



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:03 am BST

PDB ID : 1G8L  
Title : CRYSTAL STRUCTURE OF ESCHERICHIA COLI MOEA  
Authors : Xiang, S.; Nichols, J.; Rajagopalan, K.V.; Schindelin, H.  
Deposited on : 2000-11-17  
Resolution : 1.95 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

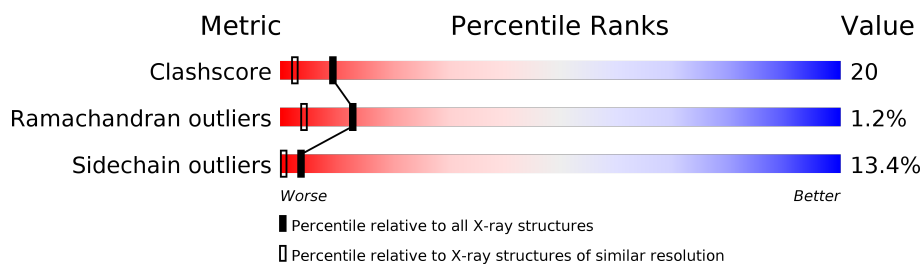
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	411	
1	B	411	

## 2 Entry composition [i](#)

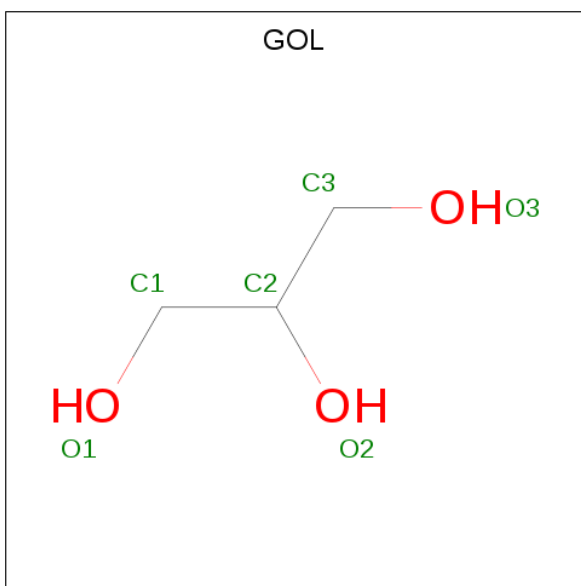
There are 3 unique types of molecules in this entry. The entry contains 6781 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MOLYBDOPTERIN BIOSYNTHESIS MOEA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	Total 3040	C 1918	N 531	O 578	S 13	0	0	0
1	B	403	Total 3040	C 1918	N 531	O 578	S 13	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
			Total	C	O		
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	312	Total O 312 312	0	0
3	B	281	Total O 281 281	0	0

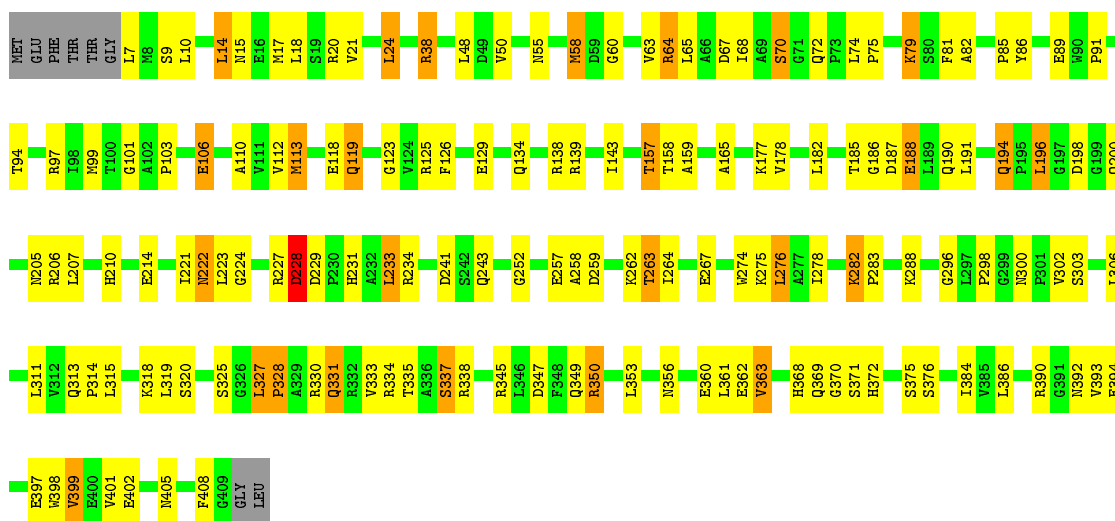
### 3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

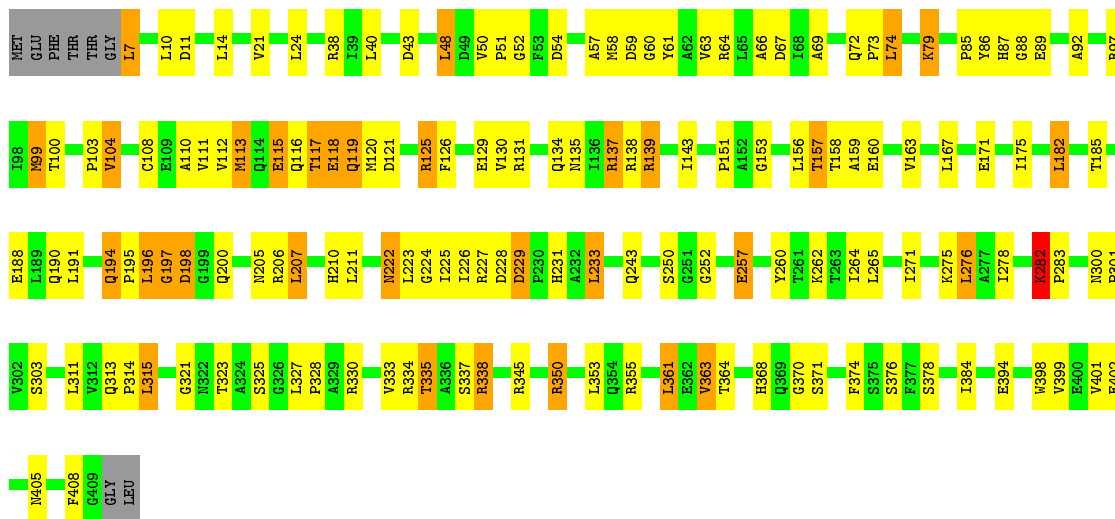
- Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS MOEA PROTEIN

Chain A: 



- Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS MOEA PROTEIN

Chain B: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.32Å 97.41Å 98.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	91.5 (20.00-1.95)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.228 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6781	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 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

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	0.67	0/3099	0.73	3/4212 (0.1%)
1	B	0.67	0/3099	0.70	0/4212
All	All	0.67	0/6198	0.71	3/8424 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	38	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	347	ASP	CB-CG-OD2	5.39	123.15	118.30

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	3040	0	3037	119	0
1	B	3040	0	3037	128	0
2	A	42	0	56	9	0
2	B	66	0	88	9	0
3	A	312	0	0	13	0
3	B	281	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6781	0	6218	244	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 20.

All (244) 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:A:356:ASN:HD21	1:A:360:GLU:HB2	1.09	1.17
1:B:368:HIS:HD2	1:B:370:GLY:H	1.00	0.95
1:B:374:PHE:H	2:B:703:GOL:H31	1.30	0.94
1:A:177:LYS:HA	2:A:706:GOL:H11	1.52	0.92
1:A:356:ASN:ND2	1:A:360:GLU:HB2	1.83	0.92
1:B:157:THR:HG22	1:B:159:ALA:H	1.36	0.90
1:A:157:THR:HG22	1:A:159:ALA:H	1.38	0.89
1:B:368:HIS:CD2	1:B:370:GLY:H	1.93	0.83
1:B:300:ASN:HD22	1:B:303:SER:H	1.26	0.80
1:B:222:ASN:HD22	1:B:224:GLY:H	1.26	0.80
1:A:300:ASN:HD22	1:A:303:SER:H	1.28	0.80
1:A:106:GLU:CD	1:A:106:GLU:H	1.83	0.79
1:B:113:MET:HE2	1:B:115:GLU:HB2	1.64	0.78
1:A:368:HIS:CD2	1:A:370:GLY:H	2.02	0.77
1:B:368:HIS:HD2	1:B:370:GLY:N	1.82	0.77
1:A:221:ILE:HD13	1:A:243:GLN:HG3	1.67	0.76
1:A:157:THR:CG2	1:A:159:ALA:H	1.99	0.76
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.34	0.75
1:B:345:ARG:HD3	3:B:961:HOH:O	1.86	0.74
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.35	0.74
2:A:704:GOL:H2	3:A:723:HOH:O	1.86	0.74
1:A:375:SER:HB3	2:A:701:GOL:H2	1.68	0.73
1:A:70:SER:HB3	1:A:72:GLN:OE1	1.88	0.72
1:B:327:LEU:HB3	3:B:918:HOH:O	1.90	0.72
1:B:222:ASN:ND2	1:B:224:GLY:H	1.87	0.72
1:B:130:VAL:HA	1:B:134:GLN:HE22	1.55	0.71
1:B:350:ARG:HD2	1:B:376:SER:OG	1.90	0.71
1:A:328:PRO:HB3	3:A:933:HOH:O	1.91	0.70
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.40	0.70
1:B:51:PRO:HG2	1:B:139:ARG:HA	1.73	0.69
1:A:368:HIS:HD2	1:A:370:GLY:H	1.41	0.68
1:A:21:VAL:HG21	1:A:315:LEU:CD1	2.23	0.68
1:B:74:LEU:CD2	1:B:74:LEU:H	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:HB3	3:A:1000:HOH:O	1.92	0.67
1:B:89:GLU:HG2	3:B:990:HOH:O	1.95	0.67
1:B:197:GLY:N	1:B:200:GLN:HB2	2.10	0.67
1:A:258:ALA:HA	1:A:262:LYS:HD3	1.76	0.67
1:A:313:GLN:HB3	1:A:314:PRO:HD3	1.76	0.65
1:B:157:THR:CG2	1:B:159:ALA:H	2.09	0.65
1:A:278:ILE:O	1:A:345:ARG:HD2	1.99	0.63
1:A:335:THR:HG22	1:A:337:SER:H	1.61	0.63
1:B:21:VAL:HG21	1:B:315:LEU:CD1	2.28	0.63
1:B:313:GLN:HE22	1:B:405:ASN:ND2	1.95	0.63
1:B:278:ILE:O	1:B:345:ARG:HD2	1.98	0.63
1:A:21:VAL:HG21	1:A:315:LEU:HD11	1.80	0.63
1:A:300:ASN:ND2	1:A:303:SER:H	1.95	0.62
1:B:74:LEU:HD21	1:B:126:PHE:CE1	2.34	0.62
1:A:350:ARG:HD2	1:A:376:SER:OG	2.00	0.62
1:B:228:ASP:HA	1:B:260:TYR:OH	1.99	0.62
1:A:222:ASN:HD22	1:A:224:GLY:H	1.46	0.62
1:B:328:PRO:HD3	3:B:967:HOH:O	1.99	0.62
1:A:333:VAL:HG21	1:A:353:LEU:HD11	1.81	0.61
1:B:110:ALA:HB1	1:B:134:GLN:HB3	1.81	0.61
1:A:263:THR:HG21	3:A:873:HOH:O	1.99	0.61
1:B:185:THR:O	1:B:252:GLY:HA3	2.00	0.61
1:A:157:THR:HG23	1:A:158:THR:N	2.15	0.60
1:B:335:THR:HG22	1:B:337:SER:H	1.67	0.60
1:A:334:ARG:HG3	1:A:398:TRP:CZ3	2.36	0.60
1:B:21:VAL:HG21	1:B:315:LEU:HD12	1.82	0.59
1:B:7:LEU:N	3:B:925:HOH:O	2.36	0.59
1:B:384:ILE:HG23	1:B:399:VAL:HG11	1.85	0.59
1:A:210:HIS:HD2	1:A:222:ASN:OD1	1.86	0.58
1:B:58:MET:SD	1:B:113:MET:HG2	2.44	0.58
1:B:74:LEU:H	1:B:74:LEU:HD23	1.69	0.58
1:A:119:GLN:HE21	1:A:119:GLN:H	1.52	0.57
1:B:300:ASN:HD21	1:B:371:SER:HB2	1.70	0.57
1:A:205:ASN:HB2	3:A:743:HOH:O	2.06	0.56
1:A:110:ALA:HB1	1:A:134:GLN:HG2	1.86	0.56
1:A:38:ARG:NH2	3:A:740:HOH:O	2.39	0.55
1:A:85:PRO:HB3	1:A:103:PRO:HG2	1.88	0.55
1:B:157:THR:HG23	1:B:158:THR:N	2.21	0.55
1:B:384:ILE:HG23	1:B:399:VAL:CG1	2.36	0.55
1:A:143:ILE:HD11	2:B:703:GOL:H2	1.88	0.55
1:B:282:LYS:HB3	1:B:283:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:NH2	3:B:877:HOH:O	2.38	0.54
1:A:368:HIS:CD2	1:A:372:HIS:HE1	2.25	0.54
1:B:345:ARG:HH22	2:B:711:GOL:H2	1.72	0.54
1:A:86:TYR:HA	2:A:715:GOL:O3	2.08	0.54
1:B:86:TYR:CZ	1:B:88:GLY:HA3	2.43	0.54
1:A:276:LEU:HD21	1:A:311:LEU:HD11	1.89	0.53
1:A:333:VAL:HG12	1:A:363:VAL:HG22	1.90	0.53
1:A:58:MET:HE2	1:A:113:MET:HB3	1.89	0.53
1:A:63:VAL:HG21	1:A:68:ILE:HD13	1.90	0.53
1:B:229:ASP:OD2	1:B:231:HIS:HB2	2.09	0.52
1:A:106:GLU:CD	1:A:106:GLU:N	2.58	0.52
1:B:157:THR:CG2	1:B:158:THR:N	2.73	0.52
1:A:60:GLY:HA3	1:A:112:VAL:O	2.09	0.52
1:B:120:MET:HG3	3:B:917:HOH:O	2.09	0.52
1:B:153:GLY:HA3	1:B:323:THR:HG23	1.92	0.52
1:A:356:ASN:N	1:A:360:GLU:O	2.36	0.51
1:B:300:ASN:ND2	1:B:303:SER:H	2.03	0.51
1:A:349:GLN:HB3	1:A:369:GLN:OE1	2.10	0.51
1:B:43:ASP:OD1	1:B:151:PRO:HA	2.09	0.51
1:A:157:THR:CG2	1:A:158:THR:N	2.73	0.51
1:B:59:ASP:OD2	1:B:99:MET:HG3	2.11	0.51
1:A:17:MET:HG3	1:A:274:TRP:CH2	2.46	0.51
1:A:231:HIS:NE2	2:A:709:GOL:H2	2.26	0.51
1:B:38:ARG:HD2	3:B:721:HOH:O	2.11	0.50
1:B:60:GLY:HA3	1:B:112:VAL:O	2.10	0.50
1:A:55:ASN:ND2	1:A:101:GLY:HA2	2.25	0.50
1:B:63:VAL:HG11	1:B:126:PHE:CZ	2.46	0.50
1:A:227:ARG:O	1:A:229:ASP:N	2.44	0.50
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.57	0.50
1:B:64:ARG:HD2	1:B:67:ASP:OD1	2.12	0.50
1:A:259:ASP:HB2	3:A:953:HOH:O	2.11	0.50
1:B:52:GLY:O	1:B:139:ARG:HB2	2.12	0.50
1:B:227:ARG:HG3	3:B:734:HOH:O	2.10	0.50
2:A:701:GOL:H32	1:B:163:VAL:HG21	1.95	0.49
1:B:194:GLN:HA	3:B:879:HOH:O	2.12	0.49
1:A:330:ARG:O	1:B:355:ARG:HD2	2.12	0.49
1:B:353:LEU:HD13	1:B:363:VAL:HG13	1.93	0.49
1:A:157:THR:HG22	1:A:159:ALA:N	2.18	0.49
1:A:18:LEU:O	1:A:318:LYS:NZ	2.40	0.49
1:A:306:LEU:C	1:A:306:LEU:HD13	2.32	0.49
1:B:79:LYS:HA	1:B:97:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLU:HG2	3:B:799:HOH:O	2.13	0.49
1:B:378:SER:O	2:B:702:GOL:H31	2.12	0.49
2:B:707:GOL:H2	3:B:862:HOH:O	2.12	0.49
2:A:706:GOL:H12	3:A:755:HOH:O	2.11	0.49
1:B:137:ARG:HD2	3:B:952:HOH:O	2.11	0.49
1:B:197:GLY:O	1:B:198:ASP:C	2.51	0.48
1:B:61:TYR:CE1	1:B:117:THR:HG21	2.48	0.48
1:B:225:ILE:HG21	2:B:708:GOL:H32	1.95	0.48
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.95	0.48
1:B:190:GLN:OE1	1:B:200:GLN:OE1	2.31	0.48
1:A:191:LEU:O	1:A:194:GLN:HG2	2.13	0.48
1:A:99:MET:HE2	3:A:937:HOH:O	2.12	0.48
1:A:335:THR:CG2	1:A:337:SER:O	2.61	0.48
1:A:320:SER:HB2	2:A:706:GOL:H2	1.95	0.48
1:B:330:ARG:HG2	1:B:402:GLU:HB2	1.95	0.48
1:A:228:ASP:HB2	3:A:1000:HOH:O	2.13	0.48
1:A:222:ASN:ND2	1:A:224:GLY:H	2.10	0.47
1:B:206:ARG:HD2	1:B:222:ASN:HD21	1.80	0.47
1:A:118:GLU:HB3	1:A:125:ARG:HB3	1.97	0.47
1:B:111:VAL:HB	1:B:135:ASN:HB2	1.96	0.47
1:A:24:LEU:HD22	1:A:178:VAL:HG22	1.96	0.47
1:A:333:VAL:CG1	1:A:363:VAL:HG22	2.45	0.47
1:A:91:PRO:HG2	1:A:94:THR:HG21	1.96	0.47
1:A:165:ALA:HB2	1:B:207:LEU:HD12	1.96	0.47
1:B:334:ARG:HG3	1:B:398:TRP:CZ3	2.50	0.47
1:A:300:ASN:HD21	1:A:371:SER:HB2	1.79	0.46
1:B:74:LEU:N	1:B:74:LEU:HD23	2.30	0.46
1:A:390:ARG:HE	1:A:393:VAL:HG22	1.81	0.46
1:B:257:GLU:O	1:B:262:LYS:HD3	2.15	0.46
1:B:350:ARG:NH2	3:B:720:HOH:O	2.42	0.46
1:B:252:GLY:O	2:B:707:GOL:H12	2.16	0.46
1:A:384:ILE:HG23	1:A:399:VAL:HG11	1.96	0.46
1:A:267:GLU:HG2	1:A:267:GLU:O	2.16	0.46
1:A:313:GLN:HE22	1:A:405:ASN:ND2	2.10	0.46
1:A:75:PRO:HA	1:A:123:GLY:HA2	1.98	0.46
1:A:186:GLY:HA3	1:A:188:GLU:OE1	2.16	0.46
1:A:85:PRO:HB3	1:A:103:PRO:CG	2.46	0.46
1:A:64:ARG:HD3	1:A:67:ASP:OD1	2.15	0.45
1:B:85:PRO:HG3	1:B:103:PRO:HG3	1.98	0.45
1:B:276:LEU:HD21	1:B:311:LEU:HD11	1.99	0.45
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:HD22	1:B:222:ASN:C	2.20	0.45
1:A:300:ASN:HD21	1:A:302:VAL:HB	1.82	0.45
1:B:157:THR:HG23	1:B:158:THR:H	1.82	0.45
1:A:190:GLN:HE21	1:A:190:GLN:HA	1.81	0.45
1:B:210:HIS:HD2	1:B:222:ASN:OD1	1.99	0.45
1:A:408:PHE:HA	1:B:157:THR:HG23	1.99	0.45
1:A:331:GLN:HB3	1:B:361:LEU:HD22	1.99	0.45
1:A:17:MET:HG3	1:A:274:TRP:CZ3	2.52	0.44
1:B:57:ALA:C	1:B:100:THR:HG23	2.37	0.44
1:B:74:LEU:CD2	1:B:74:LEU:N	2.76	0.44
1:A:394:GLU:N	1:A:397:GLU:OE2	2.41	0.44
1:B:40:LEU:HG	1:B:156:LEU:HD21	1.99	0.44
1:A:408:PHE:HA	1:B:157:THR:CG2	2.47	0.44
1:B:157:THR:HB	1:B:160:GLU:OE2	2.17	0.44
1:B:190:GLN:HE21	1:B:191:LEU:H	1.66	0.44
1:A:196:LEU:HG	1:A:200:GLN:O	2.17	0.44
1:B:206:ARG:NH1	1:B:224:GLY:HA2	2.32	0.44
1:A:263:THR:HG22	3:A:790:HOH:O	2.17	0.44
1:A:185:THR:O	1:A:252:GLY:HA3	2.18	0.44
1:A:353:LEU:HG	1:A:361:LEU:HG	1.99	0.44
1:B:229:ASP:OD2	1:B:231:HIS:N	2.51	0.44
1:B:337:SER:OG	1:B:364:THR:HG23	2.18	0.44
1:A:276:LEU:HB3	1:A:278:ILE:HG12	1.99	0.44
1:B:48:LEU:HD11	1:B:167:LEU:HA	2.00	0.44
1:B:129:GLU:HG2	1:B:130:VAL:N	2.33	0.43
1:B:112:VAL:CG2	1:B:130:VAL:HG22	2.48	0.43
1:A:384:ILE:HG22	1:A:386:LEU:HD21	2.00	0.43
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.85	0.43
1:B:271:ILE:N	1:B:271:ILE:HD12	2.33	0.43
1:B:50:VAL:HB	1:B:143:ILE:HB	2.00	0.43
1:B:66:ALA:O	1:B:69:ALA:HB3	2.17	0.43
1:B:196:LEU:HG	1:B:200:GLN:O	2.18	0.43
1:A:79:LYS:HA	1:A:97:ARG:O	2.18	0.43
1:A:234:ARG:HG3	1:A:264:ILE:HG12	1.99	0.43
1:A:81:PHE:CD2	1:A:99:MET:HG3	2.54	0.43
1:B:118:GLU:HB3	1:B:125:ARG:NH1	2.33	0.43
1:B:113:MET:CE	1:B:115:GLU:HB2	2.43	0.43
1:B:265:LEU:HD22	1:B:271:ILE:HG12	2.01	0.43
1:A:283:PRO:HG2	1:A:298:PRO:HB3	2.00	0.43
1:A:335:THR:HG21	1:A:337:SER:O	2.19	0.43
2:A:701:GOL:H32	1:B:163:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HG21	1:B:233:LEU:HA	2.01	0.43
1:B:233:LEU:HB3	1:B:264:ILE:HD13	2.01	0.43
1:A:333:VAL:HG13	1:A:362:GLU:HA	1.99	0.42
1:B:21:VAL:HG21	1:B:315:LEU:HD11	1.99	0.42
1:B:333:VAL:HG11	1:B:363:VAL:HG22	2.00	0.42
1:A:206:ARG:HD2	1:A:222:ASN:HD21	1.84	0.42
1:A:311:LEU:C	1:A:314:PRO:HD2	2.39	0.42
1:B:119:GLN:H	1:B:119:GLN:HG3	1.68	0.42
1:A:186:GLY:CA	1:A:188:GLU:OE1	2.68	0.42
1:B:61:TYR:HE1	1:B:117:THR:HG21	1.83	0.42
1:B:333:VAL:CG1	1:B:363:VAL:HG22	2.49	0.42
1:A:333:VAL:CG1	1:A:334:ARG:N	2.83	0.42
1:B:175:ILE:HD13	1:B:321:GLY:HA3	2.02	0.42
1:B:300:ASN:HD22	1:B:303:SER:N	2.06	0.42
1:A:338:ARG:NH1	1:A:392:ASN:HD22	2.17	0.42
1:A:353:LEU:HD13	1:A:401:VAL:HG11	2.01	0.42
1:B:338:ARG:NE	1:B:394:GLU:OE2	2.53	0.42
1:B:85:PRO:HB2	1:B:87:HIS:CE1	2.55	0.42
1:A:50:VAL:HB	1:A:143:ILE:HB	2.02	0.42
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.92	0.41
1:B:207:LEU:HD22	1:B:211:LEU:HG	2.02	0.41
1:B:345:ARG:HH12	2:B:711:GOL:H2	1.85	0.41
1:B:205:ASN:OD1	1:B:301:PRO:HA	2.20	0.41
1:A:14:LEU:HD22	1:A:18:LEU:HG	2.02	0.41
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.83	0.41
1:A:85:PRO:HA	1:A:103:PRO:HG2	2.03	0.41
1:B:182:LEU:HD21	1:B:250:SER:HB3	2.01	0.41
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.91	0.41
1:A:327:LEU:O	1:A:328:PRO:C	2.59	0.41
1:B:104:VAL:HG13	1:B:108:CYS:CB	2.50	0.41
1:B:195:PRO:HD2	3:B:879:HOH:O	2.21	0.41
1:A:74:LEU:HD12	1:A:126:PHE:CE1	2.56	0.41
1:A:350:ARG:HD2	1:A:376:SER:CB	2.51	0.41
1:B:54:ASP:HA	1:B:137:ARG:O	2.20	0.41
1:B:227:ARG:O	1:B:229:ASP:N	2.54	0.41
1:A:139:ARG:CZ	1:A:139:ARG:HB3	2.51	0.41
1:A:296:GLY:HA3	3:A:822:HOH:O	2.21	0.41
1:A:330:ARG:NE	1:A:402:GLU:OE1	2.48	0.40
1:B:131:ARG:HA	1:B:131:ARG:HD3	1.87	0.40
1:B:57:ALA:N	1:B:135:ASN:O	2.46	0.40
1:A:210:HIS:HE1	1:A:214:GLU:OE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:C	1:B:117:THR:H	2.24	0.40
1:B:313:GLN:HB3	1:B:314:PRO:HD3	2.03	0.40
1:A:157:THR:HG23	1:B:408:PHE:HA	2.04	0.40
1:A:338:ARG:HH12	1:A:392:ASN:HD22	1.68	0.40
1:A:38:ARG:HD2	3:A:755:HOH:O	2.20	0.40
1:B:378:SER:O	2:B:702:GOL:C3	2.70	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	401/411 (98%)	383 (96%)	13 (3%)	5 (1%)	13 4
1	B	401/411 (98%)	378 (94%)	18 (4%)	5 (1%)	13 4
All	All	802/822 (98%)	761 (95%)	31 (4%)	10 (1%)	13 4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	282	LYS
1	B	282	LYS
1	A	82	ALA
1	A	228	ASP
1	A	328	PRO
1	B	198	ASP
1	B	92	ALA
1	B	73	PRO
1	B	197	GLY

### 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	325/331 (98%)	283 (87%)	42 (13%)	4	0
1	B	325/331 (98%)	280 (86%)	45 (14%)	3	0
All	All	650/662 (98%)	563 (87%)	87 (13%)	4	0

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	SER
1	A	10	LEU
1	A	14	LEU
1	A	15	ASN
1	A	20	ARG
1	A	24	LEU
1	A	48	LEU
1	A	58	MET
1	A	64	ARG
1	A	65	LEU
1	A	70	SER
1	A	79	LYS
1	A	89	GLU
1	A	106	GLU
1	A	113	MET
1	A	119	GLN
1	A	129	GLU
1	A	138	ARG
1	A	157	THR
1	A	182	LEU
1	A	188	GLU
1	A	194	GLN
1	A	196	LEU
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	228	ASP
1	A	233	LEU
1	A	257	GLU
1	A	263	THR
1	A	275	LYS
1	A	276	LEU
1	A	288	LYS
1	A	319	LEU
1	A	325	SER
1	A	327	LEU
1	A	331	GLN
1	A	337	SER
1	A	350	ARG
1	A	363	VAL
1	A	399	VAL
1	B	7	LEU
1	B	10	LEU
1	B	11	ASP
1	B	14	LEU
1	B	24	LEU
1	B	48	LEU
1	B	72	GLN
1	B	74	LEU
1	B	79	LYS
1	B	99	MET
1	B	104	VAL
1	B	113	MET
1	B	115	GLU
1	B	116	GLN
1	B	117	THR
1	B	118	GLU
1	B	119	GLN
1	B	121	ASP
1	B	125	ARG
1	B	137	ARG
1	B	138	ARG
1	B	139	ARG
1	B	157	THR
1	B	182	LEU
1	B	188	GLU
1	B	194	GLN
1	B	196	LEU

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Mol	Chain	Res	Type
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	229	ASP
1	B	233	LEU
1	B	243	GLN
1	B	257	GLU
1	B	275	LYS
1	B	276	LEU
1	B	282	LYS
1	B	315	LEU
1	B	325	SER
1	B	335	THR
1	B	338	ARG
1	B	350	ARG
1	B	361	LEU
1	B	363	VAL
1	B	401	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	34	GLN
1	A	55	ASN
1	A	114	GLN
1	A	119	GLN
1	A	190	GLN
1	A	194	GLN
1	A	210	HIS
1	A	222	ASN
1	A	300	ASN
1	A	313	GLN
1	A	368	HIS
1	A	372	HIS
1	A	392	ASN
1	B	55	ASN
1	B	87	HIS
1	B	134	GLN
1	B	194	GLN
1	B	210	HIS
1	B	222	ASN

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Mol	Chain	Res	Type
1	B	300	ASN
1	B	313	GLN
1	B	354	GLN
1	B	368	HIS

### 5.3.3 RNA [i](#)

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	B	712	-	5,5,5	0.32	0	5,5,5	0.52	0
2	GOL	A	709	-	5,5,5	0.37	0	5,5,5	0.34	0
2	GOL	B	711	-	5,5,5	0.29	0	5,5,5	0.38	0
2	GOL	B	705	-	5,5,5	0.38	0	5,5,5	0.22	0
2	GOL	B	718	-	5,5,5	0.38	0	5,5,5	0.38	0
2	GOL	B	716	-	5,5,5	0.40	0	5,5,5	0.23	0
2	GOL	A	706	-	5,5,5	0.54	0	5,5,5	0.93	0
2	GOL	A	704	-	5,5,5	0.43	0	5,5,5	0.50	0
2	GOL	A	717	-	5,5,5	0.38	0	5,5,5	0.32	0
2	GOL	B	708	-	5,5,5	0.37	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	703	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GOL	A	714	-	5,5,5	0.38	0	5,5,5	0.25	0
2	GOL	B	707	-	5,5,5	0.31	0	5,5,5	0.32	0
2	GOL	B	713	-	5,5,5	0.35	0	5,5,5	0.42	0
2	GOL	B	702	-	5,5,5	0.48	0	5,5,5	0.74	0
2	GOL	B	710	-	5,5,5	0.34	0	5,5,5	0.45	0
2	GOL	A	701	-	5,5,5	0.58	0	5,5,5	0.76	0
2	GOL	A	715	-	5,5,5	0.42	0	5,5,5	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	712	-	-	2/4/4/4	-
2	GOL	A	709	-	-	2/4/4/4	-
2	GOL	B	711	-	-	2/4/4/4	-
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	B	718	-	-	0/4/4/4	-
2	GOL	B	716	-	-	2/4/4/4	-
2	GOL	A	706	-	-	4/4/4/4	-
2	GOL	A	704	-	-	2/4/4/4	-
2	GOL	A	717	-	-	2/4/4/4	-
2	GOL	B	708	-	-	2/4/4/4	-
2	GOL	B	703	-	-	1/4/4/4	-
2	GOL	A	714	-	-	2/4/4/4	-
2	GOL	B	707	-	-	2/4/4/4	-
2	GOL	B	713	-	-	4/4/4/4	-
2	GOL	B	702	-	-	0/4/4/4	-
2	GOL	B	710	-	-	2/4/4/4	-
2	GOL	A	701	-	-	4/4/4/4	-
2	GOL	A	715	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	711	GOL	O1-C1-C2-O2
2	B	711	GOL	O1-C1-C2-C3
2	A	709	GOL	O1-C1-C2-C3
2	B	708	GOL	C1-C2-C3-O3
2	A	714	GOL	O1-C1-C2-C3
2	B	707	GOL	O1-C1-C2-C3
2	B	713	GOL	O1-C1-C2-C3
2	B	713	GOL	C1-C2-C3-O3
2	A	706	GOL	O1-C1-C2-C3
2	A	701	GOL	O1-C1-C2-C3
2	A	706	GOL	O1-C1-C2-O2
2	B	712	GOL	O1-C1-C2-C3
2	B	705	GOL	C1-C2-C3-O3
2	B	716	GOL	C1-C2-C3-O3
2	A	704	GOL	C1-C2-C3-O3
2	A	717	GOL	O1-C1-C2-C3
2	B	710	GOL	O1-C1-C2-C3
2	A	701	GOL	C1-C2-C3-O3
2	B	712	GOL	O1-C1-C2-O2
2	A	709	GOL	O1-C1-C2-O2
2	B	708	GOL	O2-C2-C3-O3
2	A	714	GOL	O1-C1-C2-O2
2	B	707	GOL	O1-C1-C2-O2
2	B	713	GOL	O1-C1-C2-O2
2	B	710	GOL	O1-C1-C2-O2
2	A	701	GOL	O2-C2-C3-O3
2	A	704	GOL	O2-C2-C3-O3
2	B	705	GOL	O2-C2-C3-O3
2	A	717	GOL	O1-C1-C2-O2
2	A	701	GOL	O1-C1-C2-O2
2	A	706	GOL	C1-C2-C3-O3
2	B	716	GOL	O2-C2-C3-O3
2	A	706	GOL	O2-C2-C3-O3
2	B	703	GOL	C1-C2-C3-O3
2	B	713	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	709	GOL	1	0
2	B	711	GOL	2	0
2	A	706	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	704	GOL	1	0
2	B	708	GOL	1	0
2	B	703	GOL	2	0
2	B	707	GOL	2	0
2	B	702	GOL	2	0
2	A	701	GOL	3	0
2	A	715	GOL	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.