



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 08:23 am GMT

PDB ID : 4AHC  
Title : Crystal Structure of an Evolved Replicating DNA Polymerase  
Authors : Wynne, S.A.; Holliger, P.; Leslie, A.G.W.  
Deposited on : 2012-02-06  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

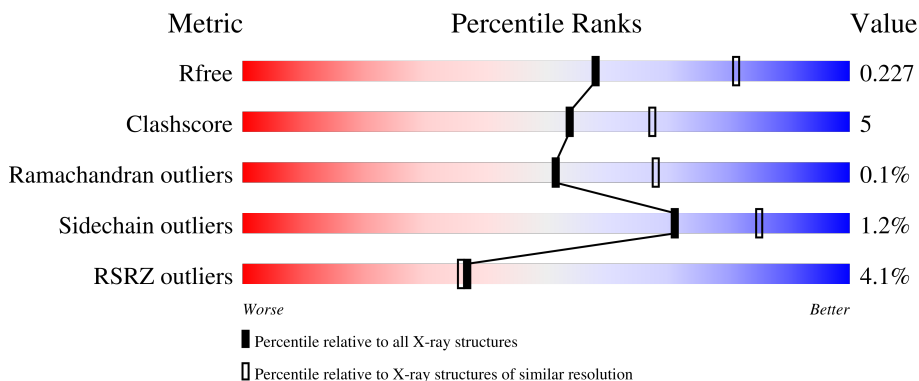
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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  $\leq 5\%$ . 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	775	 5% 80% 11% 9%
1	B	775	 3% 84% 12% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12181 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 DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	704	5786	3755	959	1059	13	0	0	0
1	B	743	6077	3941	1005	1117	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	GLN	VAL	engineered mutation	UNP P61875
A	141	ALA	ASP	engineered mutation	UNP P61875
A	143	ALA	GLU	engineered mutation	UNP P61875
A	337	ILE	VAL	engineered mutation	UNP P61875
A	399	ASP	GLU	engineered mutation	UNP P61875
A	400	ASP	ASN	engineered mutation	UNP P61875
A	407	ILE	ARG	engineered mutation	UNP P61875
A	546	HIS	TYR	engineered mutation	UNP P61875
B	93	GLN	VAL	engineered mutation	UNP P61875
B	141	ALA	ASP	engineered mutation	UNP P61875
B	143	ALA	GLU	engineered mutation	UNP P61875
B	337	ILE	VAL	engineered mutation	UNP P61875
B	399	ASP	GLU	engineered mutation	UNP P61875
B	400	ASP	ASN	engineered mutation	UNP P61875
B	407	ILE	ARG	engineered mutation	UNP P61875
B	546	HIS	TYR	engineered mutation	UNP P61875

- 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		

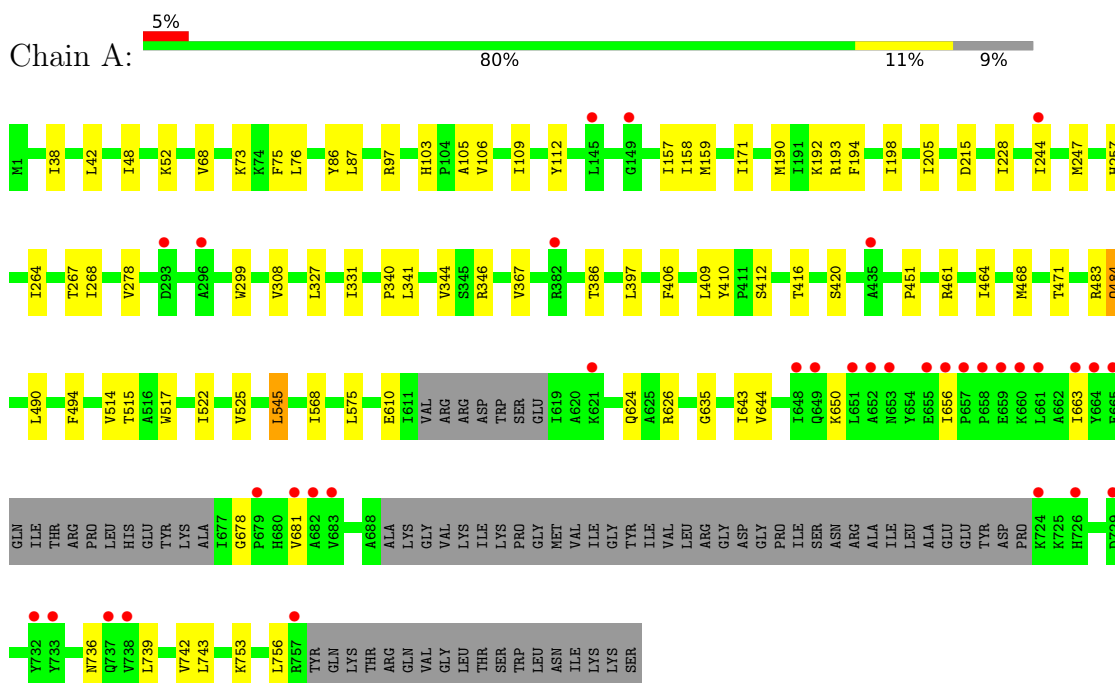
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total	O	0	0
			140	140		
3	B	154	Total	O	0	0
			154	154		

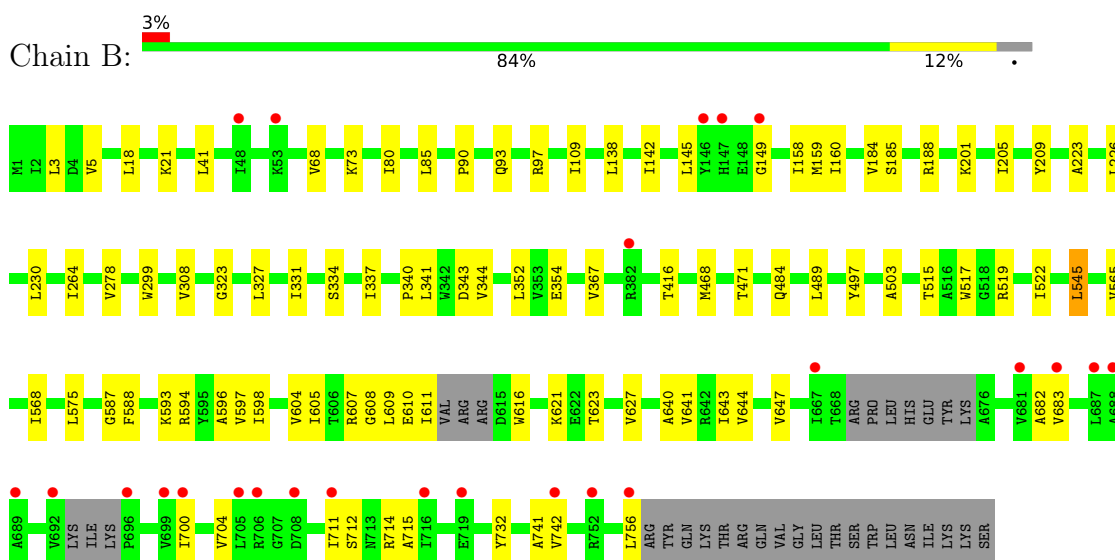
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: DNA POLYMERASE



#### • Molecule 1: DNA POLYMERASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.44Å 197.86Å 78.44Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	98.95 – 2.40 35.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.8 (98.95-2.40) 88.8 (35.88-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0002	Depositor
R, $R_{free}$	0.206 , 0.229 0.206 , 0.227	Depositor DCC
$R_{free}$ test set	3930 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 17.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.446 for l,-k,h	Xtriage
Reported twinning fraction	0.546 for H, K, L 0.454 for L, -K, H	Depositor
Outliers	0 of 78428 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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

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	0.26	0/5914	0.44	0/7970
1	B	0.26	0/6212	0.45	0/8377
All	All	0.26	0/12126	0.45	0/16347

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	5786	0	5881	59	0
1	B	6077	0	6166	68	0
2	A	12	0	16	0	0
2	B	12	0	16	1	0
3	A	140	0	0	0	0
3	B	154	0	0	0	0
All	All	12181	0	12079	127	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 5.

All (127) 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:264:ILE:HD13	1:A:278:VAL:HG11	1.52	0.91
1:B:5:VAL:HG12	1:B:18:LEU:HD23	1.60	0.83
1:B:264:ILE:HD13	1:B:278:VAL:HG11	1.62	0.82
1:B:5:VAL:CG1	1:B:18:LEU:HD23	2.11	0.81
1:A:194:PHE:CZ	1:A:198:ILE:HD11	2.24	0.72
1:A:159:MET:HE3	1:A:308:VAL:HG12	1.71	0.71
1:B:158:ILE:HG22	1:B:159:MET:HG3	1.73	0.70
1:A:97:ARG:HG3	1:A:109:ILE:HD11	1.73	0.69
1:A:267:THR:HG22	1:A:268:ILE:HG23	1.77	0.67
1:B:627:VAL:HG13	1:B:640:ALA:HB1	1.79	0.64
1:B:327:LEU:O	1:B:331:ILE:HG23	1.98	0.63
1:B:644:VAL:HG21	1:B:742:VAL:HG11	1.83	0.61
1:B:704:VAL:HG11	1:B:732:TYR:CD2	2.37	0.60
1:A:158:ILE:HG23	1:A:299:TRP:CZ3	2.37	0.60
1:A:48:ILE:HD11	1:A:68:VAL:HG11	1.84	0.59
1:A:97:ARG:CG	1:A:109:ILE:HD11	2.33	0.58
1:A:644:VAL:HG21	1:A:742:VAL:HG11	1.85	0.58
1:B:97:ARG:CG	1:B:109:ILE:HD11	2.33	0.58
1:B:337:ILE:CD1	1:B:352:LEU:HD22	2.35	0.57
1:B:158:ILE:HG23	1:B:299:TRP:CZ3	2.39	0.57
1:B:597:VAL:CG2	1:B:605:ILE:HG23	2.35	0.57
1:A:416:THR:HG22	1:A:575:LEU:H	1.69	0.56
1:A:739:LEU:HD13	1:A:756:LEU:HD12	1.86	0.56
1:A:412:SER:O	1:A:416:THR:HG23	2.06	0.56
1:A:73:LYS:HB3	1:A:367:VAL:HG23	1.88	0.56
1:B:597:VAL:HG23	1:B:605:ILE:HG23	1.88	0.55
1:B:641:VAL:HG13	1:B:756:LEU:HD23	1.89	0.55
1:A:406:PHE:CG	1:A:409:LEU:HD13	2.42	0.55
1:A:644:VAL:HG11	1:A:756:LEU:HD22	1.88	0.55
1:B:158:ILE:HG23	1:B:299:TRP:CE3	2.42	0.55
1:A:650:LYS:HB3	1:A:656:ILE:HG23	1.88	0.54
1:B:597:VAL:HG23	1:B:605:ILE:CG2	2.38	0.54
1:B:97:ARG:HG3	1:B:109:ILE:HD11	1.89	0.53
1:A:626:ARG:NH1	1:A:643:ILE:HD12	2.23	0.53
1:A:644:VAL:HG11	1:A:756:LEU:HD13	1.91	0.52
1:B:97:ARG:CD	1:B:109:ILE:HD11	2.39	0.52
1:B:323:GLY:O	1:B:327:LEU:HB2	2.10	0.52
1:B:611:ILE:HG21	1:B:621:LYS:HE3	1.91	0.52
1:B:337:ILE:HD12	1:B:352:LEU:HD22	1.91	0.52
1:A:743:LEU:HD11	1:A:753:LYS:HG2	1.93	0.51
1:A:159:MET:CE	1:A:308:VAL:HG12	2.39	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HD12	1:A:327:LEU:HD21	1.91	0.51
1:A:205:ILE:CD1	1:A:327:LEU:HD21	2.42	0.50
1:A:416:THR:CG2	1:A:575:LEU:H	2.25	0.50
1:B:5:VAL:HG11	1:B:18:LEU:HD23	1.93	0.50
1:B:97:ARG:HD2	1:B:109:ILE:HD11	1.94	0.50
1:B:545:LEU:N	1:B:545:LEU:HD12	2.27	0.49
1:A:158:ILE:HG23	1:A:299:TRP:CE3	2.48	0.49
1:B:605:ILE:HD13	2:B:801:GOL:H32	1.94	0.49
1:B:184:VAL:HG22	1:B:185:SER:H	1.77	0.49
1:B:68:VAL:HG22	1:B:85:LEU:HD22	1.94	0.49
1:A:264:ILE:HD13	1:A:278:VAL:CG1	2.35	0.48
1:B:643:ILE:O	1:B:647:VAL:HG23	2.12	0.48
1:B:90:PRO:HA	1:B:93:GLN:HE21	1.78	0.48
1:A:257:HIS:O	1:A:346:ARG:NH2	2.38	0.48
1:A:410:TYR:CD1	1:A:514:VAL:HG12	2.49	0.48
1:A:525:VAL:HG22	1:A:568:ILE:HG12	1.94	0.48
1:B:515:THR:HG22	1:B:519:ARG:NH1	2.29	0.47
1:B:138:LEU:HD13	1:B:201:LYS:HD3	1.96	0.47
1:B:145:LEU:HD22	1:B:299:TRP:CD1	2.49	0.47
1:A:739:LEU:CD1	1:A:756:LEU:HD12	2.45	0.47
1:B:159:MET:CE	1:B:308:VAL:HG12	2.45	0.47
1:B:334:SER:HA	1:B:344:VAL:HG21	1.96	0.47
1:A:490:LEU:HD13	1:A:494:PHE:HE1	1.80	0.47
1:B:588:PHE:CE1	1:B:596:ALA:HB3	2.50	0.47
1:B:68:VAL:HG13	1:B:85:LEU:HD23	1.97	0.47
1:B:683:VAL:HG22	1:B:700:ILE:HG21	1.97	0.47
1:A:545:LEU:HD12	1:A:545:LEU:N	2.30	0.46
1:A:171:ILE:HD13	1:A:193:ARG:HG3	1.97	0.46
1:B:264:ILE:HD13	1:B:278:VAL:CG1	2.41	0.46
1:B:416:THR:CG2	1:B:575:LEU:H	2.29	0.46
1:B:587:GLY:HA3	1:B:597:VAL:HG12	1.98	0.46
1:B:331:ILE:HG22	1:B:341:LEU:HD22	1.98	0.46
1:A:158:ILE:HG22	1:A:159:MET:HE2	1.98	0.45
1:B:73:LYS:HB3	1:B:367:VAL:HG23	1.97	0.45
1:A:86:TYR:O	1:A:87:LEU:HD23	2.16	0.45
1:A:386:THR:O	1:A:515:THR:HG21	2.17	0.45
1:B:598:ILE:HD12	1:B:604:VAL:HG12	1.99	0.45
1:B:340:PRO:HG2	1:B:343:ASP:OD1	2.17	0.45
1:A:38:ILE:HG22	1:A:112:TYR:HA	1.99	0.44
1:B:497:TYR:CZ	1:B:503:ALA:HB1	2.52	0.44
1:A:103:HIS:HD2	1:A:105:ALA:HB3	1.83	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:VAL:CG2	1:A:742:VAL:HG11	2.47	0.44
1:A:644:VAL:CG1	1:A:756:LEU:HD22	2.48	0.44
1:B:159:MET:HE1	1:B:308:VAL:HG12	2.00	0.44
1:A:397:LEU:HD21	1:A:635:GLY:HA2	2.00	0.44
1:A:461:ARG:NH2	1:A:484:GLN:OE1	2.50	0.44
1:A:52:LYS:HG2	1:A:68:VAL:HG21	2.00	0.44
1:A:327:LEU:O	1:A:331:ILE:HG23	2.18	0.44
1:B:565:VAL:HA	1:B:568:ILE:HG22	1.98	0.44
1:A:157:ILE:CG2	1:A:190:MET:HE3	2.48	0.44
1:B:223:ALA:HB2	1:B:230:LEU:HD21	2.00	0.44
1:B:594:ARG:HA	1:B:607:ARG:O	2.18	0.44
1:B:682:ALA:HB2	1:B:715:ALA:O	2.18	0.43
1:A:420:SER:HB3	1:A:451:PRO:HD3	1.99	0.43
1:B:641:VAL:HG13	1:B:756:LEU:CD2	2.49	0.43
1:A:42:LEU:CD2	1:A:106:VAL:HG22	2.48	0.43
1:B:416:THR:HG22	1:B:575:LEU:H	1.82	0.43
1:A:464:ILE:HD11	1:A:483:ARG:CZ	2.48	0.43
1:B:41:LEU:HD22	1:B:80:ILE:HD11	2.00	0.43
1:B:623:THR:O	1:B:627:VAL:HG23	2.20	0.42
1:A:327:LEU:HD11	1:A:341:LEU:HD21	2.01	0.42
1:A:264:ILE:CD1	1:A:278:VAL:HG11	2.35	0.42
1:A:678:GLY:O	1:A:681:VAL:HG23	2.20	0.42
1:B:608:GLY:O	1:B:609:LEU:HD23	2.20	0.42
1:A:663:ILE:HD12	1:A:663:ILE:N	2.35	0.41
1:B:522:ILE:CD1	1:B:545:LEU:HD11	2.50	0.41
1:B:522:ILE:HD11	1:B:545:LEU:HG	2.02	0.41
1:B:616:TRP:CZ3	1:B:741:ALA:HB2	2.55	0.41
1:A:468:MET:HA	1:A:471:THR:HG22	2.03	0.41
1:B:209:TYR:HE1	1:B:264:ILE:HD12	1.85	0.41
1:A:75:PHE:CD2	1:A:76:LEU:HD13	2.56	0.41
1:A:244:ILE:HD12	1:A:247:MET:CE	2.50	0.41
1:A:626:ARG:NH2	1:A:643:ILE:HG23	2.36	0.41
1:B:3:LEU:HD11	1:B:21:LYS:HB2	2.03	0.41
1:B:188:ARG:NH1	1:B:226:LEU:O	2.54	0.41
1:B:711:ILE:HG23	1:B:712:SER:N	2.36	0.41
1:B:704:VAL:HG11	1:B:732:TYR:CG	2.55	0.41
1:B:644:VAL:CG2	1:B:742:VAL:HG11	2.51	0.41
1:A:340:PRO:O	1:A:344:VAL:HG23	2.20	0.41
1:B:142:ILE:HG22	1:B:160:ILE:HG12	2.02	0.41
1:B:205:ILE:HD12	1:B:327:LEU:HD21	2.02	0.41
1:A:75:PHE:CE2	1:A:76:LEU:HD13	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HG3	1:A:228:ILE:HD12	2.03	0.41
1:A:522:ILE:HD11	1:A:545:LEU:HG	2.03	0.41
1:B:344:VAL:HG13	1:B:352:LEU:HD21	2.03	0.40
1:B:468:MET:HA	1:B:471:THR:HG22	2.04	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	696/775 (90%)	673 (97%)	23 (3%)	0	100 100
1	B	735/775 (95%)	703 (96%)	31 (4%)	1 (0%)	51 68
All	All	1431/1550 (92%)	1376 (96%)	54 (4%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	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	618/679 (91%)	611 (99%)	7 (1%)	73 87

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	648/679 (95%)	640 (99%)	8 (1%)	71 85
All	All	1266/1358 (93%)	1251 (99%)	15 (1%)	71 85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ASP
1	A	484	GLN
1	A	517	TRP
1	A	545	LEU
1	A	610	GLU
1	A	624	GLN
1	A	736	ASN
1	B	354	GLU
1	B	484	GLN
1	B	489	LEU
1	B	517	TRP
1	B	545	LEU
1	B	593	LYS
1	B	610	GLU
1	B	714	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	103	HIS
1	A	166	ASN
1	A	257	HIS
1	A	492	ASN
1	A	736	ASN
1	B	93	GLN
1	B	103	HIS
1	B	166	ASN
1	B	257	HIS
1	B	492	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	800	-	5,5,5	0.30	0	5,5,5	0.31	0
2	GOL	A	801	-	5,5,5	0.28	0	5,5,5	0.19	0
2	GOL	B	801	-	5,5,5	0.35	0	5,5,5	0.21	0
2	GOL	A	800	-	5,5,5	0.27	0	5,5,5	0.29	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	800	-	-	0/4/4/4	-
2	GOL	A	801	-	-	4/4/4/4	-
2	GOL	B	801	-	-	3/4/4/4	-
2	GOL	A	800	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
2	B	801	GOL	C1-C2-C3-O3
2	B	801	GOL	O2-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2
2	B	801	GOL	O1-C1-C2-C3
2	A	801	GOL	O2-C2-C3-O3
2	A	800	GOL	C1-C2-C3-O3
2	A	800	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	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

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	704/775 (90%)	0.32	35 (4%) 28 27	24, 44, 95, 117	0
1	B	743/775 (95%)	0.23	25 (3%) 45 44	23, 44, 89, 106	0
All	All	1447/1550 (93%)	0.28	60 (4%) 37 36	23, 44, 90, 117	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	ALA	8.3
1	A	681	VAL	8.0
1	A	656	ILE	7.3
1	A	733	TYR	7.0
1	A	663	ILE	5.8
1	A	665	GLU	5.5
1	B	687	LEU	5.3
1	B	667	ILE	5.2
1	B	700	ILE	5.0
1	B	699	VAL	4.9
1	A	659	GLU	4.6
1	A	732	TYR	4.6
1	A	664	TYR	4.5
1	B	683	VAL	4.3
1	B	149	GLY	4.1
1	B	382	ARG	4.0
1	A	661	LEU	3.9
1	B	146	TYR	3.8
1	A	658	PRO	3.8
1	A	683	VAL	3.7
1	A	679	PRO	3.7
1	A	145	LEU	3.6
1	A	244	ILE	3.5
1	A	726	HIS	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	689	ALA	3.3
1	A	737	GLN	3.2
1	A	296	ALA	3.2
1	A	653	ASN	3.2
1	B	681	VAL	3.2
1	A	149	GLY	3.1
1	B	719	GLU	3.1
1	A	652	ALA	2.9
1	B	756	LEU	2.9
1	A	651	LEU	2.8
1	A	660	LYS	2.7
1	A	724	LYS	2.7
1	A	382	ARG	2.7
1	A	757	ARG	2.6
1	A	648	ILE	2.6
1	B	752	ARG	2.6
1	A	657	PRO	2.6
1	B	696	PRO	2.5
1	A	649	GLN	2.4
1	A	729	ASP	2.4
1	B	706	ARG	2.4
1	B	53	LYS	2.4
1	A	738	VAL	2.3
1	B	692	VAL	2.3
1	B	48	ILE	2.2
1	A	293	ASP	2.2
1	A	621	LYS	2.2
1	B	705	LEU	2.2
1	B	742	VAL	2.1
1	B	147	HIS	2.1
1	A	655	GLU	2.1
1	B	711	ILE	2.1
1	B	708	ASP	2.0
1	A	435	ALA	2.0
1	B	688	ALA	2.0
1	B	716	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.



### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	GOL	B	801	6/6	0.81	0.24	39,41,41,42	0
2	GOL	A	801	6/6	0.83	0.24	49,50,50,50	0
2	GOL	B	800	6/6	0.88	0.17	31,31,32,32	0
2	GOL	A	800	6/6	0.96	0.11	30,31,32,32	0

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

There are no such residues in this entry.