



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:36 AM GMT

PDB ID : 3K5W  
Title : Crystal structure of a Carbohydrate kinase (YjeF family) from *Helicobacter pylori*  
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-10-08  
Resolution : 2.60 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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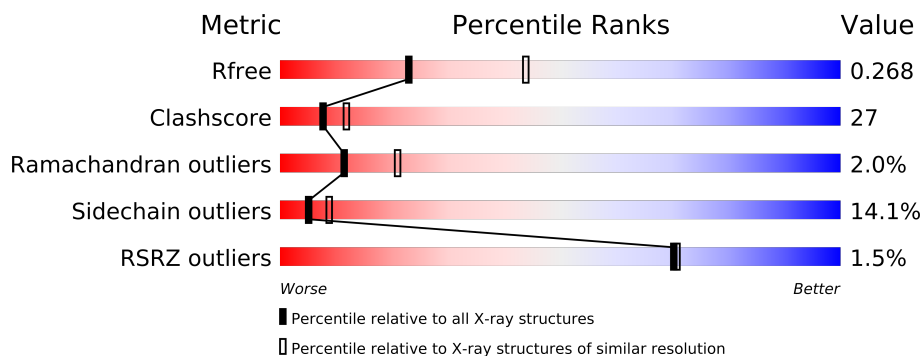
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	475	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3619 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Carbohydrate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3535	2268	597	654	9	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	expression tag	UNP P56176
A	-1	SER	-	expression tag	UNP P56176
A	73	ARG	LYS	see remark 999	UNP P56176
A	74	VAL	THR	see remark 999	UNP P56176
A	82	THR	ALA	see remark 999	UNP P56176
A	91	LYS	GLN	see remark 999	UNP P56176
A	103	THR	ALA	see remark 999	UNP P56176
A	165	ARG	GLY	see remark 999	UNP P56176
A	204	PRO	GLN	see remark 999	UNP P56176
A	227	LYS	ARG	see remark 999	UNP P56176
A	310	ARG	LYS	see remark 999	UNP P56176
A	329	ILE	VAL	see remark 999	UNP P56176
A	337	ALA	VAL	see remark 999	UNP P56176
A	338	VAL	ILE	see remark 999	UNP P56176
A	351	ASN	LYS	see remark 999	UNP P56176
A	439	LEU	SER	see remark 999	UNP P56176
A	467	GLU	-	expression tag	UNP P56176
A	468	GLY	-	expression tag	UNP P56176
A	469	HIS	-	expression tag	UNP P56176
A	470	HIS	-	expression tag	UNP P56176
A	471	HIS	-	expression tag	UNP P56176
A	472	HIS	-	expression tag	UNP P56176
A	473	HIS	-	expression tag	UNP P56176
A	474	HIS	-	expression tag	UNP P56176

- 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		

- Molecule 3 is water.

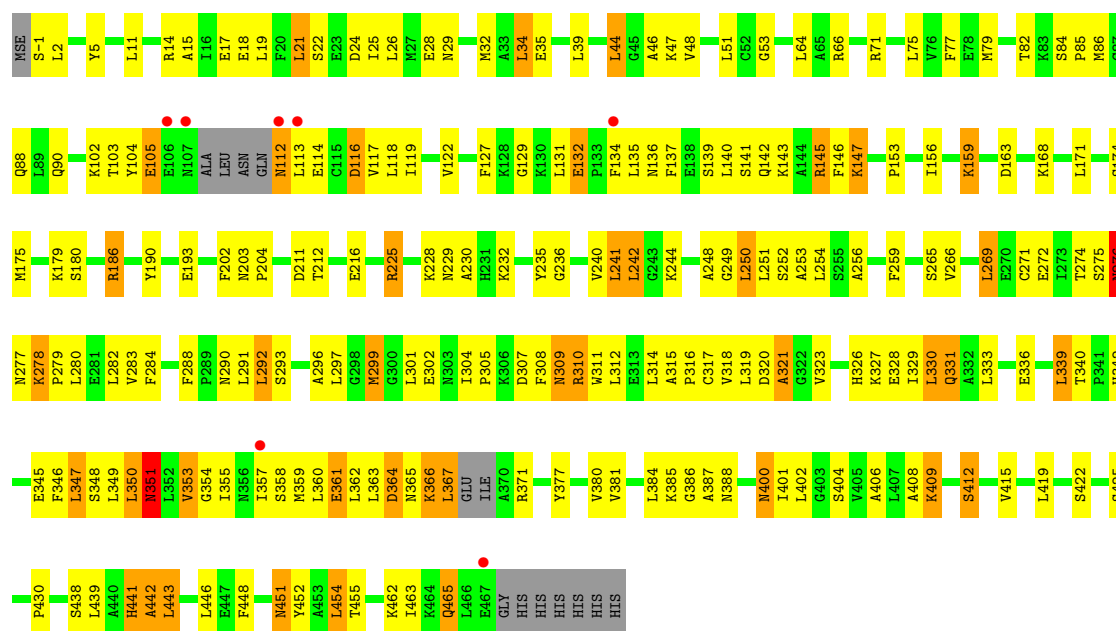
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### ● Molecule 1: Carbohydrate kinase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.95Å 119.95Å 162.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 2.60 49.30 – 2.32	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.23-2.60) 96.8 (49.30-2.32)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.262 0.228 , 0.268	Depositor DCC
$R_{free}$ test set	702 reflections (3.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.9	EDS
Estimated twinning fraction	0.007 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.016 for -1/2*h-1/2*k+1/2*l, -1/2*h-1/2*k-1/2*l, h-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48932 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3619	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 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/3582	0.69	1/4818 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	HIS	N-CA-C	-5.40	96.43	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3535	0	3664	197	0
2	A	5	0	0	0	0
3	A	79	0	0	9	0
All	All	3619	0	3664	197	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (197) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:PHE:HB3	1:A:79:MSE:HE3	1.33	1.10
1:A:366:LYS:HB2	1:A:366:LYS:NZ	1.70	1.06
1:A:276:ASN:CG	1:A:277:ASN:H	1.65	0.98
1:A:351:ASN:C	1:A:351:ASN:HD22	1.74	0.88
1:A:77:PHE:HB3	1:A:79:MSE:CE	2.04	0.88
1:A:366:LYS:HZ3	1:A:366:LYS:HB2	1.33	0.87
1:A:186:ARG:HH22	1:A:363:LEU:HD12	1.42	0.84
1:A:276:ASN:CG	1:A:277:ASN:N	2.31	0.81
1:A:340:THR:O	1:A:340:THR:HG22	1.82	0.78
1:A:136:ASN:O	1:A:140:LEU:HD13	1.83	0.78
1:A:48:VAL:HG22	1:A:117:VAL:HG13	1.68	0.76
1:A:366:LYS:HZ2	1:A:366:LYS:HB2	1.51	0.75
1:A:367:LEU:HD22	1:A:371:ARG:NH1	2.02	0.73
1:A:274:THR:C	1:A:276:ASN:H	1.90	0.72
1:A:309:ASN:H	1:A:309:ASN:ND2	1.88	0.71
1:A:28:GLU:O	1:A:32:MSE:HG3	1.91	0.71
1:A:48:VAL:HG22	1:A:117:VAL:CG1	2.21	0.70
1:A:79:MSE:HE1	1:A:104:TYR:CB	2.22	0.70
1:A:409:LYS:O	1:A:412:SER:HB3	1.92	0.70
1:A:441:HIS:O	1:A:442:ALA:HB3	1.92	0.70
1:A:357:ILE:HG23	1:A:360:LEU:HG	1.74	0.69
1:A:354:GLY:C	1:A:355:ILE:HD12	2.14	0.68
1:A:132:GLU:HG3	1:A:134:PHE:CE2	2.30	0.67
1:A:105:GLU:HA	1:A:105:GLU:OE1	1.94	0.66
1:A:326:HIS:HB3	1:A:328:GLU:OE2	1.94	0.65
1:A:409:LYS:HG3	1:A:454:LEU:O	1.95	0.65
1:A:357:ILE:CG2	1:A:360:LEU:HG	2.25	0.65
1:A:240:VAL:HG13	1:A:299:MSE:HE3	1.78	0.65
1:A:349:LEU:O	1:A:353:VAL:HG23	1.97	0.64
1:A:359:MSE:HE3	1:A:362:LEU:HD11	1.80	0.64
1:A:271:CYS:HB2	3:A:532:HOH:O	1.98	0.63
1:A:274:THR:C	1:A:276:ASN:N	2.51	0.62
1:A:244:LYS:HD2	1:A:302:GLU:OE1	1.99	0.62
1:A:225:ARG:HD2	1:A:235:TYR:CZ	2.34	0.62
1:A:292:LEU:HD12	1:A:292:LEU:H	1.64	0.62
1:A:248:ALA:HB1	1:A:299:MSE:HB2	1.82	0.62
1:A:236:GLY:HA3	1:A:425:SER:O	2.00	0.62
1:A:462:LYS:HD3	3:A:538:HOH:O	2.00	0.61
1:A:400:ASN:ND2	1:A:402:LEU:H	1.99	0.61
1:A:451:ASN:C	1:A:451:ASN:HD22	2.03	0.61
1:A:351:ASN:C	1:A:351:ASN:ND2	2.48	0.61
1:A:366:LYS:HG3	1:A:367:LEU:N	2.16	0.61
1:A:367:LEU:HD23	3:A:507:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:357:ILE:HG22	1:A:358:SER:O	2.01	0.60
1:A:75:LEU:HD11	1:A:102:LYS:HD2	1.84	0.60
1:A:79:MSE:HE1	1:A:104:TYR:HB2	1.83	0.60
1:A:454:LEU:C	1:A:454:LEU:HD13	2.22	0.60
1:A:323:VAL:HB	1:A:329:ILE:HD13	1.84	0.60
1:A:439:LEU:O	1:A:443:LEU:HB2	2.02	0.59
1:A:441:HIS:O	1:A:442:ALA:CB	2.50	0.58
1:A:317:CYS:SG	1:A:319:LEU:HD21	2.42	0.58
1:A:211:ASP:HB2	3:A:494:HOH:O	2.03	0.58
1:A:276:ASN:OD1	1:A:277:ASN:N	2.38	0.57
1:A:276:ASN:ND2	1:A:277:ASN:H	2.03	0.57
1:A:277:ASN:O	1:A:278:LYS:O	2.22	0.57
1:A:112:ASN:C	1:A:114:GLU:H	2.06	0.57
1:A:415:VAL:O	1:A:419:LEU:HG	2.05	0.56
1:A:308:PHE:CE1	1:A:312:LEU:HD11	2.40	0.56
1:A:380:VAL:HG12	1:A:381:VAL:N	2.21	0.56
1:A:311:TRP:HA	1:A:314:LEU:HD23	1.88	0.55
1:A:342:HIS:H	1:A:345:GLU:HB2	1.71	0.55
1:A:28:GLU:OE1	1:A:66:ARG:NH2	2.40	0.55
1:A:419:LEU:HD12	1:A:441:HIS:HB2	1.90	0.54
1:A:309:ASN:OD1	1:A:331:GLN:NE2	2.40	0.54
1:A:5:TYR:O	1:A:179:LYS:HA	2.08	0.54
1:A:292:LEU:HD13	1:A:315:ALA:HB2	1.90	0.54
1:A:367:LEU:HD13	1:A:371:ARG:HD2	1.90	0.54
1:A:159:LYS:HE3	1:A:364:ASP:OD1	2.08	0.54
1:A:127:PHE:CE1	1:A:131:LEU:HD13	2.43	0.54
1:A:293:SER:O	1:A:316:PRO:HD2	2.08	0.53
1:A:116:ASP:HA	1:A:145:ARG:HG3	1.90	0.53
1:A:292:LEU:HD13	1:A:315:ALA:CB	2.38	0.53
1:A:86:MSE:O	1:A:90:GLN:HG2	2.08	0.53
1:A:336:GLU:HG2	1:A:430:PRO:HG2	1.90	0.53
1:A:320:ASP:O	1:A:323:VAL:HG22	2.09	0.52
1:A:147:LYS:NZ	1:A:147:LYS:HB2	2.25	0.52
1:A:340:THR:CG2	1:A:385:LYS:HE3	2.40	0.52
1:A:272:GLU:HG2	1:A:272:GLU:O	2.09	0.52
1:A:329:ILE:HG13	1:A:329:ILE:O	2.09	0.52
1:A:79:MSE:HE2	1:A:79:MSE:HA	1.91	0.51
1:A:438:SER:O	1:A:441:HIS:O	2.27	0.51
1:A:319:LEU:HB3	1:A:323:VAL:HG21	1.92	0.51
1:A:296:ALA:CB	1:A:299:MSE:HE1	2.41	0.50
1:A:290:ASN:C	1:A:291:LEU:HD22	2.31	0.50
1:A:277:ASN:O	1:A:278:LYS:HB3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:454:LEU:C	1:A:454:LEU:CD1	2.79	0.50
1:A:355:ILE:N	1:A:355:ILE:HD12	2.26	0.50
1:A:380:VAL:CG1	1:A:381:VAL:N	2.75	0.50
1:A:82:THR:OG1	1:A:88:GLN:HG3	2.11	0.50
1:A:365:ASN:OD1	1:A:384:LEU:HD23	2.11	0.50
1:A:53:GLY:HA3	1:A:122:VAL:O	2.12	0.50
1:A:118:LEU:CD2	1:A:141:SER:HB3	2.42	0.50
1:A:360:LEU:HD12	1:A:360:LEU:O	2.12	0.49
1:A:388:ASN:CG	1:A:401:ILE:HG22	2.33	0.49
1:A:350:LEU:O	1:A:351:ASN:HB2	2.11	0.49
1:A:340:THR:CG2	1:A:340:THR:O	2.54	0.49
1:A:357:ILE:HG22	1:A:358:SER:N	2.26	0.49
1:A:114:GLU:HA	1:A:143:LYS:O	2.13	0.49
1:A:225:ARG:HD3	3:A:1:HOH:O	2.12	0.49
1:A:266:VAL:HG23	1:A:284:PHE:HD1	1.78	0.49
1:A:357:ILE:HG23	1:A:360:LEU:CG	2.43	0.49
1:A:180:SER:HB2	3:A:505:HOH:O	2.13	0.48
1:A:171:LEU:HD12	1:A:193:GLU:O	2.14	0.48
1:A:318:VAL:HG13	1:A:318:VAL:O	2.13	0.48
1:A:339:LEU:HD22	1:A:380:VAL:HG11	1.95	0.48
1:A:358:SER:C	1:A:360:LEU:H	2.17	0.48
1:A:29:ASN:HA	1:A:32:MSE:SE	2.64	0.47
1:A:451:ASN:ND2	1:A:451:ASN:C	2.68	0.47
1:A:168:LYS:HG3	1:A:190:TYR:CD1	2.49	0.47
1:A:401:ILE:C	1:A:401:ILE:HD12	2.34	0.47
1:A:328:GLU:O	1:A:331:GLN:HG3	2.14	0.47
1:A:448:PHE:CZ	1:A:454:LEU:HD22	2.49	0.47
1:A:77:PHE:CB	1:A:79:MSE:HE3	2.24	0.47
1:A:253:ALA:HB3	1:A:282:LEU:HD21	1.97	0.47
1:A:64:LEU:HD21	1:A:119:ILE:HD13	1.96	0.47
1:A:203:ASN:CG	1:A:204:PRO:HD3	2.35	0.47
1:A:328:GLU:C	1:A:330:LEU:H	2.18	0.47
1:A:328:GLU:H	1:A:328:GLU:CD	2.17	0.47
1:A:103:THR:HB	3:A:514:HOH:O	2.15	0.46
1:A:2:LEU:HD12	1:A:2:LEU:N	2.30	0.46
1:A:242:LEU:HB3	1:A:271:CYS:SG	2.56	0.46
1:A:35:GLU:OE1	1:A:71:ARG:NH2	2.37	0.46
1:A:366:LYS:NZ	1:A:366:LYS:CB	2.53	0.46
1:A:28:GLU:CD	1:A:66:ARG:HH22	2.19	0.46
1:A:153:PRO:HD2	1:A:156:ILE:HD12	1.98	0.46
1:A:241:LEU:HD23	1:A:297:LEU:HD13	1.98	0.46
1:A:117:VAL:HA	1:A:146:PHE:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:367:LEU:HD22	1:A:371:ARG:HH11	1.78	0.46
1:A:288:PHE:CZ	1:A:292:LEU:HD21	2.50	0.46
1:A:317:CYS:SG	1:A:319:LEU:CD2	3.04	0.46
1:A:297:LEU:CD1	1:A:301:LEU:HD22	2.45	0.46
1:A:139:SER:HA	1:A:142:GLN:HG3	1.99	0.45
1:A:454:LEU:HD13	1:A:455:THR:N	2.31	0.45
1:A:292:LEU:HD12	1:A:292:LEU:N	2.31	0.45
1:A:340:THR:HG22	1:A:385:LYS:HE3	1.97	0.45
1:A:419:LEU:HD21	1:A:463:ILE:HD13	1.98	0.45
1:A:225:ARG:HD2	1:A:235:TYR:CE1	2.51	0.45
1:A:85:PRO:HG2	3:A:479:HOH:O	2.15	0.45
1:A:448:PHE:CE2	1:A:454:LEU:CD2	3.00	0.45
1:A:179:LYS:HD2	1:A:179:LYS:N	2.31	0.45
1:A:22:SER:O	1:A:26:LEU:HD13	2.16	0.45
1:A:137:PHE:HA	1:A:140:LEU:HB2	1.99	0.45
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.87	0.44
1:A:232:LYS:HB3	1:A:232:LYS:HE2	1.79	0.44
1:A:350:LEU:O	1:A:351:ASN:CB	2.65	0.44
1:A:265:SER:HA	1:A:283:VAL:O	2.18	0.44
1:A:361:GLU:O	1:A:361:GLU:HG2	2.16	0.44
1:A:46:ALA:HB1	1:A:116:ASP:CB	2.47	0.44
1:A:269:LEU:HD21	1:A:305:PRO:HG2	2.00	0.44
1:A:275:SER:O	1:A:276:ASN:O	2.36	0.44
1:A:309:ASN:OD1	1:A:331:GLN:CD	2.56	0.44
1:A:331:GLN:H	1:A:331:GLN:HG2	1.47	0.44
1:A:250:LEU:O	1:A:254:LEU:HD13	2.18	0.44
1:A:359:MSE:CE	1:A:362:LEU:HD21	2.49	0.43
1:A:104:TYR:CG	1:A:105:GLU:N	2.85	0.43
1:A:277:ASN:HB3	1:A:278:LYS:H	1.60	0.43
1:A:131:LEU:HB2	1:A:163:ASP:OD2	2.18	0.43
1:A:11:LEU:HD12	1:A:11:LEU:N	2.33	0.43
1:A:32:MSE:CE	3:A:525:HOH:O	2.67	0.43
1:A:353:VAL:CG1	1:A:377:TYR:OH	2.66	0.43
1:A:34:LEU:HD13	1:A:175:MSE:HE1	2.01	0.43
1:A:346:PHE:CE2	1:A:350:LEU:HD11	2.54	0.42
1:A:367:LEU:CD2	1:A:371:ARG:NH1	2.79	0.42
1:A:202:PHE:CD2	1:A:204:PRO:HD2	2.54	0.42
1:A:79:MSE:CE	1:A:104:TYR:HB3	2.50	0.42
1:A:254:LEU:HD11	1:A:279:PRO:HG2	2.01	0.42
1:A:465:GLN:HE21	1:A:465:GLN:HB3	1.43	0.42
1:A:367:LEU:CD1	1:A:371:ARG:HD2	2.49	0.42
1:A:452:TYR:CD1	1:A:452:TYR:C	2.93	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:SER:C	1:A:406:ALA:N	2.72	0.42
1:A:400:ASN:HD22	1:A:401:ILE:N	2.18	0.42
1:A:274:THR:OG1	1:A:276:ASN:N	2.51	0.41
1:A:348:SER:O	1:A:351:ASN:HB3	2.20	0.41
1:A:333:LEU:HD13	1:A:377:TYR:CZ	2.56	0.41
1:A:15:ALA:O	1:A:21:LEU:HB2	2.21	0.41
1:A:327:LYS:O	1:A:330:LEU:HB2	2.21	0.41
1:A:228:LYS:C	1:A:230:ALA:H	2.23	0.41
1:A:297:LEU:HD11	1:A:301:LEU:HD22	2.03	0.41
1:A:249:GLY:O	1:A:252:SER:HB2	2.21	0.41
1:A:79:MSE:CE	1:A:104:TYR:CB	2.95	0.41
1:A:212:THR:OG1	1:A:371:ARG:NH2	2.46	0.41
1:A:147:LYS:HB2	1:A:147:LYS:HZ2	1.86	0.41
1:A:346:PHE:CD2	1:A:350:LEU:HD11	2.55	0.41
1:A:256:ALA:HA	1:A:422:SER:HB2	2.03	0.41
1:A:186:ARG:HB2	1:A:186:ARG:HE	1.59	0.41
1:A:310:ARG:O	1:A:314:LEU:HD22	2.21	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD13	1.80	0.41
1:A:320:ASP:CG	1:A:321:ALA:H	2.25	0.41
1:A:112:ASN:N	1:A:112:ASN:HD22	2.17	0.41
1:A:408:ALA:O	1:A:409:LYS:C	2.60	0.40
1:A:14:ARG:HG3	1:A:18:GLU:HB2	2.03	0.40
1:A:304:ILE:HD12	1:A:328:GLU:HB2	2.03	0.40
1:A:401:ILE:O	1:A:401:ILE:HD12	2.20	0.40
1:A:386:GLY:O	1:A:387:ALA:C	2.60	0.40
1:A:274:THR:H	1:A:276:ASN:HB3	1.86	0.40
1:A:-1:SER:N	1:A:216:GLU:HG3	2.37	0.40
1:A:112:ASN:C	1:A:112:ASN:HD22	2.25	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	455/475 (96%)	413 (91%)	33 (7%)	9 (2%)	11 21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	321	ALA
1	A	351	ASN
1	A	409	LYS
1	A	129	GLY
1	A	442	ALA
1	A	278	LYS
1	A	307	ASP
1	A	44	LEU

### 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	384/388 (99%)	330 (86%)	54 (14%)	<b>5</b> <b>9</b>

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	19	LEU
1	A	21	LEU
1	A	24	ASP
1	A	25	ILE
1	A	34	LEU
1	A	39	LEU
1	A	44	LEU
1	A	47	LYS
1	A	51	LEU
1	A	84	SER
1	A	105	GLU
1	A	112	ASN
1	A	113	LEU
1	A	116	ASP
1	A	132	GLU
1	A	135	LEU
1	A	145	ARG

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Mol	Chain	Res	Type
1	A	147	LYS
1	A	159	LYS
1	A	174	SER
1	A	186	ARG
1	A	225	ARG
1	A	229	ASN
1	A	241	LEU
1	A	242	LEU
1	A	250	LEU
1	A	251	LEU
1	A	259	PHE
1	A	269	LEU
1	A	276	ASN
1	A	280	LEU
1	A	292	LEU
1	A	299	MSE
1	A	309	ASN
1	A	310	ARG
1	A	330	LEU
1	A	331	GLN
1	A	339	LEU
1	A	347	LEU
1	A	350	LEU
1	A	351	ASN
1	A	353	VAL
1	A	361	GLU
1	A	364	ASP
1	A	366	LYS
1	A	367	LEU
1	A	400	ASN
1	A	412	SER
1	A	443	LEU
1	A	446	LEU
1	A	451	ASN
1	A	454	LEU
1	A	465	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	29	ASN

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Mol	Chain	Res	Type
1	A	41	ASN
1	A	112	ASN
1	A	136	ASN
1	A	229	ASN
1	A	267	GLN
1	A	303	ASN
1	A	309	ASN
1	A	326	HIS
1	A	331	GLN
1	A	351	ASN
1	A	400	ASN
1	A	427	ASN
1	A	451	ASN
1	A	465	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	501	-	4,4,4	0.81	0	6,6,6	0.31	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	PO4	A	501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	461/475 (97%)	-0.18	7 (1%) 70 71	24, 46, 68, 82	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	ASN	3.6
1	A	112	ASN	3.4
1	A	113	LEU	2.7
1	A	106	GLU	2.4
1	A	134	PHE	2.1
1	A	357	ILE	2.1
1	A	467	GLU	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 ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	501	5/5	0.15	0.01	98,98,99,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.