



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:59 AM GMT

PDB ID : 3QN3  
Title : Phosphopyruvate hydratase from *Campylobacter jejuni*.  
Authors : Osipiuk, J.; Gu, M.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-02-07  
Resolution : 2.13 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

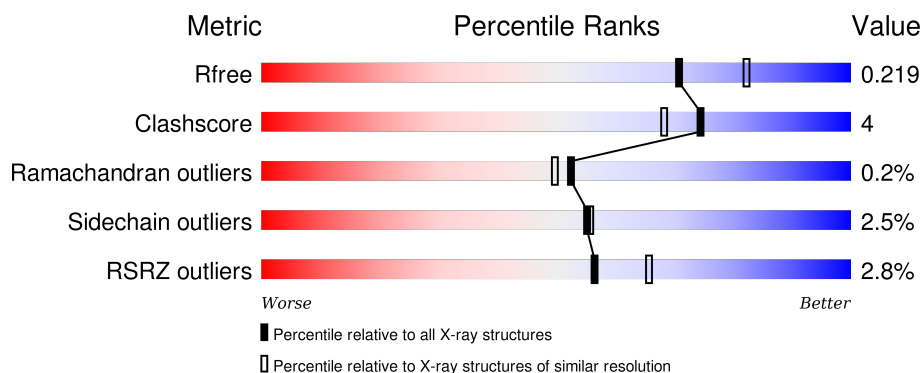
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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))
$R_{free}$	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (2.16-2.12)

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. 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	417	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	B	417	<div> <div>4%</div> <div>89%</div> <div>9%</div> </div>
1	C	417	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>
1	D	417	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>

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	MPD	A	604	X	-	-	X
3	MPD	B	603	X	-	-	X
3	MPD	C	415	X	-	-	X
3	MPD	D	602	X	-	-	X
4	GOL	C	606	-	-	-	X
5	SO4	B	609	-	-	-	X
5	SO4	D	608	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13827 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	19	0
			3266	2050	558	640	18			
1	B	415	Total	C	N	O	S	0	15	0
			3244	2036	550	640	18			
1	C	415	Total	C	N	O	S	0	17	0
			3249	2040	552	639	18			
1	D	415	Total	C	N	O	S	0	12	0
			3224	2021	548	637	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P42448
A	-1	ASN	-	EXPRESSION TAG	UNP P42448
A	0	ALA	-	EXPRESSION TAG	UNP P42448
B	-2	SER	-	EXPRESSION TAG	UNP P42448
B	-1	ASN	-	EXPRESSION TAG	UNP P42448
B	0	ALA	-	EXPRESSION TAG	UNP P42448
C	-2	SER	-	EXPRESSION TAG	UNP P42448
C	-1	ASN	-	EXPRESSION TAG	UNP P42448
C	0	ALA	-	EXPRESSION TAG	UNP P42448
D	-2	SER	-	EXPRESSION TAG	UNP P42448
D	-1	ASN	-	EXPRESSION TAG	UNP P42448
D	0	ALA	-	EXPRESSION TAG	UNP P42448

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

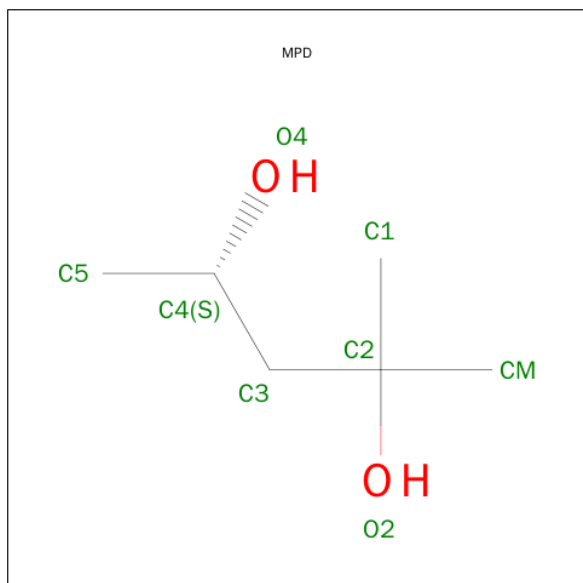
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

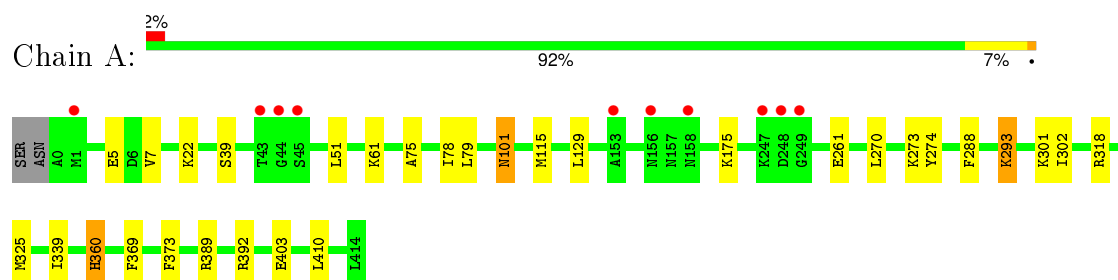
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	193	Total	O	0	1
			193	193		
6	B	178	Total	O	0	1
			178	178		
6	C	209	Total	O	0	0
			209	209		
6	D	195	Total	O	0	1
			195	195		

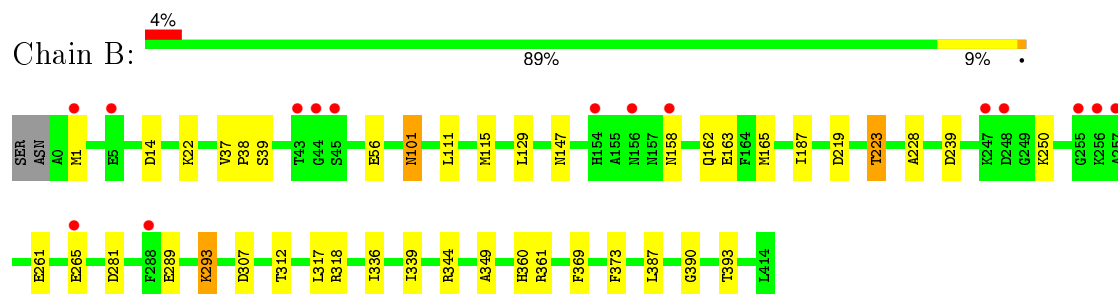
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

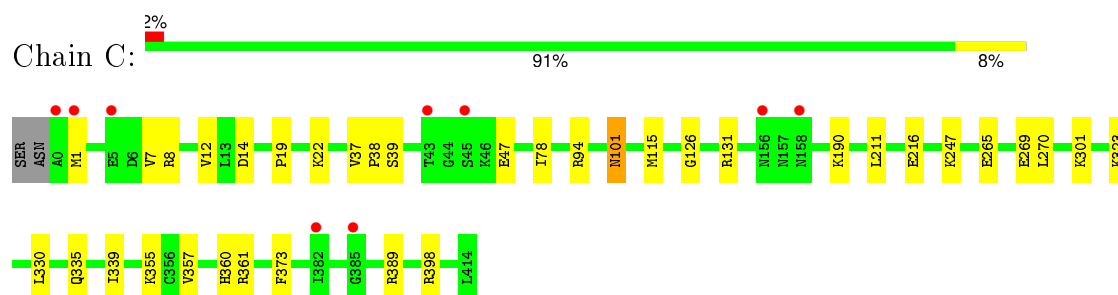
#### • Molecule 1: Enolase



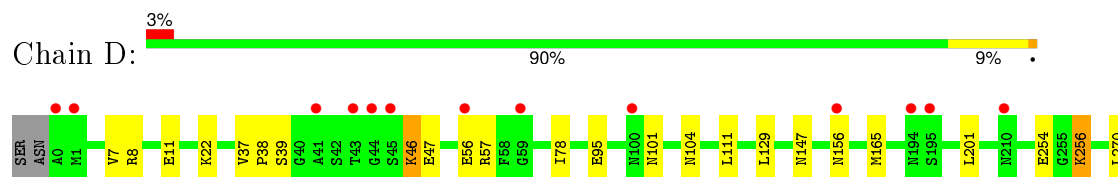
#### • Molecule 1: Enolase



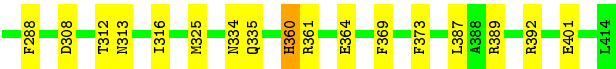
#### • Molecule 1: Enolase



#### • Molecule 1: Enolase







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.47Å 148.89Å 234.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.90 – 2.13 35.93 – 2.13	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.90-2.13) 96.2 (35.93-2.13)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.37 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.176 , 0.216 0.181 , 0.219	Depositor DCC
$R_{free}$ test set	5783 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	2 of 113808 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13827	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 2.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG, SO4, MPD

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	0.84	0/3366	0.78	0/4538
1	B	0.79	0/3332	0.79	2/4493 (0.0%)
1	C	0.82	0/3343	0.78	2/4507 (0.0%)
1	D	0.82	0/3303	0.77	1/4455 (0.0%)
All	All	0.81	0/13344	0.78	5/17993 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	D	308	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	361	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	14	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	14	ASP	CB-CG-OD1	5.11	122.89	118.30

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	3266	0	3303	25	0
1	B	3244	0	3265	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3249	0	3282	24	0
1	D	3224	0	3235	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	14	2	0
3	B	8	0	14	2	0
3	C	8	0	14	4	0
3	D	8	0	14	4	0
4	A	6	0	8	0	0
4	C	12	0	16	1	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	193	0	0	6	0
6	B	178	0	0	5	0
6	C	209	0	0	6	0
6	D	195	0	0	4	0
All	All	13827	0	13165	104	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 4.

All (104) 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:C:355:LYS:NZ	6:C:523:HOH:O	2.10	0.79
1:D:46:LYS:NZ	6:D:687:HOH:O	2.17	0.77
1:B:1:MET:HE1	1:C:126:GLY:O	1.89	0.72
1:D:7:VAL:HG21	1:D:78:ILE:HD11	1.72	0.71
1:B:219:ASP:O	1:B:223:THR:HG23	1.89	0.71
1:A:7:VAL:HG21	1:A:78:ILE:HD11	1.70	0.71
1:B:22:LYS:NZ	3:B:603:MPD:H12	2.06	0.69
1:A:22:LYS:HZ1	3:A:604:MPD:HM2	1.57	0.69
1:B:22:LYS:HZ1	3:B:603:MPD:H12	1.58	0.68
3:D:602:MPD:HM1	3:D:602:MPD:O4	1.95	0.67
3:C:415:MPD:CM	3:C:415:MPD:O4	2.43	0.66
1:C:7:VAL:HG21	1:C:78:ILE:HD11	1.78	0.66
1:D:22:LYS:NZ	3:D:602:MPD:HM2	2.14	0.62
3:C:415:MPD:HM2	3:C:415:MPD:O4	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LYS:HZ1	3:D:602:MPD:HM2	1.64	0.62
1:C:115:MET:HG2	1:C:339[A]:ILE:HD11	1.85	0.59
1:D:360:HIS:CD2	1:D:392:ARG:HH11	2.22	0.58
1:D:360:HIS:HD2	1:D:392:ARG:HH11	1.51	0.58
1:C:39[A]:SER:HB2	6:C:545:HOH:O	2.04	0.58
1:A:22:LYS:NZ	3:A:604:MPD:HM2	2.19	0.58
1:D:47:GLU:HG2	1:D:335:GLN:HG3	1.88	0.56
1:D:313:ASN:HB3	1:D:316:ILE:HD12	1.89	0.54
1:C:39[B]:SER:HB3	6:C:545:HOH:O	2.07	0.54
1:A:39[A]:SER:HB3	6:A:503:HOH:O	2.08	0.53
1:B:56[A]:GLU:H	1:B:56[A]:GLU:CD	2.11	0.53
1:D:288:PHE:HB3	1:D:325:MET:CE	2.39	0.53
1:D:254:GLU:O	1:D:256:LYS:HD3	2.09	0.53
1:C:398:ARG:HD3	4:C:607:GOL:H31	1.91	0.53
1:D:39[A]:SER:HB3	6:D:438:HOH:O	2.09	0.51
1:A:288:PHE:HB3	1:A:325:MET:CE	2.39	0.51
1:B:312:THR:O	1:B:312:THR:HG22	2.09	0.51
1:B:318:ARG:NH2	6:B:495:HOH:O	2.42	0.51
1:B:344[B]:ARG:NE	6:B:717:HOH:O	2.39	0.51
1:A:318[A]:ARG:NH2	6:A:511:HOH:O	2.36	0.50
1:A:261:GLU:OE2	1:A:293:LYS:NZ	2.33	0.50
1:C:131:ARG:HD3	6:C:422:HOH:O	2.12	0.50
1:C:190[B]:LYS:HE3	6:C:505:HOH:O	2.12	0.50
1:B:187:ILE:HD12	1:B:228:ALA:HB2	1.94	0.49
1:D:47:GLU:HG2	1:D:335:GLN:CG	2.43	0.49
1:C:115:MET:HG2	1:C:339[A]:ILE:CD1	2.41	0.49
1:C:37:VAL:HG12	1:C:38:PRO:O	2.13	0.49
1:B:281:ASP:OD2	1:B:307:ASP:HB3	2.13	0.49
1:B:39[A]:SER:HB2	6:B:651[A]:HOH:O	2.11	0.48
1:A:175[B]:LYS:NZ	1:A:403:GLU:OE2	2.42	0.48
1:C:47:GLU:OE2	6:C:574:HOH:O	2.20	0.48
1:D:288:PHE:HB3	1:D:325:MET:HE2	1.96	0.48
1:A:288:PHE:HB3	1:A:325:MET:HE2	1.96	0.47
1:A:273:LYS:HD3	1:A:274:TYR:CE2	2.49	0.47
1:A:318[A]:ARG:NE	6:A:511:HOH:O	2.33	0.47
1:A:129:LEU:HD21	1:A:369:PHE:CE2	2.50	0.47
1:D:201:LEU:HD11	6:D:546:HOH:O	2.14	0.47
1:D:37:VAL:HG12	1:D:38:PRO:O	2.15	0.47
1:D:111:LEU:HD22	1:D:334:ASN:HA	1.97	0.46
1:B:162:GLN:HG2	1:B:163:GLU:HG3	1.96	0.46
1:D:360:HIS:CD2	1:D:392:ARG:NH1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289[A]:GLU:H	1:B:289[A]:GLU:CD	2.19	0.46
3:D:602:MPD:O4	3:D:602:MPD:CM	2.61	0.46
1:C:22:LYS:NZ	3:C:415:MPD:HM3	2.30	0.46
1:C:47:GLU:HG2	1:C:335:GLN:HG3	1.98	0.45
1:A:175[B]:LYS:NZ	6:A:468:HOH:O	2.39	0.45
1:D:39[A]:SER:HB2	6:D:561[A]:HOH:O	2.17	0.45
1:B:37:VAL:HG12	1:B:38:PRO:O	2.16	0.45
1:A:318[B]:ARG:NH1	6:A:488:HOH:O	2.50	0.45
1:B:387:LEU:N	1:B:387:LEU:HD22	2.32	0.45
1:B:390:GLY:HA2	1:B:393:THR:OG1	2.17	0.45
1:D:147:ASN:HA	1:D:165:MET:HG2	1.99	0.45
1:B:163:GLU:HB2	1:B:239:ASP:HB3	1.98	0.44
1:C:22:LYS:NZ	1:D:401:GLU:OE2	2.50	0.44
1:A:115:MET:HG2	1:A:339[A]:ILE:HD11	1.98	0.44
1:B:115:MET:HG2	1:B:339[A]:ILE:HD11	1.98	0.44
1:A:301:LYS:HG2	1:A:302:ILE:HG23	2.00	0.44
1:B:101:ASN:N	1:B:101:ASN:HD22	2.15	0.44
1:A:101:ASN:HD22	1:A:101:ASN:H	1.65	0.44
1:A:101:ASN:HD22	1:A:101:ASN:N	2.15	0.43
1:B:111:LEU:HG	1:B:115:MET:HE2	2.00	0.43
1:D:129:LEU:HD21	1:D:369:PHE:CE2	2.53	0.43
1:C:211:LEU:HD22	1:C:216:GLU:OE1	2.18	0.43
1:C:22:LYS:HZ1	3:C:415:MPD:HM3	1.84	0.43
1:C:330:LEU:HD12	1:C:357:VAL:HB	2.01	0.43
1:B:261:GLU:O	1:B:265[A]:GLU:HG2	2.19	0.42
1:A:61:LYS:NZ	6:A:504:HOH:O	2.53	0.42
1:B:317:LEU:HD21	1:B:349:ALA:HB2	2.01	0.42
1:B:219:ASP:O	1:B:223:THR:CG2	2.64	0.42
1:A:273:LYS:HD3	1:A:274:TYR:CZ	2.55	0.42
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.90	0.42
1:C:339[B]:ILE:HG21	1:C:339[B]:ILE:HD13	1.78	0.42
1:A:75:ALA:O	1:A:79:LEU:HG	2.20	0.41
1:C:101:ASN:N	1:C:101:ASN:HD22	2.16	0.41
1:B:129:LEU:HD21	1:B:369:PHE:CE2	2.56	0.41
1:D:387:LEU:N	1:D:387:LEU:HD22	2.35	0.41
1:B:293:LYS:NZ	6:B:510:HOH:O	2.54	0.41
1:D:361:ARG:O	1:D:364:GLU:HG2	2.20	0.41
1:A:360:HIS:HD1	1:A:392:ARG:HH11	1.67	0.41
1:C:265:GLU:O	1:C:269[A]:GLU:HG3	2.21	0.41
1:A:7:VAL:HG21	1:A:78:ILE:CD1	2.45	0.41
1:D:11:GLU:OE1	1:D:57:ARG:NH2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASN:HA	1:B:165:MET:HG2	2.03	0.40
1:D:312:THR:HG22	1:D:312:THR:O	2.21	0.40
1:A:288:PHE:HB3	1:A:325:MET:HE1	2.03	0.40
1:C:101:ASN:HD22	1:C:101:ASN:H	1.69	0.40
1:C:12:VAL:O	1:C:19:PRO:HA	2.21	0.40
1:B:336:ILE:HA	1:B:336:ILE:HD12	1.96	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	432/417 (104%)	412 (95%)	19 (4%)	1 (0%)	52	50
1	B	428/417 (103%)	409 (96%)	19 (4%)	0	100	100
1	C	430/417 (103%)	412 (96%)	16 (4%)	2 (0%)	34	26
1	D	425/417 (102%)	403 (95%)	21 (5%)	1 (0%)	52	50
All	All	1715/1668 (103%)	1636 (95%)	75 (4%)	4 (0%)	52	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1	MET
1	A	389	ARG
1	D	389	ARG
1	C	389	ARG

### 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	351/334 (105%)	344 (98%)	7 (2%)	63	66
1	B	347/334 (104%)	340 (98%)	7 (2%)	63	66
1	C	349/334 (104%)	341 (98%)	8 (2%)	58	60
1	D	344/334 (103%)	331 (96%)	13 (4%)	40	37
All	All	1391/1336 (104%)	1356 (98%)	35 (2%)	55	56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	51	LEU
1	A	101	ASN
1	A	270	LEU
1	A	293	LYS
1	A	360	HIS
1	A	373	PHE
1	B	101	ASN
1	B	158	ASN
1	B	223	THR
1	B	250	LYS
1	B	293	LYS
1	B	360	HIS
1	B	373	PHE
1	C	8	ARG
1	C	101	ASN
1	C	247	LYS
1	C	270	LEU
1	C	301	LYS
1	C	323	LYS
1	C	360	HIS
1	C	373	PHE
1	D	8	ARG
1	D	46	LYS
1	D	56[A]	GLU
1	D	56[B]	GLU
1	D	95[A]	GLU
1	D	95[B]	GLU

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Mol	Chain	Res	Type
1	D	101	ASN
1	D	104	ASN
1	D	156	ASN
1	D	256	LYS
1	D	270	LEU
1	D	360	HIS
1	D	373	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	303	GLN
1	A	381	GLN
1	B	101	ASN
1	C	101	ASN
1	C	147	ASN
1	C	197	HIS
1	C	335	GLN
1	C	341	GLN
1	D	101	ASN
1	D	335	GLN
1	D	360	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	MPD	A	604	-	6,7,7	0.57	0	7,10,10	0.36	0
4	GOL	A	605	-	5,5,5	0.45	0	5,5,5	0.69	0
3	MPD	B	603	-	6,7,7	0.65	0	7,10,10	0.50	0
5	SO4	B	609	-	4,4,4	0.18	0	6,6,6	0.22	0
3	MPD	C	415	-	6,7,7	0.41	0	7,10,10	0.43	0
4	GOL	C	606	-	5,5,5	0.35	0	5,5,5	0.42	0
4	GOL	C	607	-	5,5,5	0.29	0	5,5,5	0.80	0
5	SO4	C	610	-	4,4,4	0.05	0	6,6,6	0.11	0
3	MPD	D	602	-	6,7,7	0.62	0	7,10,10	0.72	0
5	SO4	D	608	-	4,4,4	0.17	0	6,6,6	0.22	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	MPD	A	604	-	1/1/2/2	0/5/5/5	0/0/0/0
4	GOL	A	605	-	-	0/4/4/4	0/0/0/0
3	MPD	B	603	-	1/1/2/2	0/5/5/5	0/0/0/0
5	SO4	B	609	-	-	0/0/0/0	0/0/0/0
3	MPD	C	415	-	1/1/2/2	0/5/5/5	0/0/0/0
4	GOL	C	606	-	-	0/4/4/4	0/0/0/0
4	GOL	C	607	-	-	0/4/4/4	0/0/0/0
5	SO4	C	610	-	-	0/0/0/0	0/0/0/0
3	MPD	D	602	-	1/1/2/2	0/5/5/5	0/0/0/0
5	SO4	D	608	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	604	MPD	C4

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Mol	Chain	Res	Type	Atom
3	B	603	MPD	C4
3	D	602	MPD	C4
3	C	415	MPD	C4

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	MPD	2	0
3	B	603	MPD	2	0
3	C	415	MPD	4	0
4	C	607	GOL	1	0
3	D	602	MPD	4	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	415/417 (99%)	-0.09	10 (2%) 62 69	20, 32, 52, 64	0
1	B	415/417 (99%)	-0.01	15 (3%) 46 56	21, 34, 58, 71	0
1	C	415/417 (99%)	0.01	9 (2%) 65 72	22, 32, 51, 62	0
1	D	415/417 (99%)	-0.04	13 (3%) 52 62	22, 34, 53, 62	0
All	All	1660/1668 (99%)	-0.03	47 (2%) 56 66	20, 33, 54, 71	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	SER	5.1
1	D	44	GLY	5.1
1	A	153	ALA	4.9
1	C	45	SER	4.5
1	A	156[A]	ASN	4.4
1	D	45	SER	4.3
1	D	43	THR	4.1
1	B	44	GLY	4.0
1	D	1	MET	3.7
1	A	45	SER	3.7
1	B	43	THR	3.7
1	B	257	ALA	3.6
1	B	1	MET	3.3
1	A	43	THR	3.3
1	D	156	ASN	3.2
1	A	248	ASP	3.2
1	C	0	ALA	3.1
1	C	158	ASN	3.1
1	C	1	MET	3.1
1	A	44	GLY	3.0
1	D	210[A]	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	158[A]	ASN	2.7
1	C	5[A]	GLU	2.6
1	D	194	ASN	2.6
1	D	41	ALA	2.6
1	B	5[A]	GLU	2.5
1	A	1	MET	2.5
1	B	255	GLY	2.5
1	C	382	ILE	2.5
1	C	156	ASN	2.4
1	B	247	LYS	2.4
1	A	249	GLY	2.4
1	D	0	ALA	2.3
1	D	56[A]	GLU	2.3
1	C	385	GLY	2.3
1	C	43	THR	2.3
1	D	59	GLY	2.3
1	D	100[A]	ASN	2.1
1	B	256	LYS	2.1
1	B	154	HIS	2.1
1	B	158	ASN	2.1
1	B	265[A]	GLU	2.1
1	B	288	PHE	2.1
1	A	247	LYS	2.1
1	B	156	ASN	2.0
1	B	248	ASP	2.0
1	D	195	SER	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 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	D	602	8/8	0.80	0.27	5.82	51,55,59,60	0
5	SO4	B	609	5/5	0.77	0.33	5.45	109,110,110,110	0
3	MPD	A	604	8/8	0.88	0.21	4.01	51,54,56,57	0
3	MPD	B	603	8/8	0.91	0.22	2.57	53,57,59,59	0
3	MPD	C	415	8/8	0.95	0.19	2.54	55,57,59,60	0
4	GOL	C	606	6/6	0.73	0.22	2.07	68,69,70,70	0
5	SO4	D	608	5/5	0.89	0.24	2.06	87,88,89,89	0
4	GOL	A	605	6/6	0.94	0.20	1.74	58,59,59,60	0
5	SO4	C	610	5/5	0.86	0.19	1.21	80,80,82,82	5
4	GOL	C	607	6/6	0.92	0.15	-0.04	48,50,53,53	0
2	MG	B	601	1/1	0.96	0.10	-0.75	39,39,39,39	0
2	MG	C	601	1/1	0.98	0.09	-1.21	36,36,36,36	0
2	MG	D	601	1/1	0.97	0.09	-1.69	33,33,33,33	0
2	MG	A	601	1/1	0.95	0.05	-1.71	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.