



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:41 pm BST

PDB ID : 3F4C  
Title : Crystal structure of organophosphorus hydrolase from *Geobacillus stearothermophilus* strain 10, with glycerol bound  
Authors : Hawwa, R.; Aikens, J.; Turner, R.J.; Santarsiero, B.; Mesecar, A.  
Deposited on : 2008-10-31  
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

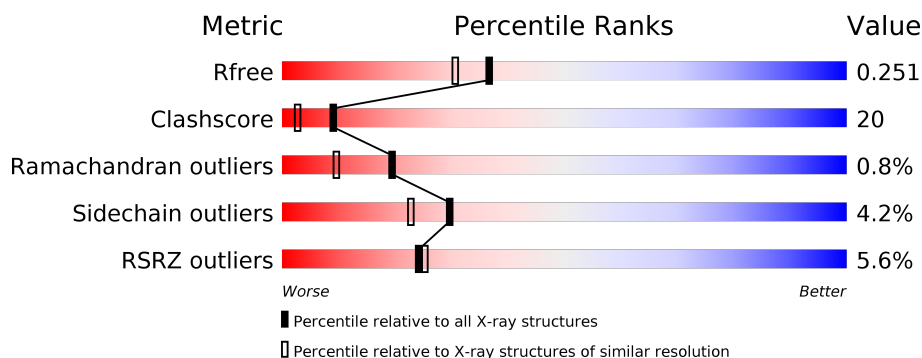
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	332	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>• •</div> </div> </div>
1	B	332	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5552 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 Organophosphorus hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2548	1623	437	474	14			
1	B	324	Total	C	N	O	S	0	0	0
			2548	1623	437	474	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	HIS	-	EXPRESSION TAG	PDB 3F4C
A	426	HIS	-	EXPRESSION TAG	PDB 3F4C
A	427	HIS	-	EXPRESSION TAG	PDB 3F4C
A	428	HIS	-	EXPRESSION TAG	PDB 3F4C
A	429	HIS	-	EXPRESSION TAG	PDB 3F4C
A	430	HIS	-	EXPRESSION TAG	PDB 3F4C
B	425	HIS	-	EXPRESSION TAG	PDB 3F4C
B	426	HIS	-	EXPRESSION TAG	PDB 3F4C
B	427	HIS	-	EXPRESSION TAG	PDB 3F4C
B	428	HIS	-	EXPRESSION TAG	PDB 3F4C
B	429	HIS	-	EXPRESSION TAG	PDB 3F4C
B	430	HIS	-	EXPRESSION TAG	PDB 3F4C

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Co	0	0
			2	2		
2	A	2	Total	Co	0	0
			2	2		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

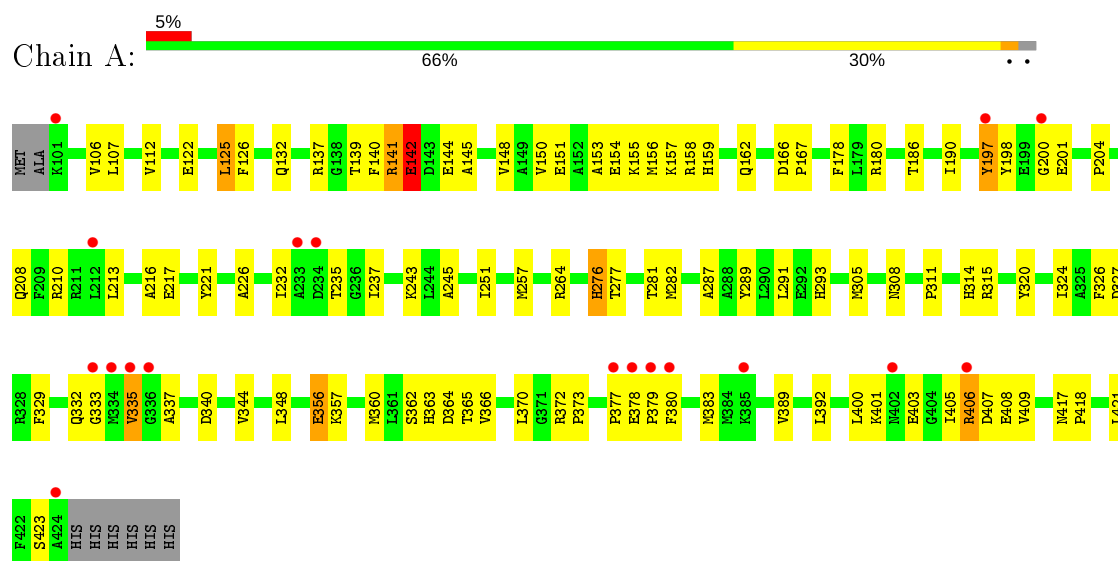
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		
4	B	250	Total	O	0	0
			250	250		

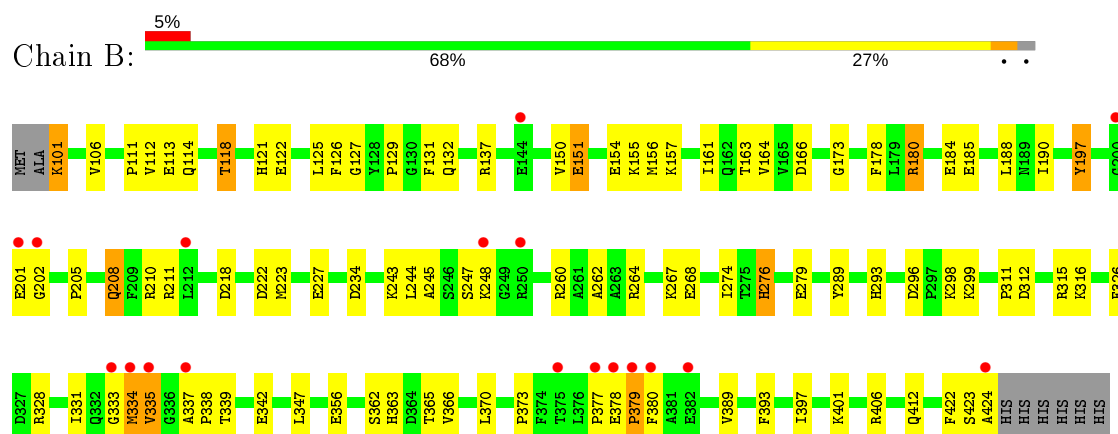
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Organophosphorus hydrolase



#### • Molecule 1: Organophosphorus hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.21Å 156.76Å 49.99Å 90.00° 116.49° 90.00°	Depositor
Resolution (Å)	20.00 – 2.07 20.03 – 2.08	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.07) 89.7 (20.03-2.08)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.45 (at 2.07Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.191 , 0.252 0.191 , 0.251	Depositor DCC
$R_{free}$ test set	1742 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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, CO, KCX

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	0.61	0/2594	0.76	2/3511 (0.1%)
1	B	0.56	0/2594	0.75	1/3511 (0.0%)
All	All	0.59	0/5188	0.75	3/7022 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	LEU	CA-CB-CG	8.68	135.26	115.30
1	B	326	PHE	N-CA-C	-6.32	93.93	111.00
1	A	326	PHE	N-CA-C	-5.26	96.80	111.00

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	2548	0	2502	103	1
1	B	2548	0	2502	106	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	7	0	0
3	B	6	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	190	0	0	21	0
4	B	250	0	0	21	0
All	All	5552	0	5018	204	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 (204) 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:334:MET:O	1:B:335:VAL:HG22	1.34	1.20
1:B:334:MET:O	1:B:335:VAL:CG2	2.00	1.09
1:A:392:LEU:HG	4:A:475:HOH:O	1.54	1.06
1:A:235:THR:HG23	1:A:237:ILE:H	1.28	0.97
1:A:232:ILE:O	1:A:235:THR:HG22	1.66	0.96
1:B:208:GLN:HE21	1:B:208:GLN:HA	1.34	0.91
1:B:180:ARG:HH11	1:B:180:ARG:HG2	1.34	0.90
1:B:378:GLU:HG3	1:B:379:PRO:HD3	1.54	0.88
1:A:125:LEU:HD13	1:A:370:LEU:HD21	1.57	0.86
1:B:132:GLN:HB2	4:B:431:HOH:O	1.76	0.85
1:B:424:ALA:HB3	4:B:575:HOH:O	1.78	0.83
1:B:129:PRO:HG2	1:B:202:GLY:HA2	1.58	0.83
1:A:148:VAL:O	1:A:151:GLU:HG3	1.79	0.82
1:A:406:ARG:H	1:A:406:ARG:NE	1.79	0.81
1:A:158:ARG:HD2	4:A:527:HOH:O	1.82	0.80
1:A:360:MET:CE	1:A:418:PRO:HG3	2.12	0.80
1:B:156:MET:HG2	1:B:389:VAL:CG1	2.12	0.79
1:B:334:MET:C	1:B:335:VAL:HG22	2.04	0.78
1:A:333:GLY:HA3	4:A:436:HOH:O	1.84	0.78
1:B:378:GLU:HG3	1:B:379:PRO:CD	2.14	0.77
1:A:363:HIS:CD2	1:A:392:LEU:HD13	2.18	0.77
1:A:360:MET:HE3	1:A:418:PRO:HG3	1.67	0.76
1:A:125:LEU:CD1	1:A:370:LEU:HD11	2.16	0.76
1:A:201:GLU:HB2	4:A:522:HOH:O	1.87	0.75
1:A:201:GLU:HA	1:B:205:PRO:HG3	1.69	0.74
1:B:377:PRO:HD3	4:B:619:HOH:O	1.87	0.73
1:A:235:THR:HG23	1:A:237:ILE:N	2.03	0.73
1:B:339:THR:OG1	1:B:342:GLU:HG3	1.89	0.73
1:A:363:HIS:NE2	1:A:392:LEU:HD13	2.06	0.70
1:B:156:MET:CG	1:B:389:VAL:HG11	2.23	0.69
1:A:122:GLU:HG3	1:A:156:MET:HE1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:O	1:B:154:GLU:HG2	1.92	0.68
1:B:268:GLU:HG2	4:B:493:HOH:O	1.92	0.68
1:B:312:ASP:O	1:B:316:LYS:HE2	1.95	0.67
1:B:334:MET:SD	1:B:337:ALA:HB3	2.35	0.67
1:B:210:ARG:HD3	4:B:65:HOH:O	1.94	0.67
1:B:248:LYS:HG3	4:B:507:HOH:O	1.94	0.67
1:B:373:PRO:CD	4:B:614:HOH:O	2.42	0.67
1:B:377:PRO:C	1:B:379:PRO:HD2	2.15	0.66
1:A:340:ASP:O	1:A:344:VAL:HG23	1.95	0.66
1:A:141:ARG:NH1	4:A:505:HOH:O	2.29	0.66
1:A:406:ARG:HG2	1:A:408:GLU:HG2	1.78	0.65
1:B:208:GLN:HE22	1:B:211:ARG:HH11	1.43	0.65
1:B:245:ALA:HB1	1:B:276:HIS:CD2	2.32	0.64
1:B:101:LYS:O	1:B:111:PRO:HA	1.97	0.64
1:B:373:PRO:HD3	4:B:614:HOH:O	1.95	0.64
1:A:141:ARG:HD3	4:A:490:HOH:O	1.97	0.64
1:A:217:GLU:N	4:A:497:HOH:O	2.28	0.64
1:A:406:ARG:HE	1:A:409:VAL:CG2	2.11	0.63
1:B:180:ARG:HG2	4:B:53:HOH:O	1.98	0.63
1:B:121:HIS:HE1	1:B:243:KCX:OQ2	1.83	0.62
1:B:423:SER:O	1:B:424:ALA:HB2	1.98	0.62
1:B:331:ILE:HG22	1:B:334:MET:HE3	1.82	0.62
1:B:125:LEU:HD13	1:B:178:PHE:CE2	2.36	0.61
1:B:379:PRO:HG2	1:B:380:PHE:HD1	1.65	0.61
1:B:245:ALA:HB1	1:B:276:HIS:HD2	1.66	0.61
1:B:156:MET:HG2	1:B:389:VAL:HG13	1.82	0.61
1:A:363:HIS:HB2	1:A:365:THR:HG23	1.83	0.60
1:A:305:MET:HG3	1:A:324:ILE:HB	1.83	0.60
1:A:198:TYR:HB3	1:A:245:ALA:HB1	1.84	0.60
1:A:406:ARG:HE	1:A:409:VAL:HG21	1.66	0.59
1:A:276:HIS:C	1:A:276:HIS:CD2	2.74	0.59
1:A:125:LEU:HD13	1:A:370:LEU:HD11	1.84	0.59
1:B:197:TYR:CD2	1:B:201:GLU:HB3	2.38	0.59
1:B:218:ASP:HB3	4:B:504:HOH:O	2.02	0.59
1:B:180:ARG:NH1	1:B:180:ARG:HG2	2.08	0.58
1:A:401:LYS:C	1:A:403:GLU:H	2.07	0.58
1:A:221:TYR:CE1	1:A:264:ARG:HG2	2.39	0.57
1:A:197:TYR:HE2	4:A:522:HOH:O	1.87	0.57
1:B:126:PHE:HB3	1:B:366:VAL:HG13	1.85	0.57
1:A:378:GLU:N	1:A:379:PRO:CD	2.68	0.57
1:B:111:PRO:HG3	1:B:114:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:HG3	1:B:389:VAL:HG11	1.85	0.56
1:B:151:GLU:O	1:B:155:LYS:HG3	2.06	0.56
1:B:121:HIS:CE1	1:B:243:KCX:OQ2	2.59	0.55
1:B:208:GLN:NE2	1:B:208:GLN:HA	2.12	0.55
1:A:251:ILE:HG13	1:A:282:MET:CE	2.37	0.55
1:B:316:LYS:N	1:B:316:LYS:HD3	2.21	0.55
1:A:141:ARG:NH2	1:A:373:PRO:HG3	2.22	0.55
1:B:379:PRO:HG2	1:B:380:PHE:CD1	2.41	0.55
1:A:141:ARG:H	1:A:141:ARG:HD3	1.72	0.55
1:B:397:ILE:HG22	1:B:401:LYS:HE3	1.88	0.55
1:B:423:SER:O	1:B:424:ALA:CB	2.54	0.54
1:A:311:PRO:O	1:A:315:ARG:HG3	2.07	0.54
1:A:405:ILE:HA	1:A:406:ARG:CZ	2.38	0.53
1:A:141:ARG:HH22	1:A:373:PRO:HG3	1.74	0.53
1:B:118:THR:HB	1:B:163:THR:HB	1.91	0.53
1:A:198:TYR:CE2	1:A:200:GLY:HA3	2.44	0.53
1:A:142:GLU:O	1:A:145:ALA:N	2.42	0.52
1:B:157:LYS:HZ2	1:B:188:LEU:HD13	1.74	0.52
1:A:125:LEU:HD13	1:A:370:LEU:CD2	2.37	0.52
1:B:311:PRO:O	1:B:315:ARG:HG3	2.10	0.52
1:B:334:MET:N	1:B:334:MET:SD	2.83	0.51
1:B:397:ILE:CG2	1:B:401:LYS:HE3	2.40	0.51
1:A:198:TYR:HB3	1:A:245:ALA:CB	2.41	0.51
1:A:406:ARG:H	1:A:406:ARG:CD	2.23	0.51
1:B:312:ASP:O	1:B:316:LYS:HG2	2.11	0.51
1:B:378:GLU:N	1:B:379:PRO:HD2	2.25	0.51
1:A:153:ALA:O	1:A:157:LYS:HG2	2.11	0.51
1:A:210:ARG:HA	1:A:213:LEU:HD12	1.92	0.51
1:A:287:ALA:O	1:A:291:LEU:HG	2.11	0.51
1:A:406:ARG:CZ	1:A:406:ARG:H	2.23	0.51
1:B:248:LYS:HB3	4:B:469:HOH:O	2.10	0.51
1:B:289:TYR:O	1:B:293:HIS:HD2	1.94	0.51
1:B:389:VAL:O	1:B:389:VAL:CG1	2.60	0.50
1:A:406:ARG:NE	1:A:409:VAL:HG21	2.27	0.49
1:B:180:ARG:HD2	4:B:470:HOH:O	2.13	0.49
1:B:184:GLU:OE2	4:B:470:HOH:O	2.20	0.49
1:B:298:LYS:NZ	4:B:617:HOH:O	2.46	0.49
1:A:150:VAL:HG12	1:A:154:GLU:OE2	2.12	0.49
1:A:251:ILE:HG13	1:A:282:MET:HE2	1.94	0.49
1:B:131:PHE:CE2	1:B:132:GLN:HG3	2.48	0.49
1:A:132:GLN:HB2	4:A:472:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:HD2	1:A:201:GLU:O	1.96	0.48
1:B:154:GLU:O	1:B:157:LYS:HB2	2.14	0.48
1:A:405:ILE:HA	1:A:406:ARG:NH2	2.29	0.48
1:B:328:ARG:NH2	3:B:601:GOL:O2	2.46	0.48
1:A:337:ALA:HB2	4:A:542:HOH:O	2.14	0.47
1:A:417:ASN:HB2	1:A:418:PRO:HD3	1.96	0.47
1:B:260:ARG:O	1:B:264:ARG:HG3	2.14	0.47
1:A:204:PRO:HG3	4:A:530:HOH:O	2.13	0.47
1:A:151:GLU:OE1	1:A:155:LYS:HE3	2.14	0.47
1:A:400:LEU:O	1:A:403:GLU:HB2	2.13	0.47
1:B:296:ASP:HB3	1:B:299:LYS:HD2	1.96	0.47
1:A:335:VAL:HG12	1:A:335:VAL:O	2.14	0.47
1:B:157:LYS:NZ	1:B:188:LEU:HD13	2.29	0.47
1:A:308:ASN:O	1:A:314:HIS:HE1	1.98	0.47
1:A:378:GLU:HG3	4:A:566:HOH:O	2.15	0.47
1:A:122:GLU:O	1:A:166:ASP:HA	2.15	0.47
1:A:329:PHE:HB2	1:A:392:LEU:HD11	1.96	0.46
1:B:334:MET:O	1:B:335:VAL:HG23	2.02	0.46
1:B:122:GLU:O	1:B:166:ASP:HA	2.16	0.46
1:B:208:GLN:NE2	1:B:211:ARG:HD3	2.30	0.46
1:B:244:LEU:HD21	1:B:262:ALA:HB2	1.97	0.46
1:A:201:GLU:HA	1:B:205:PRO:CG	2.40	0.46
1:B:223:MET:O	1:B:227:GLU:HG3	2.16	0.46
1:A:372:ARG:HD2	1:B:210:ARG:NH2	2.31	0.46
1:A:257:MET:CG	4:A:497:HOH:O	2.64	0.46
1:B:180:ARG:NH1	1:B:180:ARG:CG	2.78	0.46
1:B:197:TYR:HD1	1:B:197:TYR:HA	1.57	0.46
1:B:127:GLY:HA3	1:B:370:LEU:HB2	1.98	0.45
1:A:327:ASP:O	1:A:364:ASP:HB2	2.16	0.45
1:A:216:ALA:HB3	4:A:497:HOH:O	2.16	0.45
1:A:360:MET:HE3	1:A:418:PRO:CG	2.42	0.45
1:B:157:LYS:NZ	1:B:188:LEU:CD1	2.80	0.45
1:B:111:PRO:CG	1:B:114:GLN:NE2	2.80	0.45
1:A:154:GLU:HG2	4:A:560:HOH:O	2.17	0.44
1:A:379:PRO:O	1:A:383:MET:HG2	2.18	0.44
1:A:155:LYS:O	1:A:159:HIS:HD2	2.01	0.44
1:A:277:THR:HB	1:A:281:THR:O	2.17	0.44
1:B:208:GLN:HG3	4:B:568:HOH:O	2.18	0.44
1:B:333:GLY:HA2	4:B:607:HOH:O	2.17	0.44
1:B:377:PRO:HG2	1:B:380:PHE:HD1	1.83	0.44
1:A:180:ARG:NH2	1:A:237:ILE:HG13	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:KCX:OQ1	1:A:276:HIS:HB2	2.18	0.44
1:B:378:GLU:HB3	4:B:477:HOH:O	2.17	0.44
1:B:161:ILE:HD11	1:B:393:PHE:CZ	2.53	0.44
1:A:406:ARG:CG	1:A:408:GLU:HG2	2.47	0.43
1:A:348:LEU:HD23	1:A:405:ILE:HD11	2.00	0.43
1:A:112:VAL:HG11	1:A:423:SER:HB3	2.00	0.43
1:B:363:HIS:HB2	1:B:365:THR:HG23	2.00	0.43
1:A:107:LEU:HD23	1:A:180:ARG:HG3	2.01	0.43
1:B:337:ALA:HB1	1:B:338:PRO:HD2	2.00	0.43
1:A:137:ARG:HG3	1:B:222:ASP:OD1	2.18	0.43
1:B:137:ARG:NH1	4:B:526:HOH:O	2.28	0.43
1:A:226:ALA:HB2	1:B:137:ARG:CZ	2.48	0.43
1:B:267:LYS:NZ	4:B:466:HOH:O	2.51	0.43
1:A:289:TYR:O	1:A:293:HIS:HD2	2.01	0.43
1:B:389:VAL:HG12	1:B:389:VAL:O	2.19	0.43
1:A:126:PHE:HB3	1:A:366:VAL:HG13	2.01	0.42
1:B:106:VAL:HG13	1:B:190:ILE:O	2.20	0.42
1:A:162:GLN:HB2	4:A:451:HOH:O	2.19	0.42
1:A:332:GLN:HG3	1:A:383:MET:O	2.19	0.42
1:B:113:GLU:HG3	1:B:114:GLN:HG3	2.01	0.42
1:B:248:LYS:HG2	1:B:279:GLU:OE1	2.20	0.42
1:A:401:LYS:C	1:A:403:GLU:N	2.73	0.42
1:A:167:PRO:HB2	1:A:243:KCX:HE3	2.02	0.42
1:B:197:TYR:HD2	1:B:201:GLU:O	2.03	0.42
1:B:247:SER:HB3	4:B:507:HOH:O	2.19	0.42
1:B:129:PRO:HG2	1:B:202:GLY:CA	2.40	0.42
1:A:157:LYS:NZ	1:A:186:THR:O	2.50	0.42
1:B:156:MET:SD	1:B:164:VAL:HG21	2.60	0.42
1:A:125:LEU:HD23	1:A:178:PHE:CD2	2.55	0.42
1:A:372:ARG:HA	1:A:373:PRO:HD3	1.86	0.42
1:B:356:GLU:HG3	1:B:412:GLN:HG2	2.01	0.42
1:A:208:GLN:OE1	1:A:208:GLN:HA	2.20	0.41
1:A:257:MET:HG3	4:A:497:HOH:O	2.21	0.41
1:A:337:ALA:CB	4:A:542:HOH:O	2.68	0.41
1:A:356:GLU:HG2	1:A:357:LYS:N	2.34	0.41
1:A:180:ARG:HD2	4:A:461:HOH:O	2.20	0.41
1:A:141:ARG:HA	4:A:92:HOH:O	2.21	0.41
1:B:112:VAL:HG21	1:B:422:PHE:O	2.21	0.41
1:B:157:LYS:HZ1	1:B:188:LEU:HD12	1.84	0.41
1:B:208:GLN:NE2	1:B:211:ARG:CD	2.83	0.41
1:B:406:ARG:HD3	4:B:543:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:HA	1:A:197:TYR:HD1	1.60	0.41
1:A:380:PHE:O	1:A:383:MET:N	2.54	0.41
1:A:106:VAL:HG13	1:A:190:ILE:O	2.21	0.41
1:B:157:LYS:HZ1	1:B:188:LEU:CD1	2.34	0.41
1:A:139:THR:CG2	1:A:140:PHE:N	2.84	0.41
1:A:389:VAL:HG13	4:A:440:HOH:O	2.21	0.40
1:A:139:THR:HG22	1:A:140:PHE:N	2.35	0.40
1:B:125:LEU:CD1	1:B:178:PHE:CE2	3.04	0.40
1:B:173:GLY:HA3	1:B:370:LEU:CD1	2.51	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:320:TYR:OH	1:B:234:ASP:OD2[1_656]	2.16	0.04

## 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	321/332 (97%)	304 (95%)	14 (4%)	3 (1%)	17	8
1	B	321/332 (97%)	308 (96%)	11 (3%)	2 (1%)	25	15
All	All	642/664 (97%)	612 (95%)	25 (4%)	5 (1%)	19	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLU
1	A	335	VAL
1	A	377	PRO
1	B	335	VAL

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Mol	Chain	Res	Type
1	B	379	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	262/269 (97%)	252 (96%)	10 (4%)	33	26
1	B	262/269 (97%)	250 (95%)	12 (5%)	27	19
All	All	524/538 (97%)	502 (96%)	22 (4%)	30	23

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	142	GLU
1	A	144	GLU
1	A	197	TYR
1	A	276	HIS
1	A	356	GLU
1	A	362	SER
1	A	406	ARG
1	A	407	ASP
1	A	421	LEU
1	B	101	LYS
1	B	118	THR
1	B	151	GLU
1	B	180	ARG
1	B	185	GLU
1	B	197	TYR
1	B	208	GLN
1	B	274	ILE
1	B	276	HIS
1	B	334	MET
1	B	347	LEU
1	B	362	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	276	HIS
1	A	293	HIS
1	A	402	ASN
1	B	114	GLN
1	B	208	GLN
1	B	293	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	B	243	1,2	7,11,12	1.01	0	4,12,14	0.68	0
1	KCX	A	243	1,2	7,11,12	0.52	0	4,12,14	1.07	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
1	KCX	B	243	1,2	-	0/7/10/12	-
1	KCX	A	243	1,2	-	2/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	243	KCX	CG-CD-CE-NZ
1	A	243	KCX	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	243	KCX	2	0
1	A	243	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
3	GOL	B	601	2	5,5,5	0.86	0	5,5,5	0.33	0
3	GOL	A	601	2	5,5,5	0.94	0	5,5,5	0.40	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	B	601	2	-	0/4/4/4	-
3	GOL	A	601	2	-	0/4/4/4	-



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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	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	323/332 (97%)	0.02	18 (5%) 24 25	18, 32, 54, 75	0
1	B	323/332 (97%)	0.06	18 (5%) 24 25	18, 34, 57, 78	0
All	All	646/664 (97%)	0.04	36 (5%) 24 25	18, 33, 56, 78	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	VAL	7.3
1	B	334	MET	6.4
1	B	424	ALA	6.0
1	B	202	GLY	5.6
1	B	333	GLY	4.7
1	A	380	PHE	4.6
1	A	335	VAL	4.5
1	B	380	PHE	4.5
1	A	333	GLY	4.3
1	A	212	LEU	4.1
1	A	378	GLU	4.0
1	A	334	MET	3.6
1	A	197	TYR	3.5
1	A	379	PRO	3.4
1	A	424	ALA	3.4
1	B	212	LEU	3.3
1	B	378	GLU	3.1
1	B	379	PRO	2.9
1	B	200	GLY	2.9
1	B	337	ALA	2.7
1	B	377	PRO	2.6
1	B	375	THR	2.5
1	A	200	GLY	2.5
1	B	144	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	382	GLU	2.3
1	A	101	LYS	2.3
1	A	377	PRO	2.3
1	A	336	GLY	2.2
1	A	385	LYS	2.2
1	A	234	ASP	2.2
1	B	248	LYS	2.2
1	B	201	GLU	2.1
1	B	250	ARG	2.1
1	A	402	ASN	2.0
1	A	233	ALA	2.0
1	A	406	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	A	243	12/13	0.84	0.15	17,23,41,42	0
1	KCX	B	243	12/13	0.87	0.13	19,22,39,39	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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	B	601	6/6	0.79	0.20	53,56,58,61	0
3	GOL	A	601	6/6	0.87	0.18	37,44,45,49	0
2	CO	A	502	1/1	0.96	0.05	60,60,60,60	0
2	CO	B	502	1/1	0.96	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CO	A	501	1/1	0.99	0.05	28,28,28,28	0
2	CO	B	501	1/1	1.00	0.05	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.