



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 11:20 PM EDT

PDB ID : 6XMO  
Title : Human aldolase A I98F  
Authors : Meneely, K.M.; Lamb, A.L.  
Deposited on : 2020-06-30  
Resolution : 2.60 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>.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

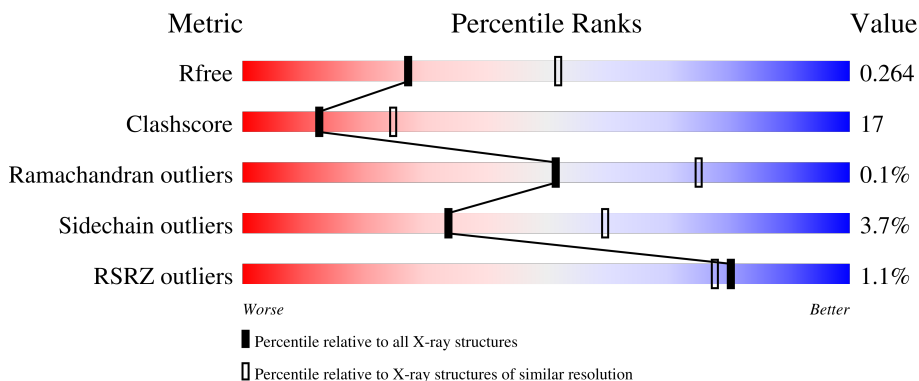
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	 63% 33% ..
1	B	364	 2% 64% 31% ..

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
3	GOL	B	404	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10941 atoms, of which 5470 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	
			Total	C	H	N	O				S
1	A	353	5405	1696	2714	474	510	11	0	0	0
1	B	353	5405	1696	2714	474	510	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	PHE	ILE	engineered mutation	UNP P04075
B	98	PHE	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
			Total	O	P		
2	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	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
			12	3	6	3		
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		

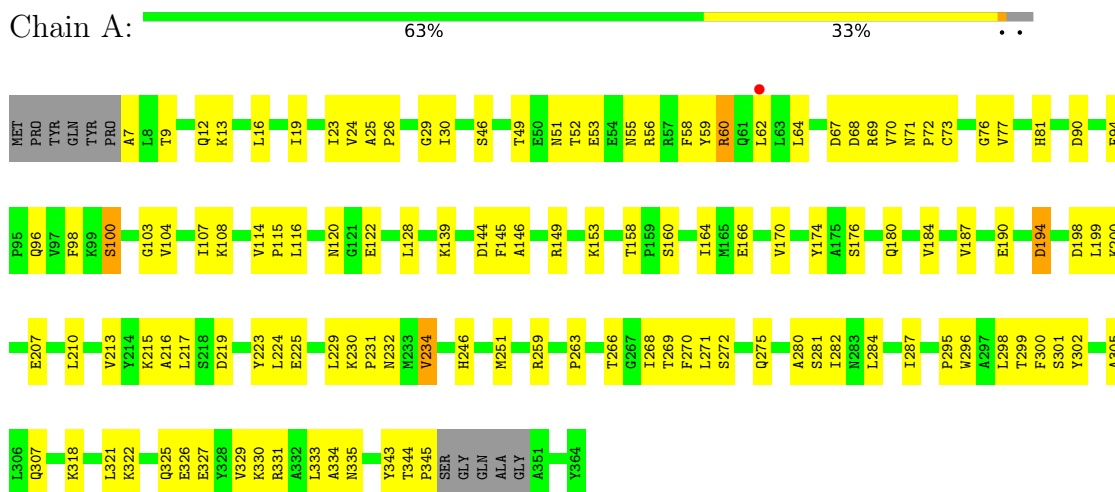
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	16	Total 16	O 16	0	0
4	B	17	Total 17	O 17	0	0

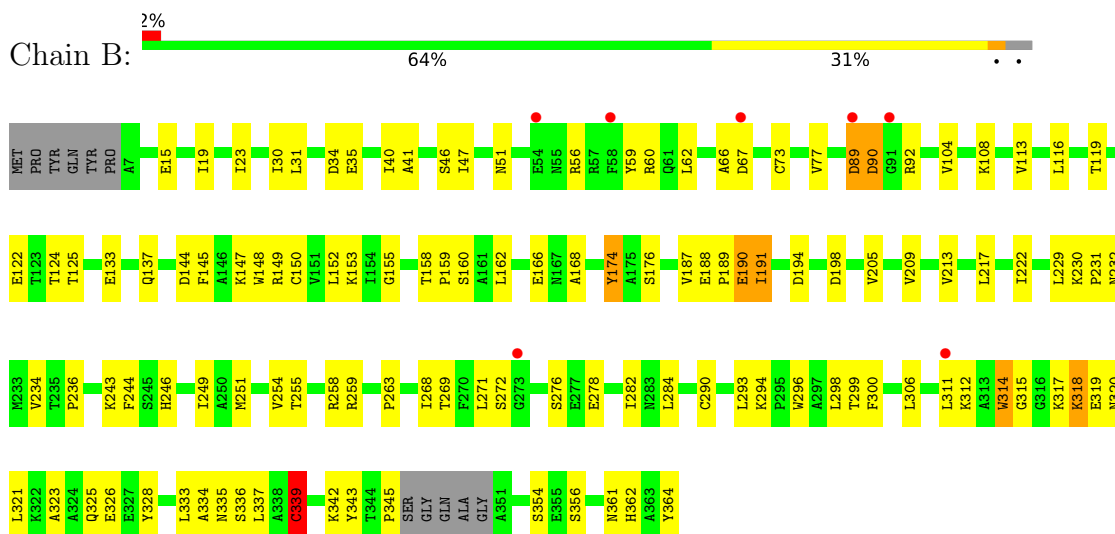
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	159.68Å 159.68Å 165.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.03 – 2.60 53.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	67.3 (53.03-2.60) 67.3 (53.03-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.61Å)	Xtrriage
Refinement program	REFMAC, PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.213 , 0.259 0.226 , 0.264	Depositor DCC
$R_{free}$ test set	1271 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtrriage
Anisotropy	0.097	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.61 % 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 1.1172e-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: PO4, 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	0.77	1/2741 (0.0%)	0.93	6/3712 (0.2%)
1	B	0.92	13/2741 (0.5%)	0.94	4/3712 (0.1%)
All	All	0.85	14/5482 (0.3%)	0.94	10/7424 (0.1%)

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	B	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	188	GLU	CD-OE2	-9.60	1.15	1.25
1	B	187	VAL	C-O	-8.43	1.07	1.23
1	B	188	GLU	CD-OE1	-8.19	1.16	1.25
1	B	326	GLU	CG-CD	7.22	1.62	1.51
1	B	339	CYS	CB-SG	-6.64	1.71	1.82
1	B	326	GLU	CB-CG	6.04	1.63	1.52
1	B	314	TRP	C-O	-5.90	1.12	1.23
1	B	319	GLU	CD-OE1	-5.60	1.19	1.25
1	B	188	GLU	C-O	-5.55	1.12	1.23
1	A	234	VAL	CB-CG2	-5.50	1.41	1.52
1	B	315	GLY	C-O	-5.25	1.15	1.23
1	B	150	CYS	CB-SG	5.14	1.91	1.82
1	B	318	LYS	C-O	-5.09	1.13	1.23
1	B	190	GLU	CD-OE2	-5.09	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	LEU	CB-CG-CD1	6.59	122.20	111.00
1	A	251	MET	CA-CB-CG	-5.57	103.83	113.30
1	A	60	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	116	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	B	190	GLU	CB-CG-CD	5.38	128.72	114.20
1	A	16	LEU	CB-CG-CD1	5.36	120.11	111.00
1	B	155	GLY	N-CA-C	-5.31	99.81	113.10
1	A	194	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	89	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	90	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	TRP	Mainchain
1	B	317	LYS	Mainchain
1	B	66	ALA	Peptide
1	B	67	ASP	Peptide

## 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	2691	2714	2713	93	0
1	B	2691	2714	2713	91	0
2	A	15	0	0	1	0
2	B	5	0	0	1	0
3	A	18	20	22	3	0
3	B	18	22	24	2	0
4	A	16	0	0	2	0
4	B	17	0	0	1	0
All	All	5471	5470	5472	182	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 17.

All (182) 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:149:ARG:NH1	1:A:190:GLU:OE2	2.00	0.94
1:B:272:SER:OG	2:B:402:PO4:O3	1.84	0.94
1:B:153:LYS:O	1:B:158:THR:HG22	1.71	0.91
1:A:24:VAL:HG23	1:A:299:THR:HG21	1.55	0.88
1:B:345:PRO:O	3:B:403:GOL:O1	1.91	0.88
1:A:160:SER:O	1:A:164:ILE:HD12	1.79	0.83
1:A:232:ASN:HA	1:A:271:LEU:HD11	1.60	0.80
1:A:70:VAL:HG11	1:A:329:VAL:HG22	1.65	0.78
1:A:70:VAL:CG1	1:A:329:VAL:HG22	2.13	0.77
1:B:23:ILE:HG12	1:B:104:VAL:HG11	1.67	0.77
1:B:19:ILE:HD13	1:B:144:ASP:HB3	1.67	0.76
1:B:290:CYS:O	1:B:294:LYS:NZ	2.21	0.74
1:B:113:VAL:HG12	1:B:125:THR:HG22	1.71	0.70
1:A:153:LYS:O	1:A:158:THR:HG22	1.90	0.70
1:A:210:LEU:HD11	1:A:229:LEU:HD21	1.75	0.69
1:B:62:LEU:HD12	1:B:321:LEU:HD12	1.75	0.69
1:B:116:LEU:O	1:B:119:THR:HG22	1.93	0.68
1:B:41:ALA:HB2	1:B:51:ASN:ND2	2.09	0.68
1:A:81:HIS:N	3:A:403:GOL:O1	2.28	0.67
1:B:90:ASP:OD2	1:B:92:ARG:NH1	2.27	0.66
1:A:62:LEU:HD12	1:A:321:LEU:HD12	1.78	0.65
1:B:125:THR:HG21	1:B:149:ARG:O	1.98	0.64
1:B:246:HIS:ND1	1:B:282:ILE:HG21	2.13	0.62
1:A:23:ILE:HD11	1:A:145:PHE:CD2	2.35	0.62
1:A:322:LYS:HA	1:A:325:GLN:HG2	1.83	0.61
1:A:59:TYR:OH	1:A:307:GLN:HB3	2.00	0.61
1:A:234:VAL:HG23	1:A:234:VAL:O	2.01	0.61
1:A:98:PHE:CE2	1:A:103:GLY:HA3	2.36	0.60
1:A:281:SER:OG	1:A:331:ARG:NH2	2.35	0.60
1:A:114:VAL:CG2	1:A:115:PRO:HD2	2.32	0.59
1:A:7:ALA:O	1:A:180:GLN:NE2	2.36	0.59
1:A:263:PRO:HD2	1:B:258:ARG:O	2.02	0.59
1:B:124:THR:HG23	1:B:166:GLU:OE2	2.03	0.58
1:A:73:CYS:SG	1:A:333:LEU:HD23	2.44	0.58
1:A:139:LYS:HE2	1:A:144:ASP:OD1	2.04	0.58
1:A:77:VAL:HG23	1:A:98:PHE:CZ	2.39	0.57
1:B:152:LEU:N	1:B:152:LEU:HD12	2.19	0.57
1:B:284:LEU:HD12	1:B:284:LEU:O	2.06	0.56
1:A:246:HIS:CD2	1:A:282:ILE:HG21	2.40	0.56
1:A:19:ILE:HD13	1:A:144:ASP:HB3	1.87	0.56
1:A:268:ILE:HD11	1:A:270:PHE:CZ	2.41	0.56
1:B:229:LEU:HG	1:B:231:PRO:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:HB3	3:B:401:GOL:H2	1.88	0.55
1:A:232:ASN:HA	1:A:271:LEU:CD1	2.33	0.55
1:A:271:LEU:C	1:A:271:LEU:HD12	2.27	0.55
1:B:124:THR:HG22	1:B:125:THR:H	1.70	0.55
1:B:251:MET:O	1:B:255:THR:HG23	2.07	0.55
1:B:40:ILE:HD13	1:B:56:ARG:HG2	1.88	0.54
1:B:148:TRP:CB	1:B:174:TYR:CE2	2.90	0.54
1:A:120:ASN:HB2	4:A:513:HOH:O	2.07	0.54
1:B:148:TRP:HB2	1:B:174:TYR:CE2	2.43	0.54
1:B:148:TRP:HB2	1:B:174:TYR:CZ	2.43	0.54
1:B:124:THR:HG22	1:B:125:THR:N	2.22	0.53
1:A:271:LEU:HD12	1:A:271:LEU:O	2.08	0.53
1:A:299:THR:OG1	1:A:300:PHE:N	2.42	0.53
1:A:343:TYR:CE2	1:A:345:PRO:HG3	2.44	0.53
1:B:113:VAL:HA	1:B:125:THR:HA	1.91	0.53
1:B:229:LEU:O	1:B:231:PRO:HD3	2.09	0.53
1:A:326:GLU:O	1:A:330:LYS:HG3	2.08	0.53
1:B:230:LYS:HA	1:B:269:THR:O	2.09	0.52
1:A:215:LYS:NZ	1:A:219:ASP:OD1	2.33	0.52
1:B:47:ILE:HD13	1:B:311:LEU:HG	1.90	0.52
1:A:153:LYS:O	1:A:158:THR:CG2	2.56	0.51
1:B:73:CYS:SG	1:B:333:LEU:HD23	2.50	0.51
1:B:23:ILE:HG12	1:B:104:VAL:CG1	2.40	0.51
1:A:269:THR:HB	1:A:301:SER:HB2	1.92	0.51
1:B:31:LEU:CD1	1:B:328:TYR:CE1	2.94	0.51
1:B:254:VAL:O	1:B:258:ARG:HG3	2.10	0.51
1:A:25:ALA:HB1	1:A:26:PRO:HD2	1.93	0.51
1:A:225:GLU:O	1:A:266:THR:OG1	2.28	0.50
1:B:23:ILE:CG1	1:B:104:VAL:HG11	2.40	0.50
1:B:251:MET:HA	1:B:251:MET:HE2	1.93	0.50
1:B:337:LEU:HD22	1:B:342:LYS:O	2.10	0.50
1:B:334:ALA:HB1	1:B:343:TYR:CE1	2.46	0.50
1:A:23:ILE:HG21	1:A:30:ILE:HD11	1.93	0.50
1:A:122:GLU:OE2	1:A:160:SER:HB3	2.12	0.50
1:B:148:TRP:HB3	1:B:174:TYR:CE2	2.46	0.50
1:A:268:ILE:HG12	1:A:298:LEU:HD12	1.93	0.50
1:A:272:SER:O	1:A:275:GLN:HG3	2.12	0.50
1:A:107:ILE:O	1:A:146:ALA:HA	2.11	0.50
1:A:114:VAL:HG23	1:A:115:PRO:HD2	1.94	0.50
1:A:334:ALA:HB1	1:A:343:TYR:CE1	2.47	0.49
1:B:217:LEU:HB3	1:B:222:ILE:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:O	1:A:64:LEU:HG	2.12	0.49
1:A:223:TYR:CZ	1:A:225:GLU:HB2	2.46	0.49
1:B:119:THR:HG23	1:B:122:GLU:H	1.78	0.49
1:B:149:ARG:NH2	1:B:362:HIS:O	2.45	0.49
1:B:191:ILE:HD11	1:B:209:VAL:HG21	1.95	0.49
1:B:31:LEU:HD12	1:B:306:LEU:HD13	1.95	0.49
1:A:25:ALA:HB1	1:A:26:PRO:CD	2.43	0.49
1:A:90:ASP:OD1	1:A:90:ASP:N	2.40	0.49
1:A:268:ILE:HG13	1:A:268:ILE:O	2.12	0.48
1:A:184:VAL:O	1:A:184:VAL:HG12	2.13	0.48
1:A:230:LYS:HE2	1:A:271:LEU:HB3	1.94	0.48
1:B:335:ASN:O	1:B:339:CYS:HB3	2.14	0.48
1:A:51:ASN:OD1	1:A:56:ARG:NH1	2.47	0.48
1:A:29:GLY:HA3	1:A:300:PHE:CZ	2.49	0.48
1:A:210:LEU:CD1	1:A:229:LEU:HD21	2.42	0.48
1:A:13:LYS:HD3	1:A:223:TYR:CE1	2.49	0.47
1:B:23:ILE:HD11	1:B:145:PHE:CD2	2.49	0.47
1:A:108:LYS:O	3:A:403:GOL:H12	2.13	0.47
1:B:251:MET:HE2	1:B:290:CYS:SG	2.54	0.47
1:A:9:THR:HG23	1:A:12:GLN:OE1	2.14	0.47
1:A:318:LYS:N	1:A:318:LYS:HD3	2.29	0.47
1:A:29:GLY:HA3	1:A:300:PHE:CE1	2.50	0.47
1:B:77:VAL:HG13	1:B:77:VAL:O	2.14	0.47
1:B:234:VAL:O	1:B:249:ILE:HG23	2.15	0.47
1:B:137:GLN:OE1	1:B:137:GLN:HA	2.14	0.47
1:B:217:LEU:HD13	1:B:222:ILE:HD11	1.97	0.47
1:B:35:GLU:OE1	1:B:60:ARG:NH2	2.47	0.47
1:A:67:ASP:O	1:A:70:VAL:HG22	2.15	0.47
1:B:59:TYR:CZ	1:B:311:LEU:HD13	2.50	0.47
1:B:232:ASN:HA	1:B:271:LEU:HD11	1.97	0.46
1:A:280:ALA:HB1	1:A:302:TYR:CZ	2.50	0.46
1:A:329:VAL:O	1:A:333:LEU:HG	2.15	0.46
1:B:168:ALA:HB1	1:B:213:VAL:HA	1.97	0.46
1:A:230:LYS:HA	1:A:269:THR:O	2.15	0.46
1:A:207:GLU:OE2	1:A:259:ARG:NH1	2.46	0.46
1:B:162:LEU:HD12	1:B:162:LEU:O	2.15	0.46
1:B:236:PRO:HG3	1:B:244:PHE:CD1	2.51	0.46
1:A:187:VAL:HG23	1:A:187:VAL:O	2.17	0.45
1:B:34:ASP:OD2	1:B:147:LYS:NZ	2.42	0.45
1:B:246:HIS:ND1	1:B:282:ILE:CG2	2.80	0.45
1:A:70:VAL:HG12	1:A:329:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:O	1:A:234:VAL:CG2	2.64	0.45
1:B:31:LEU:HD13	1:B:328:TYR:CE1	2.51	0.45
1:A:200:LYS:HE2	2:A:402:PO4:O1	2.16	0.45
1:A:272:SER:HB2	1:A:305:ALA:HB2	1.98	0.45
1:A:114:VAL:HG22	1:A:115:PRO:HD2	1.97	0.45
1:B:124:THR:CG2	1:B:166:GLU:OE2	2.65	0.45
1:A:52:THR:O	1:A:53:GLU:C	2.55	0.45
1:B:108:LYS:HE3	1:B:364:TYR:O	2.17	0.45
1:B:318:LYS:N	1:B:318:LYS:HD3	2.31	0.45
1:A:71:ASN:N	1:A:72:PRO:CD	2.80	0.45
1:A:287:ILE:CG2	1:A:298:LEU:HD23	2.47	0.44
1:B:299:THR:OG1	1:B:300:PHE:N	2.47	0.44
1:B:133:GLU:HA	1:B:133:GLU:OE2	2.18	0.44
1:A:58:PHE:CZ	1:A:321:LEU:HD13	2.53	0.44
1:A:343:TYR:O	1:A:344:THR:HG23	2.18	0.44
1:A:76:GLY:HA2	1:A:104:VAL:O	2.18	0.43
1:B:15:GLU:O	1:B:19:ILE:HG13	2.18	0.43
1:B:153:LYS:NZ	1:B:361:ASN:OD1	2.50	0.43
1:A:295:PRO:HG3	1:B:263:PRO:HG3	2.00	0.43
1:B:73:CYS:HB3	1:B:336:SER:HB2	2.00	0.43
1:A:49:THR:HG22	1:A:55:ASN:ND2	2.34	0.43
1:B:205:VAL:O	1:B:209:VAL:HG23	2.18	0.43
1:B:251:MET:CE	1:B:290:CYS:SG	3.06	0.43
1:A:71:ASN:N	1:A:72:PRO:HD2	2.33	0.43
1:A:229:LEU:C	1:A:231:PRO:HD3	2.38	0.43
1:B:229:LEU:C	1:B:231:PRO:HD3	2.39	0.43
1:B:243:LYS:HA	4:B:504:HOH:O	2.19	0.43
1:B:321:LEU:O	1:B:325:GLN:HG2	2.18	0.43
1:B:342:LYS:HE3	1:B:342:LYS:HB2	1.86	0.43
1:B:122:GLU:OE1	1:B:159:PRO:HA	2.18	0.43
1:A:23:ILE:CG2	1:A:30:ILE:HD11	2.49	0.42
1:A:53:GLU:HA	1:A:56:ARG:NH2	2.34	0.42
1:B:271:LEU:HD12	1:B:271:LEU:O	2.19	0.42
1:A:198:ASP:OD1	1:A:199:LEU:N	2.53	0.42
1:A:128:LEU:HD11	1:A:170:VAL:HG23	1.99	0.42
1:A:331:ARG:O	1:A:335:ASN:ND2	2.53	0.42
1:B:213:VAL:O	1:B:217:LEU:HG	2.19	0.42
1:A:67:ASP:OD2	1:A:69:ARG:HB2	2.19	0.42
1:B:40:ILE:O	1:B:40:ILE:HG12	2.19	0.42
1:B:276:SER:HB2	1:B:354:SER:HA	2.02	0.42
1:A:213:VAL:O	1:A:216:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLN:O	1:A:100:SER:HB3	2.19	0.41
1:A:187:VAL:O	1:A:187:VAL:CG2	2.68	0.41
1:B:278:GLU:HG3	1:B:282:ILE:CD1	2.50	0.41
3:A:406:GOL:H11	1:B:259:ARG:HD3	2.02	0.41
1:B:149:ARG:NH1	1:B:190:GLU:OE2	2.54	0.41
1:B:268:ILE:HB	1:B:298:LEU:HD23	2.02	0.41
1:B:320:ASN:O	1:B:321:LEU:C	2.58	0.41
1:A:217:LEU:HD12	1:A:217:LEU:N	2.36	0.41
1:B:320:ASN:O	1:B:323:ALA:N	2.53	0.41
1:B:23:ILE:HG21	1:B:30:ILE:HD11	2.03	0.41
1:B:119:THR:HG21	1:B:122:GLU:HB2	2.03	0.41
1:B:122:GLU:OE2	1:B:160:SER:HB3	2.21	0.41
1:A:284:LEU:HD22	1:A:300:PHE:HB3	2.03	0.40
1:A:200:LYS:NZ	4:A:501:HOH:O	2.55	0.40
1:B:258:ARG:HD2	1:B:293:LEU:O	2.21	0.40
1:B:278:GLU:HG3	1:B:282:ILE:HD12	2.04	0.40
1:B:147:LYS:NZ	1:B:364:TYR:OH	2.53	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	349/364 (96%)	322 (92%)	27 (8%)	0	100	100
1	B	349/364 (96%)	321 (92%)	27 (8%)	1 (0%)	41	64
All	All	698/728 (96%)	643 (92%)	54 (8%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/292 (97%)	274 (96%)	10 (4%)	36	62
1	B	284/292 (97%)	273 (96%)	11 (4%)	32	58
All	All	568/584 (97%)	547 (96%)	21 (4%)	34	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	68	ASP
1	A	94	PHE
1	A	100	SER
1	A	166	GLU
1	A	174	TYR
1	A	176	SER
1	A	194	ASP
1	A	296	TRP
1	A	327	GLU
1	B	46	SER
1	B	89	ASP
1	B	174	TYR
1	B	176	SER
1	B	191	ILE
1	B	194	ASP
1	B	198	ASP
1	B	296	TRP
1	B	312	LYS
1	B	339	CYS
1	B	356	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 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	A	402	-	4,4,4	0.39	0	6,6,6	1.07	0
2	PO4	A	401	-	4,4,4	0.88	0	6,6,6	1.03	0
3	GOL	A	403	-	5,5,5	1.26	0	5,5,5	1.55	2 (40%)
3	GOL	A	404	-	5,5,5	1.19	0	5,5,5	2.61	2 (40%)
2	PO4	A	405	-	4,4,4	1.00	0	6,6,6	1.10	0
3	GOL	B	404	-	5,5,5	1.96	2 (40%)	5,5,5	1.20	1 (20%)
3	GOL	B	403	-	5,5,5	0.96	0	5,5,5	0.91	0
3	GOL	B	401	-	5,5,5	1.64	2 (40%)	5,5,5	0.51	0
3	GOL	A	406	-	5,5,5	1.63	2 (40%)	5,5,5	1.88	1 (20%)
2	PO4	B	402	-	4,4,4	1.09	0	6,6,6	0.77	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
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	A	404	-	-	1/4/4/4	-
3	GOL	B	404	-	-	3/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	B	401	-	-	2/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	GOL	C3-C2	3.15	1.64	1.51
3	B	404	GOL	C1-C2	2.99	1.64	1.51
3	B	401	GOL	C3-C2	2.53	1.62	1.51
3	A	406	GOL	C3-C2	2.51	1.62	1.51
3	A	406	GOL	C1-C2	2.21	1.60	1.51
3	B	401	GOL	C1-C2	2.16	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	GOL	C3-C2-C1	-4.85	92.85	111.70
3	A	406	GOL	C3-C2-C1	-3.37	98.60	111.70
3	A	404	GOL	O2-C2-C1	2.61	120.61	109.12
3	A	403	GOL	C3-C2-C1	-2.40	102.39	111.70
3	B	404	GOL	O2-C2-C3	2.21	118.86	109.12
3	A	403	GOL	O2-C2-C3	2.01	117.98	109.12

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-C3
3	B	401	GOL	O1-C1-C2-C3
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
3	A	406	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	A	406	GOL	O1-C1-C2-O2
3	B	401	GOL	O1-C1-C2-O2
3	B	404	GOL	O2-C2-C3-O3

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

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	PO4	1	0
3	A	403	GOL	2	0
3	B	403	GOL	1	0
3	B	401	GOL	1	0
3	A	406	GOL	1	0
2	B	402	PO4	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](#)

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%)	0.12	1 (0%) 94 93	23, 41, 60, 78	0
1	B	353/364 (96%)	0.14	7 (1%) 65 60	18, 41, 62, 82	0
All	All	706/728 (96%)	0.13	8 (1%) 80 78	18, 41, 61, 82	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	ASP	3.2
1	B	89	ASP	3.2
1	B	273	GLY	2.7
1	A	62	LEU	2.3
1	B	311	LEU	2.2
1	B	54	GLU	2.2
1	B	91	GLY	2.2
1	B	58	PHE	2.1

### 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(Å <sup>2</sup> )	Q<0.9
3	GOL	A	406	6/6	0.83	0.25	51,62,79,80	0
3	GOL	B	401	6/6	0.84	0.29	46,68,79,82	0
3	GOL	B	403	6/6	0.88	0.14	43,63,79,79	0
3	GOL	B	404	6/6	0.88	0.25	42,51,62,73	0
3	GOL	A	404	6/6	0.90	0.27	49,66,83,88	0
3	GOL	A	403	6/6	0.92	0.35	45,54,61,65	0
2	PO4	A	402	5/5	0.95	0.14	50,53,58,61	0
2	PO4	A	405	5/5	0.95	0.12	47,47,65,74	0
2	PO4	B	402	5/5	0.97	0.11	34,44,53,60	0
2	PO4	A	401	5/5	0.98	0.15	41,45,51,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.