Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 – 04:24 am GMT

PDB ID	:	2WL9
Title	:	Crystal structure of catechol 2,3-dioxygenase
Authors	:	Cho, H.J.; Kim, K.J.; Kang, B.S.
Deposited on	:	2009-06-23
Resolution	:	1.90 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

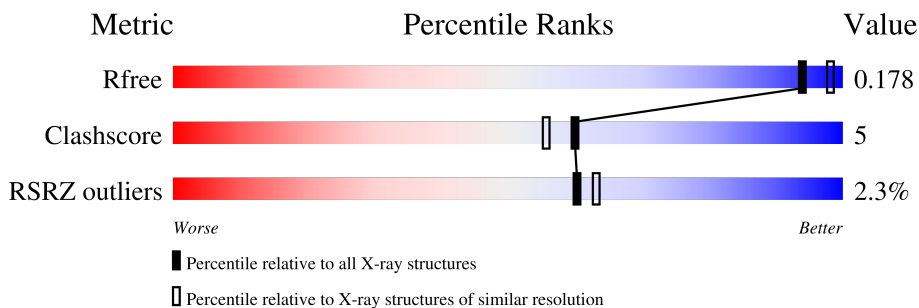|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
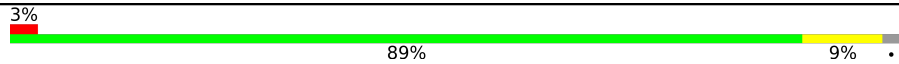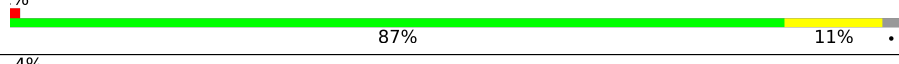*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.178
Clashscore		5
RSRZ outliers		2.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
RSRZ outliers	127900	6082 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	305	3% 89% 9% •
1	B	305	% 84% 12% •
1	C	305	% 87% 11% •
1	D	305	4% 85% 11% •

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
5	MBD	B	1301	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9772 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 CATECHOL 2,3-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	5	0
			2383	1509	415	449	10			
1	B	293	Total	C	N	O	S	0	4	0
			2346	1487	413	437	9			
1	C	299	Total	C	N	O	S	0	3	0
			2364	1497	413	444	10			
1	D	294	Total	C	N	O	S	0	4	0
			2336	1480	406	441	9			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0

- Molecule 5 is 3-METHYLCATECHOL (three-letter code: MBD) (formula: $C_7H_8O_2$).

MBD
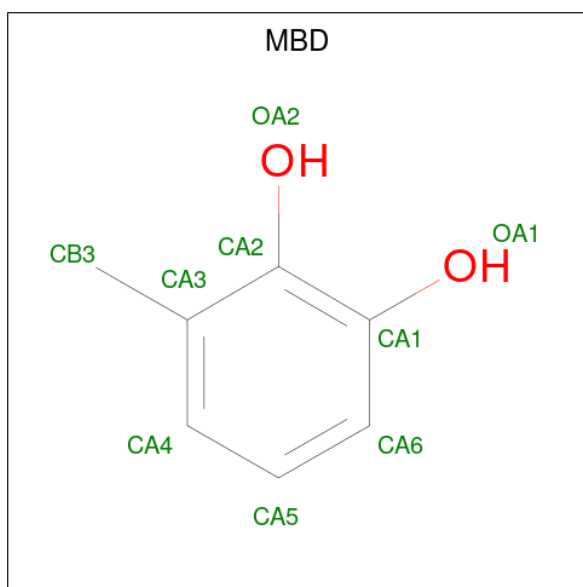
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 9	C 7	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 9	C 7	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total 89	O 89	0	0
6	B	77	Total 77	O 77	0	0
6	C	69	Total 69	O 69	0	0
6	D	67	Total 67	O 67	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 a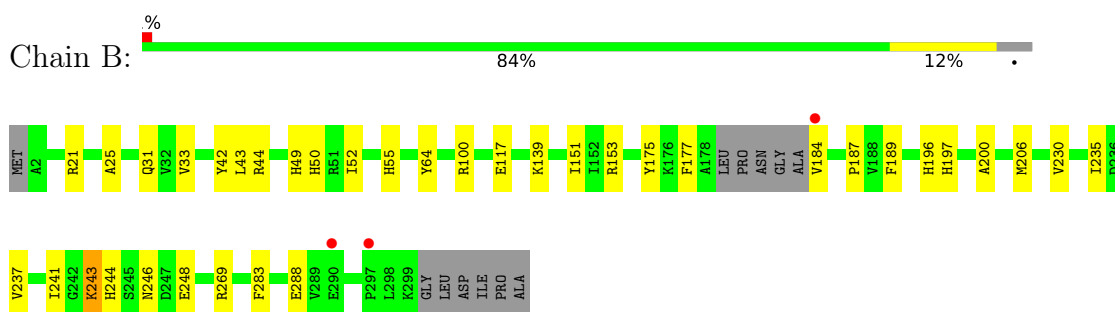re color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CATECHOL 2,3-DIOXYGENASE
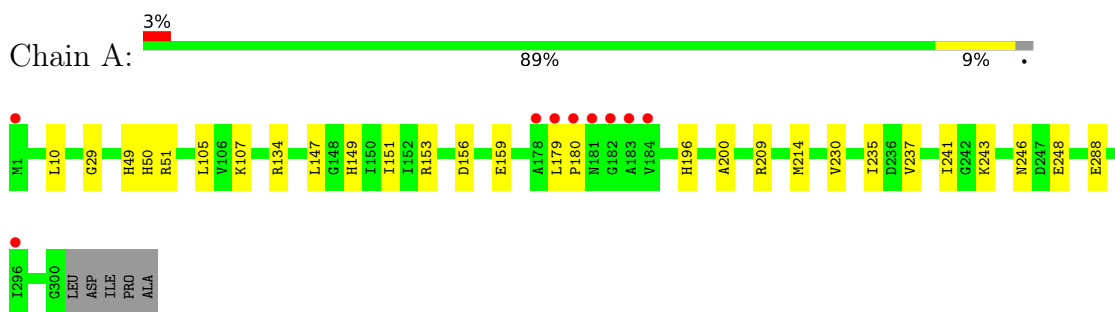
• Molecule 1: CATECHOL 2,3-DIOXYGENASE

• Molecule 1: CATECHOL 2,3-DIOXYGENASE

• Molecule 1: CATECHOL 2,3-DIOXYGENASE

MET A2 S13 R21 A25 V32 D35 G36 L43 H49 H50 R51 I52 D57 G58 S59 D76 E77 L78 L105 V106 K107 H149 I150 I151 I152 R153 L167 E174 Y175 K176 F177 ALA LEU PRO ASN GLY A183 V184 R195 H196 H197 A200 V203

M206 M214 V237 T238 K243 E248 L261 Q275 D281 H285 E288 V289 E290 D295 I296 P297 G300 LEU ASP ILE PRO ALA
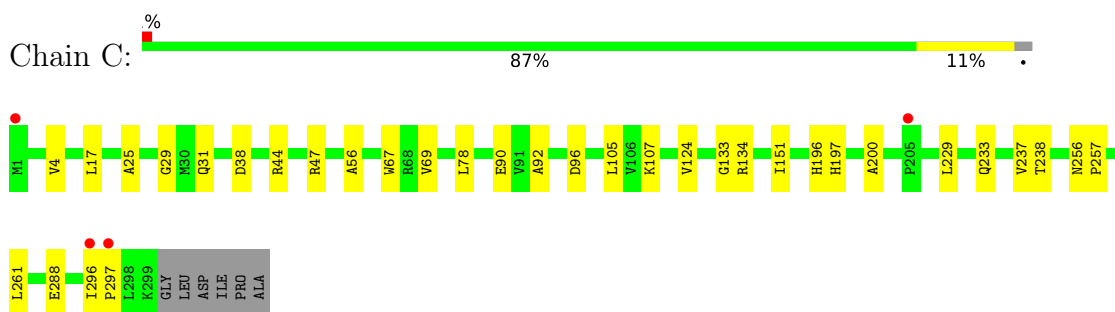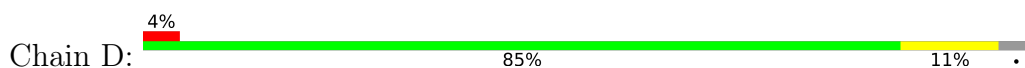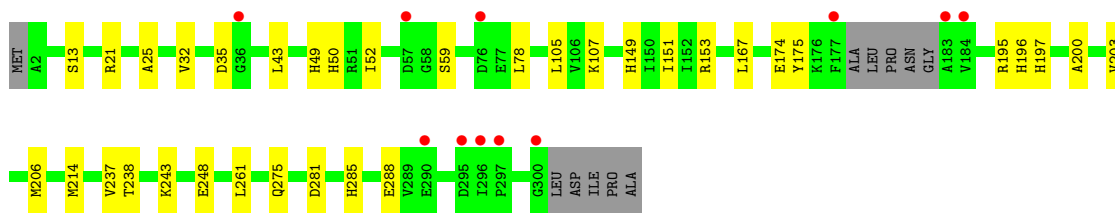
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α, β, γ	102.56Å 102.56Å 142.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	142.17 – 1.90 35.14 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (142.17-1.90) 99.7 (35.14-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.151 , 0.176 0.154 , 0.178	Depositor DCC
R_{free} test set	5775 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
Reported twinning fraction	0.508 for H, K, L 0.492 for K, H, -L	Depositor
Outliers	0 of 115161 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9772	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MBD, MG, GOL, FE

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	0.42	0/2463	0.60	1/3346 (0.0%)
1	B	0.52	1/2421 (0.0%)	0.56	0/3285
1	C	0.48	0/2438	0.60	0/3314
1	D	0.47	0/2411	0.57	0/3273
All	All	0.47	1/9733 (0.0%)	0.58	1/13218 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	LYS	CE-NZ	-5.53	1.35	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	2383	0	2262	17	0
1	B	2346	0	2234	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2364	0	2238	23	0
1	D	2336	0	2214	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
4	A	12	0	16	2	0
4	D	6	0	8	0	0
5	B	9	0	6	4	0
5	D	9	0	6	1	0
6	A	89	0	0	0	0
6	B	77	0	0	1	0
6	C	69	0	0	0	0
6	D	67	0	0	0	0
All	All	9772	0	8984	84	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 (84) 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:D:149:HIS:CE1	1:D:214:MET:HG2	2.04	0.92
1:C:196:HIS:HD2	1:C:197:HIS:HD2	1.08	0.91
1:A:149:HIS:CE1	1:A:214:MET:HG2	2.10	0.86
1:C:196:HIS:HD2	1:C:197:HIS:CD2	1.96	0.80
1:B:139:LYS:HG2	6:B:2011:HOH:O	1.78	0.80
1:C:196:HIS:CD2	1:C:197:HIS:HD2	1.99	0.74
1:D:151:ILE:HG12	1:D:200:ALA:HB3	1.70	0.72
1:A:49:HIS:HD2	1:A:50:HIS:ND1	1.93	0.66
1:D:175:TYR:CE2	5:D:1303:MBD:HA6	2.32	0.65
1:C:151:ILE:HG12	1:C:200:ALA:HB3	1.79	0.65
1:B:151:ILE:HG12	1:B:200:ALA:HB3	1.80	0.63
1:A:151:ILE:HG12	1:A:200:ALA:HB3	1.80	0.63
1:A:243:LYS:HE3	1:A:248:GLU:O	1.98	0.63
1:C:17:LEU:HD22	1:C:56:ALA:HB2	1.81	0.62
1:D:196:HIS:ND1	1:D:197:HIS:HD2	1.97	0.62
1:B:243:LYS:HE3	1:B:248:GLU:O	1.99	0.62
1:B:246:ASN:OD1	5:B:1301:MBD:HA6	2.01	0.60
1:B:49:HIS:HD2	1:B:50:HIS:ND1	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1304:GOL:H2	1:B:241:ILE:HG13	1.84	0.58
1:C:238:THR:HG21	1:C:261:LEU:HD21	1.85	0.58
1:C:69:VAL:HG11	1:C:78:LEU:HD12	1.86	0.58
1:A:241:ILE:HG13	4:A:1303:GOL:H2	1.87	0.56
1:C:4:VAL:HG11	1:C:67:TRP:HB3	1.87	0.56
1:C:4:VAL:CG1	1:C:67:TRP:HB3	2.36	0.55
1:D:49:HIS:HD2	1:D:50:HIS:ND1	2.03	0.55
1:C:92:ALA:HB1	1:C:96:ASP:HB2	1.88	0.55
1:A:153[A]:ARG:CZ	1:C:90:GLU:HG3	2.38	0.54
1:B:237:VAL:O	1:B:288:GLU:HB3	2.06	0.54
1:A:153[A]:ARG:NH2	1:C:90:GLU:HG3	2.23	0.53
1:D:13[A]:SER:OG	1:D:59:SER:HB3	2.09	0.52
1:A:179:LEU:HB3	1:A:180:PRO:HD2	1.92	0.52
1:B:196:HIS:ND1	1:B:197:HIS:HD2	2.09	0.51
1:C:237:VAL:O	1:C:288:GLU:HB3	2.11	0.50
1:D:238:THR:HG21	1:D:261:LEU:HD21	1.94	0.50
1:C:105:LEU:HD21	1:C:107:LYS:HE3	1.94	0.50
1:B:55:HIS:HE1	1:B:64:TYR:OH	1.95	0.49
1:C:38:ASP:OD1	1:C:38:ASP:N	2.44	0.48
1:A:149:HIS:CE1	1:A:214:MET:CG	2.92	0.48
1:B:153:ARG:HA	1:B:206:MET:CE	2.44	0.48
1:B:33:VAL:HB	1:B:42:TYR:HB2	1.94	0.47
1:D:174:GLU:HG2	1:D:275:GLN:HE22	1.79	0.47
1:D:43:LEU:HB2	1:D:52:ILE:HB	1.97	0.47
1:A:156:ASP:HB3	1:A:159:GLU:HB2	1.97	0.46
1:C:29:GLY:HA2	1:C:134:ARG:HG3	1.97	0.46
1:A:10:LEU:HG	1:A:147:LEU:HD21	1.97	0.46
1:D:151:ILE:HD13	1:D:203:VAL:HG11	1.98	0.46
1:D:149:HIS:HB3	1:D:197:HIS:O	2.16	0.46
1:D:105:LEU:HD21	1:D:107:LYS:HE3	1.96	0.46
1:C:256:ASN:HB2	1:C:257:PRO:CD	2.46	0.46
1:A:153[A]:ARG:NH2	1:A:209:ARG:HG2	2.32	0.45
1:A:237:VAL:O	1:A:288:GLU:HB3	2.17	0.45
1:A:230:VAL:HG13	1:A:235:ILE:HB	1.99	0.45
1:D:237:VAL:O	1:D:288:GLU:HB3	2.17	0.44
1:B:243:LYS:HD2	1:B:283:PHE:CE1	2.52	0.44
1:D:153:ARG:HA	1:D:206:MET:CE	2.47	0.44
1:B:31:GLN:HB3	1:B:44:ARG:HB3	1.99	0.43
1:C:92:ALA:HB1	1:C:96:ASP:CB	2.49	0.43
1:D:149:HIS:CE1	1:D:214:MET:CG	2.91	0.43
1:A:29:GLY:HA2	1:A:134:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TYR:CZ	5:B:1301:MBD:HA5	2.54	0.43
1:B:43:LEU:HB2	1:B:52:ILE:HB	2.01	0.43
1:B:175:TYR:CE2	5:B:1301:MBD:HA5	2.53	0.42
1:C:31:GLN:HB3	1:C:44:ARG:HB3	2.00	0.42
1:D:35:ASP:OD2	1:D:49:HIS:CE1	2.72	0.42
1:D:25:ALA:HB2	1:D:32:VAL:HG23	2.01	0.42
1:B:244:HIS:CG	5:B:1301:MBD:CA6	3.03	0.42
1:D:78:LEU:HD11	1:D:167:LEU:HA	2.02	0.42
1:D:243:LYS:HE2	1:D:248:GLU:O	2.19	0.42
1:C:296:ILE:HD12	1:C:297:PRO:HD2	2.02	0.42
1:D:21:ARG:HD3	1:D:32:VAL:HG11	2.03	0.41
1:A:196:HIS:CE1	1:A:246:ASN:HB2	2.56	0.41
1:B:230:VAL:HG13	1:B:235:ILE:HB	2.02	0.41
1:C:229:LEU:HD22	1:C:233:GLN:HE21	1.86	0.41
1:B:100:ARG:HD2	1:B:117:GLU:OE1	2.20	0.41
1:B:21:ARG:O	1:B:25:ALA:HB3	2.20	0.41
1:D:195:ARG:O	1:D:196:HIS:C	2.59	0.41
1:B:196:HIS:HB2	1:B:269:ARG:O	2.21	0.40
1:D:281:ASP:OD2	1:D:285:HIS:HD2	2.04	0.40
1:A:105:LEU:HD21	1:A:107:LYS:HE3	2.02	0.40
1:B:187:PRO:HB2	1:B:189:PHE:CE2	2.56	0.40
1:B:177:PHE:O	1:B:184:VAL:HG23	2.21	0.40
1:C:25:ALA:HB1	1:C:133:GLY:HA3	2.03	0.40
1:D:35:ASP:OD2	1:D:49:HIS:HE1	2.05	0.40
1:C:47:ARG:HB3	1:C:124:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	$\#|Z| > 2$
4	GOL	A	1303	-	5,5,5	0.33	0	5,5,5	0.38	0
4	GOL	D	1302	-	5,5,5	0.39	0	5,5,5	0.19	0
5	MBD	D	1303	2	9,9,9	2.39	3 (33%)	12,12,12	1.19	1 (8%)
4	GOL	A	1304	-	5,5,5	0.33	0	5,5,5	0.51	0
5	MBD	B	1301	2	9,9,9	2.51	1 (11%)	12,12,12	1.32	2 (16%)

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
4	GOL	A	1303	-	-	0/4/4/4	-
4	GOL	D	1302	-	-	0/4/4/4	-
5	MBD	D	1303	2	-	-	0/1/1/1
4	GOL	A	1304	-	-	2/4/4/4	-
5	MBD	B	1301	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1301	MBD	CA1-CA2	7.52	1.49	1.40
5	D	1303	MBD	CA1-CA2	4.13	1.44	1.40
5	D	1303	MBD	CA2-CA3	-4.13	1.34	1.40
5	D	1303	MBD	OA2-CA2	-2.13	1.32	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1301	MBD	CA4-CA3-CA2	2.62	120.31	117.82
5	D	1303	MBD	CA4-CA3-CA2	2.54	120.22	117.82
5	B	1301	MBD	CA1-CA2-CA3	-2.43	118.96	121.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1304	GOL	C1-C2-C3-O3
4	A	1304	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1303	GOL	1	0
5	D	1303	MBD	1	0
4	A	1304	GOL	1	0
5	B	1301	MBD	4	0

5.7 Other polymers ⓘ

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 ⓘ

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	300/305 (98%)	-0.07	9 (3%)	50	53	14, 20, 32, 45	0
1	B	293/305 (96%)	-0.17	3 (1%)	82	84	15, 21, 33, 44	0
1	C	299/305 (98%)	-0.13	4 (1%)	77	79	15, 21, 33, 47	0
1	D	294/305 (96%)	0.05	11 (3%)	41	44	16, 23, 35, 44	0
All	All	1186/1220 (97%)	-0.08	27 (2%)	60	63	14, 21, 34, 47	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	GLY	5.2
1	A	180	PRO	5.1
1	C	296	ILE	4.9
1	D	183	ALA	4.7
1	A	179	LEU	4.3
1	D	297	PRO	3.7
1	A	183	ALA	3.6
1	A	184	VAL	3.6
1	A	181	ASN	3.5
1	C	297	PRO	3.5
1	D	295	ASP	3.5
1	A	178	ALA	3.0
1	A	1	MET	2.8
1	B	184	VAL	2.8
1	B	297	PRO	2.6
1	D	296	ILE	2.4
1	D	184	VAL	2.4
1	C	205	PRO	2.4
1	D	300	GLY	2.3
1	C	1	MET	2.3
1	D	36	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	296	ILE	2.1
1	D	57	ASP	2.1
1	D	290	GLU	2.1
1	D	177	PHE	2.1
1	B	290	GLU	2.0
1	D	76[A]	ASP	2.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

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. 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	B-factors($Å^2$)	Q<0.9
4	GOL	A	1304	6/6	0.80	0.20	46,46,47,47	0
5	MBD	B	1301	9/9	0.84	0.19	31,31,31,31	0
4	GOL	A	1303	6/6	0.88	0.16	45,47,47,47	0
4	GOL	D	1302	6/6	0.91	0.12	40,42,42,43	0
5	MBD	D	1303	9/9	0.96	0.09	34,34,36,37	0
2	FE	C	1300	1/1	0.99	0.04	36,36,36,36	0
2	FE	A	1301	1/1	0.99	0.04	33,33,33,33	0
2	FE	B	1300	1/1	0.99	0.07	35,35,35,35	0
3	MG	A	1302	1/1	1.00	0.15	10,10,10,10	0
2	FE	D	1301	1/1	1.00	0.03	38,38,38,38	0

6.5   Other polymers ⓘ

There are no such residues in this entry.