



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:53 PM UTC

PDB ID : 1OX4 / pdb_00001ox4
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

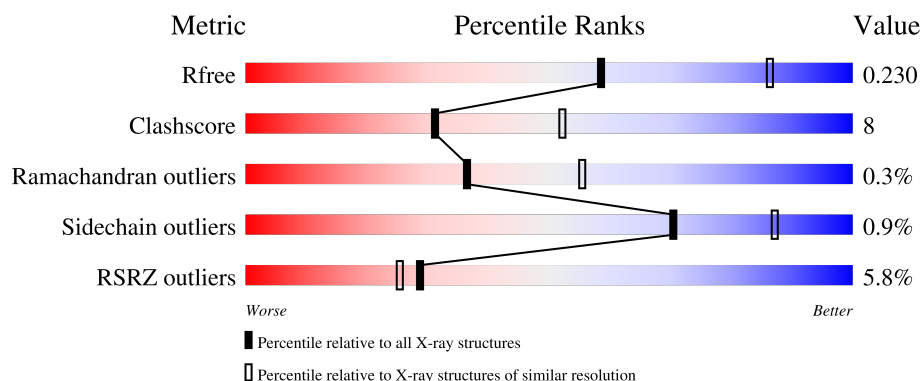
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	555	5% 74% 21% • •
2	B	555	6% 77% 19% • •

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

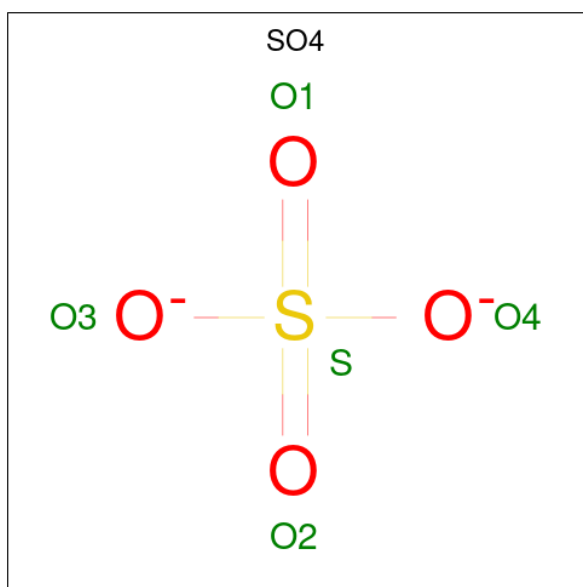
- Molecule 2 is a protein called Imidazole glycerol phosphate synthase hisHF.

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 (CCD ID: SO4) (formula: O₄S).

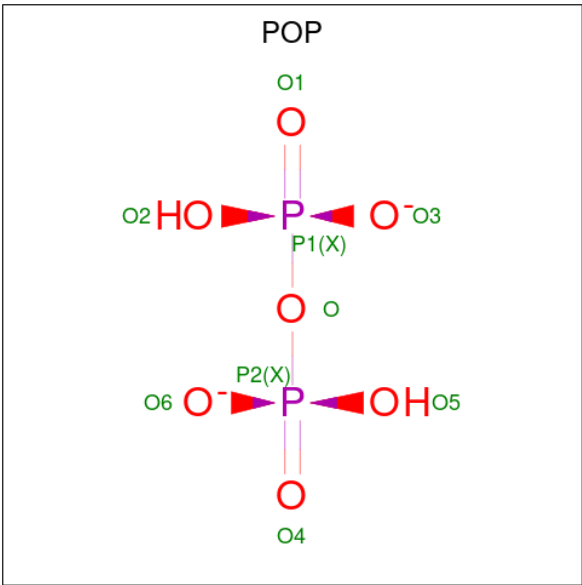


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 5 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



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		

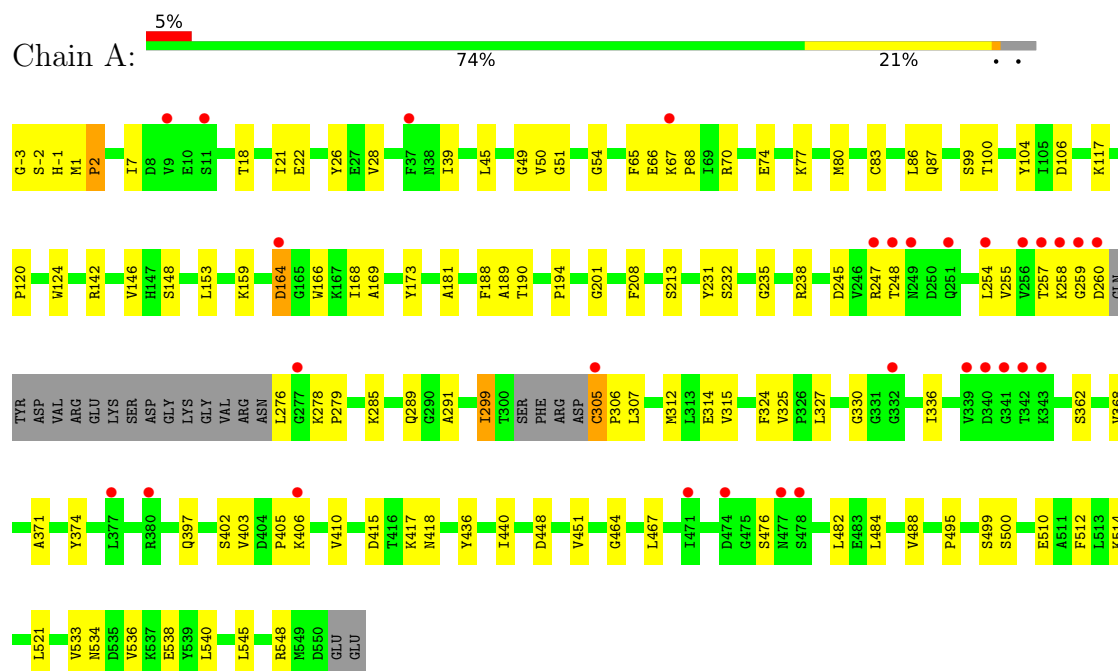
- Molecule 6 is water.

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

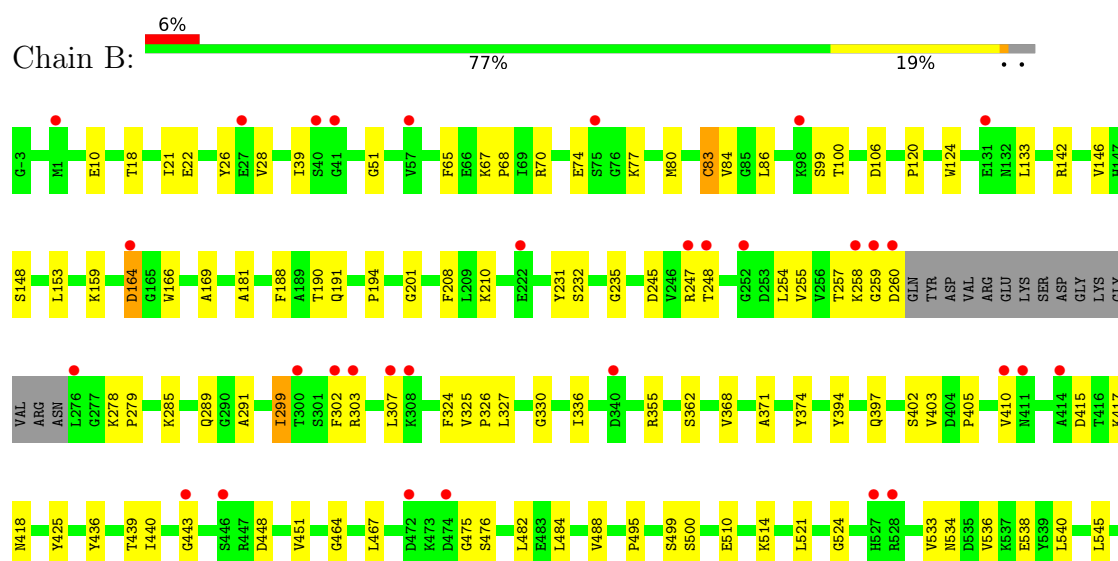
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: Imidazole glycerol phosphate synthase hisHF



- Molecule 2: Imidazole glycerol phosphate synthase hisHF



RE48	MS49
D550	GLU
GLU	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.50Å 112.00Å 115.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.50) 99.8 (50.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	2256 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8572	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CYD, POP, SO4

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	0.41	0/4235	0.92	14/5729 (0.2%)
2	B	0.41	0/4266	0.91	9/5770 (0.2%)
All	All	0.41	0/8501	0.91	23/11499 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	CYS	CA-C-N	9.47	129.53	119.78
1	A	305	CYS	C-N-CA	9.47	129.53	119.78
1	A	232	SER	N-CA-C	-8.39	98.06	110.48
1	A	106	ASP	N-CA-C	7.63	122.52	110.70
2	B	106	ASP	N-CA-C	7.59	122.47	110.70
2	B	232	SER	N-CA-C	-7.52	99.35	110.48
2	B	482	LEU	N-CA-C	6.37	118.22	111.28
1	A	2	PRO	CA-C-N	-6.06	115.28	123.10
1	A	2	PRO	C-N-CA	-6.06	115.28	123.10
2	B	153	LEU	N-CA-C	6.04	119.90	110.17
1	A	482	LEU	N-CA-C	5.87	117.68	111.28
1	A	77	LYS	CA-C-N	5.85	126.19	119.93
1	A	77	LYS	C-N-CA	5.85	126.19	119.93
1	A	153	LEU	N-CA-C	5.68	119.22	110.42
2	B	77	LYS	CA-C-N	5.65	125.98	119.93
2	B	77	LYS	C-N-CA	5.65	125.98	119.93
2	B	191	GLN	N-CA-C	-5.41	106.52	113.23
1	A	476	SER	N-CA-C	5.26	117.76	111.71
1	A	324	PHE	N-CA-C	5.19	117.19	110.65
2	B	324	PHE	N-CA-C	5.17	117.16	110.65
1	A	168	ILE	N-CA-C	5.06	115.19	108.11
1	A	104	TYR	N-CA-C	-5.04	105.88	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	99	SER	N-CA-C	5.03	117.17	110.53

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	68	1
2	B	4194	0	4132	70	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	136	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 (136) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:521:LEU:C	1:A:521:LEU:HD23	2.30	0.56
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:521:LEU:C	2:B:521:LEU:HD23	2.32	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:HG13	2:B:146:VAL:O	2.08	0.53
1:A:146:VAL:O	1:A:146:VAL:HG13	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:18:THR:HG22	2:B:28:VAL:HG11	1.91	0.52
2:B:146:VAL:CG2	2:B:397:GLN:HB2	2.39	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
2:B:245:ASP:HB3	2:B:299:ILE:HD11	1.92	0.52
2:B:291:ALA:HA	2:B:533:VAL:HG11	1.92	0.52
1:A:325:VAL:O	1:A:327:LEU:HD12	2.10	0.52
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:54:GLY:HA2	1:A:99:SER:OG	2.13	0.49
1:A:417:LYS:HE2	1:A:448:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:65:PHE:C	1:A:68:PRO:HD2	2.40	0.46
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:65:PHE:C	2:B:68:PRO:HD2	2.40	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:67:LYS:HB2	1:A:68:PRO:HD3	1.98	0.45
1:A:194:PRO:O	1:A:201:GLY:HA3	2.16	0.45
1:A:80:MET:HA	1:A:188:PHE:O	2.18	0.44
1:A:86:LEU:HD13	1:A:190:THR:C	2.42	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LEU:HD13	2:B:190:THR:C	2.43	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:66:GLU:HB3	6:A:1020:HOH:O	2.17	0.43
1:A:80:MET:HB2	1:A:208:PHE:CZ	2.54	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
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
1:A:7:ILE:HG13	1:A:45:LEU:HD11	2.01	0.41
1:A:50:VAL:HG12	1:A:51:GLY:N	2.35	0.41
1:A:248:THR:HG22	1:A:254:LEU:HD12	2.02	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
1:A:86:LEU:HD12	1:A:189:ALA:C	2.46	0.41
2:B:248:THR:HG22	2:B:254:LEU:HD12	2.01	0.41
2:B:51:GLY:HA2	2:B:394:TYR:C	2.46	0.41
2:B:402:SER:HA	2:B:467:LEU:HB3	2.03	0.41
1:A:312:MET:HE3	1:A:315:VAL:HB	2.03	0.41
1:A:368:VAL:HG21	1:A:440:ILE:HG22	2.01	0.41
1:A:410:VAL:HB	1:A:415:ASP:HB2	2.03	0.41
2:B:368:VAL:HG21	2:B:440:ILE:HG22	2.03	0.41
1:A:83:CYS:O	1:A:87:GLN:HG3	2.20	0.41
1:A:257:THR:HG22	1:A:259:GLY:H	1.85	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
1:A:-1:HIS:NE2	1:A:1:MET:HE3	2.37	0.40
2:B:80:MET:HB2	2:B:208:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HB3	1:A:512:PHE:CE2	2.57	0.40
2:B:83:CYD:HB2	2:B:84:VAL:H	1.63	0.40
2:B:439:THR:OG1	2:B:443:GLY:HA2	2.21	0.40
2:B:326:PRO:C	2:B:327:LEU:HD12	2.47	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 [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	528/555 (95%)	508 (96%)	18 (3%)	2 (0%)	30	49
2	B	533/555 (96%)	513 (96%)	19 (4%)	1 (0%)	43	63
All	All	1061/1110 (96%)	1021 (96%)	37 (4%)	3 (0%)	36	55

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 [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	448/467 (96%)	444 (99%)	4 (1%)	70	87
2	B	451/466 (97%)	447 (99%)	4 (1%)	70	87
All	All	899/933 (96%)	891 (99%)	8 (1%)	70	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	A	159	LYS
1	A	164	ASP
1	A	299	ILE
2	B	100	THR
2	B	159	LYS
2	B	164	ASP
2	B	299	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	87	GLN
1	A	183	ASN
1	A	298	ASN
2	B	38	ASN
2	B	87	GLN
2	B	132	ASN
2	B	183	ASN
2	B	289	GLN
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	13,15,16	1.32	1 (7%)	12,18,20	1.61	1 (8%)

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	-	6/15/17/19	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	83	CYD	O1-C2	3.91	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	4.87	131.47	113.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	83	CYD	C-CA-CB-SG
2	B	83	CYD	C2-C1-SG-CB
2	B	83	CYD	C3-C4-C5-N1
2	B	83	CYD	C3-C4-C5-C6
2	B	83	CYD	C2-C3-C4-C5
2	B	83	CYD	N-CA-CB-SG

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	POP	B	999	-	6,8,8	1.46	0	12,13,13	1.83	4 (33%)
5	POP	A	998	-	6,8,8	1.35	0	12,13,13	1.84	4 (33%)
3	SO4	B	804	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	B	803	-	4,4,4	0.35	0	6,6,6	0.12	0
3	SO4	A	801	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	A	806	-	4,4,4	0.42	0	6,6,6	0.09	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
5	POP	B	999	-	-	2/6/6/6	-
5	POP	A	998	-	-	3/6/6/6	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	998	POP	O5-P2-O	-3.78	91.95	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	999	POP	O5-P2-O	-3.56	92.69	104.64
5	A	998	POP	O-P2-O4	3.17	127.71	111.04
5	B	999	POP	O-P2-O4	3.00	126.84	111.04
5	B	999	POP	O5-P2-O4	-2.78	100.00	110.83
5	A	998	POP	O5-P2-O4	-2.60	100.72	110.83
5	B	999	POP	O6-P2-O4	2.44	120.34	110.83
5	A	998	POP	O6-P2-O4	2.40	120.20	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	998	POP	P2-O-P1-O2
5	A	998	POP	P2-O-P1-O3
5	B	999	POP	P2-O-P1-O3
5	B	999	POP	P2-O-P1-O1
5	A	998	POP	P2-O-P1-O1

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, 95th 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 ²)	Q<0.9
1	A	534/555 (96%)	0.41	30 (5%)	30 26	17, 36, 59, 81	0
2	B	537/555 (96%)	0.40	32 (5%)	27 24	18, 35, 59, 82	0
All	All	1071/1110 (96%)	0.41	62 (5%)	29 25	17, 35, 59, 82	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	276	LEU	4.5
1	A	471	ILE	4.1
2	B	302	PHE	4.0
1	A	406	LYS	3.9
1	A	343	LYS	3.7
1	A	258	LYS	3.5
2	B	260	ASP	3.4
1	A	9	VAL	3.4
1	A	11	SER	3.2
1	A	260	ASP	3.1
1	A	67	LYS	3.0
1	A	248	THR	3.0
1	A	254	LEU	2.9
2	B	259	GLY	2.9
1	A	259	GLY	2.9
2	B	1	MET	2.9
1	A	339	VAL	2.8
1	A	251	GLN	2.7
1	A	249	ASN	2.7
2	B	443	GLY	2.6
2	B	40	SER	2.6
2	B	258	LYS	2.6
1	A	164	ASP	2.5
2	B	41	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	477	ASN	2.5
2	B	472	ASP	2.5
1	A	37	PHE	2.5
2	B	527	HIS	2.5
1	A	256	VAL	2.4
2	B	252	GLY	2.4
2	B	308	LYS	2.4
2	B	164	ASP	2.4
2	B	474	ASP	2.4
1	A	377	LEU	2.4
1	A	257	THR	2.4
2	B	98	LYS	2.3
1	A	342	THR	2.3
1	A	277	GLY	2.3
2	B	57	VAL	2.3
1	A	341	GLY	2.2
2	B	307	LEU	2.2
1	A	247	ARG	2.2
1	A	340	ASP	2.2
2	B	27	GLU	2.2
1	A	305	CYS	2.2
2	B	247	ARG	2.2
2	B	528	ARG	2.2
2	B	446	SER	2.2
1	A	474	ASP	2.2
2	B	222	GLU	2.2
1	A	380	ARG	2.2
2	B	414	ALA	2.1
2	B	411	ASN	2.1
2	B	303	ARG	2.1
2	B	340	ASP	2.1
1	A	478	SER	2.1
2	B	131	GLU	2.0
2	B	248	THR	2.0
2	B	75	SER	2.0
2	B	410	VAL	2.0
1	A	332	GLY	2.0
2	B	300	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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(Å ²)	Q<0.9
2	CYD	B	83	16/17	0.88	0.15	27,47,50,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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(Å ²)	Q<0.9
5	POP	A	998	9/9	0.70	0.19	98,98,99,99	0
3	SO4	A	806	5/5	0.75	0.18	95,95,96,96	0
3	SO4	A	801	5/5	0.76	0.13	85,85,85,86	0
5	POP	B	999	9/9	0.84	0.18	84,85,86,86	0
3	SO4	B	804	5/5	0.85	0.12	73,73,74,75	0
3	SO4	B	803	5/5	0.94	0.11	60,60,62,62	0
4	NI	B	901	1/1	0.99	0.08	52,52,52,52	0
4	NI	A	902	1/1	1.00	0.01	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.