



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2022 – 02:24 PM EST

PDB ID : 6XML  
Title : Human aldolase A I98C  
Authors : Meneely, K.M.; Brewer, K.; Lamb, A.L.  
Deposited on : 2020-06-30  
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.

---

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)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
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) : 2.25

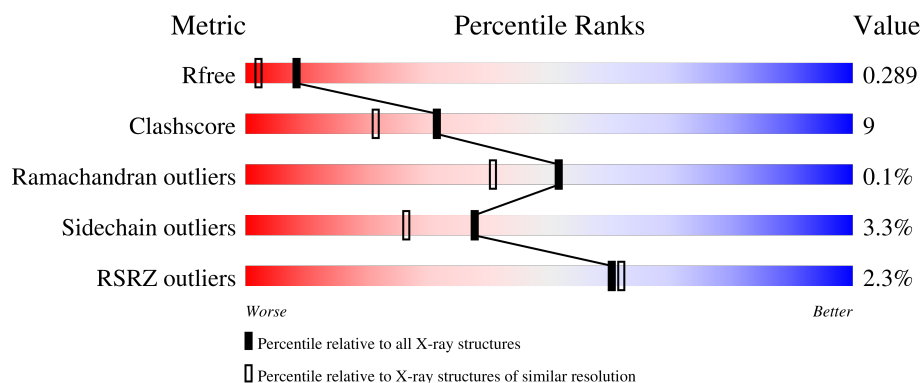
# 1 Overall quality at a glance

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))
$R_{free}$	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (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 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	364	
1	B	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	402	-	-	X	-
3	GOL	A	405	-	X	-	-
3	GOL	B	403	-	X	-	-
3	GOL	B	405	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11179 atoms, of which 5486 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.

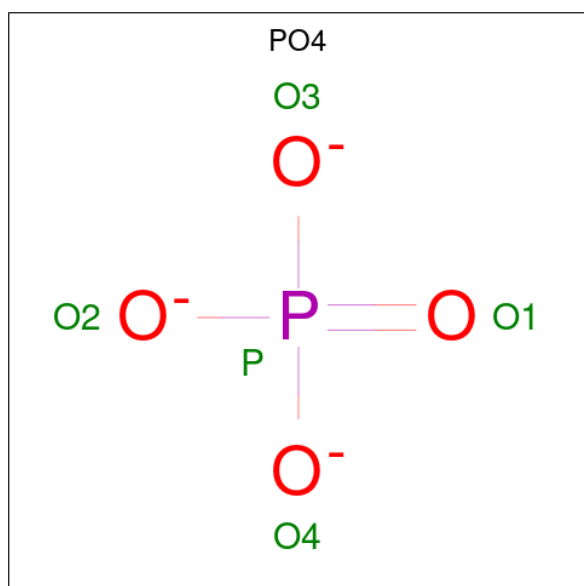
- Molecule 1 is a protein called Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	353	Total	C	H	N	O	S	0	0	0
			5380	1682	2705	472	509	12			
1	B	358	Total	C	H	N	O	S	0	0	0
			5444	1704	2733	478	517	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	CYS	ILE	engineered mutation	UNP P04075
B	98	CYS	ILE	engineered mutation	UNP P04075

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

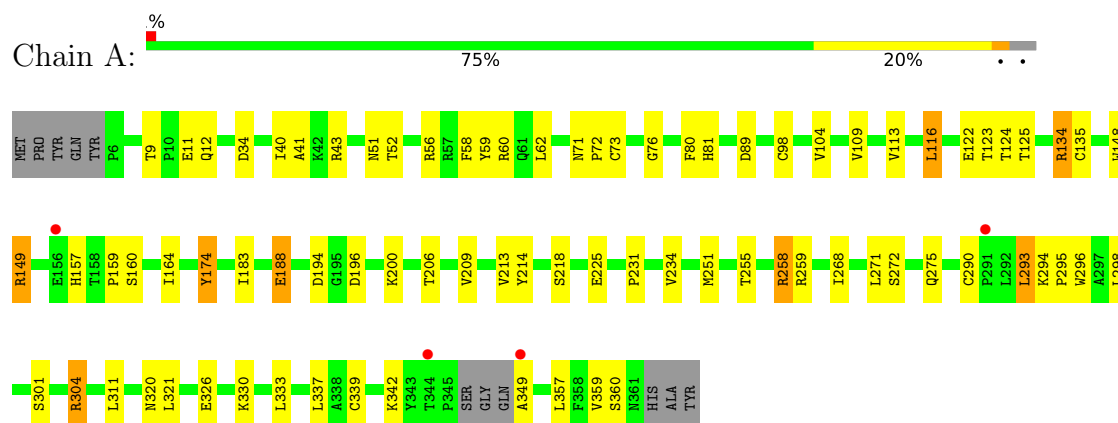
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total 126	O 126	0	0
4	B	125	Total 125	O 125	0	0

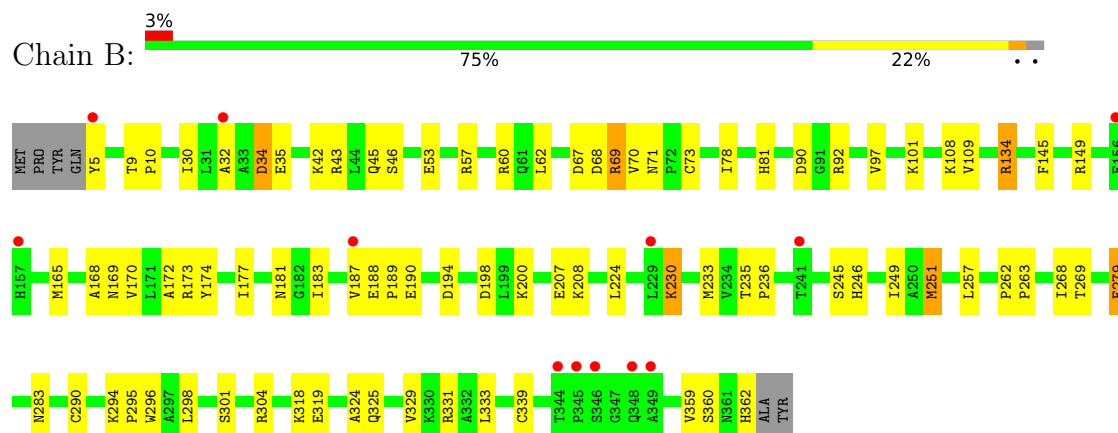
### 3 Residue-property plots

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: Fructose-bisphosphate aldolase A



#### • Molecule 1: Fructose-bisphosphate aldolase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.57Å 162.57Å 167.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.20 – 1.88 40.20 – 1.88	Depositor EDS
% Data completeness (in resolution range)	61.7 (40.20-1.88) 61.7 (40.20-1.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 1.88Å)	Xtriage
Refinement program	REFMAC 1.16_3549, PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.245 , 0.286 0.255 , 0.289	Depositor DCC
$R_{free}$ test set	3139 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0494e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	1.05	10/2723 (0.4%)	1.09	11/3687 (0.3%)
1	B	1.16	17/2761 (0.6%)	0.99	8/3741 (0.2%)
All	All	1.11	27/5484 (0.5%)	1.05	19/7428 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	GLU	CD-OE1	-12.57	1.11	1.25
1	B	279	GLU	CG-CD	10.04	1.67	1.51
1	B	188	GLU	CD-OE2	-8.63	1.16	1.25
1	B	190	GLU	CD-OE1	-8.17	1.16	1.25
1	B	9	THR	C-O	-6.88	1.10	1.23
1	B	35	GLU	CG-CD	6.63	1.61	1.51
1	B	187	VAL	C-O	-6.46	1.11	1.23
1	A	225	GLU	CG-CD	6.37	1.61	1.51
1	A	231	PRO	N-CD	-6.20	1.39	1.47
1	B	190	GLU	CD-OE2	-6.17	1.18	1.25
1	B	10	PRO	C-O	-6.11	1.11	1.23
1	A	214	TYR	CE2-CZ	6.10	1.46	1.38
1	A	11	GLU	CB-CG	6.08	1.63	1.52
1	B	207	GLU	CG-CD	6.07	1.61	1.51
1	A	214	TYR	CD2-CE2	5.75	1.48	1.39
1	A	98	CYS	CB-SG	-5.70	1.72	1.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	ASP	CB-CG	5.66	1.63	1.51
1	B	208	LYS	CE-NZ	5.65	1.63	1.49
1	A	11	GLU	CG-CD	5.53	1.60	1.51
1	A	349	ALA	CA-CB	5.53	1.64	1.52
1	B	5	TYR	CE1-CZ	5.37	1.45	1.38
1	A	89	ASP	CB-CG	5.32	1.62	1.51
1	B	5	TYR	CB-CG	5.30	1.59	1.51
1	B	230	LYS	C-N	-5.19	1.24	1.34
1	A	188	GLU	CG-CD	5.07	1.59	1.51
1	B	53	GLU	CG-CD	5.03	1.59	1.51
1	B	362	HIS	CA-CB	5.02	1.65	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	NE-CZ-NH2	-11.59	114.50	120.30
1	A	149	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	A	134	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	B	134	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	A	134	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	B	134	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	116	LEU	CB-CG-CD2	-7.90	97.57	111.00
1	B	224	LEU	CB-CG-CD1	-7.83	97.69	111.00
1	A	258	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	69	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	271	LEU	CB-CG-CD1	6.36	121.82	111.00
1	A	34	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	B	62	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	214	TYR	CA-CB-CG	-5.80	102.37	113.40
1	B	57	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	251	MET	CG-SD-CE	5.34	108.75	100.20
1	B	149	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	293	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	A	89	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	THR	Peptide

## 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	2675	2705	2704	45	0
1	B	2711	2733	2731	55	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
3	A	18	24	24	3	0
3	B	18	24	24	7	0
4	A	126	0	0	1	0
4	B	125	0	0	4	0
All	All	5693	5486	5483	98	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 9.

All (98) 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:124:THR:HG22	1:A:125:THR:H	1.00	1.09
1:B:290:CYS:O	1:B:294:LYS:NZ	1.86	1.08
1:A:124:THR:HG22	1:A:125:THR:N	1.80	0.96
1:A:124:THR:CG2	1:A:125:THR:H	1.81	0.93
1:B:319:GLU:OE1	4:B:501:HOH:O	2.01	0.78
1:B:200:LYS:NZ	2:B:402:PO4:O4	2.21	0.74
1:A:304:ARG:HB3	1:A:357:LEU:HD13	1.76	0.68
1:A:149:ARG:HG3	1:A:188:GLU:HG2	1.76	0.67
1:A:272:SER:O	1:A:275:GLN:HG3	1.96	0.66
1:B:230:LYS:HG3	1:B:269:THR:O	1.95	0.66
1:B:68:ASP:OD1	4:B:502:HOH:O	2.14	0.65
1:A:43:ARG:O	1:A:311:LEU:HD21	1.96	0.64
1:A:290:CYS:O	1:A:294:LYS:NZ	2.30	0.64
3:B:405:GOL:HO1	3:B:405:GOL:HO3	1.46	0.64
1:B:108:LYS:HE3	3:B:403:GOL:H32	1.81	0.61
1:A:326:GLU:O	1:A:330:LYS:HG3	2.03	0.59
1:B:81:HIS:HE2	3:B:405:GOL:H2	1.68	0.58
1:A:337:LEU:HD22	1:A:342:LYS:HD3	1.85	0.58
1:B:67:ASP:O	1:B:70:VAL:HG22	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:MET:HE2	4:B:624:HOH:O	2.05	0.57
1:B:318:LYS:HG3	1:B:318:LYS:O	2.05	0.56
1:A:157:HIS:HA	3:A:404:GOL:H32	1.85	0.56
1:A:304:ARG:HD3	2:A:401:PO4:O1	2.05	0.56
1:A:160:SER:O	1:A:164:ILE:HG13	2.06	0.56
1:B:109:VAL:HG21	1:B:174:TYR:HE1	1.71	0.55
1:A:116:LEU:HD13	1:A:124:THR:OG1	2.07	0.55
1:A:135:CYS:HB3	1:A:183:ILE:HD12	1.90	0.54
1:B:359:VAL:O	1:B:360:SER:C	2.46	0.54
1:B:43:ARG:NH1	1:B:43:ARG:HG2	2.23	0.54
1:B:165:MET:SD	1:B:165:MET:C	2.86	0.53
1:A:149:ARG:HG3	1:A:188:GLU:CG	2.39	0.53
1:B:90:ASP:OD1	1:B:92:ARG:HG3	2.09	0.53
1:A:41:ALA:HB2	1:A:51:ASN:ND2	2.23	0.53
1:B:257:LEU:HD13	1:B:268:ILE:HD13	1.91	0.52
1:A:293:LEU:HD22	1:B:295:PRO:HB3	1.90	0.52
1:B:169:ASN:O	1:B:172:ALA:HB3	2.11	0.51
1:A:209:VAL:O	1:A:213:VAL:HG23	2.11	0.51
1:B:359:VAL:O	1:B:359:VAL:HG23	2.11	0.51
1:B:233:MET:CE	1:B:283:ASN:HB3	2.41	0.50
1:B:170:VAL:HG12	3:B:404:GOL:H2	1.92	0.50
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.76	0.49
1:B:97:VAL:O	1:B:101:LYS:HG3	2.12	0.49
1:B:170:VAL:HG13	3:B:404:GOL:O3	2.12	0.49
1:B:109:VAL:O	1:B:134:ARG:NH2	2.42	0.48
1:B:181:ASN:OD1	4:B:503:HOH:O	2.20	0.48
1:B:67:ASP:OD2	1:B:69:ARG:HD3	2.13	0.48
1:B:81:HIS:NE2	3:B:405:GOL:H2	2.28	0.48
1:B:173:ARG:O	1:B:177:ILE:HG13	2.14	0.48
1:B:34:ASP:OD2	1:B:108:LYS:HE2	2.14	0.48
1:B:169:ASN:O	1:B:172:ALA:N	2.45	0.48
1:A:76:GLY:HA2	1:A:104:VAL:O	2.14	0.47
1:A:80:PHE:O	1:A:81:HIS:C	2.51	0.47
1:A:109:VAL:O	1:A:134:ARG:NH2	2.45	0.47
1:B:30:ILE:HB	1:B:301:SER:HA	1.96	0.47
1:B:43:ARG:O	1:B:46:SER:OG	2.31	0.47
1:A:73:CYS:SG	1:A:333:LEU:HD23	2.55	0.47
1:A:255:THR:O	1:A:259:ARG:HG3	2.15	0.46
1:A:40:ILE:O	1:A:40:ILE:HG13	2.14	0.46
1:A:295:PRO:HG3	1:B:263:PRO:HG3	1.97	0.46
1:B:32:ALA:HB1	1:B:34:ASP:OD1	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:CD2	1:A:342:LYS:HD3	2.45	0.46
1:B:294:LYS:HD2	1:B:298:LEU:HD12	1.98	0.45
1:A:157:HIS:HA	3:A:404:GOL:C3	2.46	0.45
1:B:71:ASN:OD1	1:B:101:LYS:HB3	2.16	0.45
1:A:58:PHE:CZ	1:A:321:LEU:HD12	2.52	0.45
1:A:268:ILE:HB	1:A:298:LEU:HD23	1.99	0.45
1:B:235:THR:HB	1:B:236:PRO:HD2	1.98	0.45
1:B:168:ALA:O	1:B:169:ASN:C	2.55	0.44
1:B:324:ALA:O	1:B:325:GLN:C	2.56	0.44
1:A:148:TRP:HB2	1:A:174:TYR:CE1	2.53	0.44
1:A:59:TYR:O	1:A:62:LEU:HB3	2.17	0.44
1:A:320:ASN:O	1:A:321:LEU:C	2.55	0.44
1:B:30:ILE:HG21	1:B:78:ILE:HD11	2.00	0.44
1:A:258:ARG:O	1:B:263:PRO:HD2	2.18	0.44
1:A:218:SER:O	3:A:405:GOL:H12	2.18	0.44
1:B:70:VAL:CG1	1:B:329:VAL:HG22	2.48	0.43
1:A:71:ASN:N	1:A:72:PRO:CD	2.82	0.43
1:A:294:LYS:HD2	1:A:298:LEU:CD1	2.48	0.43
1:B:73:CYS:SG	1:B:333:LEU:HD23	2.59	0.43
1:B:246:HIS:NE2	1:B:279:GLU:OE2	2.51	0.43
1:B:262:PRO:HA	1:B:263:PRO:HD3	1.83	0.43
1:A:122:GLU:OE1	1:A:159:PRO:HA	2.20	0.42
1:A:359:VAL:HG12	1:A:360:SER:N	2.34	0.42
1:A:206:THR:OG1	1:A:234:VAL:HG22	2.20	0.42
1:A:9:THR:HG23	1:A:12:GLN:OE1	2.19	0.42
1:A:41:ALA:HB2	1:A:51:ASN:HD22	1.85	0.41
1:B:183:ILE:HD13	1:B:183:ILE:HG21	1.78	0.41
1:B:235:THR:HG22	1:B:249:ILE:HD13	2.02	0.41
1:B:78:ILE:HG12	1:B:145:PHE:CE1	2.55	0.41
1:B:109:VAL:HG21	1:B:174:TYR:CE1	2.52	0.41
1:A:52:THR:O	1:A:56:ARG:HG3	2.21	0.41
1:A:113:VAL:HA	1:A:124:THR:O	2.20	0.41
1:B:169:ASN:HD22	3:B:404:GOL:C3	2.34	0.41
1:B:233:MET:HE1	1:B:283:ASN:CB	2.50	0.41
1:B:198:ASP:C	1:B:198:ASP:OD1	2.57	0.41
1:A:122:GLU:HG2	4:A:531:HOH:O	2.19	0.41
1:B:230:LYS:HD2	1:B:301:SER:CB	2.51	0.41
1:B:200:LYS:NZ	2:B:402:PO4:P	2.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/364 (96%)	332 (95%)	17 (5%)	0	100	100
1	B	356/364 (98%)	340 (96%)	15 (4%)	1 (0%)	41	30
All	All	705/728 (97%)	672 (95%)	32 (4%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	PRO

### 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	283/292 (97%)	273 (96%)	10 (4%)	36	24
1	B	286/292 (98%)	277 (97%)	9 (3%)	40	29
All	All	569/584 (97%)	550 (97%)	19 (3%)	38	26

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	174	TYR
1	A	194	ASP
1	A	196	ASP
1	A	200	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	251	MET
1	A	296	TRP
1	A	301	SER
1	A	304	ARG
1	A	339	CYS
1	B	42	LYS
1	B	45	GLN
1	B	60	ARG
1	B	194	ASP
1	B	245	SER
1	B	296	TRP
1	B	304	ARG
1	B	331	ARG
1	B	339	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	B	96	GLN
1	B	320	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](#)

10 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	PO4	B	401	-	4,4,4	1.47	1 (25%)	6,6,6	1.03	0
3	GOL	A	403	-	5,5,5	1.51	0	5,5,5	1.15	0
3	GOL	A	405	-	5,5,5	1.83	2 (40%)	5,5,5	1.50	1 (20%)
3	GOL	B	403	-	5,5,5	2.28	2 (40%)	5,5,5	1.00	0
2	PO4	B	402	-	4,4,4	1.17	1 (25%)	6,6,6	0.75	0
2	PO4	A	401	-	4,4,4	1.01	0	6,6,6	1.27	0
2	PO4	A	402	-	4,4,4	0.96	0	6,6,6	0.74	0
3	GOL	A	404	-	5,5,5	0.95	0	5,5,5	1.21	0
3	GOL	B	405	-	5,5,5	2.20	3 (60%)	5,5,5	0.70	0
3	GOL	B	404	-	5,5,5	1.85	1 (20%)	5,5,5	1.83	2 (40%)

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
3	GOL	B	403	-	-	4/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
3	GOL	A	405	-	-	4/4/4/4	-
3	GOL	A	404	-	-	1/4/4/4	-
3	GOL	B	405	-	-	4/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	405	GOL	C3-C2	3.90	1.67	1.51
3	B	404	GOL	O1-C1	3.81	1.58	1.42
3	B	403	GOL	C3-C2	3.79	1.67	1.51
3	A	405	GOL	C3-C2	3.13	1.64	1.51
3	B	403	GOL	C1-C2	2.96	1.63	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	GOL	C1-C2	2.45	1.61	1.51
2	B	401	PO4	P-O1	2.42	1.56	1.50
2	B	402	PO4	P-O1	2.29	1.56	1.50
3	B	405	GOL	C1-C2	2.15	1.60	1.51
3	B	405	GOL	O2-C2	2.05	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	GOL	C3-C2-C1	-2.84	100.66	111.70
3	A	405	GOL	C3-C2-C1	-2.37	102.50	111.70
3	B	404	GOL	O1-C1-C2	-2.36	98.91	110.20

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	GOL	C1-C2-C3-O3
3	B	404	GOL	C1-C2-C3-O3
3	B	405	GOL	O1-C1-C2-O2
3	B	405	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	B	405	GOL	C1-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
3	B	405	GOL	O2-C2-C3-O3
3	A	404	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3
3	A	405	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	GOL	1	0
3	B	403	GOL	1	0
2	B	402	PO4	2	0
2	A	401	PO4	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	GOL	2	0
3	B	405	GOL	3	0
3	B	404	GOL	3	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](#)

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	353/364 (96%)	0.08	4 (1%) 80 82	24, 41, 58, 63	0
1	B	358/364 (98%)	0.19	12 (3%) 45 46	25, 41, 57, 83	0
All	All	711/728 (97%)	0.14	16 (2%) 60 62	24, 41, 57, 83	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	ALA	3.9
1	B	5	TYR	3.8
1	B	156	GLU	3.5
1	B	346	SER	3.5
1	B	349	ALA	3.5
1	B	348	GLN	3.1
1	A	156	GLU	3.1
1	B	157	HIS	2.9
1	B	345	PRO	2.7
1	A	344	THR	2.7
1	B	241	THR	2.5
1	B	229	LEU	2.3
1	B	32	ALA	2.1
1	A	291	PRO	2.1
1	B	187	VAL	2.1
1	B	344	THR	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 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	405	6/6	0.71	0.40	61,74,83,93	0
3	GOL	B	403	6/6	0.77	0.26	47,61,76,80	0
3	GOL	A	403	6/6	0.77	0.38	48,64,78,85	0
3	GOL	A	405	6/6	0.84	0.14	43,52,57,60	14
3	GOL	A	404	6/6	0.88	0.16	62,75,80,89	14
3	GOL	B	404	6/6	0.90	0.14	37,53,64,65	0
2	PO4	A	401	5/5	0.94	0.12	47,50,60,66	0
2	PO4	B	401	5/5	0.95	0.14	51,53,53,65	0
2	PO4	B	402	5/5	0.97	0.10	52,54,64,73	0
2	PO4	A	402	5/5	0.98	0.09	47,56,59,59	0

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

There are no such residues in this entry.