



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:29 am GMT

PDB ID : 1GQG  
Title : QUERCETIN 2,3-DIOXYGENASE IN COMPLEX WITH THE INHIBITOR  
DIETHYLDITHIOCARBAMATE  
Authors : Steiner, R.A.; Dijkstra, B.W.  
Deposited on : 2001-11-23  
Resolution : 1.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

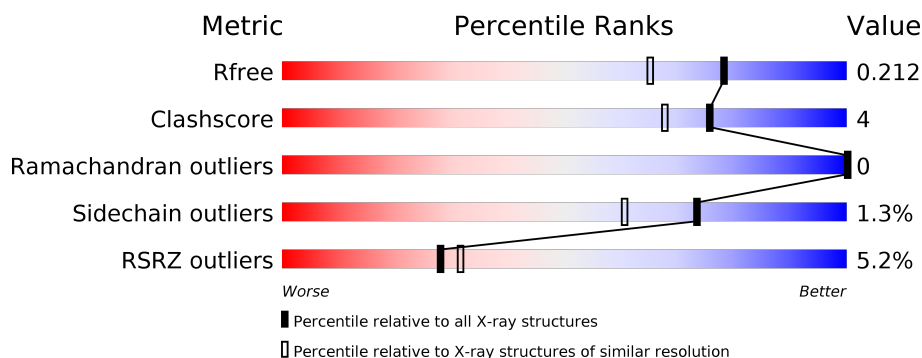
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	350	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	350	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	C	350	<div> <div>9%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	D	350	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DCD	C	1351	-	-	-	X
4	NAG	A	1356	-	-	-	X
4	NAG	A	1357	-	-	-	X
4	NAG	B	1355	-	-	-	X
4	NAG	C	1356	-	-	-	X
4	NAG	D	1356	-	-	-	X
5	NAG	A	1355	-	-	-	X
5	NAG	C	1354	-	-	-	X
5	NAG	C	1355	-	-	-	X

## 2 Entry composition [i](#)

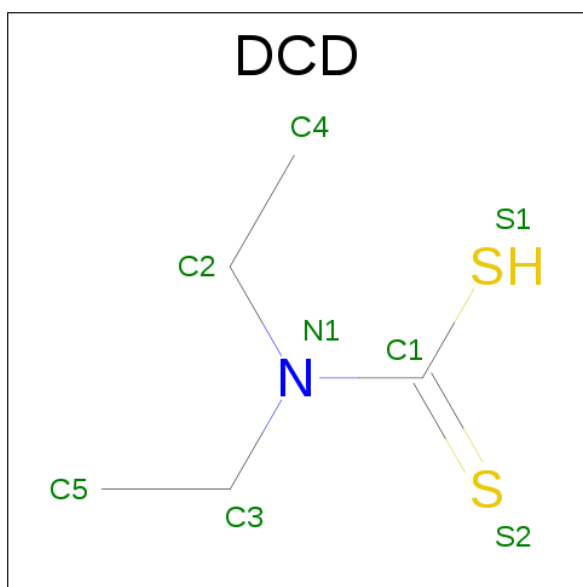
There are 7 unique types of molecules in this entry. The entry contains 12136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 QUERCETIN 2,3-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	8	0
			2595	1654	420	515	6			
1	B	334	Total	C	N	O	S	0	4	0
			2590	1648	421	516	5			
1	C	337	Total	C	N	O	S	0	3	0
			2605	1655	424	521	5			
1	D	333	Total	C	N	O	S	0	3	0
			2578	1642	419	512	5			

- Molecule 2 is DIETHYLCARBAMODITHIOIC ACID (three-letter code: DCD) (formula:  $C_5H_{11}NS_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			8	5	1	2		
2	B	1	Total	C	N	S	0	0
			8	5	1	2		

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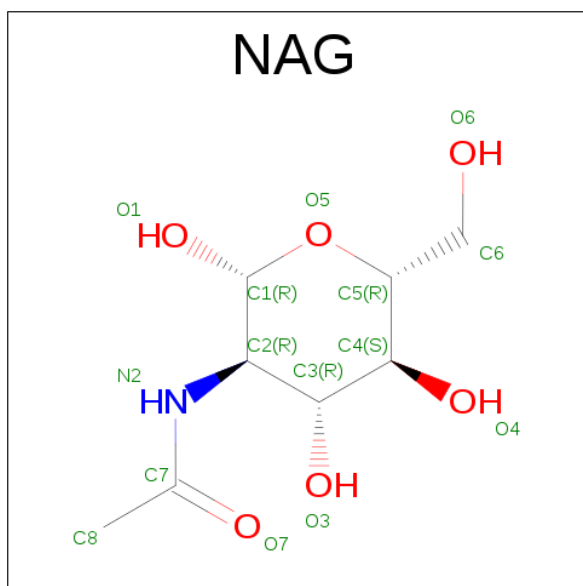
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	S	0	0
			8	5	1	2		
2	D	1	Total	C	N	S	0	0
			8	5	1	2		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cu	0	0
			1	1		
3	A	1	Total	Cu	0	0
			1	1		
3	D	1	Total	Cu	0	0
			1	1		
3	C	1	Total	Cu	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	411	Total	O	0	0
			411	411		
7	B	346	Total	O	0	0
			346	346		

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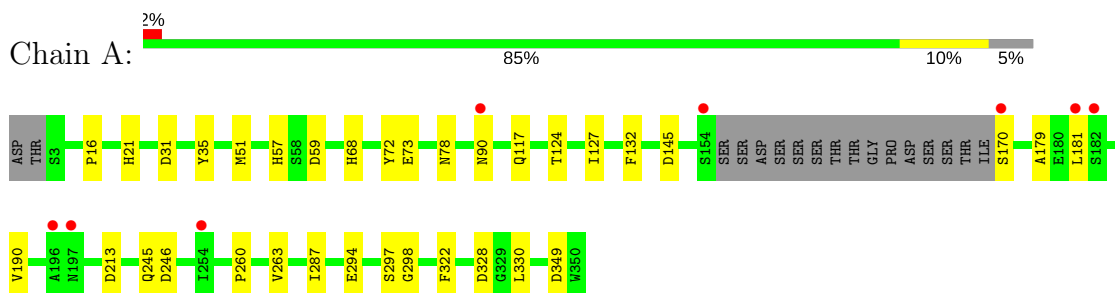
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	345	Total 345	O 345	0	0
7	D	342	Total 342	O 342	0	0

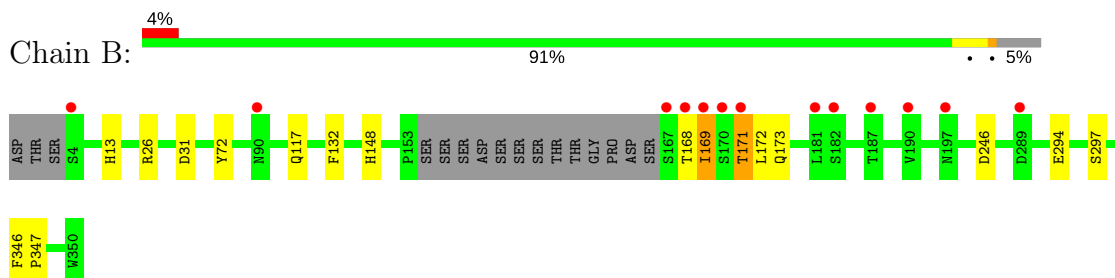
### 3 Residue-property plots [i](#)

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.

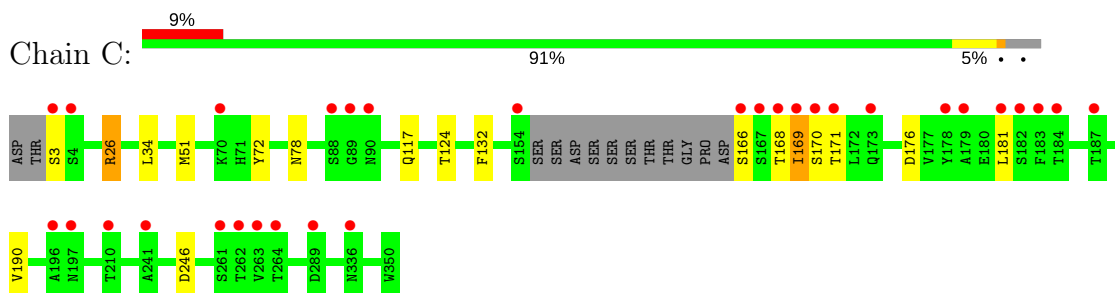
#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE



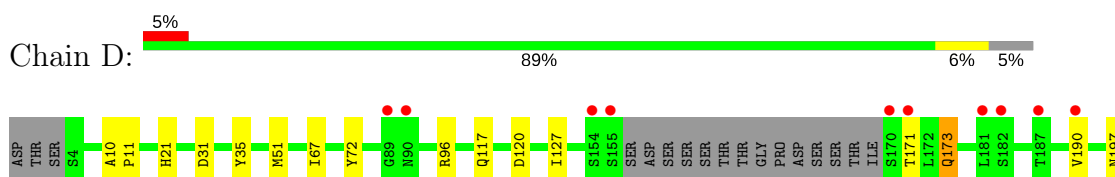
#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE



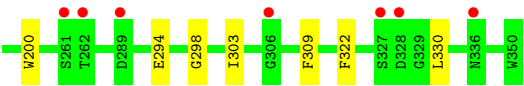
#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE



#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.94Å 55.65Å 123.86Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	19.92 – 1.70 19.89 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.92-1.70) 91.3 (19.89-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.64 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.161 , 0.183 0.198 , 0.212	Depositor DCC
$R_{free}$ test set	7417 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: DCD, BMA, NAG, CU

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	0.49	0/2710	0.78	6/3713 (0.2%)
1	B	0.43	0/2687	0.77	2/3684 (0.1%)
1	C	0.41	0/2698	0.73	2/3698 (0.1%)
1	D	0.43	0/2670	0.75	2/3660 (0.1%)
All	All	0.44	0/10765	0.76	12/14755 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	31	ASP	CB-CG-OD2	5.86	123.58	118.30
1	D	31	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	31	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	120	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	246	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	145	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	328	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	246	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	213	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	349	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	246	ASP	CB-CG-OD2	5.07	122.87	118.30

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	2595	0	2405	28	0
1	B	2590	0	2399	13	0
1	C	2605	0	2411	20	0
1	D	2578	0	2385	15	0
2	A	8	0	10	1	0
2	B	8	0	11	0	0
2	C	8	0	10	3	0
2	D	8	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	42	0	39	0	0
4	B	56	0	52	0	0
4	C	42	0	39	0	0
4	D	42	0	39	0	0
5	A	39	0	34	1	0
5	C	39	0	34	1	0
6	D	28	0	25	1	0
7	A	411	0	0	8	0
7	B	346	0	0	4	0
7	C	345	0	0	5	0
7	D	342	0	0	4	0
All	All	12136	0	9904	75	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 4.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78[A]:ASN:OD1	7:C:2112:HOH:O	1.74	1.04
1:D:171:THR:HA	1:D:173:GLN:OE1	1.68	0.93
1:A:73:GLU:HG3	1:A:127[A]:ILE:HD12	1.55	0.86
1:A:181[B]:LEU:HD23	7:A:2103:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78[B]:ASN:ND2	1:A:124:THR:OG1	2.12	0.82
1:B:297:SER:HB3	7:B:2270:HOH:O	1.86	0.76
1:A:78[A]:ASN:OD1	7:A:2125:HOH:O	2.05	0.73
1:A:260[B]:PRO:HG2	1:A:263:VAL:CG2	2.19	0.71
1:A:245:GLN:HG3	7:A:2285:HOH:O	1.91	0.71
1:A:57:HIS:HE1	1:A:59:ASP:OD1	1.75	0.68
1:C:190:VAL:HG11	5:C:1354:NAG:H82	1.79	0.65
1:C:117:GLN:HB2	7:C:2155:HOH:O	1.97	0.65
1:D:173:GLN:H	1:D:173:GLN:CD	2.03	0.62
1:A:170:SER:HB3	1:A:179:ALA:HB2	1.84	0.60
1:A:78[B]:ASN:HD21	1:A:124:THR:CB	2.15	0.60
1:C:169:ILE:CG2	1:C:170:SER:N	2.64	0.59
1:B:148:HIS:HE1	7:B:2004:HOH:O	1.86	0.59
1:C:181:LEU:HD12	1:C:181:LEU:H	1.69	0.58
1:B:169:ILE:O	1:B:173:GLN:HG3	2.04	0.57
1:B:117:GLN:HG3	7:D:2212:HOH:O	2.03	0.56
1:C:181:LEU:HD12	1:C:181:LEU:N	2.22	0.54
1:A:73:GLU:CG	1:A:127[A]:ILE:HD12	2.35	0.54
1:D:190:VAL:HG11	6:D:1354:NAG:H82	1.89	0.54
1:A:179:ALA:HB1	1:A:181[A]:LEU:CD1	2.37	0.54
1:C:51:MET:CE	2:C:1351:DCD:H3C2	2.39	0.53
1:A:68:HIS:CE1	1:A:132:PHE:HZ	2.27	0.53
1:A:127[A]:ILE:HD11	2:A:1351:DCD:H5C1	1.92	0.52
1:A:190:VAL:HG11	5:A:1354:NAG:H82	1.92	0.51
1:C:132:PHE:HB3	7:C:2081:HOH:O	2.10	0.51
1:A:35:TYR:HD2	1:A:51[B]:MET:CE	2.25	0.50
1:A:179:ALA:HB1	1:A:181[A]:LEU:HD12	1.94	0.50
1:A:260[B]:PRO:HG2	1:A:263:VAL:HG23	1.93	0.50
1:C:78[B]:ASN:ND2	1:C:124:THR:OG1	2.37	0.50
1:B:132:PHE:HB3	7:B:2066:HOH:O	2.11	0.49
1:C:166:SER:O	1:C:169:ILE:HG22	2.13	0.49
1:A:16:PRO:HB3	1:A:287:ILE:HG21	1.96	0.48
1:C:132:PHE:CB	7:C:2081:HOH:O	2.62	0.47
1:A:294:GLU:HG2	7:A:2339:HOH:O	2.14	0.47
1:D:67:ILE:HD11	7:D:2145:HOH:O	2.14	0.46
1:B:13:HIS:HB2	1:C:171:THR:HG23	1.97	0.46
1:B:168:THR:O	1:B:171:THR:N	2.49	0.46
1:B:294:GLU:HG2	7:B:2284:HOH:O	2.17	0.45
1:A:322:PHE:CZ	1:A:330:LEU:HB3	2.52	0.45
1:D:294:GLU:HG2	7:D:2288:HOH:O	2.17	0.45
1:C:169:ILE:HD12	1:C:169:ILE:HA	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:CB	7:A:2179:HOH:O	2.65	0.44
1:B:171:THR:HG22	7:C:2026:HOH:O	2.16	0.44
1:A:57:HIS:CE1	1:A:59:ASP:OD1	2.63	0.44
1:B:168:THR:O	1:B:169:ILE:C	2.55	0.44
1:D:171:THR:CA	1:D:173:GLN:OE1	2.54	0.43
1:C:169:ILE:HG22	1:C:170:SER:H	1.84	0.43
1:A:132:PHE:HB2	7:A:2179:HOH:O	2.18	0.43
1:A:170:SER:CB	1:A:179:ALA:HB2	2.49	0.42
1:D:21:HIS:CG	1:D:298:GLY:HA3	2.53	0.42
1:B:346:PHE:HB2	1:B:347:PRO:HD2	2.00	0.42
1:C:169:ILE:HG22	1:C:170:SER:N	2.33	0.42
1:D:35:TYR:HD2	1:D:51:MET:CE	2.32	0.42
1:C:51:MET:HE1	2:C:1351:DCD:H3C2	2.01	0.42
1:D:322:PHE:CZ	1:D:330:LEU:HB3	2.55	0.41
1:A:181[A]:LEU:CD1	7:A:2221:HOH:O	2.67	0.41
1:D:10:ALA:HA	1:D:11:PRO:HD3	1.90	0.41
1:C:169:ILE:HG23	1:C:170:SER:N	2.36	0.41
1:D:96:ARG:HD2	1:D:200:TRP:CD2	2.56	0.41
1:B:346:PHE:HB2	1:B:347:PRO:CD	2.50	0.41
1:C:34:LEU:C	1:C:34:LEU:HD23	2.40	0.41
1:A:57:HIS:HD2	1:A:117:GLN:O	2.02	0.41
1:D:197:ASN:O	1:D:197:ASN:CG	2.59	0.41
1:A:117:GLN:HB2	7:A:2166:HOH:O	2.20	0.41
1:A:21:HIS:CG	1:A:298:GLY:HA3	2.56	0.41
1:C:51:MET:HE2	2:C:1351:DCD:H3C2	2.02	0.41
1:B:172:LEU:HA	1:B:172:LEU:HD23	1.94	0.40
1:D:117:GLN:NE2	7:D:2149:HOH:O	2.54	0.40
1:C:26:ARG:HG2	1:C:26:ARG:HH11	1.86	0.40
1:D:303:ILE:HG21	1:D:309:PHE:CD1	2.56	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	337/350 (96%)	329 (98%)	8 (2%)	0	100	100
1	B	334/350 (95%)	325 (97%)	9 (3%)	0	100	100
1	C	336/350 (96%)	324 (96%)	12 (4%)	0	100	100
1	D	332/350 (95%)	323 (97%)	9 (3%)	0	100	100
All	All	1339/1400 (96%)	1301 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	284/294 (97%)	280 (99%)	4 (1%)	71	58
1	B	282/294 (96%)	278 (99%)	4 (1%)	71	58
1	C	284/294 (97%)	279 (98%)	5 (2%)	64	47
1	D	279/294 (95%)	277 (99%)	2 (1%)	87	81
All	All	1129/1176 (96%)	1114 (99%)	15 (1%)	73	60

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	TYR
1	A	90	ASN
1	A	297[A]	SER
1	A	297[B]	SER
1	B	26	ARG
1	B	72	TYR
1	B	169	ILE
1	B	171	THR
1	C	3	SER
1	C	26	ARG
1	C	72	TYR
1	C	168	THR
1	C	169	ILE

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Mol	Chain	Res	Type
1	D	72	TYR
1	D	173	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	332	GLN
1	A	336	ASN
1	B	83	GLN
1	B	117	GLN
1	B	148	HIS
1	B	173	GLN
1	B	332	GLN
1	B	336	ASN
1	C	83	GLN
1	C	332	GLN
1	C	336	ASN
1	D	332	GLN
1	D	336	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

8 carbohydrates 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
5	NAG	A	1354	1,5	14,14,15	0.45	0	15,19,21	1.26	1 (6%)
5	NAG	A	1355	5	14,14,15	0.48	0	15,19,21	1.10	2 (13%)
5	BMA	A	1358	5	11,11,12	0.59	0	13,15,17	0.59	0
5	NAG	C	1354	1,5	14,14,15	0.49	0	15,19,21	0.96	0
5	NAG	C	1355	5	14,14,15	0.50	0	15,19,21	1.10	1 (6%)
5	BMA	C	1358	5	11,11,12	0.63	0	13,15,17	0.61	0
6	NAG	D	1354	1,6	14,14,15	0.53	0	15,19,21	1.39	2 (13%)
6	NAG	D	1355	6	14,14,15	0.57	0	15,19,21	0.91	1 (6%)

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	NAG	A	1354	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1355	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1358	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1354	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1355	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1358	5	-	0/2/19/22	0/1/1/1
6	NAG	D	1354	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	1355	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1354	NAG	O5-C1-C2	-3.60	106.46	111.47
5	A	1354	NAG	O5-C1-C2	-3.53	106.56	111.47
6	D	1354	NAG	C2-N2-C7	-3.11	118.41	122.94
5	A	1355	NAG	O5-C1-C2	-2.35	108.21	111.47
5	A	1355	NAG	O4-C4-C3	-2.19	105.60	110.36
5	C	1355	NAG	O5-C1-C2	-2.04	108.64	111.47
6	D	1355	NAG	O5-C1-C2	-2.02	108.66	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1354	NAG	1	0
5	C	1354	NAG	1	0
6	D	1354	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	DCD	A	1351	3	5,7,7	0.88	0	6,8,8	0.88	0
4	NAG	A	1353	1	14,14,15	0.45	0	15,19,21	0.84	0
4	NAG	A	1356	1	14,14,15	0.58	0	15,19,21	0.91	1 (6%)
4	NAG	A	1357	1	14,14,15	0.62	0	15,19,21	0.81	0
2	DCD	B	1351	3	5,7,7	1.48	1 (20%)	6,8,8	0.87	0
4	NAG	B	1353	1	14,14,15	0.60	0	15,19,21	0.90	0
4	NAG	B	1354	1	14,14,15	0.54	0	15,19,21	1.30	2 (13%)
4	NAG	B	1355	1	14,14,15	0.64	0	15,19,21	1.62	2 (13%)
4	NAG	B	1356	1	14,14,15	0.58	0	15,19,21	0.70	0
2	DCD	C	1351	3	5,7,7	1.18	1 (20%)	6,8,8	0.55	0
4	NAG	C	1353	1	14,14,15	0.47	0	15,19,21	0.50	0
4	NAG	C	1356	1	14,14,15	0.58	0	15,19,21	1.11	1 (6%)
4	NAG	C	1357	1	14,14,15	0.64	0	15,19,21	1.34	1 (6%)
2	DCD	D	1351	3	5,7,7	1.69	1 (20%)	6,8,8	1.39	1 (16%)
4	NAG	D	1353	1	14,14,15	0.52	0	15,19,21	1.30	2 (13%)
4	NAG	D	1356	1	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
4	NAG	D	1357	1	14,14,15	0.63	0	15,19,21	1.15	1 (6%)

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	DCD	A	1351	3	-	0/8/8/8	0/0/0/0
4	NAG	A	1353	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1356	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1357	1	-	0/6/23/26	0/1/1/1
2	DCD	B	1351	3	-	0/8/8/8	0/0/0/0
4	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1354	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1355	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1356	1	-	0/6/23/26	0/1/1/1
2	DCD	C	1351	3	-	0/8/8/8	0/0/0/0
4	NAG	C	1353	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1356	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1357	1	-	0/6/23/26	0/1/1/1
2	DCD	D	1351	3	-	0/8/8/8	0/0/0/0
4	NAG	D	1353	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1356	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1357	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1351	DCD	C1-S2	-3.60	1.59	1.66
2	B	1351	DCD	C1-S2	-3.10	1.60	1.66
2	C	1351	DCD	C1-S2	-2.38	1.61	1.66

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1355	NAG	O5-C1-C2	-5.04	104.46	111.47
4	C	1357	NAG	O5-C1-C2	-3.84	106.14	111.47
4	B	1354	NAG	C2-N2-C7	-3.80	117.40	122.94
2	D	1351	DCD	S2-C1-N1	-3.02	117.98	123.71
4	D	1353	NAG	C6-C5-C4	-3.00	105.98	113.00
4	D	1357	NAG	O5-C1-C2	-2.98	107.33	111.47
4	C	1356	NAG	O5-C1-C2	-2.91	107.42	111.47
4	B	1355	NAG	C2-N2-C7	-2.72	118.97	122.94
4	D	1356	NAG	O5-C1-C2	-2.18	108.44	111.47
4	A	1356	NAG	O5-C1-C2	-2.17	108.46	111.47
4	D	1353	NAG	C4-C3-C2	-2.07	107.99	111.02
4	B	1354	NAG	O5-C1-C2	-2.06	108.61	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1351	DCD	1	0
2	C	1351	DCD	3	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	333/350 (95%)	0.10	8 (2%) 59 64	12, 15, 20, 27	0
1	B	334/350 (95%)	0.04	13 (3%) 40 46	12, 15, 19, 28	0
1	C	337/350 (96%)	0.37	31 (9%) 10 11	12, 15, 20, 34	0
1	D	333/350 (95%)	0.16	17 (5%) 29 33	12, 15, 20, 34	0
All	All	1337/1400 (95%)	0.17	69 (5%) 28 31	12, 15, 20, 34	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	167	SER	9.3
1	B	167	SER	8.9
1	D	155	SER	7.6
1	B	169	ILE	7.5
1	C	169	ILE	6.8
1	C	3	SER	6.7
1	C	166	SER	6.7
1	B	181	LEU	5.8
1	C	168	THR	5.5
1	C	4	SER	5.3
1	D	90	ASN	5.2
1	A	90	ASN	5.1
1	C	178	TYR	4.9
1	A	154	SER	4.9
1	B	187	THR	4.8
1	D	181	LEU	4.7
1	D	262	THR	4.7
1	D	154	SER	4.7
1	D	170	SER	4.6
1	C	182	SER	4.5
1	C	89	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	154	SER	4.1
1	B	168	THR	4.1
1	D	182	SER	4.1
1	C	90	ASN	4.0
1	C	181	LEU	3.9
1	C	261	SER	3.9
1	D	171	THR	3.8
1	C	210	THR	3.7
1	C	289	ASP	3.6
1	A	170	SER	3.6
1	D	261	SER	3.3
1	C	262	THR	3.2
1	C	197	ASN	3.1
1	B	4	SER	3.1
1	A	181[A]	LEU	3.1
1	C	170	SER	3.0
1	D	190	VAL	3.0
1	B	182	SER	3.0
1	B	190	VAL	2.9
1	C	264	THR	2.9
1	B	197	ASN	2.9
1	B	289	ASP	2.9
1	D	89	GLY	2.8
1	D	289	ASP	2.8
1	C	187	THR	2.7
1	A	182	SER	2.7
1	A	254	ILE	2.7
1	B	170	SER	2.7
1	C	70	LYS	2.6
1	C	171	THR	2.6
1	C	88	SER	2.6
1	C	196	ALA	2.6
1	A	197	ASN	2.6
1	D	306	GLY	2.5
1	D	187	THR	2.4
1	C	241	ALA	2.4
1	A	196	ALA	2.4
1	B	90[A]	ASN	2.3
1	D	327	SER	2.2
1	C	179	ALA	2.2
1	D	328	ASP	2.1
1	C	173	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	336	ASN	2.1
1	D	336	ASN	2.1
1	B	171	THR	2.1
1	C	183	PHE	2.1
1	C	263	VAL	2.0
1	C	184	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](#)

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(Å <sup>2</sup> )	Q<0.9
5	NAG	C	1355	14/15	0.67	0.22	5.33	35,40,43,48	0
5	NAG	A	1355	14/15	0.78	0.24	2.15	36,41,44,46	0
5	NAG	C	1354	14/15	0.82	0.17	2.11	31,36,42,45	0
5	NAG	A	1354	14/15	0.78	0.20	1.37	31,36,39,40	0
6	NAG	D	1355	14/15	0.80	0.23	1.15	36,39,43,45	0
6	NAG	D	1354	14/15	0.80	0.14	-0.28	31,36,39,40	0
5	BMA	C	1358	11/12	0.66	0.37	-	52,55,56,56	0
5	BMA	A	1358	11/12	0.77	0.32	-	48,49,50,50	0

## 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(Å <sup>2</sup> )	Q<0.9
4	NAG	D	1356	14/15	0.78	0.17	6.89	29,33,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	1355	14/15	0.83	0.20	5.75	28,34,45,46	0
4	NAG	C	1356	14/15	0.80	0.22	3.91	34,39,46,46	0
4	NAG	A	1357	14/15	0.80	0.18	3.52	32,36,42,44	0
4	NAG	A	1356	14/15	0.88	0.13	2.66	27,32,41,43	0
2	DCD	C	1351	8/8	0.93	0.13	2.66	20,21,22,23	0
4	NAG	D	1357	14/15	0.84	0.17	0.89	32,38,44,45	0
4	NAG	B	1354	14/15	0.87	0.17	0.80	40,45,47,48	0
4	NAG	D	1353	14/15	0.82	0.16	0.06	33,39,42,43	0
2	DCD	B	1351	8/8	0.97	0.07	-0.67	22,23,24,24	0
2	DCD	A	1351	8/8	0.97	0.07	-1.07	17,18,20,20	0
2	DCD	D	1351	8/8	0.98	0.05	-2.12	19,20,23,23	0
4	NAG	C	1353	14/15	0.76	0.16	-	34,39,44,46	0
4	NAG	C	1357	14/15	0.86	0.13	-	32,39,42,43	0
3	CU	B	1352	1/1	0.99	0.04	-	17,17,17,17	0
4	NAG	A	1353	14/15	0.88	0.11	-	26,32,35,36	0
4	NAG	B	1353	14/15	0.90	0.15	-	29,34,38,38	0
3	CU	C	1352	1/1	0.98	0.05	-	17,17,17,17	0
3	CU	A	1352	1/1	0.99	0.06	-	17,17,17,17	0
3	CU	D	1352	1/1	0.99	0.02	-	17,17,17,17	0
4	NAG	B	1356	14/15	0.88	0.15	-	35,42,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.