



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H1I
Title : CRYSTAL STRUCTURE OF QUERCETIN 2,3-DIOXYGENASE ANAEROBICALLY COMPLEXED WITH THE SUBSTRATE QUERCETIN
Authors : Steiner, R.A.; Dijkstra, B.W.
Deposited on : 2002-07-15
Resolution : 1.75 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

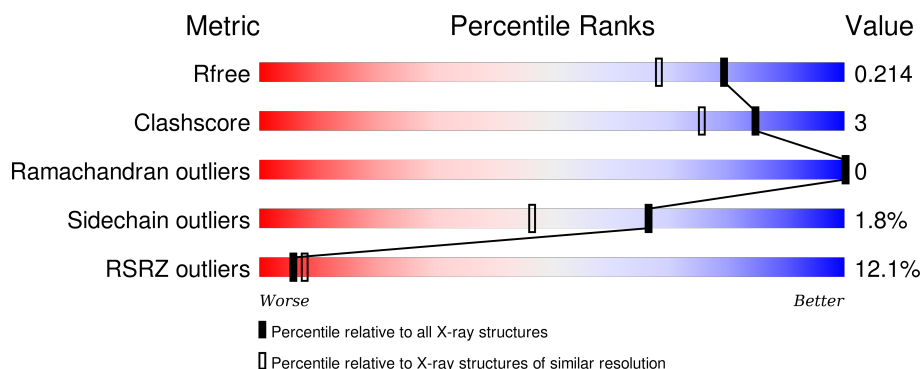
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 ≥ 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	 8% 92% 6% ..
1	B	350	 11% 93% 5% ..
1	C	350	 15% 91% 6% ..
1	D	350	 13% 93% 5% .

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	B	1353	-	-	-	X
3	NAG	C	1354	-	-	-	X
6	MPD	A	1359	-	-	-	X
6	MPD	B	1357	-	-	-	X
6	MPD	B	1358	-	-	X	X
6	MPD	C	1351	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12575 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	7	0
			2665	1687	433	540	5			
1	B	346	Total	C	N	O	S	0	7	0
			2674	1692	433	543	6			
1	C	343	Total	C	N	O	S	0	2	0
			2642	1676	429	532	5			
1	D	343	Total	C	N	O	S	0	3	0
			2651	1681	431	534	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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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	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 (2-MER).

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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

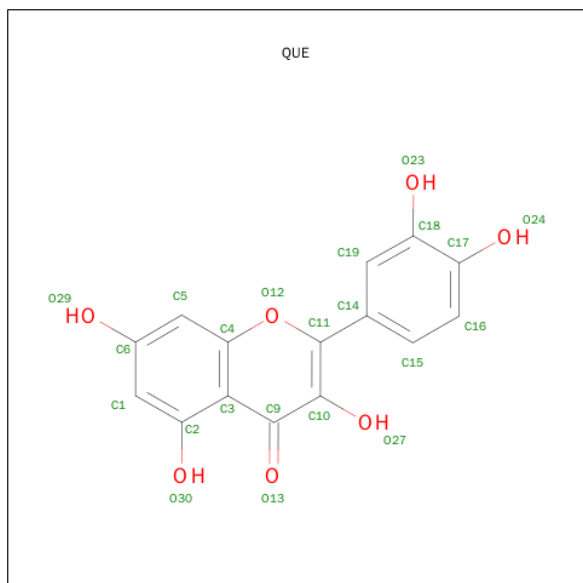
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		
4	A	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cu	0	0
			1	1		
4	C	1	Total	Cu	0	0
			1	1		

- Molecule 5 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: $C_{15}H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	15	7		
5	B	1	Total	C	O	0	0
			22	15	7		
5	C	1	Total	C	O	0	0
			22	15	7		
5	D	1	Total	C	O	0	0
			22	15	7		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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		

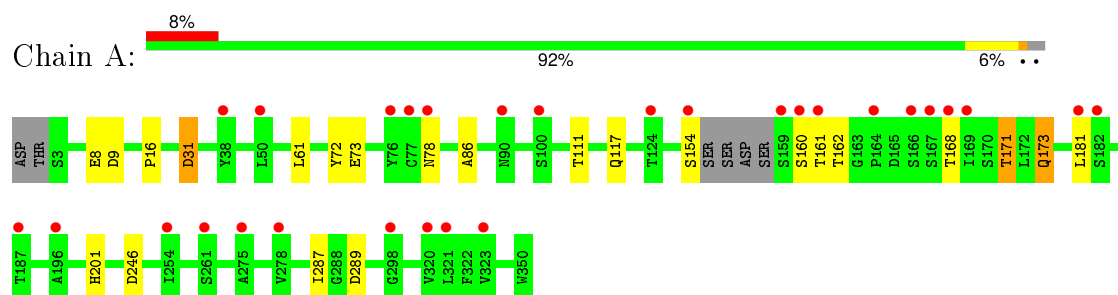
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	427	Total	O	0	0
			427	427		
7	B	378	Total	O	0	0
			378	378		
7	C	370	Total	O	0	0
			370	370		
7	D	364	Total	O	0	0
			364	364		

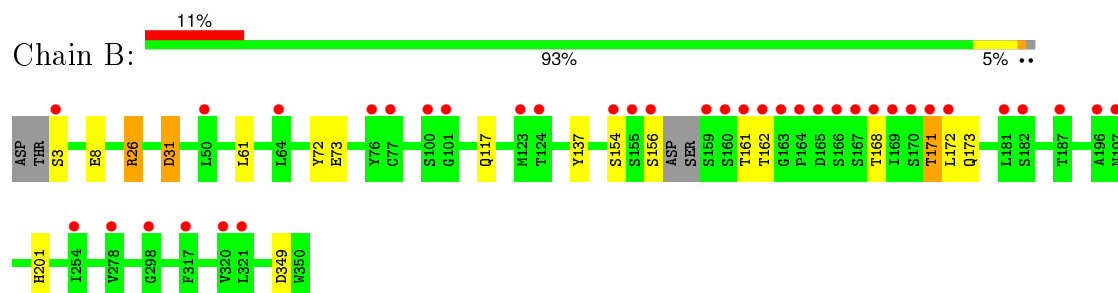
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

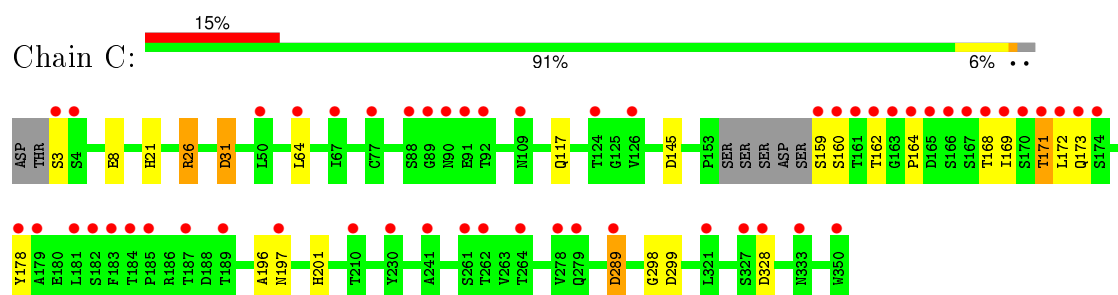
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE



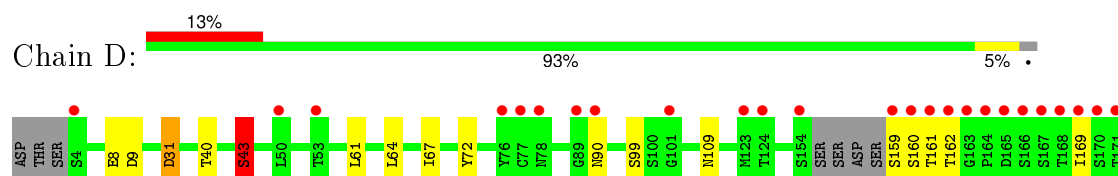
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE

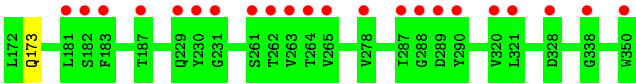


• Molecule 1: QUERCETIN 2,3-DIOXYGENASE



• 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, α , β , γ	109.30Å 55.74Å 124.16Å 90.00° 98.39° 90.00°	Depositor
Resolution (Å)	49.39 – 1.75 47.02 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.39-1.75) 99.5 (47.02-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.148 , 0.183 0.190 , 0.214	Depositor DCC
R_{free} test set	7473 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 148815 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12575	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, QUE, 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	0.84	0/2777	0.86	4/3806 (0.1%)
1	B	0.74	0/2788	0.82	2/3820 (0.1%)
1	C	0.73	0/2732	0.81	5/3746 (0.1%)
1	D	0.74	0/2746	0.80	3/3764 (0.1%)
All	All	0.77	0/11043	0.82	14/15136 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ASP	CB-CG-OD2	6.47	124.12	118.30
1	D	31	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	31	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	31	ASP	CB-CG-OD2	6.15	123.84	118.30
1	C	289	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	299	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	328	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	43	SER	CA-CB-OG	-5.36	96.73	111.20
1	B	349	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	9	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	145	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	9	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	289	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	31	ASP	CB-CG-OD2	5.02	122.82	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	2665	0	2460	16	0
1	B	2674	0	2475	14	0
1	C	2642	0	2447	16	0
1	D	2651	0	2453	9	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
3	A	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	22	0	5	2	0
5	B	22	0	5	2	0
5	C	22	0	5	1	0
5	D	22	0	5	0	0
6	A	8	0	14	3	0
6	B	16	0	28	6	0
6	C	8	0	14	3	0
7	A	427	0	0	5	0
7	B	378	0	0	3	0
7	C	370	0	0	5	0
7	D	364	0	0	5	0
All	All	12575	0	10168	62	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 (62) 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:196:ALA:O	1:C:197:ASN:HB3	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1357:MPD:H32	6:B:1358:MPD:H32	1.50	0.93
1:B:8[A]:GLU:HG2	7:B:2003:HOH:O	1.73	0.88
1:D:8[A]:GLU:HG2	7:D:2010:HOH:O	1.74	0.87
1:A:173:GLN:HE21	1:A:173:GLN:H	1.21	0.84
1:A:8[A]:GLU:HG2	7:A:2014:HOH:O	1.78	0.82
6:B:1357:MPD:C3	6:B:1358:MPD:H32	2.11	0.81
1:C:8:GLU:HG2	7:C:2009:HOH:O	1.79	0.81
1:B:201:HIS:CE1	6:B:1358:MPD:HM1	2.26	0.71
1:A:171:THR:HG23	7:A:2215:HOH:O	1.94	0.68
6:A:1359:MPD:H32	6:C:1351:MPD:H32	1.78	0.66
1:A:173:GLN:NE2	1:A:173:GLN:H	1.95	0.64
1:C:197:ASN:O	1:C:197:ASN:ND2	2.30	0.63
1:B:31:ASP:HB2	1:B:162:THR:HG23	1.80	0.63
1:D:8[A]:GLU:CG	7:D:2010:HOH:O	2.41	0.62
1:C:172:LEU:HA	7:C:2202:HOH:O	2.02	0.59
1:D:31:ASP:HB2	1:D:162:THR:HG23	1.85	0.58
1:C:64:LEU:HB2	1:C:169:ILE:HD13	1.85	0.57
1:C:196:ALA:O	1:C:197:ASN:CB	2.34	0.56
1:C:8:GLU:CG	7:C:2009:HOH:O	2.44	0.56
1:B:168:THR:O	1:B:171:THR:HB	2.09	0.53
1:B:171:THR:HG22	1:B:172:LEU:HD23	1.91	0.52
1:D:40:THR:H	1:D:43:SER:HB2	1.75	0.52
6:A:1359:MPD:C3	6:C:1351:MPD:H32	2.39	0.51
1:D:173:GLN:HG3	7:D:2195:HOH:O	2.10	0.51
1:A:31:ASP:HB2	1:A:162:THR:HG23	1.93	0.51
1:A:117:GLN:HG3	7:C:2225:HOH:O	2.11	0.51
1:C:168:THR:O	1:C:171:THR:HB	2.11	0.50
1:B:26:ARG:HD3	1:B:137:TYR:CE1	2.47	0.49
1:C:31:ASP:HB2	1:C:162:THR:HG23	1.95	0.49
1:A:201:HIS:CE1	6:A:1359:MPD:HM1	2.47	0.49
1:C:289:ASP:CG	1:C:289:ASP:O	2.51	0.48
1:C:173:GLN:HG2	1:C:178:TYR:CE2	2.48	0.48
1:B:117:GLN:HG3	7:D:2220:HOH:O	2.12	0.48
1:C:201:HIS:CE1	6:C:1351:MPD:HM1	2.48	0.48
1:C:164:PRO:HG2	1:C:169:ILE:HD12	1.96	0.47
5:A:1358:QUE:O27	5:A:1358:QUE:H19	2.15	0.46
1:B:73:GLU:CD	5:B:1356:QUE:H19	2.35	0.46
1:B:8[A]:GLU:CG	7:B:2003:HOH:O	2.45	0.46
1:A:78[B]:ASN:ND2	7:A:2110:HOH:O	2.34	0.46
1:C:26:ARG:HD2	7:C:2053:HOH:O	2.16	0.46
6:B:1357:MPD:H31	6:B:1358:MPD:H32	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:SER:HB2	7:B:2170:HOH:O	2.17	0.45
1:B:61:LEU:HB2	1:B:161:THR:HG23	1.99	0.45
6:B:1358:MPD:H11	1:D:99:SER:HB3	1.99	0.44
1:A:168:THR:O	1:A:171:THR:HB	2.19	0.43
1:A:61:LEU:HB2	1:A:161:THR:HG23	2.00	0.43
6:B:1357:MPD:H4	6:B:1358:MPD:H13	2.01	0.43
1:A:8[A]:GLU:CG	7:A:2014:HOH:O	2.51	0.43
5:C:1358:QUE:O27	5:C:1358:QUE:H19	2.20	0.42
1:B:73:GLU:OE2	5:B:1356:QUE:H19	2.19	0.42
1:A:16:PRO:HB3	1:A:287:ILE:HG21	2.01	0.42
1:C:21:HIS:CG	1:C:298:GLY:HA3	2.55	0.42
1:A:73:GLU:OE2	5:A:1358:QUE:H19	2.20	0.41
1:D:64:LEU:HB2	1:D:169:ILE:HD13	2.02	0.41
1:A:201:HIS:HB3	1:C:117:GLN:NE2	2.36	0.41
1:D:61:LEU:HB2	1:D:161:THR:HG23	2.02	0.41
1:A:154:SER:HB2	7:A:2202:HOH:O	2.20	0.40
1:A:86:ALA:HA	1:A:111:THR:O	2.21	0.40
1:D:109:ASN:HB3	7:D:2133:HOH:O	2.21	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	347/350 (99%)	340 (98%)	7 (2%)	0	100	100
1	B	349/350 (100%)	340 (97%)	9 (3%)	0	100	100
1	C	341/350 (97%)	329 (96%)	12 (4%)	0	100	100
1	D	342/350 (98%)	332 (97%)	10 (3%)	0	100	100
All	All	1379/1400 (98%)	1341 (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	295/294 (100%)	290 (98%)	5 (2%)	68	49
1	B	297/294 (101%)	292 (98%)	5 (2%)	68	49
1	C	289/294 (98%)	284 (98%)	5 (2%)	68	49
1	D	290/294 (99%)	284 (98%)	6 (2%)	61	37
All	All	1171/1176 (100%)	1150 (98%)	21 (2%)	66	46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	TYR
1	A	160	SER
1	A	171	THR
1	A	173	GLN
1	A	181	LEU
1	B	3	SER
1	B	26	ARG
1	B	72	TYR
1	B	156	SER
1	B	171	THR
1	C	3	SER
1	C	26	ARG
1	C	159	SER
1	C	160	SER
1	C	171	THR
1	D	43	SER
1	D	67	ILE
1	D	72	TYR
1	D	90	ASN
1	D	159	SER
1	D	160	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	173	GLN
1	A	245	GLN
1	B	83	GLN
1	C	197	ASN
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 ⓘ

6 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	0.54	0	15,19,21	0.90	0
3	NAG	A	1353	3	14,14,15	0.53	0	15,19,21	1.10	1 (6%)
3	NAG	C	1353	1,3	14,14,15	0.65	0	15,19,21	1.14	1 (6%)
3	NAG	C	1354	3	14,14,15	0.40	0	15,19,21	1.17	2 (13%)
3	NAG	D	1352	1,3	14,14,15	0.51	0	15,19,21	1.08	1 (6%)
3	NAG	D	1353	3	14,14,15	0.54	0	15,19,21	1.16	2 (13%)

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	NAG	C	1353	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1354	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1352	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1353	3	-	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(°)
3	C	1354	NAG	O7-C7-C8	-2.61	117.27	122.06
3	C	1353	NAG	O4-C4-C5	-2.43	102.81	109.24
3	D	1352	NAG	C2-N2-C7	-2.04	120.42	123.04
3	A	1353	NAG	O4-C4-C5	2.16	114.97	109.24
3	D	1353	NAG	C1-O5-C5	2.32	115.19	112.25
3	C	1354	NAG	O7-C7-N2	2.49	126.94	121.86
3	D	1353	NAG	O7-C7-N2	2.53	127.01	121.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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	0.45	0	15,19,21	1.10	1 (6%)
2	NAG	A	1354	1	14,14,15	0.73	1 (7%)	15,19,21	1.03	1 (6%)
2	NAG	A	1355	1	14,14,15	0.62	0	15,19,21	1.12	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1356	1	14,14,15	0.83	0	15,19,21	1.66	1 (6%)
5	QUE	A	1358	4	20,24,24	2.67	7 (35%)	27,36,36	1.52	4 (14%)
6	MPD	A	1359	-	6,7,7	0.48	0	7,10,10	2.07	3 (42%)
2	NAG	B	1351	1	14,14,15	0.56	0	15,19,21	0.77	0
2	NAG	B	1352	1	14,14,15	0.44	0	15,19,21	1.21	1 (6%)
2	NAG	B	1353	1	14,14,15	0.71	0	15,19,21	1.05	1 (6%)
2	NAG	B	1354	1	14,14,15	0.65	0	15,19,21	1.10	1 (6%)
5	QUE	B	1356	4	20,24,24	2.58	4 (20%)	27,36,36	1.48	6 (22%)
6	MPD	B	1357	-	6,7,7	0.38	0	7,10,10	2.15	1 (14%)
6	MPD	B	1358	-	6,7,7	0.43	0	7,10,10	1.73	2 (28%)
6	MPD	C	1351	-	6,7,7	0.46	0	7,10,10	2.30	3 (42%)
2	NAG	C	1352	1	14,14,15	0.37	0	15,19,21	1.31	2 (13%)
2	NAG	C	1355	1	14,14,15	0.71	1 (7%)	15,19,21	0.93	1 (6%)
2	NAG	C	1356	1	14,14,15	0.61	0	15,19,21	0.99	1 (6%)
5	QUE	C	1358	4	20,24,24	2.36	4 (20%)	27,36,36	1.58	5 (18%)
2	NAG	D	1351	1	14,14,15	0.43	0	15,19,21	1.22	3 (20%)
2	NAG	D	1354	1	14,14,15	0.82	1 (7%)	15,19,21	1.20	1 (6%)
2	NAG	D	1355	1	14,14,15	0.75	1 (7%)	15,19,21	0.83	0
5	QUE	D	1357	4	20,24,24	2.60	5 (25%)	27,36,36	1.66	5 (18%)

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
5	QUE	A	1358	4	-	0/4/4/4	0/3/3/3
6	MPD	A	1359	-	-	0/5/5/5	0/0/0/0
2	NAG	B	1351	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1352	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1354	1	-	0/6/23/26	0/1/1/1
5	QUE	B	1356	4	-	0/4/4/4	0/3/3/3
6	MPD	B	1357	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	B	1358	-	-	0/5/5/5	0/0/0/0
6	MPD	C	1351	-	-	0/5/5/5	0/0/0/0
2	NAG	C	1352	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1355	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1356	1	-	0/6/23/26	0/1/1/1
5	QUE	C	1358	4	-	0/4/4/4	0/3/3/3
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
5	QUE	D	1357	4	-	0/4/4/4	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1358	QUE	O29-C6	-2.07	1.32	1.37
2	D	1355	NAG	C1-C2	2.03	1.55	1.52
5	A	1358	QUE	C5-C6	2.08	1.41	1.37
2	A	1354	NAG	C1-C2	2.18	1.55	1.52
2	D	1354	NAG	C1-C2	2.20	1.55	1.52
2	C	1355	NAG	C1-C2	2.23	1.55	1.52
5	D	1357	QUE	C2-C3	2.71	1.48	1.43
5	C	1358	QUE	C14-C11	2.89	1.50	1.46
5	D	1357	QUE	C14-C11	2.91	1.50	1.46
5	A	1358	QUE	C2-C3	3.08	1.49	1.43
5	A	1358	QUE	C14-C11	3.08	1.50	1.46
5	B	1356	QUE	C14-C11	4.20	1.51	1.46
5	C	1358	QUE	C18-C17	4.29	1.47	1.40
5	B	1356	QUE	C18-C17	4.43	1.47	1.40
5	D	1357	QUE	C3-C4	4.94	1.47	1.41
5	A	1358	QUE	C18-C17	4.97	1.48	1.40
5	A	1358	QUE	C3-C4	5.07	1.47	1.41
5	B	1356	QUE	C3-C4	5.11	1.47	1.41
5	C	1358	QUE	C3-C4	5.51	1.48	1.41
5	C	1358	QUE	C9-C3	5.95	1.49	1.41
5	D	1357	QUE	C18-C17	6.08	1.50	1.40
5	D	1357	QUE	C9-C3	6.43	1.50	1.41
5	B	1356	QUE	C9-C3	6.88	1.50	1.41
5	A	1358	QUE	C9-C3	7.42	1.51	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1351	MPD	CM-C2-C1	-4.92	99.52	110.24
6	B	1357	MPD	CM-C2-C1	-4.64	100.12	110.24
6	A	1359	MPD	CM-C2-C1	-4.12	101.25	110.24
6	B	1358	MPD	CM-C2-C1	-3.29	103.07	110.24
5	D	1357	QUE	C14-C19-C18	-3.15	118.32	120.98
2	B	1354	NAG	C1-O5-C5	-3.11	108.30	112.25
5	B	1356	QUE	O12-C4-C3	-2.93	118.13	121.15
5	C	1358	QUE	C10-C9-C3	-2.88	117.09	121.25
2	C	1356	NAG	O4-C4-C3	-2.78	104.08	110.34
5	C	1358	QUE	O12-C4-C3	-2.73	118.33	121.15
5	D	1357	QUE	C10-C9-C3	-2.70	117.35	121.25
5	D	1357	QUE	O12-C4-C3	-2.63	118.44	121.15
5	A	1358	QUE	O12-C4-C3	-2.50	118.57	121.15
2	C	1355	NAG	C2-N2-C7	-2.47	119.86	123.04
5	C	1358	QUE	C1-C2-C3	-2.46	118.72	120.84
5	A	1358	QUE	C15-C16-C17	-2.36	118.07	120.49
2	D	1351	NAG	O7-C7-C8	-2.23	117.96	122.06
2	A	1351	NAG	O7-C7-C8	-2.19	118.05	122.06
2	A	1354	NAG	C2-N2-C7	-2.15	120.27	123.04
5	B	1356	QUE	C10-C9-C3	-2.09	118.23	121.25
2	A	1355	NAG	O7-C7-C8	-2.06	118.29	122.06
5	B	1356	QUE	C1-C2-C3	-2.05	119.07	120.84
2	B	1353	NAG	C2-N2-C7	-2.05	120.41	123.04
2	C	1352	NAG	O7-C7-C8	-2.02	118.36	122.06
2	D	1351	NAG	C2-N2-C7	2.09	125.73	123.04
6	A	1359	MPD	O2-C2-CM	2.11	115.84	108.09
5	B	1356	QUE	O23-C18-C19	2.21	125.36	119.42
2	D	1351	NAG	C1-O5-C5	2.23	115.08	112.25
6	A	1359	MPD	C2-C3-C4	2.33	127.66	116.66
6	C	1351	MPD	O2-C2-CM	2.34	116.68	108.09
6	C	1351	MPD	C2-C3-C4	2.36	127.83	116.66
6	B	1358	MPD	C2-C3-C4	2.50	128.47	116.66
5	A	1358	QUE	C14-C11-C10	3.01	125.75	120.04
5	C	1358	QUE	C14-C11-C10	3.04	125.80	120.04
5	D	1357	QUE	C14-C11-C10	3.08	125.88	120.04
5	B	1356	QUE	C14-C11-C10	3.16	126.03	120.04
2	C	1352	NAG	C2-N2-C7	3.38	127.38	123.04
5	B	1356	QUE	O12-C4-C5	3.59	120.76	116.18
2	B	1352	NAG	C1-O5-C5	3.92	117.22	112.25
2	D	1354	NAG	C1-O5-C5	3.94	117.25	112.25
5	C	1358	QUE	O12-C4-C5	4.21	121.54	116.18
5	A	1358	QUE	O12-C4-C5	4.67	122.13	116.18
5	D	1357	QUE	O12-C4-C5	4.74	122.22	116.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1356	NAG	C1-O5-C5	5.43	119.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1358	QUE	2	0
6	A	1359	MPD	3	0
5	B	1356	QUE	2	0
6	B	1357	MPD	4	0
6	B	1358	MPD	6	0
6	C	1351	MPD	3	0
5	C	1358	QUE	1	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, 95th 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 ²)	Q<0.9
1	A	344/350 (98%)	0.51	29 (8%) 14 16	7, 10, 18, 31	0
1	B	346/350 (98%)	0.55	37 (10%) 8 10	5, 10, 18, 41	0
1	C	343/350 (98%)	0.87	54 (15%) 3 4	6, 10, 18, 32	0
1	D	343/350 (98%)	0.73	47 (13%) 4 6	6, 10, 17, 34	0
All	All	1376/1400 (98%)	0.66	167 (12%) 6 8	5, 10, 18, 41	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	ILE	10.4
1	C	159	SER	8.4
1	C	160	SER	8.2
1	B	159	SER	7.9
1	D	159	SER	7.9
1	C	169	ILE	7.9
1	B	155	SER	7.1
1	D	160	SER	6.3
1	B	160	SER	6.2
1	B	3	SER	6.1
1	A	160	SER	6.0
1	C	181	LEU	5.9
1	B	156	SER	5.9
1	B	168	THR	5.9
1	D	169	ILE	5.6
1	C	168	THR	5.6
1	C	163	GLY	5.5
1	C	170	SER	5.4
1	C	289	ASP	5.3
1	C	165	ASP	5.2
1	C	197	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	167	SER	5.0
1	B	165	ASP	5.0
1	B	181	LEU	5.0
1	C	166	SER	4.8
1	D	262	THR	4.8
1	B	161	THR	4.7
1	B	170	SER	4.7
1	A	169	ILE	4.7
1	C	3	SER	4.7
1	A	90	ASN	4.7
1	C	164	PRO	4.7
1	B	166	SER	4.7
1	B	162	THR	4.6
1	D	4	SER	4.6
1	D	263	VAL	4.5
1	C	90	ASN	4.5
1	C	89	GLY	4.5
1	A	161	THR	4.4
1	C	4	SER	4.4
1	C	167	SER	4.4
1	D	181	LEU	4.3
1	B	187	THR	4.3
1	D	164	PRO	4.2
1	D	166	SER	4.2
1	B	164	PRO	4.2
1	C	162	THR	4.2
1	C	161	THR	4.2
1	B	163	GLY	4.1
1	D	289	ASP	4.0
1	D	168	THR	4.0
1	A	321	LEU	4.0
1	D	170	SER	3.9
1	B	278	VAL	3.8
1	C	321	LEU	3.8
1	D	77	CYS	3.8
1	B	321	LEU	3.7
1	C	171	THR	3.7
1	C	187	THR	3.7
1	D	264	THR	3.7
1	D	321	LEU	3.6
1	C	182	SER	3.6
1	C	178	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	350	TRP	3.6
1	C	210	THR	3.6
1	A	78[A]	ASN	3.5
1	A	168	THR	3.5
1	A	278	VAL	3.4
1	D	171	THR	3.4
1	D	182	SER	3.4
1	D	320	VAL	3.4
1	C	184	THR	3.3
1	B	64	LEU	3.3
1	B	154	SER	3.2
1	B	197	ASN	3.2
1	A	320	VAL	3.2
1	D	265	VAL	3.2
1	D	161	THR	3.2
1	D	154	SER	3.1
1	D	261	SER	3.1
1	D	162	THR	3.1
1	A	159	SER	3.1
1	A	167	SER	3.1
1	D	167	SER	3.1
1	A	154	SER	3.1
1	D	163	GLY	3.0
1	A	77	CYS	3.0
1	C	262	THR	3.0
1	B	76	TYR	3.0
1	B	182	SER	3.0
1	C	327	SER	3.0
1	A	76	TYR	2.9
1	C	278	VAL	2.9
1	D	230	TYR	2.9
1	A	181	LEU	2.9
1	B	320	VAL	2.9
1	D	278	VAL	2.9
1	B	171	THR	2.9
1	A	323	VAL	2.8
1	C	67	ILE	2.8
1	D	76	TYR	2.7
1	C	241	ALA	2.7
1	D	50	LEU	2.7
1	A	196	ALA	2.7
1	C	88	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	165	ASP	2.7
1	C	261	SER	2.7
1	D	90	ASN	2.6
1	D	78	ASN	2.6
1	A	254	ILE	2.5
1	B	101	GLY	2.5
1	D	290	TYR	2.5
1	C	230	TYR	2.5
1	A	166	SER	2.5
1	C	179	ALA	2.5
1	B	123[A]	MET	2.4
1	B	254	ILE	2.4
1	C	264	THR	2.4
1	C	185	PRO	2.4
1	C	172	LEU	2.4
1	D	183	PHE	2.4
1	C	350	TRP	2.4
1	B	196	ALA	2.4
1	A	124	THR	2.4
1	C	189	THR	2.4
1	D	53	THR	2.4
1	B	77	CYS	2.3
1	B	298	GLY	2.3
1	A	164	PRO	2.3
1	D	187	THR	2.3
1	D	338	GLY	2.3
1	C	77	CYS	2.3
1	C	183	PHE	2.3
1	C	174	SER	2.3
1	A	50	LEU	2.3
1	C	333	ASN	2.3
1	D	101	GLY	2.3
1	C	92	THR	2.2
1	D	287	ILE	2.2
1	B	100[A]	SER	2.2
1	D	89	GLY	2.2
1	C	173	GLN	2.2
1	C	50	LEU	2.2
1	D	328	ASP	2.1
1	A	187	THR	2.1
1	D	124	THR	2.1
1	A	261	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	298	GLY	2.1
1	A	38	TYR	2.1
1	B	124	THR	2.1
1	A	275	ALA	2.1
1	A	182	SER	2.1
1	D	229	GLN	2.1
1	C	109	ASN	2.1
1	C	91	GLU	2.1
1	A	100[A]	SER	2.1
1	D	231	GLY	2.1
1	C	64	LEU	2.1
1	C	328	ASP	2.1
1	C	124	THR	2.0
1	B	317	PHE	2.0
1	B	172	LEU	2.0
1	D	123	MET	2.0
1	C	126	VAL	2.0
1	D	288	GLY	2.0
1	B	50	LEU	2.0
1	C	279	GLN	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, 95th 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 ²)	Q<0.9
3	NAG	C	1354	14/15	0.75	0.22	2.76	34,44,47,50	0
3	NAG	A	1353	14/15	0.66	0.26	1.57	43,48,52,54	0
3	NAG	D	1353	14/15	0.80	0.20	0.87	36,42,45,46	0
3	NAG	C	1353	14/15	0.86	0.14	0.44	28,35,44,44	0
3	NAG	A	1352	14/15	0.86	0.12	-0.15	31,38,42,42	0
3	NAG	D	1352	14/15	0.82	0.11	-0.54	31,36,40,40	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, 95th 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 ²)	Q<0.9
6	MPD	B	1358	8/8	0.70	0.31	5.82	34,41,44,45	0
6	MPD	B	1357	8/8	0.86	0.24	4.24	26,36,40,41	0
6	MPD	A	1359	8/8	0.84	0.24	3.74	22,36,41,42	0
2	NAG	B	1353	14/15	0.84	0.18	3.71	26,35,45,48	0
6	MPD	C	1351	8/8	0.84	0.20	2.45	25,34,39,41	0
2	NAG	B	1352	14/15	0.83	0.19	1.78	36,44,49,49	0
2	NAG	A	1355	14/15	0.82	0.26	1.73	22,33,39,43	0
2	NAG	D	1351	14/15	0.82	0.21	1.26	39,44,50,50	0
2	NAG	A	1354	14/15	0.91	0.11	1.09	22,28,39,39	0
5	QUE	A	1358	22/22	0.87	0.16	0.78	15,21,25,27	0
2	NAG	C	1355	14/15	0.87	0.17	0.60	29,36,45,46	0
2	NAG	A	1356	14/15	0.73	0.22	0.55	27,35,40,43	0
2	NAG	D	1355	14/15	0.85	0.13	0.51	30,36,46,47	0
2	NAG	D	1354	14/15	0.87	0.15	0.22	26,30,38,39	0
5	QUE	B	1356	22/22	0.89	0.14	-0.09	17,21,25,28	0
5	QUE	D	1357	22/22	0.85	0.14	-0.10	16,20,23,26	0
5	QUE	C	1358	22/22	0.89	0.11	-0.33	14,18,22,25	0
4	CU	C	1357	1/1	0.97	0.10	-	17,17,17,17	1
4	CU	A	1357	1/1	0.99	0.06	-	19,19,19,19	1
2	NAG	B	1351	14/15	0.90	0.17	-	25,33,37,37	0
2	NAG	C	1352	14/15	0.90	0.16	-	29,36,43,45	0
2	NAG	C	1356	14/15	0.88	0.12	-	31,40,46,47	0
2	NAG	A	1351	14/15	0.88	0.21	-	26,31,38,39	0
2	NAG	B	1354	14/15	0.86	0.13	-	32,39,45,46	0
4	CU	D	1356	1/1	0.98	0.11	-	18,18,18,18	1
4	CU	B	1355	1/1	0.99	0.07	-	17,17,17,17	1

6.5 Other polymers ⓘ

There are no such residues in this entry.