



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:35 am GMT

PDB ID : 1H1M  
Title : CRYSTAL STRUCTURE OF QUERCETIN 2,3-DIOXYGENASE ANAEROBICALLY COMPLEXED WITH THE SUBSTRATE KAEMPFEROL  
Authors : Steiner, R.A.; Dijkstra, B.W.  
Deposited on : 2002-07-19  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : trunk28620  
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

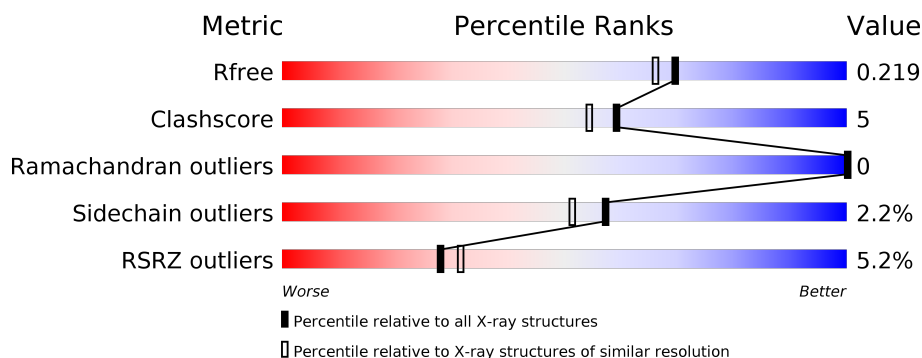
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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	350	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	B	350	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	C	350	<div> <div>6%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	D	350	<div> <div>7%</div> <div>89%</div> <div>9%</div> <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	NAG	A	1354	-	-	-	X
2	NAG	B	1354	-	-	-	X
2	NAG	C	1354	-	-	-	X
6	MPD	A	1362	-	-	-	X
6	MPD	B	1360	-	-	-	X
6	MPD	B	1361	-	-	X	X
6	MPD	C	1360	-	-	X	X

## 2 Entry composition [i](#)

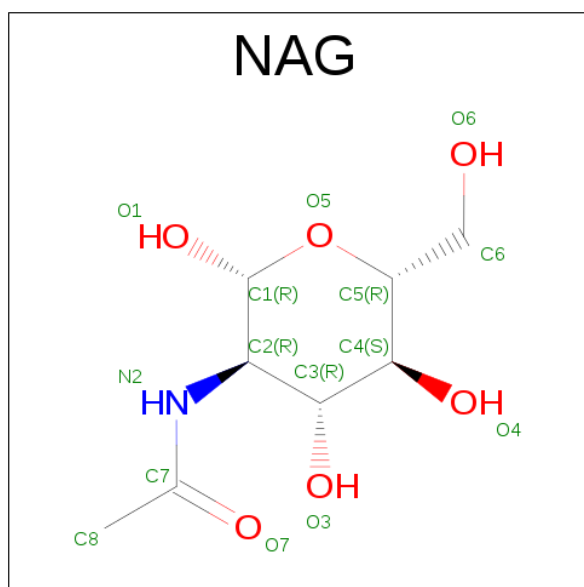
There are 9 unique types of molecules in this entry. The entry contains 12645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	344	Total	C	N	O	S	0	5	0
			2657	1682	431	539	5			
1	B	344	Total	C	N	O	S	0	4	0
			2654	1681	431	537	5			
1	C	343	Total	C	N	O	S	0	4	0
			2648	1678	430	535	5			
1	D	343	Total	C	N	O	S	0	5	0
			2648	1678	430	535	5			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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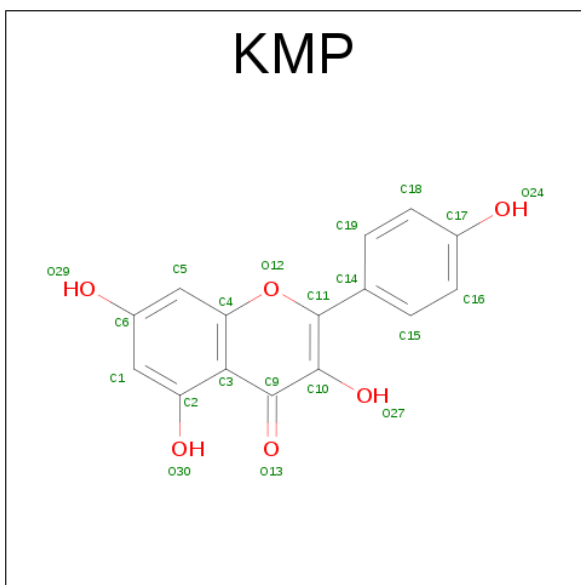
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
	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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is 3,5,7-TRIHIDROXY-2-(4-HYDROXYPHENYL)-4H-CHROMEN-4-ONE (three-letter code: KMP) (formula: C<sub>15</sub>H<sub>10</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	15	6		
4	B	1	Total	C	O	0	0
			21	15	6		
4	C	1	Total	C	O	0	0
			21	15	6		
4	D	1	Total	C	O	0	0
			21	15	6		

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	4	Total	C	N	O	0	0
			50	28	2	20		
7	C	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 9 is water.

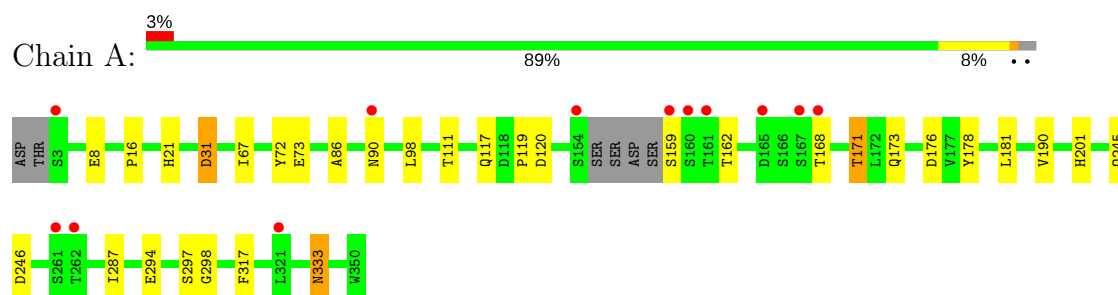
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	416	Total 416	O 416	0	0
9	B	387	Total 387	O 387	0	0
9	C	381	Total 381	O 381	0	0
9	D	363	Total 363	O 363	0	0



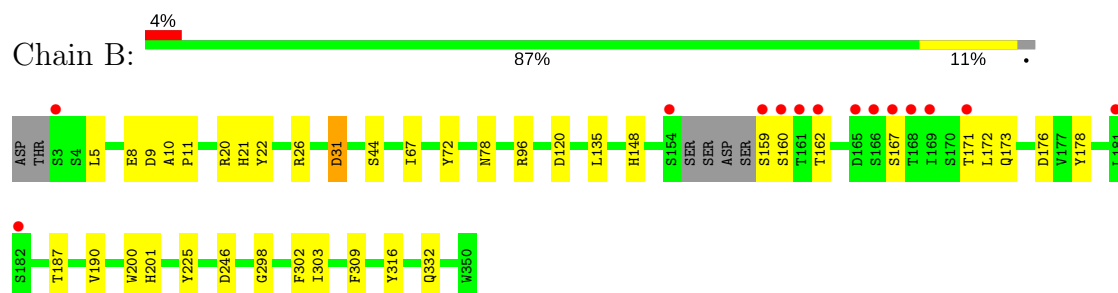
### 3 Residue-property plots [i](#)

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.

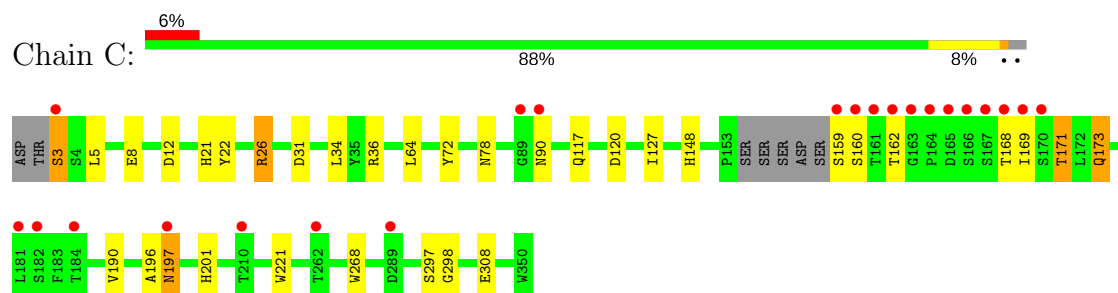
#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE



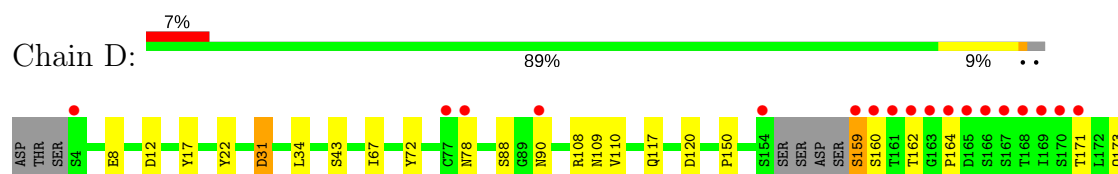
#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE

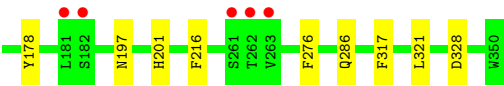


#### • Molecule 1: QUERCETIN 2,3-DIOXYGENASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	109.27Å 55.38Å 123.93Å 90.00° 98.33° 90.00°	Depositor
Resolution (Å)	49.39 – 1.90 39.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.39-1.90) 96.5 (39.72-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.154 , 0.204 0.179 , 0.219	Depositor DCC
$R_{free}$ test set	5608 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, KMP, CU, MAN

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	0.95	0/2762	0.94	4/3786 (0.1%)
1	B	0.91	0/2754	0.93	7/3775 (0.2%)
1	C	0.92	0/2748	0.87	2/3767 (0.1%)
1	D	0.90	0/2748	0.88	4/3767 (0.1%)
All	All	0.92	0/11012	0.91	17/15095 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ASP	CB-CG-OD2	8.07	125.56	118.30
1	A	246	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	9	ASP	CB-CG-OD2	7.60	125.14	118.30
1	A	176	ASP	CB-CG-OD2	7.37	124.93	118.30
1	C	120	ASP	CB-CG-OD2	7.01	124.61	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2657	0	2453	32	0
1	B	2654	0	2454	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2648	0	2449	26	0
1	D	2648	0	2445	25	0
2	A	56	0	52	0	0
2	B	42	0	39	0	0
2	C	42	0	39	4	0
2	D	42	0	39	0	0
3	A	61	0	52	1	0
4	A	21	0	6	1	0
4	B	21	0	6	1	0
4	C	21	0	6	0	0
4	D	21	0	7	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	8	0	14	4	0
6	B	16	0	28	7	0
6	C	8	0	14	6	0
7	B	50	0	43	1	0
7	C	50	0	43	1	0
8	D	28	0	25	1	0
9	A	416	0	0	14	0
9	B	387	0	0	12	0
9	C	381	0	0	6	0
9	D	363	0	0	11	0
All	All	12645	0	10214	115	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 5.

The worst 5 of 115 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)
6:B:1360:MPD:H32	6:B:1361:MPD:H32	1.26	1.14
1:A:8[A]:GLU:HG2	9:A:2018:HOH:O	1.55	1.05
1:D:117:GLN:HG3	9:D:2141:HOH:O	1.66	0.95
1:D:78[D]:ASN:HB3	9:D:2151:HOH:O	1.66	0.94
6:B:1360:MPD:C3	6:B:1361:MPD:H32	2.02	0.89

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	345/350 (99%)	333 (96%)	12 (4%)	0	100	100
1	B	344/350 (98%)	332 (96%)	12 (4%)	0	100	100
1	C	343/350 (98%)	334 (97%)	9 (3%)	0	100	100
1	D	343/350 (98%)	334 (97%)	9 (3%)	0	100	100
All	All	1375/1400 (98%)	1333 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	293/294 (100%)	287 (98%)	6 (2%)	60	55
1	B	292/294 (99%)	287 (98%)	5 (2%)	66	62
1	C	291/294 (99%)	282 (97%)	9 (3%)	45	36
1	D	291/294 (99%)	285 (98%)	6 (2%)	59	53
All	All	1167/1176 (99%)	1141 (98%)	26 (2%)	57	51

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	SER
1	C	159	SER
1	D	159	SER

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Mol	Chain	Res	Type
1	C	26	ARG
1	C	72	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	332	GLN
1	C	83	GLN
1	D	83	GLN
1	B	286	GLN
1	D	90	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 ⓘ

15 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	$\# Z  > 2$
3	NAG	A	1352	1,3	14,14,15	0.87	1 (7%)	15,19,21	1.33	2 (13%)
3	NAG	A	1353	3	14,14,15	0.70	0	15,19,21	1.29	2 (13%)
3	BMA	A	1357	3	11,11,12	0.96	0	13,15,17	0.97	1 (7%)
3	MAN	A	1358	3	11,11,12	0.59	0	13,15,17	1.35	1 (7%)
3	MAN	A	1359	3	11,11,12	0.79	0	13,15,17	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	1352	1,7	14,14,15	0.88	1 (7%)	15,19,21	1.58	1 (6%)
7	NAG	B	1353	7	14,14,15	0.61	0	15,19,21	1.98	6 (40%)
7	BMA	B	1356	7	11,11,12	0.71	0	13,15,17	1.71	2 (15%)
7	MAN	B	1357	7	11,11,12	0.86	0	13,15,17	1.08	0
7	NAG	C	1352	1,7	14,14,15	0.45	0	15,19,21	1.62	4 (26%)
7	NAG	C	1353	7	14,14,15	0.50	0	15,19,21	1.58	4 (26%)
7	BMA	C	1356	7	11,11,12	1.08	1 (9%)	13,15,17	1.02	0
7	MAN	C	1357	7	11,11,12	0.68	0	13,15,17	0.87	0
8	NAG	D	1352	1,8	14,14,15	0.76	1 (7%)	15,19,21	1.02	1 (6%)
8	NAG	D	1353	8	14,14,15	0.85	0	15,19,21	1.85	4 (26%)

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
3	NAG	A	1352	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1353	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1357	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1358	3	-	0/2/19/22	0/1/1/1
3	MAN	A	1359	3	-	0/2/19/22	0/1/1/1
7	NAG	B	1352	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1353	7	-	0/6/23/26	0/1/1/1
7	BMA	B	1356	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1357	7	-	0/2/19/22	0/1/1/1
7	NAG	C	1352	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1353	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1356	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1357	7	-	0/2/19/22	0/1/1/1
8	NAG	D	1352	1,8	-	0/6/23/26	0/1/1/1
8	NAG	D	1353	8	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1356	BMA	O5-C1	-2.91	1.39	1.43
7	B	1352	NAG	C1-C2	2.09	1.55	1.52
8	D	1352	NAG	C1-C2	2.32	1.55	1.52
3	A	1352	NAG	C1-C2	2.33	1.55	1.52



The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1353	NAG	O5-C1-C2	-4.25	105.56	111.47
8	D	1353	NAG	O7-C7-C8	-4.20	114.41	122.06
7	C	1352	NAG	O5-C1-C2	-3.42	106.72	111.47
3	A	1352	NAG	O5-C1-C2	-3.26	106.94	111.47
7	B	1353	NAG	O6-C6-C5	-2.89	101.61	111.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1352	NAG	1	0
7	B	1352	NAG	1	0
7	C	1352	NAG	1	0
8	D	1353	NAG	1	0

## 5.6 Ligand geometry

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	NAG	A	1351	1	14,14,15	0.64	0	15,19,21	1.04	1 (6%)
2	NAG	A	1354	1	14,14,15	0.72	0	15,19,21	1.58	2 (13%)
2	NAG	A	1355	1	14,14,15	0.99	1 (7%)	15,19,21	1.60	3 (20%)
2	NAG	A	1356	1	14,14,15	0.93	0	15,19,21	1.52	1 (6%)
4	KMP	A	1360	5	21,23,23	2.11	5 (23%)	25,34,34	2.01	6 (24%)
6	MPD	A	1362	-	7,7,7	0.69	0	9,10,10	1.76	1 (11%)
2	NAG	B	1351	1	14,14,15	0.47	0	15,19,21	1.05	1 (6%)
2	NAG	B	1354	1	14,14,15	0.73	0	15,19,21	1.24	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	1355	1	14,14,15	0.78	1 (7%)	15,19,21	1.26	2 (13%)
4	KMP	B	1358	5	21,23,23	1.96	6 (28%)	25,34,34	1.47	5 (20%)
6	MPD	B	1360	-	7,7,7	0.61	0	9,10,10	1.89	3 (33%)
6	MPD	B	1361	-	7,7,7	0.67	0	9,10,10	1.77	2 (22%)
2	NAG	C	1351	1	14,14,15	0.51	0	15,19,21	1.01	0
2	NAG	C	1354	1	14,14,15	0.93	1 (7%)	15,19,21	1.39	2 (13%)
2	NAG	C	1355	1	14,14,15	0.75	0	15,19,21	2.02	4 (26%)
4	KMP	C	1358	5	21,23,23	2.12	4 (19%)	25,34,34	1.69	7 (28%)
6	MPD	C	1360	-	7,7,7	0.63	0	9,10,10	1.39	1 (11%)
2	NAG	D	1351	1	14,14,15	0.80	1 (7%)	15,19,21	1.47	3 (20%)
2	NAG	D	1354	1	14,14,15	1.08	1 (7%)	15,19,21	2.12	2 (13%)
2	NAG	D	1355	1	14,14,15	0.85	1 (7%)	15,19,21	1.78	3 (20%)
4	KMP	D	1356	5	21,23,23	2.34	4 (19%)	25,34,34	1.86	6 (24%)

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	NAG	A	1351	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1354	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1355	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1356	1	-	0/6/23/26	0/1/1/1
4	KMP	A	1360	5	-	0/4/4/4	0/3/3/3
6	MPD	A	1362	-	-	0/5/5/5	0/0/0/0
2	NAG	B	1351	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1354	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1355	1	-	0/6/23/26	0/1/1/1
4	KMP	B	1358	5	-	0/4/4/4	0/3/3/3
6	MPD	B	1360	-	-	0/5/5/5	0/0/0/0
6	MPD	B	1361	-	-	0/5/5/5	0/0/0/0
2	NAG	C	1351	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1354	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1355	1	-	0/6/23/26	0/1/1/1
4	KMP	C	1358	5	-	0/4/4/4	0/3/3/3
6	MPD	C	1360	-	-	0/5/5/5	0/0/0/0
2	NAG	D	1351	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1354	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1355	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	KMP	D	1356	5	-	0/4/4/4	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1360	KMP	O24-C17	-2.21	1.31	1.37
4	B	1358	KMP	O29-C6	-2.18	1.32	1.37
2	B	1355	NAG	C1-C2	2.07	1.55	1.52
4	B	1358	KMP	C14-C11	2.08	1.50	1.46
2	D	1351	NAG	C1-C2	2.09	1.55	1.52

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1354	NAG	O5-C1-C2	-5.72	103.51	111.47
2	C	1355	NAG	C1-O5-C5	-4.60	105.82	112.17
6	A	1362	MPD	CM-C2-C1	-4.54	100.29	110.42
4	A	1360	KMP	C5-C4-C3	-4.51	118.06	123.05
6	B	1361	MPD	CM-C2-C1	-4.33	100.77	110.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1360	KMP	1	0
6	A	1362	MPD	4	0
4	B	1358	KMP	1	0
6	B	1360	MPD	5	0
6	B	1361	MPD	6	0
2	C	1355	NAG	4	0
6	C	1360	MPD	6	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	344/350 (98%)	-0.14	12 (3%) 44 48	4, 9, 16, 30	0
1	B	344/350 (98%)	-0.15	14 (4%) 38 42	3, 9, 17, 31	0
1	C	343/350 (98%)	0.13	22 (6%) 20 23	3, 9, 17, 31	0
1	D	343/350 (98%)	0.08	23 (6%) 19 21	4, 9, 16, 31	1 (0%)
All	All	1374/1400 (98%)	-0.02	71 (5%) 28 31	3, 9, 17, 31	1 (0%)

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	ILE	7.0
1	C	159	SER	5.8
1	B	3	SER	5.6
1	D	159	SER	5.4
1	D	160	SER	5.2

### 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( $\text{\AA}^2$ )	Q<0.9
7	NAG	B	1353	14/15	0.82	0.15	0.61	24,32,40,44	0
8	NAG	D	1353	14/15	0.93	0.10	0.20	18,29,34,35	0
7	NAG	C	1353	14/15	0.94	0.08	-0.20	21,25,30,33	0
7	NAG	B	1352	14/15	0.94	0.10	-0.37	21,24,29,31	0
7	NAG	C	1352	14/15	0.95	0.08	-0.38	19,23,34,36	0
3	NAG	A	1352	14/15	0.95	0.09	-0.41	19,25,28,30	0
8	NAG	D	1352	14/15	0.96	0.09	-0.73	20,25,31,33	0
3	NAG	A	1353	14/15	0.94	0.09	-0.95	24,29,35,39	0
3	MAN	A	1358	11/12	0.80	0.26	-	60,61,62,65	0
7	BMA	B	1356	11/12	0.65	0.22	-	46,48,54,59	0
7	MAN	B	1357	11/12	0.57	0.26	-	61,62,64,65	0
3	MAN	A	1359	11/12	0.73	0.31	-	67,68,68,69	0
7	BMA	C	1356	11/12	0.86	0.15	-	35,41,43,44	0
3	BMA	A	1357	11/12	0.86	0.14	-	45,48,54,58	0
7	MAN	C	1357	11/12	0.61	0.20	-	43,46,48,49	0

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
6	MPD	B	1361	8/8	0.70	0.33	5.98	26,36,39,43	0
6	MPD	B	1360	8/8	0.75	0.31	5.51	24,34,37,39	0
6	MPD	C	1360	8/8	0.80	0.23	3.94	24,34,38,42	0
2	NAG	B	1354	14/15	0.89	0.17	2.91	22,31,42,43	0
6	MPD	A	1362	8/8	0.84	0.22	2.77	20,29,31,34	0
2	NAG	C	1354	14/15	0.88	0.14	2.50	28,36,46,47	0
2	NAG	A	1354	14/15	0.91	0.10	2.22	20,32,41,41	0
2	NAG	D	1355	14/15	0.88	0.13	1.30	27,35,44,46	0
2	NAG	A	1355	14/15	0.91	0.24	1.04	28,37,44,46	0
2	NAG	D	1351	14/15	0.85	0.17	0.43	30,40,42,44	0
2	NAG	A	1356	14/15	0.79	0.15	0.06	26,33,36,39	0
2	NAG	D	1354	14/15	0.89	0.13	-0.02	22,28,32,36	0
4	KMP	B	1358	21/21	0.94	0.10	-0.13	15,18,21,21	0
4	KMP	C	1358	21/21	0.93	0.10	-0.40	17,18,20,23	0
4	KMP	D	1356	21/21	0.94	0.09	-0.60	12,16,18,19	0
4	KMP	A	1360	21/21	0.96	0.08	-0.85	11,14,19,20	0
2	NAG	C	1355	14/15	0.83	0.15	-	34,44,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	1351	14/15	0.92	0.13	-	27,34,40,43	0
5	CU	B	1359	1/1	1.00	0.02	-	10,10,10,10	0
5	CU	A	1361	1/1	1.00	0.06	-	9,9,9,9	0
2	NAG	B	1355	14/15	0.86	0.16	-	31,41,44,47	0
5	CU	C	1359	1/1	0.99	0.02	-	11,11,11,11	0
2	NAG	B	1351	14/15	0.91	0.16	-	23,32,34,35	0
5	CU	D	1357	1/1	0.99	0.02	-	11,11,11,11	0
2	NAG	A	1351	14/15	0.87	0.14	-	26,32,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.