



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:34 PM GMT

PDB ID : 1G8R  
Title : MOEA  
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Deposited on : 2000-11-20  
Resolution : 2.65 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

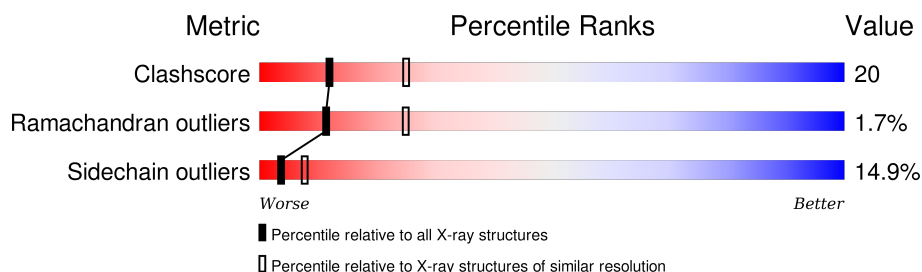
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	411	 62% 29% 6% •
1	B	411	 65% 27% 5% •

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6358 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
1	A	403	Total	C	N	O	S	0	0	0
			3040	1918	531	578	13			
1	B	403	Total	C	N	O	S	0	0	0
			3040	1918	531	578	13			

- 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	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	A	1	Total	C	O	0	0
			6	3	3		

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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	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		

- Molecule 3 is water.

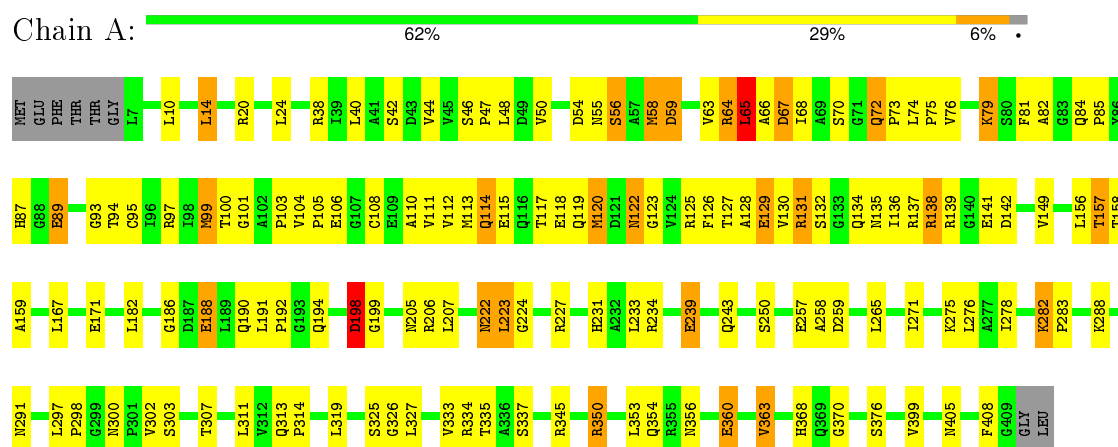
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	112	Total	O	0	0
			112	112		

### 3 Residue-property plots

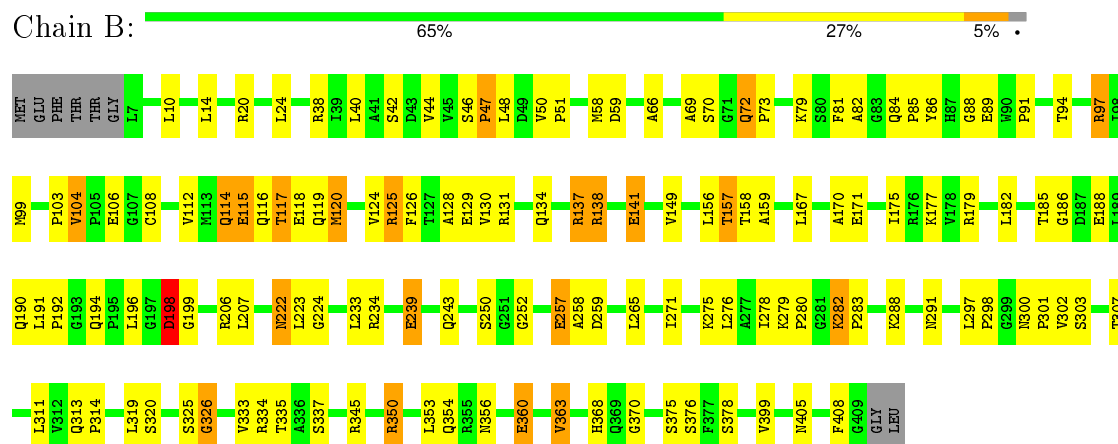
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS MOEA PROTEIN



#### • Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS MOEA PROTEIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.90 Å 98.60 Å 159.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65	Depositor
% Data completeness (in resolution range)	98.8 (50.00-2.65)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.221 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.41	0/3099	0.63	0/4212
1	B	0.41	0/3099	0.64	0/4212
All	All	0.41	0/6198	0.64	0/8424

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

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	136	1
1	B	3040	0	3037	117	1
2	A	24	0	32	1	0
2	B	48	0	64	5	0
3	A	94	0	0	11	0
3	B	112	0	0	10	0
All	All	6358	0	6170	246	1

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 (246) 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:B:157:THR:HG22	1:B:159:ALA:H	1.24	1.03
1:A:157:THR:HG22	1:A:159:ALA:H	1.21	1.02
1:B:300:ASN:HD22	1:B:303:SER:H	1.04	1.01
1:B:179:ARG:HD2	3:B:506:HOH:O	1.64	0.95
1:A:368:HIS:HD2	1:A:370:GLY:H	1.17	0.93
1:A:300:ASN:HD22	1:A:303:SER:H	1.03	0.92
1:B:368:HIS:HD2	1:B:370:GLY:H	1.18	0.89
3:A:418:HOH:O	1:B:192:PRO:HB3	1.70	0.89
1:A:300:ASN:ND2	1:A:303:SER:H	1.71	0.88
1:B:300:ASN:ND2	1:B:303:SER:H	1.72	0.88
1:B:72:GLN:NE2	1:B:72:GLN:H	1.75	0.85
1:B:265:LEU:HD22	1:B:271:ILE:HG13	1.57	0.84
1:A:265:LEU:HD22	1:A:271:ILE:HG13	1.57	0.84
1:B:335:THR:HG22	1:B:337:SER:H	1.45	0.79
1:B:257:GLU:HG2	3:B:525:HOH:O	1.82	0.78
1:A:120:MET:HE1	1:A:125:ARG:HE	1.48	0.78
1:A:335:THR:HG22	1:A:337:SER:H	1.47	0.77
1:B:138:ARG:O	1:B:141:GLU:HG2	1.84	0.77
1:B:79:LYS:O	1:B:86:TYR:HB2	1.86	0.76
1:B:81:PHE:HD2	1:B:99:MET:HG3	1.51	0.76
1:B:114:GLN:O	1:B:117:THR:HG22	1.87	0.74
1:A:97:ARG:HH22	1:A:114:GLN:HE22	1.37	0.73
1:B:137:ARG:HD3	3:B:420:HOH:O	1.89	0.73
1:A:157:THR:CG2	1:A:158:THR:N	2.52	0.72
1:B:177:LYS:HA	2:B:413:GOL:H32	1.73	0.71
1:A:113:MET:HB2	1:A:115:GLU:OE1	1.91	0.71
1:A:368:HIS:CD2	1:A:370:GLY:H	2.06	0.71
1:A:97:ARG:HH12	1:A:114:GLN:HE21	1.37	0.71
1:A:59:ASP:HB3	1:A:99:MET:HG3	1.72	0.70
1:B:222:ASN:HD22	1:B:224:GLY:H	1.40	0.70
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.56	0.70
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.57	0.70
1:B:115:GLU:N	1:B:115:GLU:OE2	2.25	0.69
1:A:105:PRO:HD2	1:A:108:CYS:HB2	1.75	0.69
1:A:157:THR:HG23	1:A:158:THR:H	1.57	0.68
1:B:350:ARG:HD2	1:B:376:SER:OG	1.94	0.68
1:B:157:THR:CG2	1:B:158:THR:N	2.56	0.67
1:B:368:HIS:CD2	1:B:370:GLY:H	2.07	0.67
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.40	0.67
1:A:72:GLN:HG2	1:A:73:PRO:CD	2.25	0.67
1:B:157:THR:HG23	1:B:158:THR:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:GLU:H	1:B:115:GLU:CD	1.97	0.66
1:B:72:GLN:H	1:B:72:GLN:HE21	1.42	0.66
1:A:234:ARG:HD2	3:A:454:HOH:O	1.94	0.66
1:A:117:THR:HG22	1:A:126:PHE:HA	1.77	0.66
1:B:91:PRO:HG2	1:B:94:THR:HG21	1.77	0.65
1:A:234:ARG:CD	3:A:454:HOH:O	2.44	0.65
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.44	0.65
1:B:86:TYR:CZ	1:B:88:GLY:HA3	2.32	0.65
1:A:222:ASN:HD22	1:A:224:GLY:H	1.44	0.65
1:A:191:LEU:HB2	1:A:194:GLN:HG3	1.78	0.65
1:B:191:LEU:HB2	1:B:194:GLN:HG3	1.77	0.65
1:B:104:VAL:HG13	1:B:108:CYS:HB3	1.78	0.64
1:A:157:THR:HG23	1:A:158:THR:N	2.13	0.64
1:A:64:ARG:NH1	1:A:64:ARG:HB2	2.12	0.64
1:B:116:GLN:HB3	1:B:128:ALA:HB3	1.80	0.64
1:A:65:LEU:HD11	1:A:130:VAL:O	1.98	0.64
1:B:114:GLN:HB2	3:B:472:HOH:O	1.96	0.63
1:A:74:LEU:HD22	1:A:93:GLY:O	1.99	0.63
1:A:50:VAL:O	1:A:142:ASP:HB2	1.99	0.63
1:A:38:ARG:HD2	3:A:439:HOH:O	1.99	0.63
1:A:97:ARG:HH12	1:A:114:GLN:NE2	1.96	0.63
1:A:76:VAL:HA	1:A:95:CYS:O	1.99	0.62
1:A:120:MET:CE	1:A:125:ARG:HE	2.12	0.61
1:A:72:GLN:HG2	1:A:73:PRO:HD2	1.82	0.61
1:A:350:ARG:HD2	1:A:376:SER:OG	1.99	0.61
1:B:157:THR:HG23	1:B:158:THR:N	2.15	0.61
1:B:72:GLN:HB2	1:B:73:PRO:HD2	1.83	0.61
1:A:353:LEU:HD13	1:A:363:VAL:HG13	1.81	0.61
1:A:97:ARG:HH22	1:A:114:GLN:NE2	1.97	0.61
1:A:115:GLU:H	1:A:115:GLU:CD	2.05	0.60
1:A:75:PRO:O	1:A:94:THR:HB	2.01	0.60
1:B:114:GLN:NE2	3:B:478:HOH:O	2.33	0.60
1:A:55:ASN:ND2	1:A:101:GLY:HA2	2.15	0.60
1:B:206:ARG:HD2	1:B:222:ASN:HD21	1.66	0.60
1:A:408:PHE:HA	1:B:157:THR:CG2	2.32	0.59
1:B:368:HIS:HD2	1:B:370:GLY:N	1.96	0.59
1:A:112:VAL:HG22	1:A:134:GLN:NE2	2.18	0.59
1:A:131:ARG:O	1:A:134:GLN:HB3	2.02	0.59
1:A:356:ASN:HD21	1:A:360:GLU:HG3	1.66	0.58
1:B:353:LEU:HD13	1:B:363:VAL:HG13	1.85	0.58
1:B:79:LYS:HG2	1:B:97:ARG:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG21	1:B:126:PHE:CD2	2.39	0.58
1:A:59:ASP:OD2	1:A:59:ASP:N	2.31	0.58
1:B:72:GLN:NE2	1:B:72:GLN:N	2.49	0.58
1:A:64:ARG:HH11	1:A:64:ARG:HB2	1.69	0.58
1:B:81:PHE:CD2	1:B:99:MET:HG3	2.35	0.57
1:B:190:GLN:NE2	1:B:194:GLN:NE2	2.52	0.57
1:B:40:LEU:HG	1:B:156:LEU:HD21	1.85	0.57
1:A:67:ASP:HB3	1:A:93:GLY:HA2	1.85	0.57
1:A:206:ARG:HD2	1:A:222:ASN:HD21	1.69	0.56
1:B:50:VAL:HA	1:B:51:PRO:C	2.24	0.56
1:B:72:GLN:N	1:B:72:GLN:HE21	2.04	0.56
1:B:73:PRO:HA	1:B:124:VAL:O	2.06	0.56
1:A:353:LEU:CD1	1:A:363:VAL:HG13	2.36	0.56
1:B:114:GLN:OE1	1:B:114:GLN:N	2.38	0.56
1:A:190:GLN:NE2	1:A:194:GLN:NE2	2.53	0.56
1:B:222:ASN:ND2	1:B:224:GLY:H	2.02	0.56
1:A:54:ASP:HA	1:A:137:ARG:O	2.06	0.56
1:B:356:ASN:HD21	1:B:360:GLU:HG3	1.69	0.56
1:A:84:GLN:HA	3:A:483:HOH:O	2.06	0.55
1:B:112:VAL:HG21	1:B:126:PHE:HD2	1.72	0.55
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.88	0.55
1:A:368:HIS:HD2	1:A:370:GLY:N	1.96	0.55
1:A:58:MET:HG3	1:A:135:ASN:ND2	2.21	0.55
1:A:55:ASN:HD22	1:A:101:GLY:CA	2.20	0.55
1:A:138:ARG:O	1:A:141:GLU:CB	2.55	0.55
1:B:69:ALA:O	1:B:70:SER:C	2.44	0.55
1:A:192:PRO:HB2	1:B:170:ALA:HB2	1.89	0.54
1:A:40:LEU:HG	1:A:156:LEU:HD21	1.89	0.54
1:B:114:GLN:OE1	1:B:114:GLN:CA	2.54	0.54
1:A:408:PHE:HA	1:B:157:THR:HG21	1.89	0.54
1:A:222:ASN:ND2	1:A:224:GLY:H	2.04	0.54
1:B:282:LYS:HB3	1:B:283:PRO:HD3	1.89	0.54
1:A:120:MET:HE1	1:A:125:ARG:NE	2.18	0.54
1:A:97:ARG:NH1	1:A:114:GLN:HE21	2.05	0.54
1:A:75:PRO:HD2	1:A:94:THR:HA	1.90	0.54
1:A:130:VAL:HG13	1:A:134:GLN:NE2	2.23	0.54
2:B:413:GOL:H31	3:B:515:HOH:O	2.08	0.54
1:A:190:GLN:HE21	1:A:194:GLN:CB	2.21	0.54
1:B:300:ASN:HD21	1:B:302:VAL:HB	1.73	0.53
1:B:40:LEU:HD11	1:B:44:VAL:HG23	1.90	0.53
1:A:63:VAL:HG11	1:A:126:PHE:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ALA:HB1	1:A:134:GLN:HG2	1.92	0.52
1:A:137:ARG:HD2	3:A:442:HOH:O	2.10	0.52
1:A:105:PRO:HD2	1:A:108:CYS:CB	2.40	0.52
1:B:120:MET:HE2	1:B:125:ARG:HB2	1.92	0.52
1:B:353:LEU:CD1	1:B:363:VAL:HG13	2.40	0.51
1:B:234:ARG:NH1	3:B:431:HOH:O	2.43	0.51
1:A:138:ARG:O	1:A:141:GLU:HB2	2.11	0.51
1:B:85:PRO:HB3	1:B:103:PRO:HG2	1.91	0.51
1:B:375:SER:HA	3:B:529:HOH:O	2.10	0.51
1:A:118:GLU:HA	3:A:502:HOH:O	2.10	0.51
1:A:356:ASN:ND2	1:A:360:GLU:HG3	2.25	0.51
1:A:111:VAL:HB	1:A:135:ASN:HB2	1.93	0.50
1:A:79:LYS:NZ	1:A:84:GLN:HG3	2.25	0.50
1:A:300:ASN:HD21	1:A:302:VAL:HB	1.76	0.50
1:B:278:ILE:O	1:B:345:ARG:HD2	2.12	0.50
1:A:76:VAL:HG23	1:A:76:VAL:O	2.12	0.50
1:B:190:GLN:HE21	1:B:194:GLN:CB	2.24	0.49
1:A:73:PRO:HB2	1:A:123:GLY:HA3	1.93	0.49
1:B:186:GLY:HA2	2:B:417:GOL:H2	1.94	0.49
1:B:138:ARG:HH11	1:B:138:ARG:CG	2.23	0.49
1:A:40:LEU:HD11	1:A:44:VAL:HG23	1.94	0.49
1:A:408:PHE:C	1:B:157:THR:HG21	2.32	0.49
1:B:66:ALA:O	1:B:69:ALA:HB3	2.13	0.48
1:B:356:ASN:ND2	1:B:360:GLU:HG3	2.28	0.48
1:A:81:PHE:HB2	1:A:84:GLN:CG	2.43	0.48
1:B:104:VAL:HG13	1:B:108:CYS:CB	2.44	0.48
1:A:72:GLN:HG2	1:A:73:PRO:N	2.25	0.48
1:B:118:GLU:OE2	1:B:120:MET:HE1	2.14	0.47
1:A:227:ARG:NH1	3:A:471:HOH:O	2.44	0.47
1:B:378:SER:O	2:B:414:GOL:H2	2.14	0.47
1:B:333:VAL:HG12	1:B:363:VAL:HG22	1.96	0.47
1:A:333:VAL:HG12	1:A:363:VAL:HG22	1.97	0.47
1:A:234:ARG:HD3	3:A:454:HOH:O	2.10	0.47
1:A:85:PRO:HB3	1:A:103:PRO:HG2	1.97	0.47
1:A:356:ASN:OD1	1:A:360:GLU:HG3	2.14	0.47
1:A:278:ILE:O	1:A:345:ARG:HD2	2.16	0.46
1:A:89:GLU:H	1:A:89:GLU:HG3	1.34	0.46
1:B:190:GLN:HG3	1:B:194:GLN:HB2	1.97	0.46
1:A:149:VAL:HG21	1:A:167:LEU:HD11	1.98	0.46
3:A:418:HOH:O	1:B:192:PRO:CB	2.46	0.46
1:A:335:THR:HA	1:A:363:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HD2	3:B:515:HOH:O	2.15	0.46
1:B:356:ASN:OD1	1:B:360:GLU:HG3	2.15	0.46
1:A:275:LYS:NZ	1:A:282:LYS:NZ	2.64	0.46
1:A:283:PRO:HG2	1:A:298:PRO:HB3	1.98	0.46
1:B:326:GLY:N	3:B:430:HOH:O	2.49	0.46
1:A:120:MET:HB2	1:A:123:GLY:O	2.16	0.46
1:A:190:GLN:HG3	1:A:194:GLN:HB2	1.98	0.46
1:A:104:VAL:HG11	1:A:136:ILE:HG23	1.98	0.45
1:B:46:SER:HA	1:B:47:PRO:HD3	1.80	0.45
1:B:320:SER:HB2	2:B:413:GOL:H2	1.99	0.45
1:A:333:VAL:CG1	1:A:334:ARG:N	2.79	0.45
1:A:63:VAL:HG11	1:A:126:PHE:CZ	2.51	0.45
1:A:157:THR:CG2	1:B:408:PHE:HA	2.46	0.45
1:B:104:VAL:CG1	1:B:108:CYS:HB3	2.47	0.45
1:A:275:LYS:HZ3	1:A:282:LYS:NZ	2.15	0.45
1:B:149:VAL:HG21	1:B:167:LEU:HD11	1.99	0.45
1:A:72:GLN:CG	1:A:73:PRO:HD2	2.46	0.44
1:A:58:MET:HE3	1:A:135:ASN:HD21	1.82	0.44
1:A:157:THR:HG22	1:A:158:THR:N	2.31	0.44
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.66	0.44
1:B:307:THR:HG23	1:B:311:LEU:HD12	1.99	0.44
1:B:258:ALA:O	1:B:259:ASP:HB3	2.18	0.44
1:A:350:ARG:NH2	3:A:455:HOH:O	2.50	0.44
1:B:250:SER:HA	1:B:297:LEU:HD12	1.99	0.44
1:B:335:THR:HA	1:B:363:VAL:HG23	1.98	0.44
1:B:185:THR:HG22	1:B:252:GLY:HA3	1.99	0.44
1:A:128:ALA:O	1:A:129:GLU:C	2.55	0.44
1:A:79:LYS:HZ2	1:A:84:GLN:HG3	1.82	0.44
1:B:259:ASP:OD1	1:B:259:ASP:C	2.56	0.44
1:B:333:VAL:CG1	1:B:334:ARG:N	2.80	0.43
1:A:70:SER:C	1:A:72:GLN:N	2.71	0.43
1:B:279:LYS:HD2	1:B:345:ARG:NH2	2.33	0.43
1:A:313:GLN:HB3	1:A:314:PRO:HD3	2.00	0.43
1:B:300:ASN:HA	1:B:301:PRO:HD3	1.91	0.43
1:B:307:THR:O	1:B:311:LEU:HB2	2.19	0.43
1:A:313:GLN:HB3	1:A:314:PRO:CD	2.48	0.43
1:A:120:MET:HE1	1:A:125:ARG:HG3	1.99	0.43
1:A:205:ASN:CG	2:A:415:GOL:H2	2.39	0.43
1:A:300:ASN:HD22	1:A:303:SER:N	1.89	0.43
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.82	0.43
1:B:114:GLN:O	1:B:117:THR:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.14	0.42
1:A:137:ARG:HB3	1:A:141:GLU:OE2	2.19	0.42
1:A:198:ASP:HB3	1:A:199:GLY:H	1.71	0.42
1:A:275:LYS:HZ3	1:A:282:LYS:HZ1	1.65	0.42
1:A:157:THR:HG21	1:B:408:PHE:C	2.40	0.42
1:A:157:THR:HG21	1:B:408:PHE:HA	2.01	0.42
1:B:313:GLN:HB3	1:B:314:PRO:HD3	2.01	0.42
1:A:259:ASP:OD1	1:A:259:ASP:C	2.57	0.42
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.87	0.42
1:A:250:SER:HA	1:A:297:LEU:HD12	2.01	0.42
1:A:408:PHE:CA	1:B:157:THR:HG21	2.50	0.42
1:B:138:ARG:NH1	1:B:138:ARG:CG	2.83	0.42
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.66	0.42
1:A:56:SER:OG	1:A:111:VAL:HG11	2.19	0.42
1:B:275:LYS:HZ3	1:B:282:LYS:NZ	2.17	0.42
1:B:196:LEU:HA	1:B:196:LEU:HD12	1.77	0.42
1:B:190:GLN:HE21	1:B:194:GLN:NE2	2.18	0.42
1:A:46:SER:HA	1:A:47:PRO:HD3	1.82	0.42
1:A:64:ARG:O	1:A:66:ALA:N	2.53	0.41
1:B:119:GLN:HG3	1:B:120:MET:N	2.36	0.41
1:B:275:LYS:NZ	1:B:282:LYS:NZ	2.69	0.41
1:A:307:THR:HG23	1:A:311:LEU:HD12	2.02	0.41
1:B:280:PRO:HG3	1:B:302:VAL:HG12	2.02	0.41
1:A:130:VAL:HG13	1:A:134:GLN:CD	2.41	0.41
1:A:110:ALA:HA	1:A:136:ILE:HD11	2.02	0.41
1:B:190:GLN:NE2	1:B:194:GLN:HE21	2.19	0.41
1:A:258:ALA:O	1:A:259:ASP:HB3	2.21	0.41
1:A:186:GLY:HA3	1:A:188:GLU:OE1	2.20	0.41
1:B:198:ASP:HB3	1:B:199:GLY:H	1.70	0.41
1:A:157:THR:HG22	1:A:159:ALA:N	2.06	0.41
1:A:67:ASP:N	1:A:67:ASP:OD1	2.47	0.41
1:A:335:THR:CG2	1:A:337:SER:O	2.69	0.41
1:A:111:VAL:O	1:A:134:GLN:HG3	2.21	0.41
1:B:283:PRO:HG2	1:B:298:PRO:HB3	2.02	0.41
1:B:350:ARG:HD2	1:B:376:SER:CB	2.51	0.40
1:B:157:THR:HG22	1:B:158:THR:N	2.36	0.40
1:B:112:VAL:CG1	1:B:130:VAL:HG22	2.51	0.40
1:B:275:LYS:HZ3	1:B:282:LYS:HZ1	1.69	0.40
1:A:327:LEU:HA	1:A:327:LEU:HD12	1.85	0.40
1:B:335:THR:CG2	1:B:337:SER:O	2.69	0.40
1:A:223:LEU:HD21	1:A:239:GLU:HG2	2.03	0.40

All (1) 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)
1:A:231:HIS:O	1:B:239:GLU:OE2[3_545]	2.19	0.01

## 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%)	359 (90%)	32 (8%)	10 (2%)	7	15
1	B	401/411 (98%)	370 (92%)	27 (7%)	4 (1%)	19	41
All	All	802/822 (98%)	729 (91%)	59 (7%)	14 (2%)	11	25

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	282	LYS
1	B	198	ASP
1	B	282	LYS
1	A	82	ALA
1	A	100	THR
1	B	82	ALA
1	A	65	LEU
1	A	122	ASN
1	A	127	THR
1	A	129	GLU
1	A	119	GLN
1	A	326	GLY
1	B	326	GLY

### 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	325/331 (98%)	277 (85%)	48 (15%)	4	8
1	B	325/331 (98%)	276 (85%)	49 (15%)	3	7
All	All	650/662 (98%)	553 (85%)	97 (15%)	4	8

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	LEU
1	A	20	ARG
1	A	24	LEU
1	A	42	SER
1	A	48	LEU
1	A	56	SER
1	A	58	MET
1	A	59	ASP
1	A	64	ARG
1	A	65	LEU
1	A	67	ASP
1	A	68	ILE
1	A	72	GLN
1	A	79	LYS
1	A	87	HIS
1	A	89	GLU
1	A	99	MET
1	A	106	GLU
1	A	114	GLN
1	A	120	MET
1	A	122	ASN
1	A	131	ARG
1	A	132	SER
1	A	138	ARG
1	A	139	ARG
1	A	157	THR

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Mol	Chain	Res	Type
1	A	171	GLU
1	A	182	LEU
1	A	188	GLU
1	A	198	ASP
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	233	LEU
1	A	239	GLU
1	A	243	GLN
1	A	257	GLU
1	A	276	LEU
1	A	288	LYS
1	A	291	ASN
1	A	319	LEU
1	A	325	SER
1	A	350	ARG
1	A	354	GLN
1	A	360	GLU
1	A	363	VAL
1	A	399	VAL
1	B	10	LEU
1	B	14	LEU
1	B	20	ARG
1	B	24	LEU
1	B	42	SER
1	B	47	PRO
1	B	48	LEU
1	B	58	MET
1	B	59	ASP
1	B	72	GLN
1	B	84	GLN
1	B	89	GLU
1	B	97	ARG
1	B	104	VAL
1	B	106	GLU
1	B	114	GLN
1	B	115	GLU
1	B	117	THR
1	B	120	MET
1	B	125	ARG
1	B	129	GLU

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Mol	Chain	Res	Type
1	B	131	ARG
1	B	134	GLN
1	B	137	ARG
1	B	138	ARG
1	B	141	GLU
1	B	157	THR
1	B	171	GLU
1	B	175	ILE
1	B	182	LEU
1	B	188	GLU
1	B	198	ASP
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	233	LEU
1	B	239	GLU
1	B	243	GLN
1	B	257	GLU
1	B	276	LEU
1	B	288	LYS
1	B	291	ASN
1	B	319	LEU
1	B	325	SER
1	B	350	ARG
1	B	354	GLN
1	B	360	GLU
1	B	363	VAL
1	B	399	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	114	GLN
1	A	119	GLN
1	A	122	ASN
1	A	190	GLN
1	A	194	GLN
1	A	210	HIS
1	A	222	ASN
1	A	243	GLN
1	A	300	ASN

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	368	HIS
1	B	72	GLN
1	B	119	GLN
1	B	135	ASN
1	B	190	GLN
1	B	194	GLN
1	B	210	HIS
1	B	222	ASN
1	B	243	GLN
1	B	300	ASN
1	B	313	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](#)

12 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	412	-	5,5,5	0.53	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	413	-	5,5,5	0.56	0	5,5,5	0.64	0
2	GOL	A	414	-	5,5,5	0.43	0	5,5,5	0.55	0
2	GOL	A	415	-	5,5,5	0.47	0	5,5,5	0.62	0
2	GOL	B	412	-	5,5,5	0.46	0	5,5,5	0.41	0
2	GOL	B	413	-	5,5,5	0.53	0	5,5,5	0.43	0
2	GOL	B	414	-	5,5,5	0.38	0	5,5,5	0.57	0
2	GOL	B	415	-	5,5,5	0.43	0	5,5,5	0.58	0
2	GOL	B	416	-	5,5,5	0.54	0	5,5,5	0.47	0
2	GOL	B	417	-	5,5,5	1.04	0	5,5,5	0.53	0
2	GOL	B	418	-	5,5,5	0.36	0	5,5,5	0.44	0
2	GOL	B	419	-	5,5,5	0.39	0	5,5,5	0.45	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	A	412	-	-	0/4/4/4	0/0/0/0
2	GOL	A	413	-	-	0/4/4/4	0/0/0/0
2	GOL	A	414	-	-	0/4/4/4	0/0/0/0
2	GOL	A	415	-	-	0/4/4/4	0/0/0/0
2	GOL	B	412	-	-	0/4/4/4	0/0/0/0
2	GOL	B	413	-	-	0/4/4/4	0/0/0/0
2	GOL	B	414	-	-	0/4/4/4	0/0/0/0
2	GOL	B	415	-	-	0/4/4/4	0/0/0/0
2	GOL	B	416	-	-	0/4/4/4	0/0/0/0
2	GOL	B	417	-	-	0/4/4/4	0/0/0/0
2	GOL	B	418	-	-	0/4/4/4	0/0/0/0
2	GOL	B	419	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	413	GOL	3	0
2	B	414	GOL	1	0
2	B	417	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.