285	CME	CE-SD-SG-CB
1	A	285	CME	SD-CE-CZ-OH
1	B	285	CME	SD-CE-CZ-OH
1	B	285	CME	N-CA-CB-SG
1	B	285	CME	CZ-CE-SD-SG
1	A	285	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	CME	1	0
1	B	285	CME	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	ET0	A	1	-	13,17,17	1.19	1 (7%)	14,23,23	1.83	3 (21%)
3	GLC	B	2	-	12,12,12	1.20	1 (8%)	17,17,17	1.78	4 (23%)

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	ET0	A	1	-	-	2/5/7/7	0/2/2/2
3	GLC	B	2	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ET0	C1-C4	-2.45	1.36	1.42
3	B	2	GLC	C1-C2	2.08	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ET0	C6-C1-C4	4.34	124.19	118.26
3	B	2	GLC	O5-C1-C2	4.18	117.74	110.28
3	B	2	GLC	C4-C3-C2	-3.86	104.08	110.82
3	B	2	GLC	C1-O5-C5	3.31	119.90	113.66
2	A	1	ET0	C7-C2-C3	3.23	134.01	127.19
2	A	1	ET0	C1-C4-N1	2.18	112.76	107.92
3	B	2	GLC	C1-C2-C3	2.01	114.49	110.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ET0	C1-C2-C7-C9
2	A	1	ET0	C3-C2-C7-C9

There are no ring outliers.

2 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ET0	1	0
3	B	2	GLC	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	259/292 (88%)	-0.14	10 (3%) 39 38	40, 60, 104, 158	0
1	B	258/292 (88%)	-0.04	18 (6%) 16 15	39, 61, 125, 178	0
All	All	517/584 (88%)	-0.09	28 (5%) 25 24	39, 61, 119, 178	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	8.5
1	B	461	THR	7.1
1	B	242	THR	6.1
1	B	243	ASP	4.0
1	B	241	THR	4.0
1	B	459	THR	3.7
1	B	476	LEU	3.6
1	A	358	LYS	3.5
1	A	262	ILE	3.2
1	B	452	LEU	3.2
1	B	454	GLN	3.1
1	B	363	PHE	3.0
1	B	451	GLN	3.0
1	A	256	MET	2.9
1	B	262	ILE	2.9
1	A	241	THR	2.9
1	B	436	LEU	2.9
1	B	240	LYS	2.8
1	A	259	GLU	2.7
1	A	240	LYS	2.6
1	A	206	MET	2.5
1	B	462	ASP	2.5
1	A	244	LYS	2.4
1	A	253	ASN	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	463	MET	2.3
1	B	439	MET	2.1
1	B	358	LYS	2.1
1	B	294	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	CME	B	285	10/11	0.89	0.18	58,70,99,136	0
1	CME	A	285	10/11	0.94	0.20	60,67,137,138	0

## 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(Å <sup>2</sup> )	Q<0.9
3	GLC	B	2	12/12	0.81	0.26	68,79,106,107	0
2	ET0	A	1	16/16	0.86	0.21	66,84,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.