



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 02:38 pm GMT

PDB ID : 3QWF  
Title : Crystal structure of the 17beta-hydroxysteroid dehydrogenase from *Cochliobolus lunatus*  
Authors : Cassetta, A.; Lamba, D.; Krastanova, I.; Stojan, J.; Lanisnik-Rizner, T.; Kristan, K.; Brunskole, M.  
Deposited on : 2011-02-28  
Resolution : 1.88 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

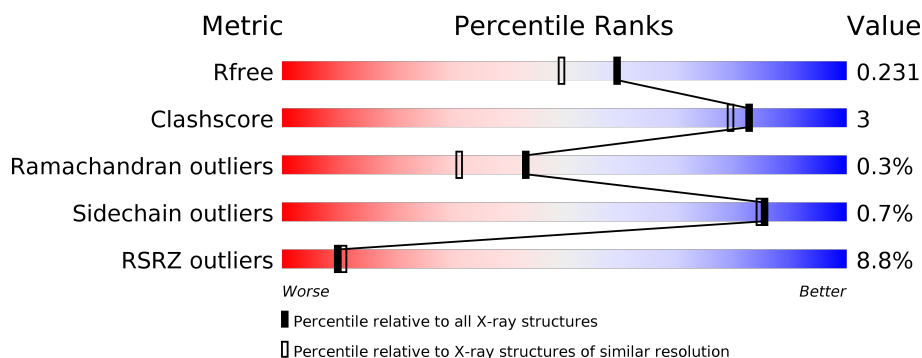
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	111664	8255 (1.90-1.86)
Clashscore	122126	9028 (1.90-1.86)
Ramachandran outliers	120053	8930 (1.90-1.86)
Sidechain outliers	120020	8930 (1.90-1.86)
RSRZ outliers	108989	8087 (1.90-1.86)

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	270	<div> <div>9%</div> <div>91%</div> <div>6%</div> </div>
1	B	270	<div> <div>7%</div> <div>88%</div> <div>8%</div> </div>
1	C	270	<div> <div>6%</div> <div>92%</div> <div>2%</div> </div>
1	D	270	<div> <div>10%</div> <div>89%</div> <div>8%</div> </div>
1	E	270	<div> <div>9%</div> <div>94%</div> <div>2%</div> </div>
1	F	270	<div> <div>8%</div> <div>90%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	270	<div><div></div><div>9%</div><div>92%</div><div>5%</div><div></div></div>
1	H	270	<div><div></div><div>9%</div><div>89%</div><div>7%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17526 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 17beta-hydroxysteroid dehydrogenase.

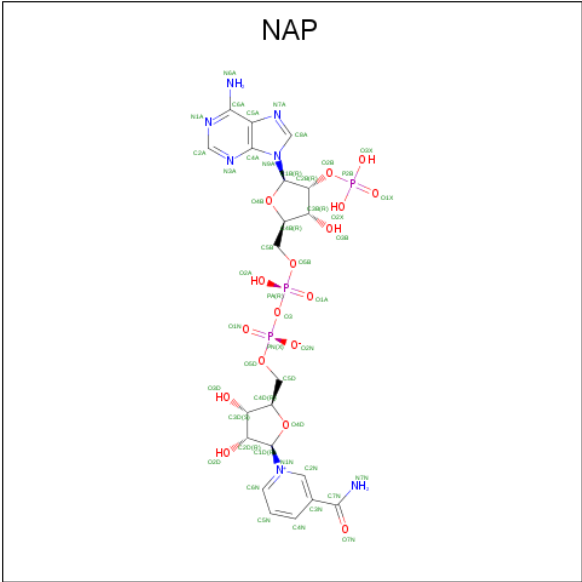
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	B	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	C	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	D	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	E	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	F	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	G	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0
1	H	261	Total 1971	C 1240	N 354	O 374	S 3	0	0	0

- 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	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	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	179	Total	O	0	0
			179	179		
4	C	191	Total	O	0	0
			191	191		
4	D	133	Total	O	0	0
			133	133		

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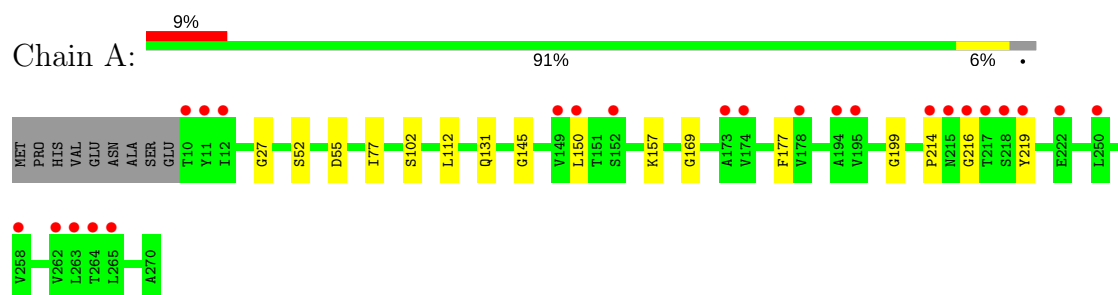
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	155	Total 155	O 155	0	0
4	F	157	Total 157	O 157	0	0
4	G	157	Total 157	O 157	0	0
4	H	149	Total 149	O 149	0	0

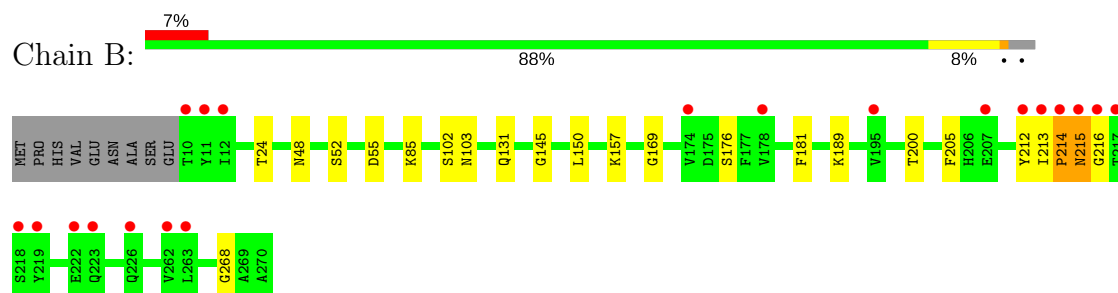
### 3 Residue-property plots [i](#)

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.

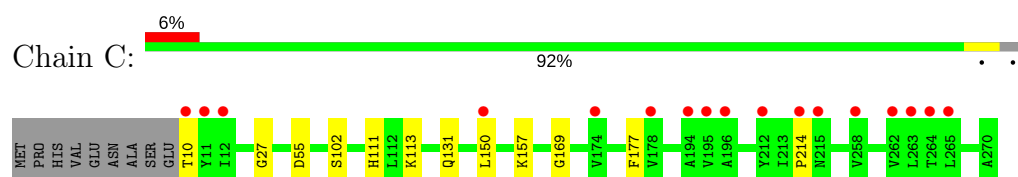
- Molecule 1: 17beta-hydroxysteroid dehydrogenase



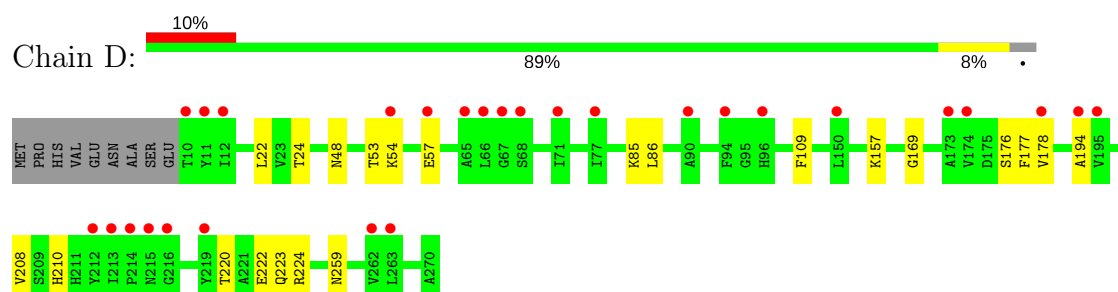
- Molecule 1: 17beta-hydroxysteroid dehydrogenase



- Molecule 1: 17beta-hydroxysteroid dehydrogenase

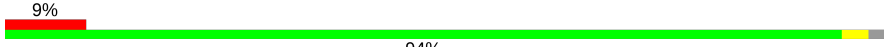


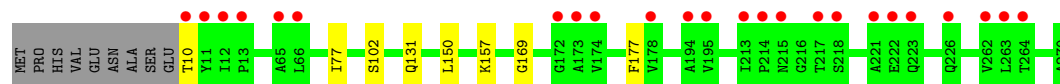
- Molecule 1: 17beta-hydroxysteroid dehydrogenase






- Molecule 1: 17beta-hydroxysteroid dehydrogenase

Chain E: 




- Molecule 1: 17beta-hydroxysteroid dehydrogenase

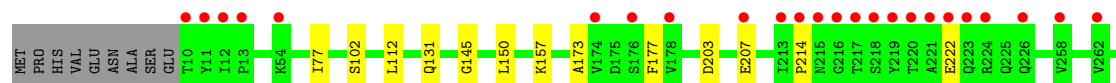
Chain F: 



A270


- Molecule 1: 17beta-hydroxysteroid dehydrogenase

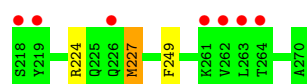
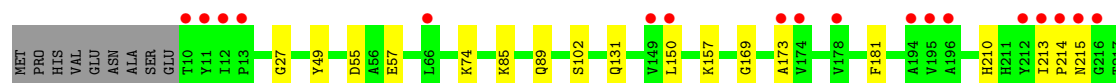
Chain G: 



A270

- Molecule 1: 17beta-hydroxysteroid dehydrogenase

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.52Å 67.83Å 138.89Å 84.20° 85.31° 66.57°	Depositor
Resolution (Å)	37.45 – 1.88 37.45 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.0 (37.45-1.88) 95.9 (37.45-1.88)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0094	Depositor
R, $R_{free}$	0.165 , 0.194 0.208 , 0.231	Depositor DCC
$R_{free}$ test set	8540 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, NAP

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	0.52	0/2010	0.55	0/2720
1	B	0.47	0/2010	0.54	0/2720
1	C	0.47	0/2010	0.54	0/2720
1	D	0.44	0/2010	0.52	0/2720
1	E	0.45	0/2010	0.53	0/2720
1	F	0.46	0/2010	0.55	0/2720
1	G	0.44	0/2010	0.53	0/2720
1	H	0.44	0/2010	0.51	0/2720
All	All	0.46	0/16080	0.53	0/21760

There are no bond length outliers.

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	1971	0	1952	15	0
1	B	1971	0	1952	21	0
1	C	1971	0	1952	9	0
1	D	1971	0	1952	15	0
1	E	1971	0	1952	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1971	0	1952	12	0
1	G	1971	0	1952	10	0
1	H	1971	0	1952	18	0
2	A	12	0	16	4	0
2	B	12	0	16	1	0
2	C	6	0	8	0	0
2	D	6	0	8	2	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
2	G	6	0	8	1	0
2	H	6	0	8	2	0
3	A	48	0	25	1	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
3	D	48	0	25	0	0
3	E	48	0	25	1	0
3	F	48	0	25	0	0
3	G	48	0	25	1	0
3	H	48	0	25	0	0
4	A	193	0	0	1	0
4	B	179	0	0	2	0
4	C	191	0	0	0	0
4	D	133	0	0	0	0
4	E	155	0	0	0	0
4	F	157	0	0	0	0
4	G	157	0	0	0	0
4	H	149	0	0	1	0
All	All	17526	0	15896	88	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 (88) 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:E:157:LYS:HE3	1:F:157:LYS:HE3	1.22	1.12
1:C:157:LYS:HE3	1:D:157:LYS:HE3	1.13	1.08
1:A:157:LYS:HE3	1:B:157:LYS:HE3	1.37	1.02
1:B:214:PRO:O	1:B:215:ASN:CG	2.04	0.96
2:A:302:GOL:H32	4:A:561:HOH:O	1.64	0.95
1:G:157:LYS:HE3	1:H:157:LYS:HE3	1.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:LYS:CE	1:D:157:LYS:HE3	2.05	0.80
1:A:145:GLY:O	2:A:301:GOL:H32	1.88	0.73
1:B:189:LYS:HE2	4:B:558:HOH:O	1.95	0.67
1:B:214:PRO:O	1:B:215:ASN:ND2	2.29	0.66
1:D:222:GLU:HB2	2:D:301:GOL:H11	1.78	0.66
1:A:216:GLY:HA2	1:A:219:TYR:HD2	1.62	0.64
1:B:145:GLY:O	2:B:302:GOL:H32	1.98	0.64
1:E:157:LYS:HE3	1:F:157:LYS:CE	2.14	0.64
1:H:57:GLU:HG3	4:H:536:HOH:O	1.99	0.63
1:G:131:GLN:HB3	1:G:150:LEU:HD13	1.81	0.63
1:B:215:ASN:OD1	1:B:216:GLY:N	2.25	0.63
1:H:224:ARG:HA	1:H:227:MET:HE2	1.80	0.62
1:E:77:ILE:HG12	3:E:302:NAP:H2A	1.82	0.61
1:B:215:ASN:CG	1:B:216:GLY:H	2.04	0.61
1:F:109:PHE:CE2	1:F:208:VAL:HB	2.36	0.60
1:F:215:ASN:HB2	1:F:219:TYR:HE2	1.67	0.60
1:B:214:PRO:O	1:B:215:ASN:OD1	2.19	0.59
1:E:131:GLN:HB3	1:E:150:LEU:HD13	1.84	0.59
1:F:213:ILE:HG22	1:F:216:GLY:H	1.65	0.59
1:B:212:TYR:O	1:B:213:ILE:HG13	2.05	0.56
1:A:199:GLY:HA3	2:A:302:GOL:H11	1.86	0.56
1:A:131:GLN:HB3	1:A:150:LEU:HD13	1.88	0.55
1:H:131:GLN:HB3	1:H:150:LEU:HD13	1.88	0.55
1:H:249:PHE:N	2:H:301:GOL:H32	2.22	0.55
1:H:213:ILE:HG21	1:H:227:MET:HE1	1.90	0.54
1:C:111:HIS:ND1	1:C:113:LYS:HG2	2.23	0.54
1:D:53:THR:O	1:D:57:GLU:HG2	2.08	0.53
1:D:220:THR:HG23	1:D:223:GLN:HE21	1.73	0.53
1:G:177:PHE:CE1	1:H:169:GLY:HA3	2.43	0.53
1:H:213:ILE:HG21	1:H:227:MET:CE	2.39	0.52
1:B:24:THR:HA	1:B:48:ASN:HB3	1.92	0.52
1:H:85:LYS:HE2	1:H:89:GLN:NE2	2.25	0.52
1:A:157:LYS:CE	1:B:157:LYS:HE3	2.26	0.51
1:C:131:GLN:HB3	1:C:150:LEU:HD13	1.93	0.51
1:A:102:SER:HB3	1:A:150:LEU:HD22	1.91	0.51
1:D:222:GLU:CB	2:D:301:GOL:H11	2.42	0.50
1:C:102:SER:HB3	1:C:150:LEU:HD22	1.94	0.50
1:E:169:GLY:HA3	1:F:177:PHE:CE1	2.47	0.49
1:H:249:PHE:HA	2:H:301:GOL:H12	1.95	0.48
1:H:210:HIS:HA	1:H:224:ARG:HD2	1.94	0.48
1:B:214:PRO:C	1:B:215:ASN:CG	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:HB3	1:B:55:ASP:HB2	1.94	0.48
1:G:145:GLY:O	2:G:301:GOL:H32	2.13	0.48
1:A:77:ILE:HG12	3:A:303:NAP:H2A	1.96	0.47
1:E:177:PHE:CE1	1:F:169:GLY:HA3	2.49	0.47
1:G:77:ILE:HG12	3:G:302:NAP:H2A	1.95	0.47
1:B:268:GLY:HA2	1:D:259:ASN:O	2.13	0.47
1:A:177:PHE:CE1	1:B:169:GLY:HA3	2.50	0.47
1:B:102:SER:HB3	1:B:150:LEU:HD22	1.98	0.46
1:C:169:GLY:HA3	1:D:177:PHE:CE1	2.50	0.46
1:A:199:GLY:HA3	2:A:302:GOL:C1	2.46	0.45
1:H:102:SER:HB3	1:H:150:LEU:HD22	1.98	0.45
1:C:177:PHE:CE1	1:D:169:GLY:HA3	2.51	0.45
1:G:203:ASP:O	1:G:207:GLU:HG2	2.16	0.45
1:F:213:ILE:HG22	1:F:216:GLY:N	2.32	0.45
1:G:173:ALA:HB2	1:H:173:ALA:HB2	1.98	0.45
1:G:157:LYS:CE	1:H:157:LYS:HE3	2.34	0.44
1:B:131:GLN:HB3	1:B:150:LEU:HD13	2.00	0.44
1:F:27:GLY:O	1:F:55:ASP:HB3	2.18	0.43
1:C:27:GLY:O	1:C:55:ASP:HB3	2.19	0.43
1:G:102:SER:HB3	1:G:150:LEU:HD22	1.99	0.43
1:E:102:SER:HB3	1:E:150:LEU:HD22	2.00	0.43
1:H:49:TYR:CZ	1:H:74:LYS:HB2	2.53	0.43
1:B:85:LYS:HB3	4:B:574:HOH:O	2.18	0.42
1:D:210:HIS:HA	1:D:224:ARG:HD2	2.01	0.42
1:F:24:THR:HA	1:F:48:ASN:HB3	2.01	0.42
1:A:52:SER:HB3	1:A:55:ASP:HB2	2.02	0.42
1:F:109:PHE:HE2	1:F:208:VAL:HB	1.84	0.42
1:B:200:THR:O	1:B:205:PHE:HB2	2.20	0.42
1:A:27:GLY:O	1:A:55:ASP:HB3	2.20	0.42
1:H:85:LYS:HE2	1:H:89:GLN:HE22	1.85	0.41
1:C:169:GLY:HA2	1:D:176:SER:HB2	2.02	0.41
1:A:112:LEU:HD13	1:B:181:PHE:CE1	2.55	0.41
1:G:112:LEU:HD13	1:H:181:PHE:CE1	2.56	0.41
1:H:27:GLY:O	1:H:55:ASP:HB3	2.20	0.41
1:D:109:PHE:CE2	1:D:208:VAL:HB	2.55	0.41
1:D:22:LEU:HD11	1:D:86:LEU:HG	2.02	0.41
1:A:169:GLY:HA2	1:B:176:SER:HB2	2.02	0.41
1:D:178:VAL:HG11	1:D:194:ALA:HB2	2.03	0.41
1:D:24:THR:HA	1:D:48:ASN:HB3	2.02	0.41
1:F:189:LYS:HA	1:F:189:LYS:HD3	1.83	0.40
1:A:216:GLY:HA2	1:A:219:TYR:CD2	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	259/270 (96%)	250 (96%)	8 (3%)	1 (0%)	36	24
1	B	259/270 (96%)	250 (96%)	8 (3%)	1 (0%)	36	24
1	C	259/270 (96%)	248 (96%)	10 (4%)	1 (0%)	36	24
1	D	259/270 (96%)	251 (97%)	8 (3%)	0	100	100
1	E	259/270 (96%)	252 (97%)	7 (3%)	0	100	100
1	F	259/270 (96%)	251 (97%)	6 (2%)	2 (1%)	21	9
1	G	259/270 (96%)	250 (96%)	8 (3%)	1 (0%)	36	24
1	H	259/270 (96%)	249 (96%)	9 (4%)	1 (0%)	36	24
All	All	2072/2160 (96%)	2001 (97%)	64 (3%)	7 (0%)	43	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	214	PRO
1	A	214	PRO
1	G	214	PRO
1	B	215	ASN
1	C	214	PRO
1	F	216	GLY
1	F	214	PRO

### 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	208/216 (96%)	208 (100%)	0	100	100
1	B	208/216 (96%)	206 (99%)	2 (1%)	78	76
1	C	208/216 (96%)	207 (100%)	1 (0%)	90	89
1	D	208/216 (96%)	206 (99%)	2 (1%)	78	76
1	E	208/216 (96%)	207 (100%)	1 (0%)	90	89
1	F	208/216 (96%)	205 (99%)	3 (1%)	69	65
1	G	208/216 (96%)	207 (100%)	1 (0%)	90	89
1	H	208/216 (96%)	206 (99%)	2 (1%)	78	76
All	All	1664/1728 (96%)	1652 (99%)	12 (1%)	85	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	ASN
1	B	214	PRO
1	C	10	THR
1	D	54	LYS
1	D	85	LYS
1	E	10	THR
1	F	215	ASN
1	F	222	GLU
1	F	226	GLN
1	G	222	GLU
1	H	215	ASN
1	H	227	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	223	GLN
1	H	89	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	301	-	5,5,5	0.32	0	5,5,5	0.57	0
2	GOL	A	302	-	5,5,5	0.40	0	5,5,5	0.26	0
3	NAP	A	303	-	44,52,52	1.38	3 (6%)	53,80,80	1.49	3 (5%)
2	GOL	B	301	-	5,5,5	0.41	0	5,5,5	0.41	0
2	GOL	B	302	-	5,5,5	0.35	0	5,5,5	0.50	0
3	NAP	B	303	-	44,52,52	1.38	5 (11%)	53,80,80	1.50	5 (9%)
2	GOL	C	301	-	5,5,5	0.38	0	5,5,5	0.30	0
3	NAP	C	302	-	44,52,52	1.28	5 (11%)	53,80,80	1.60	6 (11%)
2	GOL	D	301	-	5,5,5	0.45	0	5,5,5	0.57	0
3	NAP	D	302	-	44,52,52	1.39	4 (9%)	53,80,80	1.56	5 (9%)
2	GOL	E	301	-	5,5,5	0.34	0	5,5,5	0.22	0
3	NAP	E	302	-	44,52,52	1.27	3 (6%)	53,80,80	1.45	5 (9%)
2	GOL	F	301	-	5,5,5	0.32	0	5,5,5	0.22	0
3	NAP	F	302	-	44,52,52	1.28	4 (9%)	53,80,80	1.52	3 (5%)
2	GOL	G	301	-	5,5,5	0.33	0	5,5,5	0.49	0
3	NAP	G	302	-	44,52,52	1.48	6 (13%)	53,80,80	1.51	3 (5%)
2	GOL	H	301	-	5,5,5	0.43	0	5,5,5	0.31	0
3	NAP	H	302	-	44,52,52	1.31	4 (9%)	53,80,80	1.42	2 (3%)

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	301	-	-	0/4/4/4	0/0/0/0
2	GOL	A	302	-	-	0/4/4/4	0/0/0/0
3	NAP	A	303	-	-	0/27/67/67	0/5/5/5
2	GOL	B	301	-	-	0/4/4/4	0/0/0/0
2	GOL	B	302	-	-	0/4/4/4	0/0/0/0
3	NAP	B	303	-	-	0/27/67/67	0/5/5/5
2	GOL	C	301	-	-	0/4/4/4	0/0/0/0
3	NAP	C	302	-	-	0/27/67/67	0/5/5/5
2	GOL	D	301	-	-	0/4/4/4	0/0/0/0
3	NAP	D	302	-	-	0/27/67/67	0/5/5/5
2	GOL	E	301	-	-	0/4/4/4	0/0/0/0
3	NAP	E	302	-	-	0/27/67/67	0/5/5/5
2	GOL	F	301	-	-	0/4/4/4	0/0/0/0
3	NAP	F	302	-	-	0/27/67/67	0/5/5/5
2	GOL	G	301	-	-	0/4/4/4	0/0/0/0
3	NAP	G	302	-	-	0/27/67/67	0/5/5/5
2	GOL	H	301	-	-	0/4/4/4	0/0/0/0
3	NAP	H	302	-	-	0/27/67/67	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	NAP	C8A-N9A	-2.50	1.33	1.36
3	D	302	NAP	C8A-N9A	-2.38	1.34	1.36
3	C	302	NAP	C8A-N9A	-2.27	1.34	1.36
3	F	302	NAP	C8A-N9A	-2.19	1.34	1.36
3	E	302	NAP	C8A-N9A	-2.10	1.34	1.36
3	G	302	NAP	C8A-N9A	-2.01	1.34	1.36
3	C	302	NAP	C3N-C7N	2.10	1.53	1.50
3	F	302	NAP	C6N-N1N	2.26	1.41	1.35
3	B	303	NAP	C3N-C7N	2.27	1.54	1.50
3	F	302	NAP	P2B-O2B	2.27	1.63	1.59
3	B	303	NAP	P2B-O2B	2.29	1.63	1.59
3	C	302	NAP	O4B-C1B	2.36	1.44	1.41
3	D	302	NAP	O4B-C1B	2.37	1.44	1.41
3	G	302	NAP	C6N-N1N	2.38	1.41	1.35
3	H	302	NAP	C6N-N1N	2.40	1.41	1.35
3	H	302	NAP	O4B-C1B	2.44	1.44	1.41
3	B	303	NAP	O4D-C1D	2.51	1.44	1.41
3	C	302	NAP	O4D-C1D	2.55	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	NAP	O4B-C1B	2.75	1.45	1.41
3	H	302	NAP	O4D-C1D	2.88	1.45	1.41
3	G	302	NAP	P2B-O2B	2.90	1.64	1.59
3	G	302	NAP	O4B-C1B	3.08	1.45	1.41
3	E	302	NAP	O4D-C1D	3.19	1.45	1.41
3	A	303	NAP	O4D-C1D	3.24	1.45	1.41
3	G	302	NAP	O4D-C1D	3.30	1.45	1.41
3	D	302	NAP	O4D-C1D	3.42	1.46	1.41
3	C	302	NAP	O7N-C7N	4.82	1.33	1.24
3	E	302	NAP	O7N-C7N	5.31	1.34	1.24
3	H	302	NAP	O7N-C7N	5.46	1.35	1.24
3	B	303	NAP	O7N-C7N	5.54	1.35	1.24
3	F	302	NAP	O7N-C7N	5.65	1.35	1.24
3	A	303	NAP	O7N-C7N	5.65	1.35	1.24
3	D	302	NAP	O7N-C7N	5.90	1.36	1.24
3	G	302	NAP	O7N-C7N	5.99	1.36	1.24

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	NAP	N3A-C2A-N1A	-8.76	121.36	128.86
3	G	302	NAP	N3A-C2A-N1A	-8.60	121.50	128.86
3	C	302	NAP	N3A-C2A-N1A	-8.56	121.53	128.86
3	F	302	NAP	N3A-C2A-N1A	-8.53	121.56	128.86
3	B	303	NAP	N3A-C2A-N1A	-8.34	121.72	128.86
3	E	302	NAP	N3A-C2A-N1A	-8.19	121.86	128.86
3	A	303	NAP	N3A-C2A-N1A	-8.07	121.96	128.86
3	H	302	NAP	N3A-C2A-N1A	-8.00	122.02	128.86
3	A	303	NAP	C4A-C5A-N7A	-3.09	106.42	109.41
3	D	302	NAP	C4D-O4D-C1D	-3.08	106.61	109.83
3	F	302	NAP	C4B-O4B-C1B	-2.82	106.89	109.83
3	C	302	NAP	C4B-O4B-C1B	-2.76	106.95	109.83
3	G	302	NAP	C4B-O4B-C1B	-2.55	107.17	109.83
3	D	302	NAP	C4A-C5A-N7A	-2.47	107.02	109.41
3	A	303	NAP	C4B-O4B-C1B	-2.41	107.31	109.83
3	B	303	NAP	C4B-O4B-C1B	-2.40	107.32	109.83
3	B	303	NAP	C5B-C4B-C3B	-2.36	106.41	115.29
3	G	302	NAP	C4D-O4D-C1D	-2.36	107.37	109.83
3	D	302	NAP	C4B-O4B-C1B	-2.30	107.43	109.83
3	D	302	NAP	PN-O3-PA	-2.26	125.05	132.63
3	B	303	NAP	PN-O3-PA	-2.25	125.08	132.63
3	H	302	NAP	PN-O3-PA	-2.22	125.18	132.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	NAP	O4B-C1B-C2B	-2.19	102.79	106.60
3	E	302	NAP	C4A-C5A-N7A	-2.15	107.33	109.41
3	C	302	NAP	C4D-O4D-C1D	-2.12	107.62	109.83
3	C	302	NAP	PN-O3-PA	-2.12	125.52	132.63
3	C	302	NAP	C5B-C4B-C3B	-2.10	107.39	115.29
3	E	302	NAP	PN-O3-PA	-2.07	125.66	132.63
3	F	302	NAP	C4A-C5A-N7A	-2.05	107.43	109.41
3	B	303	NAP	O4B-C1B-C2B	-2.03	103.07	106.60
3	E	302	NAP	C2N-C3N-C4N	2.11	120.70	118.26
3	C	302	NAP	C2N-C3N-C4N	2.28	120.89	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	GOL	1	0
2	A	302	GOL	3	0
3	A	303	NAP	1	0
2	B	302	GOL	1	0
2	D	301	GOL	2	0
3	E	302	NAP	1	0
2	G	301	GOL	1	0
3	G	302	NAP	1	0
2	H	301	GOL	2	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	261/270 (96%)	0.53	24 (9%) 9 10	16, 28, 50, 60	0
1	B	261/270 (96%)	0.41	20 (7%) 13 15	17, 31, 65, 87	0
1	C	261/270 (96%)	0.34	17 (6%) 19 20	17, 30, 48, 65	0
1	D	261/270 (96%)	0.62	28 (10%) 6 6	20, 40, 69, 84	0
1	E	261/270 (96%)	0.43	24 (9%) 9 10	22, 33, 56, 72	0
1	F	261/270 (96%)	0.26	22 (8%) 11 12	22, 31, 55, 70	0
1	G	261/270 (96%)	0.41	24 (9%) 9 10	22, 34, 64, 86	0
1	H	261/270 (96%)	0.46	25 (9%) 8 9	22, 34, 58, 71	0
All	All	2088/2160 (96%)	0.43	184 (8%) 10 11	16, 33, 60, 87	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	ASN	8.7
1	G	213	ILE	8.0
1	G	214	PRO	7.7
1	D	10	THR	7.6
1	E	12	ILE	7.3
1	H	10	THR	6.7
1	F	10	THR	6.7
1	D	66	LEU	6.1
1	H	12	ILE	6.1
1	A	215	ASN	6.1
1	A	214	PRO	5.9
1	E	10	THR	5.9
1	F	11	TYR	5.8
1	E	213	ILE	5.7
1	B	10	THR	5.2
1	G	10	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	G	12	ILE	5.0
1	A	10	THR	5.0
1	H	214	PRO	5.0
1	B	214	PRO	4.9
1	B	11	TYR	4.8
1	E	11	TYR	4.7
1	F	219	TYR	4.6
1	D	214	PRO	4.6
1	H	11	TYR	4.5
1	B	218	SER	4.5
1	G	11	TYR	4.4
1	B	217	THR	4.4
1	C	10	THR	4.4
1	D	213	ILE	4.3
1	D	11	TYR	4.2
1	B	212	TYR	4.1
1	B	12	ILE	4.1
1	A	219	TYR	4.0
1	G	221	ALA	4.0
1	A	11	TYR	4.0
1	E	66	LEU	4.0
1	H	218	SER	4.0
1	B	213	ILE	4.0
1	F	215	ASN	4.0
1	H	213	ILE	3.9
1	C	262	VAL	3.8
1	E	262	VAL	3.8
1	A	216	GLY	3.8
1	G	226	GLN	3.8
1	D	215	ASN	3.8
1	F	220	THR	3.7
1	A	12	ILE	3.7
1	A	262	VAL	3.7
1	H	263	LEU	3.7
1	H	262	VAL	3.6
1	E	215	ASN	3.6
1	E	214	PRO	3.6
1	G	222	GLU	3.6
1	G	218	SER	3.5
1	B	219	TYR	3.5
1	F	214	PRO	3.5
1	H	226	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	216	GLY	3.4
1	B	262	VAL	3.4
1	E	222	GLU	3.3
1	A	263	LEU	3.3
1	H	215	ASN	3.3
1	F	217	THR	3.3
1	G	262	VAL	3.3
1	G	219	TYR	3.2
1	E	178	VAL	3.2
1	H	216	GLY	3.2
1	F	226	GLN	3.2
1	D	68	SER	3.2
1	A	258	VAL	3.2
1	C	215	ASN	3.2
1	D	12	ILE	3.1
1	C	212	TYR	3.1
1	A	195	VAL	3.0
1	F	262	VAL	3.0
1	D	262	VAL	3.0
1	H	174	VAL	3.0
1	B	226	GLN	2.9
1	C	195	VAL	2.9
1	F	263	LEU	2.9
1	G	217	THR	2.9
1	B	223	GLN	2.9
1	A	178	VAL	2.9
1	D	219	TYR	2.8
1	B	174	VAL	2.8
1	D	150	LEU	2.8
1	G	216	GLY	2.8
1	D	212	TYR	2.8
1	H	13	PRO	2.8
1	H	195	VAL	2.8
1	F	156	SER	2.7
1	D	216	GLY	2.7
1	C	214	PRO	2.7
1	E	195	VAL	2.7
1	F	258	VAL	2.7
1	F	222	GLU	2.7
1	G	215	ASN	2.7
1	C	150	LEU	2.7
1	B	216	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	57	GLU	2.7
1	C	263	LEU	2.7
1	D	263	LEU	2.7
1	E	13	PRO	2.7
1	C	194	ALA	2.6
1	E	172	GLY	2.6
1	C	174	VAL	2.6
1	E	221	ALA	2.6
1	F	194	ALA	2.6
1	D	71	ILE	2.6
1	F	213	ILE	2.6
1	B	195	VAL	2.6
1	G	224	ARG	2.6
1	G	54	LYS	2.6
1	E	194	ALA	2.6
1	D	178	VAL	2.6
1	E	217	THR	2.6
1	D	67	GLY	2.6
1	A	250	LEU	2.6
1	D	96	HIS	2.5
1	A	173	ALA	2.5
1	G	223	GLN	2.5
1	H	66	LEU	2.5
1	E	226	GLN	2.5
1	G	13	PRO	2.5
1	D	174	VAL	2.5
1	G	178	VAL	2.5
1	B	178	VAL	2.4
1	H	178	VAL	2.4
1	C	258	VAL	2.4
1	B	222	GLU	2.4
1	H	219	TYR	2.4
1	D	54	LYS	2.4
1	C	12	ILE	2.4
1	G	220	THR	2.4
1	E	174	VAL	2.4
1	A	194	ALA	2.4
1	A	217	THR	2.4
1	F	195	VAL	2.4
1	G	258	VAL	2.4
1	G	176	SER	2.3
1	A	150	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	265	LEU	2.3
1	D	173	ALA	2.3
1	F	223	GLN	2.3
1	E	173	ALA	2.3
1	H	194	ALA	2.3
1	A	264	THR	2.3
1	H	264	THR	2.3
1	A	174	VAL	2.3
1	F	196	ALA	2.3
1	H	173	ALA	2.3
1	A	152	SER	2.3
1	H	212	TYR	2.3
1	B	263	LEU	2.3
1	E	223	GLN	2.2
1	A	218	SER	2.2
1	D	94	PHE	2.2
1	F	264	THR	2.2
1	E	263	LEU	2.2
1	C	264	THR	2.2
1	G	174	VAL	2.2
1	H	150	LEU	2.2
1	H	196	ALA	2.2
1	E	264	THR	2.1
1	D	195	VAL	2.1
1	G	207	GLU	2.1
1	D	77	ILE	2.1
1	F	12	ILE	2.1
1	E	65	ALA	2.1
1	B	207	GLU	2.1
1	F	173	ALA	2.1
1	A	149	VAL	2.1
1	C	178	VAL	2.1
1	C	196	ALA	2.1
1	D	65	ALA	2.1
1	D	90	ALA	2.1
1	D	194	ALA	2.1
1	C	11	TYR	2.0
1	E	218	SER	2.0
1	H	149	VAL	2.0
1	A	265	LEU	2.0
1	A	222	GLU	2.0
1	H	261	LYS	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	302	6/6	0.57	0.24	46,49,50,51	0
2	GOL	B	301	6/6	0.76	0.13	37,41,42,44	0
2	GOL	H	301	6/6	0.76	0.15	43,47,48,49	0
2	GOL	G	301	6/6	0.78	0.19	49,51,51,52	0
2	GOL	D	301	6/6	0.79	0.20	30,36,37,38	0
2	GOL	E	301	6/6	0.79	0.13	44,49,50,51	0
2	GOL	A	301	6/6	0.88	0.11	42,45,47,48	0
2	GOL	F	301	6/6	0.90	0.16	37,39,40,42	0
2	GOL	C	301	6/6	0.90	0.11	32,37,37,38	0
2	GOL	B	302	6/6	0.91	0.13	31,32,33,34	0
3	NAP	D	302	48/48	0.94	0.12	9,11,12,13	0
3	NAP	H	302	48/48	0.95	0.12	9,11,12,14	0
3	NAP	G	302	48/48	0.96	0.15	10,12,13,14	0
3	NAP	E	302	48/48	0.96	0.11	10,12,14,14	0
3	NAP	B	303	48/48	0.96	0.08	23,29,35,35	0
3	NAP	C	302	48/48	0.97	0.09	19,25,29,30	0
3	NAP	F	302	48/48	0.97	0.08	7,11,12,13	0
3	NAP	A	303	48/48	0.97	0.06	8,10,12,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.