



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:16 AM GMT

PDB ID : 2WJ4  
Title : CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE (HOD) FROM ARTHROBACTER NITROGUAJACOLICUS RU61A ANAEROBICALLY COMPLEXED WITH ITS NATURAL SUBSTRATE 1-H-3-HYDROXY-4-OXOQUINALDINE  
Authors : Steiner, R.A.  
Deposited on : 2009-05-20  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

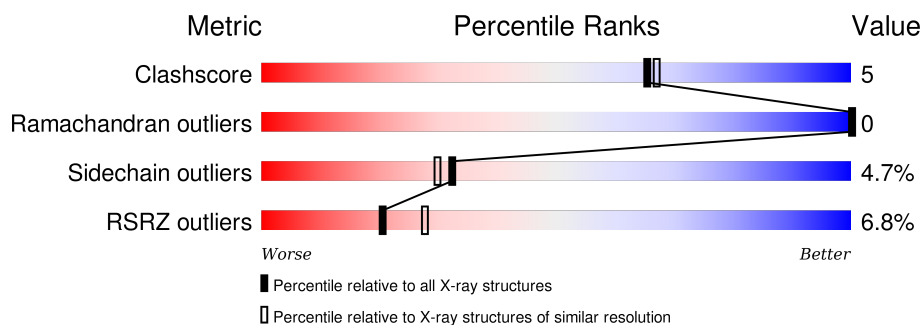
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	<div> <div>6%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	B	276	<div> <div>6%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	C	276	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	D	276	<div> <div>9%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	1276	-	-	-	X
2	GOL	D	1275	-	-	X	-
2	GOL	D	1276	-	-	X	-
5	SRT	A	1283	-	-	-	X
5	SRT	A	1284	-	-	-	X
5	SRT	B	1279	-	-	-	X
5	SRT	B	1280	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9483 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 1H-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	273	Total	C	N	O	S	0	0	0
			2227	1422	390	407	8			
1	C	273	Total	C	N	O	S	0	1	0
			2236	1428	391	409	8			
1	D	273	Total	C	N	O	S	0	0	0
			2230	1424	390	408	8			

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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



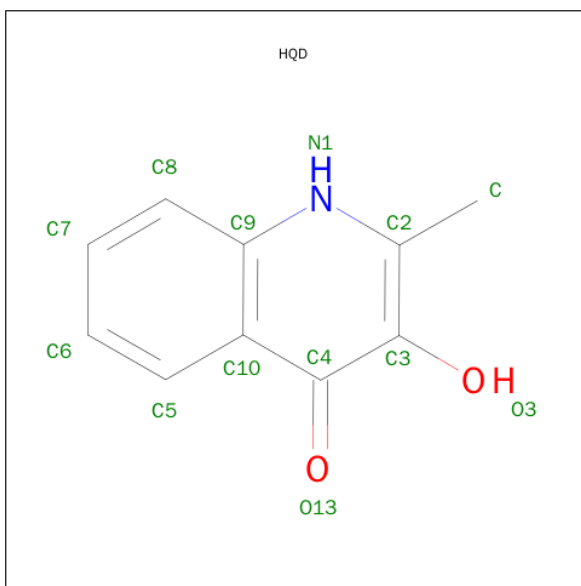
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

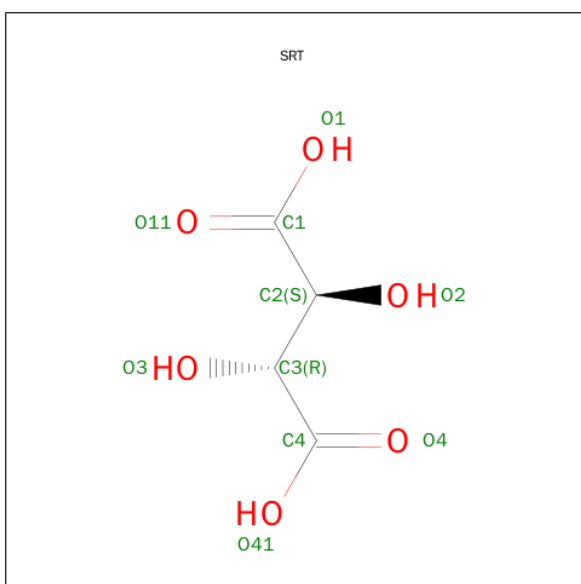
- Molecule 4 is 3-HYDROXY-2-METHYLQUINOLIN-4(1H)-ONE (three-letter code: HQD)

(formula:  $C_{10}H_9NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	10	1	2		
4	B	1	Total	C	N	O	0	0
			13	10	1	2		
4	C	1	Total	C	N	O	0	0
			13	10	1	2		
4	D	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula:  $C_4H_6O_6$ ).



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

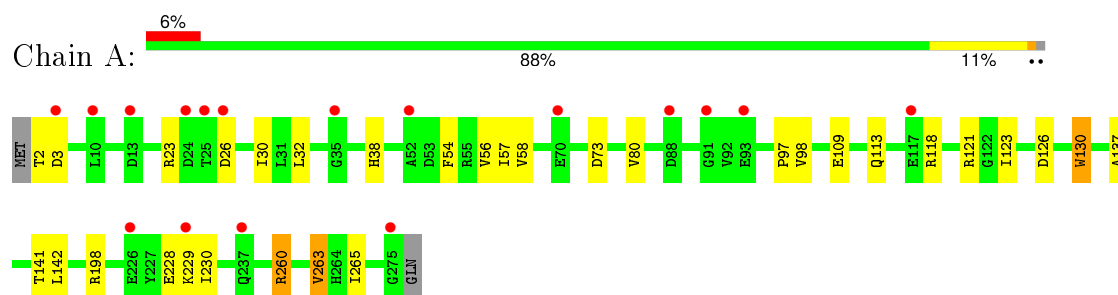
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	101	Total O 101 101	0	0
6	B	99	Total O 99 99	0	0
6	C	108	Total O 108 108	0	0
6	D	79	Total O 79 79	0	0

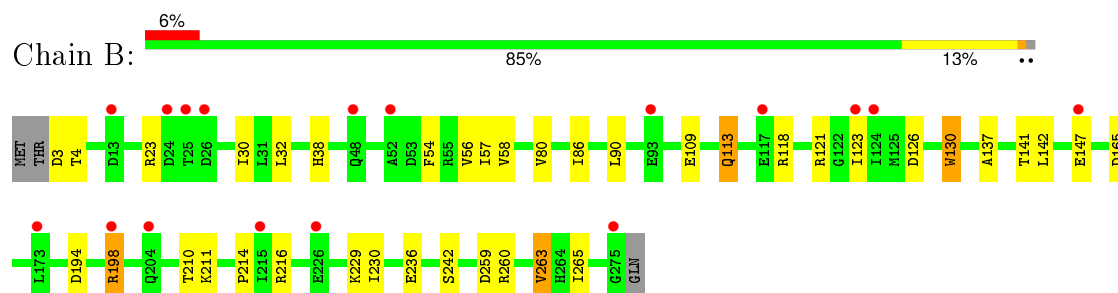
### 3 Residue-property plots [i](#)

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.

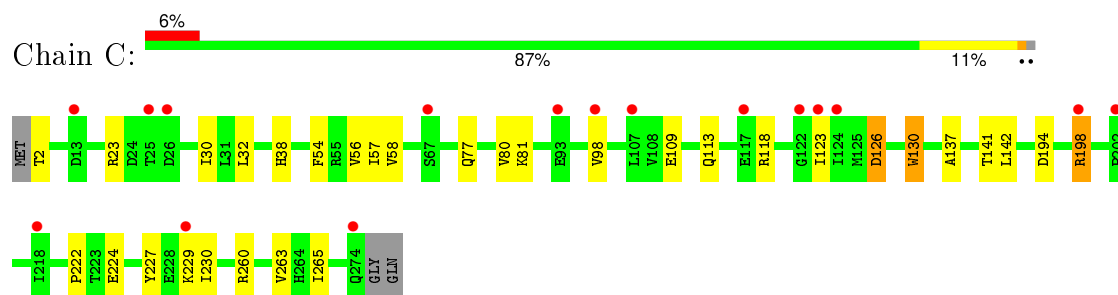
- Molecule 1: 1H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



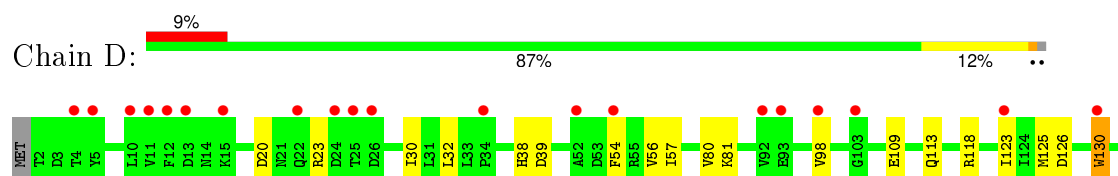
- Molecule 1: 1H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



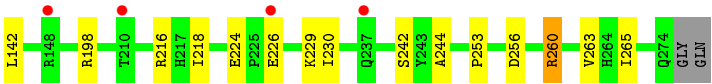
- Molecule 1: 1H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



- Molecule 1: 1H-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, $\alpha$ , $\beta$ , $\gamma$	44.81Å 167.20Å 167.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.84 – 2.10 37.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.84-2.10) 93.5 (37.39-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.176 , 0.204 0.227 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.1	EDS
Estimated twinning fraction	0.577 for H, K, L 0.423 for -H, L, K 0.138 for -h,l,k	Xtriage
Reported twinning fraction	0.577 for H, K, L 0.423 for -H, L, K	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	3 of 70128 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 23.51 % 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 4.5991e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: GOL, K, HQD, SRT

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	0.88	2/2305 (0.1%)	1.05	4/3137 (0.1%)
1	B	0.90	4/2298 (0.2%)	1.09	6/3127 (0.2%)
1	C	0.89	1/2310 (0.0%)	0.83	5/3144 (0.2%)
1	D	0.90	0/2301	0.88	4/3132 (0.1%)
All	All	0.89	7/9214 (0.1%)	0.96	19/12540 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	VAL	CB-CG1	-11.32	1.29	1.52
1	B	263	VAL	CB-CG2	-8.72	1.34	1.52
1	A	113	GLN	CG-CD	-7.13	1.34	1.51
1	C	263	VAL	CB-CG2	-6.85	1.38	1.52
1	B	113	GLN	CD-OE1	-6.63	1.09	1.24
1	A	263	VAL	CB-CG2	-5.23	1.41	1.52
1	B	147	GLU	CD-OE2	-5.17	1.20	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ARG	NE-CZ-NH2	28.88	134.74	120.30
1	B	260	ARG	NE-CZ-NH1	-27.34	106.63	120.30
1	A	260	ARG	NE-CZ-NH1	-27.09	106.76	120.30
1	A	260	ARG	NE-CZ-NH2	26.62	133.61	120.30
1	B	260	ARG	CD-NE-CZ	15.21	144.90	123.60
1	D	260	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	D	260	ARG	NE-CZ-NH2	-14.19	113.21	120.30
1	A	260	ARG	CD-NE-CZ	13.55	142.57	123.60
1	C	260	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	C	260	ARG	NE-CZ-NH2	-11.38	114.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	ARG	CD-NE-CZ	9.64	137.10	123.60
1	C	260	ARG	CD-NE-CZ	9.30	136.62	123.60
1	B	263	VAL	CG1-CB-CG2	-7.79	98.43	110.90
1	A	260	ARG	CG-CD-NE	6.71	125.90	111.80
1	B	260	ARG	CG-CD-NE	6.47	125.39	111.80
1	B	147	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	C	126	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	260	ARG	CG-CD-NE	5.47	123.28	111.80
1	D	260	ARG	CG-CD-NE	5.04	122.38	111.80

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	14	0
1	B	2227	0	2118	23	0
1	C	2236	0	2130	18	0
1	D	2230	0	2122	22	0
2	A	18	0	22	2	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	12	0	16	11	0
3	A	2	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	13	0	9	0	0
4	B	13	0	8	0	0
4	C	13	0	8	0	0
4	D	13	0	9	0	0
5	A	30	0	11	0	0
5	B	20	0	7	2	0
5	C	10	0	4	0	0
5	D	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	101	0	0	0	1
6	B	99	0	0	5	1
6	C	108	0	0	4	1
6	D	79	0	0	4	1
All	All	9483	0	8609	89	2

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 (89) 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:224:GLU:OE2	6:C:2090:HOH:O	1.97	0.81
1:D:226:GLU:HB2	6:D:2063:HOH:O	1.90	0.70
2:D:1275:GOL:C2	2:D:1276:GOL:H32	2.22	0.69
2:D:1275:GOL:H2	2:D:1276:GOL:H32	1.76	0.66
2:D:1275:GOL:C2	2:D:1276:GOL:C3	2.73	0.66
1:C:81:LYS:HE2	6:C:2026:HOH:O	1.95	0.66
2:D:1275:GOL:O2	2:D:1276:GOL:H31	1.95	0.65
2:A:1276:GOL:H12	6:C:2097:HOH:O	1.97	0.65
1:C:30:ILE:HD12	1:C:54:PHE:HB3	1.78	0.64
2:D:1275:GOL:O2	2:D:1276:GOL:C3	2.45	0.64
1:D:130:TRP:CE3	1:D:230:ILE:HD13	2.33	0.63
1:B:211:LYS:NZ	6:B:2069:HOH:O	2.34	0.61
1:B:30:ILE:HD12	1:B:54:PHE:HB3	1.82	0.60
5:B:1280:SRT:C1	6:B:2099:HOH:O	2.49	0.59
1:A:30:ILE:HD12	1:A:54:PHE:HB3	1.85	0.59
2:D:1275:GOL:O1	2:D:1276:GOL:H32	2.03	0.58
1:D:81:LYS:NZ	6:D:2022:HOH:O	2.36	0.57
1:C:56:VAL:C	1:C:57:ILE:HD13	2.26	0.56
1:D:30:ILE:HD12	1:D:54:PHE:HB3	1.86	0.55
1:C:80:VAL:HG21	1:C:109:GLU:HB3	1.88	0.55
1:B:165:ASP:O	2:D:1276:GOL:O3	2.21	0.55
1:A:30:ILE:HD12	1:A:54:PHE:CB	2.37	0.54
1:D:56:VAL:C	1:D:57:ILE:HD13	2.27	0.54
1:C:130:TRP:CE3	1:C:230:ILE:HD13	2.42	0.54
1:D:130:TRP:HE3	1:D:230:ILE:HD13	1.71	0.54
1:B:30:ILE:HD12	1:B:54:PHE:CB	2.38	0.53
1:B:259:ASP:O	1:B:263:VAL:HG23	2.08	0.53
1:D:98:VAL:CG1	1:D:125:MET:HE2	2.38	0.53
1:C:30:ILE:HD12	1:C:54:PHE:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1276:GOL:C1	6:C:2097:HOH:O	2.54	0.51
5:B:1280:SRT:H2	6:B:2098:HOH:O	2.10	0.51
1:A:32:LEU:HB2	1:A:58:VAL:HG22	1.94	0.50
1:C:32:LEU:HD23	1:C:98:VAL:HB	1.94	0.50
1:D:80:VAL:HG21	1:D:109:GLU:HB3	1.93	0.50
1:D:30:ILE:HD12	1:D:54:PHE:CB	2.41	0.50
1:B:130:TRP:CE3	1:B:230:ILE:HD13	2.46	0.50
1:B:165:ASP:H	2:D:1276:GOL:H11	1.76	0.50
1:C:30:ILE:HD11	1:C:54:PHE:CD1	2.47	0.49
1:C:130:TRP:HE3	1:C:230:ILE:HD13	1.78	0.49
1:B:80:VAL:HG21	1:B:109:GLU:HB3	1.95	0.49
1:B:56:VAL:C	1:B:57:ILE:HD13	2.34	0.48
1:B:236:GLU:HG3	6:B:2080:HOH:O	2.13	0.48
1:D:32:LEU:HD23	1:D:98:VAL:HB	1.95	0.48
1:A:32:LEU:HD23	1:A:98:VAL:HB	1.96	0.48
1:D:260:ARG:O	1:D:263:VAL:HG22	2.12	0.48
1:B:30:ILE:HD11	1:B:54:PHE:CD1	2.48	0.47
1:D:218:ILE:HG22	1:D:244:ALA:HB3	1.95	0.47
1:A:97:PRO:HD2	1:A:121:ARG:O	2.15	0.47
1:C:56:VAL:O	1:C:57:ILE:HD13	2.15	0.47
1:D:98:VAL:CG1	1:D:125:MET:CE	2.94	0.46
1:A:30:ILE:HD11	1:A:54:PHE:CD1	2.51	0.46
1:A:56:VAL:C	1:A:57:ILE:HD13	2.37	0.46
1:A:130:TRP:CE3	1:A:230:ILE:HD13	2.52	0.45
1:D:56:VAL:O	1:D:57:ILE:HD13	2.17	0.45
1:B:56:VAL:O	1:B:57:ILE:HD13	2.17	0.45
1:A:137:ALA:O	1:A:141:THR:HG23	2.17	0.44
1:B:216:ARG:HA	1:B:242:SER:O	2.17	0.44
1:B:137:ALA:O	1:B:141:THR:HG23	2.18	0.44
1:D:216:ARG:HA	1:D:242:SER:O	2.17	0.44
2:D:1275:GOL:C1	2:D:1276:GOL:H32	2.47	0.44
1:C:30:ILE:CD1	1:C:54:PHE:CG	3.01	0.44
1:C:32:LEU:HB2	1:C:58:VAL:HG22	2.00	0.44
1:C:222:PRO:HD2	1:C:227:TYR:CE2	2.53	0.44
1:C:123:ILE:CD1	1:C:265:ILE:HA	2.47	0.44
1:B:123:ILE:CD1	1:B:265:ILE:HA	2.48	0.44
1:D:30:ILE:HD11	1:D:54:PHE:CD1	2.53	0.43
1:B:30:ILE:CD1	1:B:54:PHE:CG	3.02	0.43
1:A:260:ARG:O	1:A:263:VAL:HG22	2.18	0.43
1:D:130:TRP:CE3	1:D:230:ILE:CD1	3.02	0.43
2:D:1275:GOL:C1	6:D:2077:HOH:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ASP:OD1	1:D:57:ILE:HD11	2.18	0.42
1:A:80:VAL:HG21	1:A:109:GLU:HB3	2.00	0.42
1:A:30:ILE:CD1	1:A:54:PHE:CG	3.02	0.42
1:A:123:ILE:CD1	1:A:265:ILE:HA	2.49	0.42
1:B:130:TRP:HE3	1:B:230:ILE:HD13	1.85	0.42
1:B:165:ASP:N	2:D:1276:GOL:H11	2.34	0.42
1:C:194:ASP:OD2	1:C:198:ARG:NH1	2.51	0.42
1:B:32:LEU:HB2	1:B:58:VAL:HG22	2.02	0.42
1:A:56:VAL:O	1:A:57:ILE:HD13	2.20	0.42
1:B:121:ARG:HG2	1:B:214:PRO:HB2	2.01	0.42
1:C:137:ALA:O	1:C:141:THR:HG23	2.20	0.41
1:B:210:THR:OG1	6:B:2068:HOH:O	2.21	0.41
1:C:77[B]:GLN:H	1:C:77[B]:GLN:HG2	1.62	0.41
1:D:20:ASP:OD1	1:D:57:ILE:CD1	2.68	0.41
1:D:224:GLU:HG3	6:D:2062:HOH:O	2.21	0.41
1:D:253:PRO:HA	1:D:256:ASP:OD1	2.20	0.41
1:B:194:ASP:OD2	1:B:198:ARG:NH1	2.51	0.41
1:D:123:ILE:CD1	1:D:265:ILE:HA	2.51	0.40
1:B:86:ILE:O	1:B:90:LEU:HG	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2088:HOH:O	6:C:2053:HOH:O[4_456]	2.04	0.16
6:A:2098:HOH:O	6:D:2045:HOH:O[4_456]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	272/276 (99%)	265 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	271/276 (98%)	265 (98%)	6 (2%)	0	100	100
1	C	272/276 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	271/276 (98%)	263 (97%)	8 (3%)	0	100	100
All	All	1086/1104 (98%)	1059 (98%)	27 (2%)	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	236/238 (99%)	223 (94%)	13 (6%)	27	23
1	B	235/238 (99%)	224 (95%)	11 (5%)	32	30
1	C	237/238 (100%)	227 (96%)	10 (4%)	36	35
1	D	236/238 (99%)	226 (96%)	10 (4%)	36	35
All	All	944/952 (99%)	900 (95%)	44 (5%)	32	30

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	ASP
1	A	23	ARG
1	A	26	ASP
1	A	38	HIS
1	A	73	ASP
1	A	118	ARG
1	A	126	ASP
1	A	130	TRP
1	A	142	LEU
1	A	198	ARG
1	A	228	GLU
1	A	229	LYS

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Mol	Chain	Res	Type
1	B	3	ASP
1	B	4	THR
1	B	23	ARG
1	B	38	HIS
1	B	113	GLN
1	B	118	ARG
1	B	126	ASP
1	B	130	TRP
1	B	142	LEU
1	B	198	ARG
1	B	229	LYS
1	C	2	THR
1	C	23	ARG
1	C	38	HIS
1	C	113	GLN
1	C	118	ARG
1	C	126	ASP
1	C	130	TRP
1	C	142	LEU
1	C	198	ARG
1	C	229	LYS
1	D	23	ARG
1	D	38	HIS
1	D	39	ASP
1	D	113	GLN
1	D	118	ARG
1	D	126	ASP
1	D	130	TRP
1	D	142	LEU
1	D	198	ARG
1	D	229	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 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	GOL	A	1276	3	5,5,5	0.72	0	5,5,5	0.93	0
2	GOL	A	1277	3	5,5,5	0.28	0	5,5,5	1.72	1 (20%)
2	GOL	A	1278	-	5,5,5	0.38	0	5,5,5	0.83	0
4	HQD	A	1281	-	12,14,14	3.32	6 (50%)	17,20,20	1.12	2 (11%)
5	SRT	A	1282	-	3,9,9	1.39	0	6,12,12	1.30	2 (33%)
5	SRT	A	1283	3	3,9,9	1.60	1 (33%)	6,12,12	2.26	4 (66%)
5	SRT	A	1284	-	3,9,9	1.13	0	6,12,12	1.46	1 (16%)
2	GOL	B	1276	3	5,5,5	0.77	0	5,5,5	0.69	0
4	HQD	B	1278	-	12,14,14	3.88	6 (50%)	17,20,20	1.13	2 (11%)
5	SRT	B	1279	-	3,9,9	1.26	0	6,12,12	2.19	2 (33%)
5	SRT	B	1280	-	3,9,9	1.49	1 (33%)	6,12,12	4.04	4 (66%)
2	GOL	C	1275	3	5,5,5	0.21	0	5,5,5	0.67	0
4	HQD	C	1277	-	12,14,14	5.85	8 (66%)	17,20,20	1.14	2 (11%)
5	SRT	C	1278	-	3,9,9	0.62	0	6,12,12	1.46	1 (16%)
2	GOL	D	1275	-	5,5,5	0.37	0	5,5,5	1.19	0
2	GOL	D	1276	-	5,5,5	0.57	0	5,5,5	0.97	0
4	HQD	D	1278	-	12,14,14	5.51	8 (66%)	17,20,20	1.13	2 (11%)
5	SRT	D	1279	-	3,9,9	0.33	0	6,12,12	2.32	3 (50%)

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	GOL	A	1276	3	-	0/4/4/4	0/0/0/0
2	GOL	A	1277	3	-	0/4/4/4	0/0/0/0
2	GOL	A	1278	-	-	0/4/4/4	0/0/0/0
4	HQD	A	1281	-	-	0/0/0/0	0/2/2/2
5	SRT	A	1282	-	-	0/4/12/12	0/0/0/0
5	SRT	A	1283	3	-	0/4/12/12	0/0/0/0
5	SRT	A	1284	-	-	0/4/12/12	0/0/0/0
2	GOL	B	1276	3	-	0/4/4/4	0/0/0/0
4	HQD	B	1278	-	-	0/0/0/0	0/2/2/2
5	SRT	B	1279	-	-	0/4/12/12	0/0/0/0
5	SRT	B	1280	-	-	0/4/12/12	0/0/0/0
2	GOL	C	1275	3	-	0/4/4/4	0/0/0/0
4	HQD	C	1277	-	-	0/0/0/0	0/2/2/2
5	SRT	C	1278	-	-	0/4/12/12	0/0/0/0
2	GOL	D	1275	-	-	0/4/4/4	0/0/0/0
2	GOL	D	1276	-	-	0/4/4/4	0/0/0/0
4	HQD	D	1278	-	-	0/0/0/0	0/2/2/2
5	SRT	D	1279	-	-	0/4/12/12	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1278	HQD	C8-C9	-3.17	1.36	1.41
4	B	1278	HQD	C5-C10	-3.01	1.34	1.41
4	A	1281	HQD	C8-C9	-2.29	1.37	1.41
4	A	1281	HQD	C5-C10	-2.29	1.36	1.41
4	A	1281	HQD	C4-C10	-2.12	1.38	1.41
5	B	1280	SRT	O2-C2	2.03	1.46	1.42
4	D	1278	HQD	C7-C8	2.03	1.41	1.36
4	A	1281	HQD	C10-C9	2.04	1.45	1.41
4	C	1277	HQD	C7-C8	2.09	1.41	1.36
4	D	1278	HQD	C4-C10	2.24	1.44	1.41
4	C	1277	HQD	C7-C6	2.38	1.44	1.38
4	B	1278	HQD	C10-C9	2.38	1.46	1.41
4	D	1278	HQD	C7-C6	2.46	1.44	1.38
5	A	1283	SRT	O3-C3	2.74	1.48	1.42
4	C	1277	HQD	C4-C10	2.82	1.45	1.41
4	D	1278	HQD	C6-C5	2.97	1.43	1.36
4	B	1278	HQD	C9-N1	3.07	1.42	1.37
4	C	1277	HQD	C9-N1	3.08	1.42	1.37
4	D	1278	HQD	C10-C9	3.16	1.48	1.41
4	C	1277	HQD	C6-C5	3.16	1.43	1.36
4	C	1277	HQD	C10-C9	3.22	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1278	HQD	C9-N1	3.28	1.43	1.37
4	A	1281	HQD	C2-N1	5.05	1.36	1.32
4	B	1278	HQD	C2-N1	8.06	1.39	1.32
4	B	1278	HQD	C3-C2	8.66	1.46	1.40
4	A	1281	HQD	C3-C2	8.87	1.46	1.40
4	D	1278	HQD	C2-N1	9.59	1.41	1.32
4	C	1277	HQD	C2-N1	10.09	1.41	1.32
4	D	1278	HQD	C3-C2	14.96	1.50	1.40
4	C	1277	HQD	C3-C2	16.03	1.51	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1280	SRT	O3-C3-C4	-6.42	95.00	111.21
5	B	1279	SRT	C4-C3-C2	-3.67	105.83	113.35
5	B	1279	SRT	C1-C2-C3	-3.55	106.07	113.35
5	D	1279	SRT	O3-C3-C2	-3.02	100.10	108.61
5	A	1283	SRT	C1-C2-C3	-2.98	107.25	113.35
2	A	1277	GOL	O3-C3-C2	-2.64	97.37	110.18
5	A	1283	SRT	O3-C3-C4	-2.43	105.09	111.21
5	C	1278	SRT	O3-C3-C2	-2.41	101.81	108.61
5	A	1283	SRT	O2-C2-C1	-2.18	105.72	111.21
5	B	1280	SRT	O2-C2-C3	-2.17	102.49	108.61
5	A	1282	SRT	C4-C3-C2	-2.08	109.08	113.35
5	A	1282	SRT	C1-C2-C3	-2.03	109.19	113.35
4	B	1278	HQD	C-C2-N1	2.16	119.93	116.94
5	B	1280	SRT	C1-C2-C3	2.17	117.80	113.35
4	A	1281	HQD	C-C2-N1	2.18	119.95	116.94
4	D	1278	HQD	C-C2-N1	2.18	119.96	116.94
4	C	1277	HQD	C-C2-N1	2.18	119.96	116.94
5	A	1284	SRT	O3-C3-C2	2.26	114.97	108.61
4	B	1278	HQD	C2-N1-C9	2.41	120.15	118.40
4	C	1277	HQD	C2-N1-C9	2.42	120.16	118.40
4	A	1281	HQD	C2-N1-C9	2.44	120.17	118.40
4	D	1278	HQD	C2-N1-C9	2.44	120.17	118.40
5	A	1283	SRT	O2-C2-C3	2.56	115.83	108.61
5	D	1279	SRT	O2-C2-C3	2.87	116.70	108.61
5	D	1279	SRT	C4-C3-C2	3.55	120.63	113.35
5	B	1280	SRT	O3-C3-C2	6.57	127.14	108.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1276	GOL	2	0
5	B	1280	SRT	2	0
2	D	1275	GOL	8	0
2	D	1276	GOL	10	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	274/276 (99%)	0.50	17 (6%) 24 32	20, 30, 40, 49	0
1	B	273/276 (98%)	0.45	17 (6%) 24 32	20, 30, 40, 46	0
1	C	273/276 (98%)	0.45	16 (5%) 26 34	21, 30, 39, 50	0
1	D	273/276 (98%)	0.61	24 (8%) 12 17	21, 30, 40, 52	0
All	All	1093/1104 (99%)	0.50	74 (6%) 20 28	20, 30, 40, 52	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	THR	5.6
1	A	24	ASP	5.5
1	A	25	THR	5.0
1	B	24	ASP	4.5
1	D	24	ASP	4.5
1	A	275	GLY	4.2
1	B	26	ASP	4.0
1	D	5	TYR	4.0
1	D	123	ILE	4.0
1	A	117	GLU	3.9
1	D	10	LEU	3.9
1	B	275	GLY	3.9
1	D	92	VAL	3.8
1	D	52	ALA	3.7
1	D	4	THR	3.7
1	A	13	ASP	3.7
1	A	3	ASP	3.6
1	D	26	ASP	3.5
1	A	26	ASP	3.4
1	C	26	ASP	3.4
1	D	98	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	226	GLU	3.4
1	D	12	PHE	3.3
1	C	124	ILE	3.3
1	B	13	ASP	3.3
1	C	93	GLU	3.3
1	C	123	ILE	3.2
1	D	237	GLN	3.2
1	C	198	ARG	3.2
1	B	123	ILE	3.1
1	A	10	LEU	3.1
1	C	13	ASP	3.1
1	D	148	ARG	3.1
1	D	11	VAL	3.1
1	D	13	ASP	2.9
1	B	48	GLN	2.9
1	A	91	GLY	2.9
1	D	22	GLN	2.9
1	A	70	GLU	2.8
1	D	93	GLU	2.8
1	A	52	ALA	2.7
1	B	124	ILE	2.6
1	C	67	SER	2.6
1	B	52	ALA	2.5
1	A	88	ASP	2.5
1	B	93	GLU	2.5
1	D	210	THR	2.5
1	B	173	LEU	2.4
1	D	54	PHE	2.4
1	A	93	GLU	2.4
1	A	229	LYS	2.4
1	D	15	LYS	2.4
1	D	34	PRO	2.4
1	C	98	VAL	2.3
1	B	198	ARG	2.3
1	C	274	GLN	2.3
1	B	147	GLU	2.3
1	C	25	THR	2.2
1	C	218	ILE	2.2
1	C	122	GLY	2.2
1	A	35	GLY	2.2
1	A	237	GLN	2.2
1	B	226	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	117	GLU	2.2
1	B	204	GLN	2.1
1	B	117	GLU	2.1
1	D	130	TRP	2.1
1	D	226	GLU	2.1
1	B	25	THR	2.0
1	C	107	LEU	2.0
1	C	229	LYS	2.0
1	B	215	ILE	2.0
1	C	202	PRO	2.0
1	D	103	GLY	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](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	B	1276	6/6	0.65	0.31	3.66	46,47,47,48	0
5	SRT	B	1280	10/10	0.88	0.25	3.52	18,35,39,40	0
5	SRT	A	1283	10/10	0.84	0.21	3.14	22,32,38,38	0
5	SRT	A	1284	10/10	0.84	0.21	2.42	15,34,38,39	0
5	SRT	B	1279	10/10	0.68	0.20	2.24	32,36,39,42	0
5	SRT	C	1278	10/10	0.86	0.20	1.48	30,37,41,41	0
4	HQD	D	1278	13/13	0.92	0.18	1.14	23,27,31,32	0
2	GOL	A	1276	6/6	0.88	0.15	0.36	29,35,37,39	0
4	HQD	B	1278	13/13	0.93	0.15	0.28	15,18,21,21	0
5	SRT	D	1279	10/10	0.80	0.17	0.26	31,40,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	C	1275	6/6	0.92	0.15	0.24	33,35,35,38	0
2	GOL	D	1276	6/6	0.79	0.13	-0.01	15,20,27,28	0
4	HQD	A	1281	13/13	0.96	0.14	-0.02	14,19,22,23	0
2	GOL	A	1277	6/6	0.87	0.12	-0.08	24,29,31,33	0
4	HQD	C	1277	13/13	0.93	0.13	-0.28	19,24,27,28	0
5	SRT	A	1282	10/10	0.91	0.14	-0.41	24,30,37,37	0
3	K	A	1279	1/1	0.95	0.07	-1.38	38,38,38,38	0
3	K	D	1277	1/1	0.98	0.06	-1.45	33,33,33,33	0
3	K	C	1276	1/1	0.99	0.07	-2.44	25,25,25,25	0
3	K	B	1277	1/1	0.98	0.06	-3.15	30,30,30,30	0
2	GOL	D	1275	6/6	0.80	0.19	-	31,32,37,38	0
2	GOL	A	1278	6/6	0.73	0.25	-	52,53,53,53	0
3	K	A	1280	1/1	0.95	0.06	-	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.