



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:23 am BST

PDB ID : 1GG1  
Title : CRYSTAL STRUCTURE ANALYSIS OF DAHP SYNTHASE IN COMPLEX  
WITH MN<sup>2+</sup> AND 2-PHOSPHOGLYCOLATE  
Authors : Wagner, T.; Shumilin, I.A.; Bauerle, R.; Kretsinger, R.H.  
Deposited on : 2000-08-04  
Resolution : 2.00 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

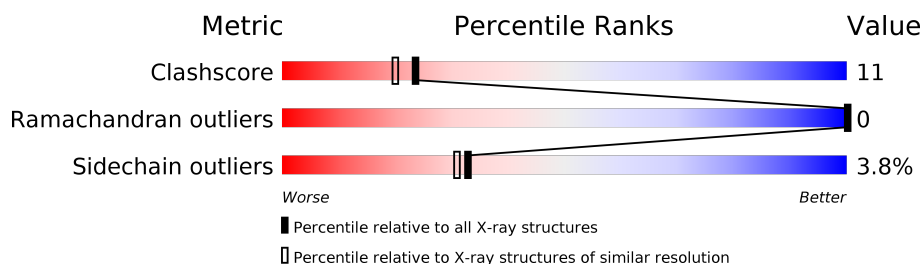
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	350	
1	B	350	
1	C	350	
1	D	350	

## 2 Entry composition [i](#)

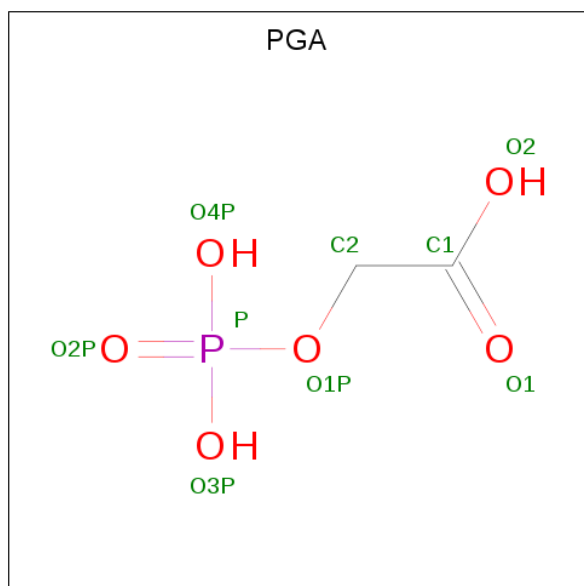
There are 5 unique types of molecules in this entry. The entry contains 10970 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2521	1584	449	474	14			
1	B	343	Total	C	N	O	S	0	0	0
			2586	1624	461	487	14			
1	C	339	Total	C	N	O	S	0	0	0
			2507	1578	446	469	14			
1	D	340	Total	C	N	O	S	0	0	0
			2536	1595	452	475	14			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula:  $C_2H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			9	2	6	1		
2	D	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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



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

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

- Molecule 5 is water.

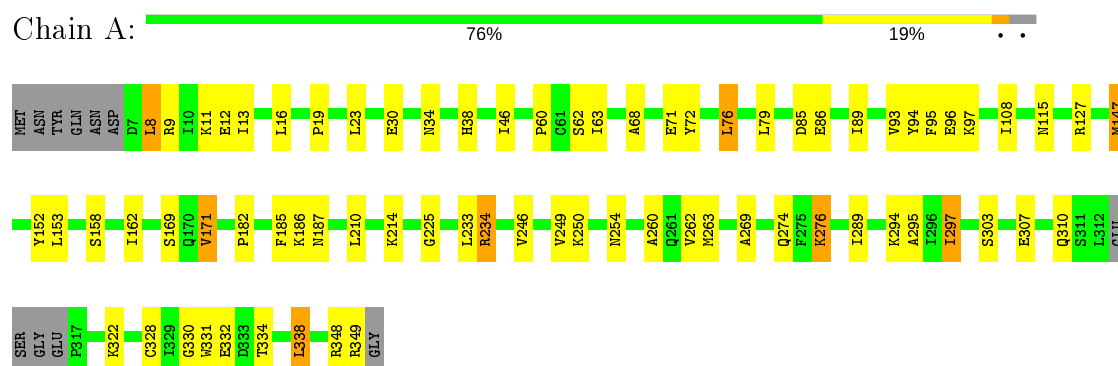
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	146	Total	O	0	0
			146	146		
5	B	299	Total	O	0	0
			299	299		
5	C	114	Total	O	0	0
			114	114		
5	D	181	Total	O	0	0
			181	181		

### 3 Residue-property plots

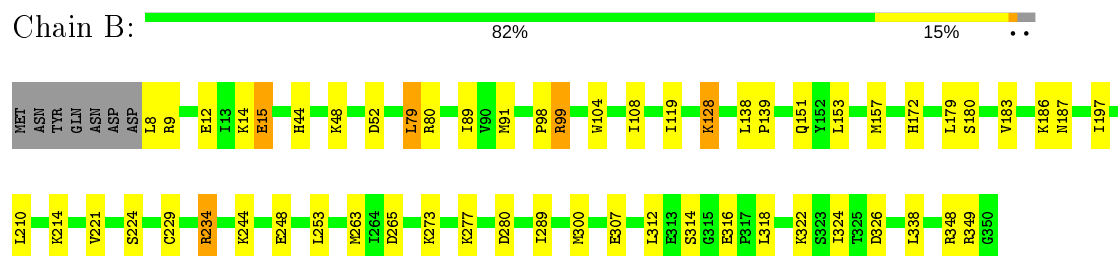
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

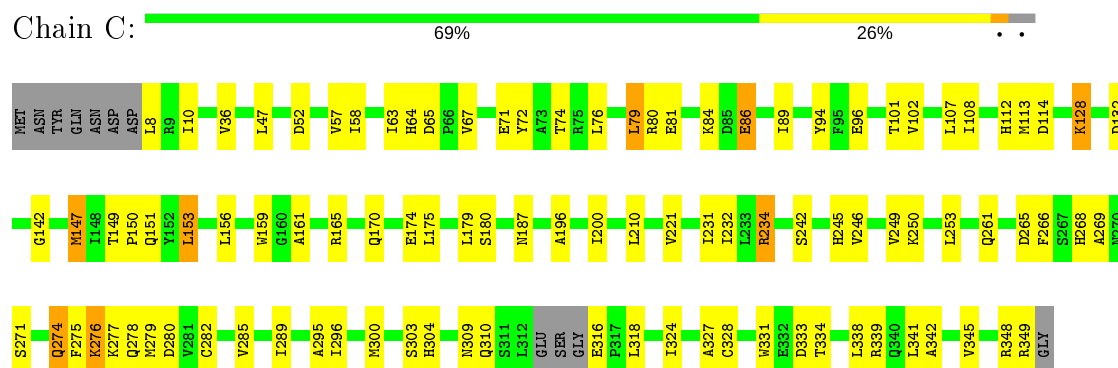
#### • Molecule 1: 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE



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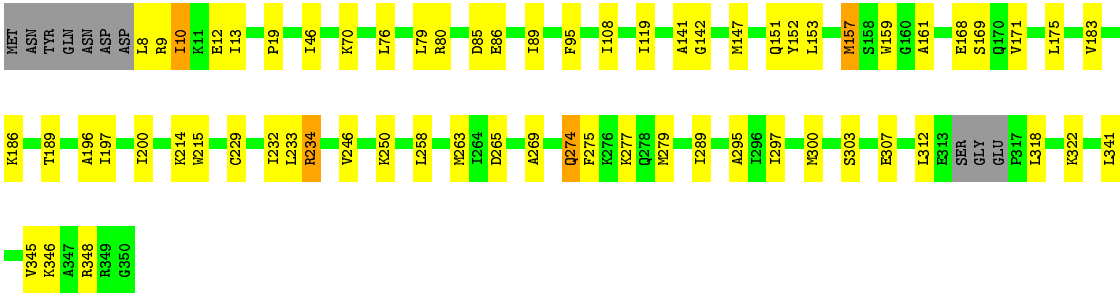
#### • Molecule 1: 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE

Chain D: 

79%

17%

••



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.36 Å   53.19 Å   149.39 Å 90.00°   116.09°   90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP



## 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: MN, SO4, PGA

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	0.47	0/2565	0.66	2/3483 (0.1%)
1	B	0.69	0/2631	0.81	4/3562 (0.1%)
1	C	0.44	0/2550	0.67	1/3465 (0.0%)
1	D	0.53	0/2580	0.71	3/3498 (0.1%)
All	All	0.54	0/10326	0.72	10/14008 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	MET	CG-SD-CE	6.19	110.11	100.20
1	A	263	MET	CG-SD-CE	5.87	109.58	100.20
1	D	263	MET	CG-SD-CE	5.85	109.56	100.20
1	B	263	MET	CG-SD-CE	5.80	109.49	100.20
1	B	91	MET	CG-SD-CE	5.79	109.47	100.20
1	A	147	MET	CG-SD-CE	5.78	109.44	100.20
1	B	157	MET	CG-SD-CE	5.50	109.00	100.20
1	D	157	MET	CG-SD-CE	5.40	108.84	100.20
1	C	147	MET	CG-SD-CE	5.39	108.83	100.20
1	B	99	ARG	NE-CZ-NH2	-5.30	117.65	120.30

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	2521	0	2481	70	0
1	B	2586	0	2594	48	0
1	C	2507	0	2470	76	0
1	D	2536	0	2518	48	0
2	A	9	0	2	0	0
2	B	9	0	2	1	0
2	C	9	0	2	0	0
2	D	9	0	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	1	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	146	0	0	10	0
5	B	299	0	0	9	0
5	C	114	0	0	3	0
5	D	181	0	0	5	0
All	All	10970	0	10071	227	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 11.

All (227) 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:276:LYS:H	1:A:276:LYS:CD	1.55	1.20
1:A:63:ILE:HD11	1:A:93:VAL:HA	1.44	1.00
1:A:276:LYS:HD2	1:A:276:LYS:H	1.31	0.94
1:A:276:LYS:HD3	1:A:276:LYS:H	1.32	0.93
1:C:86:GLU:HG3	1:C:342:ALA:HB1	1.51	0.90
1:B:273:LYS:HE2	5:B:2419:HOH:O	1.72	0.89
1:A:276:LYS:N	1:A:276:LYS:CD	2.37	0.84
1:A:254:ASN:HD21	1:A:260:ALA:HB2	1.44	0.81
1:C:274:GLN:HB3	1:C:276:LYS:HE3	1.60	0.81
1:C:72:TYR:HE2	1:C:76:LEU:HD22	1.46	0.80
1:C:81:GLU:O	1:C:84:LYS:HG2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LEU:O	1:C:345:VAL:HG23	1.83	0.78
1:A:276:LYS:N	1:A:276:LYS:HD3	2.00	0.74
1:C:309:ASN:HB3	1:C:327:ALA:HA	1.68	0.73
1:D:169:SER:OG	1:D:171:VAL:HG22	1.88	0.72
1:C:64:HIS:HB2	1:C:113:MET:HE2	1.70	0.72
1:D:151:GLN:OE1	1:D:214:LYS:HG2	1.92	0.69
1:D:234:ARG:O	1:D:269:ALA:HB3	1.91	0.69
1:A:62:SER:HB3	1:A:97:LYS:HD2	1.74	0.68
1:D:8:LEU:HD23	1:D:10:ILE:CD1	2.24	0.67
1:D:289:ILE:O	1:D:348:ARG:HB2	1.95	0.66
1:D:246:VAL:O	1:D:250:LYS:HG3	1.94	0.66
1:A:63:ILE:CD1	1:A:93:VAL:HA	2.24	0.65
1:A:63:ILE:HD12	5:A:1408:HOH:O	1.95	0.64
1:A:147:MET:HE2	5:A:1427:HOH:O	1.96	0.64
1:A:310:GLN:NE2	1:A:322:LYS:HB3	2.11	0.64
1:A:234:ARG:O	1:A:269:ALA:HB3	1.97	0.64
1:C:274:GLN:CB	1:C:276:LYS:HE3	2.28	0.63
1:B:151:GLN:OE1	1:B:214:LYS:HE3	1.99	0.63
1:A:152:TYR:C	1:A:153:LEU:HD12	2.19	0.62
1:A:254:ASN:ND2	1:A:260:ALA:HB2	2.14	0.62
1:D:152:TYR:O	1:D:153:LEU:HD12	1.99	0.62
1:C:80:ARG:HA	1:C:89:ILE:HD12	1.81	0.62
1:C:246:VAL:O	1:C:250:LYS:HG3	2.00	0.62
1:C:52:ASP:OD2	1:C:349:ARG:NE	2.26	0.62
1:A:76:LEU:HD22	1:A:89:ILE:HG21	1.82	0.62
1:B:80:ARG:HA	1:B:89:ILE:HD12	1.80	0.62
1:A:250:LYS:HD3	1:A:295:ALA:CB	2.30	0.61
1:D:147:MET:HE2	1:D:175:LEU:HD22	1.81	0.61
1:A:115:ASN:ND2	5:A:1419:HOH:O	2.32	0.61
1:A:11:LYS:HE2	1:B:224:SER:HB3	1.83	0.61
1:C:274:GLN:HA	1:C:276:LYS:HE3	1.83	0.61
1:B:128:LYS:HE3	5:B:2667:HOH:O	2.01	0.60
1:A:274:GLN:HA	1:A:276:LYS:HZ3	1.67	0.60
1:B:314:SER:C	1:B:316:GLU:H	2.05	0.60
1:D:85:ASP:HB2	5:D:4533:HOH:O	2.02	0.59
1:A:16:LEU:HD22	1:B:210:LEU:HD22	1.84	0.59
1:D:141:ALA:C	1:D:157:MET:HE1	2.22	0.59
1:A:310:GLN:HE21	1:A:322:LYS:HB3	1.67	0.59
1:D:141:ALA:HB1	1:D:159:TRP:HE3	1.67	0.59
1:C:128:LYS:HE2	1:C:132:ASP:OD2	2.02	0.58
1:A:97:LYS:CE	5:A:1414:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD21	1:D:119:ILE:HG21	1.84	0.58
1:D:147:MET:CE	1:D:175:LEU:HD22	2.33	0.58
1:A:11:LYS:HE2	1:B:224:SER:CB	2.34	0.58
1:C:234:ARG:O	1:C:269:ALA:HB3	2.04	0.58
1:A:152:TYR:HB2	1:A:153:LEU:HD12	1.85	0.57
1:A:86:GLU:HG3	1:A:349:ARG:NH2	2.19	0.57
1:C:79:LEU:HD23	1:C:338:LEU:HD12	1.86	0.57
1:A:147:MET:SD	1:A:171:VAL:HG23	2.44	0.57
1:C:276:LYS:HD2	5:C:3377:HOH:O	2.03	0.57
1:A:63:ILE:CD1	5:A:1408:HOH:O	2.52	0.56
1:C:8:LEU:HD23	1:C:10:ILE:HB	1.88	0.56
1:C:289:ILE:O	1:C:348:ARG:HB2	2.04	0.56
1:C:275:PHE:HA	1:C:278:GLN:HE21	1.69	0.56
1:A:68:ALA:HB2	5:A:1410:HOH:O	2.04	0.56
1:A:85:ASP:HB2	5:A:1412:HOH:O	2.06	0.56
1:C:277:LYS:HD3	1:C:280:ASP:OD2	2.06	0.55
1:C:303:SER:HA	1:C:328:CYS:HB3	1.87	0.55
1:C:274:GLN:CA	1:C:276:LYS:HE3	2.37	0.55
1:A:246:VAL:O	1:A:250:LYS:HG3	2.07	0.55
1:D:12:GLU:O	1:D:13:ILE:HD13	2.07	0.55
1:D:214:LYS:HG3	5:D:4498:HOH:O	2.07	0.55
1:D:250:LYS:HD3	1:D:295:ALA:CB	2.37	0.55
1:C:266:PHE:O	1:C:271:SER:HB3	2.08	0.54
1:B:8:LEU:N	5:B:2514:HOH:O	2.39	0.54
1:A:95:PHE:HB3	1:A:108:ILE:HG13	1.88	0.54
1:C:250:LYS:HD3	1:C:295:ALA:HB2	1.90	0.54
1:C:285:VAL:HG13	1:C:296:ILE:HD13	1.90	0.54
1:A:276:LYS:HD2	1:A:276:LYS:N	2.12	0.53
1:C:250:LYS:HD3	1:C:295:ALA:CB	2.37	0.53
1:B:15:GLU:OE1	1:D:215:TRP:NE1	2.42	0.53
1:A:210:LEU:HD21	1:B:119:ILE:HG21	1.91	0.53
1:D:10:ILE:HD13	1:D:10:ILE:O	2.08	0.53
1:C:128:LYS:HD2	1:C:128:LYS:C	2.30	0.53
1:A:152:TYR:HB2	1:A:153:LEU:CD1	2.39	0.53
1:C:309:ASN:HB3	1:C:327:ALA:CA	2.38	0.53
1:C:170:GLN:O	1:C:174:GLU:HG3	2.09	0.52
1:D:147:MET:HA	1:D:147:MET:HE2	1.91	0.52
1:B:186:LYS:HD3	1:B:234:ARG:HG2	1.92	0.52
1:A:30:GLU:O	1:A:34:ASN:ND2	2.43	0.52
1:A:12:GLU:HG3	1:A:13:ILE:N	2.25	0.52
1:A:97:LYS:HE3	5:A:1414:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:O	1:C:74:THR:HB	2.09	0.52
1:B:265:ASP:HA	1:B:300:MET:HB3	1.92	0.52
1:D:151:GLN:HG2	5:D:4511:HOH:O	2.10	0.52
1:D:80:ARG:HA	1:D:89:ILE:HD12	1.92	0.51
1:B:128:LYS:O	1:B:128:LYS:CD	2.59	0.51
1:C:165:ARG:HB3	1:D:168:GLU:HG2	1.93	0.51
1:D:152:TYR:C	1:D:153:LEU:HD12	2.31	0.51
1:D:275:PHE:HA	5:D:4446:HOH:O	2.10	0.51
1:C:265:ASP:OD2	1:C:268:HIS:ND1	2.35	0.51
1:D:141:ALA:C	1:D:157:MET:CE	2.79	0.51
1:C:128:LYS:HD2	1:C:128:LYS:O	2.11	0.51
1:A:63:ILE:N	1:A:63:ILE:HD12	2.27	0.50
1:A:8:LEU:HD23	1:B:180:SER:HA	1.92	0.50
1:D:197:ILE:HG23	1:D:258:LEU:HD12	1.93	0.49
1:A:233:LEU:HD11	1:A:249:VAL:HG21	1.95	0.49
1:B:99:ARG:HD2	4:B:2373:SO4:O3	2.13	0.49
1:B:79:LEU:HD23	1:B:338:LEU:HD12	1.94	0.49
1:C:221:VAL:HG22	1:D:13:ILE:HD12	1.94	0.49
1:A:13:ILE:CD1	1:B:221:VAL:HG22	2.42	0.49
1:C:64:HIS:O	1:C:113:MET:HE1	2.12	0.49
1:C:159:TRP:CH2	1:C:161:ALA:HB2	2.47	0.49
1:C:76:LEU:HA	1:C:331:TRP:HH2	1.77	0.49
1:A:23:LEU:HD23	1:A:127:ARG:CZ	2.42	0.49
1:A:334:THR:O	1:A:338:LEU:HD22	2.12	0.49
1:A:294:LYS:HD3	1:A:348:ARG:HD2	1.92	0.49
1:D:8:LEU:HD23	1:D:10:ILE:HD11	1.94	0.49
1:B:52:ASP:OD2	1:B:349:ARG:NH1	2.45	0.49
1:D:186:LYS:HD3	1:D:234:ARG:HG2	1.95	0.49
1:A:13:ILE:HD13	1:B:221:VAL:HG22	1.94	0.49
1:B:248:GLU:HG2	5:B:2580:HOH:O	2.12	0.49
1:B:128:LYS:O	1:B:128:LYS:HD3	2.13	0.48
1:D:46:ILE:HG22	1:D:297:ILE:HG13	1.95	0.48
1:A:153:LEU:N	1:A:153:LEU:HD12	2.27	0.48
1:D:142:GLY:N	1:D:157:MET:CE	2.76	0.48
1:C:159:TRP:CZ3	1:C:161:ALA:HB2	2.48	0.48
1:B:289:ILE:O	1:B:348:ARG:HB2	2.14	0.48
1:D:265:ASP:HA	1:D:300:MET:HB3	1.96	0.48
1:A:60:PRO:HB3	5:A:1471:HOH:O	2.13	0.48
1:C:8:LEU:HG	5:D:4460:HOH:O	2.14	0.47
1:A:225:GLY:O	1:B:9:ARG:HD3	2.14	0.47
1:D:151:GLN:OE1	1:D:214:LYS:CG	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:SER:OG	1:D:8:LEU:HD12	2.15	0.47
1:A:63:ILE:HD13	1:A:94:TYR:N	2.30	0.47
1:A:152:TYR:CB	1:A:153:LEU:HD12	2.45	0.47
1:A:76:LEU:CD2	1:A:89:ILE:HG21	2.45	0.47
1:B:108:ILE:HD11	1:B:153:LEU:HD11	1.96	0.47
1:B:248:GLU:CG	5:B:2580:HOH:O	2.62	0.47
1:C:64:HIS:HB2	1:C:113:MET:CE	2.44	0.47
1:A:158:SER:O	1:A:182:PRO:HD2	2.16	0.46
1:B:244:LYS:O	1:B:248:GLU:HG3	2.14	0.46
1:D:19:PRO:HG3	1:D:152:TYR:CE1	2.50	0.46
1:C:57:VAL:O	1:C:300:MET:HA	2.15	0.46
1:A:186:LYS:HD3	1:A:234:ARG:HG2	1.98	0.46
1:B:98:PRO:HG3	5:B:2546:HOH:O	2.14	0.46
1:C:64:HIS:O	1:C:113:MET:CE	2.64	0.46
1:C:47:LEU:O	1:C:261:GLN:NE2	2.33	0.46
1:D:234:ARG:HD3	1:D:234:ARG:C	2.36	0.46
1:A:303:SER:HA	1:A:328:CYS:HB3	1.98	0.46
1:A:233:LEU:HD23	1:A:262:VAL:HB	1.98	0.46
1:C:310:GLN:O	1:C:324:ILE:HA	2.15	0.46
1:A:19:PRO:HD2	1:A:214:LYS:O	2.16	0.46
1:A:169:SER:OG	1:A:171:VAL:HG13	2.16	0.45
1:A:289:ILE:O	1:A:348:ARG:HB2	2.17	0.45
1:D:183:VAL:O	1:D:229:CYS:HA	2.16	0.45
1:C:242:SER:OG	1:C:245:HIS:ND1	2.48	0.45
1:D:95:PHE:HB3	1:D:108:ILE:HG13	1.98	0.45
1:C:65:ASP:OD1	1:C:67:VAL:HB	2.16	0.45
1:B:128:LYS:HD3	1:B:128:LYS:HA	1.85	0.45
2:B:372:PGA:H22	5:B:2546:HOH:O	2.17	0.45
1:D:196:ALA:O	1:D:200:ILE:HG13	2.16	0.45
1:A:233:LEU:N	1:A:233:LEU:HD22	2.32	0.44
1:C:112:HIS:HB2	1:C:114:ASP:OD1	2.17	0.44
1:C:149:THR:N	1:C:150:PRO:CD	2.79	0.44
1:C:79:LEU:HD23	1:C:338:LEU:CD1	2.47	0.44
1:C:147:MET:CE	1:C:175:LEU:HD22	2.46	0.44
1:D:159:TRP:CZ3	1:D:161:ALA:HB2	2.53	0.44
1:A:332:GLU:HB2	5:A:1503:HOH:O	2.18	0.44
1:B:273:LYS:NZ	1:B:326:ASP:OD1	2.50	0.44
1:B:8:LEU:HD13	5:B:2513:HOH:O	2.16	0.44
1:A:71:GLU:O	1:A:72:TYR:C	2.57	0.43
1:C:151:GLN:HE21	1:C:151:GLN:CA	2.30	0.43
1:C:234:ARG:HD3	1:C:234:ARG:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:TYR:CE2	1:C:76:LEU:HD22	2.37	0.43
1:D:341:LEU:O	1:D:345:VAL:HG23	2.17	0.43
1:C:309:ASN:OD1	1:C:327:ALA:HB2	2.18	0.43
1:B:307:GLU:O	1:B:322:LYS:HE3	2.18	0.43
1:C:151:GLN:HE21	1:C:151:GLN:HA	1.82	0.43
1:D:152:TYR:HB2	1:D:153:LEU:HD13	1.99	0.43
1:C:231:ILE:HG12	1:C:232:ILE:N	2.34	0.43
1:C:36:VAL:HG21	1:C:156:LEU:HA	2.00	0.43
1:A:34:ASN:O	1:A:38:HIS:ND1	2.51	0.43
1:C:289:ILE:HG23	1:C:348:ARG:HD3	2.00	0.43
1:C:79:LEU:HD22	1:C:331:TRP:CZ2	2.54	0.43
1:C:179:LEU:O	1:D:9:ARG:HD2	2.19	0.43
1:D:274:GLN:HG3	1:D:277:LYS:HD2	2.01	0.43
1:A:63:ILE:CD1	1:A:94:TYR:N	2.82	0.43
1:B:277:LYS:HD3	1:B:280:ASP:OD2	2.19	0.43
1:A:307:GLU:HB3	1:A:330:GLY:N	2.34	0.42
1:C:245:HIS:HE1	5:C:3486:HOH:O	2.02	0.42
1:C:58:ILE:HD11	1:C:334:THR:HG23	2.00	0.42
1:A:171:VAL:HG11	1:B:172:HIS:HE1	1.84	0.42
1:A:79:LEU:HD11	1:A:331:TRP:CZ2	2.54	0.42
1:D:186:LYS:HG2	1:D:232:ILE:HB	2.01	0.42
1:B:128:LYS:CD	1:B:128:LYS:C	2.88	0.42
1:B:314:SER:C	1:B:316:GLU:N	2.71	0.42
1:B:273:LYS:NZ	1:B:326:ASP:CG	2.73	0.42
1:C:101:THR:OG1	1:C:102:VAL:N	2.53	0.42
1:B:12:GLU:CD	1:B:14:LYS:HE2	2.40	0.42
1:B:316:GLU:OE1	1:B:316:GLU:HA	2.19	0.42
1:C:108:ILE:HD11	1:C:153:LEU:HD21	2.02	0.42
1:C:333:ASP:OD2	5:C:3484:HOH:O	2.22	0.42
1:A:162:ILE:HG13	1:A:185:PHE:CE2	2.55	0.41
1:B:44:HIS:CE1	1:B:48:LYS:HE2	2.55	0.41
1:C:279:MET:O	1:C:282:CYS:HB3	2.21	0.41
1:B:197:ILE:HG12	1:B:253:LEU:HD23	2.03	0.41
1:B:98:PRO:CG	5:B:2546:HOH:O	2.69	0.41
1:B:104:TRP:CZ3	1:B:324:ILE:HD11	2.55	0.41
1:C:94:TYR:CE1	1:C:142:GLY:HA2	2.55	0.41
1:C:196:ALA:O	1:C:200:ILE:HG13	2.20	0.41
1:B:138:LEU:HA	1:B:139:PRO:HD3	1.96	0.41
1:B:183:VAL:O	1:B:229:CYS:HA	2.20	0.41
1:C:151:GLN:NE2	1:C:151:GLN:HA	2.35	0.41
1:A:46:ILE:HG22	1:A:297:ILE:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:O	1:C:253:LEU:HG	2.20	0.41
1:C:285:VAL:O	1:C:289:ILE:HG13	2.20	0.41
1:D:307:GLU:O	1:D:322:LYS:HE2	2.21	0.41
1:C:107:LEU:HD23	1:C:107:LEU:C	2.41	0.41
1:A:9:ARG:HD2	1:B:179:LEU:O	2.21	0.40
1:B:128:LYS:O	1:B:128:LYS:HD2	2.21	0.40
1:B:338:LEU:HA	1:B:338:LEU:HD23	1.95	0.40
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.87	0.40
1:D:86:GLU:HG2	1:D:346:LYS:HG3	2.03	0.40
1:C:147:MET:HE2	1:C:175:LEU:HD22	2.04	0.40
1:D:141:ALA:HB1	1:D:159:TRP:CE3	2.52	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	335/350 (96%)	322 (96%)	13 (4%)	0	100	100
1	B	341/350 (97%)	334 (98%)	7 (2%)	0	100	100
1	C	335/350 (96%)	319 (95%)	16 (5%)	0	100	100
1	D	336/350 (96%)	324 (96%)	12 (4%)	0	100	100
All	All	1347/1400 (96%)	1299 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	258/283 (91%)	249 (96%)	9 (4%)	36	35
1	B	271/283 (96%)	264 (97%)	7 (3%)	46	48
1	C	255/283 (90%)	242 (95%)	13 (5%)	24	19
1	D	261/283 (92%)	250 (96%)	11 (4%)	30	27
All	All	1045/1132 (92%)	1005 (96%)	40 (4%)	33	31

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	76	LEU
1	A	96	GLU
1	A	171	VAL
1	A	187	ASN
1	A	234	ARG
1	A	276	LYS
1	A	297	ILE
1	A	338	LEU
1	B	15	GLU
1	B	79	LEU
1	B	128	LYS
1	B	187	ASN
1	B	234	ARG
1	B	312	LEU
1	B	318	LEU
1	C	63	ILE
1	C	79	LEU
1	C	86	GLU
1	C	96	GLU
1	C	128	LYS
1	C	153	LEU
1	C	187	ASN
1	C	234	ARG
1	C	274	GLN
1	C	276	LYS
1	C	304	HIS
1	C	316	GLU
1	C	318	LEU
1	D	10	ILE

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Mol	Chain	Res	Type
1	D	70	LYS
1	D	76	LEU
1	D	79	LEU
1	D	189	THR
1	D	233	LEU
1	D	234	ARG
1	D	274	GLN
1	D	303	SER
1	D	312	LEU
1	D	318	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	115	ASN
1	A	151	GLN
1	A	254	ASN
1	A	261	GLN
1	B	34	ASN
1	B	50	ASN
1	C	151	GLN
1	D	254	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z  > 2$
4	SO4	D	4373	-	4,4,4	0.21	0	6,6,6	0.10	0
4	SO4	D	4374	-	4,4,4	0.38	0	6,6,6	0.23	0
4	SO4	A	1374	-	4,4,4	0.35	0	6,6,6	0.14	0
4	SO4	A	1373	-	4,4,4	0.26	0	6,6,6	0.12	0
2	PGA	A	372	3	5,8,8	0.93	0	6,11,11	1.00	0
2	PGA	B	372	3	5,8,8	0.93	0	6,11,11	1.86	3 (50%)
2	PGA	C	372	3	5,8,8	0.71	0	6,11,11	1.00	0
2	PGA	D	372	3	5,8,8	0.89	0	6,11,11	1.15	0
4	SO4	B	2373	-	4,4,4	0.27	0	6,6,6	0.15	0
4	SO4	C	3373	-	4,4,4	0.22	0	6,6,6	0.17	0
4	SO4	B	2374	-	4,4,4	0.41	0	6,6,6	0.25	0
4	SO4	C	3374	-	4,4,4	0.41	0	6,6,6	0.12	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	PGA	C	372	3	-	2/4/6/6	-
2	PGA	D	372	3	-	3/4/6/6	-
2	PGA	A	372	3	-	2/4/6/6	-
2	PGA	B	372	3	-	3/4/6/6	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	PGA	O4P-P-O1P	-2.69	99.58	106.73
2	B	372	PGA	O4P-P-O3P	2.62	117.65	107.64
2	B	372	PGA	O3P-P-O1P	-2.09	101.18	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	372	PGA	C2-O1P-P-O4P
2	B	372	PGA	C2-O1P-P-O3P
2	B	372	PGA	C2-O1P-P-O4P
2	C	372	PGA	C2-O1P-P-O3P
2	C	372	PGA	C2-O1P-P-O4P
2	D	372	PGA	C2-O1P-P-O2P
2	D	372	PGA	C2-O1P-P-O3P
2	D	372	PGA	C2-O1P-P-O4P
2	A	372	PGA	C2-O1P-P-O3P
2	B	372	PGA	C2-O1P-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	372	PGA	1	0
4	B	2373	SO4	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.