



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:53 PM UTC

PDB ID : 2WM2 / pdb_00002wm2
Title : CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4- OXOQUINALDINE 2,4-DIOXYGENASE (HOD) FROM ARTHROBACTER NITROGUAJACOLICUS RU61A IN COMPLEX WITH CHLORIDE
Authors : Steiner, R.A.
Deposited on : 2009-06-29
Resolution : 2.70 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

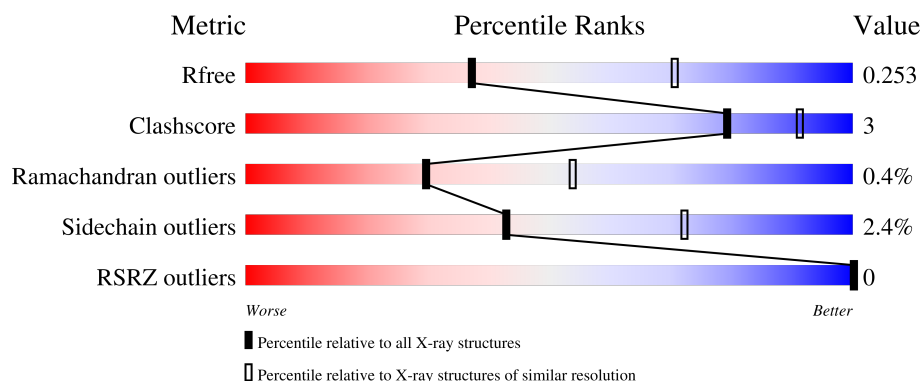
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	279	
1	B	279	
1	C	279	
1	D	279	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9316 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 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2234	1426	391	409	8			
1	B	275	Total	C	N	O	S	0	1	0
			2248	1435	393	411	9			
1	C	277	Total	C	N	O	S	0	1	0
			2264	1444	397	414	9			
1	D	277	Total	C	N	O	S	0	1	0
			2266	1445	399	413	9			

There are 4 discrepancies between the modelled and reference sequences:

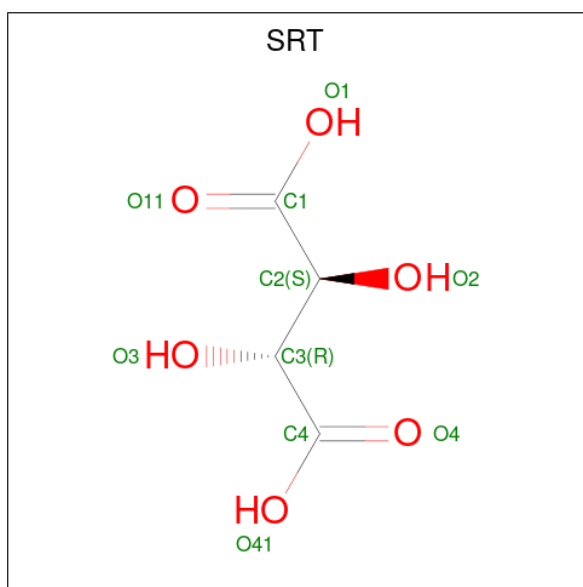
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	CYS	engineered mutation	UNP A4V8M9
B	69	SER	CYS	engineered mutation	UNP A4V8M9
C	69	SER	CYS	engineered mutation	UNP A4V8M9
D	69	SER	CYS	engineered mutation	UNP A4V8M9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: C₄H₆O₆).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	3	Total Na 3 3	0	0
5	C	4	Total Na 4 4	0	0
5	D	4	Total Na 4 4	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Cl 4 4	0	0
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0
6	D	2	Total Cl 2 2	0	0

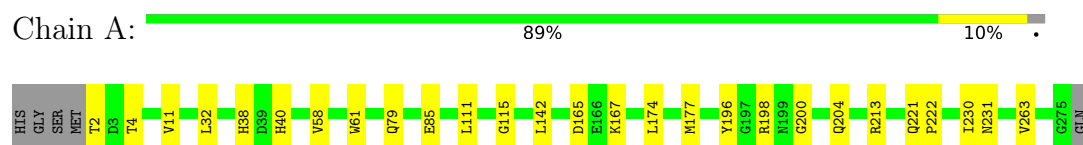
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	41	Total O 41 41	0	0
7	C	50	Total O 50 50	0	0
7	D	24	Total O 24 24	0	0

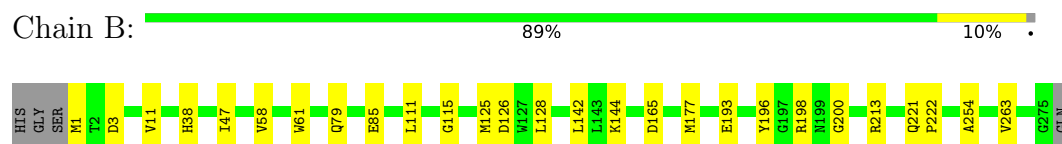
3 Residue-property plots [i](#)

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 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.

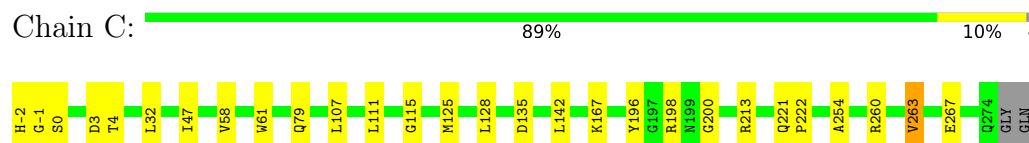
- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



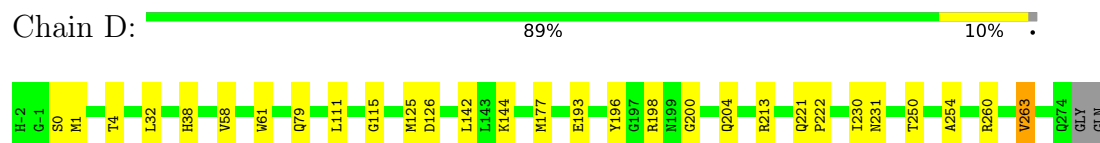
- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



- Molecule 1: 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.77Å 167.00Å 166.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.38 – 2.70 46.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.38-2.70) 97.8 (46.38-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.211 , 0.246 0.218 , 0.253	Depositor DCC
R_{free} test set	1787 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.447 for -h,l,k	Xtriage
Reported twinning fraction	0.527 for H, K, L 0.473 for -H, L, K	Depositor
Outliers	1 of 35417 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9316	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6643e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SRT, NA, K, GOL, CL

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	0.59	0/2305	0.81	2/3137 (0.1%)
1	B	0.57	0/2322	0.80	2/3159 (0.1%)
1	C	0.58	0/2339	0.80	2/3182 (0.1%)
1	D	0.57	0/2341	0.81	3/3184 (0.1%)
All	All	0.58	0/9307	0.81	9/12662 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	GLY	CA-C-N	5.52	125.61	119.87
1	C	115	GLY	C-N-CA	5.52	125.61	119.87
1	A	115	GLY	CA-C-N	5.34	125.42	119.87
1	A	115	GLY	C-N-CA	5.34	125.42	119.87
1	D	115	GLY	CA-C-N	5.31	125.39	119.87
1	D	115	GLY	C-N-CA	5.31	125.39	119.87
1	D	250	THR	N-CA-C	5.09	117.02	109.69
1	B	115	GLY	CA-C-N	5.01	125.08	119.87
1	B	115	GLY	C-N-CA	5.01	125.08	119.87

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	2234	0	2125	11	0
1	B	2248	0	2145	12	0
1	C	2264	0	2157	15	0
1	D	2266	0	2162	12	0
2	A	12	0	16	2	0
2	B	12	0	16	1	0
2	C	12	0	16	1	0
2	D	12	0	16	0	0
3	A	40	0	16	1	0
3	B	20	0	8	2	0
3	C	10	0	4	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	1	0	0	0	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
7	A	47	0	0	1	0
7	B	41	0	0	1	0
7	C	50	0	0	2	0
7	D	24	0	0	0	0
All	All	9316	0	8681	48	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 (48) 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)
3:A:1285:SRT:O1	1:C:263:VAL:HG11	1.85	0.76
1:A:167:LYS:HG2	7:A:2028:HOH:O	1.86	0.76
1:C:128:LEU:HD11	2:C:1276:GOL:H2	1.79	0.63
1:C:135:ASP:HB2	7:C:2019:HOH:O	1.97	0.63
1:A:174:LEU:HD22	2:A:1276:GOL:H32	1.84	0.58
1:A:111:LEU:HD22	1:A:213:ARG:HD2	1.92	0.52
1:D:38:HIS:HB3	1:D:177:MET:HE2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:HD22	1:B:213:ARG:HD2	1.93	0.51
2:A:1276:GOL:H31	1:C:267:GLU:HA	1.92	0.51
1:B:128:LEU:CD1	2:B:1276:GOL:H11	2.41	0.50
1:C:111:LEU:HD22	1:C:213:ARG:HD2	1.93	0.50
1:C:167:LYS:HB2	7:C:2027:HOH:O	2.11	0.50
1:A:165:ASP:OD2	1:C:260:ARG:HD3	2.12	0.49
1:B:38:HIS:HB3	1:B:177:MET:HE2	1.95	0.48
1:D:111:LEU:HD22	1:D:213:ARG:HD2	1.95	0.48
1:A:38:HIS:HB3	1:A:177:MET:HE2	1.95	0.48
3:B:1283:SRT:O1	1:D:263:VAL:CG1	2.62	0.48
3:B:1283:SRT:O1	1:D:263:VAL:HG13	2.14	0.48
1:D:32:LEU:HB2	1:D:58:VAL:HG22	1.96	0.47
1:A:61:TRP:CG	1:A:79:GLN:HE21	2.32	0.47
1:D:61:TRP:CG	1:D:79:GLN:HE21	2.32	0.47
1:A:32:LEU:HB2	1:A:58:VAL:HG22	1.97	0.46
1:B:61:TRP:CG	1:B:79:GLN:HE21	2.34	0.46
1:B:165:ASP:OD2	1:D:260:ARG:HD3	2.16	0.45
1:C:125:MET:HE1	1:C:254:ALA:HB2	1.97	0.45
1:B:125:MET:HE1	1:B:254:ALA:HB2	1.99	0.45
1:C:32:LEU:HB2	1:C:58:VAL:HG22	1.99	0.45
1:D:125:MET:HE1	1:D:254:ALA:HB2	1.98	0.45
1:C:-2:HIS:CG	1:C:-1:GLY:H	2.35	0.44
1:B:47:ILE:HD11	1:B:58:VAL:HG21	1.98	0.44
1:C:47:ILE:HD11	1:C:58:VAL:HG21	2.00	0.44
1:C:61:TRP:CG	1:C:79:GLN:HE21	2.36	0.43
1:B:196:TYR:O	1:B:200:GLY:N	2.51	0.43
1:C:196:TYR:O	1:C:200:GLY:N	2.50	0.43
1:D:144:LYS:NZ	1:D:193:GLU:OE2	2.51	0.43
1:A:196:TYR:O	1:A:200:GLY:N	2.52	0.43
1:B:11:VAL:HG13	1:B:85:GLU:HG2	2.02	0.42
1:B:38:HIS:CD2	7:B:2005:HOH:O	2.73	0.42
1:A:230:ILE:HG13	1:A:231:ASN:N	2.35	0.42
1:B:221:GLN:HA	1:B:222:PRO:C	2.44	0.41
1:C:221:GLN:HA	1:C:222:PRO:C	2.44	0.41
1:A:221:GLN:HA	1:A:222:PRO:C	2.44	0.41
1:D:221:GLN:HA	1:D:222:PRO:C	2.45	0.41
1:B:144:LYS:NZ	1:B:193:GLU:OE2	2.51	0.41
1:D:230:ILE:HG13	1:D:231:ASN:N	2.36	0.41
1:D:196:TYR:O	1:D:200:GLY:N	2.53	0.41
1:A:11:VAL:HG13	1:A:85:GLU:HG2	2.03	0.40
1:C:107:LEU:C	1:C:107:LEU:HD23	2.47	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	272/279 (98%)	262 (96%)	9 (3%)	1 (0%)	30	54
1	B	274/279 (98%)	264 (96%)	8 (3%)	2 (1%)	18	41
1	C	276/279 (99%)	263 (95%)	13 (5%)	0	100	100
1	D	276/279 (99%)	263 (95%)	12 (4%)	1 (0%)	30	54
All	All	1098/1116 (98%)	1052 (96%)	42 (4%)	4 (0%)	30	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	B	3	ASP
1	D	126	ASP
1	B	126	ASP

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	236/240 (98%)	230 (98%)	6 (2%)	42	71
1	B	238/240 (99%)	234 (98%)	4 (2%)	53	79
1	C	240/240 (100%)	234 (98%)	6 (2%)	42	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	240/240 (100%)	233 (97%)	7 (3%)	37	67
All	All	954/960 (99%)	931 (98%)	23 (2%)	43	72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	4	THR
1	A	142	LEU
1	A	198	ARG
1	A	204	GLN
1	A	263	VAL
1	B	1	MET
1	B	142	LEU
1	B	198	ARG
1	B	263	VAL
1	C	0	SER
1	C	3	ASP
1	C	4	THR
1	C	142	LEU
1	C	198	ARG
1	C	263	VAL
1	D	0	SER
1	D	1	MET
1	D	4	THR
1	D	142	LEU
1	D	198	ARG
1	D	204	GLN
1	D	263	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	199	ASN
1	B	7	HIS
1	B	221	GLN
1	B	238	HIS
1	C	7	HIS
1	D	7	HIS
1	D	221	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 24 are monoatomic - leaving 15 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	$\# Z > 2$
3	SRT	A	1285	-	9,9,9	1.18	0	12,12,12	1.15	1 (8%)
2	GOL	C	1276	-	5,5,5	0.41	0	5,5,5	0.34	0
3	SRT	C	1283	-	9,9,9	1.18	0	12,12,12	1.05	1 (8%)
3	SRT	B	1283	-	9,9,9	1.22	0	12,12,12	1.16	1 (8%)
2	GOL	A	1278	-	5,5,5	0.40	0	5,5,5	0.20	0
3	SRT	A	1277	-	9,9,9	1.18	0	12,12,12	1.02	1 (8%)
3	SRT	A	1286	-	9,9,9	1.13	0	12,12,12	1.28	2 (16%)
3	SRT	B	1284	5	9,9,9	1.18	0	12,12,12	1.47	2 (16%)
2	GOL	D	1276	-	5,5,5	0.74	0	5,5,5	1.09	0
2	GOL	C	1275	-	5,5,5	0.36	0	5,5,5	0.29	0
3	SRT	A	1287	5	9,9,9	1.09	0	12,12,12	1.51	2 (16%)
2	GOL	A	1276	-	5,5,5	0.49	0	5,5,5	0.58	0
2	GOL	D	1275	-	5,5,5	0.33	0	5,5,5	0.55	0
2	GOL	B	1277	-	5,5,5	0.47	0	5,5,5	0.29	0
2	GOL	B	1276	-	5,5,5	0.27	0	5,5,5	0.43	0

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	SRT	A	1285	-	-	8/12/12/12	-
2	GOL	C	1276	-	-	4/4/4/4	-
3	SRT	C	1283	-	-	7/12/12/12	-
3	SRT	B	1283	-	-	5/12/12/12	-
2	GOL	A	1278	-	-	2/4/4/4	-
3	SRT	A	1277	-	-	6/12/12/12	-
3	SRT	A	1286	-	-	6/12/12/12	-
3	SRT	B	1284	5	-	7/12/12/12	-
2	GOL	D	1276	-	-	4/4/4/4	-
2	GOL	C	1275	-	-	2/4/4/4	-
3	SRT	A	1287	5	-	8/12/12/12	-
2	GOL	A	1276	-	-	2/4/4/4	-
2	GOL	D	1275	-	-	3/4/4/4	-
2	GOL	B	1277	-	-	2/4/4/4	-
2	GOL	B	1276	-	-	4/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1287	SRT	C3-C2-C1	3.01	116.50	109.82
3	B	1284	SRT	O41-C4-C3	2.90	121.38	113.31
3	A	1287	SRT	O1-C1-C2	2.58	120.48	113.31
3	A	1285	SRT	O1-C1-C2	2.50	120.26	113.31
3	B	1284	SRT	C2-C3-C4	2.48	115.33	109.82
3	A	1286	SRT	O41-C4-C3	2.40	119.99	113.31
3	C	1283	SRT	C2-C3-C4	2.33	114.99	109.82
3	A	1286	SRT	O1-C1-C2	2.05	119.02	113.31
3	A	1277	SRT	C2-C3-C4	2.04	114.35	109.82
3	B	1283	SRT	O41-C4-C3	2.02	118.93	113.31

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1276	GOL	O1-C1-C2-C3
2	A	1278	GOL	O1-C1-C2-C3
2	C	1276	GOL	O1-C1-C2-C3
2	D	1275	GOL	C1-C2-C3-O3
2	D	1276	GOL	O1-C1-C2-C3
2	D	1276	GOL	C1-C2-C3-O3
3	A	1277	SRT	O3-C3-C4-O4
3	A	1277	SRT	O3-C3-C4-O41
3	A	1285	SRT	O2-C2-C3-O3
3	A	1285	SRT	O2-C2-C3-C4
3	B	1283	SRT	C2-C3-C4-O4
3	B	1283	SRT	C2-C3-C4-O41
3	B	1284	SRT	C2-C3-C4-O4
3	B	1284	SRT	C2-C3-C4-O41
3	B	1284	SRT	O3-C3-C4-O4
3	C	1283	SRT	O1-C1-C2-O2
3	C	1283	SRT	O11-C1-C2-O2
3	A	1285	SRT	C1-C2-C3-C4
3	A	1286	SRT	O1-C1-C2-O2
3	A	1286	SRT	O11-C1-C2-O2
3	A	1287	SRT	O3-C3-C4-O4
3	A	1287	SRT	O3-C3-C4-O41
3	B	1283	SRT	O3-C3-C4-O4
3	B	1283	SRT	O3-C3-C4-O41
3	B	1284	SRT	O3-C3-C4-O41
3	A	1277	SRT	C2-C3-C4-O4
3	A	1277	SRT	C2-C3-C4-O41
3	A	1287	SRT	C2-C3-C4-O4
3	A	1287	SRT	C2-C3-C4-O41
3	A	1285	SRT	C1-C2-C3-O3
3	A	1286	SRT	O2-C2-C3-C4
3	B	1284	SRT	O1-C1-C2-O2
3	B	1284	SRT	O11-C1-C2-O2
3	C	1283	SRT	O3-C3-C4-O41
3	A	1287	SRT	O1-C1-C2-O2
3	A	1287	SRT	O11-C1-C2-O2
3	C	1283	SRT	O3-C3-C4-O4
3	A	1286	SRT	O1-C1-C2-C3
2	A	1278	GOL	O1-C1-C2-O2
3	A	1287	SRT	O2-C2-C3-C4
3	B	1284	SRT	O2-C2-C3-O3
2	B	1276	GOL	O1-C1-C2-C3
2	B	1276	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1277	GOL	O1-C1-C2-C3
2	C	1275	GOL	C1-C2-C3-O3
2	C	1276	GOL	C1-C2-C3-O3
3	A	1286	SRT	C1-C2-C3-C4
2	A	1276	GOL	O1-C1-C2-O2
2	B	1276	GOL	O2-C2-C3-O3
2	B	1277	GOL	O1-C1-C2-O2
2	C	1275	GOL	O2-C2-C3-O3
2	C	1276	GOL	O1-C1-C2-O2
2	D	1275	GOL	O2-C2-C3-O3
2	D	1276	GOL	O1-C1-C2-O2
2	D	1276	GOL	O2-C2-C3-O3
3	A	1277	SRT	C1-C2-C3-O3
3	C	1283	SRT	C1-C2-C3-O3
3	A	1285	SRT	C2-C3-C4-O4
3	A	1285	SRT	C2-C3-C4-O41
3	A	1286	SRT	O11-C1-C2-C3
3	A	1287	SRT	C1-C2-C3-C4
2	B	1276	GOL	O1-C1-C2-O2
2	D	1275	GOL	O1-C1-C2-O2
3	A	1277	SRT	C1-C2-C3-C4
3	C	1283	SRT	C1-C2-C3-C4
3	B	1283	SRT	O2-C2-C3-O3
3	A	1285	SRT	O3-C3-C4-O41
3	A	1285	SRT	O3-C3-C4-O4
3	C	1283	SRT	C2-C3-C4-O4
2	C	1276	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1285	SRT	1	0
2	C	1276	GOL	1	0
3	B	1283	SRT	2	0
2	A	1276	GOL	2	0
2	B	1276	GOL	1	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 [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, 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	274/279 (98%)	-1.21	0 100 100	31, 40, 49, 53	0
1	B	275/279 (98%)	-1.18	0 100 100	25, 40, 50, 57	1 (0%)
1	C	277/279 (99%)	-1.17	0 100 100	23, 40, 50, 59	1 (0%)
1	D	277/279 (99%)	-1.23	0 100 100	21, 40, 50, 54	1 (0%)
All	All	1103/1116 (98%)	-1.20	0 100 100	21, 40, 50, 59	3 (0%)

There are no RSRZ outliers to report.

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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	SRT	A	1285	10/10	0.96	0.06	56,58,58,59	0
5	NA	B	1281	1/1	0.96	0.07	21,21,21,21	0
2	GOL	C	1276	6/6	0.97	0.08	37,38,39,41	0
2	GOL	D	1276	6/6	0.97	0.09	34,35,35,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	1276	6/6	0.97	0.08	38,40,41,41	0
5	NA	B	1279	1/1	0.97	0.11	27,27,27,27	0
2	GOL	C	1275	6/6	0.97	0.09	59,61,61,62	0
5	NA	C	1278	1/1	0.97	0.08	19,19,19,19	0
5	NA	C	1279	1/1	0.97	0.10	19,19,19,19	0
5	NA	C	1281	1/1	0.97	0.08	51,51,51,51	0
5	NA	D	1278	1/1	0.97	0.10	14,14,14,14	0
6	CL	D	1302	1/1	0.97	0.09	53,53,53,53	0
3	SRT	B	1284	10/10	0.98	0.05	61,62,62,62	0
3	SRT	C	1283	10/10	0.98	0.08	47,49,50,51	0
4	K	B	1278	1/1	0.98	0.05	51,51,51,51	0
2	GOL	D	1275	6/6	0.98	0.07	49,51,52,53	0
5	NA	B	1280	1/1	0.98	0.04	24,24,24,24	0
2	GOL	B	1276	6/6	0.98	0.06	53,53,54,54	0
3	SRT	A	1277	10/10	0.98	0.03	32,37,37,38	0
2	GOL	B	1277	6/6	0.98	0.06	37,40,40,40	0
5	NA	C	1280	1/1	0.98	0.12	27,27,27,27	0
3	SRT	A	1286	10/10	0.98	0.08	76,77,78,79	0
3	SRT	A	1287	10/10	0.98	0.06	74,75,76,77	0
5	NA	D	1300	1/1	0.98	0.04	19,19,19,19	0
5	NA	D	1301	1/1	0.98	0.04	24,24,24,24	0
6	CL	A	1281	1/1	0.98	0.11	44,44,44,44	0
6	CL	A	1282	1/1	0.98	0.10	37,37,37,37	0
6	CL	A	1283	1/1	0.98	0.10	40,40,40,40	0
6	CL	B	1282	1/1	0.98	0.10	59,59,59,59	0
6	CL	C	1282	1/1	0.98	0.04	47,47,47,47	0
3	SRT	B	1283	10/10	0.98	0.05	58,60,61,61	0
4	K	A	1279	1/1	0.99	0.03	50,50,50,50	0
2	GOL	A	1278	6/6	0.99	0.06	51,52,52,52	0
4	K	C	1277	1/1	0.99	0.04	55,55,55,55	0
6	CL	A	1284	1/1	0.99	0.03	31,31,31,31	0
5	NA	D	1279	1/1	0.99	0.04	21,21,21,21	0
4	K	D	1277	1/1	0.99	0.04	56,56,56,56	0
6	CL	D	1280	1/1	0.99	0.04	43,43,43,43	0
5	NA	A	1280	1/1	0.99	0.02	15,15,15,15	0

6.5 Other polymers

There are no such residues in this entry.