



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:41 PM GMT

PDB ID : 1GQH
Title : QUERCETIN 2,3-DIOXYGENASE IN COMPLEX WITH THE INHIBITOR
KOJIC ACID
Authors : Steiner, R.A.; Dijkstra, B.W.
Deposited on : 2001-11-23
Resolution : 2.15 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

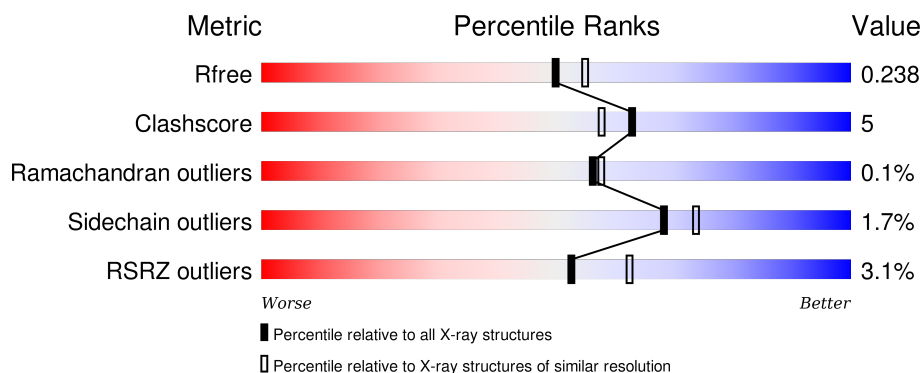
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>• •</div> </div>
1	B	350	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>• 5%</div> </div>
1	C	350	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
1	D	350	<div> <div>3%</div> <div>83%</div> <div>12%</div> <div>5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KOJ	B	1351	-	-	-	X
4	NAG	A	1357	-	-	-	X
4	NAG	B	1356	-	-	-	X
5	MAN	A	1361	X	-	-	-
6	MAN	B	1358	X	-	-	-
6	MAN	C	1359	X	-	-	-

2 Entry composition [i](#)

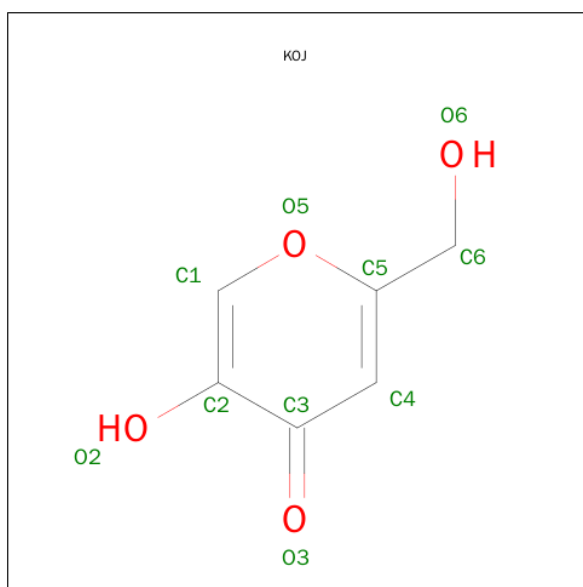
There are 8 unique types of molecules in this entry. The entry contains 11746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	341	Total	C	N	O	S	0	3	0
			2633	1671	428	529	5			
1	B	334	Total	C	N	O	S	0	0	0
			2581	1644	420	512	5			
1	C	333	Total	C	N	O	S	0	2	0
			2573	1636	419	513	5			
1	D	331	Total	C	N	O	S	0	0	0
			2561	1631	417	508	5			

- Molecule 2 is 5-HYDROXY-2-(HYDROXYMETHYL)-4H-PYRAN-4-ONE (three-letter code: KOJ) (formula: C₆H₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		

- 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: C₈H₁₅NO₆).



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	A	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		

- 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		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

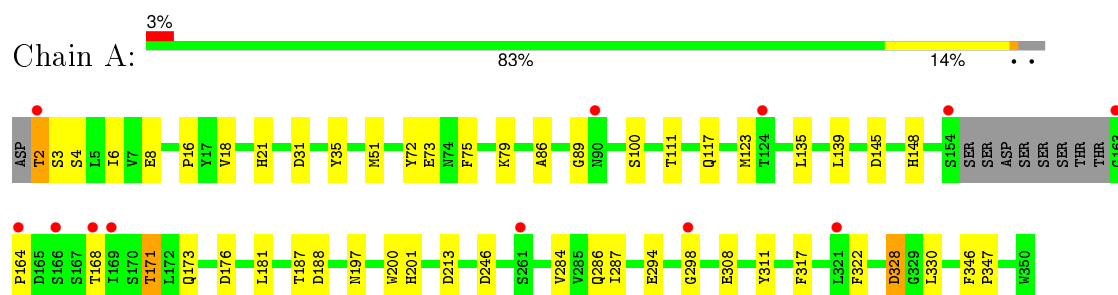
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	294	Total 294	O 294	0	0
8	B	251	Total 251	O 251	0	0
8	C	251	Total 251	O 251	0	0
8	D	223	Total 223	O 223	0	0

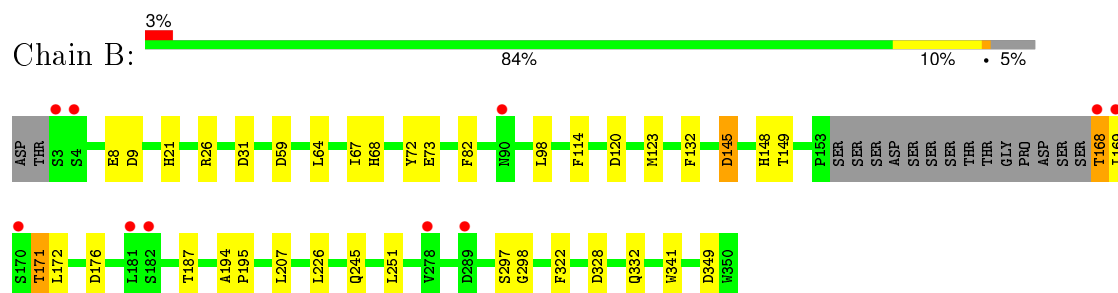
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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.

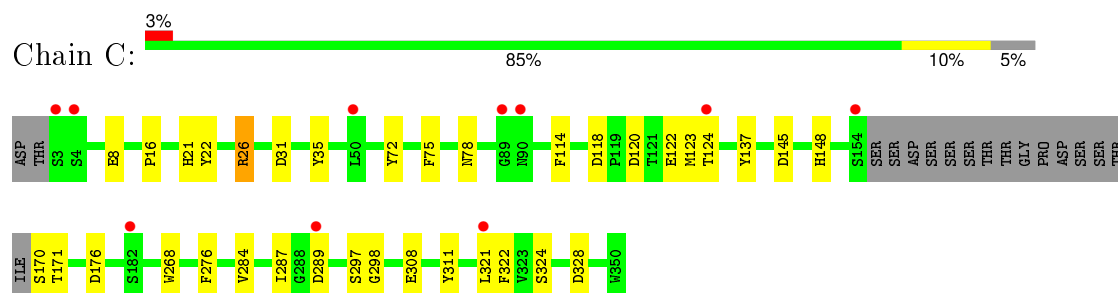
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE



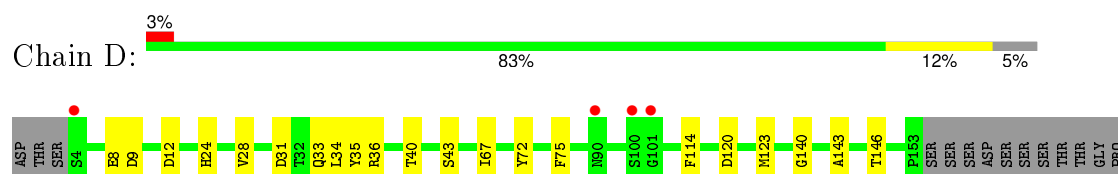
• Molecule 1: QUERCETIN 2,3-DIOXYGENASE

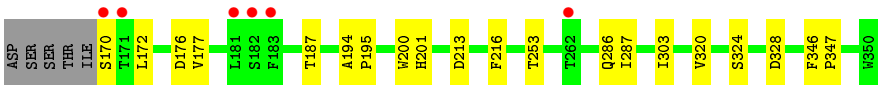


• Molecule 1: QUERCETIN 2,3-DIOXYGENASE



• 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	108.64Å 55.40Å 124.42Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	49.39 – 2.15 37.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	89.2 (49.39-2.15) 89.2 (37.95-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.178 , 0.228 0.195 , 0.238	Depositor DCC
R_{free} test set	3587 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	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 71715 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11746	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KOJ, NAG, 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	0.51	0/2728	0.79	6/3740 (0.2%)
1	B	0.49	0/2660	0.82	8/3647 (0.2%)
1	C	0.46	0/2662	0.79	7/3648 (0.2%)
1	D	0.48	0/2640	0.80	6/3619 (0.2%)
All	All	0.49	0/10690	0.80	27/14654 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	1	0
6	B	1	0
6	C	1	0
All	All	3	0

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	ASP	CB-CG-OD2	7.39	124.96	118.30
1	D	31	ASP	CB-CG-OD2	7.23	124.81	118.30
1	D	120	ASP	CB-CG-OD2	7.01	124.61	118.30
1	C	176	ASP	CB-CG-OD2	6.80	124.42	118.30
1	B	145	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	176	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	31	ASP	CB-CG-OD2	6.12	123.80	118.30
1	C	120	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	328	ASP	CB-CG-OD2	5.89	123.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	145	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	31	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	213	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	289	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	349	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	188	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	59	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	213	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	246	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	118	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	120	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	328	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	9	ASP	CB-CG-OD2	5.06	122.86	118.30
1	D	12	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	145	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	176	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	328	ASP	CB-CG-OD2	5.01	122.81	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1361	MAN	C1
6	B	1358	MAN	C1
6	C	1359	MAN	C1

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	2633	0	2432	39	0
1	B	2581	0	2392	25	0
1	C	2573	0	2380	20	0
1	D	2561	0	2373	27	0
2	A	10	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	4	3	0
2	C	10	0	4	3	0
2	D	10	0	4	1	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	56	0	52	0	0
4	B	42	0	39	0	0
4	C	42	0	39	0	0
4	D	28	0	26	0	0
5	A	39	0	34	0	0
6	B	50	0	43	2	0
6	C	50	0	43	0	0
7	D	28	0	25	0	0
8	A	294	0	0	10	0
8	B	251	0	0	10	0
8	C	251	0	0	3	0
8	D	223	0	0	4	0
All	All	11746	0	9894	110	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.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8[A]:GLU:OE2	1:A:148:HIS:HE1	1.44	0.99
1:A:8[A]:GLU:OE2	1:A:148:HIS:CE1	2.31	0.82
1:C:114:PHE:CE1	2:C:1351:KOJ:H4	2.15	0.81
1:B:245:GLN:HG2	8:B:2172:HOH:O	1.80	0.81
1:A:139:LEU:HD13	1:A:164:PRO:HG3	1.66	0.76
1:C:8:GLU:OE2	1:C:148:HIS:HE1	1.67	0.76
1:B:8:GLU:OE2	1:B:148:HIS:HE1	1.72	0.72
1:B:168:THR:O	1:B:172:LEU:HG	1.92	0.69
1:A:173:GLN:HG3	8:A:2143:HOH:O	1.92	0.69
1:A:8[B]:GLU:OE2	8:A:2006:HOH:O	2.10	0.68
1:B:332:GLN:NE2	8:B:2231:HOH:O	2.28	0.65
1:A:197:ASN:OD1	1:A:197:ASN:O	2.14	0.65
1:A:171:THR:HG23	8:A:2141:HOH:O	1.96	0.65
1:D:75:PHE:CD2	1:D:123:MET:HE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:CG2	1:A:171:THR:O	2.47	0.63
1:D:33:GLN:NE2	1:D:35:TYR:OH	2.34	0.61
1:A:308:GLU:HB2	8:A:2248:HOH:O	2.00	0.61
8:B:2013:HOH:O	1:C:171:THR:HG23	2.00	0.60
1:A:117:GLN:HG3	8:C:2156:HOH:O	2.02	0.60
1:B:168:THR:HA	1:B:171:THR:HG23	1.84	0.59
1:B:114:PHE:CE1	2:B:1351:KOJ:H4	2.37	0.59
1:D:28:VAL:HG21	1:D:140:GLY:HA3	1.84	0.59
1:D:75:PHE:HD2	1:D:123:MET:HE1	1.69	0.58
1:D:28:VAL:CG2	1:D:140:GLY:HA3	2.32	0.58
1:A:86:ALA:HA	1:A:111:THR:O	2.05	0.56
1:C:26:ARG:NH1	8:C:2025:HOH:O	2.38	0.56
1:D:24:HIS:HE1	1:D:143:ALA:O	1.89	0.55
1:D:287:ILE:HD13	1:D:303:ILE:HG13	1.88	0.55
1:D:75:PHE:HD2	1:D:123:MET:CE	2.21	0.53
8:B:2013:HOH:O	1:C:171:THR:CG2	2.55	0.53
1:A:294:GLU:HG2	8:A:2240:HOH:O	2.08	0.53
1:C:35:TYR:HE2	2:C:1351:KOJ:H6C2	1.74	0.53
1:D:40:THR:H	1:D:43:SER:HB3	1.75	0.52
1:B:8:GLU:HG2	8:B:2002:HOH:O	2.08	0.52
1:A:73:GLU:OE2	2:A:1351:KOJ:O2	2.28	0.51
1:D:8:GLU:HG2	8:D:2005:HOH:O	2.10	0.51
1:A:16:PRO:HB3	1:A:287:ILE:HG21	1.92	0.51
1:D:146:THR:HG22	8:D:2112:HOH:O	2.10	0.51
1:B:82:PHE:CE2	1:B:123:MET:HG2	2.45	0.51
1:A:197:ASN:C	1:A:197:ASN:OD1	2.49	0.50
1:A:2:THR:OG1	1:A:3:SER:N	2.40	0.50
1:B:73:GLU:OE2	2:B:1351:KOJ:C1	2.60	0.50
1:C:114:PHE:HE1	2:C:1351:KOJ:H4	1.75	0.50
1:C:26:ARG:HD2	8:C:2025:HOH:O	2.12	0.49
1:A:21:HIS:CG	1:A:298:GLY:HA3	2.47	0.49
1:A:328:ASP:HB2	8:A:2264:HOH:O	2.11	0.49
1:A:4:SER:HB3	8:A:2003:HOH:O	2.12	0.49
1:C:26:ARG:HD3	1:C:137:TYR:OH	2.13	0.49
1:B:73:GLU:OE2	2:B:1351:KOJ:C2	2.60	0.49
1:D:67:ILE:HD11	8:D:2084:HOH:O	2.12	0.48
1:C:78[A]:ASN:ND2	1:C:124:THR:OG1	2.45	0.48
1:C:8:GLU:OE2	1:C:148:HIS:CE1	2.58	0.48
1:D:9:ASP:OD1	1:D:24:HIS:HD2	1.96	0.48
1:A:35:TYR:HD2	1:A:51:MET:CE	2.27	0.47
1:D:114:PHE:CE2	2:D:1351:KOJ:H4	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG23	1:A:171:THR:O	2.14	0.46
1:D:172:LEU:HB2	1:D:177:VAL:HB	1.97	0.46
1:B:251:LEU:HD12	1:B:322:PHE:O	2.16	0.46
1:B:297:SER:HB2	8:B:2199:HOH:O	2.16	0.46
1:B:297:SER:HB3	8:B:2200:HOH:O	2.15	0.45
1:C:78[A]:ASN:HB2	1:C:122:GLU:HB3	1.99	0.45
1:C:21:HIS:CG	1:C:298:GLY:HA3	2.51	0.45
1:A:284:VAL:O	1:A:311:TYR:HA	2.16	0.45
1:D:216:PHE:CD1	1:D:216:PHE:N	2.85	0.45
1:B:21:HIS:CG	1:B:298:GLY:HA3	2.52	0.45
1:B:8:GLU:OE2	1:B:148:HIS:CE1	2.62	0.44
1:A:73:GLU:CD	2:A:1351:KOJ:O2	2.55	0.44
1:B:82:PHE:CD2	1:B:123:MET:HG2	2.53	0.44
1:D:346:PHE:HB2	1:D:347:PRO:HD2	1.99	0.44
1:D:253:THR:HA	1:D:320:VAL:O	2.17	0.44
6:B:1358:MAN:H62	1:D:187:THR:OG1	2.18	0.44
1:C:268:TRP:O	1:C:308:GLU:HA	2.19	0.43
1:A:317:PHE:HB3	1:C:22:TYR:CE2	2.53	0.43
1:A:346:PHE:HB2	1:A:347:PRO:CD	2.48	0.43
1:B:98:LEU:N	1:B:98:LEU:HD12	2.33	0.43
1:D:75:PHE:CE2	1:D:123:MET:HE1	2.54	0.43
1:A:187:THR:HG23	8:A:2154:HOH:O	2.18	0.43
1:D:200:TRP:O	1:D:201:HIS:HB2	2.18	0.43
1:D:346:PHE:HB2	1:D:347:PRO:CD	2.49	0.42
1:B:132:PHE:CB	8:B:2098:HOH:O	2.67	0.42
1:A:75:PHE:HD2	1:A:123:MET:HE2	1.83	0.42
1:C:322:PHE:CZ	1:C:324:SER:HB2	2.54	0.42
1:A:8[A]:GLU:HG2	8:A:2007:HOH:O	2.18	0.42
1:C:16:PRO:HB3	1:C:287:ILE:HG21	2.02	0.42
1:B:145:ASP:OD2	1:B:149:THR:O	2.37	0.42
1:A:168:THR:O	1:A:171:THR:HB	2.19	0.42
1:B:226:LEU:HB2	1:B:341:TRP:CG	2.54	0.42
1:B:67:ILE:CG2	1:B:68:HIS:N	2.82	0.42
1:D:40:THR:OG1	1:D:43:SER:HB2	2.20	0.42
1:C:75:PHE:HD2	1:C:123:MET:CE	2.33	0.42
1:D:286:GLN:HA	8:D:2178:HOH:O	2.19	0.42
1:A:322:PHE:CZ	1:A:330:LEU:HB3	2.55	0.42
1:C:284:VAL:O	1:C:311:TYR:HA	2.20	0.42
1:A:75:PHE:CD2	1:A:123:MET:HE2	2.54	0.41
1:A:79:LYS:HA	1:A:100[B]:SER:OG	2.20	0.41
1:D:34:LEU:HD22	1:D:36:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG22	1:A:171:THR:O	2.20	0.41
6:B:1358:MAN:H62	1:D:187:THR:HG21	2.02	0.41
1:A:346:PHE:HB2	1:A:347:PRO:HD2	2.01	0.41
1:D:194:ALA:HA	1:D:195:PRO:C	2.40	0.41
1:B:132:PHE:HB3	8:B:2098:HOH:O	2.20	0.41
1:B:187:THR:HG22	8:B:2131:HOH:O	2.21	0.41
1:B:207:LEU:N	1:B:207:LEU:HD12	2.36	0.41
1:A:286:GLN:NE2	8:A:2233:HOH:O	2.54	0.41
1:A:200:TRP:O	1:A:201:HIS:HB2	2.20	0.41
1:C:276:PHE:HA	1:C:321:LEU:O	2.21	0.40
1:A:75:PHE:HD2	1:A:123:MET:CE	2.34	0.40
1:A:6:ILE:HA	1:A:18:VAL:O	2.21	0.40
1:B:194:ALA:HA	1:B:195:PRO:C	2.41	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	340/350 (97%)	329 (97%)	10 (3%)	1 (0%)	46	42
1	B	330/350 (94%)	319 (97%)	11 (3%)	0	100	100
1	C	331/350 (95%)	318 (96%)	13 (4%)	0	100	100
1	D	327/350 (93%)	320 (98%)	7 (2%)	0	100	100
All	All	1328/1400 (95%)	1286 (97%)	41 (3%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	GLY

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	287/294 (98%)	281 (98%)	6 (2%)	61	65
1	B	278/294 (95%)	272 (98%)	6 (2%)	60	63
1	C	279/294 (95%)	275 (99%)	4 (1%)	74	80
1	D	276/294 (94%)	273 (99%)	3 (1%)	80	85
All	All	1120/1176 (95%)	1101 (98%)	19 (2%)	68	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	72	TYR
1	A	135	LEU
1	A	171	THR
1	A	181	LEU
1	A	328	ASP
1	B	26	ARG
1	B	64	LEU
1	B	72	TYR
1	B	168	THR
1	B	169	ILE
1	B	171	THR
1	C	26	ARG
1	C	72	TYR
1	C	170	SER
1	C	297	SER
1	D	72	TYR
1	D	170	SER
1	D	324	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	117	GLN
1	A	148	HIS
1	A	173	GLN
1	A	332	GLN
1	A	336	ASN
1	B	83	GLN
1	B	148	HIS
1	B	286	GLN
1	B	332	GLN
1	C	83	GLN
1	C	148	HIS
1	D	24	HIS
1	D	33	GLN
1	D	83	GLN
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 ⓘ

13 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	5	14,14,15	0.61	0	15,19,21	0.77	0
5	NAG	A	1355	1,5	14,14,15	0.53	0	15,19,21	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	A	1361	5	11,11,12	0.78	0	14,15,17	0.88	0
6	NAG	B	1354	1,6	14,14,15	0.72	0	15,19,21	1.00	0
6	NAG	B	1355	6	14,14,15	0.74	0	15,19,21	0.74	0
6	MAN	B	1358	6	11,11,12	0.60	0	14,15,17	1.09	1 (7%)
6	MAN	B	1359	6	11,11,12	0.53	0	14,15,17	1.13	1 (7%)
6	NAG	C	1355	1,6	14,14,15	0.67	0	15,19,21	0.87	1 (6%)
6	NAG	C	1356	6	14,14,15	0.52	0	15,19,21	1.00	0
6	MAN	C	1359	6	11,11,12	0.72	0	14,15,17	1.29	2 (14%)
6	MAN	C	1360	6	11,11,12	0.64	0	14,15,17	1.28	3 (21%)
7	NAG	D	1354	1,7	14,14,15	0.51	0	15,19,21	0.80	0
7	NAG	D	1355	7	14,14,15	0.57	0	15,19,21	1.40	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	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1355	1,5	-	0/6/23/26	0/1/1/1
5	MAN	A	1361	5	1/1/4/5	0/2/19/22	0/1/1/1
6	NAG	B	1354	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1355	6	-	0/6/23/26	0/1/1/1
6	MAN	B	1358	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	B	1359	6	-	0/2/19/22	0/1/1/1
6	NAG	C	1355	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1356	6	-	0/6/23/26	0/1/1/1
6	MAN	C	1359	6	1/1/4/5	0/2/19/22	0/1/1/1
6	MAN	C	1360	6	-	0/2/19/22	0/1/1/1
7	NAG	D	1354	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	1355	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1355	NAG	C2-N2-C7	-2.29	120.10	123.04
6	B	1359	MAN	C3-C4-C5	-2.25	106.27	110.20
6	C	1360	MAN	C1-C2-C3	-2.02	107.15	109.54
6	C	1355	NAG	C1-O5-C5	2.03	114.82	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1358	MAN	O5-C5-C6	2.13	111.96	107.35
6	C	1359	MAN	C3-C4-C5	2.20	114.03	110.20
6	C	1360	MAN	O3-C3-C2	2.25	114.07	110.00
5	A	1355	NAG	C1-O5-C5	2.39	115.28	112.25
6	C	1359	MAN	C1-C2-C3	2.59	112.60	109.54
6	C	1360	MAN	O5-C5-C6	2.76	113.33	107.35
7	D	1355	NAG	C1-O5-C5	4.48	117.93	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1361	MAN	C1
6	C	1359	MAN	C1
6	B	1358	MAN	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1358	MAN	2	0

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	KOJ	A	1351	3	6,10,10	3.67	2 (33%)	4,13,13	1.52	1 (25%)
4	NAG	A	1353	1	14,14,15	0.71	0	15,19,21	1.21	1 (6%)
4	NAG	A	1356	1	14,14,15	0.60	0	15,19,21	1.37	2 (13%)
4	NAG	A	1357	1	14,14,15	0.62	0	15,19,21	1.45	2 (13%)
4	NAG	A	1358	1	14,14,15	0.46	0	15,19,21	1.39	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KOJ	B	1351	3	6,10,10	3.47	2 (33%)	4,13,13	2.13	1 (25%)
4	NAG	B	1353	1	14,14,15	0.62	0	15,19,21	0.85	0
4	NAG	B	1356	1	14,14,15	0.66	0	15,19,21	1.41	3 (20%)
4	NAG	B	1357	1	14,14,15	0.61	0	15,19,21	0.87	0
2	KOJ	C	1351	3	6,10,10	3.42	2 (33%)	4,13,13	1.76	1 (25%)
4	NAG	C	1354	1	14,14,15	0.63	0	15,19,21	1.22	2 (13%)
4	NAG	C	1357	1	14,14,15	0.72	0	15,19,21	0.97	1 (6%)
4	NAG	C	1358	1	14,14,15	0.61	0	15,19,21	1.97	4 (26%)
2	KOJ	D	1351	3	6,10,10	3.86	2 (33%)	4,13,13	1.19	0
4	NAG	D	1353	1	14,14,15	0.50	0	15,19,21	1.27	2 (13%)
4	NAG	D	1356	1	14,14,15	0.59	0	15,19,21	1.12	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
2	KOJ	A	1351	3	-	0/1/2/2	0/1/1/1
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
4	NAG	A	1358	1	-	0/6/23/26	0/1/1/1
2	KOJ	B	1351	3	-	0/1/2/2	0/1/1/1
4	NAG	B	1353	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1356	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1357	1	-	0/6/23/26	0/1/1/1
2	KOJ	C	1351	3	-	0/1/2/2	0/1/1/1
4	NAG	C	1354	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1357	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1358	1	-	0/6/23/26	0/1/1/1
2	KOJ	D	1351	3	-	0/1/2/2	0/1/1/1
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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1351	KOJ	O5-C5	-8.67	1.24	1.35
2	A	1351	KOJ	O5-C5	-8.23	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1351	KOJ	O5-C5	-7.58	1.25	1.35
2	C	1351	KOJ	O5-C5	-7.37	1.26	1.35
2	A	1351	KOJ	C4-C5	2.50	1.39	1.35
2	D	1351	KOJ	C4-C5	2.67	1.39	1.35
2	C	1351	KOJ	C4-C5	3.01	1.40	1.35
2	B	1351	KOJ	C4-C5	3.11	1.40	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1358	NAG	C2-N2-C7	-4.64	117.08	123.04
4	C	1358	NAG	C1-O5-C5	-4.15	106.98	112.25
4	A	1353	NAG	C2-N2-C7	-3.51	118.53	123.04
4	B	1356	NAG	C2-N2-C7	-3.08	119.08	123.04
4	A	1356	NAG	C2-N2-C7	-2.64	119.65	123.04
4	D	1356	NAG	C2-N2-C7	-2.60	119.70	123.04
4	C	1354	NAG	C3-C4-C5	-2.53	105.78	110.20
4	C	1357	NAG	C2-N2-C7	-2.28	120.11	123.04
4	D	1353	NAG	C2-N2-C7	-2.18	120.23	123.04
4	A	1358	NAG	O7-C7-C8	-2.17	118.07	122.06
4	B	1356	NAG	C4-C3-C2	-2.06	108.03	111.23
4	D	1356	NAG	C1-O5-C5	2.32	115.20	112.25
4	C	1358	NAG	O5-C5-C6	2.50	112.76	107.35
4	A	1358	NAG	C2-N2-C7	2.52	126.28	123.04
4	D	1353	NAG	C1-O5-C5	2.59	115.53	112.25
4	C	1354	NAG	O5-C5-C6	2.61	113.00	107.35
4	A	1357	NAG	C3-C4-C5	2.66	114.83	110.20
4	C	1358	NAG	C4-C3-C2	2.80	115.59	111.23
2	A	1351	KOJ	O6-C6-C5	2.93	118.69	112.37
4	B	1356	NAG	C1-O5-C5	3.06	116.13	112.25
2	C	1351	KOJ	O6-C6-C5	3.13	119.13	112.37
4	A	1356	NAG	C1-O5-C5	3.27	116.40	112.25
4	A	1357	NAG	C1-O5-C5	3.31	116.45	112.25
2	B	1351	KOJ	O6-C6-C5	4.26	121.57	112.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1351	KOJ	2	0
2	B	1351	KOJ	3	0
2	C	1351	KOJ	3	0
2	D	1351	KOJ	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(Å²)	Q<0.9
1	A	341/350 (97%)	-0.07	12 (3%)	48	58	6, 11, 17, 25	0
1	B	334/350 (95%)	-0.14	10 (2%)	54	64	6, 11, 16, 26	0
1	C	333/350 (95%)	-0.03	10 (3%)	54	64	7, 11, 16, 24	0
1	D	331/350 (94%)	-0.02	10 (3%)	54	64	7, 11, 16, 24	0
All	All	1339/1400 (95%)	-0.07	42 (3%)	52	62	6, 11, 16, 26	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	SER	4.8
1	B	3	SER	4.7
1	D	181	LEU	4.1
1	A	90	ASN	4.0
1	D	182	SER	3.6
1	B	170	SER	3.3
1	C	4	SER	3.1
1	A	169	ILE	3.1
1	B	181	LEU	3.0
1	A	154	SER	2.8
1	D	170	SER	2.8
1	A	168	THR	2.8
1	B	168	THR	2.6
1	D	90	ASN	2.6
1	C	89	GLY	2.6
1	B	169	ILE	2.5
1	C	90	ASN	2.5
1	D	171	THR	2.5
1	D	262	THR	2.5
1	A	321	LEU	2.4
1	A	163	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	4	SER	2.3
1	D	183	PHE	2.3
1	B	4	SER	2.3
1	C	289	ASP	2.3
1	B	289	ASP	2.3
1	C	50	LEU	2.3
1	C	321	LEU	2.3
1	C	182	SER	2.2
1	D	100	SER	2.2
1	A	164	PRO	2.2
1	A	261	SER	2.2
1	C	3	SER	2.2
1	A	2	THR	2.2
1	B	278	VAL	2.2
1	A	166	SER	2.1
1	B	90	ASN	2.1
1	A	298	GLY	2.1
1	D	101	GLY	2.1
1	A	124	THR	2.1
1	B	182	SER	2.1
1	C	124	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, 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(\AA^2)	Q<0.9
5	NAG	A	1354	14/15	0.89	0.13	1.17	26,30,35,35	0
6	NAG	C	1356	14/15	0.94	0.12	0.68	25,30,34,34	0
7	NAG	D	1355	14/15	0.87	0.13	0.63	24,30,34,35	0
6	NAG	B	1355	14/15	0.90	0.13	0.00	27,35,38,41	0
6	NAG	B	1354	14/15	0.94	0.12	-0.26	24,29,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	1355	14/15	0.95	0.09	-0.39	22,26,27,29	0
7	NAG	D	1354	14/15	0.96	0.10	-0.77	22,26,29,30	0
6	NAG	C	1355	14/15	0.96	0.08	-0.83	23,26,32,33	0
5	MAN	A	1361	11/12	0.91	0.13	-	37,40,41,43	0
6	MAN	B	1358	11/12	0.86	0.24	-	43,45,47,50	0
6	MAN	C	1359	11/12	0.89	0.19	-	37,40,42,43	0
6	MAN	C	1360	11/12	0.72	0.27	-	41,42,44,44	0
6	MAN	B	1359	11/12	0.84	0.24	-	46,48,50,50	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(\AA^2)	Q<0.9
4	NAG	B	1356	14/15	0.83	0.28	4.80	29,35,40,41	0
2	KOJ	B	1351	10/10	0.95	0.18	2.70	29,30,31,32	0
4	NAG	A	1357	14/15	0.83	0.19	2.52	30,34,37,38	0
4	NAG	A	1358	14/15	0.80	0.31	1.84	31,37,40,40	0
4	NAG	A	1356	14/15	0.90	0.14	1.76	25,31,37,38	0
2	KOJ	C	1351	10/10	0.93	0.16	1.74	30,30,32,32	0
2	KOJ	D	1351	10/10	0.95	0.15	1.45	25,28,32,34	0
4	NAG	D	1356	14/15	0.94	0.15	1.38	30,34,41,42	0
4	NAG	C	1357	14/15	0.91	0.16	1.13	31,35,41,41	0
4	NAG	D	1353	14/15	0.89	0.16	0.59	31,36,39,39	0
2	KOJ	A	1351	10/10	0.93	0.13	0.24	21,24,26,27	0
3	CU	D	1352	1/1	1.00	0.01	-	12,12,12,12	0
3	CU	B	1352	1/1	1.00	0.03	-	14,14,14,14	0
3	CU	A	1352	1/1	1.00	0.04	-	12,12,12,12	0
4	NAG	A	1353	14/15	0.93	0.13	-	24,27,30,34	0
4	NAG	C	1358	14/15	0.78	0.21	-	36,43,45,46	0
4	NAG	B	1357	14/15	0.90	0.16	-	33,39,41,41	0
3	CU	C	1352	1/1	0.99	0.02	-	13,13,13,13	0
4	NAG	C	1354	14/15	0.90	0.15	-	30,35,40,40	0
4	NAG	B	1353	14/15	0.91	0.13	-	25,29,32,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.