



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:53 PM BST

PDB ID : 5ZBN  
Title : Structure of glycolate oxidase without FMN from *Nicotiana benthamiana*  
Authors : Chen, Z.; Liu, Y.  
Deposited on : 2018-02-12  
Resolution : 2.32 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

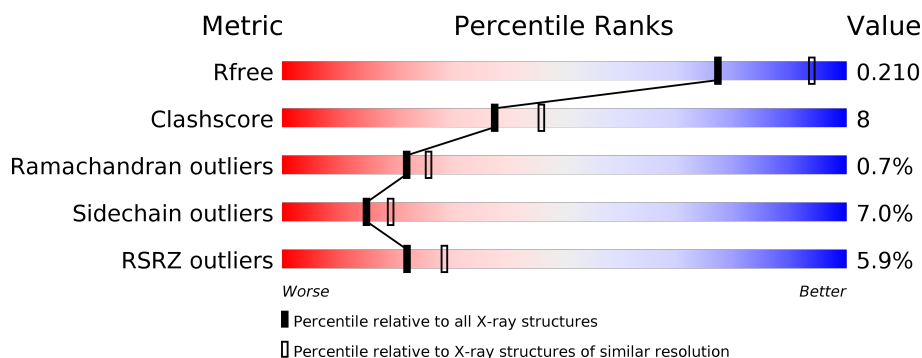
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	371	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	371	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	C	371	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>• 10%</div> </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
2	PO4	A	401	-	-	X	-
2	PO4	C	401	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8438 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 Glycolate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2734	1755	469	498	12			
1	B	347	Total	C	N	O	S	0	0	0
			2618	1677	447	483	11			
1	C	333	Total	C	N	O	S	0	0	0
			2483	1594	421	457	11			

- 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		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

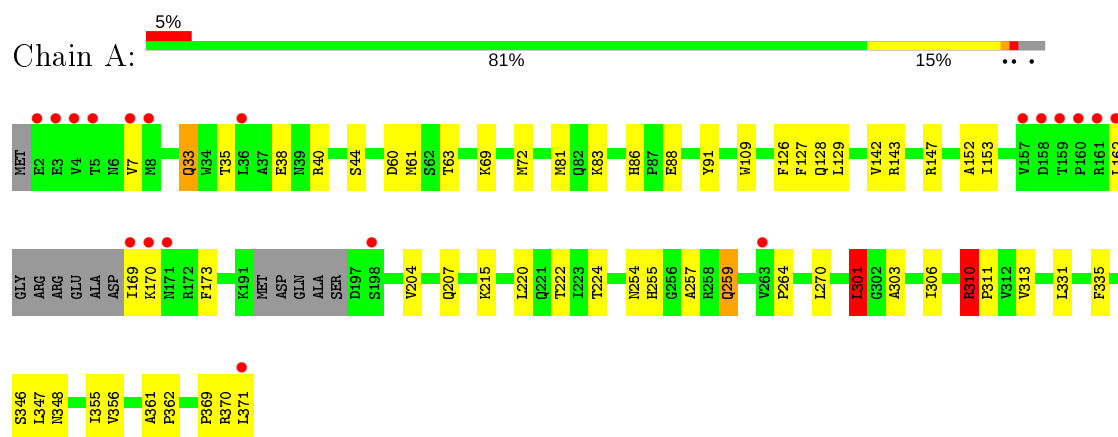
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	193	Total 193	O 193	0	0
3	B	195	Total 195	O 195	0	0
3	C	200	Total 200	O 200	0	0

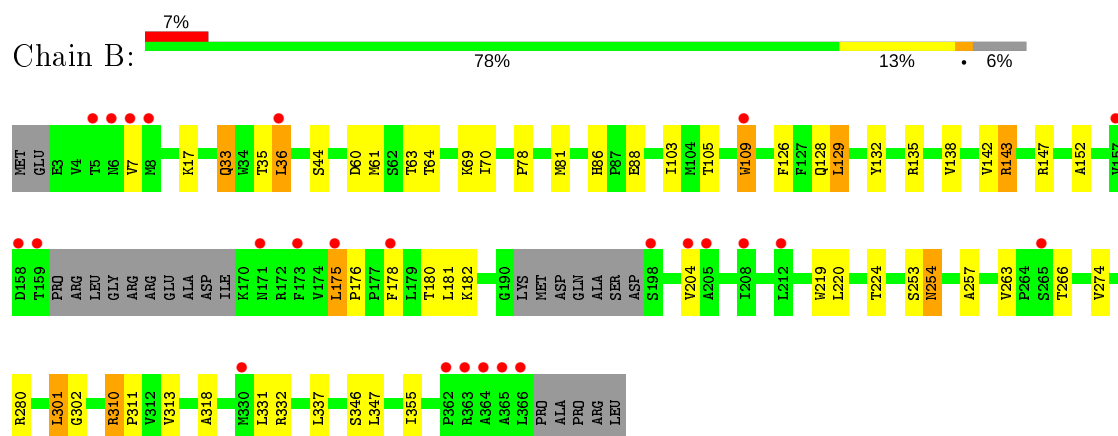
### 3 Residue-property plots

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

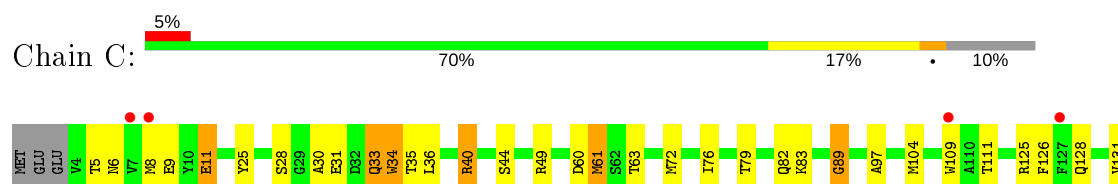
- Molecule 1: Glycolate oxidase

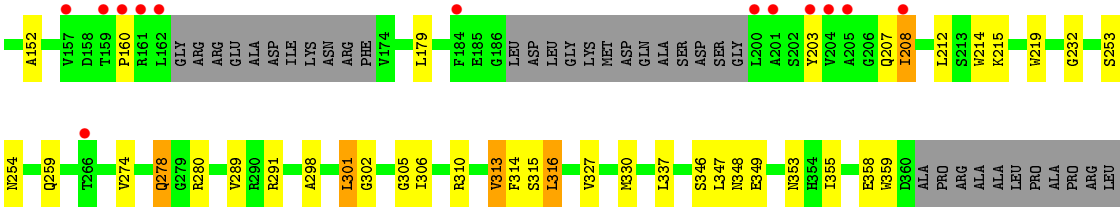


- Molecule 1: Glycolate oxidase



- Molecule 1: Glycolate oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.35Å 145.35Å 156.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.32 49.21 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.32) 98.5 (49.21-2.32)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.215 0.196 , 0.210	Depositor DCC
$R_{free}$ test set	3443 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.387 for -h,k,-l	Xtriage
Reported twinning fraction	0.644 for H, K, L 0.356 for K, H, -L	Depositor
Outliers	0 of 69316 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 ⓘ

### 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	0.50	1/2787 (0.0%)	0.64	2/3776 (0.1%)
1	B	0.49	0/2664	0.65	1/3612 (0.0%)
1	C	0.52	5/2528 (0.2%)	0.64	0/3436
All	All	0.50	6/7979 (0.1%)	0.64	3/10824 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	359	TRP	CD2-CE2	5.41	1.47	1.41
1	C	214	TRP	CD2-CE2	5.16	1.47	1.41
1	A	109	TRP	CD2-CE2	5.15	1.47	1.41
1	C	34	TRP	CD2-CE2	5.06	1.47	1.41
1	C	219	TRP	CD2-CE2	5.05	1.47	1.41
1	C	109	TRP	CD2-CE2	5.00	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	310	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	301	LEU	CA-CB-CG	5.21	127.30	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	PRO	Peptide

## 5.2 Too-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 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	2734	0	2771	37	0
1	B	2618	0	2630	38	0
1	C	2483	0	2451	49	0
2	A	5	0	0	2	0
2	B	5	0	0	1	0
2	C	5	0	0	2	0
3	A	193	0	0	5	0
3	B	195	0	0	4	0
3	C	200	0	0	5	0
All	All	8438	0	7852	121	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 8.

All (121) 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:79:THR:HB	3:C:518:HOH:O	1.57	1.04
1:C:33:GLN:HE21	1:C:33:GLN:HA	1.35	0.89
1:A:127[B]:PHE:CZ	1:A:153:ILE:HD13	2.12	0.84
1:A:310:ARG:HD3	2:A:401:PO4:O1	1.77	0.84
1:B:310:ARG:HD3	2:B:401:PO4:O4	1.77	0.83
1:C:298:ALA:CB	1:C:306:ILE:HD11	2.10	0.82
1:C:33:GLN:HE22	1:C:259:GLN:H	1.25	0.82
1:A:127[B]:PHE:CE2	1:A:153:ILE:HD13	2.15	0.82
1:A:86:HIS:HD2	1:A:88:GLU:H	1.35	0.73
1:B:109:TRP:CZ3	1:B:132:TYR:OH	2.42	0.72
1:B:181:LEU:HD13	1:B:204:VAL:HG21	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:HIS:CD2	1:A:88:GLU:H	2.08	0.71
1:B:86:HIS:HD2	1:B:88:GLU:H	1.39	0.71
1:B:109:TRP:CH2	1:B:132:TYR:OH	2.43	0.71
1:C:291:ARG:NH1	3:C:501:HOH:O	2.23	0.70
1:C:33:GLN:HE21	1:C:33:GLN:CA	2.02	0.70
1:A:61:MET:HE2	1:A:72:MET:HB3	1.76	0.68
1:C:79:THR:HG21	1:C:313:VAL:HG22	1.76	0.67
1:A:127[B]:PHE:CZ	1:A:153:ILE:CD1	2.77	0.67
1:A:63:THR:HB	1:A:347:LEU:HD12	1.78	0.64
1:C:33:GLN:NE2	1:C:33:GLN:HA	2.08	0.64
1:C:8:MET:O	1:C:11:GLU:HB2	1.98	0.64
1:B:36:LEU:H	1:B:36:LEU:HD23	1.63	0.64
1:A:33:GLN:HB3	1:A:257:ALA:HA	1.80	0.62
1:A:61:MET:HE2	1:A:72:MET:CB	2.29	0.62
1:B:109:TRP:HH2	1:B:132:TYR:HH	1.42	0.62
1:C:301:LEU:HD13	1:C:355:ILE:HD11	1.82	0.62
1:C:310:ARG:HD3	2:C:401:PO4:O1	2.00	0.62
1:A:259:GLN:HA	1:A:259:GLN:HE21	1.65	0.60
1:B:17:LYS:HD2	1:B:318:ALA:HA	1.83	0.60
1:C:36:LEU:CB	3:C:567:HOH:O	2.49	0.60
1:B:86:HIS:CD2	1:B:88:GLU:H	2.20	0.60
1:C:358:GLU:CG	3:C:605:HOH:O	2.49	0.60
1:C:298:ALA:HB1	1:C:306:ILE:HD11	1.83	0.60
1:A:207:GLN:HB3	3:A:610:HOH:O	2.02	0.59
1:A:301:LEU:HD13	1:A:355:ILE:HD11	1.84	0.59
1:B:147:ARG:HD3	3:B:506:HOH:O	2.04	0.57
1:B:301:LEU:HD13	1:B:355:ILE:HD11	1.86	0.57
1:A:169:ILE:HG13	1:A:170:LYS:H	1.70	0.57
1:B:176:PRO:HB2	1:B:178:PHE:CE1	2.39	0.57
1:B:78:PRO:HD3	1:B:105:THR:HB	1.87	0.57
1:C:33:GLN:NE2	1:C:259:GLN:H	2.01	0.57
1:B:280:ARG:HD3	1:C:280:ARG:CZ	2.36	0.56
1:A:371:LEU:HG	3:A:575:HOH:O	2.05	0.56
1:C:298:ALA:HB3	1:C:306:ILE:HD11	1.86	0.56
1:A:61:MET:CE	1:A:72:MET:CB	2.85	0.55
1:A:142:VAL:HG11	1:A:224:THR:HB	1.87	0.55
1:C:104:MET:HG2	1:C:125:ARG:HG2	1.88	0.55
1:A:301:LEU:HD13	1:A:355:ILE:CD1	2.37	0.55
1:A:61:MET:HE1	1:A:335:PHE:HD2	1.71	0.54
1:C:33:GLN:HE22	1:C:259:GLN:N	2.01	0.53
1:A:61:MET:CE	1:A:72:MET:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HA	1:B:310:ARG:NH2	2.24	0.53
1:A:69:LYS:HE2	3:A:630:HOH:O	2.08	0.53
1:C:83:LYS:HD2	1:C:179:LEU:HD22	1.91	0.52
1:C:203:TYR:O	1:C:207:GLN:HB2	2.10	0.51
1:A:63:THR:HB	1:A:347:LEU:CD1	2.41	0.51
1:C:126:PHE:CD1	1:C:152:ALA:HB3	2.46	0.51
1:B:70:ILE:HG21	1:B:103:ILE:HG13	1.93	0.51
1:C:61:MET:HG2	1:C:72:MET:HB3	1.93	0.51
1:C:289:VAL:HG11	1:C:306:ILE:HG21	1.94	0.50
1:A:60:ASP:O	1:A:346:SER:HA	2.13	0.49
1:B:86:HIS:CD2	1:B:88:GLU:HB2	2.47	0.49
1:C:63:THR:HB	1:C:347:LEU:HD12	1.95	0.49
1:C:25:TYR:CE2	1:C:30:ALA:HB2	2.48	0.49
1:B:63:THR:HB	1:B:347:LEU:HD12	1.95	0.49
1:A:310:ARG:CD	2:A:401:PO4:O1	2.57	0.49
1:B:142:VAL:HG11	1:B:224:THR:HB	1.95	0.48
1:B:64:THR:HG22	3:B:548:HOH:O	2.13	0.48
1:B:280:ARG:HD3	1:C:280:ARG:NH2	2.29	0.48
1:B:109:TRP:HZ3	1:B:132:TYR:HH	1.55	0.48
1:B:60:ASP:O	1:B:346:SER:HA	2.13	0.48
1:A:126:PHE:CD1	1:A:152:ALA:HB3	2.49	0.47
1:B:274:VAL:HG11	1:B:302:GLY:HA3	1.96	0.47
1:B:266:THR:HG22	3:B:580:HOH:O	2.14	0.47
1:C:89:GLY:HA2	1:C:316:LEU:HD11	1.96	0.47
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.80	0.47
1:C:315:SER:HB3	1:C:327:VAL:HG21	1.97	0.46
1:C:31:GLU:HG3	1:C:33:GLN:HB2	1.96	0.46
1:B:33:GLN:HB3	1:B:257:ALA:HA	1.97	0.46
1:A:38:GLU:OE2	1:A:255:HIS:ND1	2.48	0.46
1:C:49:ARG:HD3	1:C:353:ASN:O	2.16	0.46
1:C:76:ILE:HD12	1:C:97:ALA:HB2	1.97	0.46
1:A:7:VAL:HG13	1:A:311:PRO:HB3	1.98	0.46
1:A:81:MET:HE1	1:A:173:PHE:CE2	2.51	0.46
1:C:40:ARG:NH1	3:C:502:HOH:O	2.44	0.46
1:C:310:ARG:HB3	1:C:314:PHE:CE2	2.51	0.45
1:C:232:GLY:HA2	1:C:253:SER:O	2.17	0.45
3:B:643:HOH:O	1:C:278:GLN:HG2	2.17	0.45
1:A:61:MET:CE	1:A:72:MET:HB3	2.44	0.45
1:C:131:VAL:HB	1:C:212:LEU:HD21	1.98	0.44
1:C:208:ILE:HG13	1:C:208:ILE:H	1.54	0.44
1:C:310:ARG:CD	2:C:401:PO4:O1	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:VAL:HG11	1:C:302:GLY:HA3	1.99	0.44
1:B:126:PHE:CD1	1:B:152:ALA:HB3	2.53	0.43
1:C:79:THR:HG23	1:C:82:GLN:HE21	1.83	0.43
1:C:79:THR:CG2	1:C:82:GLN:HE21	2.31	0.43
1:C:60:ASP:O	1:C:346:SER:HA	2.19	0.43
1:B:7:VAL:CG1	1:B:311:PRO:HB3	2.48	0.43
1:A:88:GLU:O	1:A:91:TYR:HB2	2.19	0.42
1:A:147:ARG:HD2	3:A:584:HOH:O	2.20	0.42
1:C:305:GLY:O	1:C:306:ILE:HD12	2.19	0.42
1:B:61:MET:HE1	1:B:332:ARG:HG3	2.01	0.42
1:B:181:LEU:HD13	1:B:204:VAL:CG2	2.47	0.42
1:C:298:ALA:HB3	1:C:306:ILE:CD1	2.48	0.42
1:C:79:THR:CG2	1:C:82:GLN:NE2	2.83	0.42
1:A:83:LYS:NZ	3:A:502:HOH:O	2.44	0.41
1:B:129:LEU:HD11	1:B:138:VAL:HG13	2.02	0.41
1:B:132:TYR:H	1:B:138:VAL:CG2	2.34	0.41
1:B:109:TRP:HZ3	1:B:132:TYR:OH	1.96	0.41
1:B:81:MET:SD	1:B:175:LEU:HD13	2.60	0.41
1:B:253:SER:O	1:B:254:ASN:HB2	2.20	0.41
1:C:5:THR:N	1:C:9:GLU:OE1	2.50	0.41
1:B:135:ARG:HD2	1:B:219:TRP:CH2	2.55	0.41
1:A:361:ALA:HA	1:A:362:PRO:HD3	1.91	0.41
1:B:86:HIS:HD2	1:B:88:GLU:HB2	1.86	0.40
1:A:81:MET:CE	1:A:173:PHE:CE2	3.05	0.40
1:C:28:SER:HA	1:C:34:TRP:HB2	2.03	0.40
1:C:6:ASN:ND2	1:C:8:MET:HB2	2.36	0.40
1:A:222:THR:O	1:B:143:ARG:HD2	2.21	0.40
1:A:270:LEU:HD11	1:A:303:ALA:HB2	2.04	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	354/371 (95%)	345 (98%)	6 (2%)	3 (1%)	19	23
1	B	341/371 (92%)	329 (96%)	11 (3%)	1 (0%)	41	50
1	C	327/371 (88%)	312 (95%)	12 (4%)	3 (1%)	17	19
All	All	1022/1113 (92%)	986 (96%)	29 (3%)	7 (1%)	22	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	ARG
1	C	160	PRO
1	B	254	ASN
1	C	254	ASN
1	A	264	PRO
1	C	89	GLY
1	A	254	ASN

### 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	276/298 (93%)	257 (93%)	19 (7%)	15	20
1	B	265/298 (89%)	247 (93%)	18 (7%)	16	20
1	C	245/298 (82%)	227 (93%)	18 (7%)	14	17
All	All	786/894 (88%)	731 (93%)	55 (7%)	15	19

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	35	THR
1	A	40	ARG
1	A	44	SER
1	A	128	GLN
1	A	129	LEU

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Mol	Chain	Res	Type
1	A	143	ARG
1	A	162	LEU
1	A	204	VAL
1	A	215	LYS
1	A	220	LEU
1	A	259	GLN
1	A	301	LEU
1	A	306	ILE
1	A	310	ARG
1	A	313	VAL
1	A	331	LEU
1	A	348	ASN
1	A	356	VAL
1	B	33	GLN
1	B	35	THR
1	B	36	LEU
1	B	44	SER
1	B	69	LYS
1	B	109	TRP
1	B	128	GLN
1	B	129	LEU
1	B	143	ARG
1	B	175	LEU
1	B	180	THR
1	B	182	LYS
1	B	220	LEU
1	B	263	VAL
1	B	301	LEU
1	B	313	VAL
1	B	331	LEU
1	B	337	LEU
1	C	11	GLU
1	C	33	GLN
1	C	35	THR
1	C	40	ARG
1	C	44	SER
1	C	61	MET
1	C	111	THR
1	C	128	GLN
1	C	208	ILE
1	C	215	LYS
1	C	278	GLN

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Mol	Chain	Res	Type
1	C	301	LEU
1	C	313	VAL
1	C	316	LEU
1	C	330	MET
1	C	337	LEU
1	C	348	ASN
1	C	349	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	86	HIS
1	A	221	GLN
1	A	259	GLN
1	B	33	GLN
1	B	86	HIS
1	B	128	GLN
1	B	218	GLN
1	B	221	GLN
1	C	6	ASN
1	C	33	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

3 ligands are modelled in this entry.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	B	401	-	4,4,4	1.23	0	6,6,6	1.06	0
2	PO4	A	401	-	4,4,4	1.13	0	6,6,6	0.97	0
2	PO4	C	401	-	4,4,4	1.08	0	6,6,6	0.98	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PO4	1	0
2	A	401	PO4	2	0
2	C	401	PO4	2	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	359/371 (96%)	0.31	19 (5%)	26 33	15, 28, 65, 122	0
1	B	347/371 (93%)	0.37	25 (7%)	15 20	16, 29, 64, 110	0
1	C	333/371 (89%)	0.28	17 (5%)	28 35	17, 28, 57, 87	1 (0%)
All	All	1039/1113 (93%)	0.32	61 (5%)	22 29	15, 28, 64, 122	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	PHE	8.2
1	C	162	LEU	7.5
1	C	204	VAL	6.6
1	B	366	LEU	6.0
1	A	161	ARG	5.8
1	B	364	ALA	5.8
1	A	160	PRO	5.4
1	A	3	GLU	5.3
1	B	158	ASP	5.0
1	C	7	VAL	5.0
1	A	162	LEU	5.0
1	C	205	ALA	4.8
1	C	157	VAL	4.7
1	A	2	GLU	4.5
1	C	8	MET	4.3
1	A	171	ASN	4.2
1	B	365	ALA	4.1
1	B	36	LEU	4.1
1	C	200	LEU	4.1
1	C	160	PRO	4.0
1	A	5	THR	4.0
1	A	159	THR	3.9
1	B	362	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	159	THR	3.9
1	B	7	VAL	3.8
1	A	4	VAL	3.6
1	A	169	ILE	3.4
1	B	8	MET	3.4
1	B	171	ASN	3.2
1	A	7	VAL	3.1
1	C	208	ILE	3.1
1	B	157	VAL	3.1
1	C	184	PHE	3.0
1	A	157	VAL	3.0
1	B	208	ILE	3.0
1	B	159	THR	2.9
1	C	203	TYR	2.9
1	C	266	THR	2.8
1	A	8	MET	2.7
1	B	175	LEU	2.7
1	B	6	ASN	2.7
1	C	109	TRP	2.7
1	B	363	ARG	2.6
1	A	36	LEU	2.6
1	A	198	SER	2.6
1	B	265	SER	2.5
1	B	173	PHE	2.5
1	C	127	PHE	2.5
1	A	158	ASP	2.5
1	A	371	LEU	2.4
1	B	212	LEU	2.4
1	A	170	LYS	2.4
1	C	201	ALA	2.3
1	B	5	THR	2.3
1	B	109	TRP	2.2
1	B	330	MET	2.1
1	A	263	VAL	2.1
1	B	205	ALA	2.1
1	B	198	SER	2.1
1	C	161	ARG	2.1
1	B	204	VAL	2.1

## 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 [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	401	5/5	0.98	0.15	19,20,22,22	0
2	PO4	A	401	5/5	0.98	0.14	19,20,21,21	0
2	PO4	C	401	5/5	0.99	0.13	17,17,18,18	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.