



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:56 pm GMT

PDB ID : 2WJ6  
Title : CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE (HOD) FROM ARTHROBACTER NITROGUAJACOLICUS RU61A COMPLEXED WITH ITS NATURAL PRODUCT N-ACETYLANTHRANILATE  
Authors : Steiner, R.A.  
Deposited on : 2009-05-22  
Resolution : 2.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

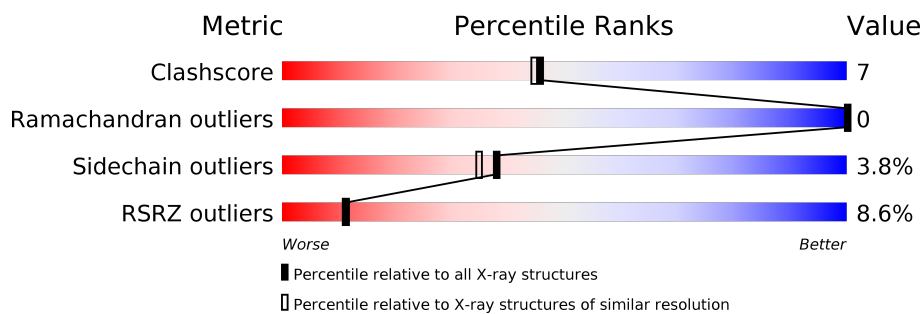
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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>9%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	276	<div> <div>6%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
1	C	276	<div> <div>8%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	D	276	<div> <div>11%</div> <div>84%</div> <div>13%</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	A	1278	-	-	X	X
2	GOL	A	1279	-	-	X	-
2	GOL	A	1280	-	-	X	-
2	GOL	A	1281	-	-	X	-
2	GOL	B	1277	-	-	X	-
2	GOL	B	1278	-	-	X	-
2	GOL	B	1279	-	-	X	-
2	GOL	B	1280	-	-	X	-
2	GOL	C	1277	-	-	X	-
2	GOL	D	1276	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9896 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	274	Total	C	N	O	S	0	0	0
			2234	1426	391	409	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	2	0
			2242	1432	390	412	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	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	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	C	1	Total	C	O	0	0
			6	3	3		

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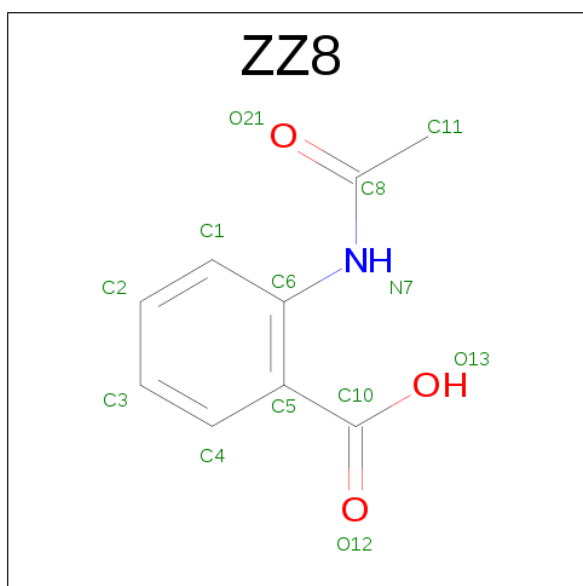
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- 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 2-(ACETYLAMINO)BENZOIC ACID (three-letter code: ZZ8) (formula: C<sub>9</sub>H<sub>9</sub>NO<sub>3</sub>).



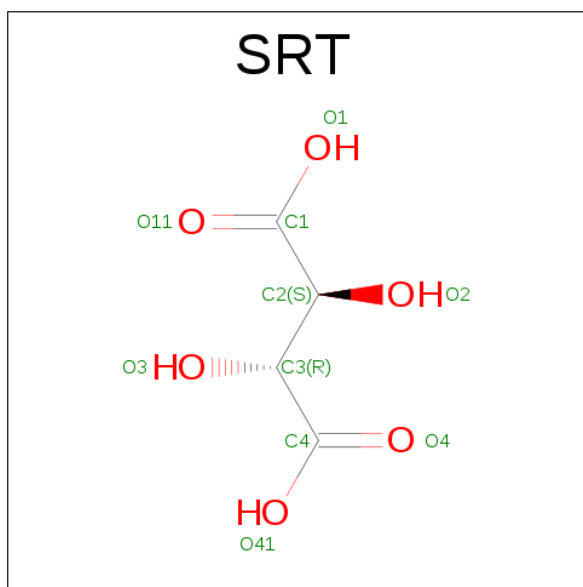
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	9	1	3		
4	B	1	Total	C	N	O	0	0
			13	9	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			13	9	1	3		
4	D	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	179	Total	O	0	0
			179	179		
6	B	190	Total	O	0	0
			190	190		

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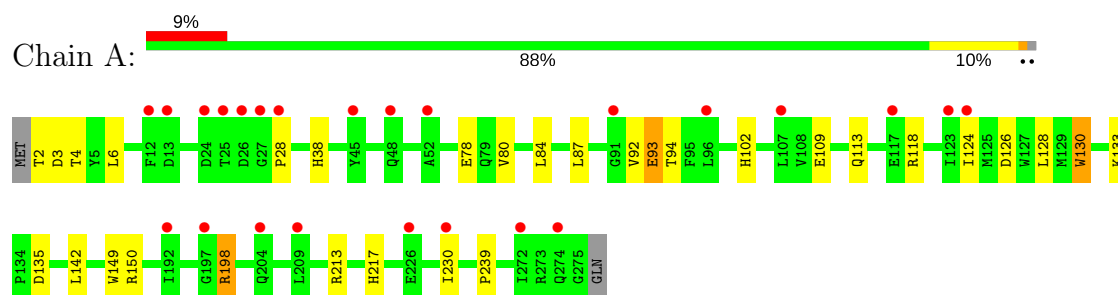
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	216	Total 216	O 216	0	0
6	D	156	Total 156	O 156	0	0



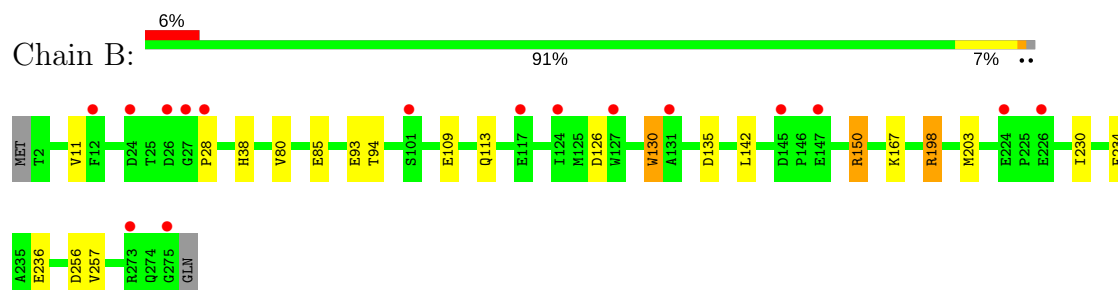
### 3 Residue-property plots [i](#)

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

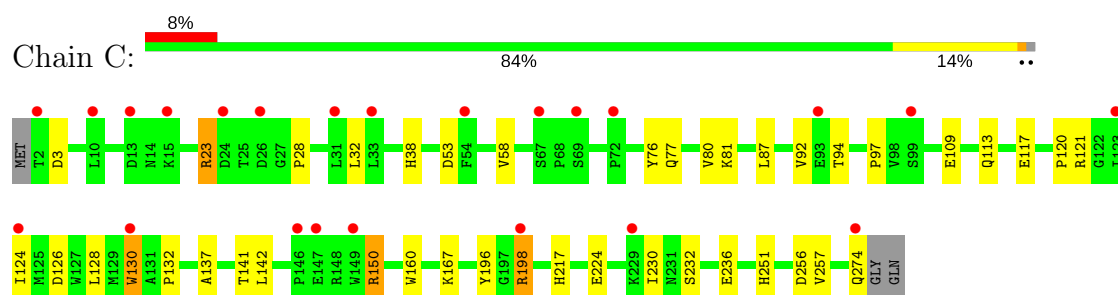
#### • Molecule 1: 1H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



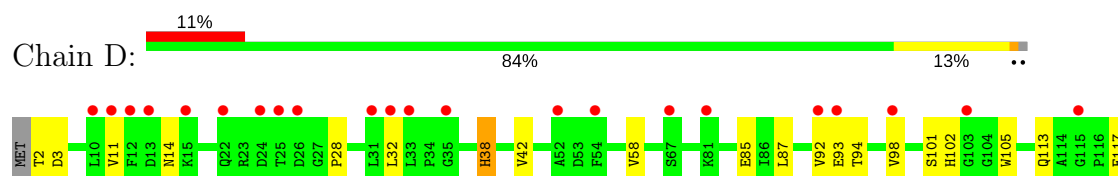
#### • Molecule 1: 1H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE

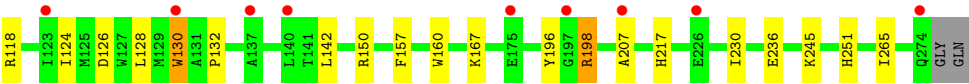


#### • Molecule 1: 1H-3-HYDROXY-4-OXOQUINALDINE 2,4-DIOXYGENASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	44.94Å 167.09Å 167.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.52 – 2.00 28.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.52-2.00) 94.1 (28.74-2.00)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.179 , 0.216 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.137 for -h,l,k	Xtriage
Reported twinning fraction	0.486 for H, K, L 0.514 for -H, L, K	Depositor
Outliers	6 of 81829 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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 29.58 % 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 1.5134e-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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, K, SRT, ZZ8

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	0.71	0/2305	0.72	0/3137
1	B	0.70	1/2305 (0.0%)	0.70	0/3137
1	C	0.75	1/2310 (0.0%)	0.71	0/3144
1	D	0.71	1/2319 (0.0%)	0.71	0/3157
All	All	0.72	3/9239 (0.0%)	0.71	0/12575

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	LYS	CB-CG	-7.12	1.33	1.52
1	D	167	LYS	CB-CG	-5.21	1.38	1.52
1	C	167	LYS	CD-CE	-5.05	1.38	1.51

There are no bond angle outliers.

There are no chirality outliers.

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	2234	0	2125	34	0
1	B	2234	0	2125	17	0
1	C	2236	0	2130	31	0
1	D	2242	0	2134	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	47	20	0
2	B	30	0	40	10	0
2	C	24	0	32	12	0
2	D	12	0	16	9	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	8	0	0
4	B	13	0	8	1	0
4	C	13	0	8	0	0
4	D	13	0	8	1	0
5	A	20	0	8	0	0
5	B	10	0	4	0	0
5	C	10	0	4	0	0
5	D	10	0	4	0	0
6	A	179	0	0	9	0
6	B	190	0	0	6	0
6	C	216	0	0	9	0
6	D	156	0	0	2	0
All	All	9896	0	8701	130	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 7.

All (130) 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)
2:B:1277:GOL:O1	2:B:1280:GOL:H12	1.43	1.19
2:B:1277:GOL:O2	2:B:1280:GOL:H32	1.54	1.06
1:A:128:LEU:HD13	2:A:1278:GOL:H32	1.05	1.03
1:A:128:LEU:HD13	2:A:1278:GOL:C3	1.88	1.02
1:A:128:LEU:CD1	2:A:1278:GOL:H32	1.96	0.95
1:C:77[B]:GLN:OE1	6:C:2074:HOH:O	1.91	0.88
2:B:1278:GOL:O2	2:B:1279:GOL:H2	1.78	0.84
1:B:94:THR:HG21	6:B:2068:HOH:O	1.76	0.83
1:C:128:LEU:CD1	2:C:1277:GOL:H2	2.12	0.79
1:C:128:LEU:HD12	2:C:1277:GOL:H2	1.69	0.74
2:A:1279:GOL:H11	6:A:2141:HOH:O	1.89	0.71
1:C:128:LEU:HG	2:C:1277:GOL:H31	1.74	0.70
1:D:101:SER:OG	2:D:1276:GOL:H32	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:HIS:CE1	2:C:1277:GOL:H32	2.30	0.67
1:C:76:TYR:CE1	2:C:1278:GOL:H31	2.31	0.66
2:B:1277:GOL:HO1	2:B:1280:GOL:H12	1.56	0.66
2:B:1278:GOL:O1	2:B:1279:GOL:H12	1.96	0.65
2:A:1280:GOL:O1	2:A:1281:GOL:H32	1.98	0.64
1:D:101:SER:HG	2:D:1276:GOL:H32	1.63	0.63
1:D:207:ALA:HB1	2:D:1275:GOL:H11	1.80	0.63
1:C:232:SER:O	1:C:236:GLU:HG3	1.99	0.63
1:A:128:LEU:HD11	2:A:1279:GOL:C2	2.29	0.63
1:D:128:LEU:CD1	2:D:1276:GOL:H2	2.28	0.62
1:A:2:THR:HG23	6:A:2030:HOH:O	1.98	0.62
1:B:135:ASP:HB2	6:B:2091:HOH:O	1.99	0.61
2:B:1278:GOL:O2	2:B:1279:GOL:C2	2.48	0.61
1:A:133:LYS:HG2	2:A:1278:GOL:O2	1.99	0.61
2:B:1278:GOL:H11	2:B:1279:GOL:O2	1.99	0.61
1:A:28:PRO:HA	1:A:94:THR:HG23	1.84	0.59
1:B:150:ARG:NH1	6:B:2099:HOH:O	2.36	0.58
1:B:28:PRO:HB3	1:B:94:THR:HG23	1.86	0.58
2:A:1280:GOL:H11	2:A:1281:GOL:O3	2.03	0.57
1:C:87:LEU:HD22	1:C:92:VAL:HG11	1.88	0.56
1:D:28:PRO:HA	1:D:94:THR:HG23	1.88	0.55
1:A:78:GLU:CD	6:A:2050:HOH:O	2.45	0.54
1:A:239:PRO:HA	6:A:2169:HOH:O	2.06	0.54
1:D:28:PRO:HB3	1:D:94:THR:HG23	1.89	0.54
1:A:4:THR:O	1:A:4:THR:CG2	2.55	0.54
1:C:130:TRP:CE3	1:C:230:ILE:HD13	2.43	0.54
1:D:128:LEU:HD12	2:D:1276:GOL:H2	1.89	0.54
2:C:1277:GOL:H11	6:C:2173:HOH:O	2.08	0.54
2:B:1277:GOL:O1	2:B:1280:GOL:C1	2.36	0.53
1:C:28:PRO:HB3	1:C:94:THR:HG23	1.90	0.52
2:A:1279:GOL:C1	6:A:2141:HOH:O	2.52	0.52
1:C:76:TYR:CD1	2:C:1278:GOL:H31	2.45	0.52
1:D:87:LEU:HD22	1:D:92:VAL:HG11	1.91	0.52
1:A:128:LEU:HD11	2:A:1279:GOL:H2	1.90	0.52
1:D:28:PRO:CB	1:D:94:THR:HG23	2.39	0.52
2:A:1280:GOL:C1	2:A:1281:GOL:H32	2.40	0.51
1:B:28:PRO:CB	1:B:94:THR:HG23	2.40	0.51
1:C:81:LYS:HG2	6:C:2033:HOH:O	2.10	0.51
1:A:133:LYS:H	2:A:1278:GOL:C2	2.24	0.51
4:B:1282:ZZ8:C10	4:B:1282:ZZ8:O21	2.59	0.51
1:C:128:LEU:HG	2:C:1277:GOL:C3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:HIS:CE1	2:D:1276:GOL:H31	2.46	0.51
1:C:274:GLN:OE1	6:C:2213:HOH:O	2.19	0.51
1:D:160:TRP:HE1	2:D:1276:GOL:C1	2.23	0.51
1:A:28:PRO:CA	1:A:94:THR:HG23	2.41	0.50
1:D:28:PRO:CA	1:D:94:THR:HG23	2.41	0.50
1:B:198:ARG:CZ	1:B:198:ARG:HB2	2.42	0.50
1:A:128:LEU:HB3	2:A:1278:GOL:H31	1.94	0.49
1:D:157:PHE:HB2	6:D:2084:HOH:O	2.11	0.49
1:D:130:TRP:CE3	1:D:230:ILE:HD13	2.48	0.49
4:D:1278:ZZ8:O21	4:D:1278:ZZ8:C10	2.61	0.48
2:B:1278:GOL:H2	1:D:245:LYS:O	2.13	0.48
1:B:93:GLU:HG3	6:B:2066:HOH:O	2.14	0.48
1:C:28:PRO:CB	1:C:94:THR:HG23	2.44	0.47
1:A:87:LEU:HD22	1:A:92:VAL:HG11	1.97	0.47
1:A:128:LEU:HD11	2:A:1279:GOL:H32	1.97	0.47
2:C:1277:GOL:H31	6:C:2100:HOH:O	2.13	0.47
1:A:213:ARG:NH2	6:A:2139:HOH:O	2.48	0.47
1:A:28:PRO:HA	1:A:94:THR:CG2	2.45	0.47
1:A:28:PRO:CB	1:A:94:THR:HG23	2.45	0.47
1:C:198:ARG:CZ	1:C:198:ARG:HB2	2.44	0.47
1:C:224:GLU:OE2	6:C:2176:HOH:O	2.20	0.47
1:D:28:PRO:HA	1:D:94:THR:CG2	2.45	0.47
1:C:160:TRP:HE1	2:C:1277:GOL:H12	1.79	0.46
2:A:1280:GOL:O2	2:A:1281:GOL:H11	2.16	0.46
1:A:130:TRP:NE1	2:A:1278:GOL:O2	2.48	0.46
1:A:149:TRP:HE1	2:A:1277:GOL:H2	1.80	0.46
1:A:93:GLU:O	1:A:118:ARG:HG2	2.16	0.46
1:D:32:LEU:HB2	1:D:58:VAL:HG22	1.98	0.45
1:C:160:TRP:HE1	2:C:1277:GOL:C1	2.29	0.45
1:A:28:PRO:HB3	1:A:94:THR:HG23	1.98	0.45
1:B:28:PRO:HA	1:B:94:THR:HG23	1.98	0.45
1:C:80:VAL:HG21	1:C:109:GLU:HB3	1.99	0.45
1:C:120:PRO:HD2	6:C:2092:HOH:O	2.17	0.45
1:A:102:HIS:HB2	6:A:2172:HOH:O	2.17	0.45
1:A:135:ASP:HB2	6:A:2076:HOH:O	2.17	0.44
1:D:102:HIS:HD1	1:D:105:TRP:HE1	1.63	0.44
1:B:256:ASP:OD1	1:B:257:VAL:HG22	2.17	0.44
1:C:28:PRO:HA	1:C:94:THR:HG23	1.99	0.44
1:D:11:VAL:HG13	1:D:85:GLU:CG	2.47	0.44
1:C:150:ARG:NH2	6:C:2119:HOH:O	2.42	0.44
1:A:128:LEU:HD11	2:A:1279:GOL:H12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:OE1	6:B:2159:HOH:O	2.21	0.44
1:C:97:PRO:HD2	1:C:121:ARG:O	2.18	0.44
1:C:124:ILE:HG13	1:C:217:HIS:HA	2.00	0.44
1:A:124:ILE:HG13	1:A:217:HIS:HA	1.99	0.43
1:C:23:ARG:HD3	6:C:2030:HOH:O	2.18	0.43
1:B:203:MET:HE1	1:B:234:PHE:HB2	2.00	0.43
1:D:98:VAL:HG11	1:D:265:ILE:HD11	2.00	0.43
1:B:28:PRO:CA	1:B:94:THR:HG23	2.49	0.43
1:A:109:GLU:OE1	6:A:2063:HOH:O	2.21	0.43
1:A:130:TRP:CE3	1:A:230:ILE:HD13	2.53	0.43
1:A:84:LEU:HA	1:A:84:LEU:HD23	1.91	0.42
1:B:28:PRO:HA	1:B:94:THR:CG2	2.49	0.42
1:A:3:ASP:OD1	1:A:6:LEU:HD22	2.20	0.42
1:D:93:GLU:O	1:D:118:ARG:HG2	2.18	0.42
1:A:198:ARG:CZ	1:A:198:ARG:HB2	2.50	0.42
1:C:137:ALA:O	1:C:141:THR:HG23	2.20	0.42
1:A:80:VAL:HG21	1:A:109:GLU:HB3	2.02	0.42
1:D:198:ARG:HB2	1:D:198:ARG:CZ	2.49	0.42
1:D:124:ILE:HG13	1:D:217:HIS:HA	2.02	0.42
1:C:53:ASP:HB3	2:C:1275:GOL:H12	2.02	0.41
1:B:80:VAL:HG21	1:B:109:GLU:HB3	2.02	0.41
1:B:130:TRP:CE3	1:B:230:ILE:HD13	2.54	0.41
1:C:32:LEU:HB2	1:C:58:VAL:HG22	2.02	0.41
1:D:14:ASN:OD1	6:D:2009:HOH:O	2.21	0.41
2:B:1278:GOL:C1	2:B:1279:GOL:O2	2.67	0.41
1:D:160:TRP:HE1	2:D:1276:GOL:H12	1.86	0.41
1:C:132:PRO:HD3	1:C:196:TYR:CD2	2.56	0.41
1:C:256:ASP:OD1	1:C:257:VAL:HG22	2.20	0.41
1:D:251:HIS:CE1	2:D:1276:GOL:C3	3.04	0.41
1:A:128:LEU:HD11	2:A:1279:GOL:C3	2.50	0.40
1:D:132:PRO:HD3	1:D:196:TYR:CD2	2.56	0.40
1:D:38:HIS:CE1	1:D:42:VAL:HG21	2.56	0.40
1:B:150:ARG:HG2	6:B:2101:HOH:O	2.20	0.40
2:A:1280:GOL:H11	2:A:1281:GOL:C3	2.50	0.40
1:B:11:VAL:HG13	1:B:85:GLU:CG	2.52	0.40

There are no symmetry-related clashes.



## 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
1	B	272/276 (99%)	265 (97%)	7 (3%)	0	100	100
1	C	272/276 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
All	All	1089/1104 (99%)	1063 (98%)	26 (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%)	228 (97%)	8 (3%)	42	40
1	B	236/238 (99%)	229 (97%)	7 (3%)	46	46
1	C	237/238 (100%)	227 (96%)	10 (4%)	34	30
1	D	238/238 (100%)	226 (95%)	12 (5%)	28	23
All	All	947/952 (100%)	910 (96%)	37 (4%)	38	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	93	GLU

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	126	ASP
1	A	130	TRP
1	A	142	LEU
1	A	150	ARG
1	A	198	ARG
1	B	38	HIS
1	B	113	GLN
1	B	126	ASP
1	B	130	TRP
1	B	142	LEU
1	B	150	ARG
1	B	198	ARG
1	C	3	ASP
1	C	23	ARG
1	C	38	HIS
1	C	113	GLN
1	C	117	GLU
1	C	126	ASP
1	C	130	TRP
1	C	142	LEU
1	C	150	ARG
1	C	198	ARG
1	D	2	THR
1	D	3	ASP
1	D	38	HIS
1	D	113	GLN
1	D	117	GLU
1	D	126	ASP
1	D	130	TRP
1	D	142	LEU
1	D	150	ARG
1	D	198	ARG
1	D	236[A]	GLU
1	D	236[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	ASN
1	C	7	HIS
1	C	22	GLN

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Mol	Chain	Res	Type
1	D	14	ASN
1	D	113	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 5 are monoatomic - leaving 26 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	0.60	0	5,5,5	1.11	0
2	GOL	A	1277	-	5,5,5	0.37	0	5,5,5	0.48	0
2	GOL	A	1278	-	5,5,5	0.71	0	5,5,5	1.17	0
2	GOL	A	1279	-	5,5,5	0.58	0	5,5,5	0.95	0
2	GOL	A	1280	-	5,5,5	0.59	0	5,5,5	1.05	0
2	GOL	A	1281	-	5,5,5	0.77	0	5,5,5	1.32	0
4	ZZ8	A	1284	-	10,13,13	2.15	2 (20%)	13,17,17	2.30	5 (38%)
5	SRT	A	1285	-	3,9,9	0.55	0	6,12,12	2.58	5 (83%)
5	SRT	A	1286	3	3,9,9	1.56	1 (33%)	6,12,12	3.29	3 (50%)
2	GOL	B	1276	-	5,5,5	0.45	0	5,5,5	0.30	0
2	GOL	B	1277	-	5,5,5	0.41	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	1278	-	5,5,5	0.78	0	5,5,5	2.08	2 (40%)
2	GOL	B	1279	-	5,5,5	0.59	0	5,5,5	1.44	1 (20%)
2	GOL	B	1280	-	5,5,5	0.62	0	5,5,5	0.86	0
4	ZZ8	B	1282	-	10,13,13	2.67	3 (30%)	13,17,17	1.80	4 (30%)
5	SRT	B	1283	-	3,9,9	0.59	0	6,12,12	1.72	2 (33%)
2	GOL	C	1275	-	5,5,5	0.36	0	5,5,5	0.31	0
2	GOL	C	1276	3	5,5,5	0.37	0	5,5,5	0.54	0
2	GOL	C	1277	-	5,5,5	1.03	0	5,5,5	0.96	0
2	GOL	C	1278	-	5,5,5	0.93	0	5,5,5	1.06	0
4	ZZ8	C	1280	-	10,13,13	2.94	2 (20%)	13,17,17	2.22	4 (30%)
5	SRT	C	1281	-	3,9,9	0.49	0	6,12,12	2.19	2 (33%)
2	GOL	D	1275	-	5,5,5	0.39	0	5,5,5	0.65	0
2	GOL	D	1276	-	5,5,5	0.83	0	5,5,5	0.77	0
4	ZZ8	D	1278	-	10,13,13	2.31	2 (20%)	13,17,17	2.00	4 (30%)
5	SRT	D	1279	-	3,9,9	1.20	1 (33%)	6,12,12	2.29	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	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1278	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1279	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1280	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1281	-	-	0/4/4/4	0/0/0/0
4	ZZ8	A	1284	-	-	0/4/8/8	0/1/1/1
5	SRT	A	1285	-	-	0/4/12/12	0/0/0/0
5	SRT	A	1286	3	-	0/4/12/12	0/0/0/0
2	GOL	B	1276	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1277	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1278	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1279	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1280	-	-	0/4/4/4	0/0/0/0
4	ZZ8	B	1282	-	-	0/4/8/8	0/1/1/1
5	SRT	B	1283	-	-	0/4/12/12	0/0/0/0
2	GOL	C	1275	-	-	0/4/4/4	0/0/0/0
2	GOL	C	1276	3	-	0/4/4/4	0/0/0/0
2	GOL	C	1277	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	1278	-	-	0/4/4/4	0/0/0/0
4	ZZ8	C	1280	-	-	0/4/8/8	0/1/1/1
5	SRT	C	1281	-	-	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	ZZ8	D	1278	-	-	0/4/8/8	0/1/1/1
5	SRT	D	1279	-	-	0/4/12/12	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1282	ZZ8	C6-N7	-3.18	1.35	1.41
4	D	1278	ZZ8	C6-N7	-3.02	1.35	1.41
4	A	1284	ZZ8	C6-N7	-2.80	1.36	1.41
4	C	1280	ZZ8	C6-N7	-2.33	1.37	1.41
4	B	1282	ZZ8	C8-N7	-2.13	1.32	1.35
5	D	1279	SRT	O2-C2	2.07	1.46	1.42
5	A	1286	SRT	O2-C2	2.42	1.47	1.42
4	A	1284	ZZ8	C5-C6	5.86	1.48	1.40
4	D	1278	ZZ8	C5-C6	6.01	1.49	1.40
4	B	1282	ZZ8	C5-C6	7.06	1.50	1.40
4	C	1280	ZZ8	C5-C6	8.77	1.52	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1286	SRT	O2-C2-C1	-6.17	96.12	111.13
5	A	1285	SRT	C1-C2-C3	-4.35	103.75	113.11
5	D	1279	SRT	O3-C3-C4	-4.03	101.31	111.13
5	C	1281	SRT	O3-C3-C2	-3.99	96.85	108.88
2	B	1278	GOL	C3-C2-C1	-3.23	98.70	111.52
5	A	1286	SRT	C1-C2-C3	-3.11	106.42	113.11
4	C	1280	ZZ8	C1-C6-N7	-3.10	114.53	121.84
4	B	1282	ZZ8	C1-C6-N7	-3.09	114.56	121.84
4	C	1280	ZZ8	C4-C5-C10	-2.96	115.68	120.23
4	B	1282	ZZ8	C11-C8-N7	-2.89	110.78	115.02
4	A	1284	ZZ8	C1-C6-N7	-2.77	115.31	121.84
5	B	1283	SRT	O2-C2-C1	-2.68	104.62	111.13
5	A	1285	SRT	C4-C3-C2	-2.35	108.06	113.11
4	D	1278	ZZ8	C11-C8-N7	-2.34	111.58	115.02
5	B	1283	SRT	C1-C2-C3	-2.31	108.13	113.11
5	A	1285	SRT	O3-C3-C2	-2.28	102.01	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1281	SRT	C1-C2-C3	-2.24	108.29	113.11
4	A	1284	ZZ8	C1-C6-C5	-2.23	116.75	119.86
4	D	1278	ZZ8	C1-C6-N7	-2.12	116.84	121.84
4	A	1284	ZZ8	O21-C8-C11	-2.08	118.28	122.06
5	A	1285	SRT	O2-C2-C1	-2.04	106.16	111.13
2	B	1279	GOL	C3-C2-C1	2.03	119.59	111.52
5	D	1279	SRT	C4-C3-C2	2.13	117.68	113.11
2	B	1278	GOL	O2-C2-C1	2.38	120.08	108.84
5	A	1285	SRT	O3-C3-C4	2.45	117.10	111.13
4	B	1282	ZZ8	O21-C8-N7	2.59	126.43	123.06
5	D	1279	SRT	O2-C2-C3	2.69	116.98	108.88
4	D	1278	ZZ8	C5-C6-N7	2.78	124.54	119.45
4	C	1280	ZZ8	O21-C8-N7	3.42	127.51	123.06
5	A	1286	SRT	O2-C2-C3	3.79	120.30	108.88
4	B	1282	ZZ8	C5-C6-N7	3.85	126.48	119.45
4	A	1284	ZZ8	C5-C6-N7	4.49	127.65	119.45
4	C	1280	ZZ8	C5-C6-N7	4.56	127.78	119.45
4	A	1284	ZZ8	O21-C8-N7	4.74	129.22	123.06
4	D	1278	ZZ8	O21-C8-N7	4.87	129.40	123.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1277	GOL	1	0
2	A	1278	GOL	7	0
2	A	1279	GOL	7	0
2	A	1280	GOL	5	0
2	A	1281	GOL	5	0
2	B	1277	GOL	4	0
2	B	1278	GOL	6	0
2	B	1279	GOL	5	0
2	B	1280	GOL	4	0
4	B	1282	ZZ8	1	0
2	C	1275	GOL	1	0
2	C	1277	GOL	9	0
2	C	1278	GOL	2	0
2	D	1275	GOL	1	0
2	D	1276	GOL	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1278	ZZ8	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, 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%)	0.72	24 (8%) <b>11</b> <b>11</b>	12, 20, 29, 34	0
1	B	274/276 (99%)	0.66	16 (5%) <b>24</b> <b>24</b>	12, 20, 29, 34	0
1	C	273/276 (98%)	0.82	23 (8%) <b>12</b> <b>12</b>	12, 20, 29, 36	0
1	D	273/276 (98%)	0.78	31 (11%) <b>6</b> <b>6</b>	12, 20, 29, 36	0
All	All	1094/1104 (99%)	0.74	94 (8%) <b>11</b> <b>11</b>	12, 20, 29, 36	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ASP	6.1
1	B	24	ASP	6.1
1	B	26	ASP	6.1
1	A	13	ASP	5.5
1	D	54	PHE	5.2
1	C	274	GLN	5.0
1	A	91	GLY	4.9
1	D	24	ASP	4.5
1	A	24	ASP	4.5
1	D	13	ASP	4.5
1	A	226	GLU	4.4
1	A	230	ILE	3.6
1	B	275	GLY	3.4
1	A	25	THR	3.4
1	D	25	THR	3.4
1	C	67	SER	3.4
1	D	274	GLN	3.2
1	C	146	PRO	3.2
1	B	226	GLU	3.2
1	B	117	GLU	3.1
1	D	93	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	33	LEU	2.9
1	A	117	GLU	2.9
1	B	12	PHE	2.9
1	D	137	ALA	2.8
1	C	93	GLU	2.8
1	A	27	GLY	2.8
1	D	92	VAL	2.8
1	B	147	GLU	2.8
1	A	107	LEU	2.7
1	D	98	VAL	2.7
1	D	123	ILE	2.7
1	B	28	PRO	2.7
1	A	52	ALA	2.7
1	C	123	ILE	2.6
1	D	12	PHE	2.6
1	A	124	ILE	2.6
1	C	15	LYS	2.6
1	C	69	SER	2.5
1	B	27	GLY	2.5
1	C	124	ILE	2.5
1	A	204	GLN	2.5
1	B	224	GLU	2.5
1	A	274	GLN	2.5
1	C	229	LYS	2.5
1	B	145	ASP	2.5
1	D	26	ASP	2.5
1	C	26	ASP	2.4
1	D	11	VAL	2.4
1	B	273	ARG	2.4
1	D	103	GLY	2.4
1	D	81	LYS	2.4
1	A	272	ILE	2.4
1	A	197	GLY	2.4
1	C	72	PRO	2.3
1	C	198	ARG	2.3
1	B	101	SER	2.3
1	D	197	GLY	2.3
1	D	10	LEU	2.3
1	C	2	THR	2.3
1	A	48	GLN	2.3
1	B	124	ILE	2.3
1	A	209	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	24	ASP	2.3
1	B	131	ALA	2.3
1	C	149	TRP	2.3
1	D	35	GLY	2.2
1	D	32	LEU	2.2
1	A	28	PRO	2.2
1	C	31	LEU	2.2
1	A	45	TYR	2.2
1	C	54	PHE	2.2
1	C	99	SER	2.2
1	B	127	TRP	2.2
1	A	96	LEU	2.2
1	C	33	LEU	2.2
1	D	175	GLU	2.2
1	C	13	ASP	2.2
1	A	123	ILE	2.1
1	A	12	PHE	2.1
1	D	22	GLN	2.1
1	C	147	GLU	2.1
1	C	10	LEU	2.1
1	D	52	ALA	2.1
1	D	130	TRP	2.1
1	D	115	GLY	2.1
1	D	31	LEU	2.1
1	D	67	SER	2.1
1	D	15	LYS	2.1
1	C	130	TRP	2.0
1	A	192	ILE	2.0
1	D	207	ALA	2.0
1	D	226	GLU	2.0
1	D	140	LEU	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

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	A	1278	6/6	0.87	0.31	5.50	24,28,30,33	0
2	GOL	B	1280	6/6	0.52	0.27	1.83	19,20,20,22	0
5	SRT	B	1283	10/10	0.90	0.17	1.73	19,24,27,27	0
2	GOL	B	1278	6/6	0.89	0.15	1.37	8,15,18,19	0
2	GOL	B	1276	6/6	0.79	0.23	1.09	32,36,38,38	0
2	GOL	C	1277	6/6	0.96	0.20	0.99	16,19,21,22	0
5	SRT	A	1286	10/10	0.84	0.18	0.96	15,20,23,25	0
2	GOL	A	1279	6/6	0.93	0.18	0.96	19,22,24,26	0
5	SRT	A	1285	10/10	0.90	0.19	0.90	14,18,22,24	0
2	GOL	C	1278	6/6	0.88	0.19	0.86	20,22,23,24	0
5	SRT	D	1279	10/10	0.86	0.20	0.42	16,24,30,34	0
4	ZZ8	B	1282	13/13	0.95	0.19	0.24	8,11,13,14	0
2	GOL	A	1281	6/6	0.90	0.15	0.21	4,16,16,19	0
2	GOL	D	1276	6/6	0.92	0.15	0.06	17,20,22,24	0
2	GOL	A	1276	6/6	0.93	0.14	-0.09	15,20,22,26	0
4	ZZ8	A	1284	13/13	0.95	0.16	-0.09	8,12,15,18	0
5	SRT	C	1281	10/10	0.92	0.13	-0.48	13,23,26,26	0
4	ZZ8	C	1280	13/13	0.95	0.16	-0.57	9,12,14,14	0
4	ZZ8	D	1278	13/13	0.94	0.15	-0.70	2,12,16,16	0
2	GOL	D	1275	6/6	0.91	0.16	-0.75	30,31,32,32	0
2	GOL	C	1276	6/6	0.94	0.12	-0.96	19,21,24,26	0
3	K	D	1277	1/1	0.98	0.07	-1.96	27,27,27,27	0
3	K	A	1282	1/1	0.99	0.06	-3.03	19,19,19,19	0
3	K	C	1279	1/1	0.99	0.04	-3.24	22,22,22,22	0
3	K	B	1281	1/1	0.99	0.06	-3.56	18,18,18,18	0
2	GOL	A	1277	6/6	0.76	0.20	-	34,39,40,42	0
3	K	A	1283	1/1	0.98	0.06	-	21,21,21,21	0
2	GOL	A	1280	6/6	0.90	0.15	-	18,19,21,22	0
2	GOL	B	1277	6/6	0.90	0.18	-	23,26,30,35	0
2	GOL	B	1279	6/6	0.89	0.19	-	14,20,21,26	0
2	GOL	C	1275	6/6	0.79	0.20	-	40,40,41,41	0

## 6.5 Other polymers

There are no such residues in this entry.