



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:03 pm GMT

PDB ID : 1OX4  
Title : TOWARDS UNDERSTANDING THE MECHANISM OF THE COM-  
PLEX CYCLIZATION REACTION CATALYZED BY IMIDAZOLE GLYC-  
EROPHOSPHATE SYNTHASE  
Authors : Chaudhuri, B.N.; Smith, J.L.  
Deposited on : 2003-04-01  
Resolution : 2.50 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

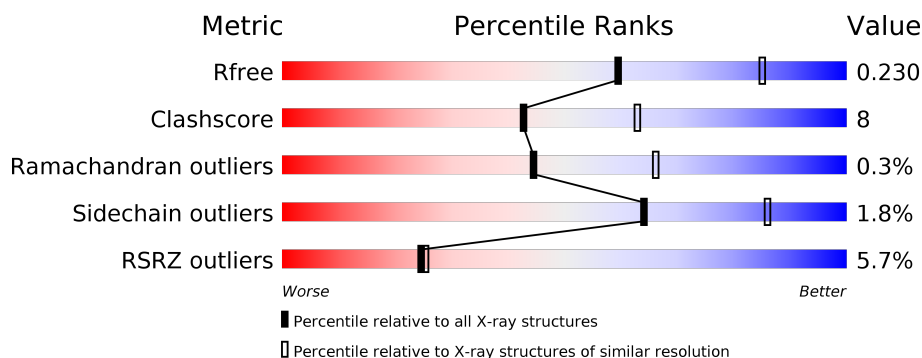
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	555	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div></div> </div> <div></div> </div>
2	B	555	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8572 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 Imidazole glycerol phosphate synthase hisHF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4148	2640	694	799	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	CLONING ARTIFACT	UNP P33734
A	-2	SER	-	CLONING ARTIFACT	UNP P33734
A	-1	HIS	-	CLONING ARTIFACT	UNP P33734

- Molecule 2 is a protein called Imidazole glycerol phosphate synthase hisHF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	538	Total	C	N	O	S	0	0	0
			4194	2668	702	809	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	CLONING ARTIFACT	UNP P33734
B	-2	SER	-	CLONING ARTIFACT	UNP P33734
B	-1	HIS	-	CLONING ARTIFACT	UNP P33734
B	83	CYD	CYS	MODIFIED RESIDUE	UNP P33734

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

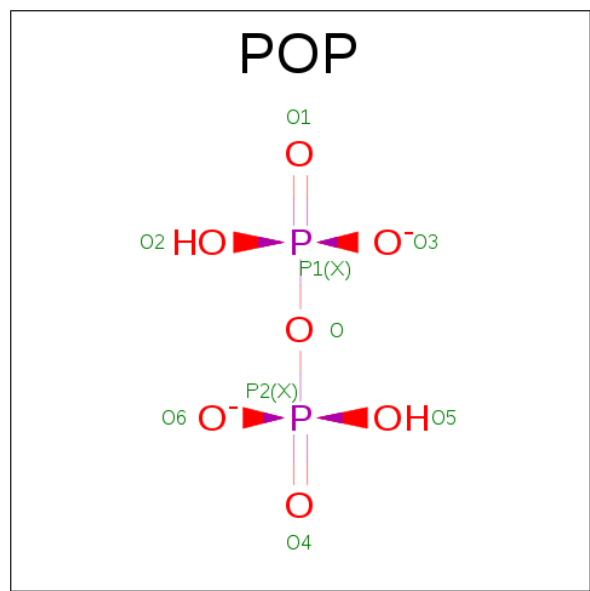


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ni	0	0
			1	1		
4	A	1	Total	Ni	0	0
			1	1		

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		
5	B	1	Total	O	P	0	0
			9	7	2		

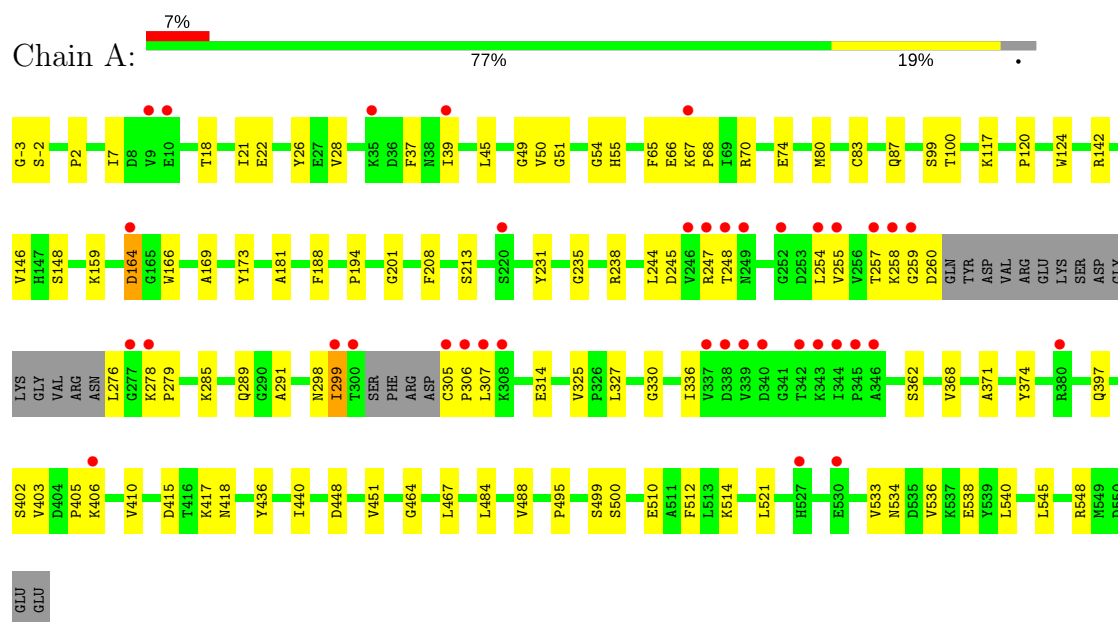
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total	O	0	0
			98	98		
6	B	92	Total	O	0	0
			92	92		

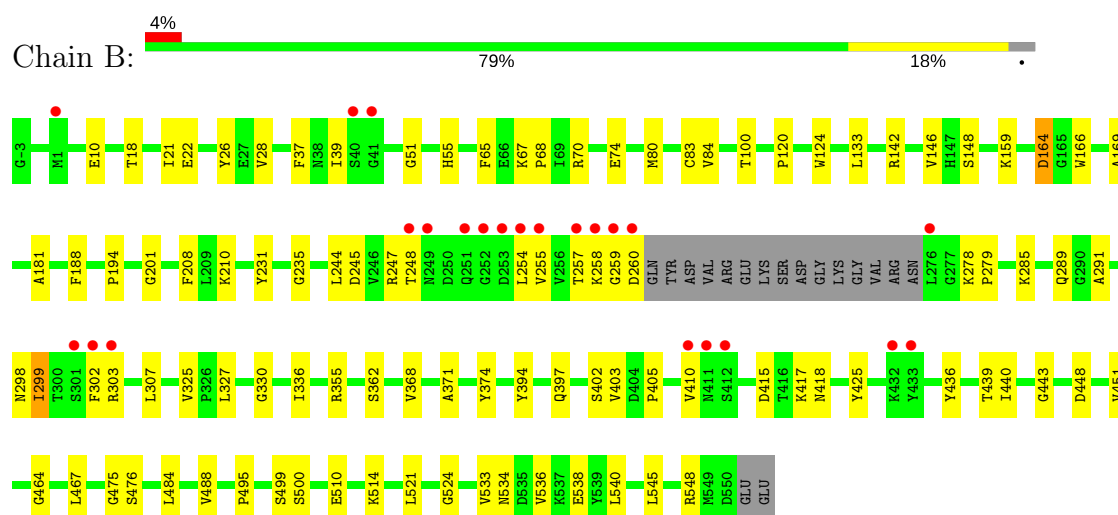
### 3 Residue-property plots [i](#)

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

- Molecule 1: Imidazole glycerol phosphate synthase hisHF



- Molecule 2: Imidazole glycerol phosphate synthase hisHF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.50Å 112.00Å 115.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 73.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.50) 99.7 (73.96-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.53 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.260 0.229 , 0.230	Depositor DCC
$R_{free}$ test set	2255 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: NI, SO4, POP, CYD

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	0.36	0/4235	0.59	0/5729
2	B	0.37	0/4266	0.60	0/5770
All	All	0.37	0/8501	0.60	0/11499

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4148	0	4093	64	1
2	B	4194	0	4132	67	1
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	9	0	0	0	0
5	B	9	0	0	2	0
6	A	98	0	0	2	0
6	B	92	0	0	1	0
All	All	8572	0	8225	129	1



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (129) 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)
2:B:403:VAL:HG12	2:B:405:PRO:HD3	1.57	0.85
2:B:83:CYD:H32	2:B:84:VAL:HG22	1.58	0.85
1:A:403:VAL:HG12	1:A:405:PRO:HD3	1.57	0.84
1:A:278:LYS:HB2	1:A:279:PRO:HD3	1.72	0.70
2:B:278:LYS:HB2	2:B:279:PRO:HD3	1.75	0.69
2:B:21:ILE:HG22	2:B:26:TYR:HB2	1.79	0.65
1:A:21:ILE:HG22	1:A:26:TYR:HB2	1.81	0.63
2:B:83:CYD:H32	2:B:84:VAL:CG2	2.30	0.62
2:B:307:LEU:HD22	2:B:336:ILE:HD11	1.83	0.61
2:B:510:GLU:HG3	2:B:514:LYS:HD2	1.83	0.60
1:A:307:LEU:HD22	1:A:336:ILE:HD11	1.83	0.59
1:A:464:GLY:O	1:A:495:PRO:HD2	2.02	0.59
2:B:464:GLY:O	2:B:495:PRO:HD2	2.04	0.58
1:A:510:GLU:HG3	1:A:514:LYS:HD2	1.84	0.58
1:A:405:PRO:HB2	1:A:436:TYR:HB3	1.89	0.55
2:B:257:THR:HB	2:B:260:ASP:OD2	2.07	0.54
1:A:257:THR:HB	1:A:260:ASP:OD2	2.07	0.54
2:B:403:VAL:HG11	2:B:451:VAL:HG23	1.89	0.54
2:B:405:PRO:HB2	2:B:436:TYR:HB3	1.88	0.54
1:A:-3:GLY:HA3	2:B:425:TYR:CE2	2.43	0.53
1:A:499:SER:O	1:A:500:SER:HB2	2.06	0.53
2:B:146:VAL:O	2:B:146:VAL:HG13	2.08	0.53
1:A:146:VAL:HG13	1:A:146:VAL:O	2.09	0.53
2:B:231:TYR:HA	2:B:235:GLY:HA2	1.91	0.53
2:B:80:MET:HA	2:B:188:PHE:O	2.08	0.53
1:A:231:TYR:HA	1:A:235:GLY:HA2	1.91	0.53
2:B:146:VAL:CG2	2:B:397:GLN:HB2	2.39	0.52
2:B:18:THR:HG22	2:B:28:VAL:HG11	1.91	0.52
1:A:124:TRP:CE3	1:A:548:ARG:HD2	2.44	0.52
1:A:247:ARG:O	1:A:254:LEU:HA	2.09	0.52
2:B:70:ARG:O	2:B:74:GLU:HG3	2.09	0.52
1:A:70:ARG:O	1:A:74:GLU:HG3	2.09	0.52
2:B:499:SER:O	2:B:500:SER:HB2	2.08	0.52
1:A:521:LEU:C	1:A:521:LEU:HD23	2.30	0.52
2:B:291:ALA:HA	2:B:533:VAL:HG11	1.92	0.52
2:B:245:ASP:HB3	2:B:299:ILE:HD11	1.92	0.52
1:A:325:VAL:O	1:A:327:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:VAL:HG22	2:B:397:GLN:HB2	1.91	0.52
1:A:403:VAL:HG11	1:A:451:VAL:HG23	1.92	0.52
2:B:247:ARG:O	2:B:254:LEU:HA	2.10	0.52
1:A:245:ASP:HB3	1:A:299:ILE:HD11	1.92	0.51
2:B:285:LYS:O	2:B:289:GLN:HG3	2.10	0.51
1:A:169:ALA:HB3	1:A:181:ALA:HB3	1.93	0.51
2:B:169:ALA:HB3	2:B:181:ALA:HB3	1.93	0.51
1:A:285:LYS:O	1:A:289:GLN:HG3	2.11	0.51
2:B:371:ALA:O	2:B:374:TYR:HB3	2.12	0.50
1:A:18:THR:HG22	1:A:28:VAL:HG11	1.93	0.49
1:A:417:LYS:HE2	1:A:448:ASP:OD2	2.13	0.49
1:A:54:GLY:HA2	1:A:99:SER:OG	2.13	0.49
2:B:521:LEU:C	2:B:521:LEU:HD23	2.32	0.49
2:B:325:VAL:O	2:B:327:LEU:HD12	2.11	0.49
1:A:2:PRO:HB3	2:B:476:SER:HB2	1.95	0.49
2:B:451:VAL:HG12	6:B:1006:HOH:O	2.12	0.49
1:A:330:GLY:HA3	1:A:362:SER:HB3	1.95	0.48
1:A:371:ALA:O	1:A:374:TYR:HB3	2.13	0.48
2:B:248:THR:HG21	2:B:302:PHE:CD1	2.48	0.48
2:B:51:GLY:HA2	2:B:394:TYR:O	2.13	0.47
2:B:248:THR:HG21	2:B:302:PHE:CE1	2.49	0.47
1:A:164:ASP:HB3	1:A:166:TRP:HD1	1.79	0.47
2:B:417:LYS:HE2	2:B:448:ASP:OD2	2.15	0.47
1:A:417:LYS:HG3	1:A:418:ASN:N	2.30	0.47
2:B:164:ASP:HB3	2:B:166:TRP:HD1	1.80	0.47
2:B:303:ARG:HH11	2:B:303:ARG:HG3	1.79	0.47
1:A:540:LEU:HD22	1:A:545:LEU:HD12	1.97	0.47
1:A:291:ALA:HA	1:A:533:VAL:HG11	1.97	0.46
2:B:475:GLY:HA2	5:B:999:POP:O2	2.15	0.46
2:B:67:LYS:HB2	2:B:68:PRO:HD3	1.98	0.46
2:B:534:ASN:O	2:B:538:GLU:HG2	2.16	0.46
2:B:124:TRP:HB3	2:B:142:ARG:HB3	1.97	0.45
1:A:276:LEU:HD11	1:A:314:GLU:HG3	1.98	0.45
1:A:146:VAL:CG2	1:A:397:GLN:HB2	2.46	0.45
2:B:327:LEU:HD12	2:B:327:LEU:N	2.32	0.45
2:B:540:LEU:HD22	2:B:545:LEU:HD12	1.99	0.45
2:B:417:LYS:HG3	2:B:418:ASN:N	2.31	0.45
1:A:124:TRP:HB3	1:A:142:ARG:HB3	1.99	0.45
1:A:194:PRO:O	1:A:201:GLY:HA3	2.16	0.45
1:A:67:LYS:HB2	1:A:68:PRO:HD3	1.98	0.45
1:A:80:MET:HA	1:A:188:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LYS:O	2:B:258:LYS:HG2	2.17	0.44
1:A:21:ILE:CG2	1:A:26:TYR:HB2	2.48	0.44
1:A:49:GLY:O	1:A:83:CYS:HB3	2.17	0.44
2:B:330:GLY:HA3	2:B:362:SER:HB3	1.99	0.44
1:A:327:LEU:HD12	1:A:327:LEU:N	2.33	0.43
2:B:524:GLY:HA3	5:B:999:POP:O1	2.18	0.43
1:A:117:LYS:HE3	1:A:173:TYR:O	2.18	0.43
1:A:436:TYR:CD2	1:A:484:LEU:HD13	2.54	0.43
1:A:484:LEU:O	1:A:488:VAL:HG23	2.18	0.43
1:A:258:LYS:O	1:A:258:LYS:HG2	2.17	0.43
2:B:436:TYR:CD2	2:B:484:LEU:HD13	2.54	0.43
1:A:402:SER:HA	1:A:467:LEU:HB3	2.00	0.43
1:A:80:MET:HB2	1:A:208:PHE:CZ	2.54	0.43
1:A:66:GLU:HB3	6:A:1020:HOH:O	2.17	0.43
2:B:21:ILE:CG2	2:B:26:TYR:HB2	2.48	0.43
1:A:120:PRO:HB3	1:A:148:SER:OG	2.19	0.43
2:B:83:CYD:HN11	2:B:397:GLN:HE22	1.66	0.43
2:B:124:TRP:CE3	2:B:548:ARG:HD2	2.54	0.43
1:A:213:SER:HB3	6:A:1027:HOH:O	2.20	0.42
1:A:534:ASN:O	1:A:538:GLU:HG2	2.20	0.42
1:A:255:VAL:HG12	1:A:278:LYS:HD2	2.00	0.42
1:A:330:GLY:CA	1:A:362:SER:HB3	2.49	0.42
2:B:120:PRO:HB3	2:B:148:SER:OG	2.20	0.42
2:B:255:VAL:HG12	2:B:278:LYS:HD2	2.02	0.42
1:A:65:PHE:C	1:A:68:PRO:HD2	2.40	0.42
2:B:410:VAL:HB	2:B:415:ASP:HB2	2.02	0.42
1:A:305:CYS:HA	1:A:306:PRO:HD3	1.73	0.41
2:B:65:PHE:C	2:B:68:PRO:HD2	2.40	0.41
1:A:248:THR:HG22	1:A:254:LEU:HD12	2.02	0.41
1:A:50:VAL:HG12	1:A:51:GLY:N	2.35	0.41
1:A:7:ILE:HG13	1:A:45:LEU:HD11	2.01	0.41
2:B:10:GLU:HA	2:B:355:ARG:HH12	1.85	0.41
2:B:194:PRO:O	2:B:201:GLY:HA3	2.19	0.41
2:B:484:LEU:O	2:B:488:VAL:HG23	2.19	0.41
2:B:22:GLU:HA	2:B:26:TYR:O	2.20	0.41
1:A:536:VAL:O	1:A:540:LEU:HG	2.20	0.41
2:B:248:THR:HG22	2:B:254:LEU:HD12	2.01	0.41
2:B:402:SER:HA	2:B:467:LEU:HB3	2.03	0.41
1:A:368:VAL:HG21	1:A:440:ILE:HG22	2.01	0.41
2:B:368:VAL:HG21	2:B:440:ILE:HG22	2.03	0.41
1:A:410:VAL:HB	1:A:415:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:THR:HG22	1:A:259:GLY:H	1.85	0.41
1:A:83:CYS:O	1:A:87:GLN:HG3	2.20	0.41
2:B:257:THR:HG22	2:B:259:GLY:H	1.85	0.41
2:B:536:VAL:O	2:B:540:LEU:HG	2.21	0.41
1:A:22:GLU:HA	1:A:26:TYR:O	2.21	0.40
2:B:133:LEU:HD23	2:B:133:LEU:HA	1.90	0.40
2:B:80:MET:HB2	2:B:208:PHE:CZ	2.57	0.40
1:A:238:ARG:HB3	1:A:512:PHE:CE2	2.57	0.40
2:B:439:THR:OG1	2:B:443:GLY:HA2	2.21	0.40
2:B:83:CYD:HB2	2:B:84:VAL:H	1.63	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:NZ	2:B:210:LYS:O[1_545]	2.19	0.01

## 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	528/555 (95%)	508 (96%)	18 (3%)	2 (0%)	38	59
2	B	533/555 (96%)	513 (96%)	19 (4%)	1 (0%)	51	73
All	All	1061/1110 (96%)	1021 (96%)	37 (4%)	3 (0%)	44	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	39	ILE
2	B	39	ILE

### 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	448/467 (96%)	440 (98%)	8 (2%)	64	86
2	B	451/466 (97%)	443 (98%)	8 (2%)	64	86
All	All	899/933 (96%)	883 (98%)	16 (2%)	64	86

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	55	HIS
1	A	100	THR
1	A	159	LYS
1	A	164	ASP
1	A	244	LEU
1	A	298	ASN
1	A	299	ILE
2	B	37	PHE
2	B	55	HIS
2	B	100	THR
2	B	159	LYS
2	B	164	ASP
2	B	244	LEU
2	B	298	ASN
2	B	299	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
2	B	298	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	CYD	B	83	2	10,15,16	1.41	1 (10%)	8,18,20	2.81	1 (12%)

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	CYD	B	83	2	-	0/11/17/19	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	CYD	O1-C2	3.87	1.28	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	83	CYD	CA-CB-SG	7.38	131.47	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	83	CYD	4	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	SO4	A	801	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	A	806	-	4,4,4	0.39	0	6,6,6	0.09	0
5	POP	A	998	-	8,8,8	1.16	0	8,13,13	1.62	3 (37%)
3	SO4	B	803	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	B	804	-	4,4,4	0.37	0	6,6,6	0.09	0
5	POP	B	999	-	8,8,8	1.42	0	8,13,13	1.63	3 (37%)

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	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	SO4	A	806	-	-	0/0/0/0	0/0/0/0
5	POP	A	998	-	-	0/6/6/6	0/0/0/0
3	SO4	B	803	-	-	0/0/0/0	0/0/0/0
3	SO4	B	804	-	-	0/0/0/0	0/0/0/0
5	POP	B	999	-	-	0/6/6/6	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	999	POP	O5-P2-O4	-2.68	100.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	998	POP	O5-P2-O4	-2.50	100.72	110.50
5	A	998	POP	O6-P2-O4	2.48	120.20	110.50
5	B	999	POP	O-P2-O4	2.50	126.84	111.44
5	B	999	POP	O6-P2-O4	2.51	120.34	110.50
5	A	998	POP	O-P2-O4	2.65	127.71	111.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	999	POP	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	534/555 (96%)	0.32	38 (7%) 17 17	17, 36, 59, 81	0
2	B	537/555 (96%)	0.28	23 (4%) 36 38	18, 35, 59, 82	0
All	All	1071/1110 (96%)	0.30	61 (5%) 24 25	17, 35, 59, 82	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	PHE	6.1
1	A	339	VAL	6.1
2	B	251	GLN	5.7
2	B	303	ARG	4.9
1	A	342	THR	4.8
1	A	308	LYS	4.8
1	A	343	LYS	4.3
1	A	344	ILE	4.2
1	A	305	CYS	4.2
1	A	258	LYS	4.1
1	A	340	ASP	3.9
1	A	259	GLY	3.8
2	B	41	GLY	3.7
1	A	247	ARG	3.7
2	B	411	ASN	3.7
1	A	255	VAL	3.6
2	B	253	ASP	3.5
1	A	254	LEU	3.4
2	B	276	LEU	3.4
1	A	248	THR	3.4
1	A	257	THR	3.3
1	A	307	LEU	3.2
2	B	257	THR	3.2
2	B	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	410	VAL	3.2
1	A	35	LYS	3.1
2	B	249	ASN	3.1
1	A	338	ASP	3.1
1	A	306	PRO	3.0
2	B	40	SER	3.0
2	B	260	ASP	3.0
2	B	254	LEU	2.9
2	B	412	SER	2.9
2	B	258	LYS	2.9
1	A	380	ARG	2.8
2	B	252	GLY	2.7
2	B	259	GLY	2.7
1	A	530	GLU	2.7
2	B	248	THR	2.6
2	B	432	LYS	2.6
1	A	337	VAL	2.5
1	A	249	ASN	2.5
1	A	406	LYS	2.4
1	A	278	LYS	2.3
1	A	67	LYS	2.3
1	A	345	PRO	2.3
1	A	299	ILE	2.3
1	A	277	GLY	2.3
1	A	300	THR	2.3
1	A	527	HIS	2.2
1	A	39	ILE	2.2
1	A	252	GLY	2.2
1	A	346	ALA	2.2
2	B	301	SER	2.1
1	A	10	GLU	2.1
1	A	220	SER	2.1
1	A	9	VAL	2.1
1	A	164	ASP	2.1
1	A	246	VAL	2.0
2	B	255	VAL	2.0
2	B	433	TYR	2.0

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

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(Å <sup>2</sup> )	Q<0.9
2	CYD	B	83	16/17	0.90	0.19	-	27,47,50,52	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
5	POP	B	999	9/9	0.91	0.24	1.82	84,85,86,86	0
5	POP	A	998	9/9	0.81	0.23	0.99	98,98,99,99	0
3	SO4	A	806	5/5	0.75	0.20	0.48	95,95,96,96	0
3	SO4	B	804	5/5	0.94	0.14	0.19	73,73,74,75	0
3	SO4	A	801	5/5	0.93	0.11	-0.91	85,85,85,86	0
4	NI	A	902	1/1	0.99	0.09	-3.30	33,33,33,33	0
4	NI	B	901	1/1	0.99	0.04	-	52,52,52,52	0
3	SO4	B	803	5/5	0.96	0.17	-	60,60,62,62	0

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

There are no such residues in this entry.